



**HAL**  
open science

# The Photon Wave Function in Principle and in Practice

Vincent Debierre

► **To cite this version:**

Vincent Debierre. The Photon Wave Function in Principle and in Practice. Optics [physics.optics]. Ecole Centrale Marseille; École centrale de Marseille, 2015. English. NNT: 2015ECDM0004. tel-01406401

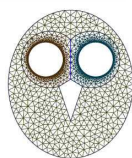
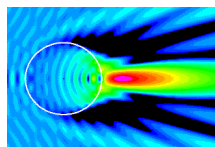
**HAL Id: tel-01406401**

**<https://theses.hal.science/tel-01406401>**

Submitted on 1 Dec 2016

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Thèse présentée à  
l'École Centrale de Marseille  
pour obtenir le grade de Docteur

École Doctorale : Physique et Sciences de la Matière  
Spécialité : Optique, Photonique et Traitement d'Image

# LA FONCTION D'ONDE DU PHOTON EN PRINCIPE ET EN PRATIQUE

Vincent DEBIERRE

Institut Fresnel (Équipes CLARTÉ et ATHÉNA)—CNRS

Soutenue publiquement le 25 Septembre 2015 devant un jury composé de

Pascal	DEGIOVANNI	Rapporteur	DR CNRS—Labo. Physique ÉNS Lyon
Margaret	HAWTON	Rapporteur	Professor Emeritus—Lakehead University
Paolo	FACCHI	Examineur	Prof. Associato—Univ. Bari
Evgueni	KARPOV	Examineur	Senior Researcher—Univ. Libre de Bruxelles
Alexandre	MATZKIN	Examineur	CR CNRS—Labo. Phys. Théor. Modélisation
Frédéric	ZOLLA	Examineur	PR—Aix-Marseille Université
Thomas	DURT	Directeur de Thèse	PR—École Centrale de Marseille
André	NICOLET	Co-directeur de Thèse	PR—Aix-Marseille Université

**This page intentionally left blank**

# TABLE OF CONTENTS

---

<b>Introduction</b>	<b>1</b>
<b>I Photon Wave Function &amp; Localisability</b>	<b>5</b>
<b>Introduction to Part I</b>	<b>7</b>
<b>1 Canonical Quantisation of the Electromagnetic Field</b>	<b>11</b>
1.1 The Poincaré group . . . . .	13
1.2 Wigner-Bargmann equation for the Maxwell field . . . . .	16
1.3 Canonical quantisation of the Maxwell field: some preliminaries . . . . .	21
1.4 Coulomb gauge quantisation . . . . .	24
1.A Representations of the Poincaré group and Poincaré-invariant quantisation . . . . .	35
<b>2 The Photon Position Operator</b>	<b>59</b>
2.1 A brief history of the photon position operator . . . . .	60
2.2 The Hawton position operator . . . . .	61
2.A Commutation of the components of the photon position operator . . . . .	65
<b>3 Photon Wave Functions</b>	<b>69</b>
3.1 Photon wave function in momentum space . . . . .	70
3.2 Wave equation . . . . .	71
3.3 Energy and number densities—Nonlocality issues . . . . .	71
3.4 Photon wave functions through Glauber’s extraction rule . . . . .	73
3.5 Advanced topics . . . . .	75
3.6 Photon trajectories in the Bohmian picture of wave mechanics . . . . .	79
3.7 Outlook on the photon wave function . . . . .	83
3.A Kernel computation in spherical coordinates . . . . .	84
<b>4 An Overview of Nonclassicality in Quantum Optics</b>	<b>91</b>
4.1 Elements of photodetection theory . . . . .	93
4.2 Single-mode quantum optics: physical modes . . . . .	95
4.3 Single-mode quantum optics: quantum optics . . . . .	99
4.4 Interlude: $n$ -photon wave functions . . . . .	106
4.5 Single mode quantum optics: effective one-point wave function . . . . .	110
4.6 Quantum optics and classical electrodynamics: an informal overview . . . . .	112
4.A Completeness relation for coherent states . . . . .	113

<b>II Quantum Electrodynamics &amp; Light Emission</b>	<b>117</b>
<b>Introduction to Part II</b>	<b>119</b>
<b>5 Simple Interacting Systems</b>	<b>123</b>
5.1 Nuclear decay and Gamow states . . . . .	125
5.2 On the two-level Friedrichs model . . . . .	130
5.3 A toy-model for the description of losses in cavity quantum electrodynamics . . . . .	134
5.A Quantum scattering: complex poles and their eigenfunctions . . . . .	141
<b>6 Transient Regime in the Atom-Field Interaction</b>	<b>145</b>
6.1 Interaction of light with nonrelativistic matter . . . . .	147
6.2 The dipole approximation and its shortcomings . . . . .	154
6.3 Improving on the dipole approximation: exact atom-field coupling . . . . .	158
6.4 Bonus: the ideal cutoff frequency for the dipole approximation . . . . .	163
6.5 Discussion . . . . .	164
6.A Some useful results of distribution theory . . . . .	166
<b>7 Causality in Spontaneous Emission and Hegerfeldt's Theorem</b>	<b>171</b>
7.1 Hegerfeldt's theorem as a Paley-Wiener theorem . . . . .	172
7.2 Photon propagation in spontaneous emission . . . . .	175
7.3 Discussion . . . . .	184
7.A The Paley-Wiener theorem . . . . .	185
<b>Conclusion</b>	<b>189</b>

# WORD OF THANKS

---

*“After all, science is essentially international, and it is only through lack of the historical sense that national qualities have been attributed to it.”*

Marie Curie

First of all, of course, I wish to thank my thesis advisors. A PhD project is always a collaborative affair, and I am glad to have worked under the supervision of Profs. Thomas Durt and André Nicolet. I have truly enjoyed academic freedom without being left on my own. Both Thomas and André were always interested in what I had to say, or at least, that is the impression I had! I found that Thomas’s style of investigation, radically different from mine, often made us a very complementary pair. Meanwhile, along with “third man” Frédéric Zolla, André provided very helpful suggestions along the way.

I am of course also indebted to the members of the defense committee and especially to the two reviewers of this work who kindly accepted the time-consuming task of reading the present manuscript.

Warm thanks also go to other collaborators outside and inside the lab, especially Édouard Brainis, Brian Stout and Guillaume Demésy and to past and present officemates Brice Rolly, Victor Grigoriev and Mahmoud Elsayy—*not* least for coping up with my frequent mumbling to myself.

During my stay in Institut Fresnel I am lucky to have met many fellow students, some of them scientific collaborators, and all of them friendly co-workers. A list of all the people I’m thinking about while writing these lines would be too long—and I do mean that—but I want to mention Yoann Brûlé and Isabelle Goessens who were—I feel—the closest to me.

I embarked on this PhD adventure at the same time and on the same campus as friends Arnaud Demion, Laurent Chôné and Pierre Manas. Thanks for the shared adventure and the shared moments, guys.

A PhD project lives and dies by intellectual curiosity, and I owe mine to my parents, who always encouraged me. Thanks for all the help, and for having so many books at home.

Maybe in spite of the epigraph with which I open these acknowledgments, I wish to express my gratitude to the French taxpayer who, whether they liked it or not, provided for me during these three years. As I see it, there’s no better arrangement than being paid to perform calculations.

And also a mention to the people at CUMSJ badminton, with whom I shared most of my weeknights. Especially to Vladyslav Atavin who very generously took two full days to sit down with me and patiently translate a paper by Shirokov from Russian.

# AN INCOMPLETE GUIDE TO NOTATIONS

---

## General conventions

Throughout this work we endeavoured to keep the following conventions:

The prime notation	$x'$	is used to denote the image of a quantity $x$ under a Poincaré transformation.
The boldface notation	$\mathbf{x}$	is used to denote three-vectors.
The hat notation	$\hat{x}$	is used to denote quantum operators on Hilbert spaces.
The overbar notation	$\bar{x}$	is used to denote the Fourier transform of a quantity $x$ .
The star notation	$x^*$	is used to denote complex conjugation.
The upper plus/minus notation	$x^\pm$	is used to denote the positive or negative frequency part of a quantity $x$ .
The longitudinal part	$\mathbf{F}_\parallel(\mathbf{x})$	of a vector field is the inverse Fourier transform of (6.1.6a).
The transverse part	$\mathbf{F}_\perp(\mathbf{x})$	of a vector field is the inverse Fourier transform of (6.1.6b).
The brace notation	$\{x, y\}$	is used to denote the Poisson bracket of two quantities $x$ and $y$ .
The square bracket notation	$[\hat{x}, \hat{y}]$	is used to denote the commutator of two operators $\hat{x}$ and $\hat{y}$ .
Latin indices such as	$i$	run over 1,2,3.
Greek indices such as	$\mu$	run over 0,1,2,3.

## Tensor algebra and the Poincaré group

The following notations are especially relevant to chapter 1:

The twice covariant metric tensor	$\eta_{\mu\nu}$	is defined at (1.1.1a).
The twice contravariant metric tensor	$\eta^{\mu\nu}$	is defined at (1.1.1d).
The mixed metric tensor	$\eta^\mu_\nu$	is defined at (1.1.2).
The covariant Levi-Civita symbol	$\epsilon_{\mu\nu\rho\sigma}$	is the totally antisymmetric tensor.
The Poincaré generator	$P^\mu$	generates spacetime translations.
The Poincaré generator	$J^{\mu\nu}$	generates Lorentz transf. ( <i>i.e.</i> , space rot. and Lorentz boosts).
The Pauli-Lubański four-pseudovector	$W_\mu$	is defined at (1.1.12).
The invariant volume element on the lightcone	$\tilde{d}k$	is defined at (1.4.23).

## Electrodynamics

The four-vector potential	$A^\mu$	is formed by the scalar pot. $A^0$ and the vector pot. $\mathbf{A}$ .
The Faraday tensor	$F^{\mu\nu}$	is defined at (1.2.20) in terms of the electric $\mathbf{E}$ and magnetic $\mathbf{B}$ fields.
The charge density-current four-vector	$J^\mu$	is formed by the charge density $\rho$ and the current density $\mathbf{j}$ .
The polarisation vectors	$\epsilon_{(\lambda)}(\mathbf{k})$	in the Coulomb gauge are defined at (1.4.19).
The polarisation four-vectors	$\epsilon_{(\lambda)}^\mu(\mathbf{k})$	in the Lorenz gauge are defined at (1.A.51), (1.A.54) and (1.A.55).
The connection	$\alpha(\mathbf{k})$	on the lightcone is defined at (1.4.28).
The generators	$\hat{S}_i$	of the rotation group $SO(3)$ are defined at (2.1.2).
The photon wave function	$\psi_{(\lambda)}^{(+1/2)}$	is the Riemann-Silberstein wave function (see sects. 3.3 and 3.4).
The photon wave function	$\psi_{(\lambda)}^{(0)}$	is the Landau-Peierls wave function (see sect. 3.3).
The photon wave function	$\psi_{(\lambda)}^{(-1/2)}$	is the Gross-Hawton wave function (see sect. 3.4).

## Schwartz distributions

The Dirac delta distribution	$\delta$	has its usual definition.
The Heaviside step distribution	$\theta$	is the antiderivative of $\delta$ .
The Cauchy principal value distribution	$\text{vp}(1/.)$	is defined at (6.A.1).

## Special integral functions

The following notations are especially relevant to chapters 6 and 7:

The cosine integral function	Ci	is defined at (6.2.5a).
The sine integral function	Si	is defined at (6.2.5b).
The exponential integral function	Ei	is defined at (6.3.15).





# INTRODUCTION

---

*“Before we start, however, keep in mind that although fun and learning are the primary goals of all Enrichment Center activities, serious injuries may occur.”*  
GLaDOS in Portal™

This work is concerned with various topics in quantum electrodynamics, with an emphasis on photon wave mechanics, and hence, the photon wave function. We deal with both formal, definitional issues (chiefly in Part I) and more operational questions (chiefly in Part II).

The history of the photon wave function is fairly old but not very dense, so to say. The photon wave function in reciprocal (momentum) space is a firmly established, widely used notion (see, *e.g.*, [1]). This is so essentially because the photon linear momentum operator is a clearly defined object. It is indeed the generator of translations in direct space. The various vector components of the momentum operator commute, which means that their eigenvectors are common. The photon position operator is, on the other hand, a more problematic object. Newton and Wigner announced [4], in a famous 1948 paper, that no localised states exist for relativistic fields with zero mass and helicity  $\pm 1$ , in other words, for photons. This confirmed previous works by Kemmer [5] and Pryce [6]. This is in contrast to the case of massive particles, the description of which in direct space has always been common. However, investigations of the coherence properties of electromagnetic fields in quantum optics drove Titulaer and Glauber to introduce [7] the object

$$\langle 0 | \hat{\mathbf{E}}^+(\mathbf{x}, t) | 1_{\vec{f}} \rangle \quad (0.1)$$

where  $|0\rangle$  is the vacuum state of the electromagnetic field,  $\hat{\mathbf{E}}^+(\mathbf{x}, t)$  is the positive frequency (annihilation) part of the electric field operator and  $|1_{\vec{f}}\rangle$  is a one-photon state. For many practical purposes, the object (0.1) can be considered to be the wave function of the single photon described by the state vector  $|1_{\vec{f}}\rangle$ . It is, among others, directly linked to the density of electromagnetic energy carried by the single photon in question.

In Part I of this Thesis we show how to get from the usual relativistic quantum field theoretical picture of photons as objects with a definite momentum (wave vector) and helicity to a more wave mechanical paradigm where a wave function in direct space can be defined for photons [8–12]. We discuss Hawton’s overcoming [11, 13] of the Newton-Wigner result mentioned above. We show that the wave equation for single photons is simply the Maxwell equations, which shows the formal equivalence between single-photon wave mechanics and classical electrodynamics. This has been exploited in [14] for instance where classical electromagnetic codes were used to study the frequency and lifetime of photons in the quantum electrodynamical cavity used by Serge Haroche and his collaborators at ÉNS in Paris [2]. Numerical investigations of this system are ongoing [22]. We show in Part I how photon wave functions relate to Poynting’s local density of electromagnetic energy and to the more difficult local density of photons, for which several definitions can be given, none of them being entirely satisfactory. We discuss the relevance of the object obtained through Glauber’s extraction rule (0.1), and show

that it is one of the (best) possible choices for the photon wave function. A brief summary of our findings on photon wave mechanics is found in Tab. 3.1, which spells out the main advantages and drawbacks of the three most natural choices for the photon wave function. We also discuss the extension of the wave function formalism to several photon states and, ultimately, arbitrary states of the electromagnetic field. As argued in [21], the photon wave function is a very handy tool in physical situations where “the number of photons [...] is small, fixed and known”. We see for instance that when the physical situation is such that the description of the electromagnetic field only requires to take into account a single polychromatic mode, then for  $n$ -photon Fock states of that mode all  $n$  photons have the same wave function [7, 15]. We give a more detailed introduction to Part I below.

In Part II we turn to the interaction of the electromagnetic field with charged matter. The main focus is on the spontaneous emission of light by quantum-level transitions of atomic electrons. Theoretical investigations of spontaneous emission and similar problems in atomic physics and quantum electrodynamics are often dominated by the computation of transition rates from an atomic level to another one. Behind this lies the assumption that the decay of excited states is exponential in time. This exponential decay can only ever be an approximation [16, 17], as we discuss. However, it is very often a successful approximation, in spite of its discrepancy with the short-time dynamics of quantum systems. We study the very short-time dynamics of spontaneous emission from the point of view of the decaying electron and discuss the relevance of exponential decay (well approximated at reasonably short times by Fermi’s golden rule) and that of the ubiquitous dipole approximation for the atom-field interaction in detail. Our study of the short-time dynamics of spontaneous emission was largely motivated by our curiosity about the causality of the emitted field. Indeed, there exist [3, 18, 19] “proofs” that the emitted field propagates causally, but these “proofs” involve several approximations. One such approximation is the Wigner-Weisskopf approximation: the decay of the radiating electron is assumed to be strictly exponential in time. As such, these “proofs” are *a priori* not relevant to the description of the emitted field immediately after the onset of the decay, since at such short times the Wigner-Weisskopf approximation is not relevant. Using what we learn about the dynamics of the decaying electron, we look carefully at the spacetime dependence of the electromagnetic field emitted during the atomic transition, and discuss the causality of the propagation of that emitted field. In that task the insights gained on the photon wave function in Part I prove very helpful. This is just one illustration among many that the photon wave function is not only a matter of purely formal inquiry. It can for instance prove a valuable tool to carry out computations without resorting to the heavy apparatus of ladder operators (and integrals over wave vectors) at every step (see *e.g.* [21] where the authors make use of the photon wave function formalism to describe among others, Hong-Ou-Mandel interferometry (see sect. 4.4.4 for a different—and brief—discussion of that topic), or [20] where the Lindblad master equation is established for photons in an open cavity entirely in terms of photon wave functions and states (also see sect. 5.3.3.3)). We give a more detailed introduction to Part II below.

# REFERENCES

---

## Books

- [1] A.I. Akhiezer and V.B. Berestetskii, *Quantum Electrodynamics*, edited by R.E. Marshak, 2nd ed. (Interscience Publishers, 1965) (cit. on p. 1).
- [2] S. Haroche and J.M. Raimond, *Exploring the Quantum - Atoms, Cavities and Photons* (Oxford University Press, 2007) (cit. on p. 1).
- [3] M.O. Scully and M.S. Zubairy, *Quantum Optics* (Cambridge University Press, 1997) (cit. on p. 2).

## Articles

- [4] T.D. Newton and E.P. Wigner, ‘Localized States for Elementary Systems’, *Rev. Mod. Phys.* **21**, 400 (1949) (cit. on p. 1).
- [5] N. Kemmer, ‘The Particle Aspect of Meson Theory’, *Proc. R. Soc. Lond. A* **173**, 91 (1939) (cit. on p. 1).
- [6] M.H.L. Pryce, ‘The Mass-Centre in the Restricted Theory of Relativity and Its Connexion with the Quantum Theory of Elementary Particles’, *Proc. R. Soc. Lond. A* **195**, 62 (1948) (cit. on p. 1).
- [7] U.M. Titulaer and R.J. Glauber, ‘Density Operators for Coherent Fields’, *Phys. Rev.* **145**, 1041 (1966) (cit. on pp. 1, 2).
- [8] I. Białynicki-Birula, ‘Photon Wave Function’, *Prog. Opt.* **36**, 245 (1996) (cit. on p. 1).
- [9] J.E. Sipe, ‘Photon Wave Functions’, *Phys. Rev. A* **52**, 1875 (1995) (cit. on p. 1).
- [10] M. Hawton, ‘Photon wave functions in a localized coordinate space basis’, *Phys. Rev. A* **59**, 3223 (1999) (cit. on p. 1).
- [11] M. Hawton and W.E. Baylis, ‘Photon position operators and localized bases’, *Phys. Rev. A* **64**, 012101 (2001) (cit. on p. 1).
- [12] M. Hawton, ‘Photon wave mechanics and position eigenvectors’, *Phys. Rev. A* **75**, 062107 (2007) (cit. on p. 1).
- [13] M. Hawton, ‘Photon position operator with commuting components’, *Phys. Rev. A* **59**, 954 (1999) (cit. on p. 1).
- [14] V. Debievre, G. Demésy, T. Durt, A. Nicolet, B. Vial and F. Zolla, ‘Absorption in quantum electrodynamic cavities in terms of a quantum jump operator’, *Phys. Rev. A* **90**, 033806 (2014) (cit. on p. 1).
- [15] B.J. Smith and M.G. Raymer, ‘Photon wave functions, wave-packet quantization of light, and coherence theory’, *New J. Phys.* **9**, 414 (2007) (cit. on p. 2).
- [16] L.A. Khalfin, *Sov. Phys. JETP* **96**, 1053 (1958) (cit. on p. 2).
- [17] B. Misra and E.C.G. Sudarshan, ‘The Zeno’s paradox in quantum theory’, *J. Math. Phys.* **18**, 756 (1977) (cit. on p. 2).

- [18] E. Fermi, 'Quantum Theory of Radiation', *Rev. Mod. Phys.* **4**, 87 (1932) (cit. on p. 2).
- [19] M.I. Shirokov, 'Signal velocity in quantum electrodynamics', *Sov. Phys. Usp.* **21**, 345 (1978) (cit. on p. 2).
- [20] T. Durt and V. Debieuvre, 'Coherent states and the classical-quantum limit considered from the point of view of entanglement', *Int. J. Mod. Phys. B* **27**, 1345014 (2013) (cit. on p. 2).

## Conference Proceedings

- [21] É. Brainis and P. Emplit, Wave function formalism in quantum optics and generalized Huygens-Fresnel principle for  $N$  photon-states: derivation and applications, in *Proc. SPIE*, Vol. 1, edited by V.N. Zadkov and T. Durt (2010), p. 77270 (cit. on p. 2).

## Theses

- [22] N. Marsic, *Solveurs électromagnétiques éléments finis massivement parallèles*, PhD Thesis (Université de Liège, ongoing) (cit. on p. 1).

PART I

PHOTON WAVE FUNCTION & LOCALISABILITY



# INTRODUCTION TO PART I

---

For monochromatic light (of frequency  $\omega_0$ ), the words “light” and “photons” can arguably be used interchangeably: a beam of energy  $E$  consists of

$$n_\gamma = \frac{E}{\omega_0} \quad (\text{I.1})$$

photons. But in the vacuum, there is no such thing as a beam of monochromatic light, as it would be equally intense everywhere in space and thus of infinite energy. To make physical sense, we must give up mathematical convenience and consider light as the irretrievably polychromatic object that it is. In that framework, it is natural to wonder what becomes of the simple relation (I.1). Surely we can invoke spectral densities and keep the notion of a number of photons present in the electromagnetic field.

That paradigm arises, some readers will no doubt know, naturally in the framework of relativistic quantum field theory. The comprehensive formalism of that theory features such a quantity as the total photon number operator, which is most easily expressed as a sum (integral) over all electromagnetic frequencies (and, as it happens, a sum over the two usual transverse polarisations of electrodynamics). In quantum field theory, photons are described as the excitations of the electromagnetic field (or four-potential) over its vacuum state, in which there are no photons present. These excitations are most often labelled by their wave vector (and hence frequency) and, once again, their polarisations.

In that respect, the notion of a photon is seemingly always restricted to the reciprocal space of wave vectors. Questions such as where photons are located in configuration space are very rarely even asked, even in the simplest case where a single photon is present in the electromagnetic field. We emphasise again that for strictly monochromatic light (of frequency  $\omega_0$ ), there is no problem. We can simply divide Poynting’s electromagnetic energy density

$$w(\mathbf{x}, t) = \frac{\epsilon_0}{2} [\mathbf{E}^2(\mathbf{x}, t) + c^2 \mathbf{B}^2(\mathbf{x}, t)] \quad (\text{I.2})$$

by the single-photon energy  $\hbar\omega_0$  to obtain the number density of photons. This prescription, however, does not carry directly, to say the least, to the physical, polychromatic case. Nonlocal expressions arise, pointing to the difficulty of defining a local density of photons.

This difficulty is linked to the main formal reason why photons are so seldom considered in configuration space, namely, the fact that the photon position operator is a problematic object, to say the least. The most direct route by far to a discussion of configuration space localisation in quantum mechanics revolves around the use of that (in the case of photons, “hypothetical” at this point of the discussion) position operator and its eigenstates, the existence of which was ruled out by Newton and Wigner in a 1948 article [2] on the localisation of relativistic particles. This result stood for decades as an argument against the description of photons in configuration space.

In a series of articles [3–5] at the turn of the century, Hawton constructed a position operator for photons, overcom-



ing the Newton-Wigner no-go prescription. This result gave further credence to the regained interest in photon wave mechanics, the relevance of which was explored (or reviewed) in the mid-1990s by Białynicki-Birula [6] and Sipe [7]. All these contributions extended the relevance of photon wave mechanics, which had historically been confined to wave vector space [1], to configuration space.

In chapter 1 we review how photons emerge—from the canonical quantisation of electrodynamics—naturally as objects of definite (polarisation and) wave vector. We show that the solidity of the idea of “photons” is crucially based on the fact that polarisation and masslessness are invariant properties under Lorentz transformations and spacetime translations.

The construction and discussion of Hawton’s photon position operator are undertaken in chapter 2. The key property of this operator is that it has commuting vector components, which allows for simultaneous localisation of photons in all three directions of space.

Chapter 3 is a thorough investigation of photon wave mechanics. We carefully examine the issue of the relevance of single-photon wave functions, as well as the connections of that object, or, more accurately, that family of objects, to the local density of electromagnetic energy (I.2) and the more elusive and problematic local density of photons, for which it is shown that no entirely satisfactory definition can be given: either, this photon number density is positive but does not transform under any representation of the Poincaré group, or, it transforms as the zeroth component of a four-vector but is not positive definite.

Chapter 4 veers off of the central topic of this first part of the dissertation which is photon localisation. This chapter can be seen as an inexhaustive look into the question of which quantum states of the electromagnetic field can be thought of as almost “classical” and which ones absolutely cannot. It is noteworthy that the most systematic approach to answer this question—namely, the examination of the correlation functions of the electromagnetic field—has connections to chapter 3, as it makes use of a generalisation of Glauber’s extraction rule, which links single-photon states to single-photon wave functions, as well as connections to chapters 6 and 7, as it is based on the theory of light-matter interaction.

# REFERENCES

---

## Books

- [1] A.I. Akhiezer and V.B. Berestetskii, *Quantum Electrodynamics*, edited by R.E. Marshak, 2nd ed. (Interscience Publishers, 1965) (cit. on p. 8).

## Articles

- [2] T.D. Newton and E.P. Wigner, 'Localized States for Elementary Systems', *Rev. Mod. Phys.* **21**, 400 (1949) (cit. on p. 7).
- [3] M. Hawton, 'Photon position operator with commuting components', *Phys. Rev. A* **59**, 954 (1999) (cit. on p. 7).
- [4] M. Hawton, 'Photon wave functions in a localized coordinate space basis', *Phys. Rev. A* **59**, 3223 (1999) (cit. on p. 7).
- [5] M. Hawton and W.E. Baylis, 'Photon position operators and localized bases', *Phys. Rev. A* **64**, 012101 (2001) (cit. on p. 7).
- [6] I. Białynicki-Birula, 'Photon Wave Function', *Prog. Opt.* **36**, 245 (1996) (cit. on p. 8).
- [7] J.E. Sipe, 'Photon Wave Functions', *Phys. Rev. A* **52**, 1875 (1995) (cit. on p. 8).



## CHAPTER 1

---

# CANONICAL QUANTISATION OF THE ELECTROMAGNETIC FIELD

---

*“[Gallileo] was much on my mind as I came here tonight. I thought here I am, facing the anti-Galilean forces once again. . . And I expected them to be very, very old.”*

Philip Gourevitch during the Intelligence<sup>2</sup> US Debate: ‘Freedom of expression must include the license to offend’

The natural framework for studying photons is relativistic quantum field theory. The study of the symmetries of the four-dimensional Minkowski spacetime and the canonical quantisation of field degrees of freedom allow us to define photons as the excitations of a vector field, the electromagnetic four-vector potential, over the relativistically invariant vacuum state of the field. In this chapter we present these topics, which we feel provide the valid definition of a photon, in detail. Sect. 1.1 is a quick introduction to the formalism of special relativity. Covariant notation is introduced and some important results on the representation theory of the Poincaré group are given. A more thorough discussion of the latter topic can be found in the appendix 1.A to this chapter, where we also review the (Poincaré-invariant) Lorenz gauge quantisation procedure. In sect. 1.2 we establish the link between the behaviour of a vector field under Poincaré transformations and the fact that its wave equations are the Maxwell equations. In sect. 1.3 we give some preliminaries to the canonical quantisation of the vector potential in the Coulomb gauge, which is undertaken in sect. 1.4.

---

## Contents of the Chapter

1.1	The Poincaré group . . . . .	13
1.1.1	Minkowski metric and index gymnastics . . . . .	13
1.1.2	Formal definition of the Lorentz group . . . . .	13
1.1.3	Key elements of the representation theory of the Poincaré group . . . . .	15
1.2	Wigner-Bargmann equation for the Maxwell field . . . . .	16
1.2.1	General vector field . . . . .	17
1.2.2	Massive vector field: a quick detour . . . . .	18
1.2.2.1	Massive vector field of spin 1 . . . . .	18
1.2.2.2	Massive vector field of spin 0 . . . . .	18
1.2.3	Massless vector field: Maxwell equation . . . . .	19
1.2.4	Fields, potentials, and gauges: degrees of freedom . . . . .	20
1.3	Canonical quantisation of the Maxwell field: some preliminaries . . . . .	21

1.3.1	Relativistic field theory: a brief introduction . . . . .	21
1.3.1.1	The principle of least action . . . . .	21
1.3.1.2	Hamilton's canonical formalism . . . . .	21
1.3.1.3	Poisson brackets . . . . .	22
1.3.2	Fields, potentials, and gauges: when to quantise . . . . .	23
1.4	Coulomb gauge quantisation . . . . .	24
1.4.1	Conjugate momenta . . . . .	24
1.4.2	Excursion: constraints and Dirac brackets . . . . .	24
1.4.3	Excursion continued: Dirac bracket of the electromagnetic field . . . . .	25
1.4.4	Canonical commutator . . . . .	26
1.4.5	Formal solution of the source-free Maxwell equations . . . . .	26
1.4.6	More on polarisation vectors . . . . .	29
1.4.7	Quantisation—Fock space . . . . .	29
1.4.8	Poincaré generators . . . . .	30
1.4.9	States of definite momentum and helicity . . . . .	34
1.4.10	Hamiltonian of the field . . . . .	34
1.A	Representations of the Poincaré group and Poincaré-invariant quantisation . . . . .	35
1.A.1	The Poincaré algebra . . . . .	35
1.A.2	Casimir invariants of the Poincaré algebra . . . . .	36
1.A.2.1	Representations and irreducible representations . . . . .	36
1.A.2.2	Casimir invariants . . . . .	37
1.A.3	Wigner representations of the Poincaré algebra . . . . .	39
1.A.3.1	Hilbert space representation of Poincaré transformations . . . . .	39
1.A.3.2	Momentum eigenstates . . . . .	40
1.A.3.3	Massive particles . . . . .	41
1.A.3.4	Massless particles . . . . .	42
1.A.4	Lorenz gauge quantisation . . . . .	44
1.A.4.1	Stückelberg Lagrangian . . . . .	44
1.A.4.2	Excursion: Lagrange multipliers . . . . .	44
1.A.4.3	Canonical analysis: momenta and commutation relations . . . . .	45
1.A.4.4	Formal solution of the Stückelberg equations . . . . .	45
1.A.4.5	Quantisation from auxiliary Poisson brackets . . . . .	48
1.A.4.6	The Gupta-Bleuler condition . . . . .	48
1.A.4.7	Quotient space . . . . .	50
1.A.4.8	Gauge arbitrariness and physical observables . . . . .	52
1.A.4.9	Poincaré generators . . . . .	53
1.A.4.10	States of definite momentum and helicity . . . . .	55

---

## 1.1 The Poincaré group

The Poincaré group is the fundamental symmetry group of special relativity and thus a symmetry group for any relativistic theory. As such, the study of its properties and that of its representations (see appendix 1.A) is very instructive. We try in the present section to give the key results presented in that appendix.

### 1.1.1 Minkowski metric and index gymnastics

We introduce Greek indices which run over the four spacetime coordinates of objects, as well as the Minkowski metric tensor  $\eta_{\mu\nu}$  which has components

$$\eta_{\mu\nu} = \begin{cases} 1 & \text{if } \mu = \nu = 0, \\ -1 & \text{if } \mu = \nu = 1, 2, \text{ or } 3, \\ 0 & \text{if } \mu \neq \nu. \end{cases} \quad (1.1.1a)$$

From here on out, we will be talking about the contravariant components  $A^\mu$  and the covariant components  $A_\mu$  of a four-vector. They are related by the fundamental relation

$$A_\mu = \eta_{\mu\nu} A^\nu \quad (1.1.1b)$$

where Einstein's summation convention—that is, an index which appears twice in an expression (once as a contravariant—upper—index and once as a covariant—lower—index) is summed over—is implied (unless explicitly mentioned, it will be implied throughout this document). This index-lowering rule can be extended to objects with an arbitrary number of indices, and is completed by the corresponding index-raising rule

$$A^\mu = \eta^{\mu\nu} A_\nu \quad (1.1.1c)$$

with

$$\eta^{\mu\nu} = \begin{cases} 1 & \text{if } \mu = \nu = 0, \\ -1 & \text{if } \mu = \nu = 1, 2, \text{ or } 3, \\ 0 & \text{if } \mu \neq \nu. \end{cases} \quad (1.1.1d)$$

Contracting the metric tensor with itself by  $\eta^\mu_\nu = \eta^{\mu\lambda} \eta_{\lambda\nu}$  yields

$$\eta^\mu_\nu = \begin{cases} 1 & \text{if } \mu = \nu, \\ 0 & \text{if } \mu \neq \nu. \end{cases} \quad (1.1.2)$$

Because of that last equation (1.1.2), the following notation is often employed:  $\eta^\mu_\nu \equiv \delta^\mu_\nu$ . Once all these rules have been introduced, we define the square (pseudo)norm of a four-vector as

$$\boxed{\mathcal{A}^2 = A_\mu A^\mu = \eta_{\mu\nu} A^\mu A^\nu}. \quad (1.1.3)$$

### 1.1.2 Formal definition of the Lorentz group

Special relativity has as its central axiom that observers at rest in all inertial frames of reference measure the same speed of light. Considering any two observers  $O$  and  $O'$ , the following four situations are compatible with this paradigm:

1.  $O$  and  $O'$  are in uniform translatory motion relatively to each other. In that case they measure different values for the time intervals and distances between events in Minkowski space, the values of the distances and intervals for the two observers being linked by the Lorentz boost equations [1].

2.  $O$  and  $O'$  do not move relatively to each other, and sit at the same point in space, but use different—that is, rotated—sets of axes to measure positions (but the same clock). Of course rotation of space axes does not affect the measurement of distances.
3.  $O$  and  $O'$  do not move relatively to each other, but sit at different points in space (but use the same clock). This does not affect their respective measurements of distance either.
4.  $O$  and  $O'$  do not move relatively to each other, and sit at the same point in space, but have a different time origin for their clocks. This does not affect their measurement of time intervals.

All these four subsets—Lorentz boosts, space rotations, space translations, time translations—form the **proper orthochronous Poincaré group**, which is the fundamental symmetry group of special relativity. It consists of all the space orientation- and time direction-conserving transformations which allow to build an inertial frame of reference from another one through changes of the space and time axes (Lorentz boosts, rotation) and shifts in the spatiotemporal origin of the frames (space and time translations). The other two possible transformations of space and time coordinates, which leave the speed of light invariant, are space reflections with respect to a plane, and time inversion, the so-called discrete symmetries of special relativity. The **proper orthochronous Poincaré group** consists of the Poincaré transformations which conserve the direction of time and the orientation of space. The full Poincaré group consists of four disconnected components [1], one of which is the proper orthochronous Poincaré group. Elements of disconnected components of the full Poincaré group cannot be transformed into one another by a continuous change of parameters (boost velocities, rotation angles, translation four-vectors), as is the case for elements of the same component (see sect. 1.A). However elements of disconnected components can be accessed from the proper orthochronous Poincaré group by time reversal and space inversion.

Using covariant notation, we can regroup the action of both Lorentz boosts and rotations on four-vectors in the same equation

$$A'^{\mu} = \Lambda^{\mu}_{\nu} A^{\nu}. \quad (1.1.4)$$

Here  $\Lambda^{\mu}_{\nu}$  is a matrix describing a Lorentz transformation, that is, an arbitrary combination of rotations and Lorentz boosts which link the primed frame of reference to the unprimed one.  $A^{\mu}$  and  $A'^{\mu}$  are the contravariant coordinates of the same four-vector in these two inertial frames of reference. The transformation law of covariant coordinates is given by

$$\begin{aligned} A'_{\mu} &= \eta_{\mu\nu} A'^{\nu} \\ &= \eta_{\mu\nu} \Lambda^{\nu}_{\zeta} A^{\zeta} \\ &= \eta_{\mu\nu} \eta^{\zeta\lambda} \Lambda^{\nu}_{\zeta} A_{\lambda} \\ &= \Lambda^{\lambda}_{\mu} A_{\lambda}. \end{aligned}$$

The invariance of the Minkowski norm can be translated in terms of Lorentz matrices:

$$\begin{aligned} A'_{\mu} A'^{\mu} &= A_{\mu} A^{\mu}. \\ \eta_{\mu\nu} A'^{\mu} A'^{\nu} &= \eta_{\mu\nu} A^{\mu} A^{\nu}. \\ \eta_{\mu\nu} \Lambda^{\mu}_{\zeta} \Lambda^{\nu}_{\lambda} A^{\zeta} A^{\lambda} &= \eta_{\mu\nu} \delta^{\zeta}_{\mu} \delta^{\lambda}_{\nu} A^{\zeta} A^{\lambda}. \\ \eta_{\mu\nu} \Lambda^{\mu}_{\zeta} \Lambda^{\nu}_{\lambda} &= \eta_{\mu\nu} \delta^{\zeta}_{\mu} \delta^{\lambda}_{\nu}. \\ \eta_{\mu\nu} \Lambda^{\mu}_{\zeta} \Lambda^{\nu}_{\lambda} &= \eta_{\zeta\lambda}. \\ (\Lambda^{\top})^{\mu}_{\zeta} \eta_{\mu\nu} \Lambda^{\nu}_{\lambda} &= \eta_{\zeta\lambda}. \end{aligned}$$

This yields the following identity, which is in fact the **definition of the Lorentz group**:

$$\boxed{(\Lambda^\top \eta \Lambda)_{\mu\nu} = \eta_{\mu\nu}}. \quad (1.1.5)$$

In that light, the Lorentz group is formally defined as the group of all transformations of Minkowski space that leave the norm of four-vectors invariant. It consists, as mentioned above (1.1.4), of Lorentz boosts and rotations. The Poincaré group consists of the set of all transformations of the Lorentz groups to which one “adds” spacetime translations. We mention that the identity (1.1.5) ensures that the Kronecker form  $\delta_\nu^\mu \equiv \eta_\nu^\mu$  defined above and the well known completely antisymmetric Levi-Civita form  $\epsilon_{\mu\nu\rho\sigma}$  are invariant under Lorentz transformations.

It can be checked [1] from (1.1.5) that  $\text{Det}\Lambda = \pm 1$  and that  $|\Lambda_0^0| \geq 1$ . The proper orthochronous Lorentz group consists of Lorentz transformations for which  $\text{Det}\Lambda = +1$  and  $\Lambda_0^0 \geq 1$ , and contains the identity transformation  $\delta_\mu^\nu$ . From then on, we will only focus on the proper orthochronous Lorentz and Poincaré groups, but for the sake of simplicity will refer to them simply as the Lorentz and Poincaré groups.

We write, around the identity transformation,  $\Lambda^{\mu\nu} = \delta^{\mu\nu} + \omega^{\mu\nu}$ . It is easy to show that (1.1.5) demands that  $\omega^{\mu\nu} = -\omega^{\nu\mu}$ . Such antisymmetric  $(4 \times 4)$  matrices have six independent components and can be expanded [18] over the basis

$$(M^{\rho\sigma})^{\mu\nu} = \eta^{\rho\mu}\eta^{\sigma\nu} - \eta^{\rho\nu}\eta^{\sigma\mu} \quad (1.1.6)$$

as

$$\omega^{\mu\nu} = \frac{1}{2}\Omega_{\rho\sigma}(M^{\rho\sigma})^{\mu\nu}. \quad (1.1.7)$$

The six  $M$  matrices obey the commutation relations

$$[M^{\alpha\beta}, M^{\mu\nu}] = -\eta^{\alpha\mu}M^{\beta\nu} + \eta^{\alpha\nu}M^{\beta\mu} + \eta^{\beta\mu}M^{\alpha\nu} - \eta^{\beta\nu}M^{\alpha\mu}. \quad (1.1.8)$$

### 1.1.3 Key elements of the representation theory of the Poincaré group

Here we try and give a summary of what is developed in the appendix 1.A to this chapter. While Lorentz transformations keep the square-norm of any four-vector invariant, the Poincaré group is the group of all the transformations of Minkowski space that keep the square-norm of the difference of any two four-vectors invariant<sup>1</sup>. The invariance of the speed of light under Poincaré transformations is a special case of that property.

The Poincaré group is a Lie group, that is, a group which is also a smooth manifold for which the group operations are smooth maps. The tangent space to that manifold at the identity element of the group is called the Lie algebra of the group. Explicitly, an element  $g$  of the Poincaré group  $G$  is obtained by the exponentiation of an element of the Poincaré algebra (*i.e.* the Lie algebra of the Poincaré group). Hence the group law of a Lie group is determined by the Lie brackets of its Lie algebra (see sect. 1.A.1), which means that for our purposes we can restrain our study to the Lie algebra of the Poincaré group. This algebra is generated by ten elements: four translations  $P_\mu$  and six Lorentz transformations  $J_{\mu\nu} = -J_{\nu\mu}$ . Lorentz transformations can be further split into three spatial rotations  $J_{ij}$  and three Lorentz boosts  $J_{0i}$ . This means that any element  $m$  of the Poincaré algebra  $\mathfrak{g}$  is a linear superposition of the form

$$\boxed{\mathfrak{g} \ni m = ib^\mu P_\mu + \frac{i}{2}\Omega^{\mu\nu} J_{\mu\nu}}. \quad (1.1.9)$$

The structure of the Poincaré algebra is defined by the following Lie brackets:

$$[P_\mu, P_\nu] = 0, \quad (1.1.10a)$$

<sup>1</sup>This comes from the fact that the Poincaré group consists of Lorentz transformations and spacetime translations.



$$[P_\mu, J_{\nu\rho}] = i(\eta_{\mu\nu}P_\rho - \eta_{\mu\rho}P_\nu), \quad (1.1.10b)$$

$$[J_{\mu\nu}, J_{\rho\sigma}] = i(\eta_{\mu\rho}J_{\sigma\nu} - \eta_{\nu\rho}J_{\sigma\mu} - \eta_{\mu\sigma}J_{\rho\nu} + \eta_{\nu\sigma}J_{\rho\mu}). \quad (1.1.10c)$$

A representation  $T$  of a Lie algebra  $\mathfrak{g}$  on a vector space  $X$  is a linear application which to every element of  $\mathfrak{g}$  associates an element of the endomorphisms of  $X$  (see sect. 1.A.2.1). Extensive study of the representations of the Poincaré algebra has been carried out by Wigner [12]. Probably the most important outgrowth of this work is the classification of all admissible relativistic wave equations. This was again done by Wigner, this time collaborating with Bargmann [13]. They started from the possible representations of the Poincaré algebra found by Wigner in [12] and wrote the corresponding wave equations, known as the Wigner-Bargmann equations. The Klein-Gordon, Dirac, Weyl, Proca, Maxwell, etc. equations are all Wigner-Bargmann equations, classified according to mass and spin. To build a relativistic field theory we are led to study the irreducible representations (see sect. 1.A.2.1) of the Poincaré algebra. Classifying these representations is done by the way of examining the Casimir operators  $\mathcal{C}_\alpha$  of the algebra which are defined as

$$\forall m \in \mathfrak{g} \quad [\mathcal{C}_\alpha, m] = 0. \quad (1.1.11)$$

We can show, and this is done in sect. 1.A.2.2, that there are two such Casimir operators for the Poincaré algebra:

- $P^2 = P^\mu P_\mu \equiv \mathcal{C}_1$  where  $P_\mu$  is the generator of spacetime translations.
- $W^2 = W^\mu W_\mu \equiv \mathcal{C}_2$  where  $W_\mu$  is the Pauli-Lubański four-pseudovector:

$$W_\mu \equiv -\frac{1}{2}\epsilon_{\mu\nu\rho\sigma}J^{\nu\rho}P^\sigma \quad (1.1.12)$$

with  $\epsilon_{\mu\nu\rho\sigma}$  the totally antisymmetric tensor.

From the definition (1.1.11) of these Casimir operators, we understand the importance of their corresponding physical quantities: the latter are conserved under all transformations of the Poincaré group.

Important information about the particles is given by the action of the Hilbert space-representatives of these Casimir invariants on one-particle states. Since  $\hat{P}^2$  and  $\hat{W}^2$  commute with all the elements of the Poincaré algebra, they commute with each other and can be diagonalised simultaneously. One obtains, for massive particles (see sect. 1.A.3.3)  $\hat{P}^2 |p, s, \zeta\rangle = m^2 |p, s, \zeta\rangle$  and  $\hat{W}^2 |p, s, \zeta\rangle = -m^2 s(s+1) |p, s, \zeta\rangle$  where  $s$  is positive and is either an integer or a half-integer. Here  $\zeta$  refers to the quantum numbers necessary to describe a one-particle state, in addition to its momentum  $p$  and spin  $s$ . Since  $\hat{P}^2$  and  $\hat{W}^2$  are (Casimir invariants and hence) conserved under Poincaré transformations, the invariant mass  $m$  and the spin  $s$  of a (massive) particle are Poincaré invariants. For massless particles  $\hat{P}^2$  and  $\hat{W}^2$  both vanish, but it is possible to show (see sect. 1.A.3.4) that  $\hat{W}_\mu |k, \lambda, \zeta\rangle = \lambda \hat{P}_\mu |k, \lambda, \zeta\rangle$  where  $\lambda$  is an integer. Since  $\hat{P}^2$  is conserved under Poincaré transformations, the invariant mass remains zero in all inertial frames of reference. Since  $\hat{P}^\mu$  is a vector and  $\hat{W}^\mu$  a pseudovector,  $\lambda$  is, up to a sign, conserved under Poincaré transformations, and conserved (without any change of sign) under transformations of the proper orthochronous Poincaré group. It corresponds to the helicity of the massless one-particle state  $|k, \lambda, \zeta\rangle$ . Representation theory of the Poincaré group thus classifies particles by mass and spin or, in the case of massless particles, by helicity. As can be seen from (1.A.26) and (1.A.29), helicity is the component of the angular momentum of a particle along its linear momentum. We investigate in the impending sect. 1.2 the case of the vector field, which we shall see corresponds, for massless particles, to helicities  $\lambda = \pm 1$ , that is, to photons.

## 1.2 Wigner-Bargmann equation for the Maxwell field

Experiments tell us that photons are massless [14] particles of helicity  $\lambda = \pm 1$ . But a one-particle theory is ill-adapted to a fully relativistic framework. We must thus make steps towards a field theory. The first step is to

establish the equivalence between the behaviour of vector fields under Poincaré transformations and the Proca (here, it will be Maxwell since we will focus on the massless case) equations. This exercise amounts to a pedestrian construction of the Wigner-Bargmann field equation for a massless, helicity  $\pm 1$  representation of the Poincaré group.

## 1.2.1 General vector field

A vector field  $A_\mu$  is defined by its behaviour under Poincaré transformations  $(\Lambda, a)$ :

$$\boxed{A'_\mu(x') = \Lambda_\mu^\nu A_\nu(x)} \quad (1.2.1)$$

where  $x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu$  and  $A'_\mu$  describes the vector field as observed in the primed frame of reference.

For an infinitesimal transformation  $\Lambda_\mu^\nu = \delta_\mu^\nu + \omega_\mu^\nu$  around the identity, the relation (1.2.1) is rewritten

$$A'_\mu(x) + \delta x^\nu \partial_\nu A'_\mu(x) = A_\mu(x) + \omega_\mu^\nu A_\nu(x) \quad (1.2.2)$$

to first order. Hence the field variation:

$$A'_\mu(x) - A_\mu(x) = -\delta x^\nu \partial_\nu A_\mu(x) + \omega_\mu^\nu A_\nu(x). \quad (1.2.3)$$

This variation is generated by an infinitesimal Poincaré transformation, that is, by the corresponding element of the Poincaré algebra. Explicitly (see (1.1.9))

$$A'_\mu(x) - A_\mu(x) = \left( i a^\nu T(P_\nu) + \frac{i}{2} \Omega^{\nu\tau} T(J_{\nu\tau}) \right) A_\mu(x) \quad (1.2.4)$$

where  $T(m)$  is the representative of  $m$  on the space of vector fields (sect. 1.A.2.1). From what we wrote above it is easy to see that

$$\delta x^\mu = a^\mu + \omega^\mu_\nu x^\nu, \quad (1.2.5)$$

from which we have

$$-(a^\nu + \omega^\nu_\tau x^\tau) \partial_\nu A_\mu + \omega_\mu^\nu A_\nu = \left( i a^\nu T(P_\nu) + \frac{i}{2} \Omega^{\nu\tau} T(J_{\nu\tau}) \right) A_\mu. \quad (1.2.6)$$

Use (1.1.6) and (1.1.7) to write

$$-a^\nu \partial_\nu A_\mu - \frac{1}{2} \Omega^{\nu\tau} (x_\tau \partial_\nu - x_\nu \partial_\tau) A_\mu - \frac{1}{2} \Omega^{\nu\tau} (\eta_{\tau\mu} A_\nu - \eta_{\nu\mu} A_\tau) = \left( i a^\nu T(P_\nu) + \frac{i}{2} \Omega^{\nu\tau} T(J_{\nu\tau}) \right) A_\mu. \quad (1.2.7)$$

The action of the representatives of the generators of the Poincaré algebra for a vector field is then deduced:

$$T(P_\mu) = i \partial_\mu, \quad (1.2.8a)$$

$$(T(J_{\mu\nu}))^\sigma_\rho = -i [(x_\mu \partial_\nu - x_\nu \partial_\mu) \delta_\rho^\sigma + (\eta_{\mu\rho} \delta_\nu^\sigma - \eta_{\nu\rho} \delta_\mu^\sigma)]. \quad (1.2.8b)$$

Now take a look at the Casimir invariants. For  $P^2$  we have, by definition (see sect. 1.A.3),  $T(P^2) = m^2$ . This yields the Klein-Gordon equation

$$(\partial^\nu \partial_\nu + m^2) A_\mu = 0. \quad (1.2.9)$$

which, as we have shown, appears simply by the study of the symmetries of Minkowski space.

As for  $W^2$ , we have (see sect. 1.A.3)  $T(W^2) = -m^2 s(s+1)$  for massive particles and  $T(W^2) = 0$  for massless

particles. We compute, now dropping the heavy  $T(\cdot)$  notation for representatives

$$\begin{aligned}
W^\mu W_\mu A^\nu &= W^\mu \left( -\frac{1}{2} \right) \epsilon_{\mu\rho\sigma\tau} (J^{\rho\sigma})^\nu_\lambda P^\tau A^\lambda \\
&= W^\mu \left( \frac{1}{2} \right) \epsilon_{\mu\rho\sigma\tau} (i(x^\rho \partial^\sigma - x^\sigma \partial^\rho) \delta^\nu_\lambda - i(\eta^{\rho\nu} \delta^\sigma_\lambda - \eta^{\sigma\nu} \delta^\rho_\lambda)) P^\tau A^\lambda \\
&= W^\mu \left( -\frac{i}{2} \right) \epsilon_{\mu\rho\sigma\tau} (\eta^{\rho\nu} \delta^\sigma_\lambda - \eta^{\sigma\nu} \delta^\rho_\lambda) P^\tau A^\lambda \\
&= W^\mu \left( -\frac{i}{2} \right) [\epsilon_\mu^{\nu\lambda\tau} - \epsilon_\mu^{\lambda\nu\tau}] P_\tau A_\lambda \\
&= W^\mu i \epsilon_\mu^{\nu\tau\lambda} P_\tau A_\lambda \\
&= -\epsilon_\mu^{\nu\tau\lambda} \epsilon_{\lambda\sigma\rho}^\mu P_\tau P^\sigma A^\rho \\
&= 2 (\delta_\sigma^\nu \delta_\rho^\tau - \delta_\sigma^\tau \delta_\rho^\nu) P_\tau P^\sigma A^\rho \\
&= 2 (P^\nu P^\mu A_\mu - P^\mu P_\mu A^\nu). \tag{1.2.10}
\end{aligned}$$

where we made use of (1.2.8) and of the antisymmetry of the Levi-Civita form. At this point it is hard to read anything clear from (1.2.10). For massive particles we try and contract it with  $P_\nu$ :

$$\begin{aligned}
2 (P^2 P_\nu A^\nu - P^2 P_\nu A^\nu) &= -m^2 s (s+1) P_\nu A^\nu, \\
\text{hence } 0 &= -m^2 s (s+1) P_\nu A^\nu. \tag{1.2.11}
\end{aligned}$$

Thus there are two possibilities for a massive vector field: either  $s = 0$ , or  $P^\mu A_\mu = 0$ . We only very briefly explore these cases in the following sect. 1.2.2, and then focus on the massless case, where (1.2.10) can be rewritten

$$0 = P^\nu P^\mu A_\mu - P^\mu P_\mu A^\nu. \tag{1.2.12}$$

## 1.2.2 Massive vector field: a quick detour

### 1.2.2.1 Massive vector field of spin 1

For a massive vector field, we first look at the case  $s \neq 0$ . In that case we have  $P^\mu A_\mu = 0$  from (1.2.11). With the action (1.2.10) of the Casimir operator  $W^2$  on the field in mind, we remember the general result  $W^2 A^\mu = -m^2 s (s+1) A^\mu$  and deduce

$$P^\nu P_\nu A_\mu = \frac{1}{2} m^2 s (s+1) A_\mu. \tag{1.2.13}$$

Upon comparing this with the general action  $P^\mu P_\mu A^\nu = m^2 A^\nu$  of the other Casimir operator  $P^2$ , we see that the massive vector field has spin  $s = 1$ . We can then write the final form of the field equation, the Proca equation:

$$\partial^\nu \partial_\nu A_\mu = -m^2 A_\mu. \tag{1.2.14}$$

In this form, it is just the Klein-Gordon equation, but we already knew (see (1.2.9)) that it is a constraint which  $A_\mu$  should obey.

### 1.2.2.2 Massive vector field of spin 0

We then explore the second case, for which  $s = 0$ . In this case we see from (1.2.10) that

$$P^\nu P_\nu A_\mu - P_\mu P^\nu A_\nu = 0, \tag{1.2.15}$$

which can be cast as

$$P^2 \left( \delta_\mu^\nu - \frac{P_\mu P^\nu}{P^2} \right) A_\nu = 0. \quad (1.2.16)$$

This massive, spinless case will be of no further interest to us, but we will see that the massless case features the same wave equation as (1.2.15).

### 1.2.3 Massless vector field: Maxwell equation

In the latter, massless case, the field equation (1.2.12) is written, expliciting the action (1.2.8) of the generators of the Poincaré algebra

$$\boxed{\partial^\nu \partial_\nu A_\mu - \partial^\nu \partial_\mu A_\nu = 0}. \quad (1.2.17)$$

This is the (source-free) Maxwell equation(s). But it is not sufficient to determine  $A_\mu$ : for a solution  $A_\mu$  and an arbitrary—though sufficiently differentiable—function  $\Xi$  of spacetime coordinates we can make the transformation

$$A_\mu \rightarrow A_\mu + \partial_\mu \Xi \equiv \check{A}_\mu \quad (1.2.18)$$

and  $\check{A}_\mu$  is a new solution to (1.2.17). This is the well known gauge invariance of electrodynamics when we use the potentials instead of the field: the four-vector  $A^\mu = (A^0, \mathbf{A})$  is the object formed by the scalar potential  $A^0$  and the vector potential  $\mathbf{A}$  of classical electrodynamics. The transformation (1.2.18) is called a **gauge transformation**.

For those unused to covariant notation—or forgetful—we remind that the electromagnetic field is described by an antisymmetric second-rank tensor sometimes—including in this work—called the Faraday tensor. It is defined by

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu \quad (1.2.19)$$

and its nonzero components are given by

$$F^{0i} = -\frac{E^i}{c}, \quad (1.2.20a)$$

$$F^{jk} = -\epsilon^{0ijk} B_i. \quad (1.2.20b)$$

In terms of the Faraday tensor, the source-free Maxwell equations read

$$\partial_\mu F^{\mu\nu} = 0 \quad (1.2.21a)$$

as seen from (1.2.17) and

$$\partial^\mu F^{\rho\sigma} + \partial^\rho F^{\sigma\mu} + \partial^\sigma F^{\mu\rho} = 0 \quad (1.2.21b)$$

as seen from (1.2.19). Here (1.2.21a) corresponds to the (source-free) Maxwell-Gauß and Maxwell-Ampère equations, while (1.2.21b) corresponds to the Maxwell-Faraday and Maxwell-Thomson equations. Notice that the Faraday tensor is unaffected by gauge transformations (1.2.18):  $\partial^\mu \check{A}^\nu - \partial^\nu \check{A}^\mu \equiv \check{F}^{\mu\nu} = F^{\mu\nu}$ . We end this section by writing the two relativistic invariants [2] of the electromagnetic field:

$$-F^{\mu\nu} F_{\mu\nu} = 2 \left( \frac{\mathbf{E}^2}{c^2} - \mathbf{B}^2 \right), \quad (1.2.22a)$$

$$-\epsilon_{\mu\nu\rho\sigma} F^{\mu\nu} F^{\rho\sigma} = \frac{4}{c} (\mathbf{E} \cdot \mathbf{B}) \quad (1.2.22b)$$

## 1.2.4 Fields, potentials, and gauges: degrees of freedom

The electric and magnetic fields are not subject to the gauge freedom of the four-vector potential, which makes them more agreeable to the intuition, but they are less straightforward to work with than the potential four-vector. Ultimately, the interactions of the electromagnetic field with matter are expressed in terms of the potential. To accommodate our working with the potential, the gauge can (and should) be fixed, for instance through the Lorenz<sup>2</sup> gauge condition  $\partial^\mu A_\mu = 0$  or the Coulomb gauge condition  $A^0 = 0, \nabla \cdot \mathbf{A} = 0$ . In sect. 1.3 we will study the quantisation of the Maxwell field  $A^\mu$  in both these gauges.

The massless vector field  $A^\mu$  obeying the Maxwell equation (1.2.17) describes massless particles of helicities  $\pm 1$ <sup>3</sup>. The fact that particles with helicities of equal magnitude but opposite sign are described by the same field is due [1] to the requirement that electrodynamics be invariant under space inversions<sup>4</sup>. As a consequence we expect that in the massless case  $A^\mu$  carries only two degrees of freedom. But does it? The answer, of course, is no—otherwise why would we even ask the question?—as we now discuss.

Let us, once again, begin by examining the easier massive case. We saw in sect. 1.2.2.1 that for the  $s \neq 0$  massive case the vector field is constrained to be orthogonal to the momentum:  $P^\mu A_\mu = 0$ , and that it should obey the Proca equations  $(\partial^\mu \partial_\mu + m^2) A^\nu = 0$ . A priori each component of  $A^\mu$  carries a degree of freedom, but the orthogonality constraint kills one degree of freedom, because it tells us that there are only three independent components of the field. The Proca equations, on the other hand, form a set of four equations solved separately by the various components of the field. Thus they do not reduce the number of degrees of freedom. This means that in the end the massive, spin 1 vector field carries three degrees of freedom. They correspond, for instance, to the three eigenvalues values  $+1, 0, -1$  of the projection operator  $\hat{J}_3$  of the angular momentum on the  $z$  axis. Indeed,  $\hat{J}_3$  and the Casimir operator  $\hat{W}^2 = -m^2 \hat{\mathbf{J}}^2$  can be simultaneously diagonalised (see appendix 1.A). This corresponds to the usual [3, 4] quantum physics of angular momentum.

In the massless case the Maxwell equations (1.2.17) do kill a degree of freedom, because of the index structure of the second term  $\partial^\nu \partial_\mu A_\nu$  on the left-hand side<sup>5</sup>. But this is—except for the nonviolent Klein-Gordon equation<sup>6</sup> (1.2.9), which does not kill any degrees of freedom—the only equation the field should obey, and we are left with three field degrees of freedom compared to two expected helicity states. Of course now gauge fixing should somehow fix this problem.

- It readily does if we choose the Coulomb gauge condition  $A^0 = 0, \nabla \cdot \mathbf{A} = 0$ , which kills two degrees of freedom. In that case the Maxwell equations (1.2.17) are reduced to  $\partial^\mu \partial_\mu A_i = 0$ , which is simply the zero mass Klein-Gordon equation and does not kill any further degree of freedom.
- On the other hand, if we choose the Lorenz gauge condition  $\partial^\mu A_\mu = 0$ , this kills one degree of freedom and the Maxwell equations read, again,  $\partial^\mu \partial_\mu A_\nu = 0$ . Thus the total number of degrees of freedom is three. This is problematic, but, as we shall see in sect. 1.A.4, is solved when quantising the field.

<sup>2</sup>It is indeed “Lorenz” for Ludvig Lorenz, a Danish physicist who first introduced this gauge fixing scheme. As for Dutchman Hendrik Lorentz, he wrote the equations for the change of reference frames compatible with electrodynamics. The Lorenz gauge condition is invariant under Lorentz transformations, the source of endless confusion.

<sup>3</sup>At this point, we have enforced the masslessness to go from (1.2.10) to (1.2.12), but have not encountered helicity in sect. 1.2. We will see that helicities  $\pm 1$  are the only possibility for a massless field transforming as (1.2.1) under Poincaré transformations.

<sup>4</sup>Ultimately, this is again linked to the structure of the full Lorentz group (remember that it consists of four disconnected components).

<sup>5</sup>Which has the consequence that the four components of  $A^\mu$  are not independent from each other.

<sup>6</sup>Here, with zero mass.

## 1.3 Canonical quantisation of the Maxwell field: some preliminaries

We are now getting closer to the satisfactory definition of a photon. For this, we need to quantise the massless vector field studied in sect. 1.2. This means that the field will become a linear operator acting on a Hilbert space. The nature of this operator is determined by the canonical Poisson bracket of the classical field theory which, upon quantisation, becomes a commutator.

### 1.3.1 Relativistic field theory: a brief introduction

#### 1.3.1.1 The principle of least action

Classical—in the sense of non-quantum—physics can be and often is formulated in terms of the principle of least action. This principle states that for a physical system there is a certain quantity, called the action, to be defined below, which, expressed in function of an arbitrary generalised trajectory of the system, reaches its extremal values for the actual generalised trajectory of the system. In classical mechanics, for instance, the generalised trajectory is the trajectory of an assembly of particles in three-dimensional space, the Lagrangian is the difference between the kinetic energy and the potential energy of the system, and the principle of least action is equivalent to Newton's second law. Once we switch to fields, the fundamental degrees of freedom are no longer the positions and momenta of a collection of particles, but the values of a field  $\varphi$  at every point in space. The action  $S$  of the field over the spacetime domain  $\Omega$  is then defined by

$$S_{\Omega}[\varphi] = \int_{\Omega} d^4x \mathcal{L}(x, \varphi(x)) \quad (1.3.1a)$$

where  $\mathcal{L}$  is the Lagrangian density of the field. One then asks that this quantity be extremal to find the actual value of the field  $\varphi$ . If the Lagrangian is only a functional of the field and its first space-and-time derivatives, and also a functional of the spacetime coordinates, then we write

$$S_{\Omega}[\varphi] = \int_{\Omega} d^4x \mathcal{L}\left(x, \varphi(x), \frac{\partial\varphi}{\partial t}(x), \frac{\partial\varphi}{\partial x^i}(x)\right). \quad (1.3.1b)$$

and for the action to be extremal  $\varphi$  should solve the Euler-Lagrange field equations [5]

$$\frac{\partial\mathcal{L}}{\partial\varphi(x)} - \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\varphi}{\partial t}(x)\right)}\right) - \frac{d}{dx^i}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\varphi}{\partial x^i}(x)\right)}\right) = 0. \quad (1.3.2)$$

In covariant notation, this reads

$$\boxed{\frac{\partial\mathcal{L}}{\partial\varphi(x)} - d_{\mu}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\varphi}{\partial x^{\mu}}(x)\right)}\right) = 0.} \quad (1.3.3)$$

Here the seldom-used notation  $d_{\mu}$  stands for a total derivative with respect to  $x^{\mu}$ . If the Lagrangian density is a function of several—say,  $n$ —fields, then there are  $n$  such Euler-Lagrange equations of motion, one for each field.

#### 1.3.1.2 Hamilton's canonical formalism

If for electrodynamics we choose

$$\mathcal{L}(A^{\mu}, \partial^{\nu}A^{\mu}) = \frac{1}{2}\left(\epsilon_0\mathbf{E}^2 - \frac{1}{\mu_0}\mathbf{B}^2\right) = -\frac{1}{4\mu_0}F^{\rho\sigma}F_{\rho\sigma} = -\frac{1}{4\mu_0}(\partial^{\rho}A^{\sigma} - \partial^{\sigma}A^{\rho})(\partial_{\rho}A_{\sigma} - \partial_{\sigma}A_{\rho}) \quad (1.3.4)$$

then the Euler-Lagrange equations are the Maxwell equations (1.2.17). We may therefore ask why the introduction of the action is necessary, since we derived the Maxwell equations from the representation theory of the Poincaré group. In that sense, we deduced the action from the field equation, and not the opposite. The answer is that this so-called canonical formalism is needed to know how to promote the massless vector field  $A^\mu$  to a linear operator on a Hilbert space, which is the way to obtain the quantum theory of the electromagnetic field.

In the generic case define the **canonically conjugate momentum**  $\pi_j$  to the field  $\varphi_j$  (here  $j$  can stand for any type of index or set of indices, including Mikowski indices) as

$$\pi_j(x) \equiv \frac{\partial \mathcal{L}}{\partial (\partial_t \varphi^j(x))} \quad (1.3.5)$$

where the difference between the upper and lower position of the index is only meaningful for Minkowski indices. The Hamiltonian  $\mathcal{H}$  density is then defined by

$$\mathcal{H}(\varphi_j, \pi_j) \equiv \left[ \sum_i (\partial_t \varphi^i) \pi_i \right] - \mathcal{L}(\varphi_j, \partial^\mu \varphi_j). \quad (1.3.6)$$

Note that though the Lagrangian and Hamiltonian densities are rather easier to work with than the actual Lagrangian and Hamiltonian, we can define such objects with

$$L[\varphi_j, \partial^\mu \varphi_j](t) \equiv \int dx \mathcal{L}(\varphi_j(x), \partial^\mu \varphi_j(x)) \quad \text{and} \quad H[\varphi_j, \pi_j](t) \equiv \int dx \mathcal{H}(\varphi_j(x), \pi_j(x)). \quad (1.3.7)$$

Here the square brackets indicate functional dependence:  $L$  and  $H$  depend on the value of the field, its derivatives (only for  $L$ ) or its conjugate momentum (only for  $H$ ) at every point in space. The abstract, infinite-dimensional space of all the values of  $\varphi_j$  and  $\pi_j$  at every point in space is known as phase space.

The Euler-Lagrange equations can be rewritten in terms of the canonical variables  $\varphi_j$  and  $\pi_j$ , yielding the so-called Hamilton equations

$$\frac{\partial \varphi_j}{\partial t}(x) = \frac{\delta \mathcal{H}}{\delta \pi^j(x)}, \quad (1.3.8a)$$

$$\frac{\partial \pi^j}{\partial t}(x) = -\frac{\delta \mathcal{H}}{\delta \varphi_j(x)}. \quad (1.3.8b)$$

For all practical purposes, the functional derivative can be understood [5] here as

$$\frac{\delta}{\delta \eta} \equiv \frac{\partial}{\partial \eta} - d_\mu \frac{\partial}{\partial (\partial_\mu \eta)}. \quad (1.3.9)$$

### 1.3.1.3 Poisson brackets

For any two sufficiently differentiable functionals  $F$  and  $G$  defined over phase space, we can define their Poisson bracket  $\{F, G\}$ , which is another functional over phase space, as follows:

$$\{F, G\}[\varphi_j, \pi_j](t) \equiv \sum_j \int dx \left[ \frac{\delta F}{\delta \varphi_j(x)} \frac{\delta G}{\delta \pi^j(x)} - \frac{\delta F}{\delta \pi^j(x)} \frac{\delta G}{\delta \varphi_j(x)} \right]. \quad (1.3.10)$$

One such Poisson bracket is the central object of the quantisation procedure. Luckily, it is the easiest one to calculate (except for the cases where  $F$  and/or  $G$  are/is identically zero, of course). It is called the **canonical**

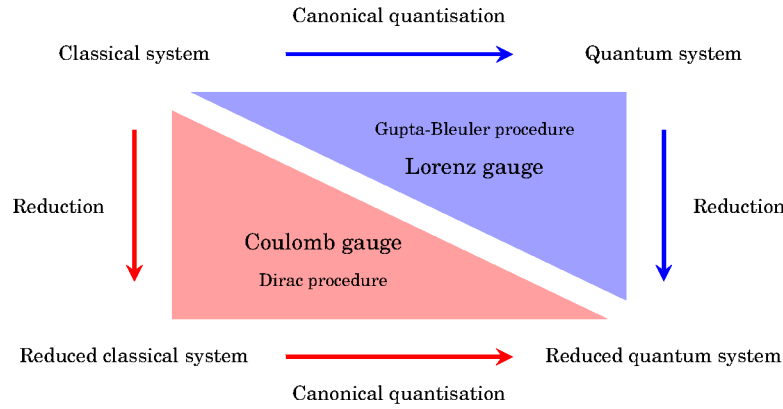


Fig. 1.3.1 – Quantisation of the electromagnetic field: two possible paths.

**Poisson bracket** and reads

$$\begin{aligned}
 \{\varphi_m(\mathbf{x}_1, t), \pi^n(\mathbf{x}_2, t)\} &= \sum_j \int d\mathbf{x} \left[ \frac{\delta\varphi_m(\mathbf{x}_1, t)}{\delta\varphi_j(\mathbf{x}, t)} \frac{\delta\pi^n(\mathbf{x}_2, t)}{\delta\pi^j(\mathbf{x}, t)} - \frac{\delta\varphi_m(\mathbf{x}_1, t)}{\delta\pi^j(\mathbf{x}, t)} \frac{\delta\pi^n(\mathbf{x}_2, t)}{\delta\varphi_j(\mathbf{x}, t)} \right] \\
 &= \sum_j \int d\mathbf{x} [\delta_m^j \delta_j^n \delta(\mathbf{x} - \mathbf{x}_1) \delta(\mathbf{x} - \mathbf{x}_2) - 0] \\
 &= \delta_m^n \delta(\mathbf{x}_1 - \mathbf{x}_2).
 \end{aligned} \tag{1.3.11}$$

where we made use of (1.3.9). When the theory is quantised, the field  $\varphi_j$  and its canonical momentum  $\pi_j$  become operators on a Hilbert space, and their commutator or their anticommutator is given—up to a factor  $i$ —the value of the canonical Poisson bracket (1.3.11). This is **canonical quantisation**.

## 1.3.2 Fields, potentials, and gauges: when to quantise

We learned in sects. 1.3.1.2 and 1.3.1.3 how to build a **field operator**, that is, a Hilbert space-operator corresponding to a classical field. For a massless vector field, we will see, however, that this method cannot be implemented directly. This is due to what we discussed at length in the twin sect. 1.2.4 of the present section, namely, the problem of the gauge degree of freedom carried by the field.

In sect. 1.2.4 we asserted that gauge fixing was the solution to the issue. We know that if we enforce the Coulomb gauge condition, the number of degrees of freedom is reduced to two. The quantisation of the field can then be carried from there, as we do in sect. 1.4. The price to pay for enforcing that two of the four components of  $A^\mu$  carry redundant information is that it causes complications in applying Hamilton’s canonical formalism. But invoking Dirac’s work on the quantisation of such constrained systems—here the constraint is the gauge fixing condition—saves the day. If we enforce the Lorenz gauge condition, however, we realise that the vector space of one-photon states we are able to build is not a Hilbert space, which makes the use of the Born rule (1.A.17) problematic as it yields negative probabilities for some couples of state vectors ( $|m\rangle, |n\rangle$ ). Gupta [15] and Bleuler [16], however, showed that this problem of negative probabilities and the issue of degrees of freedom could be solved together<sup>7</sup>. Their method is exposed in sect. 1.A.4. These two possibilities are represented on Fig. 1.3.1, where the diagram highlights that the enforcement of constraints and canonical quantisation are performed in reversed orders.

<sup>7</sup>One could even go as far as to say that they solve each other.



## 1.4 Coulomb gauge quantisation

Here we follow Dirac's procedure to quantise a constrained system. The constraints are  $A_0 = 0$ ,  $\partial^i A_i = 0$ . Notice that these conditions are not Lorentz invariant: **the Coulomb gauge condition may only be imposed in a single frame of reference** for  $A^\mu$  to be a four-vector. This means that the Coulomb gauge is a smart choice if there is a reason to consider that some frame of reference should be privileged. It is the case for many physical systems. The Coulomb gauge condition, of course, is not invariant under Lorentz boosts. This is discussed in sect. 1.4.8.

### 1.4.1 Conjugate momenta

The Maxwell-Faraday Lagrangian density which we wrote at (1.3.4) reads  $\mathcal{L} = -1/(4\mu_0) F_{\mu\nu} F^{\mu\nu}$ , with the Faraday tensor  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ . The corresponding Euler-Lagrange equations are the Maxwell equations (1.2.21). To canonically quantise the free electromagnetic field we need to compute the conjugate momenta to the potential four-vector:

$$\begin{aligned}\pi^0 &= \frac{\partial \mathcal{L}}{\partial \dot{A}_0} = 0, \\ \pi^i &= \frac{\partial \mathcal{L}}{\partial \dot{A}_i} = -\frac{F^{0i}}{\mu_0 c} = \epsilon_0 E^i.\end{aligned}\tag{1.4.1}$$

On the one hand, (1.4.1) is incompatible with  $\{A_0(t, \mathbf{x}), \pi^0(t, \mathbf{y})\} = \delta(\mathbf{x} - \mathbf{y})$  because  $\pi^0 = 0$ . On the other hand, the canonical Poisson bracket for the spatial components should read  $\{A_i(t, \mathbf{x}), \pi^j(t, \mathbf{y})\} = \delta_i^j \delta(\mathbf{x} - \mathbf{y})$ , but differentiation with respect to  $\mathbf{x}$  yields

$$\epsilon_0 \{\partial^i A_i(t, \mathbf{x}), E^j(t, \mathbf{y})\} = \partial_{\mathbf{x}}^j \delta(\mathbf{x} - \mathbf{y}),\tag{1.4.2}$$

which is not compatible with the constraint  $\partial^i A_i = 0$ .

Clearly, canonical quantisation will not be straightforward in these circumstances. Since we have  $A_0$  and  $\pi^0$  both vanishing, we understand that these variables can be ignored from the treatment as they do not appear to play a part in the dynamics of the system. The incompatibility between the Poisson bracket (1.4.2) and the Coulomb gauge condition, however, is more problematic. A nice and easy way to solve the latter issue is proposed to the interested reader in sect. 4.4 of Ryder's book [6]. However, we choose to go slightly more in depth and catch a glimpse of Dirac's solution to these problems.

### 1.4.2 Excursion: constraints and Dirac brackets

Dirac developed his formalism for the study of constraints in [17], but once again we follow [1], trying to keep the treatment as simple as possible. Getting back to the general case of fields  $\varphi_j$  and their momenta  $\pi^j$ , we write a general constraint simply by the condition  $\chi_n = 0$ . We shall refer to  $\chi_n$ , which is a functional of the  $\varphi_j$  and the  $\pi^j$ , as a constraint functional. Now we define two classes of constraints:

1. First class constraints are the constraints for which the functional  $\chi_n$  has a vanishing Poisson bracket with all other constraint functionals  $\chi_m$ , when we impose the constraints after computing the Poisson brackets.
2. Second class constraints are all constraints which do not verify this axiom.

In the case where all constraints are second class, Dirac gives a prescription for modifying the canonical Poisson bracket (1.3.11). To the author's limited knowledge, there is no general procedure for first class constraints. But this is not a problem here, since we show that the relevant constraints are second class.

Note that to the Coulomb gauge constraints  $A_0 = 0$ ,  $\partial^i A_i = 0$ , we have added, through (1.4.1), two new constraints:  $\pi^0 = 0$ , and, resulting from the injection of this very constraint in the Maxwell equations (1.2.21),  $\partial^i \pi_i = 0$ . But as we mentioned at the end of the previous sect. 1.4.1,  $A_0$  and  $\pi^0$  are not dynamical variables and can be ignored altogether. The two remaining constraints, it can be shown, are second class. Indeed, keeping (1.3.9) in mind

$$\begin{aligned}
\left\{ \partial_1^i A_i(\mathbf{x}_1, t), \partial_2^j E_j(\mathbf{x}_2, t) \right\} &= \int d\mathbf{x} \left[ \frac{\delta \partial_1^i A_i(\mathbf{x}_1, t)}{\delta A_\mu(\mathbf{x}, t)} \frac{\delta \partial_2^j E_j(\mathbf{x}_2, t)}{\delta E^\mu(\mathbf{x}, t)} - \frac{\delta \partial_1^i A_i(\mathbf{x}_1, t)}{\delta E^\mu(\mathbf{x}, t)} \frac{\delta \partial_2^j E_j(\mathbf{x}_2, t)}{\delta A_\mu(\mathbf{x}, t)} \right] \\
&= \int d\mathbf{x} \left[ d_\rho \left( \frac{\partial (\partial_1^i A_i(\mathbf{x}_1, t))}{\partial (\partial_\rho A_\mu(\mathbf{x}, t))} \right) d_\sigma \left( \frac{\partial (\partial_2^j E_j(\mathbf{x}_2, t))}{\partial (\partial_\sigma E^\mu(\mathbf{x}, t))} \right) \right] \\
&= \int d\mathbf{x} [d_\rho (\eta^{i\rho} \delta_i^\mu \delta(\mathbf{x} - \mathbf{x}_1)) d_\sigma (\eta^{j\sigma} \eta_{j\mu} \delta(\mathbf{x} - \mathbf{x}_2))] \\
&= \eta_{ij} \int d\mathbf{x} d^i(\delta(\mathbf{x} - \mathbf{x}_1)) d^j(\delta(\mathbf{x} - \mathbf{x}_2)) \\
&= -\nabla_1^2 \delta(\mathbf{x}_1 - \mathbf{x}_2) = -\nabla_2^2 \delta(\mathbf{x}_1 - \mathbf{x}_2)
\end{aligned} \tag{1.4.3}$$

through an integration by parts. This Poisson bracket is thus, obviously, nonzero, and we can use Dirac's prescription. When dealing with second class constraints, Dirac advises that instead of quantising the theory in the usual canonical way

$$\begin{array}{ccc}
\varphi_j & \rightarrow & \hat{\varphi}_j, \\
\delta_m^n \delta(\mathbf{x}_1 - \mathbf{x}_2) & = & \{ \varphi_m(\mathbf{x}_1, t), \pi^n(\mathbf{x}_2, t) \} = -\frac{i}{\hbar} [ \hat{\varphi}_m(\mathbf{x}_1, t), \hat{\pi}^n(\mathbf{x}_2, t) ]
\end{array} \tag{1.4.4}$$

we use, instead of the Poisson bracket, the modified bracket (known as Dirac bracket)

$$\{ \varphi_m(\mathbf{x}_1, t), \pi^n(\mathbf{x}_2, t) \}_{\text{Dirac}} \equiv \{ \varphi_m(\mathbf{x}_1, t), \pi^n(\mathbf{x}_2, t) \} - \sum_j \sum_k \int d\mathbf{y} \int d\mathbf{z} \{ \varphi_m(\mathbf{x}_1, t), \chi_j(\mathbf{y}) \} (C^{-1})^{jk}(\mathbf{y}, \mathbf{z}) \{ \chi_k(\mathbf{z}), \pi^n(\mathbf{x}_2, t) \} \tag{1.4.5}$$

where the matrix  $C$  is defined by

$$C^{jk}(\mathbf{y}, \mathbf{z}) \equiv \{ \chi_j(\mathbf{y}), \chi_k(\mathbf{z}) \}. \tag{1.4.6}$$

The inverse matrix  $C^{-1}$  should verify

$$\sum_l \int d\mathbf{w} C^{jl}(\mathbf{y}, \mathbf{w}) (C^{-1})^{lk}(\mathbf{w}, \mathbf{z}) = \delta^{jk} \delta(\mathbf{y} - \mathbf{z}). \tag{1.4.7}$$

### 1.4.3 Excursion continued: Dirac bracket of the electromagnetic field

Armed with this new tool, we compute the quantities in the second summand on the right-hand side of (1.4.5). We already computed (see (1.4.3))  $C^{jk}(\mathbf{y}, \mathbf{z})$ . Write  $\chi_1 \equiv \partial^i A_i$  and  $\chi_2 \equiv \partial^j E_j$ . Since  $C^{jk}(\mathbf{y}, \mathbf{z})$  has zero diagonal elements and  $C^{12}(\mathbf{y}, \mathbf{z}) = -C^{21}(\mathbf{y}, \mathbf{z})$ , we directly know that  $(C^{-1})^{11}(\mathbf{y}, \mathbf{z}) = (C^{-1})^{22}(\mathbf{y}, \mathbf{z}) = 0$  and  $(C^{-1})^{12}(\mathbf{y}, \mathbf{z}) = -(C^{-1})^{21}(\mathbf{y}, \mathbf{z}) \equiv \eta(\mathbf{y}, \mathbf{z})$ , for which we solve by integrating by parts (see (1.4.7)):

$$\begin{aligned}
\delta(\mathbf{y} - \mathbf{z}) &= \int d\mathbf{w} (-\nabla_{\mathbf{w}}^2 \delta(\mathbf{y} - \mathbf{w})) (-\eta(\mathbf{w}, \mathbf{z})) \\
&= \int d\mathbf{w} \delta(\mathbf{y} - \mathbf{w}) (\nabla_{\mathbf{w}}^2 \eta(\mathbf{w}, \mathbf{z}))
\end{aligned}$$

and it is clear, that, if  $\nabla_{\mathbf{w}}^2 \eta(\mathbf{w}, \mathbf{z}) = \delta(\mathbf{w} - \mathbf{z})$ , this equation is satisfied. Distribution theory [7] gives us such a quantity:

$$\eta(\mathbf{w}, \mathbf{z}) = -\frac{1}{4\pi \|\mathbf{w} - \mathbf{z}\|}. \tag{1.4.8}$$

Now, we compute the Poisson brackets of the field and its momentum with the constraint functionals. We find

$$\begin{aligned}
\{A_i(\mathbf{y}, t), \partial_{\mathbf{z}}^j A_j(\mathbf{z})\} &= 0, \\
\{A_i(\mathbf{y}, t), \partial_{\mathbf{z}}^j E_j(\mathbf{z})\} &= \partial_{\mathbf{y}i} \delta(\mathbf{y} - \mathbf{z}), \\
\{E_i(\mathbf{y}, t), \partial_{\mathbf{z}}^j A_j(\mathbf{z})\} &= -\partial_{\mathbf{y}i} \delta(\mathbf{y} - \mathbf{z}), \\
\{E_i(\mathbf{y}, t), \partial_{\mathbf{z}}^j E_j(\mathbf{z})\} &= 0.
\end{aligned} \tag{1.4.9}$$

Putting everything together following Dirac's prescription (1.4.5) yields

$$\begin{aligned}
\epsilon_0 \{A_i(\mathbf{x}, t), E^j(\mathbf{y}, t)\}_{\text{Dirac}} &= \delta_i^j \delta(\mathbf{x} - \mathbf{y}) + \int d\mathbf{w} \int d\mathbf{z} \eta(\mathbf{w}, \mathbf{z}) \partial_{\mathbf{x}i} \delta(\mathbf{x} - \mathbf{w}) \partial_{\mathbf{y}}^j \delta(\mathbf{z} - \mathbf{y}) \\
&= \delta_i^j \delta(\mathbf{x} - \mathbf{y}) - \frac{1}{4\pi} \partial_{\mathbf{x}i} \partial_{\mathbf{y}}^j \int d\mathbf{w} \int d\mathbf{z} \delta(\mathbf{x} - \mathbf{w}) \delta(\mathbf{z} - \mathbf{y}) \frac{1}{\|\mathbf{w} - \mathbf{z}\|} \\
&= \delta_i^j \delta(\mathbf{x} - \mathbf{y}) - \frac{1}{4\pi} \partial_{\mathbf{x}i} \partial_{\mathbf{y}}^j \frac{1}{\|\mathbf{x} - \mathbf{y}\|}.
\end{aligned} \tag{1.4.10}$$

### 1.4.4 Canonical commutator

This last expression (1.4.10) is probably better understood in Fourier space: writing

$$[\hat{A}_i(\mathbf{x}, t), \hat{E}^j(\mathbf{y}, t)] = i\hbar \{A_i(\mathbf{x}, t), E^j(\mathbf{y}, t)\}_{\text{Dirac}}, \tag{1.4.11}$$

we define the **transverse Delta function** as

$$\Delta_{ij}(\mathbf{k}) = -\eta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \tag{1.4.12a}$$

to rewrite the canonical commutator as

$$\epsilon_0 [\hat{A}_i(\mathbf{x}, t), \hat{E}^j(\mathbf{y}, t)] = -i\hbar \int \frac{d\mathbf{k}}{(2\pi)^3} \Delta_{ij}^j(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})}. \tag{1.4.12b}$$

Indeed this yields

$$\begin{aligned}
\epsilon_0 [\hat{A}_i(\mathbf{x}, t), \hat{E}^j(\mathbf{y}, t)] &= i\hbar \int \frac{d\mathbf{k}}{(2\pi)^3} \left( \delta_i^j + \frac{k_i k_j}{\mathbf{k}^2} \right) e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \\
&= i\hbar \left[ \delta_i^j \delta(\mathbf{x} - \mathbf{y}) - \partial_{\mathbf{x}i} \partial_{\mathbf{y}}^j \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})}}{\mathbf{k}^2} \right] \\
&= i\hbar \left[ \delta_i^j \delta(\mathbf{x} - \mathbf{y}) - \frac{1}{4\pi} \partial_{\mathbf{x}i} \partial_{\mathbf{y}}^j \frac{1}{\|\mathbf{x} - \mathbf{y}\|} \right]
\end{aligned} \tag{1.4.13}$$

where we used the result (3.A.7) of appendix 3.A. This is, up to the factor  $i\hbar$  expected from (1.4.11), equal to (1.4.10). The proof is thus complete, and, with the canonical commutator (1.4.12) and the equations of motion (1.2.17), we have the two ingredients needed to quantise the massless vector field  $A^\mu$ . Notice that  $k_i \Delta^{ij}(\mathbf{k}) = 0$ , which ensures that  $\partial^i A_i = 0$  is compatible with our Poisson bracket.

### 1.4.5 Formal solution of the source-free Maxwell equations

The Maxwell equations read, in the Coulomb gauge,  $\partial^\nu \partial_\nu A^\mu = 0$ . We solve them following the method of [19]. In Fourier space, this is rewritten (with the overbar standing for the Fourier transform)

$$(k_0^2 - \mathbf{k}^2) \bar{A}^\mu(k_0, \mathbf{k}) = 0 \tag{1.4.14}$$

which is solved straightforwardly by

$$\bar{A}^\mu(k_0, \mathbf{k}) = 2\pi \delta(k_0^2 - \mathbf{k}^2) a^\mu(\text{sgn}(k_0), \mathbf{k}). \quad (1.4.15)$$

Now we turn to a crucial argument: **the four-vector potential  $A^\mu$  is a real function of spacetime.** This is enforced so that its derivatives, which correspond to the electromagnetic field, be real quantities. Accordingly [7] its Fourier transform is Hermitian:  $\bar{A}^\mu(k_0, \mathbf{k}) = (\bar{A}^\mu)^*(-k_0, -\mathbf{k})$ . Accordingly we rewrite (1.4.15) as

$$\bar{A}^\mu(k_0, \mathbf{k}) = 2\pi \delta(k_0^2 - \mathbf{k}^2) (\theta(k_0) a^\mu(\mathbf{k}) + \theta(-k_0) (a^\mu)^*(-\mathbf{k})) \quad (1.4.16)$$

where  $\theta$  denotes the Heaviside step distribution. Now, we need to learn more about the function  $a^\mu$ . With the Coulomb gauge conditions  $A_0 = 0, \partial^i A_i = 0$  in mind, we conclude that  $a^0(\mathbf{k}) = 0$  and  $k_i a^i(\mathbf{k}) = 0$ . Accordingly  $a^i$  can be expanded over two vectors  $\epsilon_{(\lambda)}(\mathbf{k})$  (we choose  $\lambda$  to take the values  $\pm 1$ ) which are orthogonal to  $\mathbf{k}$  and orthogonal to one another:

$$a^i(\mathbf{k}) = \sum_{\lambda=\pm} a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}). \quad (1.4.17)$$

Using spherical coordinates with  $\mathbf{k}$  as the radial vector (see Fig. 1.4.1), we easily understand that the unit vectors  $\mathbf{e}_1(\mathbf{k})$  and  $\mathbf{e}_2(\mathbf{k})$  constitute a valid choice for the  $\epsilon_{(\lambda)}(\mathbf{k})$  vectors. Remember that the unit vectors in a spherical basis are defined by

$$\begin{aligned} \mathbf{e}_1(\mathbf{k}) &= \cos\theta \cos\varphi \mathbf{e}_x + \cos\theta \sin\varphi \mathbf{e}_y - \sin\theta \mathbf{e}_z, \\ \mathbf{e}_2(\mathbf{k}) &= -\sin\varphi \mathbf{e}_x + \cos\varphi \mathbf{e}_y, \\ \mathbf{e}_3(\mathbf{k}) &= \sin\theta \cos\varphi \mathbf{e}_x + \sin\theta \sin\varphi \mathbf{e}_y + \cos\theta \mathbf{e}_z. \end{aligned} \quad (1.4.18)$$

Here  $\mathbf{e}_3(\mathbf{k})$  is the unit vector in the direction of  $\mathbf{k}$ . For reasons that will come apparent later, we do not choose  $\mathbf{e}_1(\mathbf{k})$  and  $\mathbf{e}_2(\mathbf{k})$  but the linear combinations

$$\epsilon_{(\lambda)}(\mathbf{k}) \equiv \frac{e^{-i\lambda\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{\sqrt{2}} (\mathbf{e}_1(\mathbf{k}) + i\lambda\mathbf{e}_2(\mathbf{k})) \quad (1.4.19)$$

where  $\lambda = \pm 1$  and  $\chi$  is an arbitrary function of  $\theta$  and  $\varphi$ . These are equally valid. For future reference we give the following identities:

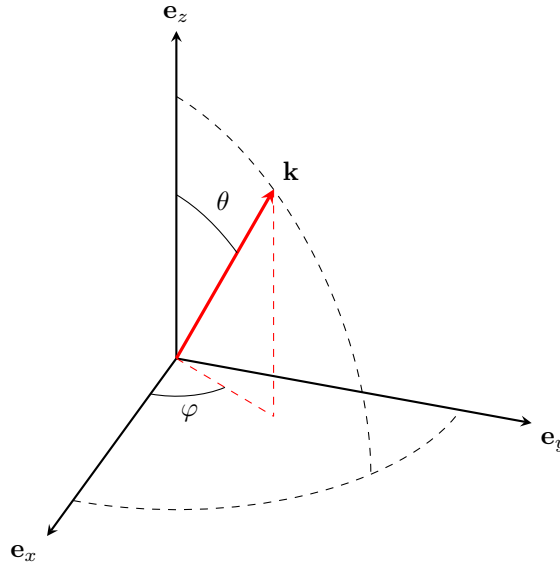
$$\begin{aligned} \epsilon_{(\lambda)}^*(\mathbf{k}) \cdot \epsilon_{(\varkappa)}(\mathbf{k}) &= \frac{e^{i(\lambda-\varkappa)\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{2} (\mathbf{e}_1(\mathbf{k}) - i\lambda\mathbf{e}_2(\mathbf{k})) \cdot (\mathbf{e}_1(\mathbf{k}) + i\varkappa\mathbf{e}_2(\mathbf{k})) \\ &= \frac{e^{i(\lambda-\varkappa)\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{2} (1 + \lambda\varkappa) \\ &= \delta_{\lambda\varkappa} \end{aligned} \quad (1.4.20a)$$

and

$$\begin{aligned} \epsilon_{(\lambda)}^*(\mathbf{k}) \times \epsilon_{(\varkappa)}(\mathbf{k}) &= \frac{e^{i(\lambda-\varkappa)\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{2} (\mathbf{e}_1(\mathbf{k}) - i\lambda\mathbf{e}_2(\mathbf{k})) \times (\mathbf{e}_1(\mathbf{k}) + i\varkappa\mathbf{e}_2(\mathbf{k})) \\ &= \frac{i e^{i(\lambda-\varkappa)\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{2} (\varkappa + \lambda) \frac{\mathbf{k}}{\|\mathbf{k}\|} \\ &= i \delta_{\lambda\varkappa} \lambda \frac{\mathbf{k}}{\|\mathbf{k}\|}. \end{aligned} \quad (1.4.20b)$$

The complex nature of the polarisation vectors (1.4.19) results in the counter-intuitive, but very powerful identity

$$\frac{\mathbf{k}}{\|\mathbf{k}\|} \times \epsilon_{(\lambda)}(\mathbf{k}) = -i\lambda\epsilon_{(\lambda)}(\mathbf{k}). \quad (1.4.21)$$

Fig. 1.4.1 – Spherical coordinates for the vector  $\mathbf{k}$ .

Of high importance is the readily proved closure relation

$$\sum_{\lambda=\pm} \epsilon_{(\lambda)}^i(\mathbf{k}) \epsilon_{(\lambda)}^{*j}(\mathbf{k}) = -\eta^{ij} - \frac{k^i k^j}{\mathbf{k}^2} = \Delta^{ij}(\mathbf{k}). \quad (1.4.22)$$

We now have all the ingredients to reverse-Fourier transform our solution:

$$\begin{aligned} A^i(x) &= \sum_{\lambda=\pm} \int \frac{d^4 k}{(2\pi)^4} 2\pi \delta(k_0^2 - \mathbf{k}^2) \left[ \theta(k_0) a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}) + \theta(-k_0) a_{(\lambda)}^*(-\mathbf{k}) \epsilon_{(\lambda)}^{*i}(-\mathbf{k}) \right] e^{-ik^\mu x_\mu} \\ &= \sum_{\lambda=\pm} \int \frac{d^4 k}{(2\pi)^4} 2\pi \delta(k_0^2 - \mathbf{k}^2) \theta(k_0) \left[ a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}) e^{-ik^\mu x_\mu} + a_{(\lambda)}^*(\mathbf{k}) \epsilon_{(\lambda)}^{*i}(\mathbf{k}) e^{ik^\mu x_\mu} \right]. \end{aligned}$$

The volume element

$$\boxed{d\tilde{k} \equiv \frac{d^4 k}{(2\pi)^4} 2\pi \delta(k_0^2 - \mathbf{k}^2) \theta(k_0)} \quad (1.4.23)$$

might look scary, but it proves a worthy ally as it is Lorentz-invariant. Indeed, by definition,  $k_0^2 - \mathbf{k}^2$  is conserved under Lorentz transformations, and the fact that  $k^\mu$  transforms according to  $k'^\mu = \Lambda^\mu_\nu k^\nu$  with  $\Lambda$  a unit-determinant matrix—this is a consequence of (1.1.5)—ensures that  $d^4 k' = d^4 k$ . As for the Heaviside step distribution  $\theta(k_0)$ , its invariance is ensured by the fact that transformations of the proper orthochronous Lorentz group never change the sign of the zeroth component of a four-vector. We call  $d\tilde{k}$  the **invariant volume element on the lightcone**. In sect. 4.1 of [6] is given this nice step-by-step calculation:

$$\begin{aligned} \frac{d^4 k}{(2\pi)^4} 2\pi \delta(k_0^2 - \mathbf{k}^2) \theta(k_0) &= \frac{d\mathbf{k} dk_0}{(2\pi)^3} \delta[(k_0 + \|\mathbf{k}\|)(k_0 - \|\mathbf{k}\|)] \theta(k_0) \\ &= \frac{d\mathbf{k} dk_0}{(2\pi)^3} \frac{1}{2\|\mathbf{k}\|} [\delta(k_0 + \|\mathbf{k}\|) + \delta(k_0 - \|\mathbf{k}\|)] \theta(k_0) \\ &= \frac{d\mathbf{k} dk_0}{(2\pi)^3} \frac{1}{2\|\mathbf{k}\|} \delta(k_0 - \|\mathbf{k}\|). \end{aligned} \quad (1.4.24)$$

Using this we rewrite the general solution as

$$A^i(\mathbf{x}, t) = \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \left[ a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} + a_{(\lambda)}^*(\mathbf{k}) \epsilon_{(\lambda)}^{*i}(\mathbf{k}) e^{i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right]. \quad (1.4.25)$$

We know that  $E^i = -\partial^0 A^i - \partial^i A^0 = -\partial^0 A^i$  in the Coulomb gauge. Hence

$$E^i(\mathbf{x}, t) = ic \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} - a_{(\lambda)}^*(\mathbf{k}) \epsilon_{(\lambda)}^{*i}(\mathbf{k}) e^{i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right]. \quad (1.4.26)$$

## 1.4.6 More on polarisation vectors

*“Calvin wakes up one morning to find he no longer exists in the third dimension! He is 2-D! Thinner than a sheet of paper, Calvin has no surface area on the bottom of his feet! He is immobile! Only by waving his body can Calvin create enough friction with the ground to move! Having width but no thickness, Calvin is vulnerable to the slightest gust of wind!”*

Calvin in Calvin & Hobbes—Yukon Ho!, by Bill Watterson (Andrews McMeel, 1989)

Following [8] we write  $\epsilon(\mathbf{k}) \equiv \epsilon_{(+1)}(\mathbf{k}) = \epsilon_{(-1)}^*(\mathbf{k})$ . From (1.4.20) we can deduce that

$$\partial_{\mathbf{k}i} \epsilon(\mathbf{k}) = -i\alpha_i(\mathbf{k}) \epsilon(\mathbf{k}) + \beta_i(\mathbf{k}) \frac{\mathbf{k}}{\|\mathbf{k}\|}$$

with  $\alpha(\mathbf{k})$  a real vector. Then, using the closure relation (1.4.22), we can see that

$$\partial_{\mathbf{k}i} \epsilon(\mathbf{k}) = -i\alpha_i(\mathbf{k}) \epsilon(\mathbf{k}) - \epsilon_i(\mathbf{k}) \frac{\mathbf{k}}{\mathbf{k}^2}. \quad (1.4.27)$$

The quantity

$$\alpha_i(\mathbf{k}) \equiv i\epsilon^*(\mathbf{k}) \cdot \partial_{\mathbf{k}i} \epsilon(\mathbf{k}) \quad (1.4.28)$$

is not directly constrained, but we can easily compute its curl, which reads:

$$\nabla_{\mathbf{k}} \times \alpha(\mathbf{k}) = -\frac{\mathbf{k}}{\|\mathbf{k}\|^3}. \quad (1.4.29)$$

## 1.4.7 Quantisation—Fock space

Now all we have to do to canonically quantise the theory is to rewrite the field and its canonically conjugate momentum as operators. This simply amounts to writing

$$\hat{A}^i(\mathbf{x}, t) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} + \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)}^{*i}(\mathbf{k}) e^{i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right] \quad (1.4.30)$$

and

$$\hat{E}^i(\mathbf{x}, t) = i\sqrt{\frac{\hbar c}{\epsilon_0}} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^i(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} - \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)}^{*i}(\mathbf{k}) e^{i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right]. \quad (1.4.31)$$

where we introduced dimensional constants. In order to satisfy the canonical commutation relations (1.4.12) we “guess” that the following commutation relation has to be enforced:

$$\boxed{\left[ \hat{a}_{(\varkappa)}(\mathbf{k}), \hat{a}_{(\lambda)}^\dagger(\mathbf{q}) \right] = 2 \|\mathbf{k}\| (2\pi)^3 \delta(\mathbf{k} - \mathbf{q}) \delta_{\varkappa\lambda}}. \quad (1.4.32)$$

Indeed, if this is true, then, with the use of (1.4.22) we can compute

$$\begin{aligned} \epsilon_0 \left[ \hat{A}_i(\mathbf{x}, t), \hat{E}^j(\mathbf{y}, t) \right] &= i\hbar \sum_{\varkappa=\pm} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \int \frac{d\mathbf{q}}{2(2\pi)^3 \|\mathbf{q}\|} \|\mathbf{q}\| \left[ 2 \|\mathbf{k}\| (2\pi)^3 \delta(\mathbf{k} - \mathbf{q}) \delta_{\varkappa\lambda} \right] \\ &\quad \left[ -\epsilon_{(\varkappa)i}(\mathbf{k}) \epsilon_{(\lambda)}^{*j}(\mathbf{q}) e^{-i[c(\|\mathbf{k}\| - \|\mathbf{q}\|)t - (\mathbf{k}\cdot\mathbf{x} - \mathbf{q}\cdot\mathbf{y})]} - \epsilon_{(\varkappa)i}^*(\mathbf{k}) \epsilon_{(\lambda)}^j(\mathbf{q}) e^{i[c(\|\mathbf{k}\| - \|\mathbf{q}\|)t - (\mathbf{k}\cdot\mathbf{x} - \mathbf{q}\cdot\mathbf{y})]} \right] \\ &= -i\hbar \sum_{\varkappa=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ \epsilon_{(\varkappa)i}(\mathbf{k}) \epsilon_{(\varkappa)}^{*j}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} + \epsilon_{(\varkappa)i}^*(\mathbf{k}) \epsilon_{(\varkappa)}^j(\mathbf{k}) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \right] \\ &= -i\hbar \sum_{\varkappa=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3} \left( \epsilon_{(\varkappa)i}(\mathbf{k}) \epsilon_{(\varkappa)}^{*j}(\mathbf{k}) + \epsilon_{(\varkappa)i}^*(\mathbf{k}) \epsilon_{(\varkappa)}^j(\mathbf{k}) \right) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \\ &= -i\hbar \int \frac{d\mathbf{k}}{(2\pi)^3} \Delta_i^j(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \end{aligned} \quad (1.4.33)$$

since  $\Delta_{ij}(-\mathbf{k}) = \Delta_{ij}(\mathbf{k})$ . This matches (1.4.12), so (1.4.32) is valid. With (1.4.32) we wrote the commutator between an operator and its Hermitian conjugate as a number (times the identity matrix), which is reminding of the quantum harmonic oscillator. We now introduce the **vacuum state**  $|0\rangle$  of the theory as a state which is destroyed by all  $\hat{a}_{(\lambda)}(\mathbf{k})$  operators:

$$\boxed{\forall \lambda \in \{1, 2\} \forall \mathbf{k} \in \mathbb{R}^3 \hat{a}_{(\lambda)}(\mathbf{k}) |0\rangle = 0}. \quad (1.4.34)$$

We also define the **number operator** as

$$\boxed{\hat{N} = \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k})}. \quad (1.4.35)$$

Following the technique [3] used for the quantum harmonic oscillator, it can be proved that the spectrum of this operator is the set of positive integers  $\mathbb{N}$ . Hence **quantum field theory provides the electromagnetic field with a particle interpretation**:  $\hat{N}$  counts the total number of particles in the field. These particles are called photons. The usual Fock space rules are then applicable for each couple  $(\lambda, \mathbf{k})$ . We refer to this couple as a **mode of the electromagnetic field**.

## 1.4.8 Poincaré generators

Up to that point, we have not commented on the meaning of the  $\lambda$  of sect. 1.4.5. The choice of notation, of course, is not innocent. It corresponds, as we shall see here, to the helicity of one-photon states.

Since the field operator is a vector, we ask that, under a Poincaré transformation  $(\Lambda, a)$ , it transform as

$$\hat{U}(\Lambda, a) \Lambda_\nu^\mu \hat{A}^\nu(x) \hat{U}^\dagger(\Lambda, a) = \hat{A}^\mu(\Lambda x + a) \quad (1.4.36)$$

where  $\hat{U}(\Lambda, a)$  is a unitary operator. Compare with (1.2.1). Manipulation of (1.4.36) yields

$$\begin{aligned} \hat{U}^\dagger(\Lambda, a) \hat{A}^\nu(\Lambda x + a) \hat{U}(\Lambda, a) &= \Lambda_\nu^\mu \hat{A}^\mu(x) = \hat{A}'^\mu(\Lambda x + a). \\ \hat{U}^\dagger(\Lambda, a) \hat{A}^\nu(x) \hat{U}(\Lambda, a) &= \Lambda_\nu^\mu \hat{A}^\mu(\Lambda^{-1}(x - a)) = \hat{A}'^\mu(x). \end{aligned} \quad (1.4.37)$$

This allows us to work out the explicit expression for the unitary operators  $\hat{U}(\Lambda, a)$ . It is seen from (1.A.20) that they can be written ( $\hat{P}_\mu$  and  $\hat{J}_{\mu\nu}$  are Hermitian operators)

$$\hat{U}(\Lambda, a) = e^{ia^\mu \hat{P}_\mu + \frac{i}{2} \Omega^{\mu\nu} \hat{J}_{\mu\nu}}, \quad (1.4.38a)$$

$$\hat{U}^\dagger(\Lambda, a) = e^{-ia^\mu \hat{P}_\mu - \frac{i}{2} \Omega^{\mu\nu} \hat{J}_{\mu\nu}} \quad (1.4.38b)$$

Now, assume that  $a^\mu$  and  $\Omega^{\mu\nu}$  are infinitesimal parameters. To first order in these parameters the rightmost expression in (1.4.37) reads (using our analysis of sect. 1.2.1)

$$\begin{aligned} (\delta_\nu^\mu + \omega_\nu^\mu) \hat{A}^\nu(\Lambda^{-1}(x-a)) &= \hat{A}^\mu(x) + \omega_\nu^\mu \hat{A}^\nu(x) - \left[ x^\nu - (\Lambda^{-1}(x-a))^\nu \right] \partial_\nu \hat{A}^\mu(x) \\ \text{(first order)} &= \hat{A}^\mu(x) + \omega_\nu^\mu \hat{A}^\nu(x) - (a^\rho + \omega_\sigma^\rho x^\sigma) \partial_\rho \hat{A}^\mu(x). \end{aligned} \quad (1.4.39)$$

To first order in  $a^\mu$  and  $\Omega^{\mu\nu}$  the leftmost expression in (1.4.37) reads

$$\hat{U}^\dagger(\Lambda, a) \hat{A}^\mu(x) \hat{U}(\Lambda, a) = \hat{A}^\mu(x) - ia_\nu \left[ \hat{P}^\nu, \hat{A}^\mu(x) \right] - \frac{i}{2} \Omega_{\rho\sigma} \left[ \hat{J}^{\rho\sigma}, \hat{A}^\mu(x) \right], \quad (1.4.40)$$

as seen from (1.4.38). Now all there is to do is equate (1.4.39) with (1.4.40). As was done in sect. 1.2.1, we use (1.1.6) and (1.1.7) to find

$$\left[ \hat{P}^\nu, \hat{A}^\mu(x) \right] = -i \partial^\nu \hat{A}^\mu(x), \quad (1.4.41a)$$

$$\left[ \hat{J}^{\rho\sigma}, \hat{A}^\mu(x) \right] = i \left[ (x^\rho \partial^\sigma - x^\sigma \partial^\rho) \hat{A}^\mu(x) + \left( \eta^{\rho\mu} \hat{A}^\sigma(x) - \eta^{\sigma\mu} \hat{A}^\rho(x) \right) \right]. \quad (1.4.41b)$$

Compare with (1.2.8).

We are on the verge of building the operators  $\hat{P}_\mu$  and  $\hat{J}_{\mu\nu}$ . The final argument needed [19] is that they annihilate the vacuum state  $|0\rangle$  of the electromagnetic field. Indeed, it is a natural requirement that the vacuum state of the theory be invariant under Poincaré transformations. Accordingly  $\hat{U}(\Lambda, a) |0\rangle = |0\rangle$ , which, to first order, yields

$$\hat{P}_\mu |0\rangle = 0, \quad (1.4.42a)$$

$$\hat{J}_{\mu\nu} |0\rangle = 0. \quad (1.4.42b)$$

This allows us to build the Hilbert-space representatives of the Poincaré generators.  $\hat{P}_\mu$  is easy enough:

$$\hat{P}_\mu = \sum_{\lambda=\pm} \int d\tilde{k} k_\mu \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}). \quad (1.4.43)$$

On the other hand, the generators  $\hat{J}_{\mu\nu}$  of Lorentz transformations are pretty hard to determine. Let us focus directly on

$$\hat{J}_i \equiv -\frac{1}{2} \epsilon_{0ijk} \hat{J}^{jk}, \quad (1.4.44a)$$

$$\hat{K}_i \equiv -\hat{J}_{0i}, \quad (1.4.44b)$$

the respective generators for rotations and boosts. According to (1.4.41) and (1.4.44) we should build these operators so that they verify

$$\left[ \hat{J}_i, \hat{A}^p(x) \right] = -\frac{i}{2} \epsilon_{0ijk} \left[ 2x^j \partial^k \hat{A}^p(x) + \left( \eta^{jp} \hat{A}^k(x) - \eta^{kp} \hat{A}^j(x) \right) \right], \quad (1.4.45a)$$

$$\left[ \hat{K}_i, \hat{A}^p(x) \right] = -i \left[ (x_0 \partial_i - x_i \partial_0) \hat{A}^p(x) + \left( \delta_0^p \hat{A}_i(x) - \delta_i^p \hat{A}_0(x) \right) \right]. \quad (1.4.45b)$$



Using (1.4.20b) and (1.4.22) we can compute the second summands on the right-hand side of both equalities in (1.4.45). This yields

$$\frac{i}{2} \epsilon_{0ijk} \left[ \eta^{jp} \epsilon_{(\lambda)}^k(\mathbf{k}) - \eta^{kp} \epsilon_{(\lambda)}^j(\mathbf{k}) \right] = \frac{\lambda}{\|\mathbf{k}\|} \left( \epsilon_{(\lambda)}^p(\mathbf{k}) k_i - \epsilon_{(\lambda)i}(\mathbf{k}) k^p \right), \quad (1.4.46a)$$

$$i \left[ \delta_0^p \epsilon_{(\lambda)i}(\mathbf{k}) - \delta_i^p \epsilon_{(\lambda)0}(\mathbf{k}) \right] = 0. \quad (1.4.46b)$$

Using what we know of the easier case of the scalar field [9], we attempt the naive guess consisting of

$$\hat{J}_i^{\text{naive}} = i \epsilon_{0ijk} \sum_{\lambda=\pm} \int \tilde{d}k \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) k^j \frac{\partial}{\partial k_k} \hat{a}_{(\lambda)}(\mathbf{k}) \quad (1.4.47a)$$

and

$$\hat{K}_i^{\text{naive}} = i \sum_{\lambda=\pm} \int \tilde{d}k \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \|\mathbf{k}\| \frac{\partial}{\partial k^i} \hat{a}_{(\lambda)}(\mathbf{k}), \quad (1.4.47b)$$

knowing that it cannot work, but merely as a starting point. Going further requires us to recall the behaviour of the polarisation vectors (1.4.19) under differentiation with respect to  $\mathbf{k}$ . As was done in sect. 1.4.6, we write  $\epsilon(\mathbf{k}) \equiv \epsilon_{(1)}(\mathbf{k}) = \epsilon_{(-1)}^*(\mathbf{k})$ . Remember that

$$\partial_{\mathbf{k}i} \epsilon(\mathbf{k}) = -i \alpha_i(\mathbf{k}) \epsilon(\mathbf{k}) - \epsilon_i(\mathbf{k}) \frac{\mathbf{k}}{k^2}. \quad (1.4.48)$$

Let us treat the rotation generators  $\hat{J}_i$  first. The commutators of the corresponding naive generator (1.4.47a) with the field reads

$$\begin{aligned} \left[ \hat{J}_i^{\text{naive}}, \hat{A}^p(x) \right] &= -i \epsilon_{0ijk} x^j \partial^k \hat{A}^p(x) + \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}k \lambda \left[ \epsilon_{0ijk} k^j \alpha^k(\mathbf{k}) \epsilon_{(\lambda)}^p(\mathbf{k}) - \epsilon_{(\lambda)i}(\mathbf{k}) \frac{k^p}{\|\mathbf{k}\|} \right] \hat{a}_{(\lambda)}(\mathbf{k}) e^{-ik^\mu x_\mu} \\ &+ \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}k \lambda \left[ \epsilon_{0ijk} k^j \alpha^k(\mathbf{k}) \epsilon_{(\lambda)}^{*p}(\mathbf{k}) - \epsilon_{(\lambda)i}^*(\mathbf{k}) \frac{k^p}{\|\mathbf{k}\|} \right] \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) e^{ik^\mu x_\mu}. \end{aligned} \quad (1.4.49)$$

Accordingly we can guess, upon comparing (1.4.46a) with (1.4.49), the correct expression for the generators. Introducing the **covariant derivative**  $D_{\mathbf{k}(\lambda)}^j$  on the lightcone [8] as

$$\boxed{D_{\mathbf{k}(\lambda)}^j = \frac{\partial}{\partial k_j} + i \lambda \alpha^j(\mathbf{k})}, \quad (1.4.50)$$

we get

$$\hat{J}_i = \sum_{\lambda=\pm} \int \tilde{d}k \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \left( i \epsilon_{0ijk} k^j D_{\mathbf{k}(\lambda)}^k + \lambda \frac{k_i}{\|\mathbf{k}\|} \right) \hat{a}_{(\lambda)}(\mathbf{k}) \quad (1.4.51)$$

which is in agreement with the result obtained in [8] by computing the energy-momentum tensor of the electromagnetic field. Things are not as simple for the boost generators  $\hat{K}_i$ . The commutators of the corresponding naive generator (1.4.47b) with the field reads

$$\begin{aligned} \left[ \hat{K}_i^{\text{naive}}, \hat{A}^p(x) \right] &= -i (x_0 \partial_i - x_i \partial_0) \hat{A}^p(x) + i \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}k \|\mathbf{k}\| \left( -i \lambda \alpha_i(\mathbf{k}) \epsilon_{(\lambda)}^p(\mathbf{k}) - \epsilon_{(\lambda)i}(\mathbf{k}) \frac{k^p}{k^2} \right) \hat{a}_{(\lambda)}(\mathbf{k}) e^{-ik^\mu x_\mu} \\ &+ i \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}k \|\mathbf{k}\| \left( i \lambda \alpha_i(\mathbf{k}) \epsilon_{(\lambda)}^{*p}(\mathbf{k}) - \epsilon_{(\lambda)i}^*(\mathbf{k}) \frac{k^p}{k^2} \right) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) e^{ik^\mu x_\mu}. \end{aligned} \quad (1.4.52)$$

Compare this last equality with (1.4.45b) and (1.4.46b). To build the correct  $\hat{K}_i$  from  $\hat{K}_i^{\text{naive}}$ , we would need to add to the latter a term the commutator of which with the potential four-vector is minus the second and third

summands on the right-hand side of (1.4.52), *i.e.*, the two complicated sum-integrals. As far as we know, this is not possible. Let us, however, consider the boost generator given in [8], namely

$$\hat{\mathcal{K}}_i = i \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \|\mathbf{k}\| \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) D_{\mathbf{k}(\lambda)i} \hat{a}_{(\lambda)}(\mathbf{k}). \quad (1.4.53)$$

A different font is used here to emphasise the fact that (1.4.53) does not fulfill (1.4.45b). The corresponding commutator reads

$$[\hat{\mathcal{K}}_i, \hat{A}^p(x')] = -i \left[ (x_0 \partial_i - x_i \partial_0) \hat{A}^p(x) + \left( \eta_{0i} \hat{A}^p(x) - \delta_i^p \hat{A}_0(x) \right) \right] + \hat{G}_i^p(x) \quad (1.4.54)$$

where

$$\hat{G}_i^p(x) \equiv -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \frac{k^p}{\|\mathbf{k}\|} \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)i}(\mathbf{k}) e^{-ik^\mu x_\mu} - \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)i}^*(\mathbf{k}) e^{ik^\mu x_\mu} \right]. \quad (1.4.55)$$

This term is best understood when investigating the transformation properties of the Coulomb gauge condition under a pure Lorentz boost. Compute, from (1.4.37), the three-divergence of the vector field in a frame of reference linked to that in which the Coulomb condition is imposed through a pure (infinitesimal) Lorentz boost of parameters  $\Omega_{0j}$ . If we accept that (1.4.53) is the boost generator, then we write, making use of (1.4.37)

$$\begin{aligned} \partial'_i \hat{A}^i(x') &= (\delta_i^\nu + \omega_i^\nu) \partial_\nu \left\{ \hat{A}^i(x') - i\Omega_{0q} \left[ \hat{\mathcal{K}}^q, \hat{A}^i(x') \right] \right\} \\ &= (\delta_i^\nu + \omega_i^\nu) \partial_\nu \left\{ \hat{A}^i(x') - i\Omega_{0q} \hat{G}^{qi}(x) - i\Omega_{0q} \left( -i \left[ (x^0 \partial^q - x^q \partial^0) \hat{A}^i(x) + \left( \eta^{0i} \hat{A}^q(x) - \eta^{qi} \hat{A}^0(x) \right) \right] \right) \right\}. \end{aligned} \quad (1.4.56)$$

Analysis similar to that used in the derivation of (1.4.39) yields, with use of (1.4.55) in the last step,

$$\begin{aligned} \partial'_i \hat{A}^i(x') &= \partial_i \hat{A}^i(x) - \Omega_{0q} \partial^0 \hat{A}^q(x) - i\Omega_{0q} \partial_i \hat{G}^{qi}(x) \\ &= \partial_i \hat{A}^i(x). \end{aligned} \quad (1.4.57)$$

Hence if we use the “wrong” generator (1.4.53), we find that the Coulomb gauge condition remains valid after a boost. This result calls for the following dichotomy: either we choose the potential four-vector to transform as a Lorentz vector (see (1.4.37)), and hence to obey the Coulomb gauge condition in one frame of reference only. In that case, no explicit form for the boost generator can be written. At best, we can use  $\hat{\mathcal{K}}_i$  and discard  $\hat{G}^{pi}$  when writing the action of Lorentz boosts on  $\hat{A}^i$ , so that (1.4.45b) will be fulfilled. Or, we choose the potential four-vector to transform as a Lorentz vector only up to an extra term  $\hat{G}^{pi}$  that corrects for the fact that the Coulomb gauge condition is not invariant under boosts. The latter choice is made in [1] and [10], and can be explained thusly: since the physical observable of free quantum electrodynamics is the gauge-invariant Faraday tensor  $\hat{F}^{\mu\nu} = \partial^\mu \hat{A}^\nu - \partial^\nu \hat{A}^\mu$ , we can relax (1.4.37) to

$$\hat{U}^\dagger(\Lambda, a) \hat{A}^\mu(x) \hat{U}(\Lambda, a) = \Lambda^\mu_\nu \hat{A}^\nu(\Lambda^{-1}(x-a)) + \partial^\mu \hat{\lambda}(x) \quad (1.4.58)$$

without affecting the fact that  $\hat{F}^{\mu\nu}$  transforms as a second-rank tensor under Lorentz transformations. Choosing the Coulomb gauge and the generator (1.4.53) amounts to choosing (1.4.58) with  $\partial^i \hat{\lambda}(x) = i\Omega_{0q} \hat{G}^{qi}(x)$ . Hence

$$\hat{\lambda}(t, \mathbf{x}) = \frac{\Omega_{0q}}{4\pi c} \int \frac{d\mathbf{y}}{\|\mathbf{x} - \mathbf{y}\|} \partial_t \hat{A}^q(t, \mathbf{y}) \quad (1.4.59)$$

as can be shown from (1.4.55) and some elementary distribution theory (also see [10] (exercise 2 of chapter 14)).

The possibility to preserve the Coulomb gauge in all frames of reference is a very nice feature of the theory of

electrodynamics, and we will therefore use this gauge in chapters 2 and 3.

### 1.4.9 States of definite momentum and helicity

Define

$$|k, \lambda\rangle = \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |0\rangle. \quad (1.4.60)$$

Using (1.4.43), (1.4.51) and (1.4.53) in the frame of reference where the momentum reads  $k^\mu = (k, 0, 0, k)$  (see sect. 1.A.3.4), it is very easy to see that we have

$$\hat{W}^\mu |k, \lambda\rangle = \lambda \hat{P}^\mu |k, \lambda\rangle = \lambda k^\mu |k, \lambda\rangle \quad (1.4.61)$$

which means, according to the discussion of sect. 1.A.3.4, that the  $\lambda$  introduced in sect. 1.4.5 to define polarisation vectors is the helicity of the single-photon state built by applying the creation operator  $\hat{a}_{(\lambda)}^\dagger(\mathbf{k})$  on the vacuum state of the theory.

### 1.4.10 Hamiltonian of the field

By definition (see (1.3.6) and (1.3.7)) the Hamiltonian reads (from (1.3.4))

$$\begin{aligned} H &= \int d\mathbf{x} (\partial_t A_i(\mathbf{x}, t) \epsilon_0 E^i(\mathbf{x}, t) - \mathcal{L}(\mathbf{x}, t)) \\ &= \int d\mathbf{x} \left( \epsilon_0 \mathbf{E}^2(\mathbf{x}, t) - \frac{\epsilon_0}{2} (\mathbf{E}^2(\mathbf{x}, t) - c^2 \mathbf{B}^2(\mathbf{x}, t)) \right) \\ &= \frac{\epsilon_0}{2} \int d\mathbf{x} (\mathbf{E}^2(\mathbf{x}, t) + c^2 \mathbf{B}^2(\mathbf{x}, t)) \end{aligned}$$

which is Poynting's usual expression. Rewriting this in terms of the vector potential we get

$$H = \frac{\epsilon_0}{2} \int d\mathbf{x} \left[ (\partial_t \mathbf{A}(\mathbf{x}, t))^2 + c^2 (\nabla \times \mathbf{A}(\mathbf{x}, t))^2 \right].$$

Substituting (1.4.30) to get the quantised Hamiltonian, we find, after a cumbersome but straightforward calculation, the following expression for the Hamiltonian operator:

$$\hat{H} = \hbar c \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3} \frac{||\mathbf{k}||}{2} \left( \hat{a}_{(\lambda)}(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) + \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) \right).$$

This expression is pretty problematic, because if we compute the expectation value  $\langle 0 | \hat{H} | 0 \rangle$  in the vacuum state, we get an infinite quantity. Indeed, from (1.4.32) we can rewrite

$$\hat{H} = \hbar c \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3} ||\mathbf{k}|| \left( \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) + ||\mathbf{k}|| (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}) \right)$$

and

$$\langle 0 | \hat{H} | 0 \rangle = \hbar c \int d\mathbf{k} ||\mathbf{k}|| \delta(\mathbf{k} - \mathbf{k})$$

which is clearly an ill-defined integral. The solution is to simply “decide” that this vacuum energy is unphysical<sup>8</sup>, and choose the Wick prescription, which states that, when writing field operators which feature products of creation and annihilation operators, all creation operators should be put on the left of all annihilation operators. This is the

<sup>8</sup>As might be clear by now, canonical analysis has shown the electromagnetic field to be no more than a collection of harmonic oscillators. Each electromagnetic mode  $(\lambda, \mathbf{k})$  is described by a quantum harmonic oscillator. Accordingly the existence of a vacuum energy is not a surprise. But since here we have an infinity of such oscillators, the vacuum energy is infinite, and we drop it.

so-called Wick ordering, or normal ordering. It yields

$$\hat{H} = \hbar c \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}). \quad (1.4.62)$$

## 1.A Representations of the Poincaré group and Poincaré-invariant quantisation

We can write the action of an element  $(\Lambda, a)$  of the Poincaré group on position four-vectors as

$$[(\Lambda, a) A]^\mu = \Lambda^\mu_\nu A^\nu + a^\mu. \quad (1.A.1)$$

We give the group law of the Poincaré group

$$(\Lambda_1, a_1) (\Lambda_2, a_2) = (\Lambda_1 \Lambda_2, a_1 + \Lambda_1 a_2) \quad (1.A.2a)$$

and the expression of an inverse element

$$(\Lambda, a)^{-1} = (\Lambda^{-1}, -\Lambda a). \quad (1.A.2b)$$

They can both be easily deduced from (1.A.1).

### 1.A.1 The Poincaré algebra

The Poincaré group is a Lie group, that is, a group which is also a smooth manifold for which the group operations are smooth maps. The tangent space to that manifold at the identity element of the group is called the Lie algebra of the group. A Lie algebra  $\mathfrak{g}$  is defined by the following axioms [20]:

1.  $\mathfrak{g}$  is a vector space over some field  $\mathbb{K}$ .
2. There exists a binary operation

$$\begin{aligned} \mathfrak{g} \times \mathfrak{g} &\rightarrow \mathfrak{g} \\ (m, n) \in (\mathfrak{g} \times \mathfrak{g}) &\mapsto [m, n] \in \mathfrak{g} \end{aligned} \quad (1.A.3)$$

called the Lie bracket, endowed with the following properties:

(a) Bilinearity:

$$\begin{aligned} \forall (m, n, p) \in \mathfrak{g}^3 \forall (\lambda, \mu) \in \mathbb{K}^2 \quad [\lambda m + \mu n, p] &= \lambda [m, p] + \mu [n, p] \\ \text{and } [m, \lambda n + \mu p] &= \lambda [m, n] + \mu [m, p] \end{aligned} \quad (1.A.4a)$$

(b) Alternation:

$$\forall m \in \mathfrak{g} \quad [m, m] = 0. \quad (1.A.4b)$$

(c) The Jacobi identity:

$$\forall (m, n, p) \in \mathfrak{g}^3 \quad [m, [n, p]] + [n, [p, m]] + [p, [m, n]] = 0. \quad (1.A.4c)$$

A direct consequence of bilinearity and alternation is the antisymmetry of the Lie bracket:  $[m, n] = -[n, m]$ .

The group law of a Lie group is determined by the Lie brackets of its Lie algebra, which means that for our purposes we can restrain our study to the Lie algebra of the Poincaré group. This algebra is generated by ten elements: four

translations  $P_\mu$  and six Lorentz transformations  $J_{\mu\nu} = -J_{\nu\mu}$ . This means that any element  $m$  of the Poincaré algebra  $\mathfrak{g}$  is a linear superposition of the form

$$\mathfrak{g} \ni m = ib^\mu P_\mu + \frac{i}{2} \Omega^{\mu\nu} J_{\mu\nu}. \quad (1.A.5)$$

Lorentz transformations can be further split into three spatial rotations  $J_{ij}$  and three Lorentz boosts  $J_{0i}$ . One often defines

$$K_i \equiv -J_{0i} \quad (1.A.6)$$

as well as

$$J_i \equiv -\frac{1}{2} \epsilon_{0ijk} J^{jk} \quad (1.A.7a)$$

which is inverted by

$$J_{ij} = -\epsilon_{0ijk} J^k. \quad (1.A.7b)$$

The structure of the Poincaré algebra is defined by the following Lie brackets:

$$[P_\mu, P_\nu] = 0, \quad (1.A.8a)$$

$$[P_\mu, J_{\nu\rho}] = i(\eta_{\mu\nu} P_\rho - \eta_{\mu\rho} P_\nu), \quad (1.A.8b)$$

$$[J_{\mu\nu}, J_{\rho\sigma}] = i(\eta_{\mu\rho} J_{\sigma\nu} - \eta_{\nu\rho} J_{\sigma\mu} - \eta_{\mu\sigma} J_{\rho\nu} + \eta_{\nu\sigma} J_{\rho\mu}). \quad (1.A.8c)$$

The Poincaré algebra is closed since the Lie brackets (which are the equivalent, for a Lie algebra, of the group law) of two elements of  $\mathfrak{g}$  can be expressed in terms of elements of  $\mathfrak{g}$  only. This closure ensures that **the Poincaré algebra generates a group by exponentiation of its elements**. Note that the six generators  $J_{\mu\nu}$  of the Lorentz transformations form a subalgebra: the Lie bracket of two such generators is given in terms of other Lorentz transformation generators  $J_{\rho\sigma}$  only, without any translation intervening. This means that—as already stated—Lorentz transformations themselves form a group, but we added Minkowski space translations  $P_\mu$  in order to consider all light speed-preserving transformations (that is, transformations that preserve the norm of the difference of two four-vectors).

## 1.A.2 Casimir invariants of the Poincaré algebra

### 1.A.2.1 Representations and irreducible representations

We now define the representation of a Lie algebra on a vector space  $X$  over a field  $\mathbb{K}$ . A representation  $T$  of  $\mathfrak{g}$  on  $X$  is a linear application which to every element of  $\mathfrak{g}$  associates an element of the endomorphisms of  $X$ :

$$\begin{aligned} \mathfrak{g} &\rightarrow M_n(\mathbb{K}) \\ m \in \mathfrak{g} &\mapsto T(m) \in \text{End}(X) \end{aligned} \quad (1.A.9)$$

where  $\text{End}(X) = \{f : X \rightarrow X \mid f \text{ is linear}\}$ , such that

$$\forall (m, n) \in \mathfrak{g}^2 \quad T([m, n]) = [T(m), T(n)] \quad (1.A.10)$$

where on the right-hand side, the square brackets stand for the matrix commutator (on the left-hand side, they still stand for the Lie bracket). The representation  $T$  of a group  $G$  on  $X$  is defined likewise: denoting the group law by  $*_G$ , it is a linear application which to every element of  $G$  associates an element of the endomorphisms of  $X$ :

$$\begin{aligned} G &\rightarrow M_n(\mathbb{K}) \\ g \in G &\mapsto T(g) \in \text{End}(X) \end{aligned} \quad (1.A.11)$$

where  $\text{End}(X) = \{f : X \rightarrow X \mid f \text{ is linear}\}$ , such that

$$\forall (g, h) \in G^2 \quad T(g *_{G} h) = T(g) T(h). \quad (1.A.12)$$

Both for algebras and groups, the elements of  $\text{End}(X)$  are called the representatives:  $T(m)$  (resp.  $T(g)$ ) is the representative of  $m$  (resp.  $g$ ) on  $X$ . We give a final formal definition: an irreducible representation  $T$  of a Lie algebra  $\mathfrak{g}$  on a finite-dimensional vector space  $X$  is a representation for which the only two subspaces  $Y_i$  of  $X$  such that

$$\forall m \in \mathfrak{g} \quad \forall y \in Y_i \quad T(m)y \in Y_i \quad (1.A.13)$$

are the one-element set consisting of the zero vector of  $X$  and  $X$  itself. We will focus on irreducible representations because reducible representations can be decomposed into irreducible representations. Hence the study of irreducible representations is enough to build the complete representation theory of the Poincaré algebra. Of course we should specify on what vector space we will represent the Poincaré algebra. That space is the one-particle quantum mechanical Hilbert space.

### 1.A.2.2 Casimir invariants

To build a relativistic field theory we are thus led to study the irreducible representations of the Poincaré algebra. Classifying these representations is done by the way of examining the Casimir operators  $C_\alpha$  of the algebra which are defined as

$$\forall m \in \mathfrak{g} \quad [C_\alpha, m] = 0. \quad (1.A.14)$$

We show below that there are two such Casimir operators for the Poincaré algebra:

- $P^2 = P^\mu P_\mu \equiv C_1$  where  $P_\mu$  (still) is the generator of spacetime translations.
- $W^2 = W^\mu W_\mu \equiv C_2$  where  $W_\mu$  is the Pauli-Lubański four-pseudovector:

$$W_\mu \equiv -\frac{1}{2} \epsilon_{\mu\nu\rho\sigma} J^{\nu\rho} P^\sigma. \quad (1.A.15)$$

Note that the antisymmetry of the Levi-Civita form ensures that  $W^\mu P_\mu = 0$ . A well known result of group theory known as Schur's lemma ensures that since we are studying irreducible representations, the representatives  $T(C_\alpha)$  will be multiples of the identity operator.

We now prove that  $P^2$  and  $W^2$  are indeed Casimir invariants for the Poincaré algebra. We make extensive use of the Lie brackets (1.A.8). Starting with the invariant mass operator  $P^2$ :

$$\begin{aligned} [P_\lambda, P^2] &= \eta^{\mu\nu} [P_\lambda, P_\mu P_\nu] \\ &= \eta^{\mu\nu} \{ [P_\lambda, P_\mu] P_\nu + P_\mu [P_\lambda, P_\nu] \} \\ &= 0, \\ [J_{\rho\sigma}, P^2] &= \eta^{\mu\nu} [J_{\rho\sigma}, P_\mu P_\nu] \\ &= \eta^{\mu\nu} \{ [J_{\rho\sigma}, P_\mu] P_\nu + P_\mu [J_{\rho\sigma}, P_\nu] \} \\ &= i \eta^{\mu\nu} \{ (\eta_{\mu\sigma} P_\rho - \eta_{\mu\rho} P_\sigma) P_\nu + P_\mu (\eta_{\nu\sigma} P_\rho - \eta_{\nu\rho} P_\sigma) \} \\ &= i (\delta_\sigma^\nu P_\rho P_\nu - \delta_\rho^\nu P_\sigma P_\nu + \delta_\sigma^\mu P_\mu P_\rho - \delta_\rho^\mu P_\mu P_\sigma) \\ &= i (P_\rho P_\sigma - P_\sigma P_\rho + P_\sigma P_\rho - P_\rho P_\sigma) \\ &= 0. \end{aligned}$$

Now on to the spin/helicity operator  $W^2$ :

$$\begin{aligned}
[W_\mu, P_\tau] &= -\frac{1}{2}\epsilon_{\mu\nu\rho\sigma}\eta_{\lambda\tau}[J^{\nu\rho}P^\sigma, P^\lambda] \\
&= -\frac{1}{2}\epsilon_{\mu\nu\rho\sigma}\eta_{\lambda\tau}[J^{\nu\rho}, P^\lambda]P^\sigma \\
&= \frac{i}{2}\epsilon_{\mu\nu\rho\sigma}\eta_{\lambda\tau}P^\sigma(\eta^{\lambda\nu}P^\rho - \eta^{\lambda\rho}P^\nu) \\
&= \frac{i}{2}\epsilon_{\mu\nu\rho\sigma}(\delta_\tau^\nu P^\sigma P^\rho - \delta_\tau^\rho P^\sigma P^\nu) \\
&= 0
\end{aligned}$$

through the antisymmetry of the Levi-Civita form, and (this is where it gets quite tricky)

$$\begin{aligned}
[W_\mu, J_{\varkappa\lambda}] &= -\frac{1}{2}\epsilon_{\mu\nu\rho\sigma}\eta^{\alpha\nu}\eta^{\beta\rho}\eta^{\xi\sigma}[J_{\alpha\beta}P_\xi, J_{\varkappa\lambda}] \\
&= \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}\eta^{\alpha\nu}\eta^{\beta\rho}\eta^{\xi\sigma}\{[J_{\varkappa\lambda}, J_{\alpha\beta}]P_\xi + J_{\alpha\beta}[J_{\varkappa\lambda}, P_\xi]\} \\
&= \frac{i}{2}\epsilon_{\mu\nu\rho\sigma}\eta^{\alpha\nu}\eta^{\beta\rho}\eta^{\xi\sigma}\{(\eta_{\varkappa\alpha}J_{\beta\lambda} - \eta_{\lambda\alpha}J_{\beta\varkappa} - \eta_{\varkappa\beta}J_{\alpha\lambda} + \eta_{\lambda\beta}J_{\alpha\varkappa})P_\xi + J_{\alpha\beta}(\eta_{\xi\lambda}P_\varkappa - \eta_{\xi\varkappa}P_\lambda)\} \\
&= \frac{i}{2}\epsilon_{\mu\nu\rho\sigma}\{[\delta_\varkappa^\nu\eta^{\beta\rho}J_{\beta\lambda} - \delta_\lambda^\nu\eta^{\beta\rho}J_{\beta\varkappa} - \delta_\varkappa^\rho\eta^{\alpha\nu}J_{\alpha\lambda} + \delta_\lambda^\rho\eta^{\alpha\nu}J_{\alpha\varkappa}]P^\sigma + J^{\nu\rho}(\delta_\varkappa^\sigma P_\lambda - \delta_\lambda^\sigma P_\varkappa)\} \\
&= \frac{i}{2}\{\eta_{\tau\lambda}(\epsilon_{\mu\varkappa\rho\sigma}J^{\rho\tau}P^\sigma - \epsilon_{\mu\nu\varkappa\sigma}J^{\nu\tau}P^\sigma - \epsilon_{\mu\nu\rho\varkappa}J^{\nu\rho}P^\tau)\} \\
&\quad - \frac{i}{2}\{\eta_{\tau\varkappa}(\epsilon_{\mu\lambda\rho\sigma}J^{\rho\tau}P^\sigma - \epsilon_{\mu\nu\lambda\sigma}J^{\nu\tau}P^\sigma - \epsilon_{\mu\nu\rho\lambda}J^{\nu\rho}P^\tau)\} \\
&= \frac{i}{2}\{\eta_{\tau\lambda}(\epsilon_{\mu\varkappa\rho\sigma}J^{\rho\tau}P^\sigma + \epsilon_{\mu\sigma\varkappa\rho}J^{\tau\sigma}P^\rho - \epsilon_{\mu\rho\varkappa\sigma}J^{\sigma\rho}P^\tau)\} \\
&\quad - \frac{i}{2}\{\eta_{\tau\varkappa}(\epsilon_{\mu\lambda\rho\sigma}J^{\rho\tau}P^\sigma + \epsilon_{\mu\sigma\lambda\rho}J^{\tau\sigma}P^\rho - \epsilon_{\mu\rho\lambda\sigma}J^{\sigma\rho}P^\tau)\} \\
&= \frac{i}{2}\{(2\eta_{\tau\lambda}\epsilon_{\mu\varkappa\rho\sigma} + \eta_{\sigma\lambda}\epsilon_{\mu\tau\rho\varkappa}) - (2\eta_{\tau\varkappa}\epsilon_{\mu\lambda\rho\sigma} + \eta_{\sigma\varkappa}\epsilon_{\mu\tau\rho\lambda})\}J^{\rho\tau}P^\sigma.
\end{aligned}$$

Going further requires a fairly subtle trick. The key argument is that since Minkowski space is four-dimensional, any expression that is antisymmetrised over five indices automatically vanishes. It is not too hard to convince oneself that this is the case for the following expression:

$$\eta_{\tau\lambda}\epsilon_{\mu\varkappa\rho\sigma} + \eta_{\mu\lambda}\epsilon_{\varkappa\rho\sigma\tau} + \eta_{\varkappa\lambda}\epsilon_{\rho\sigma\tau\mu} + \eta_{\rho\lambda}\epsilon_{\sigma\tau\mu\varkappa} + \eta_{\sigma\lambda}\epsilon_{\tau\mu\varkappa\rho} = 0. \quad (1.A.16)$$

Contracting with  $J^{\rho\tau}P^\sigma$  yields

$$[(2\eta_{\tau\lambda}\epsilon_{\mu\varkappa\rho\sigma} + \eta_{\sigma\lambda}\epsilon_{\rho\mu\tau\varkappa}) + (\eta_{\mu\lambda}\epsilon_{\varkappa\tau\rho\sigma} + \eta_{\varkappa\lambda}\epsilon_{\tau\mu\rho\sigma})]J^{\rho\tau}P^\sigma = 0.$$

This enables us to complete the calculation:

$$\begin{aligned}
[W_\mu, J_{\varkappa\lambda}] &= -\frac{i}{2}\{(\eta_{\mu\lambda}\epsilon_{\varkappa\tau\rho\sigma} + \eta_{\varkappa\lambda}\epsilon_{\tau\mu\rho\sigma}) - (\eta_{\mu\varkappa}\epsilon_{\lambda\tau\rho\sigma} + \eta_{\lambda\varkappa}\epsilon_{\tau\mu\rho\sigma})\}J^{\rho\tau}P^\sigma \\
&= -\frac{i}{2}(\eta_{\mu\lambda}\epsilon_{\varkappa\tau\rho\sigma} - \eta_{\mu\varkappa}\epsilon_{\lambda\tau\rho\sigma})J^{\rho\tau}P^\sigma \\
&= -\frac{i}{2}(-\eta_{\mu\lambda}\epsilon_{\varkappa\rho\tau\sigma} + \eta_{\mu\varkappa}\epsilon_{\lambda\rho\tau\sigma})J^{\rho\tau}P^\sigma \\
&= -i(\eta_{\mu\lambda}W_\varkappa - \eta_{\mu\varkappa}W_\lambda).
\end{aligned}$$

Hence

$$[P_\tau, W^2] = \eta^{\mu\nu}([P_\tau, W_\mu]W_\nu + W_\mu[P_\tau, W_\nu])$$

$$= 0$$

and

$$\begin{aligned} [J_{\varkappa\lambda}, W^2] &= \eta^{\mu\nu} ([J_{\varkappa\lambda}, W_\mu] W_\nu + W_\mu [J_{\varkappa\lambda}, W_\nu]) \\ &= i\eta^{\mu\nu} ((\eta_{\mu\lambda} W_\varkappa - \eta_{\mu\varkappa} W_\lambda) W_\nu + W_\mu (\eta_{\nu\lambda} W_\varkappa - \eta_{\nu\varkappa} W_\lambda)) \\ &= i((\delta_\lambda^\nu W_\varkappa - \delta_\varkappa^\nu W_\lambda) W_\nu + W_\mu (\delta_\lambda^\mu W_\varkappa - \delta_\varkappa^\mu W_\lambda)) \\ &= i(W_\varkappa W_\lambda - W_\lambda W_\varkappa + W_\lambda W_\varkappa - W_\varkappa W_\lambda) \\ &= 0 \end{aligned}$$

and the proof is complete.

## 1.A.3 Wigner representations of the Poincaré algebra

### 1.A.3.1 Hilbert space representation of Poincaré transformations

Up to this point we have not done any quantum mechanics in this appendix. The proper way [1] to introduce the quantum formalism here is to ask that the measurable quantities of quantum theory, that is, probabilities, be independent of the observer. We call quantum probability any object defined through the Born rule, that is, any object of the form

$$P(m \leftrightarrow n) = |\langle m | n \rangle|^2 \quad (1.A.17)$$

where (following Dirac's fantastically convenient notation)  $|n\rangle$  is a state of the one-particle Hilbert  $\mathcal{H}_1$  space,  $\langle m|$  is a state of the dual space of linear forms over  $\mathcal{H}_1$ , and, accordingly, the Hilbert scalar product  $\langle m | n \rangle \equiv (|m\rangle, |n\rangle)$  is a complex number.

The central requirement is that, even though states will be changed when we consider two different inertial reference frames—say, as usual, one “unprimed” and one “primed” frame—the Born probabilities (1.A.17) should remain the same. In other words, these probabilities are required to be invariant under transformations of the Poincaré group. A theorem proved by Wigner [11] states that to satisfy this requirement, only two types of transformations of the Hilbert space states are possible, namely:

- The state seen in the primed frame is given by  $|\psi'\rangle = \hat{L} |\psi\rangle$  where  $\hat{L}$  is a linear ( $\forall \lambda \in \mathbb{C} \hat{L}\lambda = \lambda\hat{L}$ ) and unitary ( $(\hat{L} |m\rangle, \hat{L} |n\rangle) = \langle m | n \rangle$ ) operator.
- The state seen in the primed frame is given by  $|\psi'\rangle = \hat{\Lambda} |\psi\rangle$  where  $\hat{\Lambda}$  is an antilinear ( $\forall \lambda \in \mathbb{C} \hat{\Lambda}\lambda = \lambda^*\hat{\Lambda}$ ) and antiunitary ( $(\hat{\Lambda} |m\rangle, \hat{\Lambda} |n\rangle) = \langle m | n \rangle^*$ ) operator.

Poincaré transformations will act upon the Hilbert space  $\mathcal{H}_1$  with such transformations. The operators  $\hat{L}$  and/or  $\hat{\Lambda}$  are called the representatives of the elements of the Poincaré group. Since proper orthochronous Poincaré transformations are continuous (see sect. 1.A.1) functions of some parameters, it is required that their representatives can be continuously deformed into the representative of the identity element, which is the identity operator on  $\mathcal{H}_1$ . This operator is linear and unitary, and thus the representatives of Poincaré transformations must be linear and unitary.

Explicitly, an element  $g$  of the (proper orthochronous) Poincaré group  $G$  is obtained by the exponentiation of an element of the Poincaré algebra:

$$G \ni g = e^{ib^\mu P_\mu + \frac{i}{2}\Omega^{\mu\nu} J_{\mu\nu}}. \quad (1.A.18)$$

Here  $g$  is a two-part object formed by a second rank tensor  $\Lambda$  corresponding to a Lorentz transformation and a



translation four-vector  $b$ . The  $J_{\mu\nu}$  are given by (1.A.6) and (1.A.7) with

$$J_1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix}, \quad J_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix}, \quad J_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$K_1 = \begin{bmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad K_2 = \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad K_3 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}. \quad (1.A.19)$$

The same equation as (1.A.18) holds in a given representation for the representatives of the group and of its Lie algebra. Note that the resemblance of (1.A.18) with what we wrote in (1.A.1) is not obvious, but it must be understood that (1.A.1) corresponded to the representation of the Poincaré group on the Minkowski space of four-vectors. Getting back to the point, the representative of an element of the Poincaré group on  $\mathcal{H}_1$  is thus given by

$$\hat{U}(\Lambda, b) = e^{ib^\mu T(P_\mu) + \frac{i}{2}\Omega^{\mu\nu} T(J_{\mu\nu})} \quad (1.A.20)$$

where  $T(P_\mu)$  and  $T(J_{\mu\nu})$  are the representatives of the elements of the Poincaré algebra in that same representation. From here on out, we drop this heavy notation and simply write  $\hat{P}_\mu$  and  $\hat{J}_{\mu\nu}$  as we will chiefly work directly with the representatives, which are operators on  $\mathcal{H}_1$  (hence the hat). Note that the expression (1.A.20) means that for  $\hat{U}(\Lambda, b)$  to be unitary,  $\hat{P}_\mu$  and  $\hat{J}_{\mu\nu}$  should act as Hermitian operators on the Hilbert space.

We know from nonrelativistic quantum mechanics [4] that linear momentum generates space translations, energy generates time translations, while angular momentum generates rotations. With the addition of the “moment of energy”  $J_{i0}$  as the generator of Lorentz boosts, this is carried in relativistic quantum mechanics. Massive and massless particles must be studied separately, with the emphasis laid on Casimir operators.

### 1.A.3.2 Momentum eigenstates

We now introduce the eigenstates of the four-momentum  $\hat{P}^\mu$  in order to study the Casimir invariants of the Poincaré group, introduced in sect. 1.A.2.2. Since the components of  $\hat{P}^\mu$  commute, they can be diagonalised simultaneously:  $\hat{P}^\mu |p, \alpha\rangle = p^\mu |p, \alpha\rangle$  where  $\alpha$  refers to the quantum numbers necessary to describe a one-particle state, in addition to the momentum. Since we want to build irreducible representations, Schur’s lemma (see sect. 1.A.2.2) tells us that  $\hat{P}^2$  is proportional to the identity operator, with the same proportionality constant for all states. From  $p^\mu p_\mu = m^2$  we deduce that all states in a given representation must have the same invariant rest mass  $m$ .

From the Poincaré group law (1.A.2a) and the expression (1.A.20) of group transformations it is easy to find that  $\hat{U}(\Lambda^{-1}, 0) \hat{P}^\mu \hat{U}(\Lambda, 0) = \Lambda^\mu_\nu \hat{P}^\nu$ , and then deduce

$$\begin{aligned} \hat{P}^\mu \hat{U}(\Lambda, 0) |p, \alpha\rangle &= \hat{U}(\Lambda, 0) \hat{U}(\Lambda^{-1}, 0) \hat{P}^\mu \hat{U}(\Lambda, 0) |p, \alpha\rangle \\ &= \hat{U}(\Lambda, 0) \Lambda^\mu_\nu \hat{P}^\nu |p, \alpha\rangle \\ &= (\Lambda p)^\mu \hat{U}(\Lambda, 0) |p, \alpha\rangle. \end{aligned}$$

Thus we built Lorentz-transformed states of the momentum eigenstates with eigenvalue  $(\Lambda p)^\mu$ . It is then natural to write  $|\Lambda p, \alpha\rangle \equiv \hat{U}(\Lambda, 0) |p, \alpha\rangle$ . Now we define  $\Lambda_{k \rightarrow p}$  such that  $(\Lambda_{k \rightarrow p})^\mu_\nu k^\nu = p^\mu$ . From then on we write,

following [20]:

$$\begin{aligned} [\Phi(\Lambda_0, k, p)]_\nu^\mu k^\nu &\equiv [(\Lambda_{k \rightarrow \Lambda_0 p})^{-1} \Lambda_0 \Lambda_{k \rightarrow p}]_\nu^\mu k^\nu \\ &= [(\Lambda_{k \rightarrow \Lambda_0 p})^{-1}]_\nu^\mu (\Lambda_0 p)^\nu \\ &= k^\nu. \end{aligned}$$

The Lorentz transformations  $\Phi(\Lambda_0, k, p)$  defined in this way, with arbitrary  $\Lambda_0$  and  $p$ , form what is called the little group of the four-momentum  $k$ . Elements of the little group of an object leave that object unmodified when acting upon it.

Lorentz transformations  $\Phi(\Lambda_0, k, p)$  can be represented onto our Hilbert space by operators  $\hat{U}(\Phi(\Lambda_0, k, p), 0)$ . It will be crucial for sect. 1.A.3.4 to notice that

$$[\Phi(\Lambda_0, k, p)]_\nu^\mu k^\nu = k^\nu \Leftrightarrow \hat{U}(\Phi(\Lambda_0, k, p), 0) |k, \alpha\rangle = \sum_\beta \varphi(\alpha, \beta) |k, \beta\rangle. \quad (1.A.21)$$

### 1.A.3.3 Massive particles

For a massive particle we can go in the rest frame where

$$p^\mu = (m, 0, 0, 0) \quad (1.A.22)$$

and make use of the antisymmetry of the Levi-Civita tensor to write  $\hat{W}_0 |p, \alpha\rangle = 0$  because  $p^0$  is the only non-null component of  $\hat{P}^\mu$  while, using (1.A.7), we get

$$\begin{aligned} \hat{W}_i |p, \alpha\rangle &= -\frac{m}{2} \epsilon_{ijk0} \hat{J}^{jk} |p, \alpha\rangle \\ &= \frac{m}{2} \epsilon_{0ijk} \hat{J}^{jk} |p, \alpha\rangle \\ &= -m \hat{J}_i |p, \alpha\rangle, \end{aligned}$$

from which we deduce  $\hat{W}^2 |p, \alpha\rangle = \hat{W}^\mu \hat{W}_\mu |p, \alpha\rangle = -m^2 \hat{\mathbf{J}}^2 |p, \alpha\rangle$ . Again, the structure of the Poincaré group ensures that this identity is valid in all inertial frames. From (1.A.7) and (1.A.8) it can be proved that the components of  $\hat{\mathbf{J}}$  have commutators

$$[\hat{J}_i, \hat{J}_j] = -\epsilon_{0ijk} \hat{J}^k \quad (1.A.23)$$

which is well known [3, 4] to yield the spectrum

$$\boxed{\hat{W}^2 |s, \beta\rangle = -m^2 s(s+1) |s, \beta\rangle} \quad (1.A.24)$$

where  $s$  is positive and is either an integer or a half-integer. Here  $|s, \beta\rangle$  is an eigenstate of  $\hat{W}^2$ , and  $\beta$  refers to the quantum numbers necessary to describe a one-particle state, in addition to  $s$  which represents its spin. We know from sect. 1.A.2.2 that  $\hat{P}^2$  commutes with  $\hat{W}^2$ , so that they can be simultaneously diagonalised. Hence momentum is one of the quantum numbers  $\beta$ , and we can write, with similar notations,  $\hat{P}^2 |s, p, \zeta\rangle = m^2 |s, p, \zeta\rangle$ .

Since we want to construct irreducible representations, the Casimir operators must be, up to a constant, the identity operator. Accordingly, each value of  $m$  and  $s$  corresponds to a unitary representation with a unique realisation of the Casimir invariants. This representation describes a massive particle with squared invariant mass  $m^2 \neq 0$  and spin  $s$ .

### 1.A.3.4 Massless particles

For a massless particle we have the identity  $\hat{P}^2 |p, \alpha\rangle = 0$ . There is no rest frame but we can choose the inertial frame in which the four-momentum of the particle reads

$$k^\mu = (k, 0, 0, k). \quad (1.A.25)$$

Now we compute the action of the components of the Pauli-Lubański four-pseudovector on the momentum eigenstates:

$$\begin{aligned} \hat{W}_\mu |k, \alpha\rangle &= -\frac{1}{2} \epsilon_{\mu\nu\rho\sigma} \hat{J}^{\nu\rho} \hat{P}^\sigma |k, \alpha\rangle \\ &= -\frac{k^\sigma}{2} \epsilon_{\mu\nu\rho\sigma} \hat{J}^{\nu\rho} |k, \alpha\rangle. \end{aligned}$$

Explicitly:

$$\begin{aligned} \hat{W}_0 |k, \alpha\rangle &= -\frac{k^l}{2} \epsilon_{0ijl} \hat{J}^{ij} |k, \alpha\rangle \\ &= k \hat{J}_3 |k, \alpha\rangle, \\ \hat{W}_1 |k, \alpha\rangle &= -\frac{1}{2} \left[ k \left( \epsilon_{1023} \hat{J}^{02} + \epsilon_{1203} \hat{J}^{20} \right) + k \left( \epsilon_{1230} \hat{J}^{23} + \epsilon_{1320} \hat{J}^{32} \right) \right] |k, \alpha\rangle \\ &= k \left( -\hat{J}_1 + \hat{K}_2 \right) |k, \alpha\rangle, \\ \hat{W}_2 |k, \alpha\rangle &= -\frac{1}{2} \left[ k \left( \epsilon_{2013} \hat{J}^{01} + \epsilon_{1203} \hat{J}^{10} \right) + k \left( \epsilon_{2130} \hat{J}^{13} + \epsilon_{2310} \hat{J}^{31} \right) \right] |k, \alpha\rangle \\ &= k \left( -\hat{J}_2 - \hat{K}_1 \right) |k, \alpha\rangle, \\ \hat{W}_3 |k, \alpha\rangle &= -\frac{p}{2} \epsilon_{3ij0} \hat{J}^{ij} |k, \alpha\rangle \\ &= k \hat{J}_3 |k, \alpha\rangle. \end{aligned}$$

To go further, some little group algebra is needed. We expand the Lorentz transformations of the little group of  $k$  according to (1.A.5), focusing on infinitesimal transformations:

$$(\Phi(\Lambda_0, k, p))^\mu{}_\nu = \delta^\mu{}_\nu + \frac{i}{2} \Omega_{\Lambda_0, k, p}^{\rho\sigma} (J_{\rho\sigma})^\mu{}_\nu.$$

For the left-hand equality in (1.A.21) to hold for the four-vector  $k^\mu$  as given in (1.A.25) we must have

$$(\Phi(\Lambda_0, k, p))^\mu{}_\nu = \delta^\mu{}_\nu + \varkappa (J_3)^\mu{}_\nu + \lambda_1 (J_2 + K_1)^\mu{}_\nu + \lambda_2 (J_1 - K_2)^\mu{}_\nu$$

(with  $\varkappa, \lambda_1, \lambda_2$  being simply real parameters) as can be shown by a cumbersome but straightforward calculation from (1.A.19). This means that the corresponding representatives must verify

$$\begin{aligned} \hat{M} |k, \alpha\rangle &\equiv \hat{J}_3 |k, \alpha\rangle = \sum_\beta \mu(\alpha, \beta) |k, \beta\rangle, \\ \hat{L}_1 |k, \alpha\rangle &\equiv \left( \hat{J}_2 + \hat{K}_1 \right) |k, \alpha\rangle = \sum_\beta \zeta_1(\alpha, \beta) |k, \beta\rangle, \\ \hat{L}_2 |k, \alpha\rangle &\equiv \left( \hat{J}_1 - \hat{K}_2 \right) |k, \alpha\rangle = \sum_\beta \zeta_2(\alpha, \beta) |k, \beta\rangle. \end{aligned} \quad (1.A.26)$$

It can be shown from (1.A.8) that the commutation relations of these operators are given by [20]

$$\begin{aligned} \left[ \hat{M}, \hat{L}_1 \right] &= \hat{L}_2, \\ \left[ \hat{M}, \hat{L}_2 \right] &= -\hat{L}_1, \\ \left[ \hat{L}_1, \hat{L}_2 \right] &= 0. \end{aligned} \quad (1.A.27)$$

Thus we can diagonalise  $\hat{L}_1$  and  $\hat{L}_2$  simultaneously, writing

$$\hat{L}_i |\boldsymbol{\eta}, \alpha\rangle = \eta_i |\boldsymbol{\eta}, \alpha\rangle \quad (1.A.28)$$

where  $\boldsymbol{\eta}$  is an abstract two-dimensional vector and  $\alpha$ , as usual, accounts for the degeneracy of the eigenstates of  $\hat{L}_i$ . Now, realise that for a fixed (squared) length  $\boldsymbol{\eta}^2 \neq 0$  of the vector  $\boldsymbol{\eta}$  there is a continuous infinity of possibilities for its orientation. But such a continuous degree of freedom—which is often called “continuous spin”—is not known to exist in nature and, at the very least, is known not to exist for photons. Accordingly, all known massless particles must be described by eigenstates of  $\hat{L}_i$  with zero eigenvalues, thus suppressing the degeneracy.

What remains to be investigated is the action of the last generator  $\hat{M}$  of the little group. We write symbolically  $\alpha = \lambda, \zeta$  with  $\lambda$  the eigenvalue of  $\hat{M}$ :

$$\hat{M} |\lambda, \zeta\rangle = \lambda |\lambda, \zeta\rangle \quad (1.A.29)$$

where  $|\lambda, \zeta\rangle$  is expanded on the shared eigenspace of the two  $\hat{L}_i$  operators with both eigenvalues  $\eta_i$  equal to zero. What values can be taken by  $\lambda$  is determined by the topology of the Lorentz group. We will not enter this here, and refer the interested reader to the second chapter of Weinberg’s celebrated book [1]. Very crudely, we state that because of the topological structure of the Lorentz group, the action of rotations of angles of  $4n\pi$ ,  $n \in \mathbb{N}$ , should not have any effect on quantum one-particle states, making only integer and half-integer values possible for  $\lambda$ . But for half-integer values the operator  $\hat{M}$  is not part of a representation of the Poincaré group, but rather of a slightly more complicated mathematical structure which is called a projective representation. Hence  $\lambda$  **can only take integer values**. It is called the helicity.

Now we remember our initial goal which was to establish the action of the Pauli-Lubański four-pseudovector on the momentum eigenstates. Putting everything together we have (remember that  $\hat{P}^2$  and  $\hat{W}^2$  can be diagonalised simultaneously)

$$\begin{aligned} \hat{W}_0 |k, \lambda, \zeta\rangle &= \hat{W}_3 |k, \lambda, \zeta\rangle = k\lambda |k, \lambda, \zeta\rangle, \\ \hat{W}_1 |k, \lambda, \zeta\rangle &= \hat{W}_2 |k, \lambda, \zeta\rangle = 0. \end{aligned} \quad (1.A.30)$$

And finally this yields  $\hat{W}^2 |k, \lambda, \zeta\rangle = 0$ .

It is then high time to conclude: we have two lightlike operators  $\hat{W}_\mu$  and  $\hat{P}_\mu$  which—as was mentioned in sect. 1.A.2.2—are orthogonal to each other. We can write

$$\begin{aligned} \hat{W}^\mu |k, \lambda, \zeta\rangle &= (||\mathbf{W}||, \mathbf{W}) |k, \lambda, \zeta\rangle, \\ \hat{P}^\mu |k, \lambda, \zeta\rangle &= (||\mathbf{P}||, \mathbf{P}) |k, \lambda, \zeta\rangle, \end{aligned}$$

whence

$$\hat{W}^\mu \hat{P}_\mu |k, \lambda, \zeta\rangle = (||\mathbf{W}|| ||\mathbf{P}|| - \mathbf{W} \cdot \mathbf{P}) |k, \lambda, \zeta\rangle.$$

For this to be zero as it should according to (1.A.15),  $\mathbf{W}$  and  $\mathbf{P}$  should be colinear. Looking at (1.A.25) and (1.A.30), we see that we already have found this by direct explicit calculations, in which we established that the proportionality factor is helicity itself:

$$\boxed{\hat{W}_\mu |k, \lambda, \zeta\rangle = \lambda \hat{P}_\mu |k, \lambda, \zeta\rangle}. \quad (1.A.31)$$

Since we want to construct irreducible representations, the Casimir operators must be, up to a constant, the identity operator. Accordingly, each value of  $\lambda$  corresponds to a unitary representation with a unique realisation of the Pauli-Lubański four-pseudovector. This representation describes a massless particle with squared invariant mass  $m^2 = 0$  and helicity  $\lambda$ . Two states for which the helicities  $\lambda$  and  $\varkappa$  are different can nevertheless correspond to the same type of particle. They do if  $\lambda + \varkappa = 0$ , which is the case for photons which can have helicity  $\lambda = \pm 1$ .

## 1.A.4 Lorenz gauge quantisation

Here we quantise the four-vector potential  $A^\mu$  of electrodynamics in the Lorenz gauge. We follow Gupta and Bleuler's procedure to eliminate irrelevant degrees of freedom. Remember that the Lorenz gauge condition reads  $\partial^\mu A_\mu = 0$ .

### 1.A.4.1 Stückelberg Lagrangian

The *raison d'être* of the Lorenz gauge condition is that it is invariant under Lorentz transformations<sup>9</sup>. In other words, it holds all four components of the vector field  $A^\mu$  in the same regard. Accordingly, we want the canonical Poisson brackets of the theory to be given by the usual

$$\{A_\mu(t, \mathbf{x}), \pi^\nu(t, \mathbf{y})\} = -\delta_\mu^\nu \delta(\mathbf{x} - \mathbf{y}). \quad (1.A.32)$$

However, we saw in sect. 1.4.1 that this is impossible if we stick with the usual Lagrangian (1.3.4) of electrodynamics. But why (and how) would we modify a Lagrangian that yields the expected equations of motion? The answer is: these equations of motion do not constrain the vector field sufficiently so that it carries only two degrees of freedom. Consequently, the gauge must be fixed, as was discussed in sects. 1.2.4 and 1.3.2. The question, of course, is how. In sect. 1.4 we used Dirac's method to incorporate the Coulomb gauge condition in the quantised system. Here we want to impose—in a way yet to be specified—the Lorenz gauge condition—remember that it reads  $\partial^\mu A_\mu = 0$ —**and** we also want to modify the Lagrangian, because of the above discussion. Given these two requirements, it is a logical step to introduce a Lagrange multiplier  $\xi$ . This amounts to redefining the Lagrangian as follows:

$$\mathcal{L}(A^\mu, \partial^\nu A^\mu) = -\frac{1}{4\mu_0} F^{\rho\sigma} F_{\rho\sigma} \rightarrow \mathcal{L}(A^\mu, \partial^\nu A^\mu) = -\frac{1}{4\mu_0} F^{\rho\sigma} F_{\rho\sigma} - \frac{\xi}{2\mu_0} (\partial^\mu A_\mu)^2. \quad (1.A.33)$$

This is the so-called Stückelberg Lagrangian [9].

### 1.A.4.2 Excursion: Lagrange multipliers

The relevance of Lagrange multipliers can be explained following Appel [7]. For simplicity we limit the discussion to functions and not functionals, which means this does not directly apply to field theory. Thus the discussion is more suggestive than conclusive, but we hope it gives a good idea of what is being done in the Gupta-Bleuler procedure.

Imagine that we want to find the extrema of a function  $f : \mathbb{R}^n \mapsto \mathbb{R}$  on a subset  $\mathcal{S}$  of  $\mathbb{R}^n$  defined by  $k$  constraints  $C^{(i)}(\mathbf{x}) = 0$ . Let us denote by  $T_{\mathcal{S}\mathbf{a}}$  the tangent plane to  $\mathcal{S}$  at point  $\mathbf{a}$ . Now, consider the family of applications

$$\begin{aligned} dC_{\mathbf{a}}^{(i)} : \mathbb{R}^n &\rightarrow \mathbb{R} \\ \mathbf{x} \in \mathbb{R}^n &\mapsto \nabla C^{(i)}(\mathbf{a}) \cdot \mathbf{x}. \end{aligned} \quad (1.A.34)$$

Since  $\mathcal{S}$  is defined by  $C^{(i)}(\mathbf{x}) = 0$ , for all  $\mathbf{x}$  in  $T_{\mathcal{S}\mathbf{a}}$  we have  $dC_{\mathbf{a}}^{(i)}(\mathbf{x}) = 0$ . Likewise, define

$$\begin{aligned} df_{\mathbf{a}} : \mathbb{R}^n &\rightarrow \mathbb{R} \\ \mathbf{x} \in \mathbb{R}^n &\mapsto \nabla f(\mathbf{a}) \cdot \mathbf{x}. \end{aligned} \quad (1.A.35)$$

If  $\mathbf{a}$  is an extremum of  $f$  then for all  $\mathbf{x}$ , including these in  $T_{\mathcal{S}\mathbf{a}}$ , we have  $df_{\mathbf{a}}(\mathbf{x}) = 0$ .

The tangent plane  $T_{\mathcal{S}\mathbf{a}}$  is a  $n - k$  dimensional set. By exploiting all  $n - k$  degrees of freedom for  $\mathbf{x} \in T_{\mathcal{S}\mathbf{a}}$  we get

<sup>9</sup>More pragmatically, perhaps, in classical electrodynamics, it gives the Maxwell equations the particularly nice form  $\partial^\nu \partial_\nu A^\mu = \mu J^\mu$ .

the Lagrange multiplier identity

$$df_{\mathbf{a}} = \sum_{i=1}^k \xi_i dC_{\mathbf{a}}^{(i)} \quad (1.A.36)$$

where the  $\xi_i$  are auxiliary unknowns which are called Lagrange multipliers. Along with  $C^{(i)}(\mathbf{x}) = 0$ , this is what must be solved for to find the extrema of  $f$  on  $\mathcal{S}$ . The Stückelberg Lagrangian accounts for the constrained nature of the problem, and the corresponding Euler-Lagrange equations, which we write in the next sect. 1.A.4.3 are the equivalent of (1.A.36). However, the key point in the Gupta-Bleuler method consists in imposing the constraints  $C^{(i)}(\mathbf{x}) = 0$  after the field is quantised using the Stückelberg Lagrangian. Also, the constraints will be imposed in a nontrivial way (see sect. 1.A.4.6).

### 1.A.4.3 Canonical analysis: momenta and commutation relations

The Euler-Lagrange equations for the Stückelberg Lagrangian (1.A.33) read

$$\partial^\nu \partial_\nu A_\mu + (\xi - 1) \partial_\mu \partial_\nu A^\nu = 0. \quad (1.A.37)$$

The canonical momentum is given by

$$\pi^\mu = \frac{\partial \mathcal{L}}{\partial \dot{A}_\mu} = \frac{1}{\mu_0 c} (F^{\mu 0} - \xi \eta^{\mu 0} \partial_\nu A^\nu), \quad (1.A.38)$$

In contrast to what happened in the Coulomb gauge (see sect. 1.4.1),  $\pi^0 \neq 0$  and it makes sense to ask that the canonical commutation relations be

$$[\hat{A}_\mu(\mathbf{x}, t), \hat{\pi}^\nu(\mathbf{y}, t)] = i\hbar \delta_\mu^\nu \delta(\mathbf{x} - \mathbf{y}). \quad (1.A.39)$$

### 1.A.4.4 Formal solution of the Stückelberg equations

Here we solve the Stückelberg equations (1.A.37). In Fourier space they read

$$(-k^2 \delta_\mu^\nu - (\xi - 1) k_\mu k^\nu) \bar{A}^\mu(k) = 0. \quad (1.A.40)$$

At this point a possible route is to define the Stückelberg operator

$$\bar{O}_\mu^\nu(k) \equiv -(k^2 \delta_\mu^\nu + (\xi - 1) k_\mu k^\nu) \quad (1.A.41)$$

and look for its inverse (let us call it the Stückelberg resolvent) as

$$(\bar{O}^{-1})_\mu^\nu(k) = f(k^2) \delta_\mu^\nu + g(k^2) k_\mu k^\nu. \quad (1.A.42)$$

since this is the only second-rank tensor we can build out of the four-vector  $k^\mu$ . This yields

$$\begin{aligned} (\bar{O}^{-1})_\mu^\nu(k) O_\nu^\lambda(k) &= [f(k^2) \delta_\mu^\nu + g(k^2) k_\mu k^\nu] [-k^2 \delta_\nu^\lambda - (\xi - 1) k_\nu k^\lambda] \\ &= -[f(k^2) k^2 \delta_\mu^\lambda + f(k^2) (\xi - 1) k_\mu k^\lambda] - [g(k^2) k^2 k_\mu k^\lambda + g(k^2) (\xi - 1) k^2 k_\mu k^\lambda]. \end{aligned}$$

The Stückelberg resolvent should verify  $(\bar{O}^{-1})_\mu^\nu(k) \bar{O}_\nu^\lambda(k) = \delta_\mu^\lambda$ . This means we must have

$$f(k^2) = -\frac{1}{k^2},$$

$$f(k^2) (\xi - 1) + k^2 g(k^2) + g(k^2) (\xi - 1) k^2 = 0.$$

Hence

$$(\bar{O}^{-1})_{\mu}^{\nu}(k) = -\frac{1}{k^2} \left( \delta_{\mu}^{\nu} + \left( \frac{1-\xi}{\xi} \right) \frac{k_{\mu} k^{\nu}}{k^2} \right). \quad (1.A.43)$$

From  $(\bar{O}^{-1})_{\mu}^{\nu}(k) \bar{O}_{\nu}^{\lambda}(k) = \delta_{\mu}^{\lambda}$  we have  $(\bar{O}^{-1})_{\mu}^{\nu}(k) \bar{O}_{\nu}^{\lambda}(k) \bar{A}^{\mu}(k) = \bar{A}^{\lambda}(k)$  and it looks like there is no (nontrivial) solution to the Stückelberg equation  $\bar{O}_{\nu}^{\lambda}(k) \bar{A}^{\nu}(k) = 0$ . But writing  $(\bar{O}^{-1})_{\mu}^{\nu}(k) \bar{O}_{\nu}^{\lambda}(k) \bar{A}^{\mu}(k)$  only makes sense if all quantities are defined. There are points where this is not the case: if  $k^2 = 0$  then the Stückelberg resolvent (1.A.43) diverges. It is at these points that we may find solutions.

The naive solution  $\bar{A}^{\mu}(k) = 2\pi \delta(k^2) a^{\mu}(\text{sgn}(k_0), \mathbf{k})$  which solved the Coulomb-gauge Maxwell equations, will not work here. But it is clear from (1.A.43) that  $\bar{A}^{\mu}(k)$  should vanish when  $k^{\mu}$  is not on the lightcone  $k^2 = 0$ . Accordingly we can try [21]

$$\bar{A}^{\mu}(k) = 2\pi \left[ \delta(k^2) a^{\mu}(\text{sgn}(k_0), \mathbf{k}) + \frac{\partial \delta(k^2)}{\partial(k^2)} k^{\mu} b(\text{sgn}(k_0), \mathbf{k}) \right]. \quad (1.A.44)$$

A calculation naturally reminiscing of the one we performed to find the resolvent yields a relation between the coefficients  $a^{\mu}$  and  $b$ . Introducing the simpler notation  $(\partial \delta(k^2)) / (\partial(k^2)) \equiv \delta^{(1)}(k^2)$  and substituting the proposed solution (1.A.44) in the Stückelberg equation (1.A.40), we get

$$\begin{aligned} 0 &= (-k^2 \delta_{\mu}^{\nu} - (\xi - 1) k_{\mu} k^{\nu}) 2\pi \left[ \delta(k^2) a^{\mu}(\text{sgn}(k_0), \mathbf{k}) + \delta^{(1)}(k^2) k^{\mu} b(\text{sgn}(k_0), \mathbf{k}) \right] \\ &= -2\pi \left[ k^2 \delta^{(1)}(k^2) k^{\nu} b(\text{sgn}(k_0), \mathbf{k}) + (\xi - 1) \delta(k^2) k_{\mu} a^{\mu}(\text{sgn}(k_0), \mathbf{k}) k^{\nu} + (\xi - 1) k^2 \delta^{(1)}(k^2) k^{\nu} b(\text{sgn}(k_0), \mathbf{k}) \right]. \end{aligned}$$

Keep in mind that ultimately, we will integrate this Fourier-space solution over momenta. Accordingly, we can use the following property of the Dirac distribution, which we can improperly refer to as integration by parts:

$$\int d^4k \delta^{(1)}(k^2) k^2 f(k^{\mu}) = - \int d^4k \delta(k^2) f(k^{\mu}). \quad (1.A.45)$$

Hence we can factor out  $2\pi \delta(k^2)$  and solve

$$0 = (\xi - 1) k_{\mu} a^{\mu}(\text{sgn}(k_0), \mathbf{k}) k^{\nu} - \xi k^{\nu} b(\text{sgn}(k_0), \mathbf{k}).$$

Hence the solution to the Stückelberg equations is given by

$$\bar{A}^{\mu}(k) = 2\pi \left[ \delta(k^2) a^{\mu}(\text{sgn}(k_0), \mathbf{k}) - \delta^{(1)}(k^2) k^{\mu} \left( \frac{1-\xi}{\xi} \right) k_{\nu} a^{\nu}(\text{sgn}(k_0), \mathbf{k}) \right]. \quad (1.A.46)$$

Now we can repeat an argument we went over in sect. 1.4.5:  $A^{\mu}$  is a real function of spacetime and thus  $\bar{A}^{\mu}(k_0, \mathbf{k}) = (\bar{A}^{\mu})^*(-k_0, -\mathbf{k})$ . Accordingly we rewrite (1.A.46) as

$$\bar{A}^{\mu}(k_0, \mathbf{k}) = 2\pi \left[ \delta(k^2) [\theta(k_0) a^{\mu}(\mathbf{k}) + \theta(-k_0) (a^{\mu})^*(-\mathbf{k})] - \delta^{(1)}(k^2) k^{\mu} \left( \frac{1-\xi}{\xi} \right) k_{\nu} [\theta(k_0) a^{\nu}(\mathbf{k}) + \theta(-k_0) (a^{\nu})^*(-\mathbf{k})] \right]. \quad (1.A.47)$$

It is at this point that we follow textbooks in choosing  $\xi = 1$  to simplify the rest of the treatment. It is mentioned in [9] (*inter alia*) that physical results are independent of  $\xi$ , but the author is unaware of any reference treating the general case. He would be very grateful to anyone pointing such a reference out to him.

In the case where we make the so-called Fermi-Feynman choice  $\xi = 1$  the Stückelberg equations are simply

$$-k^2 \bar{A}^{\mu}(k) = 0 \quad (1.A.48)$$

and the solution (1.A.47) takes the much more agreeable form

$$\bar{A}^\mu(k_0, \mathbf{k}) = 2\pi \delta(k^2) [\theta(k_0) a^\mu(\mathbf{k}) + \theta(-k_0) (a^\mu)^*(-\mathbf{k})]. \quad (1.A.49)$$

Remember that at this point we have not enforced the Lorenz gauge condition:  $\bar{A}^\mu(k_0, \mathbf{k})$  has four independent degrees of freedom. Accordingly, the Fourier amplitudes  $a^\mu$  can be expanded over four **mutually orthogonal** vectors  $\epsilon_{(\lambda)}^\mu(\mathbf{k})$  (with  $\lambda \in \{0, 1, 2, 3\}$ ) of unit Minkowski norm as follows:

$$a^\mu(\mathbf{k}) = \sum_{\lambda=0}^3 a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)}^\mu(\mathbf{k}). \quad (1.A.50)$$

It is conventional [6, 9] to take

- $\epsilon_{(0)}^\mu(\mathbf{k})$  along a so-called timelike direction.
- $\epsilon_{(3)}^\mu(\mathbf{k})$  along a so-called spacelike direction.
- $\epsilon_{(1)}^\mu(\mathbf{k})$  and  $\epsilon_{(2)}^\mu(\mathbf{k})$  orthogonal to  $k^\mu$  and also along a spacelike direction.

This means that

$$\epsilon_{(\varepsilon)}^{*\mu}(\mathbf{k}) \epsilon_{(\lambda)\mu}(\mathbf{k}) = \eta_{\varepsilon\lambda} \text{ (this is what is meant by "timelike/spacelike" direction),} \quad (1.A.51a)$$

$$\epsilon_{(1)}^\mu(\mathbf{k}) k_\mu = \epsilon_{(2)}^\mu(\mathbf{k}) k_\mu = 0. \quad (1.A.51b)$$

It is automatically true that

$$\epsilon_{(0)}^{*\mu}(\mathbf{k}) k_\mu = -\epsilon_{(3)}^{*\mu}(\mathbf{k}) k_\mu \equiv \sigma(\mathbf{k}). \quad (1.A.52)$$

Indeed if this is verified then

$$k^\mu = \sigma(\mathbf{k}) \left( \epsilon_{(0)}^\mu(\mathbf{k}) + \epsilon_{(3)}^\mu(\mathbf{k}) \right) \quad (1.A.53)$$

and, from (1.A.51),  $k^\mu k_\mu = 0$  is retrieved. If (1.A.52) was not verified then  $k^\mu$  would have lost its lightlikeness. Also note from (1.A.53) that for  $\epsilon_{(0)}^\mu(\mathbf{k})$  and  $\epsilon_{(3)}^\mu(\mathbf{k})$  to be four-vectors,  $\sigma(\mathbf{k})$  must be a scalar. Hence it can only be a function of  $k^2 = k_0^2 - \mathbf{k}^2$  which in the free case considered here is always zero. Hence  $\sigma(\mathbf{k}) \equiv \sigma$  is a constant and we can rewrite (1.A.52) and (1.A.53) as

$$\epsilon_{(0)}^{*\mu}(\mathbf{k}) k_\mu = -\epsilon_{(3)}^{*\mu}(\mathbf{k}) k_\mu \equiv \sigma \quad (1.A.54)$$

and

$$k^\mu = \sigma \left( \epsilon_{(0)}^\mu(\mathbf{k}) + \epsilon_{(3)}^\mu(\mathbf{k}) \right). \quad (1.A.55)$$

Regardless of the choice of the vectors  $\epsilon_{(\lambda)}^\mu(\mathbf{k})$  the closure relation reads [9]

$$\sum_{\lambda=0}^3 \eta_{\lambda\lambda} \epsilon_{(\lambda)\mu}^*(\mathbf{k}) \epsilon_{(\lambda)}^\nu(\mathbf{k}) = \delta_\mu^\nu. \quad (1.A.56)$$

With all of this in mind, we write the solution to the Stückelberg equations in the Fermi-Feynman case  $\xi = 1$  as

$$A_\mu(x) = \sum_{\lambda=0}^3 \int \tilde{d}k \left[ a_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)\mu}(\mathbf{k}) e^{-ik^\nu x_\nu} + a_{(\lambda)}^*(\mathbf{k}) \epsilon_{(\lambda)\mu}^*(\mathbf{k}) e^{ik^\nu x_\nu} \right]. \quad (1.A.57)$$

This follows from (1.A.49) and (1.A.50) through the same manipulations as those performed in sect. 1.4.5.



### 1.A.4.5 Quantisation from auxiliary Poisson brackets

Instead of directly using the canonical Poisson bracket (1.A.32) to quantise the theory, it is preferred [9, 21] to use another Poisson bracket, computed with the use of (1.A.38):

$$\begin{aligned} \{A_\mu(t, \mathbf{x}), \partial_0 A^\nu(t, \mathbf{y})\} &= \{A_\mu(t, \mathbf{x}), \mu_0 c \pi^\nu(t, \mathbf{y}) + \partial^\nu A^0(t, \mathbf{y}) + \xi \delta_0^\nu \partial_\tau A^\tau(t, \mathbf{y})\} \\ &= -\mu_0 c \delta_\mu^\nu \delta(\mathbf{x} - \mathbf{y}). \end{aligned} \quad (1.A.58)$$

It must be insisted upon that this is not yet another quantisation technique, but that we simply prefer to use the time-derivative of the field instead of the momentum because it makes calculations less cumbersome. We make the Fourier expansion (1.A.57) an operator:

$$\hat{A}_\mu(x) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=0}^3 \int \tilde{d}\mathbf{k} \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)\mu}(\mathbf{k}) e^{-ik^\nu x_\nu} + \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)\mu}^*(\mathbf{k}) e^{ik^\nu x_\nu} \right], \quad (1.A.59)$$

whence the time-derivative

$$\partial_0 \hat{A}_\mu(x) = -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=0}^3 \int \tilde{d}\mathbf{k} k_0 \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)\mu}(\mathbf{k}) e^{-ik^\nu x_\nu} - \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)\mu}^*(\mathbf{k}) e^{ik^\nu x_\nu} \right] \quad (1.A.60)$$

Then in order to satisfy

$$\left[ \hat{A}_\mu(t, \mathbf{x}), \partial_0 \hat{A}^\nu(t, \mathbf{y}) \right] = -i \hbar \mu_0 c \delta_\mu^\nu \delta(\mathbf{x} - \mathbf{y}) \quad (1.A.61)$$

we “guess” that the following commutation relation has to be enforced:

$$\left[ \hat{a}_{(\lambda)}(\mathbf{k}), \hat{a}_{(\lambda')}^\dagger(\mathbf{q}) \right] = -2k_0 (2\pi)^3 \delta(\mathbf{k} - \mathbf{q}) \eta_{\lambda\lambda'}. \quad (1.A.62)$$

Indeed, if this is true, then we can compute, using the closure relation (1.A.56):

$$\begin{aligned} \left[ \hat{A}_\mu(t, \mathbf{x}), \partial_0 \hat{A}^\nu(t, \mathbf{y}) \right] &= -i \frac{\hbar}{\epsilon_0 c} \sum_{\lambda=0}^3 \sum_{\lambda'=0}^3 \int \tilde{d}\mathbf{k} \int \tilde{d}\mathbf{q} q_0 \left[ 2k_0 (2\pi)^3 \delta(\mathbf{k} - \mathbf{q}) \eta_{\lambda\lambda'} \right] \\ &\quad \left[ -\epsilon_{(\lambda)\mu}(\mathbf{k}) \epsilon_{(\lambda')\mu}^*(\mathbf{q}) e^{-i[(\mathbf{k}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{y})-c(|\mathbf{k}|-|\mathbf{q}|)t]} - \epsilon_{(\lambda)\mu}^*(\mathbf{k}) \epsilon_{(\lambda')\mu}(\mathbf{q}) e^{i[(\mathbf{k}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{y})-c(|\mathbf{k}|-|\mathbf{q}|)t]} \right] \\ &= i \hbar \mu_0 c \delta_\mu^\nu \int \tilde{d}\mathbf{k} k_0 \left( -e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} - e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \right) \\ &= i \hbar \mu_0 c \delta_\mu^\nu \int \frac{d\mathbf{k}}{2(2\pi)^3} \left( -e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} - e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \right) \\ &= -i \hbar \mu_0 c \delta_\mu^\nu \delta(\mathbf{x} - \mathbf{y}) \end{aligned}$$

and (1.A.61) is retrieved. Again we introduce the **vacuum state**  $|0\rangle$  of the theory as a state which is destroyed by all  $\hat{a}_{(\lambda)}(\mathbf{k})$  operators:

$$\forall \lambda \in \{0, 1, 2, 3\} \forall \mathbf{k} \in \mathbb{R}^3 \hat{a}_{(\lambda)}(\mathbf{k}) |0\rangle = 0. \quad (1.A.63)$$

The creation operators  $\hat{a}_{(\lambda)}^\dagger(\mathbf{k})$  are said to create scalar photons for  $\lambda = 0$ , longitudinal photons for  $\lambda = 3$ , and transverse photons for  $\lambda = 1, 2$ .

### 1.A.4.6 The Gupta-Bleuler condition

Up to this point, everything seems fine. The Fermi-Feynman choice  $\xi = 1$  has made the algebra fairly simple, and the quantisation is obviously covariant, in contrast to the situation in the Coulomb gauge. However, it must be remembered that we are yet to impose the Lorenz gauge condition  $\partial^\mu A_\mu = 0$ . This will not be the only problem

that we shall encounter.

A one-photon state of polarisation  $\lambda$  reads

$$|1, f\rangle_\lambda \equiv \int \tilde{d}k f(k) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |0\rangle. \quad (1.A.64)$$

For the quantum theory we have built by canonical quantisation to make any sense, its norm should be positive (or zero). But

$$\begin{aligned} {}_\lambda \langle 1, f | 1, f \rangle_\lambda &= \int \tilde{d}k \int \tilde{d}p f^*(k) f(p) \langle 0 | \hat{a}_{(\lambda)}(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{p}) | 0 \rangle \\ &= \int \tilde{d}k \int \tilde{d}p f^*(k) f(p) \langle 0 | -\eta_{\lambda\lambda} (2\pi)^3 2k_0 \delta(\mathbf{k} - \mathbf{p}) | 0 \rangle \\ &= - \int \tilde{d}k |f(k)|^2 \langle 0 | 0 \rangle \eta_{\lambda\lambda}. \end{aligned} \quad (1.A.65)$$

If  $\lambda = 0$  then the square norm of this state is negative: the Fock space for photons is not a Hilbert space. To fix this problem, we need to select a subspace of that Fock space, the so-called subspace of physical states  $|\psi_{\text{phys}}\rangle$ . This is done through the Lorenz gauge condition. The gauge will be fixed not directly, but through an auxiliary condition that will select physical states.

We know we cannot fix the gauge directly through  $\partial^\mu \hat{A}_\mu = 0$ , since this is incompatible with the canonical commutation relations (1.A.61). The same remark goes for the tentative condition

$$\partial^\mu \hat{A}_\mu(x) |\psi_{\text{phys}}\rangle \stackrel{?}{=} 0. \quad (1.A.66)$$

Indeed,  $\partial^\mu \hat{A}_\mu(x) = -\hat{\pi}^0(x)$ , and accordingly, there would be, if we opted for (1.A.66), an incompatibility between, on the one hand,

$$\langle \psi_{\text{phys}} | [\hat{A}^0(t, \mathbf{x}), \hat{\pi}^0(t, \mathbf{y})] | \psi_{\text{phys}} \rangle = 0$$

which comes from (1.A.66) and the hermiticity of  $\hat{\pi}^0$  and, on the other hand,

$$\langle \psi_{\text{phys}} | [\hat{A}^0(t, \mathbf{x}), \hat{\pi}^0(t, \mathbf{y})] | \psi_{\text{phys}} \rangle = -i\delta(\mathbf{x} - \mathbf{y}) \langle \psi_{\text{phys}} | \psi_{\text{phys}} \rangle$$

which comes from the canonical commutation relations (1.A.61).

The proposal that the expectation value should vanish

$$\langle \psi_{\text{phys}} | \partial^\mu \hat{A}_\mu(x) | \psi_{\text{phys}} \rangle \stackrel{?}{=} 0 \quad (1.A.67)$$

is not valid either because it is not linear with respect to state vectors: if two states  $|\psi_{\text{phys}}\rangle$  and  $|\varphi_{\text{phys}}\rangle$  verify (1.A.67) then there is no guarantee that  $(|\psi_{\text{phys}}\rangle + |\varphi_{\text{phys}}\rangle)$  does.

The right answer was given by Gupta [15] and Bleuler [16]. It reads

$$\langle \varphi_{\text{phys}} | \partial^\mu \hat{A}_\mu(x) | \psi_{\text{phys}} \rangle = 0. \quad (1.A.68)$$

It is easy to show that, upon defining the creation part

$$\hat{A}_\mu^-(x) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=0}^3 \int \tilde{d}k \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)\mu}^*(\mathbf{k}) e^{ik^\nu x_\nu}, \quad (1.A.69a)$$

and the annihilation part (beware of the  $\pm$  superscript)

$$\hat{A}_\mu^+(x) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=0}^3 \int \tilde{d}k \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)\mu}(\mathbf{k}) e^{-ik^\nu x_\nu} \quad (1.A.69b)$$

of the field, the Gupta-Bleuler auxiliary condition (1.A.68) can be rewritten as

$$\boxed{\partial^\mu \hat{A}_\mu^+(x) |\psi_{\text{phys}}\rangle = 0}. \quad (1.A.70)$$

Indeed if two states  $|\psi_{\text{phys}}\rangle$  and  $|\varphi_{\text{phys}}\rangle$  verify (1.A.70) then

$$\begin{aligned} \langle \varphi_{\text{phys}} | \partial^\mu \hat{A}_\mu(x) | \psi_{\text{phys}} \rangle &= \langle \varphi_{\text{phys}} | \partial^\mu \hat{A}_\mu^+(x) | \psi_{\text{phys}} \rangle + \langle \varphi_{\text{phys}} | \partial^\mu \hat{A}_\mu^-(x) | \psi_{\text{phys}} \rangle \\ &= \langle \varphi_{\text{phys}} | \partial^\mu \hat{A}_\mu^+(x) | \psi_{\text{phys}} \rangle + \langle \varphi_{\text{phys}} | \left( \partial^\mu \hat{A}_\mu^+ \right)^\dagger(x) | \psi_{\text{phys}} \rangle \\ &= \langle \varphi_{\text{phys}} | \partial^\mu \hat{A}_\mu^+(x) | \psi_{\text{phys}} \rangle + \langle \psi_{\text{phys}} | \partial^\mu \hat{A}_\mu^+(x) | \varphi_{\text{phys}} \rangle^* \\ &= 0 \end{aligned}$$

and (1.A.68) is retrieved. It is clear that (1.A.70) is linear with respect to state vectors. Since it only features the creation part of the field, it is not in conflict with the canonical commutation relations.

### 1.A.4.7 Quotient space

The Gupta-Bleuler condition (1.A.70) has been established as a satisfactory, nontrivial prescription to impose the Lorenz gauge condition. It remains to see, however, how—and why—it solves the problem of negative square norms highlighted in the previous sect. 1.A.4.6. To that aim, we use the relations (1.A.51) on the polarisation vectors to write the Gupta-Bleuler condition as

$$\begin{aligned} 0 &= \partial^\mu \hat{A}_\mu^+(x) |\psi_{\text{phys}}\rangle \\ &= -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \int \tilde{d}k \sum_{\lambda=0}^3 k^\mu \epsilon_{(\lambda)\mu}(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) e^{-ikx} |\psi_{\text{phys}}\rangle \\ &= -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \int \tilde{d}k e^{-ikx} [\hat{a}_{(0)}(\mathbf{k}) \epsilon_{(0)\mu}(\mathbf{k}) k^\mu + \hat{a}_{(3)}(\mathbf{k}) \epsilon_{(3)\mu}(\mathbf{k}) k^\mu] |\psi_{\text{phys}}\rangle \end{aligned}$$

We can use (1.A.55) to rewrite

$$\epsilon_{(3)}^\mu(\mathbf{k}) k_\mu = \frac{1}{k^\tau \epsilon_{(0)\tau}^*(\mathbf{k})} \left[ k^\mu k_\mu - k^\nu \epsilon_{(0)\nu}^*(\mathbf{k}) \epsilon_{(0)}^\mu(\mathbf{k}) k_\mu \right].$$

Also remember that in this integral, the four-vector  $k^\mu$  is constrained to be lightlike. Hence

$$\begin{aligned} 0 &= -i \int \tilde{d}k e^{-ikx} \left[ \hat{a}_{(0)}(\mathbf{k}) - \hat{a}_{(3)}(\mathbf{k}) \frac{k^\nu \epsilon_{(0)\nu}^*(\mathbf{k})}{k^\tau \epsilon_{(0)\tau}^*(\mathbf{k})} \right] k^\mu \epsilon_{(0)\mu}(\mathbf{k}) |\psi_{\text{phys}}\rangle \\ &= -i \int \tilde{d}k e^{-ikx} [\hat{a}_{(0)}(\mathbf{k}) - \hat{a}_{(3)}(\mathbf{k})] k^\mu \epsilon_{(0)\mu}(\mathbf{k}) |\psi_{\text{phys}}\rangle. \end{aligned}$$

Thus the Gupta-Bleuler condition is rewritten as

$$\boxed{[\hat{a}_{(0)}(\mathbf{k}) - \hat{a}_{(3)}(\mathbf{k})] |\psi_{\text{phys}}\rangle = 0}. \quad (1.A.71)$$

This means that **for each wave vector a physical state has the same number of scalar and longitudinal photons**. Consider now a non necessarily physical (in the sense of Gupta and Bleuler) state

$$|\varphi\rangle = \left[ \prod_{j=1}^p \left( \alpha_j^{(1)} \hat{a}_{(\lambda_j=1)}^\dagger(\mathbf{k}_j) + \alpha_j^{(2)} \hat{a}_{(\lambda_j=2)}^\dagger(\mathbf{k}_j) \right) \right] \left[ \prod_{l=1}^n \left( \alpha_l^{(0)} \hat{a}_{(\lambda_l=0)}^\dagger(\mathbf{k}_l) + \alpha_l^{(3)} \hat{a}_{(\lambda_l=3)}^\dagger(\mathbf{k}_l) \right) \right] |0\rangle \quad (1.A.72a)$$

$$\equiv |\chi_p^{\text{trans}}\rangle \otimes |\varphi_n\rangle \quad (1.A.72b)$$

where  $|\chi_p^{\text{trans}}\rangle$  describes the transverse polarisation part and  $|\varphi_n\rangle$  (denoted with a round bracket because it does not belong to a Hilbert space) describes the scalar and longitudinal polarisation parts. The scalar numbers  $\alpha_m^{(\lambda)}$  are completely arbitrary. We will show that the non-transverse part has no physical relevance, by computing the expectation value of the Hamiltonian operator in such a state (1.A.72). We will indeed find that—provided that we ask that  $|\varphi\rangle$  be a physical state—the contribution of  $|\varphi_n\rangle$  to that expectation value vanishes. To do that, we first need to compute the Hamiltonian. As we did for the Coulomb gauge, we succumb to laziness here and only give the result. Again, we use normal ordering (see sect. 1.4.10), the use of which we signal with columns (:).

$$\begin{aligned} \hat{H} &\equiv \hbar c \int d\mathbf{x} : \left[ \sum_{\lambda=0}^3 \hat{\pi}^\mu(x) \left( \partial_0 \hat{A}_\mu(x) \right) - \hat{\mathcal{L}} \right] : \\ &= \hbar c \int \tilde{d}k k_0 \left\{ \left[ \sum_{\lambda=1,2} \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) \right] + \left[ \hat{a}_{(3)}^\dagger(\mathbf{k}) \hat{a}_{(3)}(\mathbf{k}) - \hat{a}_{(0)}^\dagger(\mathbf{k}) \hat{a}_{(0)}(\mathbf{k}) \right] \right\}. \end{aligned} \quad (1.A.73)$$

We now specifically ask that  $|\varphi\rangle$  be a physical state:  $\partial^\mu \hat{A}_\mu^\dagger(x) |\varphi_{\text{phys}}\rangle = 0$ . What this means can be seen in what follows:

$$\begin{aligned} 0 &= [\hat{a}_{(0)}(\mathbf{k}) - \hat{a}_{(3)}(\mathbf{k})] |\varphi_{\text{phys}}\rangle \\ &= |\chi_p^{\text{trans}}\rangle \otimes [\hat{a}_{(0)}(\mathbf{k}) - \hat{a}_{(3)}(\mathbf{k})] \left[ \prod_{l=1}^n \left( \alpha_l^{(0)} \hat{a}_{(\lambda_l=0)}^\dagger(\mathbf{k}_l) + \alpha_l^{(3)} \hat{a}_{(\lambda_l=3)}^\dagger(\mathbf{k}_l) \right) \right] |0\rangle \\ &= |\chi_p^{\text{trans}}\rangle \otimes \sum_{j=1}^n \left( (2\pi)^3 2k_0 \delta(\mathbf{k} - \mathbf{k}_j) \right) \left( -\alpha_j^{(0)} - \alpha_j^{(3)} \right) \left[ \prod_{l=1, l \neq j}^n \left( \alpha_l^{(0)} \hat{a}_{(\lambda_l=0)}^\dagger(\mathbf{k}_l) + \alpha_l^{(3)} \hat{a}_{(\lambda_l=3)}^\dagger(\mathbf{k}_l) \right) \right] |0\rangle. \end{aligned}$$

If, for all  $l$ , we have  $\alpha_l^{(0)} + \alpha_l^{(3)} = 0$  then the Gupta-Bleuler condition is satisfied. We thus take

$$|\varphi_n\rangle = \left[ \prod_{l=1}^n \left( \alpha_l \left( \hat{a}_{(\lambda_l=0)}^\dagger(\mathbf{k}_l) - \hat{a}_{(\lambda_l=3)}^\dagger(\mathbf{k}_l) \right) \right) \right] |0\rangle. \quad (1.A.74)$$

The energy can then be computed:

$$\frac{\langle \varphi_{\text{phys}} | \hat{H} | \varphi_{\text{phys}} \rangle}{\langle \varphi_{\text{phys}} | \varphi_{\text{phys}} \rangle} = \hbar c \int \tilde{d}k k_0 \left[ \frac{\langle \chi_p^{\text{trans}} | \left[ \sum_{\lambda=1,2} \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) \right] | \chi_p^{\text{trans}} \rangle}{\langle \chi_p^{\text{trans}} | \chi_p^{\text{trans}} \rangle} + \frac{(\varphi_n | \left[ \hat{a}_{(3)}^\dagger(\mathbf{k}) \hat{a}_{(3)}(\mathbf{k}) - \hat{a}_{(0)}^\dagger(\mathbf{k}) \hat{a}_{(0)}(\mathbf{k}) \right] | \varphi_n)}{(\varphi_n | \varphi_n)} \right].$$

The second summand on the right-hand side reads

$$\begin{aligned} \int \tilde{d}k \frac{k_0}{(\varphi_n | \varphi_n)} \langle 0 | \left[ \prod_{l=1}^n \left( \alpha_l^* \left( \hat{a}_{(\lambda_l=0)}(\mathbf{k}_l) - \hat{a}_{(\lambda_l=3)}(\mathbf{k}_l) \right) \right) \right] \\ \left[ \hat{a}_{(3)}^\dagger(\mathbf{k}) \hat{a}_{(3)}(\mathbf{k}) - \hat{a}_{(0)}^\dagger(\mathbf{k}) \hat{a}_{(0)}(\mathbf{k}) \right] \left[ \prod_{m=1}^n \left( \alpha_m \left( \hat{a}_{(\lambda_m=0)}^\dagger(\mathbf{k}_m) - \hat{a}_{(\lambda_m=3)}^\dagger(\mathbf{k}_m) \right) \right) \right] |0\rangle \end{aligned}$$

$$\begin{aligned}
&= \int \tilde{d}\mathbf{k} \frac{k_0}{(\varphi_n | \varphi_n)} \langle 0 | \left[ \prod_{l=1}^n \prod_{m=1}^n \alpha_l^* \alpha_m \left( -\hat{a}_{(\lambda_l=0)}(\mathbf{k}_l) \hat{a}_{(0)}^\dagger(\mathbf{k}) \hat{a}_{(0)}(\mathbf{k}) \hat{a}_{(\lambda_m=0)}^\dagger(\mathbf{k}_m) + \hat{a}_{(\lambda_l=3)}(\mathbf{k}_l) \hat{a}_{(3)}^\dagger(\mathbf{k}) \hat{a}_{(3)}(\mathbf{k}) \hat{a}_{(\lambda_m=3)}^\dagger(\mathbf{k}_m) \right) \right] | 0 \rangle \\
&= 0
\end{aligned}$$

because the contributions from scalar (polarisation 0) and longitudinal (polarisation 3) states cancel each other. Hence the expectation value  $\langle \varphi_{\text{Fock}} | \hat{H} | \varphi_{\text{Fock}} \rangle / \langle \varphi_{\text{Fock}} | \varphi_{\text{Fock}} \rangle$  is independent of  $|\varphi_n\rangle$ .

This result can be extended to all so-called physical observables<sup>10</sup>: **the content of a physical state in scalar and longitudinal photons is physically irrelevant.** Remember that since we are only interested in the free electromagnetic field in this chapter, this conclusion only applies in the absence of sources. In practice, this means that to build the Hilbert space of the theory, we can take the quotient space of the total Fock space with respect to the following equivalence relation:

$$\begin{aligned}
|\phi_{\text{phys}}\rangle &= |\chi_p^{\text{trans}}\rangle \otimes |\varphi_n\rangle \sim |\psi_{\text{phys}}\rangle = |\beta_p^{\text{trans}}\rangle \otimes |\gamma_j\rangle \\
\Leftrightarrow & \quad \quad \quad |\chi_p^{\text{trans}}\rangle = |\beta_p^{\text{trans}}\rangle.
\end{aligned} \tag{1.A.75}$$

In the Hilbert space of equivalence classes thusly defined, square norms are positive definite.

#### 1.A.4.8 Gauge arbitrariness and physical observables

We stated in the previous sect. 1.A.4.7 that for physical observables, the content of a physical state in scalar and longitudinal photons is physically irrelevant. It is clear from the proof of that assertion for the Hamiltonian that all the observables which are bilinear in ladder operators  $\hat{a}_{(\lambda)}^\dagger(\mathbf{k})$  and  $\hat{a}_{(\lambda)}(\mathbf{k})$  are physical. The four-vector potential  $\hat{A}^\mu$  and the Faraday tensor  $\hat{F}^{\mu\nu}$ , however, are not bilinear in these operators. We may thus ask how the content of a physical state in scalar and longitudinal photons affects their expectation values.

$$\begin{aligned}
\frac{\langle \varphi_{\text{phys}} | \hat{A}_\mu^+(x) | \varphi_{\text{phys}} \rangle}{\langle \varphi_{\text{phys}} | \varphi_{\text{phys}} \rangle} &= \sqrt{\frac{\hbar}{\epsilon_0 c}} \int \tilde{d}\mathbf{k} e^{-ik^\tau x_\tau} \left[ \sum_{\lambda=1,2} \epsilon_{(\lambda)\mu}(\mathbf{k}) \frac{\langle \chi_p^{\text{trans}} | \hat{a}_{(\lambda)}(\mathbf{k}) | \chi_p^{\text{trans}} \rangle}{\langle \chi_p^{\text{trans}} | \chi_p^{\text{trans}} \rangle} \right. \\
&\quad \left. + \frac{(\varphi_n | [\epsilon_{(3)\mu}(\mathbf{k}) \hat{a}_{(3)}(\mathbf{k}) + \epsilon_{(0)\mu}(\mathbf{k}) \hat{a}_{(0)}(\mathbf{k})] | \varphi_n)}{(\varphi_n | \varphi_n)} \right].
\end{aligned}$$

With the use of (1.A.55) we can rewrite

$$\begin{aligned}
\epsilon_{(3)\mu}(\mathbf{k}) \hat{a}_{(3)}(\mathbf{k}) + \epsilon_{(0)\mu}(\mathbf{k}) \hat{a}_{(0)}(\mathbf{k}) &= \frac{1}{2} [(\epsilon_{(3)\mu}(\mathbf{k}) + \epsilon_{(0)\mu}(\mathbf{k})) (\hat{a}_{(3)}(\mathbf{k}) + \hat{a}_{(0)}(\mathbf{k})) \\
&\quad + (\epsilon_{(3)\mu}(\mathbf{k}) - \epsilon_{(0)\mu}(\mathbf{k})) (\hat{a}_{(3)}(\mathbf{k}) - \hat{a}_{(0)}(\mathbf{k}))] \\
&= \frac{1}{2} \left[ \frac{k_\mu}{\sigma} (\hat{a}_{(3)}(\mathbf{k}) + \hat{a}_{(0)}(\mathbf{k})) \right. \\
&\quad \left. + (\epsilon_{(3)\mu}(\mathbf{k}) - \epsilon_{(0)\mu}(\mathbf{k})) (\hat{a}_{(3)}(\mathbf{k}) - \hat{a}_{(0)}(\mathbf{k})) \right].
\end{aligned} \tag{1.A.76}$$

Since we consider physical states, the second term of the right-hand side of (1.A.76) has vanishing contribution.

This means that

$$\frac{\langle \varphi_{\text{phys}} | \hat{A}_\mu^+(x) | \varphi_{\text{phys}} \rangle}{\langle \varphi_{\text{phys}} | \varphi_{\text{phys}} \rangle} = \sqrt{\frac{\hbar}{\epsilon_0 c}} \int \tilde{d}\mathbf{k} e^{-ik^\tau x_\tau} \left[ \sum_{\lambda=1,2} \epsilon_{(\lambda)\mu}(\mathbf{k}) \frac{\langle \chi_p^{\text{trans}} | \hat{a}_{(\lambda)}(\mathbf{k}) | \chi_p^{\text{trans}} \rangle}{\langle \chi_p^{\text{trans}} | \chi_p^{\text{trans}} \rangle} + \frac{1}{2} \frac{k_\mu}{\sigma} \frac{(\varphi_n | [\hat{a}_{(3)}(\mathbf{k}) + \hat{a}_{(0)}(\mathbf{k})] | \varphi_n)}{(\varphi_n | \varphi_n)} \right] \tag{1.A.77}$$

<sup>10</sup>More about this in the next sect. 1.A.4.8.

and the second integral in (1.A.77) can be rewritten as

$$\Lambda_\mu \equiv -\frac{i}{2} \partial_\mu \int \tilde{d}k e^{-ik^\tau x_\tau} \frac{1}{\sigma} \frac{(\varphi_n | [\hat{a}_{(3)}(\mathbf{k}) + \hat{a}_{(0)}(\mathbf{k})] | \varphi_n)}{(\varphi_n | \varphi_n)}. \quad (1.A.78)$$

This is just the gradient of a scalar function of  $x$ : according to what we learned in sect. 1.2.3, this is a term corresponding to a gauge transformation of the four-vector potential  $\hat{A}^\mu$ . This means that **changing the content of a physical state in scalar and longitudinal photons amounts to performing a gauge transformation on the four-vector potential**<sup>11</sup>. It follows immediately that the expectation values of the Faraday tensor (in other words, of the electric and magnetic fields)  $\hat{F}^{\mu\nu} = \partial^\mu \hat{A}^\nu - \partial^\nu \hat{A}^\mu$  are, for states obeying the Gupta-Bleuler condition (1.A.71), completely unaffected by the presence of scalar and longitudinal photons. This means that the Faraday tensor is a physical observable. For all practical purposes, it is then correct to write the four-vector potential in the Lorenz gauge as

$$\hat{A}_\mu(x) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=1,2} \int \tilde{d}k \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \epsilon_{(\lambda)\mu}(\mathbf{k}) e^{-ik^\nu x_\nu} + \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \epsilon_{(\lambda)\mu}^*(\mathbf{k}) e^{ik^\nu x_\nu} \right]. \quad (1.A.79)$$

### 1.A.4.9 Poincaré generators

Similarly to the Coulomb case, we define

$$\epsilon_{(\pm)}^\mu(\mathbf{k}) \equiv \frac{e^{-i\lambda\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{\sqrt{2}} \left( \epsilon_{(1)}^\mu(\mathbf{k}) \pm i\epsilon_{(2)}^\mu(\mathbf{k}) \right) \quad (1.A.80)$$

and write  $\epsilon^\mu(\mathbf{k}) \equiv \epsilon_{(+)}^\mu(\mathbf{k}) = \epsilon_{(-)}^\mu(\mathbf{k})$ . We also define the corresponding relation for the ladder operators

$$\hat{a}_{(\pm)}(\mathbf{k}) \equiv \frac{e^{i\lambda\chi(\frac{\mathbf{k}}{\|\mathbf{k}\|})}}{\sqrt{2}} \left( \hat{a}_{(1)}(\mathbf{k}) \mp i\hat{a}_{(2)}(\mathbf{k}) \right) \quad (1.A.81)$$

which obey the same commutation relations as (1.A.62). From (1.A.51) and (1.A.80) we get

$$\epsilon^{*\mu}(\mathbf{k}) \epsilon_\mu(\mathbf{k}) = 1, \quad (1.A.82a)$$

$$\epsilon^\mu(\mathbf{k}) \epsilon_\mu(\mathbf{k}) = 0, \quad (1.A.82b)$$

$$\epsilon^\mu(\mathbf{k}) k_\mu = 0. \quad (1.A.82c)$$

Keeping in mind that, on the lightcone, we can write the  $\mathbf{k}$ -space derivative

$$\partial_{\mathbf{k}}^i k_\mu = \delta_\mu^i - \delta_\mu^0 k^i k^0, \quad (1.A.83)$$

we use (1.A.82a) and (1.A.82b) to find the equivalent relation to (1.4.27), namely

$$\partial_{\mathbf{k}}^i \epsilon_\mu(\mathbf{k}) = -i\alpha_X^i(\mathbf{k}) \epsilon_\mu(\mathbf{k}) + \alpha_{(0)}^i(\mathbf{k}) \epsilon_{(0)}^\mu(\mathbf{k}) + \alpha_{(3)}^i(\mathbf{k}) \epsilon_{(3)}^\mu(\mathbf{k}) \quad (1.A.84)$$

where the real vector  $\alpha_X(\mathbf{k})$  is not directly constrained (one can compute its curl but the result is less eloquent than (1.4.29)) and the coefficients  $\alpha_{(0/3)}^i(\mathbf{k})$  obey

$$\sigma^* \left( \alpha_{(0)}^i(\mathbf{k}) - \alpha_{(3)}^i(\mathbf{k}) \right) + \epsilon^i(\mathbf{k}) - \epsilon^0(\mathbf{k}) \frac{k^i}{k^0} = 0 \quad (1.A.85)$$

<sup>11</sup>This gauge transformation does not affect the fact that the vector potential still satisfies the Lorenz gauge condition in the sense of Gupta and Bleuler. Indeed,  $\partial^\mu \Lambda_\mu = 0$  is still verified, as can be seen from  $k^\mu k_\mu = 0$ . Such a transformation only really makes sense if there are no boundary conditions on the potential four-vector, which is the case here.

which is proved from (1.A.82c). Remember from the previous sects. 1.A.4.6, 1.A.4.7 and 1.A.4.8 that Gupta-Bleuler quantisation tells us that, for a given wave vector  $k^\mu$ , the component of  $A^\mu$  along  $\epsilon_{(0)}^\mu(\mathbf{k}) - \epsilon_{(3)}^\mu(\mathbf{k})$  must be discarded, while the component along  $\epsilon_{(0)}^\mu(\mathbf{k}) + \epsilon_{(3)}^\mu(\mathbf{k})$ , that is, according to (1.A.54), along  $k^\mu$ , is a gauge term and may be ignored. We shall, however, see that ignoring it leads to the apparition of gauge terms similar to the one we found (1.4.55) in the Coulomb gauge.

With the help of (1.A.56) and (1.A.54) we rewrite the second term on the right-hand side of (1.4.41b) as

$$i\eta^{\rho\mu}\epsilon^\sigma(\mathbf{k}) = -i\epsilon^{*\rho}(\mathbf{k})\epsilon^\mu(\mathbf{k})\epsilon^\sigma(\mathbf{k}) + \frac{i}{2}\left[\frac{k^\rho}{\sigma^*}\left(\epsilon_{(0)}^\mu(\mathbf{k}) - \epsilon_{(3)}^\mu(\mathbf{k})\right) + \left(\epsilon_{(0)}^{*\rho}(\mathbf{k}) - \epsilon_{(3)}^{*\rho}(\mathbf{k})\right)\frac{k^\mu}{\sigma}\right]\epsilon^\sigma(\mathbf{k}). \quad (1.A.86)$$

As was done in the Coulomb gauge, we start from the Lorentz generators for the scalar field

$$\hat{J}_{ij}^{\text{naive}} = -i\sum_{\lambda=\pm}\int\tilde{d}\mathbf{k}\hat{a}_{(\lambda)}^\dagger(\mathbf{k})\left(k^i\frac{\partial}{\partial k_j} - k^j\frac{\partial}{\partial k_i}\right)\hat{a}_{(\lambda)}(\mathbf{k}) \quad (1.A.87a)$$

and

$$\hat{J}_{0i}^{\text{naive}} = -i\sum_{\lambda=\pm}\int\tilde{d}\mathbf{k}\hat{a}_{(\lambda)}^\dagger(\mathbf{k})\|\mathbf{k}\|\frac{\partial}{\partial k^i}\hat{a}_{(\lambda)}(\mathbf{k}), \quad (1.A.87b)$$

and modify them appropriately. With the use of (1.A.84) and (1.A.85) we find that

$$\begin{aligned} \hat{J}^{ij} = -i\sum_{\lambda=\pm}\int\tilde{d}\mathbf{k}\hat{a}_{(\lambda)}^\dagger(\mathbf{k})\left[\left(k^i\left(\frac{\partial}{\partial k_j} + i\lambda\alpha_X^j(\mathbf{k})\right) - k^j\left(\frac{\partial}{\partial k_i} + i\lambda\alpha_X^i(\mathbf{k})\right)\right)\right. \\ \left. + \lambda\left(\epsilon_{(\lambda)}^{*i}(\mathbf{k})\epsilon_{(\lambda)}^j(\mathbf{k}) - \epsilon_{(\lambda)}^i(\mathbf{k})\epsilon_{(\lambda)}^{*j}(\mathbf{k})\right)\right]\hat{a}_{(\lambda)}(\mathbf{k}) \quad (1.A.88a) \end{aligned}$$

and

$$\hat{J}^{0i} = -i\sum_{\lambda=\pm}\int\tilde{d}\mathbf{k}\hat{a}_{(\lambda)}^\dagger(\mathbf{k})\left[\|\mathbf{k}\|\left(\frac{\partial}{\partial k_i} + i\lambda\alpha_X^i(\mathbf{k})\right) + \lambda\left(\epsilon_{(\lambda)}^{*0}(\mathbf{k})\epsilon_{(\lambda)}^i(\mathbf{k}) - \epsilon_{(\lambda)}^0(\mathbf{k})\epsilon_{(\lambda)}^{*i}(\mathbf{k})\right)\right]\hat{a}_{(\lambda)}(\mathbf{k}) \quad (1.A.88b)$$

have the same features as the Coulomb gauge-boost generator (1.4.53), in the sense that discrepancies between the commutators  $[\hat{J}^{\rho\sigma}, \hat{A}^\mu(x)]$  computed from (1.A.88) and the expected result (1.A.86) are terms proportional to  $k^\mu$ :

$$[\hat{J}^{\rho\sigma}, \hat{A}^\mu(x)] = i\left[(x^\rho\partial^\sigma - x^\sigma\partial^\rho)\hat{A}^\mu(x) - \left(\eta^{\rho\mu}\hat{A}^\sigma(x) - \eta^{\sigma\mu}\hat{A}^\rho(x)\right)\right] + \hat{Q}^{\rho\sigma\mu}(x) \quad (1.A.89)$$

with

$$\begin{aligned} \hat{Q}^{\rho\sigma\mu}(x) = \sqrt{\frac{\hbar}{\epsilon_0 c}}\left[i\int\tilde{d}\mathbf{k}\hat{a}_{(-)}(\mathbf{k})e^{-ik^\nu x_\nu}\left\{\left[k^\rho\left(\alpha_{(0)}^\sigma + \alpha_{(3)}^\sigma\right) + \left(\epsilon_{(0)}^{*\rho}(\mathbf{k}) - \epsilon_{(0)}^{*\rho}(\mathbf{k})\right)\epsilon_{(-)}^\sigma\right] - [\rho \leftrightarrow \sigma]\right\}\frac{k^\mu}{\sigma}\right. \\ \left. + i\int\tilde{d}\mathbf{k}\hat{a}_{(+)}(\mathbf{k})e^{ik^\nu x_\nu}\left\{\left[k^\rho\left(\alpha_{(0)}^{*\sigma}(\mathbf{k}) + \alpha_{(3)}^{*\sigma}(\mathbf{k})\right) + \left(\epsilon_{(0)}^\rho(\mathbf{k}) - \epsilon_{(0)}^\rho(\mathbf{k})\right)\epsilon_{(+)}^\sigma\right] - [\rho \leftrightarrow \sigma]\right\}\frac{k^\mu}{\sigma^*}\right] \\ - \text{h.c.} \quad (1.A.90) \end{aligned}$$

where it is understood that  $\alpha_{(0)}^0(\mathbf{k})$  and  $\alpha_{(3)}^0(\mathbf{k})$ , which had not yet been introduced, vanish. In regard to (1.A.84) this can be understood as a notational way to indicate that polarisation vectors do not depend on the magnitude of the wave vector. In the Gupta-Bleuler formalism, terms such as (1.A.90) can be ignored (they are proportional to  $k^\mu$ ). Moreover, if we perform a computation equivalent to the one that led to (1.4.57), the gauge terms are found to have no influence on the compatibility of Lorentz transformations with the Lorenz gauge condition. This is so because  $\partial_\mu\hat{Q}^{\rho\sigma\mu}(x) = 0$ .

As was the case for the Coulomb gauge, keeping only the transverse degrees of freedom in the Lorenz gauge amounts to relaxing (1.4.37) to (1.4.58) with  $\partial^\mu \hat{\lambda}(x) = -i\Omega_{\rho\sigma} \hat{Q}^{\rho\sigma\mu}(x)$ . There is no easy solution to this equation that would be equivalent to (1.4.59).

It is a good idea to check whether the Lorenz generators (1.A.88) have an appropriate action on the longitudinal component of  $\hat{A}^\mu$ , that is, the one which, for a given wave vector  $k^\mu$ , is parallel to  $k^\mu$ . We can show with use of (1.A.83) that the action of (1.A.88) on the longitudinal component of  $\hat{A}^\mu$  is consistent with (1.4.41b) up to terms which do not affect the validity of the Lorenz gauge condition (in other words, up to terms the four-divergence of which (w.r.t.  $x^\mu$ ) vanishes).

Notice that, compared to the boost generator given in [8], which we showed was relevant in the Coulomb gauge, the Lorenz gauge boost generator (1.A.88b) features an extra term (the second summand on the right-hand side of (1.A.88b)). This term clearly cancels if we switch over to the Coulomb gauge, where the polarisation four-vectors become three-vectors with a time component equal to zero. As far as we know, we obtained (1.A.88a) and (1.A.88b) for the first time here.

#### 1.A.4.10 States of definite momentum and helicity

Define, with the use of the ladder operators (1.A.81)

$$|k, \lambda\rangle = \hat{a}_{(\lambda=\pm)}^\dagger(\mathbf{k}) |0\rangle. \quad (1.A.91)$$

Using (1.4.43), (1.A.88a) and (1.A.88b) in the frame of reference where the momentum reads  $k^\mu = (k, 0, 0, k)$  (see sect. 1.A.3.4), it is easy to see that we have

$$\hat{W}^\mu |k, \lambda\rangle = \lambda \hat{P}^\mu |k, \lambda\rangle = \lambda k^\mu |k, \lambda\rangle \quad (1.A.92)$$

which means, according to the discussion of sect. 1.A.3.4, that the  $\lambda = \pm$  introduced in sect. 1.A.4.9 to define the polarisation vectors (1.A.80) is the helicity of the single-photon state built by applying the creation operator  $\hat{a}_{(\lambda=\pm)}^\dagger(\mathbf{k})$  on the vacuum state of the theory.



# REFERENCES

---

## Books

- [1] S. Weinberg, *The Quantum Theory of Fields*, 1st ed., Vol. 1 (Cambridge University Press, 1995) (cit. on pp. 13–15, 20, 24, 33, 39, 43).
- [2] J.D. Jackson, *Classical Electrodynamics*, 2nd ed. (John Wiley & Sons, 1975) (cit. on p. 19).
- [3] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Mécanique Quantique*, 2nd ed., Vol. 1 (Hermann, 1996) (cit. on pp. 20, 30, 41).
- [4] A. Messiah, *Mécanique Quantique*, 1st ed., Vol. 2 (Dunod, Paris, 1965) (cit. on pp. 20, 40, 41).
- [5] H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, 1980) (cit. on pp. 21, 22).
- [6] L.H. Ryder, *Quantum Field Theory*, 2nd ed. (Cambridge University Press, 1996) (cit. on pp. 24, 28, 47).
- [7] W. Appel, *Mathematics for Physics & Physicists*, 1st ed. (Princeton University Press, 2007) (cit. on pp. 25, 27, 44).
- [8] I. Białynicki-Birula and Z. Białynicka-Birula, *Quantum Electrodynamics*, 1st ed. (Pergamon Press, 1975) (cit. on pp. 29, 32, 33, 55).
- [9] C. Itzykson and J.B. Zuber, *Quantum Field Theory*, 1st ed. (McGraw-Hill, 1980) (cit. on pp. 32, 44, 46–48).
- [10] J.D. Bjorken and S.D. Drell, *Relativistic Quantum Fields* (McGraw-Hill, 1964) (cit. on p. 33).
- [11] E.P. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren*, 1st ed. (Braunschweig, 1931) (cit. on p. 39).

## Articles

- [12] E.P. Wigner, ‘On Unitary Representations of the Inhomogeneous Lorentz Group’, *Ann. Math* **40**, 149 (1939) (cit. on p. 16).
- [13] V. Bargmann and E.P. Wigner, ‘Group Theoretical Discussion of Relativistic Wave Equations’, *Proc. Natl. Acad. Sci. USA* **34**, 211 (1948) (cit. on p. 16).
- [14] A.C. Goldhaber and M.M. Nieto, ‘Photon and graviton mass limits’, *Rev. Mod. Phys.* **82**, 939 (2010) (cit. on p. 16).
- [15] S.N. Gupta, ‘Theory of Longitudinal Photons in Quantum Electrodynamics’, *Proc. Phys. Soc. A* **BD. 63**, 681 (1950) (cit. on pp. 23, 49).
- [16] K. Bleuler, ‘Eine neue Methode zur Behandlung der longitudinalen und skalaren Photonen’, *Helv. Phys. Acta* **23**, (the link points to an English version of the article), 567 (1950) (cit. on pp. 23, 49).
- [17] P.A.M. Dirac, ‘Generalized Hamiltonian Dynamics’, *Canad. J. Math.* **2**, 129 (1950) (cit. on p. 24).

## Unpublished Articles and Online Notes

- [18] D. Tong, *Lectures on Quantum Field Theory - Ch. 4: The Dirac Equation*, <http://www.damtp.cam.ac.uk/user/tong/qft/four.pdf> (cit. on p. 15).
- [19] F. Delduc, *Introduction à la Théorie des Champs - Ch. 1 : Systèmes Continus - Champs Classiques*, [http://perso.ens-lyon.fr/francois.delduc/Chapitre\\_1.pdf](http://perso.ens-lyon.fr/francois.delduc/Chapitre_1.pdf) (cit. on pp. 26, 31).
- [20] F. Delduc, *Introduction aux groupes de Lie destinée aux physiciens*, (2008) [http://perso.ens-lyon.fr/francois.delduc/Groupes\\_2008.pdf](http://perso.ens-lyon.fr/francois.delduc/Groupes_2008.pdf) (cit. on pp. 35, 41, 42).
- [21] T.E. Clark, *Introduction to Quantum Field Theory - Ch. 2.4: Massless Spin One Particles: Photons*, <http://www.physics.purdue.edu/~clarkt/Courses/Physics662/ps/qftch24.pdf> (cit. on pp. 46, 48).



## CHAPTER 2

---

# THE PHOTON POSITION OPERATOR

---

*“What do you say to someone who does not value evidence? What evidence could you provide that would suggest they should value evidence? What logic could you use to show the necessity of valuing logical consistency?”*

Sam Harris in his ‘The Moral Landscape’ speech

In 1948 Newton and Wigner published an article [4] on the localisation of elementary relativistic systems, and found that no localised states existed for relativistic fields with zero mass and helicity  $\pm 1$ . Since then this result has restrained the search for a photon position operator, if not the study of photons in configuration space altogether. Nevertheless, we shall present in this short chapter how a position operator that allows for pointwise localisation of photons has been obtained by Hawton and her collaborators. In sect. 2.1 we give some key steps in the history of the photon position operator. Sect. 2.2 is devoted to the computation and discussion of the Hawton position operator which, as proved in appendix 2.A, has commuting components.

---

### Contents of the Chapter

2.1	A brief history of the photon position operator . . . . .	60
2.1.1	Newton-Wigner localisability . . . . .	60
2.1.2	The Pryce position operator . . . . .	61
2.2	The Hawton position operator . . . . .	61
2.2.1	Change of basis . . . . .	62
2.2.2	Explicit computation of the position operator . . . . .	63
2.2.3	Gauge freedom of the position operator . . . . .	64
2.2.4	Localised eigenvectors and the Newton-Wigner axioms . . . . .	64
2.A	Commutation of the components of the photon position operator . . . . .	65

---

The photon wave function in reciprocal (momentum) space is a firmly-established, widely used object [1, 5]. This is so essentially because the photon momentum operator  $\mathbf{k}$  is a well-defined object. It is indeed, according to the usual rules of the representation of the Lie-Poincaré algebra, the generator of translations in configuration space (see sect. 1.2.1). The photon position operator is, on the other hand, a problematic object, as we shall see in the rest of the chapter. This means that there is a lot of work to be done before the usual [2] framework of wave mechanics can be used. In that framework the configuration space wave function at point  $\mathbf{x}$  is given by

$$\psi(\mathbf{x}) = \langle \mathbf{x} | \psi \rangle, \quad (2.0.1)$$

that is, by the projection of the state vector  $|\psi\rangle$  of the system onto the eigenstates  $|\mathbf{x}\rangle$  of the (hypothetical) position operator  $\hat{\mathbf{X}}$ . Since for photons there are problems with this position operator, the states  $|\mathbf{x}\rangle$  are problematic as well and the usual prescription (2.0.1) does not apply, at least not straightforwardly. We start this chapter with a historical outline of the present issue (sect. 2.1), and then present the solution proposed by Hawton (sect. 2.2).

## 2.1 A brief history of the photon position operator

We identify two key—almost simultaneous—events in the history of the photon position operator. The first one is the announcement by Newton and Wigner [4] that no (pointwise) localised state existed for relativistic fields with zero mass and helicity equal (in absolute value) to 1 or larger. Such a statement is equivalent to stating that a position operator cannot be built for such fields, since the operator could not be associated with localised eigenstates. The second one is the construction, by Pryce, of a photon position operator [6]. Far from contradicting Newton and Wigner’s analysis, Pryce’s result confirmed it, since the position operator he obtained prohibited the simultaneous localisation of photons in all three directions of space.

### 2.1.1 Newton-Wigner localisability

The importance of the result obtained in 1948 by Newton and Wigner calls for an examination of what exactly the authors meant by “localisable states” when they said they found no such states for—among others—the Maxwell field. Before we carry this examination, let us mention that in a very technical paper [7], Wightman extended—using advanced group theoretical techniques well beyond the author’s grasp—Newton’s and Wigner’s results, which only applied to pointwise localisation, to localisation within a region of space, and summed up their approach thusly: “If the notion of [localised] state satisfies certain nearly inevitable requirements, for a single particle it is uniquely determined by the transformation law of the wave function under inhomogeneous Lorentz transformations”.

Getting back to Newton and Wigner’s article, we now investigate the properties they assumed for their localised states. Four properties, thereafter called the **Newton-Wigner axioms**, were asked [4] of localised states at position  $\mathbf{x}_0$ :

1. They form a Hilbert subspace  $\mathcal{H}_{\mathbf{x}_0}$  within the larger Hilbert space  $\mathcal{H}$  of the quantum system.
2. The Hilbert subspace  $\mathcal{H}_{\mathbf{x}_0}$  is invariant under rotations about the localisation position as well as under time and space reflections (with the localisation position taken to be in the reflection plane for the latter).
3. They are well behaved under the action of the Poincaré algebra operators, in the sense that for any normalisable state  $|\psi\rangle$  of  $\mathcal{H}_{\mathbf{x}_0}$  and for any operator (here lazily denoted as  $\hat{A}$ ) representing an element of the Poincaré algebra on  $\mathcal{H}$ , the norm of the vector  $\hat{A}|\psi\rangle$  is a finite quantity.
4. Any spatial displacement acting on a state  $|\psi\rangle$  of  $\mathcal{H}_{\mathbf{x}_0}$  makes it orthogonal to all the states of  $\mathcal{H}_{\mathbf{x}_0}$ .

The analysis is detailed for massive particles but it is simply mentioned that no such states exist for massless particles of helicity equal (in absolute value) to 1 or larger [4].

## 2.1.2 The Pryce position operator

Through relativistic centre-of-mass calculations, Pryce obtained [6] a photon position operator which does not have commuting components. Namely, his operator verifies  $\left[ \left( \hat{X}_{\text{Pryce}} \right)_i, \left( \hat{X}_{\text{Pryce}} \right)_j \right] \neq 0$ . Pryce used relativistic one-particle wave equations to define what he called formal one-particle observables. These observables act on the manifold built from the solutions of the wave equations. This allowed him to define the centre-of-mass for relativistic quantum one-particle states.

In momentum representation the centre-of-mass operator derived by Pryce, building on a previous work by Kemmer [8], reads [6]

$$\hat{\mathbf{X}}_{\text{Pryce}} = i \nabla_{\mathbf{k}} \hat{\mathbb{1}} - \frac{i}{2} \frac{\mathbf{k}}{k^2} \hat{\mathbb{1}} + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{k^2} \quad (2.1.1)$$

where  $\nabla_{\mathbf{k}}$  is the gradient in momentum space and  $\hat{\mathbf{S}}$  is the vector operator the components of which are the representatives

$$\left( \hat{S}_i \right)_{jk} = -i \epsilon_{ijk} \quad (2.1.2)$$

of the generators of the  $SO(3)$  group of rotations in three-dimensional space. As it turns out, the different components of  $\hat{\mathbf{X}}$  do not commute. Their commutator reads

$$\left[ \left( \hat{X}_{\text{Pryce}} \right)_i, \left( \hat{X}_{\text{Pryce}} \right)_j \right] = -\frac{i^2}{(k^2)^2} \epsilon_{ijq} k_q (\mathbf{k} \cdot \hat{\mathbf{S}}) \quad (2.1.3)$$

where Einstein summation over repeated indices is implied. From this point on, since we will only work with three-vectors—except when explicitly mentioned—we do not use contravariant and covariant components, but simply the usual algebra of vectors in three-dimensional Euclidian space. Hence we write  $\mathbf{x}^2 = \mathbf{x} \cdot \mathbf{x} = x_i x_i$ . The result (2.1.3), obtained through a direct calculation from (2.1.1), is for instance found in [9] and can be rewritten [10] in terms of generators of the Poincaré group. The fact that the different vector components of  $\hat{\mathbf{X}}_{\text{Pryce}}$  do not commute means that the localisation of a photon in all three directions of space at once is impossible<sup>1</sup>.

We should then answer the question: which of the Newton-Wigner axioms do the eigenstates of the Pryce operator violate? The answer is axiom 1. Indeed, since the components of  $\hat{\mathbf{X}}_{\text{Pryce}}$  do not commute, they have different eigenvectors, and, even if we assume that we can find common eigenvectors for all three  $\left( \hat{X}_{\text{Pryce}} \right)_i$  with the same eigenvalue  $x_0$ , they will not form a Hilbert space.

However, it turns out that by modifying the Pryce operator, we can construct a position operator for photons with commuting components. This is discussed in the following sect. 2.2.

## 2.2 The Hawton position operator

For massless spin 1 objects, spin and momentum are not independent degrees of freedom, since the projection of spin on momentum—that is, helicity—is a Poincaré invariant (see sect. 1.A.3.4). As argued by Hawton and Baylis [11], the unit polarisation vectors (1.4.19) upon which the momentum space wave function for the photon is expanded (throughout the present chapter we use the Coulomb gauge) depend on the direction of the momentum, and hence the usual momentum space position operator  $i \nabla_{\mathbf{k}} \hat{\mathbb{1}}$  acts not only on the argument of the momentum

<sup>1</sup>Not technically impossible, since the fact that operators do not commute does not mean that they do not have any common eigenvectors.

space wave function, but also on the polarisation vectors and hence modifies the direction of the momentum space wave function.

A possible approach to the problem, proposed by Hawton [12], consists in building a position operator with the definite helicity vectors (1.4.19) as eigenvectors. This requirement amounts to asking that the position operator commute with the helicity operator.

## 2.2.1 Change of basis

To construct a position operator commuting with helicity, it is easier to use the direct orthogonal basis consisting of

$$\begin{aligned} \mathbf{u}_1(\mathbf{k}) &\equiv \boldsymbol{\epsilon}_{(-1)}(\mathbf{k}) = \boldsymbol{\epsilon}^*(\mathbf{k}), \\ \mathbf{u}_2(\mathbf{k}) &\equiv \boldsymbol{\epsilon}_{(+1)}(\mathbf{k}) = \boldsymbol{\epsilon}(\mathbf{k}), \\ \mathbf{u}_3(\mathbf{k}) &\equiv i \frac{\mathbf{k}}{\|\mathbf{k}\|} \end{aligned} \quad (2.2.1)$$

where the definite helicity vectors  $\boldsymbol{\epsilon}(\mathbf{k})$  and  $\boldsymbol{\epsilon}^*(\mathbf{k})$  were defined in sects. 1.4.5 and 1.4.6. In that basis, the helicity operator  $\hat{\Lambda}$  is diagonal, with  $-\Lambda_{11} = \Lambda_{22} = 1$  and  $\Lambda_{33} = 0$  (see sect. 1.4.9). Hence the momentum space gradient  $\hat{\mathbf{X}}_{ij} = i \nabla_{\mathbf{k}} \delta_{ij} \hat{\Lambda}$  commutes with  $\hat{\Lambda}$ . It will constitute our ansatz for the photon position operator. Note that we could also have chosen  $\mathbf{u}_1(\mathbf{k})$  and  $\mathbf{u}_2(\mathbf{k})$  to be the spherical unit vectors  $\mathbf{e}_1(\mathbf{k})$  and  $\mathbf{e}_2(\mathbf{k})$  defined by (1.4.18)—in which case the factor  $i$  should have been dropped from  $\mathbf{u}_3(\mathbf{k})$  to maintain a direct orthogonal basis—or, for that matter, any two mutually orthogonal linear combinations of these vectors. This does not change the form of the position operator because the Kronecker form is invariant under rotations. Now we can take everything to the Cartesian basis.

We thus transform  $\{\mathbf{u}_1(\mathbf{k}), \mathbf{u}_2(\mathbf{k}), \mathbf{u}_3(\mathbf{k})\}$  back to  $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ . This is done through the transformation matrix  $R(\varphi, \theta, \chi)$  where  $\varphi$  and  $\theta$  are the spherical coordinates of the unit vector  $\mathbf{e}_3(\mathbf{k})$  in the direction of  $\mathbf{k}$  (see Fig. 1.4.1). The  $\chi$  angle corresponds to the extra degree of freedom appearing in the most general expression (1.4.19) of the polarisation vectors: they can be rotated at will around  $\mathbf{k}$ , and  $\chi$  is the corresponding angle. The matrix  $R^{-1}(\varphi, \theta, \chi = 0)$  rotates vectors from the laboratory frame to the frame where the momentum reads  $\mathbf{k} = \|\mathbf{k}\| \mathbf{e}_z$ . In the process the unit vector  $\mathbf{e}_1(\mathbf{k})$  is rotated to  $\mathbf{e}_x$  and  $\mathbf{e}_2(\mathbf{k})$  is rotated to  $\mathbf{e}_y$ . In the more general transformation  $R^{-1}(\varphi, \theta, \chi)$ , this is preceded by a rotation of  $\chi$  about  $\mathbf{k}$ . We can thus write the rotation matrix as

$$\begin{aligned} R_{ij}(\varphi, \theta, \chi) &\equiv \mathbf{e}_i \cdot \mathbf{u}_j(\mathbf{k}), \\ (R^{-1})_{ij}(\varphi, \theta, \chi) &\equiv \mathbf{u}_i^*(\mathbf{k}) \cdot \mathbf{e}_j. \end{aligned} \quad (2.2.2)$$

The Hawton position operator is then, according to the usual rules of matrix transformations

$$\boxed{\hat{\mathbf{X}}_{\text{Hawton}} = R(\varphi, \theta, \chi) i \nabla_{\mathbf{k}} R^{-1}(\varphi, \theta, \chi)}. \quad (2.2.3)$$

Using  $R_{ik}(\varphi, \theta, \chi) R_{kj}^{-1}(\varphi, \theta, \chi) = \delta_{ij}$  we get

$$R_{ik}(\varphi, \theta, \chi) \left[ \nabla_{\mathbf{k}} R_{kj}^{-1}(\varphi, \theta, \chi) \right] + [\nabla_{\mathbf{k}} R_{ik}(\varphi, \theta, \chi)] R_{kj}^{-1}(\varphi, \theta, \chi) = \mathbf{0} \quad (2.2.4)$$

and can rewrite, with the use of the notation  $\mathbf{e}_i \cdot \mathbf{u}_j(\mathbf{k}) \equiv (\mathbf{u}_j(\mathbf{k}))_i$ ,

$$\begin{aligned}
\left(\hat{\mathbf{X}}_{\text{Hawton}}\right)_{ij} &= R_{ik}(\varphi, \theta, \chi) i \nabla_{\mathbf{k}} R_{kj}^{-1}(\varphi, \theta, \chi) \\
&= R_{ik}(\varphi, \theta, \chi) i \left[ \nabla_{\mathbf{k}} \left( R_{kj}^{-1}(\varphi, \theta, \chi) \right) + R_{kj}^{-1}(\varphi, \theta, \chi) \nabla_{\mathbf{k}} \right] \\
&= i \left[ \delta_{ij} \nabla_{\mathbf{k}} - [\nabla_{\mathbf{k}} R_{ik}(\varphi, \theta, \chi)] R_{kj}^{-1}(\varphi, \theta, \chi) \right] \\
&= i \left[ \delta_{ij} \nabla_{\mathbf{k}} - [\nabla_{\mathbf{k}} (\mathbf{e}_i \cdot \mathbf{u}_k(\mathbf{k}))] (\mathbf{e}_j \cdot \mathbf{u}_k^*(\mathbf{k})) \right] \\
&= i \left[ \delta_{ij} \nabla_{\mathbf{k}} - [\nabla_{\mathbf{k}} ((\mathbf{u}_k(\mathbf{k}))_i)] (\mathbf{u}_k^*(\mathbf{k}))_j \right].
\end{aligned} \tag{2.2.5}$$

## 2.2.2 Explicit computation of the position operator

*“What can be asserted without evidence can be dismissed without evidence.”*

Christopher Hitchens’s razor

We use the closure relation (1.4.22) as well as (1.4.27) to write the second summand in (2.2.5) as

$$[\nabla_{\mathbf{k}} ((\mathbf{u}_k(\mathbf{k}))_i)] (\mathbf{u}_k^*(\mathbf{k}))_j = i \alpha(\mathbf{k}) \left[ -\epsilon_i(\mathbf{k}) \epsilon_j^*(\mathbf{k}) + \epsilon_i^*(\mathbf{k}) \epsilon_j(\mathbf{k}) \right] + \left[ \epsilon(\mathbf{k}) \epsilon_i^*(\mathbf{k}) + \epsilon^*(\mathbf{k}) \epsilon_i(\mathbf{k}) \right] \frac{k_j}{k^2} - \frac{k_i}{k^2} \left[ \epsilon(\mathbf{k}) \epsilon_j^*(\mathbf{k}) + \epsilon^*(\mathbf{k}) \epsilon_j(\mathbf{k}) \right] \tag{2.2.6}$$

where we reintroduced Białyński-Birula’s notation  $\epsilon(\mathbf{k}) \equiv \epsilon_{(+1)}(\mathbf{k}) = \epsilon_{(-1)}^*(\mathbf{k})$  (sect. 1.4.6). Now, use (1.4.19) and (1.4.22) to notice that

$$\begin{aligned}
\left(\mathbf{k} \times \hat{\mathbf{S}}\right)_{ij} &= -i \epsilon_{mnk} \mathbf{e}_m k_n \epsilon_{kij} \\
&= -i (\delta_{mi} \delta_{nj} - \delta_{mj} \delta_{ni}) \mathbf{e}_m k_n \\
&= -i (\mathbf{e}_i k_j - k_i \mathbf{e}_j) \\
&= -i \mathbf{u}_i^*(\mathbf{k}) \left( (\mathbf{u}_l(\mathbf{k}))_i k_j - k_i (\mathbf{u}_l(\mathbf{k}))_j \right) \\
&= -i \left\{ \left[ \epsilon(\mathbf{k}) \epsilon_i^*(\mathbf{k}) + \epsilon^*(\mathbf{k}) \epsilon_i(\mathbf{k}) \right] \frac{k_j}{k^2} - \frac{k_i}{k^2} \left[ \epsilon(\mathbf{k}) \epsilon_j^*(\mathbf{k}) + \epsilon^*(\mathbf{k}) \epsilon_j(\mathbf{k}) \right] \right\}
\end{aligned} \tag{2.2.7}$$

with the  $\hat{\mathbf{S}}$  matrix given by (2.1.2) and

$$\begin{aligned}
-\epsilon_i(\mathbf{k}) \epsilon_j^*(\mathbf{k}) + \epsilon_i^*(\mathbf{k}) \epsilon_j(\mathbf{k}) &= i \left[ (\mathbf{e}_1(\mathbf{k}))_i (\mathbf{e}_2(\mathbf{k}))_j - (\mathbf{e}_2(\mathbf{k}))_i (\mathbf{e}_1(\mathbf{k}))_j \right] \\
&= -\frac{1}{\|\mathbf{k}\|} \left( \mathbf{k} \cdot \hat{\mathbf{S}} \right)_{ij}
\end{aligned} \tag{2.2.8}$$

to rewrite the position operator (2.2.5) as

$$\boxed{\hat{\mathbf{X}}_{\text{Hawton}} = i \nabla_{\mathbf{k}} \hat{\mathbf{l}} + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{k^2} - \frac{\alpha(\mathbf{k})}{\|\mathbf{k}\|} \mathbf{k} \cdot \hat{\mathbf{S}}}. \tag{2.2.9}$$

Apart from the term proportional to  $\mathbf{k} \hat{\mathbf{l}}$  in the Pryce operator (2.1.1), which amounts to a change of the momentum space normalisation and ultimately to changing the physical signification of the photon wave function (more about that in the next chapter 3), the only difference between the Hawton and Pryce operators is the last term in (2.2.9). Its signification is discussed in the next sect. 2.2.3. This term features the connection  $\alpha(\mathbf{k})$  on the lightcone, introduced in sect. 1.4.6. In the appendix 2.A to this chapter we show that the vector components of  $\hat{\mathbf{X}}_{\text{Hawton}}$  commute, which allows for the construction of pointwise-localised photon states.



Notice that the Hawton position operator (2.2.9) is Hermitian. Indeed, it is well-known [3] and easy to check by an integration by parts, that  $i\nabla_{\mathbf{k}}$  is Hermitian, while it is easily seen from (2.1.2) that  $\hat{\mathbf{S}}$  is Hermitian, and  $\alpha(\mathbf{k})$  is known to be real from sect. 2.2.3. This means that the spectrum of (2.2.9) is ensured to be real, a crucial point if we are to accept it as a position operator.

### 2.2.3 Gauge freedom of the position operator

We encounter in the Hawton position operator the connection  $\alpha(\mathbf{k})$  on the lightcone, which we introduced in sect. 1.4.6 when investigating the dependence of polarisation vectors on  $\mathbf{k}$ . In sect. 1.4.8 we defined the covariant derivative on the lightcone (1.4.50). From (1.4.20a) and (2.2.8) we see that

$$\frac{1}{\|\mathbf{k}\|} \left[ (\mathbf{k} \cdot \hat{\mathbf{S}}) \epsilon_{(\lambda)}(\mathbf{k}) \right]_i = \lambda \epsilon_{(\lambda)i}(\mathbf{k}) \quad (2.2.10)$$

which means that  $\mathbf{k} \cdot \hat{\mathbf{S}} / \|\mathbf{k}\|$  is the helicity operator. Accordingly, when acting on a Hilbert subspace of definite helicity  $\lambda = \pm 1$ , the Hawton position operator can be rewritten

$$\hat{\mathbf{X}}_{\text{Hawton}}^\lambda = i\nabla_{\mathbf{k}} \hat{\mathbb{1}} + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{\mathbf{k}^2} - \frac{1}{\|\mathbf{k}\|} \lambda \alpha(\mathbf{k}). \quad (2.2.11)$$

Reintroducing the covariant derivative on the lightcone,

$$\mathbf{D}_{\mathbf{k}(\lambda)} = \nabla_{\mathbf{k}} + i\lambda \alpha(\mathbf{k}), \quad (2.2.12)$$

first seen in sect. 1.4.8, gives the definite-helicity position operator its most elegant form:

$$\boxed{\hat{\mathbf{X}}_{\text{Hawton}}^\lambda = i\mathbf{D}_{\mathbf{k}(\lambda)} \hat{\mathbb{1}} + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{\mathbf{k}^2}}. \quad (2.2.13)$$

It must be kept in mind that, as mentioned in sect. 1.4.6, the connection  $\alpha(\mathbf{k})$  on the lightcone is not directly constrained. This is due to the fact that the spherical unit vectors  $\mathbf{e}_{1/2}(\mathbf{k})$  can be freely rotated around  $\mathbf{k}$ . Only the curl of  $\alpha(\mathbf{k})$  is completely determined:

$$\nabla_{\mathbf{k}} \times \alpha(\mathbf{k}) = -\frac{\mathbf{k}}{\|\mathbf{k}\|^3}. \quad (2.2.14)$$

The connection on the lightcone thus plays a similar role, in reciprocal space, to that of the vector potential in configuration space. Helicity here plays the role of the charge. As is well known, the vector potential of electrodynamics acts as a connection for the displacement of matter fields in configuration space. Here the connection on the lightcone generates the changes in the spherical unit vectors induced by changes in the wave vector  $\mathbf{k}$ . This is best seen in (1.4.27). A discussion of this gauge freedom is found in [11], where the properties of the Berry phase arising from the existence of a connection in momentum space are exhibited.

### 2.2.4 Localised eigenvectors and the Newton-Wigner axioms

The Hawton position operator was constructed to commute with helicity. This means that, looking for eigenvectors of the position operator, we can start from definite helicity vectors and write [13, 14]

$$\boxed{\bar{\psi}_{\mathbf{x}_0(\lambda)}(\mathbf{k}) = N e^{-i\mathbf{k} \cdot \mathbf{x}_0} \epsilon_{(\lambda)}(\mathbf{k})} \quad (2.2.15)$$

where  $N$  is a normalisation factor which will be of no relevance here. As usual, the overbar indicates that this quantity can be Fourier-transformed back to configuration space. The wave function  $\bar{\psi}_{\mathbf{x}_0(\lambda)}$  describes—in

momentum space—a photon of helicity  $\lambda$ , localised at  $\mathbf{x}_0$ . We show that it is indeed an eigenvector of  $\hat{\mathbf{X}}_{\text{Hawton}}^\lambda$ :

$$\begin{aligned}\hat{\mathbf{X}}_{\text{Hawton}}^\lambda \bar{\psi}_{\mathbf{x}_0(\lambda)}(\mathbf{k}) &= \left[ \mathbf{x}_0 \epsilon_{(\lambda)}(\mathbf{k}) + i \nabla_{\mathbf{k}} \epsilon_{(\lambda)}(\mathbf{k}) + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{\mathbf{k}^2} \epsilon_{(\lambda)}(\mathbf{k}) - \frac{1}{\|\mathbf{k}\|} \lambda \alpha(\mathbf{k}) \epsilon_{(\lambda)}(\mathbf{k}) \right] e^{-i\mathbf{k} \cdot \mathbf{x}_0} \\ &= \left[ \mathbf{x}_0 \epsilon_{(\lambda)}(\mathbf{k}) - i \epsilon_{(\lambda)}(\mathbf{k}) \frac{\mathbf{k}}{\mathbf{k}^2} + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{\mathbf{k}^2} \epsilon_{(\lambda)}(\mathbf{k}) \right] e^{-i\mathbf{k} \cdot \mathbf{x}_0}.\end{aligned}$$

where we made use of (1.4.27). The last term in the brackets is computed with the use of (2.2.7):

$$\begin{aligned}\frac{\mathbf{k} \times \hat{\mathbf{S}}}{\mathbf{k}^2} \epsilon_{(\lambda)}(\mathbf{k}) &= -i \left\{ [\epsilon(\mathbf{k}) \epsilon^*(\mathbf{k}) + \epsilon^*(\mathbf{k}) \epsilon(\mathbf{k})] \frac{k_j}{\mathbf{k}^2} - \left[ \epsilon(\mathbf{k}) \frac{\mathbf{k}}{\mathbf{k}^2} \epsilon_j^*(\mathbf{k}) + \epsilon^*(\mathbf{k}) \frac{\mathbf{k}}{\mathbf{k}^2} \epsilon_j(\mathbf{k}) \right] \right\} \epsilon_{(\lambda)j}(\mathbf{k}) \\ &= i \epsilon_{(\lambda)}(\mathbf{k}) \frac{\mathbf{k}}{\mathbf{k}^2}\end{aligned}$$

and thus we find

$$\hat{\mathbf{X}}_{\text{Hawton}}^\lambda \bar{\psi}_{\mathbf{x}_0(\lambda)}(\mathbf{k}) = \mathbf{x}_0 \bar{\psi}_{\mathbf{x}_0(\lambda)}(\mathbf{k}). \quad (2.2.16)$$

Since the eigenstates of the Hawton position operator are localised, it is natural to think that they must violate one of the Newton-Wigner axioms. However, Newton and Wigner make a corollary assumption to their axiom 2. This axiom asks that the Hilbert subspace  $\mathcal{H}_{\mathbf{x}_0}$  of states localised at  $\mathbf{x}_0$  is invariant, among others, under rotations about the localisation position. To ensure that this is verified, they assumed that  $\mathcal{H}_{\mathbf{x}_0}$  is a  $2s + 1$ -dimensional space, a dimension corresponding to the possible values of the projection of the angular momentum onto an arbitrary quantisation axis. While our analysis of sect. 1.A.3.3 vindicates this approach for massive particles, we saw in sect. 1.A.3.4 that for massless particles, only two helicity states are accessible. This means that the assumption made by Newton and Wigner is, in the massless case, unnecessarily strict. We proved in appendix 1.A that helicity is rotationally invariant. Accordingly, in the massless case, the Hilbert subspace  $\mathcal{H}_{\mathbf{x}_0}$  of states localised at  $\mathbf{x}_0$  is two-dimensional, with both helicity subspaces being separately rotationally invariant [11].

## 2.A Commutation of the components of the photon position operator

It can easily be seen from (2.2.3) that the vector components of  $\hat{\mathbf{X}}_{\text{Hawton}}$  commute. Indeed the Leibniz rule yields

$$\begin{aligned}\left[ \left( \hat{X}_{\text{Hawton}} \right)_i, \left( \hat{X}_{\text{Hawton}} \right)_j \right] &= -R \partial_{\mathbf{k}i} (R^{-1} R) \partial_{\mathbf{k}j} R^{-1} - R R^{-1} R \partial_{\mathbf{k}i} \partial_{\mathbf{k}j} R^{-1} + R \partial_{\mathbf{k}j} (R^{-1} R) \partial_{\mathbf{k}i} R^{-1} + R R^{-1} R \partial_{\mathbf{k}j} \partial_{\mathbf{k}i} R^{-1} \\ &= 0\end{aligned}$$

where we used  $R R^{-1} = \mathbb{1}$ . Proving the same result through direct calculation from (2.2.9) is far from being equally straightforward. A first step is to obtain

$$\begin{aligned}\left[ \left( \hat{X}_{\text{Hawton}} \right)_i, \left( \hat{X}_{\text{Hawton}} \right)_j \right] &= i \left\{ \partial_{\mathbf{k}i} \left( \frac{k_l}{\mathbf{k}^2} \right) \epsilon_{jlm} \hat{S}_m - \partial_{\mathbf{k}j} \left( \frac{k_l}{\mathbf{k}^2} \right) \epsilon_{ilm} \hat{S}_m - \partial_{\mathbf{k}i} \left( \frac{\alpha_j(\mathbf{k})}{\|\mathbf{k}\|} k_q \right) \hat{S}_q + \partial_{\mathbf{k}j} \left( \frac{\alpha_i(\mathbf{k})}{\|\mathbf{k}\|} k_q \right) \hat{S}_q \right\} \\ &\quad + \left[ \hat{S}_m, \hat{S}_q \right] \left[ \epsilon_{ilm} \epsilon_{j pq} \frac{k_l k_p}{(\mathbf{k}^2)^2} - \frac{k_l k_q}{\|\mathbf{k}\|^3} (\epsilon_{ilm} \alpha_j(\mathbf{k}) - \epsilon_{jlm} \alpha_i(\mathbf{k})) \right] \\ &\equiv A_{ij}(\mathbf{k}) + K_{ij}(\mathbf{k})\end{aligned} \quad (2.A.1)$$

where  $A$  corresponds to the first line of the first step on the right-hand side of (2.A.1) and  $K$  to its second line. Making use of the relations

$$\partial_{\mathbf{k}i} \left( \frac{k_l}{\mathbf{k}^2} \right) = \frac{\delta_{il}}{\mathbf{k}^2} - 2 \frac{k_i k_l}{(\mathbf{k}^2)^2} \quad (2.A.2a)$$

$$\partial_{\mathbf{k}i} \left( \frac{\alpha_j(\mathbf{k})}{\|\mathbf{k}\|} k_q \right) = \frac{1}{\|\mathbf{k}\|} \left[ k_q \partial_{\mathbf{k}i} \alpha_j(\mathbf{k}) + \alpha_j(\mathbf{k}) \left( \delta_{iq} - \frac{k_i k_q}{\mathbf{k}^2} \right) \right] \quad (2.A.2b)$$

$$\left[ \hat{S}_m, \hat{S}_q \right]_{ab} = \delta_{ma} \delta_{qb} - \delta_{mb} \delta_{qa} \quad (2.A.2c)$$

yields, after a bit of straightforward algebra and with the help of (2.2.14)

$$(A_{ij})_{ab}(\mathbf{k}) = \frac{1}{\mathbf{k}^2} \left[ (\delta_{aj} \delta_{bi} - \delta_{ai} \delta_{bj}) - \frac{1}{\mathbf{k}^2} (\delta_{aj} k_i k_b - \delta_{bj} k_i k_a - \delta_{ai} k_j k_b + \delta_{bi} k_j k_a) \right. \\ \left. - \|\mathbf{k}\| \left[ \alpha_j(\mathbf{k}) \left( \epsilon_{iab} - \epsilon_{lab} \frac{k_i k_l}{\mathbf{k}^2} \right) - \alpha_i(\mathbf{k}) \left( \epsilon_{jab} - \epsilon_{lab} \frac{k_j k_l}{\mathbf{k}^2} \right) \right] \right], \quad (2.A.3a)$$

$$(K_{ij})_{ab}(\mathbf{k}) = -\frac{1}{\mathbf{k}^2} \left[ (\delta_{aj} \delta_{bi} - \delta_{ai} \delta_{bj}) - \frac{1}{\mathbf{k}^2} (\delta_{aj} k_i k_b - \delta_{bj} k_i k_a - \delta_{ai} k_j k_b + \delta_{bi} k_j k_a) \right. \\ \left. - \frac{1}{\|\mathbf{k}\|} [\alpha_j(\mathbf{k}) (\epsilon_{ilb} k_l k_a - \epsilon_{ila} k_l k_b) - \alpha_i(\mathbf{k}) (\epsilon_{jlb} k_l k_a - \epsilon_{jla} k_l k_b)] \right]. \quad (2.A.3b)$$

The first lines cancel out, and we are left with the quantity

$$(A_{ij})_{ab}(\mathbf{k}) + (K_{ij})_{ab}(\mathbf{k}) = \frac{1}{\|\mathbf{k}\|^3} \left[ \alpha_j(\mathbf{k}) (-\epsilon_{iab} \mathbf{k}^2 + \epsilon_{lab} k_i k_l + \epsilon_{ilb} k_l k_a - \epsilon_{ila} k_l k_b) \right. \\ \left. - \alpha_i(\mathbf{k}) (-\epsilon_{jab} \mathbf{k}^2 + \epsilon_{lab} k_j k_l + \epsilon_{jlb} k_l k_a - \epsilon_{jla} k_l k_b) \right]. \quad (2.A.4)$$

Now we repeat the same trick that allowed us in sect. 1.A.2.2 to conclude that spin (or, for massless particles, helicity) is a relativistic invariant: we use the fact that since space is three-dimensional, any expression that is antisymmetrised over four indices automatically vanishes. It is not too hard to convince oneself that this is the case for the following expression:

$$\delta_{aq} \epsilon_{bil} - \delta_{bq} \epsilon_{ila} + \delta_{iq} \epsilon_{lab} - \delta_{lq} \epsilon_{abi} = 0. \quad (2.A.5)$$

Contracting this with  $k_l k_q$  yields

$$\epsilon_{ilb} k_a k_l - \epsilon_{ila} k_b k_l + \epsilon_{lab} k_i k_l - \epsilon_{iab} \mathbf{k}^2 = 0. \quad (2.A.6)$$

This is exactly what appears in the first line in the right-hand side of (2.A.4). The exact same manipulation with  $j$  substituted for  $i$  is of course valid, and the corresponding expression appears in the second line of (2.A.4). Thus, according to (2.A.6),  $(A_{ij})_{ab}(\mathbf{k}) + (K_{ij})_{ab}(\mathbf{k})$  vanishes, and this ends the proof.

# REFERENCES

---

## Books

- [1] A.I. Akhiezer and V.B. Berestetskii, *Quantum Electrodynamics*, edited by R.E. Marshak, 2nd ed. (Interscience Publishers, 1965) (cit. on p. 60).
- [2] A. Messiah, *Mécanique Quantique*, 1st ed., Vol. 1 (Dunod, Paris, 1965) (cit. on p. 60).
- [3] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Mécanique Quantique*, 2nd ed., Vol. 1 (Hermann, 1996) (cit. on p. 64).

## Articles

- [4] T.D. Newton and E.P. Wigner, ‘Localized States for Elementary Systems’, *Rev. Mod. Phys.* **21**, 400 (1949) (cit. on pp. 59–61).
- [5] I. Białynicki-Birula, ‘Photon Wave Function’, *Prog. Opt.* **36**, 245 (1996) (cit. on p. 60).
- [6] M.H.L. Pryce, ‘The Mass-Centre in the Restricted Theory of Relativity and Its Connexion with the Quantum Theory of Elementary Particles’, *Proc. R. Soc. Lond. A* **195**, 62 (1948) (cit. on pp. 60, 61).
- [7] A.S. Wightman, ‘On the Localizability of Quantum Mechanical Systems’, *Rev. Mod. Phys.* **34**, 845 (1962) (cit. on p. 60).
- [8] N. Kemmer, ‘The Particle Aspect of Meson Theory’, *Proc. R. Soc. Lond. A* **173**, 91 (1939) (cit. on p. 61).
- [9] J. Mourad, ‘Optimal photon localization’, *Phys. Lett. A* **182**, 319 (1993) (cit. on p. 61).
- [10] I. Białynicki-Birula and Z. Białynicka-Birula, ‘Uncertainty Relation for Photons’, *Phys. Rev. Lett.* **108**, 140401 (2012) (cit. on p. 61).
- [11] M. Hawton and W.E. Baylis, ‘Photon position operators and localized bases’, *Phys. Rev. A* **64**, 012101 (2001) (cit. on pp. 61, 64, 65).
- [12] M. Hawton, ‘Photon position operator with commuting components’, *Phys. Rev. A* **59**, 954 (1999) (cit. on p. 62).
- [13] M. Hawton, ‘Photon wave functions in a localized coordinate space basis’, *Phys. Rev. A* **59**, 3223 (1999) (cit. on p. 64).
- [14] M. Hawton, ‘Lorentz-invariant photon number density’, *Phys. Rev. A* **78**, 012111 (2008) (cit. on p. 64).



## CHAPTER 3

---

# PHOTON WAVE FUNCTIONS

---

*“Welcome to Aperture—Where the science is theoretical but your \$60 is fact.”*  
Aperture Science promotional poster in Portal™ 2

The satisfactory photon position operator proposed by Hawton, discussed in the previous chapter 2, opens the way for the study of free photons in configuration space, which we carry out in the present chapter. In sect. 3.1 we establish momentum space photon wave mechanics as the starting point. In the short sect. 3.2 the wave equation for the photon wave function is obtained. In sects. 3.3 and 3.4 we show how different momentum space normalisations lead to configuration space wave functions with different physical contents. Along with other formal topics, we examine in sect. 3.5 how to build a photon number density similar to Poynting’s energy density. This latter question is elaborated upon in sect. 3.6. Sect. 3.7 is a summary of our investigations of single-photon wave mechanics. In the appendix 3.A to this chapter we compute spherical integrals useful to the study of photon localisation.

---

### Contents of the Chapter

3.1	Photon wave function in momentum space . . . . .	70
3.1.1	A class of position operators . . . . .	70
3.1.2	Scalar product and orthogonality . . . . .	70
3.2	Wave equation . . . . .	71
3.3	Energy and number densities—Nonlocality issues . . . . .	71
3.4	Photon wave functions through Glauber’s extraction rule . . . . .	73
3.5	Advanced topics . . . . .	75
3.5.1	Poincaré transformation properties . . . . .	75
3.5.2	Excursion: more on the Riemann-Silberstein wave function . . . . .	75
3.5.2.1	The Riemann-Silberstein vector . . . . .	75
3.5.2.2	The Riemann-Silberstein spinor . . . . .	76
3.5.3	Photon number density through the two-wave function prescription . . . . .	77
3.6	Photon trajectories in the Bohmian picture of wave mechanics . . . . .	79
3.6.1	Some notions on the Bohmian picture . . . . .	80
3.6.2	Problems with defining Bohmian trajectories for photons . . . . .	81
3.7	Outlook on the photon wave function . . . . .	83
3.A	Kernel computation in spherical coordinates . . . . .	84

---

## 3.1 Photon wave function in momentum space

### 3.1.1 A class of position operators

The Hawton position operator (2.2.3) can be freely modified [9–11] to be

$$\hat{\mathbf{X}}_{\text{Hawton}}^{(\beta)} = R(\varphi, \theta, \chi) \|\mathbf{k}\|^\beta i \nabla_{\mathbf{k}} \|\mathbf{k}\|^{-\beta} R^{-1}(\varphi, \theta, \chi) \quad (3.1.1)$$

where  $\beta$  is a scalar that modifies the momentum space normalisation of the position eigenvectors (it obviously has nothing to do with the Lorentz boost parameter). Using what we know from sects. 2.2.1 and 2.2.2, it is straightforward to check that the position operator (3.1.1) can be rewritten similarly to (2.2.9):

$$\hat{\mathbf{X}}_{\text{Hawton}}^{(\beta)} = i \left( \nabla_{\mathbf{k}} - \beta \frac{\mathbf{k}}{\|\mathbf{k}\|^2} \right) \hat{\mathbb{1}} + \frac{\mathbf{k} \times \hat{\mathbf{S}}}{\|\mathbf{k}\|^2} - \frac{\boldsymbol{\alpha}(\mathbf{k})}{\|\mathbf{k}\|} \mathbf{k} \cdot \hat{\mathbf{S}}. \quad (3.1.2)$$

For any value of  $\beta$ , the vector components of  $\hat{\mathbf{X}}_{\text{Hawton}}^{(\beta)}$  commute, and the extra term proportional to  $\beta \mathbf{k}$  adds very little complexity to the proof of appendix 2.A. The corresponding eigenstates are simple modifications of (2.2.15)

$$\bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)}(\mathbf{k}) = N \|\mathbf{k}\|^\beta e^{-i\mathbf{k} \cdot \mathbf{x}_0} \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) \quad (3.1.3)$$

with  $N$  an unimportant normalisation constant. This means that out of the “plain” ( $\beta = 0$ ) Hawton position operator (2.2.9), a whole class of valid photon position operators (3.1.2) can be constructed. Their eigenstates localised at  $\mathbf{x}_0$  have the very simple form given by (3.1.3). We will see that only for two such position operators, namely, the ones with values  $\beta = \pm 1/2$ , do the corresponding eigenstates bear clear physical meaning.

### 3.1.2 Scalar product and orthogonality

Most of the remainder of the present chapter will be devoted to the question of the physical meaning of the photon wave function. As already announced, that meaning will depend on the value of the parameter  $\beta$  introduced in the previous sect. 3.1.1. The first step that we take is to compute the scalar product of two normalisable photon wave functions. The momentum space wave function  $\bar{\psi}_{(\lambda)}^{(\beta)}$  of a photon of definite helicity  $\lambda$  can be expanded over the basis of localised states (3.1.3) as

$$\bar{\psi}_{(\lambda)}^{(\beta)}(\mathbf{k}) = \int d\mathbf{x}_0 f_\psi(\mathbf{x}_0) \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)}(\mathbf{k}) \quad (3.1.4a)$$

with, for the sake of normalisation, the requirement that

$$\int d\mathbf{x} |f_\psi(\mathbf{x})|^2 = 1. \quad (3.1.4b)$$

One would then like to ask that

$$\langle \bar{\psi}_{(\lambda)}^{(\beta)} | \bar{\psi}_{(\lambda)}^{(\beta)} \rangle = 1 \quad (3.1.5)$$

with the scalar product in Dirac notation to be defined. From here on out, we set  $N = 1$ . Using (3.1.4b), it is easy to see that, for (3.1.5) to be valid, we need to define

$$\langle \bar{\psi}_{(\lambda)}^{(\beta)} | \bar{\psi}_{(\lambda)}^{(\beta)} \rangle \equiv \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta}} \left( \bar{\psi}_{(\lambda)}^{(\beta)} \right)^*(\mathbf{k}) \cdot \bar{\psi}_{(\lambda)}^{(\beta)}(\mathbf{k}). \quad (3.1.6)$$

Indeed, making use of (3.1.3) and (3.1.4a), we compute

$$\begin{aligned}
\int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta}} \left( \bar{\psi}_{(\lambda)}^{(\beta)} \right)^* (\mathbf{k}) \cdot \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}) &= \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta}} \int d\mathbf{x}_0 f_{\psi}^* (\mathbf{x}_0) \left( \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} \right)^* (\mathbf{k}) \cdot \int d\mathbf{y}_0 f_{\psi} (\mathbf{y}_0) \bar{\psi}_{\mathbf{y}_0(\lambda)}^{(\beta)} (\mathbf{k}) \\
&= \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta}} \int d\mathbf{x}_0 \int d\mathbf{y}_0 f_{\psi}^* (\mathbf{x}_0) f_{\psi} (\mathbf{y}_0) \|\mathbf{k}\|^{2\beta} e^{i\mathbf{k} \cdot (\mathbf{x}_0 - \mathbf{y}_0)} \boldsymbol{\epsilon}_{(\lambda)}^* (\mathbf{k}) \cdot \boldsymbol{\epsilon}_{(\lambda)} (\mathbf{k}) \\
&= \int d\mathbf{x} |f_{\psi} (\mathbf{x})|^2 \\
&= 1
\end{aligned} \tag{3.1.7}$$

where we used (1.4.20a). The configuration space wave function is simply obtained through an inverse Fourier transform

$$\psi_{(\lambda)}^{(\beta)} (\mathbf{x}, t) \equiv \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k} \cdot \mathbf{x} - c\|\mathbf{k}\|t)} \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}). \tag{3.1.8a}$$

which is uninverted by

$$\bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}) \equiv \int d\mathbf{x} e^{-i(\mathbf{k} \cdot \mathbf{x} - c\|\mathbf{k}\|t)} \psi_{(\lambda)}^{(\beta)} (\mathbf{x}, t). \tag{3.1.8b}$$

## 3.2 Wave equation

From (1.4.21) and (3.1.3) it is easy to see that

$$i\mathbf{k} \times \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} (\mathbf{k}) = \lambda \|\mathbf{k}\| \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} (\mathbf{k}). \tag{3.2.1}$$

Now integrate both sides as prescribed by (3.1.4a):

$$\begin{aligned}
i \int d\mathbf{x}_0 f_{\psi} (\mathbf{x}_0) \mathbf{k} \times \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} (\mathbf{k}) &= \lambda \int d\mathbf{x}_0 f_{\psi} (\mathbf{x}_0) \|\mathbf{k}\| \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} (\mathbf{k}). \\
i\mathbf{k} \times \int d\mathbf{x}_0 f_{\psi} (\mathbf{x}_0) \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} (\mathbf{k}) &= \lambda \|\mathbf{k}\| \int d\mathbf{x}_0 f_{\psi} (\mathbf{x}_0) \bar{\psi}_{\mathbf{x}_0(\lambda)}^{(\beta)} (\mathbf{k}). \\
i\mathbf{k} \times \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}) &= \lambda \|\mathbf{k}\| \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}).
\end{aligned} \tag{3.2.2}$$

This is the wave equation obeyed by the momentum space single-photon wave function. To obtain the wave equation in configuration space, we use the Fourier transform (3.1.8a) and write

$$\begin{aligned}
i \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k} \cdot \mathbf{x} - c\|\mathbf{k}\|t)} \mathbf{k} \times \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}) &= \lambda \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k} \cdot \mathbf{x} - c\|\mathbf{k}\|t)} \|\mathbf{k}\| \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}). \\
\nabla \times \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k} \cdot \mathbf{x} - c\|\mathbf{k}\|t)} \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}) &= i\lambda \frac{1}{c} \frac{\partial}{\partial t} \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k} \cdot \mathbf{x} - c\|\mathbf{k}\|t)} \bar{\psi}_{(\lambda)}^{(\beta)} (\mathbf{k}).
\end{aligned}$$

Hence

$$\boxed{\hbar c \lambda \nabla \times \psi_{(\lambda)}^{(\beta)} (\mathbf{x}, t) = i\hbar \frac{\partial}{\partial t} \psi_{(\lambda)}^{(\beta)} (\mathbf{x}, t)}. \tag{3.2.3}$$

This is the wave equation obeyed by the configuration space single-photon wave function. Planck's constant  $\hbar$  was introduced on both sides to facilitate the comparison with the usual Schrödinger equation for massive particles.

## 3.3 Energy and number densities—Nonlocality issues

Since we asked that  $\langle \bar{\psi}_{(\lambda)}^{(\beta)} | \bar{\psi}_{(\lambda)}^{(\beta)} \rangle = 1$ , we can consider that, if we manage to rewrite an integral of the form (3.1.6) as a single integral in configuration space, then the integrand can be thought of as the probability density for



photons.

The use of (3.1.8a) yields, for the prescription (3.1.6)

$$\begin{aligned} \langle \bar{\psi}_{(\lambda)}^{(\beta)} | \bar{\psi}_{(\lambda)}^{(\beta)} \rangle &= \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta}} \int d\mathbf{x} \int d\mathbf{y} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \left( \psi_{(\lambda)}^{(\beta)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(\beta)} (\mathbf{y}, t) \\ &= \int d\mathbf{x} \int d\mathbf{y} \left( \psi_{(\lambda)}^{(\beta)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(\beta)} (\mathbf{y}, t) \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta}} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}. \end{aligned} \quad (3.3.1)$$

The rightmost integral on the right-hand side of (3.3.1) is called a kernel. Such integrals are computed in the appendix 3.A to this chapter. Using (3.A.7), (3.A.14) and (3.A.15), we rewrite

$$\langle \bar{\psi}_{(\lambda)}^{(1)} | \bar{\psi}_{(\lambda)}^{(1)} \rangle = \frac{1}{4\pi} \int d\mathbf{x} \int d\mathbf{y} \frac{\left( \psi_{(\lambda)}^{(1)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(1)} (\mathbf{y}, t)}{\|\mathbf{x} - \mathbf{y}\|}, \quad (3.3.2a)$$

$$\langle \bar{\psi}_{(\lambda)}^{(1/2)} | \bar{\psi}_{(\lambda)}^{(1/2)} \rangle = \frac{1}{2\pi^2} \int d\mathbf{x} \int d\mathbf{y} \frac{\left( \psi_{(\lambda)}^{(1/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(1/2)} (\mathbf{y}, t)}{\|\mathbf{x} - \mathbf{y}\|} \text{vp} \frac{1}{\|\mathbf{x} - \mathbf{y}\|}, \quad (3.3.2b)$$

$$\langle \bar{\psi}_{(\lambda)}^{(0)} | \bar{\psi}_{(\lambda)}^{(0)} \rangle = \int d\mathbf{x} \left( \psi_{(\lambda)}^{(0)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(0)} (\mathbf{x}, t). \quad (3.3.2c)$$

For  $\beta \geq 3/2$  the kernel integral diverges, while for  $\beta \leq -1/2$  its expression is not especially illuminating (see in appendix 3.A). Note that only the photon wave function  $\psi_{(\lambda)}^{(0)}$  allows to build a local density of photons:  $\left| \psi_{(\lambda)}^{(0)} (\mathbf{x}, t) \right|^2 d\mathbf{x}$  is the probability to find—at time  $t$ —a photon of helicity  $\lambda$  in a differential volume  $d\mathbf{x}$  around  $\mathbf{x}$ . The wave function  $\psi_{(\lambda)}^{(0)}$  is known as the Landau-Peierls wave function [12–14].

We can perform the same exercise for the expectation value of the energy. Since, in momentum representation, the Hamiltonian is simply  $\hbar \|\mathbf{k}\| c$ , we can write,

$$\langle \bar{\psi}_{(\lambda)}^{(\beta)} | \hat{H} | \bar{\psi}_{(\lambda)}^{(\beta)} \rangle = \hbar c \int d\mathbf{x} \int d\mathbf{y} \left( \psi_{(\lambda)}^{(\beta)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(\beta)} (\mathbf{y}, t) \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{2\beta-1}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}. \quad (3.3.3)$$

whence

$$\langle \bar{\psi}_{(\lambda)}^{(3/2)} | \hat{H} | \bar{\psi}_{(\lambda)}^{(3/2)} \rangle = \frac{\hbar c}{4\pi} \int d\mathbf{x} \int d\mathbf{y} \frac{\left( \psi_{(\lambda)}^{(3/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(3/2)} (\mathbf{y}, t)}{\|\mathbf{x} - \mathbf{y}\|}, \quad (3.3.4a)$$

$$\langle \bar{\psi}_{(\lambda)}^{(1)} | \hat{H} | \bar{\psi}_{(\lambda)}^{(1)} \rangle = \frac{\hbar c}{2\pi^2} \int d\mathbf{x} \int d\mathbf{y} \frac{\left( \psi_{(\lambda)}^{(1)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(1)} (\mathbf{y}, t)}{\|\mathbf{x} - \mathbf{y}\|} \text{vp} \frac{1}{\|\mathbf{x} - \mathbf{y}\|}, \quad (3.3.4b)$$

$$\langle \bar{\psi}_{(\lambda)}^{(1/2)} | \hat{H} | \bar{\psi}_{(\lambda)}^{(1/2)} \rangle = \hbar c \int d\mathbf{x} \left( \psi_{(\lambda)}^{(1/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(1/2)} (\mathbf{x}, t). \quad (3.3.4c)$$

This time it is the photon wave function  $\psi_{(\lambda)}^{(1/2)}$  that allows to build a local density of electromagnetic energy:  $\left| \psi_{(\lambda)}^{(1/2)} (\mathbf{x}, t) \right|^2 d\mathbf{x}$  is the energy density—at time  $t$ —carried by a photon of helicity  $\lambda$  in a differential volume  $d\mathbf{x}$  around  $\mathbf{x}$ . The wave function  $\psi_{(\lambda)}^{(1/2)}$  is known as the Riemann-Silberstein wave function [12, 13, 15, 16].

## 3.4 Photon wave functions through Glauber's extraction rule

To get a better sense of what the different photon wave functions mean, it is a good idea to use Glauber's extraction rule [13]. In the generalised sense that we consider here, we call Glauber's extraction rule the equations that link direct-space photon wave functions  $\psi_{(\lambda)}^{(\beta)}$  on the one side to one-photon states  $|1, f\rangle_\lambda$  and field operators  $\hat{\mathbf{O}}^{(\beta)}$  on the other. Namely

$$\boxed{\psi_{(\lambda)}^{(\beta)}(\mathbf{x}, t) = \langle 0 | \hat{\mathbf{O}}^{(\beta)}(\mathbf{x}, t) | 1, f \rangle_\lambda} \quad (3.4.1)$$

where the one-photon state  $|1, f\rangle_\lambda$  of polarisation  $\lambda$  reads

$$|1, f\rangle_\lambda \equiv \int \frac{d\mathbf{k}}{2(2\pi)^3 ||\mathbf{k}||} \bar{f}(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |0\rangle. \quad (3.4.2)$$

Glauber first introduced the object (3.4.1) with Titulaer [17] in an effort to study the coherence properties of quantum light. From (3.1.3), (3.1.4a) and (3.1.8a) we write the configuration space photon wave function explicitly as

$$\begin{aligned} \psi_{(\lambda)}^{(\beta)}(\mathbf{x}, t) &= \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k}\cdot\mathbf{x} - c||\mathbf{k}||t)} \int d\mathbf{x}_0 f_\psi(\mathbf{x}_0) ||\mathbf{k}||^\beta e^{-i\mathbf{k}\cdot\mathbf{x}_0} \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) \\ &= \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i(\mathbf{k}\cdot\mathbf{x} - c||\mathbf{k}||t)} \bar{f}_\psi(\mathbf{k}) ||\mathbf{k}||^\beta \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}). \end{aligned} \quad (3.4.3)$$

Now compare with what the right-hand side of (3.4.1) yields when we take

$$\hat{\mathbf{O}}^{(\beta)}(\mathbf{x}, t) = \sum_{\varkappa=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 ||\mathbf{k}||} g_\beta(||\mathbf{k}||) \left[ \hat{a}_{(\varkappa)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\varkappa)}(\mathbf{k}) e^{-i(c||\mathbf{k}||t - \mathbf{k}\cdot\mathbf{x})} + \hat{a}_{(\varkappa)}^\dagger(\mathbf{k}) \boldsymbol{\epsilon}_{(\varkappa)}^*(\mathbf{k}) e^{i(c||\mathbf{k}||t - \mathbf{k}\cdot\mathbf{x})} \right], \quad (3.4.4)$$

namely, with

$$\begin{aligned} \langle 0 | \hat{\mathbf{O}}^{(\beta)}(\mathbf{x}, t) | 1, f \rangle_\lambda &= \sum_{\varkappa=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 ||\mathbf{k}||} g_\beta(||\mathbf{k}||) \int \frac{d\mathbf{q}}{2(2\pi)^3 ||\mathbf{q}||} \bar{f}(\mathbf{q}) \\ &\quad \langle 0 | \left[ \hat{a}_{(\varkappa)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\varkappa)}(\mathbf{k}) e^{-i(c||\mathbf{k}||t - \mathbf{k}\cdot\mathbf{x})} + \hat{a}_{(\varkappa)}^\dagger(\mathbf{k}) \boldsymbol{\epsilon}_{(\varkappa)}^*(\mathbf{k}) e^{i(c||\mathbf{k}||t - \mathbf{k}\cdot\mathbf{x})} \right] \hat{a}_{(\lambda)}^\dagger(\mathbf{q}) | 0 \rangle \\ &= \int \frac{d\mathbf{k}}{2(2\pi)^3 ||\mathbf{k}||} e^{i(\mathbf{k}\cdot\mathbf{x} - c||\mathbf{k}||t)} \bar{f}(\mathbf{k}) g_\beta(||\mathbf{k}||) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) \end{aligned} \quad (3.4.5)$$

where we made use of the commutation relations (1.4.32). This is not very useful at this point, since we have no relation linking  $\bar{f}_\psi(\mathbf{k})$  with  $\bar{f}(\mathbf{k})$ . This, however, is possible to get. Remember that  $\bar{f}_\psi(\mathbf{k})$  is the Fourier transform of the function that describes how a general one-photon wave function (3.1.4a) is spread over all localisation positions. Also remember that  $\bar{f}(\mathbf{k})$  describes how a general one-photon state (3.4.2) is spread over all momenta. Since we want to build the one-photon wave function (3.1.4a) from the one-photon state (3.4.2), the aforementioned relation linking  $\bar{f}_\psi(\mathbf{k})$  with  $\bar{f}(\mathbf{k})$  should be simple. And, indeed, we can equalise the norm (3.1.6) of the single-photon wave function

$$\begin{aligned} \langle \bar{\psi}_{(\lambda)}^{(\beta)} | \bar{\psi}_{(\lambda)}^{(\beta)} \rangle &= \int d\mathbf{x}_0 |f_\psi(\mathbf{x}_0)|^2 \\ &= \int \frac{d\mathbf{k}}{(2\pi)^3} |\bar{f}_\psi(\mathbf{k})|^2 \end{aligned} \quad (3.4.6a)$$

where we used (3.1.7) and Plancherel's theorem, with the norm of the single-photon state (the calculation is similar to the one which we made at (1.A.65))

$${}_\lambda \langle 1, f | 1, f \rangle_\lambda = \int \frac{d\mathbf{k}}{2(2\pi)^3 ||\mathbf{k}||} |\bar{f}(\mathbf{k})|^2 \quad (3.4.6b)$$

since they should both be equal to  $1/2$  for the sake of normalisation, which is solved by

$$\bar{f}(\mathbf{k}) = \sqrt{2} \|\mathbf{k}\| \bar{f}_\psi(\mathbf{k}) \quad (3.4.7)$$

and solving (3.4.1) with (3.4.3) and (3.4.5) requires, from (3.4.7), that we take

$$g_\beta(\|\mathbf{k}\|) = \sqrt{2} \|\mathbf{k}\|^{\frac{1}{2}+\beta} \quad (3.4.8)$$

which means that Glauber's extraction rule (3.4.1) does yield the wave function defined through (3.1.4a) if we take

$$|1, f\rangle_\lambda \equiv \int \frac{d\mathbf{k}}{\sqrt{2} (2\pi)^3 \sqrt{\|\mathbf{k}\|}} \bar{f}_\psi(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |0\rangle \quad (3.4.9)$$

and

$$\hat{\mathbf{O}}^{(\beta)}(\mathbf{x}, t) = \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{\sqrt{2} (2\pi)^3 \sqrt{\|\mathbf{k}\|}} \|\mathbf{k}\|^\beta \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right], \quad (3.4.10)$$

where we just kept the annihilation part of  $\hat{\mathbf{O}}^{(\beta)}(\mathbf{x}, t)$  (see sect. 1.A.4.6 and especially (1.A.69)) because, as we saw in (3.4.5) the creation part yields zero when sandwiched as prescribed by the extraction rule (3.4.1). Comparison of (3.4.10) with (1.4.30) and (1.4.31) tells us that

- The Gross-Hawton<sup>1</sup> wave function  $\psi_{(\lambda)}^{(-1/2)}(\mathbf{x}, t)$  is “extracted” from the corresponding one-photon state with

$$\hat{\mathbf{O}}^{(-1/2)}(\mathbf{x}, t) = \sqrt{\frac{2\epsilon_0 c}{\hbar}} \hat{\mathbf{A}}^+(\mathbf{x}, t) \quad (3.4.11)$$

- The Riemann-Silberstein wave function  $\psi_{(\lambda)}^{(+1/2)}(\mathbf{x}, t)$  is “extracted” from the corresponding one-photon state with

$$\hat{\mathbf{O}}^{(+1/2)}(\mathbf{x}, t) = -i \sqrt{\frac{2\epsilon_0}{\hbar c}} \hat{\mathbf{E}}^+(\mathbf{x}, t) \quad (3.4.12)$$

where the  $^+$  superscript stands for the annihilation part—or, a term often used in quantum optics, “positive frequency part” (hence the  $^+$ )—of the corresponding operator, that is,

$$\hat{\mathbf{A}}^+(\mathbf{x}, t) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right] \quad (3.4.13)$$

and

$$\hat{\mathbf{E}}^+(\mathbf{x}, t) = i \sqrt{\frac{\hbar c}{\epsilon_0}} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right]. \quad (3.4.14)$$

For other ( $|\beta| \neq 1/2$ ) values of  $\beta$  the field operators  $\hat{\mathbf{O}}^{(\beta)}(\mathbf{x}, t)$  do not have such a simple expression in terms of the standard field operators of quantum electrodynamics. Thus Glauber's extraction rule establishes a clear signification for the photon wave functions  $\psi_{(\lambda)}^{(\pm 1/2)}$  and only these functions. For instance, the Landau-Peierls wave function  $\psi_{(\lambda)}^{(0)}(\mathbf{x}, t)$ , which nicely allowed to define a local photon density (see (3.3.2)), has no clear physical meaning in terms of the usual quantities of electrodynamics.

<sup>1</sup>We call  $\psi_{(\lambda)}^{(-1/2)}$  the Gross-Hawton wave function not to break the symmetry of two-name denominations (Riemann-Silberstein, Landau-Peierls). The choice is motivated by [11] and its citation of [18] as a reference for the possibility to use the potential as the photon wave function. Also note that the Gross-Hawton wave function has no closer relationship than the other photon wave functions to the Hawton photon position operator presented in the previous chapter 2.

## 3.5 Advanced topics

Glauber's extraction rule selects the two photon wave functions  $\psi_{(\lambda)}^{(\pm 1/2)}$ —among the infinity of possible choices—as the physically meaningful ones. This existence of a subset of “nice and useful” wave functions, as is rather obvious from (3.4.1), will be vindicated by the investigation of the Poincaré transformation properties of the various photon wave functions (sect. 3.5.1). We then present a somewhat more detailed study of the Riemann-Silberstein wave function in sect. 3.5.2. Finally we shall introduce the two-wave function prescription (sect. 3.5.3).

### 3.5.1 Poincaré transformation properties

So far, the formalism developed in the present chapter has treated single-photon wave functions as three-vectors. This is so because we implemented the Coulomb gauge condition. As such, the formalism appears ill-suited to an investigation of Poincaré transformations. But remember that in sect. 1.4.8, we studied the behaviour of the Coulomb gauge under Poincaré transformations. The only nontrivial question is that of the effect of Lorentz boosts on the Coulomb gauge condition. We found in sect. 1.4.8 that, if we are willing to add a gauge term to the usual transformation law of the four-vector potential of electrodynamics, we can ensure that the Coulomb gauge is enforced in all inertial frames of reference. This gauge term obviously does not affect the transformation laws of the electric and magnetic fields.

This means that

- The Gross-Hawton wave function  $\psi_{(\lambda)}^{(-1/2)}$  transforms either strictly like a four-vector, in which case it can only be written as the purely transverse quantity (3.4.3) in the single frame of reference where the Coulomb gauge is enforced, or, arguably more conveniently, only like a four-vector up to a gauge term, as in (1.4.57), in which case the Coulomb gauge condition and (3.4.3) are valid in all frames of reference.
- The Riemann-Silberstein wave function  $\psi_{(\lambda)}^{(+1/2)}$  transforms, regardless of the choice we make for the Gross-Hawton wave function, as the first line (or column) of a second rank tensor (*i.e.*, the Faraday tensor  $F^{\mu\nu}$ ).

Note, finally, that the Landau-Peierls wave function  $\psi_{(\lambda)}^{(0)}$  does not transform simply under Poincaré transformations. This is easily seen from the fact that the field operator  $\hat{O}^{(0)}$  corresponding to the Landau-Peierls wave function does not transform under any particular representation of the Poincaré group. Glauber's extraction rule, we might remember from sect. 3.4, does not give  $\psi_{(\lambda)}^{(0)}$  a clear physical meaning. Thus, the Landau-Peierls wave function presents problems on a formal level as well as on a more pragmatic one, and should be considered an unsatisfactory photon wave function.

### 3.5.2 Excursion: more on the Riemann-Silberstein wave function

#### 3.5.2.1 The Riemann-Silberstein vector

The Riemann-Silberstein function is probably the most established of all the possible photon wave functions. Its use has been strongly advocated by Białynicki-Birula [12] and Sipe [19] in two important articles published in the mid-1990s. More often than not, the Riemann-Silberstein wave function is manipulated as

$$\psi_{(\lambda)}^{(\text{RS})}(\mathbf{x}, t) \equiv (1 + i\lambda) \psi_{(\lambda)}^{(+1/2)}(\mathbf{x}, t) \quad (3.5.1)$$

rather than as the plain  $\psi_{(\lambda)}^{(+1/2)}$  we called the Riemann-Silberstein wave function. Since both objects are connected through a very simple identity (3.5.1), we elect not to use different names. Using the Fourier expansion for the

(positive frequency part of the) magnetic field operator

$$\hat{\mathbf{B}}^+(\mathbf{x}, t) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \lambda \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right] \quad (3.5.2)$$

which comes from (1.4.21) and (3.4.13), it is easy to see that we can write

$$\psi_{(\lambda)}^{(\text{RS})}(\mathbf{x}, t) = -i\sqrt{\frac{2\epsilon_0}{\hbar c}} \langle 0 | \hat{\mathbf{E}}^+(\mathbf{x}, t) + ic\hat{\mathbf{B}}^+(\mathbf{x}, t) | 1, f \rangle_{\lambda}. \quad (3.5.3)$$

In classical electrodynamics

$$\mathbf{F}_{\pm}(\mathbf{x}, t) = \frac{1}{\sqrt{2}} [\mathbf{E}^+(\mathbf{x}, t) \pm ic\mathbf{B}^+(\mathbf{x}, t)] \quad (3.5.4)$$

is known as the Riemann-Silberstein vector. It can easily be shown that the Maxwell equations in free space can be rewritten as

$$\frac{i}{c} \frac{\partial \mathbf{F}_{\pm}}{\partial t}(\mathbf{x}, t) = \pm \nabla \times \mathbf{F}_{\pm}(\mathbf{x}, t) \quad (3.5.5)$$

making the Riemann-Silberstein vector a very nice object to work with. Notice that this is the same wave equation as (3.2.3). Moreover, the conserved quantities of the electromagnetic field (energy, linear momentum, angular momentum, moment of energy, see sect. 1.4.8) can easily be rewritten in terms of  $\mathbf{F}_{\pm}$  [12]. With the addition of the expression of the energy density (3.3.4), which allows to think of the Riemann-Silberstein function as an energy probability amplitude, this makes  $\psi_{(\lambda)}^{(\text{RS})}$  a very convincing candidate for the title of correct photon wave function. Studying spontaneous emission of light by a two-level atom, Sipe [19] has found that, within the Wigner-Weisskopf approximation, the Riemann-Silberstein wave function exhibited causal propagation, while the Landau-Peierls wave function did not. Such issues are discussed in chapter 7. The only drawback which we see is that the norm of the Riemann-Silberstein wave function cannot be computed through a single integral in configuration space, as seen from (3.3.2). We shall get back to this in sect. 3.5.3.

### 3.5.2.2 The Riemann-Silberstein spinor

It is interesting to note that we can construct an object which “contains” the Riemann-Silberstein function  $\psi_{(\lambda)}^{(\text{RS})}$  and transforms as a second rank spinor under Poincaré transformations [12]. The result is due to Laporte and Uhlenbeck [20]. We now try to present it in a way accessible to readers who—like the author—would be unfamiliar with the formalism of spinor calculus. If familiar with such a formalism, the interested reader can consult [12] for a condensed presentation of the results of [20].

Consider the four Dirac gamma matrices  $\gamma^{\mu}$ . They generate a so-called Clifford algebra which is determined by the anticommutators

$$\gamma^{\mu}\gamma^{\nu} + \gamma^{\nu}\gamma^{\mu} = 2\eta^{\mu\nu}. \quad (3.5.6)$$

The commutators

$$S^{\mu\nu} \equiv \frac{1}{4} [\gamma^{\mu}, \gamma^{\nu}] \quad (3.5.7)$$

can be shown [30] from (3.5.6) to obey the same commutation relations—up to a factor  $i$ —as these (1.A.8) obeyed by the generators of Lorentz transformations. Namely

$$[S_{\mu\nu}, S_{\rho\sigma}] = \eta_{\mu\rho}S_{\sigma\nu} - \eta_{\nu\rho}S_{\sigma\mu} - \eta_{\mu\sigma}S_{\rho\nu} + \eta_{\nu\sigma}S_{\rho\mu}. \quad (3.5.8)$$

The proof is straightforward. The Faraday tensor introduced in sect. 1.2.3 is an antisymmetric second rank Minkowski tensor, that is,  $F^{\mu\nu} = -F^{\nu\mu}$ . We can build, from that tensor, the  $(4 \times 4)$  matrix

$$F \equiv F_{\mu\nu} S^{\mu\nu}. \quad (3.5.9)$$

Trace identities (see, for instance, the appendix of [1]) for the Dirac gamma matrices tell us that (3.5.9) can be inverted through

$$F^{\mu\nu} = -\frac{1}{2} \text{Tr}(F S^{\mu\nu}) \quad (3.5.10)$$

while explicit computation shows that the determinant of the matrix  $F$  can be expressed in terms of the invariants (1.2.22) of the electromagnetic field as

$$\text{Det}F = \frac{1}{4} \left[ (F^{\mu\nu} F_{\mu\nu})^2 + \left( \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F^{\mu\nu} F^{\rho\sigma} \right)^2 \right] \quad (3.5.11)$$

Since both terms on the right-hand side of (3.5.11) are Lorentz scalars,  $\text{Det}F$  is invariant under Lorentz transformations. This suggests [2, 3] that we try the following behaviour for  $F$  under Lorentz transformations:

$$F'(x') = A(\Lambda) F(x) A^\dagger(\Lambda) \quad (3.5.12)$$

where  $x' = \Lambda x$  and  $A$  is a  $(4 \times 4)$  matrix of determinant  $\text{Det}(A(\Lambda)) = \pm 1$ . If we limit ourselves to the special matrices, that is, those of unit determinant, then we can use several identities on the Dirac matrices, including trace identities, to show that we can write

$$A(\Lambda) = e^{\frac{1}{2} \Omega_{\mu\nu} S^{\mu\nu}}. \quad (3.5.13)$$

Indeed  $S^{\mu\nu}$  has zero trace for all values of  $\mu$  and  $\nu$ , and we can use the identity  $\text{Det}(e^M) = e^{\text{Tr}M}$ . As usual the real coefficients  $\Omega_{\mu\nu}$  parametrise the Lorentz transformation. From  $(\gamma^\mu)^\dagger = \gamma^0 \gamma^\mu \gamma^0$  we can write

$$F'(x') = e^{\frac{1}{2} \Omega_{\mu\nu} S^{\mu\nu}} F(x) e^{-\frac{1}{2} \Omega_{\rho\sigma} \gamma^0 S^{\rho\sigma} \gamma^0} \quad (3.5.14)$$

and this is the transformation law of the matrix  $F$  under Lorentz transformations. It is easy to see from  $(\gamma^0)^2 = \mathbb{1}$  that the matrices  $\gamma^0 S^{\mu\nu} \gamma^0 = -(S^{\mu\nu})^\dagger$  obey, up to a global sign, the same commutation relations (3.5.8) as the  $S^{\mu\nu}$ , namely

$$\left[ (S_{\mu\nu})^\dagger, (S_{\rho\sigma})^\dagger \right] = - \left( \eta_{\mu\rho} (S_{\sigma\nu})^\dagger - \eta_{\nu\rho} (S_{\sigma\mu})^\dagger - \eta_{\mu\sigma} (S_{\rho\nu})^\dagger + \eta_{\nu\sigma} (S_{\rho\mu})^\dagger \right). \quad (3.5.15)$$

The matrices  $S^{\mu\nu}$  and  $(S^{\mu\nu})^\dagger$  are said to provide two inequivalent representations of the Poincaré group. Up to now, the reason for introducing this fancy formalism is not clear. But, with the usual [1] explicit realisation of the Clifford algebra (3.5.6), we see that the matrix  $F$  (3.5.9) reads

$$F = \begin{bmatrix} (E_3 + ic B_3) & [(E_1 + ic B_1) - i(E_2 + ic B_2)] & 0 & 0 \\ [(E_1 + ic B_1) + i(E_2 + ic B_2)] & -(E_3 + ic B_3) & 0 & 0 \\ 0 & 0 & -(E_3 - ic B_3) & -[(E_1 - ic B_1) - i(E_2 - ic B_2)] \\ 0 & 0 & -[(E_1 - ic B_1) + i(E_2 - ic B_2)] & (E_3 - ic B_3) \end{bmatrix} \quad (3.5.16)$$

and thus “contains” the Riemann-Silberstein vector (3.5.4). The transformation law (3.5.14) is that of a second rank spinor. Hence, we can say that the Riemann-Silberstein vector, and, through Glauber’s extraction rule (3.5.3), the Riemann-Silberstein wave function, can be cast in a form which ensures that they transform as second rank spinors under Lorentz transformations.

### 3.5.3 Photon number density through the two-wave function prescription

In sect. 3.1.2 we built a scalar product between single-photon wave functions of parameter  $\beta$ . This led to the construction of a positive definite photon number density, as seen in (3.3.2). This local number density, however, was expressed by means of the Landau-Peierls wave function  $\psi_{(\lambda)}^{(0)}$ , which has no physical meaning in relation to the usual quantities of electrodynamics. To build a photon number density that does have a simple relation with

these electro-dynamical quantities, we introduce what we call the two-wave function prescription (that is, we use two wave functions with different values of  $\beta$ ). We generalise (3.1.6) as follows

$$\langle \bar{\psi}_{(\lambda)}^{(\beta_1)} | \bar{\psi}_{(\lambda)}^{(\beta_2)} \rangle \equiv \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{\beta_1+\beta_2}} \left( \bar{\psi}_{(\lambda)}^{(\beta_1)} \right)^* (\mathbf{k}) \cdot \bar{\psi}_{(\lambda)}^{(\beta_2)} (\mathbf{k}). \quad (3.5.17)$$

We now Fourier transform this back to configuration space:

$$\langle \bar{\psi}_{(\lambda)}^{(\beta_1)} | \bar{\psi}_{(\lambda)}^{(\beta_2)} \rangle = \int d\mathbf{x} \int d\mathbf{y} \left( \psi_{(\lambda)}^{(\beta_1)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(\beta_2)} (\mathbf{y}, t) \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|^{\beta_1+\beta_2}} e^{i\mathbf{k} \cdot (\mathbf{x}-\mathbf{y})} \quad (3.5.18)$$

The same results as those obtained in (3.3.1) then hold, with  $\beta_1 + \beta_2$  substituted for  $2\beta$ . Choosing  $\beta_1 + \beta_2 \neq 0$  is of little interest but, using the two physically meaningful wave functions  $\psi_{(\lambda)}^{(\pm 1/2)}$ , we can build a local photon number density  $n_{\gamma(\lambda)}$  for photons of polarisation  $\lambda$  as follows:

$$n_{\gamma(\lambda)}^{(\pm 1/2)} (\mathbf{x}, t) = \left( \psi_{(\lambda)}^{(-1/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{+(1/2)} (\mathbf{x}, t) \quad (3.5.19a)$$

$$\text{or, alternatively,} \quad n_{\gamma(\lambda)}^{(\pm 1/2)} (\mathbf{x}, t) = \left( \psi_{(\lambda)}^{+(1/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(-1/2)} (\mathbf{x}, t) \quad (3.5.19b)$$

Summation over polarisations and “symmetrisation” over the index  $\pm 1/2$  gives the photon number density

$$n_{\gamma}^{(\pm 1/2)} (\mathbf{x}, t) = \frac{1}{2} \sum_{\lambda=\pm} \left[ \left( \psi_{(\lambda)}^{(-1/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{+(1/2)} (\mathbf{x}, t) + \left( \psi_{(\lambda)}^{+(1/2)} \right)^* (\mathbf{x}, t) \cdot \psi_{(\lambda)}^{(-1/2)} (\mathbf{x}, t) \right]. \quad (3.5.20)$$

This result was first proposed in an early form in [21] and then adapted by one of the authors of [21] to the formalism of the photon wave function in [10] and [22]. Similar expressions of  $n_{\gamma}^{(\pm\beta)}$  hold for

$$\beta_1 = -\beta_2 \equiv \beta \neq \pm \frac{1}{2} \quad (3.5.21)$$

but, for given  $\mathbf{x}$  and  $t$ , they differ from Hawton’s number density (3.5.20). Of course, the integral over configuration space of the densities  $n_{\gamma}^{(\pm\beta)}$  are equal for all  $(\beta_1, \beta_2)$  couples such that  $\beta_1 + \beta_2 = 0$ . Only in the “doubly” Landau-Peierls case  $\beta_1 = \beta_2 = 0$ , does the photon number density  $n_{\gamma}^{(0)}$  take positive values for all  $\mathbf{x}$  and  $t$ , but we know from sects. 3.4 and 3.5.1 that it comes at the heavy price of unclear physical meaning combined with disagreeable behaviour of the concerned wave functions under Poincaré transformations.

The local photon number density  $n_{\gamma}^{(\pm 1/2)}$  can be expressed as the expectation value of an operator. This operator is tantamount to the dot product of the vector potential with the electric field, as we now prove. Define the negative frequency part of a field operator as  $\hat{\mathbf{O}}^- (\mathbf{x}, t) = \left( \hat{\mathbf{O}}^+ \right)^\dagger (\mathbf{x}, t)$  and compute

$$\begin{aligned} & i_{\lambda} \langle 1, f | \frac{\epsilon_0}{\hbar} \left( \hat{\mathbf{E}}^- (\mathbf{x}, t) \cdot \hat{\mathbf{A}}^+ (\mathbf{x}, t) - \hat{\mathbf{A}}^- (\mathbf{x}, t) \cdot \hat{\mathbf{E}}^+ (\mathbf{x}, t) \right) | 1, f \rangle_{\lambda} \\ &= c \sum_{\mathcal{X}=\pm} \sum_{\zeta=\pm} \int d\tilde{\mathbf{k}} \int d\tilde{\mathbf{q}} \int d\tilde{\mathbf{p}} \int d\tilde{\mathbf{z}} f_{\lambda}^* (\mathbf{p}) f_{\lambda} (\mathbf{z}) \epsilon_{(\mathcal{X})}^* (\mathbf{k}) \cdot \epsilon_{(\zeta)} (\mathbf{q}) e^{i[c(\|\mathbf{k}\|-\|\mathbf{q}\|)t - (\mathbf{k}-\mathbf{q}) \cdot \mathbf{x}]} \\ & \quad (\|\mathbf{k}\| + \|\mathbf{q}\|) \langle 0 | \hat{a}_{(\lambda)} (\mathbf{p}) \hat{a}_{(\mathcal{X})}^\dagger (\mathbf{k}) \hat{a}_{(\zeta)} (\mathbf{q}) \hat{a}_{(\lambda)}^\dagger (\mathbf{z}) | 0 \rangle \\ &= c \int d\tilde{\mathbf{k}} \int d\tilde{\mathbf{q}} f_{\lambda}^* (\mathbf{k}) f_{\lambda} (\mathbf{q}) \epsilon_{(\lambda)}^* (\mathbf{k}) \cdot \epsilon_{(\lambda)} (\mathbf{q}) e^{i[c(\|\mathbf{k}\|-\|\mathbf{q}\|)t - (\mathbf{k}-\mathbf{q}) \cdot \mathbf{x}]} (\|\mathbf{k}\| + \|\mathbf{q}\|) \end{aligned} \quad (3.5.22)$$

which, according to the results of sect. 3.4, can easily be seen to be equal to (3.5.20). This means that we can define the photon number density operator as

$$\hat{n}_{\gamma}^{(\pm 1/2)} (\mathbf{x}, t) = i \frac{\epsilon_0}{\hbar} \left( \hat{\mathbf{E}}^- (\mathbf{x}, t) \cdot \hat{\mathbf{A}}^+ (\mathbf{x}, t) - \hat{\mathbf{A}}^- (\mathbf{x}, t) \cdot \hat{\mathbf{E}}^+ (\mathbf{x}, t) \right). \quad (3.5.23)$$

Remember that in this chapter we have been working in the Coulomb gauge. Arguably, this expression is more agreeable than that given in (3.3.2) by the square modulus of the Landau-Peierls wave function. Remember, however, that (3.5.23) is not positive definite while the square modulus of the Landau-Peierls wave function obviously is. As we know from sects. 3.4 and 3.5.1, the Landau-Peierls wave function is not a satisfactory photon wave function.

It is interesting to rewrite  $\hat{n}_\gamma^{(\pm 1/2)}$  in an explicitly covariant framework. Notice that (3.5.23) is the Coulomb gauge expression of the more general quantity

$$\hat{n}_\gamma^{(\pm 1/2)}(\mathbf{x}, t) = -i \frac{\epsilon_0 c}{\hbar} \left( \partial^0 \hat{A}^{\nu-}(\mathbf{x}, t) \hat{A}_\nu^+(\mathbf{x}, t) - \hat{A}_\nu^-(\mathbf{x}, t) \partial^0 \hat{A}^{\nu+}(\mathbf{x}, t) \right) \quad (3.5.24)$$

and it is then natural to define

$$\hat{j}_\gamma^{(\pm 1/2)i}(\mathbf{x}, t) = -i \frac{\epsilon_0 c}{\hbar} \left( \partial^i \hat{A}^{\nu-}(\mathbf{x}, t) \hat{A}_\nu^+(\mathbf{x}, t) - \hat{A}_\nu^-(\mathbf{x}, t) \partial^i \hat{A}^{\nu+}(\mathbf{x}, t) \right) \quad (3.5.25)$$

to build the four-vector field operator [22]

$$\hat{j}_\gamma^{\mu(\pm 1/2)}(\mathbf{x}, t) = \left( \hat{n}_\gamma^{(\pm 1/2)}(\mathbf{x}, t), \hat{\mathbf{j}}_\gamma^{(\pm 1/2)}(\mathbf{x}, t) \right). \quad (3.5.26)$$

For the Hawton four-vector field operator (3.5.26) to make sense as a photon number four-current, it should obey the usual conservation equation

$$\partial_\mu \hat{j}_\gamma^{\mu(\pm 1/2)} = 0. \quad (3.5.27)$$

Let us show that it is the case:

$$\begin{aligned} \partial_\mu \hat{j}_\gamma^{\mu(\pm 1/2)} &= -i \frac{\epsilon_0 c}{\hbar} \left[ \left( \partial_\mu \partial^\mu \hat{A}^{\nu-} \right) \hat{A}_\nu^+ + \left( \partial^\mu \hat{A}^{\nu-} \right) \left( \partial_\mu \hat{A}_\nu^+ \right) - \hat{A}_\nu^- \left( \partial_\mu \partial^\mu \hat{A}^{\nu+} \right) - \left( \partial_\mu \hat{A}_\nu^- \right) \left( \partial^\mu \hat{A}^{\nu+} \right) \right] \\ &= -i \frac{\epsilon_0 c}{\hbar} \left[ \left( \partial^\mu \hat{A}^{\nu-} \right) \left( \partial_\mu \hat{A}_\nu^+ \right) - \left( \partial_\mu \hat{A}_\nu^- \right) \left( \partial^\mu \hat{A}^{\nu+} \right) \right] \\ &= 0 \end{aligned} \quad (3.5.28)$$

where we enforced the Lorenz gauge condition, which reduces the Maxwell equations to  $\partial^\mu \partial_\mu \hat{A}^\nu = 0$ . Hence (3.5.27) is proved. In the Lorenz gauge, we compute the equivalent of (3.5.22) as

$$i \langle 1, f | \hat{n}_\gamma(x) | 1, f \rangle = \sum_{\lambda=\pm} \int \tilde{d}k \int \tilde{d}q f_\lambda^*(\mathbf{k}) f_\lambda(\mathbf{q}) \epsilon_{(\infty)\nu}^*(\mathbf{k}) \epsilon_{(c)}^\nu(\mathbf{q}) e^{i(k^\nu - q^\nu)x_\nu} (k^0 + q^0). \quad (3.5.29)$$

Notice that, in the framework of Bohmian wave mechanics, similar expressions to (3.5.24) and (3.5.25) have been found [29] for the particle number density and current, in the case of spin 0 bosons. We explore this path in the upcoming sect. 3.6.

## 3.6 Photon trajectories in the Bohmian picture of wave mechanics

*“[L]’immense univers dans lequel nous nous trouvons n’existe ni pour nous, ni à cause de nous. Évidemment, nos théories scientifiques sont, dans un sens, des constructions sociales. Mais elles sont basées sur des arguments empiriques, ce qu’on oublie trop souvent.”*

Jean Bricmont in “La vraie signification de l’affaire Sokal”, **Le Monde**, 14 January 1997



### 3.6.1 Some notions on the Bohmian picture

The Bohmian picture is an “interpretation” of quantum mechanics that describes actual individual events in configuration space. The average over an ensemble of individual systems can then account for the statistical character of conventional quantum mechanics [4]. In this view, the trajectories of each material system truly exist independent from the act of observation so that the need to divide the world into “systems” and “observers” becomes obsolete. In other words, quantum particles are considered, in the Bohmian picture, to have a perfectly well-defined position at all times. Their evolution in space is directed by the “pilot wave” which is none other than the wave function  $\psi$  of the particle.

The particles are guided as it were to regions where  $|\psi|^2$  is most intense [4], hence the name of “pilot wave” for  $\psi$ . For the simplest case of nonrelativistic, spinless wave mechanics, Bohm parametrises the complex wave function  $\psi$  with two real functions  $R$  and  $S$ :

$$\psi(\mathbf{x}, t) = R(\mathbf{x}, t) e^{\frac{i}{\hbar} S(\mathbf{x}, t)}, \quad (3.6.1)$$

and writes down three postulates:

“... ”

1. That the  $\psi$ -field satisfies [Schrödinger]’s equation.
2. That the particle momentum is restricted to  $\mathbf{p} = \nabla S(\mathbf{x})$ .
3. That we do not predict or control the precise location of the particle, but have, in practice, a statistical ensemble with probability density  $P(\mathbf{x}) = |\psi(\mathbf{x})|^2$ . The use of statistics is, however, not inherent in the conceptual structure, but merely a consequence of our ignorance of the precise initial conditions of the particle.

...” [23]

With the wave function  $\psi$  rewritten as (3.6.1), Schrödinger’s equation can be rewritten as

$$\begin{cases} \frac{\partial R}{\partial t} = -\nabla \cdot \left[ \frac{R^2 \nabla S}{m} \right], \\ \frac{\partial S}{\partial t} = -\left[ \frac{(\nabla S)^2}{2m} + V(\mathbf{x}) - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \right]. \end{cases} \quad (3.6.2)$$

Since we have to specify an initial condition for the wave function to solve Schrödinger’s equation, the particles trajectories will depend on the initial condition  $\psi(\mathbf{x}, t=0)$  (or equivalently:  $R(\mathbf{x}, t=0)$  and  $S(\mathbf{x}, t=0)$ ) of the wave function. The specific particle trajectories for each particle are then found [23] by integrating over

$$\dot{\mathbf{x}} = \frac{1}{m} \nabla S(\mathbf{x}, t)|_{\mathbf{x}=\mathbf{x}(t)}, \quad (3.6.3)$$

for which we have to specify the initial condition  $\mathbf{x}_0$  to find the solution. This latter equation of motion for the particle is, of course, a postulate. In Bohmian mechanics, the wave function is therefore associated with an ensemble of material points differing by initial location.

The first line of equation (3.6.2) can be seen as the conservation of probability for it is the continuity equation

$$\frac{\partial |\psi|^2}{\partial t} + \nabla \cdot \mathbf{j} = 0, \quad (3.6.4)$$

where the probability density of particles equals that of conventional quantum mechanics,  $R^2(\mathbf{x}, t) = |\psi(\mathbf{x})|^2$ , and

the mean current of particles in the ensemble is

$$\begin{aligned}
 \mathbf{j}(\mathbf{x}, t) &\equiv -i\frac{\hbar}{2m}(\psi^*(\mathbf{x})\nabla\psi(\mathbf{x}) - \psi(\mathbf{x})\nabla\psi^*(\mathbf{x})) \\
 &= R^2(\mathbf{x}, t)\frac{\nabla S}{m} \\
 &= R^2(\mathbf{x}, t)\dot{\mathbf{x}}.
 \end{aligned} \tag{3.6.5}$$

It is explained in [24] that, contrary to the usual interpretation of the probability description, these probabilities  $R^2(\mathbf{x}, t)$  arise as a consequence of the inability to precisely determine the particle trajectories. In practice the physical properties of the system will give rise to a range of possible initial values over which we will have to average. This means that we might very well never be able to test the validity of Bohmian mechanics because it leads to exactly the same predictions as “standard” quantum mechanics.

The Bohmian picture is problematic with regard to its compatibility with special relativity. Various attempts have been made, for instance, to associate a conserved density (the zeroth component of a four-vector) to the Klein-Gordon field (which represents a boson of spin 0), but this density is not positive definite [29, 4, 25]. For the Dirac field associated to the electron, however, it is possible to make such an association. Even in this case, it is not easy to formulate a Lorentz covariant, consistent Bohmian interpretation of the quantum theory of the free Dirac field, based on a “particle ontology”, but the task is not impossible. We can find several proposals in this sense [29, 5, 26, 27], which have the merit to exist at the price of being highly non trivial and difficult to manipulate in practice. In the case of an entangled  $N$ -electron wave function, non-locality is impossible to avoid because the trajectories are defined at the level of a  $3N + 1$ -dimensional configuration space and no longer at the level of the usual  $3 + 1$ -dimensional space time, which imposes to choose a privileged frame.

The problem of the non-positive definiteness for spin 0 bosons is carried over to the case of photons: the conserved density is not positive definite. This we already know from sect. 3.5.3.

### 3.6.2 Problems with defining Bohmian trajectories for photons

In the previous sect. 3.6.1 we presented the role played by the mean particle current

$$\mathbf{j}(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2 \dot{\mathbf{x}} \tag{3.6.6}$$

to define the Bohmian particle trajectories  $\mathbf{x}$  via the velocity  $\dot{\mathbf{x}}$ . When we take this idea on to special relativity, a problem arises regarding the extraction of photon trajectories. Despite the existence of a continuity equation for the electromagnetic energy, namely, Poynting’s theorem

$$\frac{\partial w(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{S}(\mathbf{x}, t) = 0 \tag{3.6.7}$$

where

$$w(\mathbf{x}, t) = \frac{\epsilon_0}{2} [\mathbf{E}^2(\mathbf{x}, t) + c^2 \mathbf{B}^2(\mathbf{x}, t)], \tag{3.6.8a}$$

$$\mathbf{S}(\mathbf{x}, t) = \frac{1}{\mu_0} \mathbf{E}(\mathbf{x}, t) \times \mathbf{B}(\mathbf{x}, t) \tag{3.6.8b}$$

we cannot define a four-current  $j^\mu$  that could account for the photon trajectories. We can rewrite (3.6.7) as

$$\partial_\mu T^{\mu 0} = 0 \tag{3.6.9}$$

using the zeroth row (or column) of the stress-energy tensor  $T^{\mu\nu}$  with components [6]

$$\begin{cases} T^{00} &= \frac{\epsilon_0}{2} [\mathbf{E}^2 + c^2 \mathbf{B}^2], \\ T^{0j} &= \frac{1}{\mu_0} (\mathbf{E} \times \mathbf{B})^j, \\ T^{ij} &= -\epsilon_0 \left[ E^i E^j + c^2 B^i B^j - \frac{\delta^{ij}}{2} (\mathbf{E}^2 + c^2 \mathbf{B}^2) \right], \end{cases} \quad (3.6.10)$$

but since  $T^{\mu 0}$  transforms like

$$T^{\mu 0} \rightarrow (T^{\mu 0})' = \Lambda^\mu_\rho \Lambda^0_\sigma T^{\rho\sigma} \quad (3.6.11a)$$

under Lorentz transformations it is an unsuitable candidate for  $j^\mu$  which should transform like

$$j^\mu \rightarrow (j^\mu)' = \Lambda^\mu_\nu j^\nu. \quad (3.6.11b)$$

Of course, this is a classical argument but it remains valid in the framework of single-photon wave mechanics, as easily seen from Glauber's extraction rule (see sect. 3.4). We can therefore use the electric and magnetic single-photon wave functions to build the equivalent tensor to (3.6.10) by substituting  $\mathbf{E}$  with  $\psi_{\mathbf{E}}^{(f)}$  and  $\mathbf{B}$  with  $\psi_{\mathbf{B}}^{(f)}$ , with

$$\psi_{\mathbf{E}}^{(f)}(\mathbf{x}, t) = \langle 0 | \hat{\mathbf{E}}^+(\mathbf{x}, t) | 1, f \rangle, \quad (3.6.12)$$

$$\psi_{\mathbf{B}}^{(f)}(\mathbf{x}, t) = \langle 0 | \hat{\mathbf{B}}^+(\mathbf{x}, t) | 1, f \rangle. \quad (3.6.13)$$

Remember once again that the general one-photon state  $|1, f\rangle$  reads

$$|1, f\rangle \equiv \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3} \frac{\bar{f}_\lambda(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k})}{\|\mathbf{k}\|} |0\rangle. \quad (3.6.14)$$

The quantum version of Poynting's theorem (3.6.7) is given by

$$\frac{\partial w_\psi}{\partial t}(\mathbf{x}, t) + \nabla \cdot \mathbf{S}_\psi(\mathbf{x}, t) = 0 \quad (3.6.15)$$

where

$$w_\psi(\mathbf{x}, t) = \frac{\epsilon_0}{2} \left[ \left| \psi_{\mathbf{E}}^{(f)}(\mathbf{x}, t) \right|^2 + c^2 \left| \psi_{\mathbf{B}}^{(f)}(\mathbf{x}, t) \right|^2 \right] \quad (3.6.16a)$$

$$\mathbf{S}_\psi = \frac{1}{2\mu_0} \left[ \psi_{\mathbf{E}}^{(f)}(\mathbf{x}, t) \times \psi_{\mathbf{B}}^{(f)*}(\mathbf{x}, t) + \psi_{\mathbf{E}}^{(f)*}(\mathbf{x}, t) \times \psi_{\mathbf{B}}^{(f)}(\mathbf{x}, t) \right]. \quad (3.6.16b)$$

Indeed

$$\begin{aligned} \frac{\partial w_\psi}{\partial t} &= \frac{\epsilon_0}{2} \left[ \left( \partial_t \psi_{\mathbf{E}}^{(f)} \right) \cdot \psi_{\mathbf{E}}^{(f)*} + \psi_{\mathbf{E}}^{(f)} \cdot \left( \partial_t \psi_{\mathbf{E}}^{(f)*} \right) + c^2 \left( \partial_t \psi_{\mathbf{B}}^{(f)} \right) \cdot \psi_{\mathbf{B}}^{(f)*} + c^2 \psi_{\mathbf{B}}^{(f)} \cdot \left( \partial_t \psi_{\mathbf{B}}^{(f)*} \right) \right] \\ &= \frac{\epsilon_0}{2} \left[ c^2 \left( \nabla \times \psi_{\mathbf{B}}^{(f)} \right) \cdot \psi_{\mathbf{E}}^{(f)*} + c^2 \psi_{\mathbf{E}}^{(f)} \cdot \left( \nabla \times \psi_{\mathbf{B}}^{(f)*} \right) - c^2 \left( \nabla \times \psi_{\mathbf{E}}^{(f)} \right) \cdot \psi_{\mathbf{B}}^{(f)*} - c^2 \psi_{\mathbf{B}}^{(f)} \cdot \left( \nabla \times \psi_{\mathbf{E}}^{(f)*} \right) \right] \\ &= -\frac{1}{2\mu_0} \left[ \nabla \cdot \left( \psi_{\mathbf{E}}^{(f)} \times \psi_{\mathbf{B}}^{(f)*} \right) + \nabla \cdot \left( \psi_{\mathbf{E}}^{(f)*} \times \psi_{\mathbf{B}}^{(f)} \right) \right] \\ &\equiv -\nabla \cdot \mathbf{S}_\psi. \end{aligned}$$

We know that  $(w_\psi, \mathbf{S}_\psi)$  is not a four-vector, and that its four-norm  $w_\psi^2 - \mathbf{S}_\psi^2$  is thus not invariant under Lorentz transformations. This means that we may not apply Bohm's prescription given in the previous sect. 3.6.1 to photons in order to define trajectories in a covariant way.

It is nonetheless interesting to briefly dwell on the three-vector velocity field

$$\mathbf{j}_\psi(\mathbf{x}, t) \equiv \frac{\mathbf{S}_\psi(\mathbf{x}, t)}{w_\psi(\mathbf{x}, t)}. \quad (3.6.17)$$

The current  $\mathbf{j}_\psi$  is built on the model of (3.6.5) or on that of the Bohmian picture for Dirac fermions [4]. In the latter, relativistic case, though, the current  $\mathbf{j}_\psi$  is the quotient of the spatial part of a four-vector by its time (zeroth) component. This is not the case here, as we argued above. Despite this important and arguably fatal shortcoming, the current (3.6.17) still has a nice property. Compute

$$\begin{aligned} \|\mathbf{j}_\psi\|^2 &= \frac{\left(\boldsymbol{\psi}_{\mathbf{E}}^{(f)} \times c^2 \boldsymbol{\psi}_{\mathbf{B}}^{(f)*}\right)^2 + 2 \left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)} \times c^2 \boldsymbol{\psi}_{\mathbf{B}}^{(f)*}\right|^2 + \left(\boldsymbol{\psi}_{\mathbf{E}}^{(f)*} \times c^2 \boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right)^2}{\left(\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 + c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2\right)^2} \\ &\leq \frac{\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)*}\right|^2 + 2 \left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)*}\right|^2 + \left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)*}\right|^2 c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2}{\left(\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 + c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2\right)^2} \\ &= 4c^2 \frac{\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2}{\left(\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 + c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2\right)^2} \end{aligned} \quad (3.6.18)$$

From

$$\begin{aligned} \left(\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 + c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2\right)^2 - 4 \left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2 &= \left(\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 - c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2\right)^2 \\ &\geq 0 \end{aligned} \quad (3.6.19)$$

we find

$$4 \frac{\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2}{\left(\left|\boldsymbol{\psi}_{\mathbf{E}}^{(f)}\right|^2 + c^2 \left|\boldsymbol{\psi}_{\mathbf{B}}^{(f)}\right|^2\right)^2} \leq 1 \quad (3.6.20)$$

and therefore  $\|\mathbf{j}_\psi\|^2 \leq c^2$ . This means that, in the naive Bohmian picture given by (3.6.17), the propagation velocity of the local electromagnetic energy density is smaller or equal to  $c$  in all frames of reference, a nice property indeed.

As far as we can tell, there is no similar argument for the four-vector photon number density-current (3.5.26), the time (zeroth) component of which is not positive definite anyway, rendering a Bohmian picture of photon wave mechanics based on this four-current impossible. The photon number density given by the square modulus of the Landau-Peierls wave function, on the other hand, is positive definite, but is not the zeroth component of a four-vector. Putting everything together, this points to the impossibility of building a positive definite local density of photons which obeys a covariant conservation equation and transforms like the zeroth component of a four-vector under Lorentz transformations.

## 3.7 Outlook on the photon wave function

The standard education process that most physics students go through runs thusly: one learns of quantum physics and the special theory of relativity separately, and at some point the teacher puts them together by constructing the Dirac equation. Problems with negative energies soon arise [7], however, and one goes on to quantum field theory. Then, after studying massive fields, one proceeds to quantise the Maxwell field. At no point is there any

	$\beta = -1/2$ (Gross-Hawton)	$\beta = 0$ (Landau-Peierls)	$\beta = +1/2$ (Riem.-Silberst.)
Energy dens.	Nonlocal	Nonlocal	<b>Local &amp; positive</b>
Number dens.	Nonlocal	<b>Local &amp; positive</b>	Nonlocal
Number dens. (alt.)	Dot prod. w/ $\beta = +1/2$ ( $\otimes$ )		Dot prod. w/ $\beta = -1/2$ ( $\otimes$ )
Poincaré trans.	<b>Vector</b>	Nothing	<b>Second Rank Spinor<sup>2</sup></b>
Glauber's extr. rule	$\hat{\mathbf{A}}^+$	Nothing	$\hat{\mathbf{E}}^+$
Conservation eq.	$\partial_\mu J^\mu = 0$	Nothing	$\partial_\mu T^{\mu 0} = 0$

**Tab. 3.1** – Strengths and weaknesses of the three most common photon wave functions.

mention of photon wave mechanics. We feel that there is no fundamental reason for that. Similarly to relativistic quantum mechanics, which, though it does not account for the annihilation and creation of particles, can be a useful formalism to tackle some problems (the hydrogen atom is a fine example of that), there is no reason to think that photon wave mechanics cannot be used in some framework. Examples of such uses can be found in [12], where the author looks at single photon wave mechanics in dielectric media and optical fibres, and [28], where the Huygens-Fresnel principle is obtained for  $n$ -photon wave functions.

On a more formal level, we may be tempted to ask what is the “true”, “genuine” wave function for the photon. The Riemann-Silberstein function, arguably, has the best case, as it allows to construct a local energy density (see sect. 3.3) as well as local densities for the other invariants of the electromagnetic field (see [8] and [12]), that is, the linear momentum, the angular momentum, and the lesser known moment of energy (the Poincaré generator  $\mathbf{K}$  in our notation, see chapter 1). The Riemann-Silberstein wave function can be arranged in the Riemann-Silberstein spinor (3.5.16), which transforms under a particular representation of the Poincaré group (3.5.14). The case has been laid perhaps most convincingly by Białyński-Birula. In [12] he argues that “it is understandable that the [localisation] of photons is associated with their energy because photons do not carry other attributes like charge, fermion number, or rest mass”. Of course, photons also carry linear and angular momenta as well as moment of energy, but these, as we just mentioned, are also accounted for by the Riemann-Silberstein wave function. In [19] Sipe makes a similar argument and later argues that “it is only meaningful to introduce a wave function describing the probability amplitude for measuring the expected energy of the photon in a given region of space”. In Tab. 3.1 we give a summary of the main properties of the Gross-Hawton, Landau-Peierls and Riemann-Silberstein photon wave functions.

To what extent the introduction of the Gross-Hawton wave function—and the subsequent construction of a photon number four-current  $\hat{J}_\gamma^\mu$  which describes photon density in configuration space and obeys a conservation equation—challenges the claims of Białyński-Birula and Sipe is, we think, debatable. Indeed  $\hat{J}_\gamma^\mu$  is not invariant under gauge transformations (1.2.18) and it is not definite positive either. This challenges its physical relevance, which was enhanced by its obeying a conservation equation.

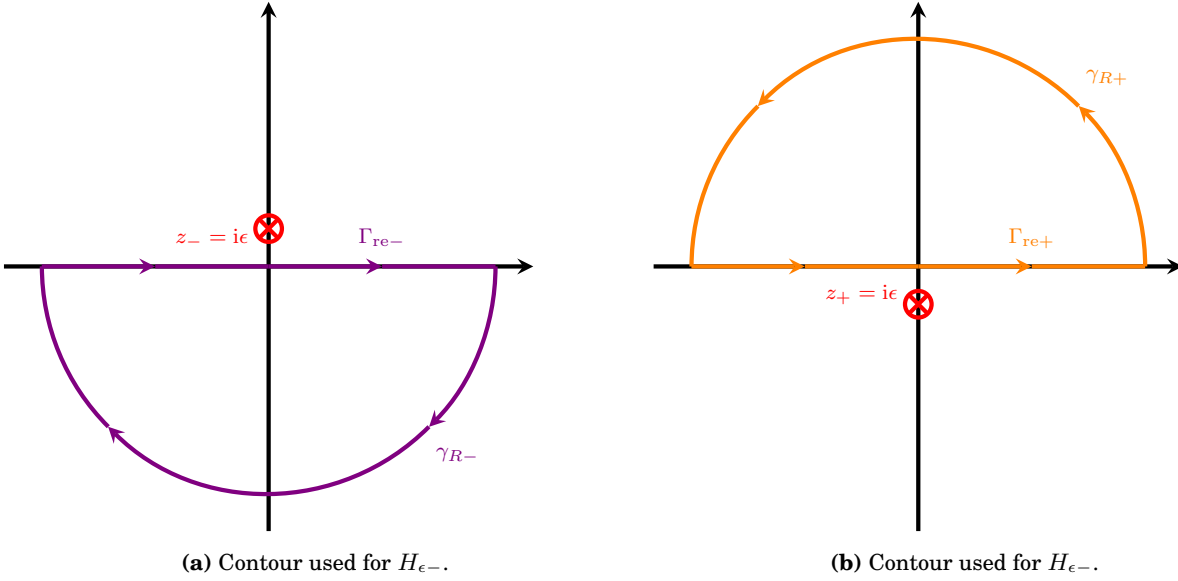
### 3.A Kernel computation in spherical coordinates

In this appendix we show how to compute kernel integrals of the form

$$I_\alpha(\mathbf{s}) \equiv \int \frac{d\mathbf{k}}{(2\pi)^3 |\mathbf{k}|^\alpha} e^{i\mathbf{k}\cdot\mathbf{s}} \quad (3.A.1)$$

in spherical coordinates. The most convenient method is to choose the spherical frame so that the so-called polar angle  $\theta$  is zero when  $\mathbf{k}$  points in the direction of  $\mathbf{s}$ : the unit vector in the direction of  $\mathbf{s}$  then plays the part of the

<sup>2</sup>As part of the Riemann-Silberstein spinor, see sect. 3.5.2.2.



**Fig. 3.A.1** – Integration contours in the complex plane used for the computation of the Dirichlet integral  $I_2(\mathbf{s})$ .

unit vector  $\mathbf{e}_z$  of usual spherical coordinates (see Fig. 1.4.1). Then we can rewrite (3.A.1) as

$$\begin{aligned}
 I_\alpha(\mathbf{s}) &= \frac{1}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta \int_0^{+\infty} dk k^{2-\alpha} e^{ik\|\mathbf{s}\|\cos\theta} \\
 &= \frac{i}{(2\pi)^2 \|\mathbf{s}\|} \int_0^{+\infty} dk k^{1-\alpha} \left[ e^{ik\|\mathbf{s}\|\cos\theta} \right]_{\theta=0}^{\theta=\pi} \\
 &= \frac{i}{(2\pi)^2 \|\mathbf{s}\|} \int_0^{+\infty} dk k^{1-\alpha} \left( e^{-ik\|\mathbf{s}\|} - e^{ik\|\mathbf{s}\|} \right) \\
 &\equiv \frac{i}{(2\pi)^2 \|\mathbf{s}\|} (J_{\alpha-}(\mathbf{s}) - J_{\alpha+}(\mathbf{s})). \tag{3.A.2}
 \end{aligned}$$

These integrals will now be computed. Note first that for  $\alpha \geq 3$  the integrand is singular at the origin, which means that  $I_{\alpha \geq 3}(\mathbf{s})$  is ill-defined. Therefore we shall only compute  $I_\alpha(\mathbf{s})$  for  $\alpha < 3$ . Even then, we will restrict ourselves to integer values of  $\alpha$ .

We start with the particular  $\alpha = 2$  case. It corresponds to the well known Dirichlet integral. Indeed

$$I_2(\mathbf{s}) = \frac{1}{(2\pi)^2 \|\mathbf{s}\|} \int_{-\infty}^{+\infty} dt \frac{\sin t}{t} \tag{3.A.3}$$

Now let

$$h_{\epsilon\pm}(t) \equiv \frac{e^{\pm it}}{t \pm i\epsilon} \tag{3.A.4a}$$

and

$$H_{\epsilon\pm} = \int_{-\infty}^{+\infty} dt h_{\epsilon\pm}(t). \tag{3.A.4b}$$

This moves the singularity of the integrand away from the real axis, to the point  $z_\pm = \mp i\epsilon$ . We then choose integration contours (see Fig. 3.A.1) that do not encircle the pole  $z_\pm$ , and, since the integral of  $h_{\epsilon\pm}$  vanishes along  $\gamma_\pm$ , Cauchy's integral theorem tells us that

$$H_{\epsilon\pm} = 0. \tag{3.A.5}$$

Taking the limit with caution is then crucial. The correct way to do that is to use the Plemelj-Sochocki theorem

(see sect. 6.A.1, especially the identity (6.A.6)), according to which we rewrite

$$\begin{aligned} \text{vp} \int_{-\infty}^{+\infty} dt \frac{e^{\pm it}}{t - t_0} \mp i\pi \int_{-\infty}^{+\infty} dt e^{\pm it} \delta(t - t_0) &= 0. \\ \text{vp} \int_{-\infty}^{+\infty} dt \frac{\sin t}{t} &= \pi. \\ \int_{-\infty}^{+\infty} dt \frac{\sin t}{t} &= \pi \end{aligned} \quad (3.A.6)$$

since the cardinal sine is well-defined at the origin and is thus equal to its principal value. Hence

$$\boxed{\int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{s}}}{\mathbf{k}^2} = \frac{1}{4\pi \|\mathbf{s}\|}}. \quad (3.A.7)$$

Now turn to the  $\alpha \leq 1$  case. In that case  $1 - \alpha \in \mathbb{N}$  and, from (6.A.14), we compute

$$\begin{aligned} J_{\alpha-}(\mathbf{s}) - J_{\alpha+}(\mathbf{s}) &= \int_0^{+\infty} dk k^{1-\alpha} \left( e^{-ik\|\mathbf{s}\|} - e^{ik\|\mathbf{s}\|} \right) \\ &= i^{1-\alpha} \frac{d^{1-\alpha}}{d\|\mathbf{s}\|^{1-\alpha}} \int_0^{+\infty} dk \left( e^{-ik\|\mathbf{s}\|} - (-1)^{1-\alpha} e^{ik\|\mathbf{s}\|} \right) \\ &= i^{1-\alpha} \frac{d^{1-\alpha}}{d\|\mathbf{s}\|^{1-\alpha}} \left[ \left( \pi \delta(\|\mathbf{s}\|) - i \text{vp} \frac{1}{\|\mathbf{s}\|} \right) + (-1)^{-\alpha} \left( \pi \delta(\|\mathbf{s}\|) + i \text{vp} \frac{1}{\|\mathbf{s}\|} \right) \right] \\ &= i^{1-\alpha} \frac{d^{1-\alpha}}{d\|\mathbf{s}\|^{1-\alpha}} \left[ \pi \left( 1 + (-1)^{-\alpha} \right) \delta(\|\mathbf{s}\|) - i \left( 1 - (-1)^{-\alpha} \right) \text{vp} \frac{1}{\|\mathbf{s}\|} \right]. \end{aligned} \quad (3.A.8)$$

Hence for  $-\alpha$  an even integer we have

$$J_{\alpha-}(\mathbf{s}) - J_{\alpha+}(\mathbf{s}) = 2\pi i^{1-\alpha} \frac{d^{1-\alpha}}{d\|\mathbf{s}\|^{1-\alpha}} \delta(\|\mathbf{s}\|) \quad (3.A.9)$$

while for  $-\alpha$  an odd integer we have

$$J_{\alpha-}(\mathbf{s}) - J_{\alpha+}(\mathbf{s}) = 2i^{-\alpha} \frac{d^{1-\alpha}}{d\|\mathbf{s}\|^{1-\alpha}} \text{vp} \frac{1}{\|\mathbf{s}\|}. \quad (3.A.10)$$

Now focus on the  $\alpha = 0$  case and notice from (3.A.2) and (3.A.9) that

$$I_0(\mathbf{s}) = -\frac{1}{2\pi \|\mathbf{s}\|} \frac{d}{d\|\mathbf{s}\|} \delta(\|\mathbf{s}\|). \quad (3.A.11)$$

Apply this distribution on a test function of  $\|\mathbf{s}\|$  while keeping in mind that, in spherical coordinates, there is a weight  $\|\mathbf{s}\|^2$  to be carried in integrations:

$$\begin{aligned} \int_0^{+\infty} dx x^2 \frac{d\delta}{dx} \frac{\varphi(x)}{x} &= \int_0^{+\infty} dx \frac{d\delta}{dx} x \varphi(x) \\ &= - \int_0^{+\infty} dx \delta(x) \left( x \frac{d\varphi}{dx} + \varphi(x) \right) \\ &= - \int_0^{+\infty} dx \delta(x) \varphi(x) \end{aligned} \quad (3.A.12)$$

so that

$$I_0(\mathbf{s}) = \frac{1}{2\pi s^2} \delta(\|\mathbf{s}\|) \quad (3.A.13)$$

which is known [31] to be equal to the usual spherical coordinate-representation of the three dimensional Dirac

delta distribution:

$$\int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{s}} = \delta(\mathbf{s}). \quad (3.A.14)$$

For  $\alpha = 1$  it is seen from (3.A.2) and (3.A.10) that

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{s}} = \frac{1}{2\pi^2} \frac{1}{|\mathbf{s}|} \text{vp} \frac{1}{|\mathbf{s}|}. \quad (3.A.15)$$



# REFERENCES

---

## Books

- [1] C. Itzykson and J.B. Zuber, *Quantum Field Theory*, 1st ed. (McGraw-Hill, 1980) (cit. on p. 77).
- [2] R.F. Streater and A.S. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin, New York, 1964) (cit. on p. 77).
- [3] G. Scharf, *Finite Quantum Electrodynamics* (Springer Verlag, 1989) (cit. on p. 77).
- [4] P.R. Holland, *The Quantum Theory of Motion* (Cambridge University Press, 1993) (cit. on pp. 80, 81, 83).
- [5] J.S. Bell, *Speakable and Unspeakable in Quantum Mechanics*, 2nd ed. (Cambridge University Press, 2004) (cit. on p. 81).
- [6] J.D. Jackson, *Classical Electrodynamics*, 2nd ed. (John Wiley & Sons, 1975) (cit. on p. 82).
- [7] A. Messiah, *Mécanique Quantique*, 1st ed., Vol. 2 (Dunod, Paris, 1965) (cit. on p. 83).
- [8] I. Białynicki-Birula and Z. Białynicka-Birula, *Quantum Electrodynamics*, 1st ed. (Pergamon Press, 1975) (cit. on p. 84).

## Articles

- [9] M. Hawton and W.E. Baylis, ‘Photon position operators and localized bases’, *Phys. Rev. A* **64**, 012101 (2001) (cit. on p. 70).
- [10] M. Hawton, ‘Photon wave mechanics and position eigenvectors’, *Phys. Rev. A* **75**, 062107 (2007) (cit. on pp. 70, 78).
- [11] M. Hawton, ‘Lorentz-invariant photon number density’, *Phys. Rev. A* **78**, 012111 (2008) (cit. on pp. 70, 74).
- [12] I. Białynicki-Birula, ‘Photon Wave Function’, *Prog. Opt.* **36**, 245 (1996) (cit. on pp. 72, 75, 76, 84).
- [13] B.J. Smith and M.G. Raymer, ‘Photon wave functions, wave-packet quantization of light, and coherence theory’, *New J. Phys.* **9**, 414 (2007) (cit. on pp. 72, 73).
- [14] L. Landau and R. Peierls, ‘Quantenelektrodynamik im Konfigurationsraum’, *Z. Phys.* **62**, 188 (1930) (cit. on p. 72).
- [15] L. Silberstein, ‘Elektromagnetische Grundgleichungen in bivectorieller Behandlung’, *Ann. Phys. (Leipzig)* **327**, (the link points to an English version of the article), 579 (1907) (cit. on p. 72).
- [16] L. Silberstein, ‘Nachtrag zur Abhandlung über ‘Elektromagnetische Grundgleichungen in bivectorieller Behandlung’, *Ann. Phys. (Leipzig)* **329**, (the link points to an English version of the article), 783 (1907) (cit. on p. 72).

- [17] U.M. Titulaer and R.J. Glauber, 'Density Operators for Coherent Fields', *Phys. Rev.* **145**, 1041 (1966) (cit. on p. 73).
- [18] L. Gross, 'Norm Invariance of Mass-Zero Equations under the Conformal Group', *J. Math. Phys.* **5**, 687 (1964) (cit. on p. 74).
- [19] J.E. Sipe, 'Photon Wave Functions', *Phys. Rev. A* **52**, 1875 (1995) (cit. on pp. 75, 76, 84).
- [20] O. Laporte and G. Uhlenbeck, 'Application of Spinor Analysis to the Maxwell and Dirac equations', *Phys. Rev.* **37**, 1380 (1931) (cit. on p. 76).
- [21] M. Hawton and T. Melde, 'Photon number density operator  $i\hat{\mathbf{E}} \cdot \hat{\mathbf{A}}$ ', *Phys. Rev. A* **51**, 4186 (1995) (cit. on p. 78).
- [22] M. Hawton, 'Photon wave functions in a localized coordinate space basis', *Phys. Rev. A* **59**, 3223 (1999) (cit. on pp. 78, 79).
- [23] D. Bohm, 'A Suggested Interpretation of the Quantum Theory in terms of "Hidden" Variables, Part I', *Phys. Rev.* **85**, 166 (1952) (cit. on p. 80).
- [24] D. Bohm, 'A Suggested Interpretation of the Quantum Theory in terms of "Hidden" Variables, Part II', *Phys. Rev.* **85**, 180 (1952) (cit. on p. 81).
- [25] D. Bohm, B.J. Hiley and P.N. Kaloyerou, 'An ontological basis for the quantum theory', *Phys. Rep.* **144**, 321 (1987) (cit. on p. 81).
- [26] S. Colin and W. Struyve, 'A Dirac sea pilot-wave model for quantum field theory', *J. Phys. A* **40**, 7309 (2007) (cit. on p. 81).
- [27] W. Struyve, 'Pilot-wave approaches to quantum field theory', *J. Phys.: Conf. Ser.* **306**, 012047 (2011) (cit. on p. 81).

## Conference Proceedings

- [28] É. Brainis and P. Emplit, Wave function formalism in quantum optics and generalized Huygens-Fresnel principle for  $N$  photon-states: derivation and applications, in *Proc. SPIE*, Vol. 1, edited by V.N. Zadkov and T. Durt (2010), p. 77270 (cit. on p. 84).

## Theses

- [29] S. Colin, Bohm-Bell Beables for Quantum Field Theory, PhD Thesis (Vrije Universiteit Brussel, 2005) (cit. on pp. 79, 81).

## Unpublished Articles and Online Notes

- [30] D. Tong, *Lectures on Quantum Field Theory - Ch. 4: The Dirac Equation*, <http://www.damtp.cam.ac.uk/user/tong/qft/four.pdf> (cit. on p. 76).
- [31] Wolfram MathWorld, *Delta Function*, <http://mathworld.wolfram.com/DeltaFunction.html> (cit. on p. 86).



## CHAPTER 4

---

# AN OVERVIEW OF NONCLASSICALITY IN QUANTUM OPTICS

---

*“You know it made me wonder why  
Why all the frequencies combine  
And form a cleaner, brighter light.”*

British Sea Power’s Jan Scott Wilkinson in “Lights Out for Darker Skies”, **Do You Like Rock Music?** (Rough Trade, 2008)

We learned in the previous chapter 3 that single-photon wave functions can be built from what we called Glauber’s extraction rule. In the present chapter we will both extend the use of the extraction rule beyond the framework of single-photon states and illustrate its relevance with respect to photodetection theory. The latter point will lead us to briefly discuss the coherence properties of the quantised electromagnetic field. Since the latter topic has already been extensively investigated, and reviewed to great length in [1], we try and discuss nonstandard approaches and topics whenever possible. In sect. 4.1 we introduce the matrix elements relevant to the description of light detection. Sect. 4.2 is mainly devoted to the construction of physical, polychromatic electromagnetic modes. In sect. 4.3 we quickly discuss the properties of the standard (Fock, coherent, thermal, etc.) single-mode states of the electromagnetic field. Sect. 4.4 deals with  $n$ -photon wave functions and correlation functions, and in sect. 4.5 we introduce effective one-point wave functions for arbitrary single-mode electromagnetic states, relevant for the discussion of the second order properties of the electromagnetic field. Finally we give in sect. 4.6 an informal summary of classicality and nonclassicality in quantum optics. The very brief appendix 4.A is devoted to the derivation of the completeness relation for coherent states.

---

### Contents of the Chapter

4.1	Elements of photodetection theory . . . . .	93
4.2	Single-mode quantum optics: physical modes . . . . .	95
4.2.1	Physical modes from normalisable states . . . . .	95
4.2.2	Excursion: discrete basis for $L^2(\mathbb{R}^3)$ . . . . .	96
4.2.3	Excursion continued: discrete basis for the space of normalised electromagnetic states . . . . .	97
4.2.4	A digression on Planck’s $E = \hbar\omega$ and Einstein’s $E = c\ \mathbf{p}\ $ . . . . .	98
4.3	Single-mode quantum optics: quantum optics . . . . .	99
4.3.1	Phase operator—Quadrature space . . . . .	99

4.3.2	Pure states . . . . .	101
4.3.2.1	Fock states . . . . .	101
4.3.2.2	Coherent states . . . . .	102
4.3.2.3	Squeezed coherent states . . . . .	102
4.3.3	Mixed states . . . . .	103
4.3.3.1	General case . . . . .	103
4.3.3.2	Blackbody radiation states . . . . .	104
4.4	Interlude: $n$ -photon wave functions . . . . .	106
4.4.1	Two-photon wave function . . . . .	106
4.4.2	Two-photon Wolf equations . . . . .	107
4.4.3	$n$ -photon wave function and $n$ -point correlation functions . . . . .	108
4.4.4	Excursion: Hong-Ou-Mandel interferometry . . . . .	109
4.5	Single mode quantum optics: effective one-point wave function . . . . .	110
4.5.1	General case . . . . .	110
4.5.2	Fock and coherent states . . . . .	111
4.6	Quantum optics and classical electrodynamics: an informal overview . . . . .	112
4.A	Completeness relation for coherent states . . . . .	113

---

## 4.1 Elements of photodetection theory

To discuss photodetection we must anticipate a bit on the content of chapter 6 and introduce, as economically as we can, the basic elements of the description of light-matter interaction. Indeed, the detection of light is made by photoabsorption, that is, the absorption of light by matter. We follow Glauber [10] and describe an ideal photodetector as a single atom with at least one electron susceptible to change atomic levels while absorbing light. For the sake of simplicity, we restrict our discussion to the case where only one such electron is present.

In nonrelativistic quantum electrodynamics, where matter is described within the framework of standard quantum mechanics, while the electromagnetic field is described by quantum field theory as done in chapter 1, the interaction Hamiltonian between an electric charge  $q$  with mass  $m$  and the field is, in the Coulomb gauge [2]

$$\hat{H}_I = -\frac{q}{m} \hat{\mathbf{p}}(t) \cdot \hat{\mathbf{A}}(\hat{\mathbf{x}}, t) + \frac{1}{2} \frac{q^2}{m} \hat{\mathbf{A}}^2(\hat{\mathbf{x}}, t) \quad (4.1.1)$$

where  $\hat{\mathbf{x}}$  is the position operator for the considered charge, and  $\hat{\mathbf{p}}$  is its linear momentum operator. The Coulomb gauge condition implies the usual identity  $\mathbf{k} \cdot \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) = 0$ , which allows us to write  $\hat{\mathbf{p}}(t) \cdot \hat{\mathbf{A}}(\hat{\mathbf{x}}, t) = \hat{\mathbf{A}}(\hat{\mathbf{x}}, t) \cdot \hat{\mathbf{p}}(t)$ , hence (4.1.1). The second summand on the right-hand side of (4.1.1) is often neglected because it only comes into play in very strong field situations [2]. In Dirac's interaction picture of quantum physics, quantum states evolve [3] according to the unitary operator

$$\hat{U}(t, t_0) = e^{-\frac{i}{\hbar} \hat{H}_I(t-t_0)}. \quad (4.1.2)$$

Now, compute the probability amplitude that an atomic electron will be excited from its initial state  $|g\rangle$  at  $t_0$  to a final state  $|e\rangle$  at  $t$ , orthogonal to  $|g\rangle$ . As seen from the structure of the first summand on the right-hand side of (4.1.1), this process will automatically take place in parallel with a change in the state of the electromagnetic field, namely from  $|\text{init}\rangle$  to  $|\text{fin}\rangle$ . To first order in time-dependent perturbation theory the probability amplitude of the process is

$$\langle e, \text{fin} | \hat{U}(t, t_0) | g, \text{init} \rangle = i \frac{q}{\hbar m} \int_{t_0}^t du \langle e, \text{fin} | \hat{\mathbf{p}}(u) \cdot \hat{\mathbf{A}}(\hat{\mathbf{x}}, u) | g, \text{init} \rangle. \quad (4.1.3)$$

The goal of photodetection theory is then to use the experimental, or theoretical data of the transition probability  $|\langle e, \text{fin} | \hat{U}(t, t_0) | g, \text{init} \rangle|^2$  to gain knowledge on the initial state  $|\text{init}\rangle$  of the electromagnetic field.

In some sense, considering this transition to take place between times  $t_0$  and  $t$  amounts to taking the light-matter interaction into account only between  $t_0$  and  $t$ . The simplest physical situation which corresponds to this is the following. Before  $t_0$ , the atom is, to quote Glauber directly, “shielded from the [electromagnetic] field we are investigating by a shutter of some sort which opens at time  $t_0$ ” [10]. As for what happens after  $t$ , we see two equivalent possibilities. Either, as proposed by Glauber [10], the shutter is closed again at  $t$ , and the state of the atom is measured at some later instant  $t_{\text{meas}}^1$ , or the state of the atom is measured directly at time  $t$ .

In the framework of light-matter interaction, the dipole approximation is often made. It consists, to adapt Shirokov's formulation [11] to the case of light absorption, in considering that the electron does not absorb light at its own position but rather at the position of the nucleus to which it is bound. In this context, we replace the dependence of the vector potential on the position operator  $\hat{\mathbf{x}}$  of the electron with a dependence on the nucleus position  $\mathbf{x}_0$ , which is considered to be a constant  $\mathbb{R}^3$ -number and not an operator (the nucleus is considered to be at rest at all times). Then the operator  $\hat{\mathbf{A}}(\mathbf{x}_0, t)$  does not feature any electronic degrees of freedom. The dipole approximation is discussed at great length in chapter 6. Since the electronic momentum operator is proportional to the identity operator in the electromagnetic Hilbert space, and, because of the dipole approximation, the

<sup>1</sup>The value of  $t_{\text{meas}} > t$  is not important as long as it is substantially smaller than the radiative lifetime of the atomic level  $|e\rangle$ .

electromagnetic potential operator is diagonal in the electronic Hilbert space, we rewrite (4.1.3) as

$$\langle e, \text{fin} | \hat{U}(t, t_0) | g, \text{init} \rangle = i \frac{q}{\hbar m} \int_{t_0}^t du e^{i(\omega_e - \omega_g)u} \langle e | \hat{\mathbf{p}}(0) | g \rangle \cdot \langle \text{fin} | \hat{\mathbf{A}}(\mathbf{x}_0, u) | \text{init} \rangle \quad (4.1.4)$$

where we used the fact that, in Dirac's interaction picture, the time evolution of operators follows the interaction-less (free) operator, for which atomic states  $|g\rangle$  and  $|e\rangle$  are eigenstates with time-oscillating exponential eigenvalues. We now rewrite

$$\int_{t_0}^t du e^{i(\omega_e - \omega_g)u} \langle \text{fin} | \hat{\mathbf{A}}(\mathbf{x}_0, u) | \text{init} \rangle = \int_{t_0}^t du e^{i(\omega_e - \omega_g)u} \langle \text{fin} | \hat{\mathbf{A}}^+(\mathbf{x}_0, u) + \hat{\mathbf{A}}^-(\mathbf{x}_0, u) | \text{init} \rangle \quad (4.1.5)$$

where  $\hat{\mathbf{A}}^+(\mathbf{x}, t)$  stands for the annihilation part—or, a term often used in quantum optics, “positive frequency part”—(3.4.13) of the vector potential and  $\hat{\mathbf{A}}^-(\mathbf{x}, t) = \left(\hat{\mathbf{A}}^+\right)^\dagger(\mathbf{x}, t)$  is the creation part, or, in the quantum optical convention, the negative frequency part. We see from (3.4.13) that the summand on the right-hand side of (4.1.5) which features  $\hat{\mathbf{A}}^+(\mathbf{x}_0, u)$  is a sum of integrals of the type  $\int_{t_0}^t du \exp(i(\omega_e - \omega_g - c\|\mathbf{k}\|)u)$  while that which features  $\hat{\mathbf{A}}^-(\mathbf{x}_0, u)$  is a sum of integrals of the type  $\int_{t_0}^t du \exp(i(\omega_e - \omega_g + c\|\mathbf{k}\|)u)$ . Since  $\omega_e - \omega_g$  and  $c\|\mathbf{k}\|$  are both positive, the integrals corresponding to the positive frequency part  $\hat{\mathbf{A}}^+(\mathbf{x}_0, u)$  are much larger than the ones corresponding to the negative frequency part  $\hat{\mathbf{A}}^-(\mathbf{x}_0, u)$  of the vector potential. This is so because  $\exp(i(\omega_e - \omega_g + c\|\mathbf{k}\|)u)$  oscillates much faster than  $\exp(i(\omega_e - \omega_g - c\|\mathbf{k}\|)u)$ . Hence, we discard the former [10], which is known as the rotating wave approximation.

What is physically measured in an experiment is the squared modulus of the probability amplitude (4.1.3), summed over all possible final states of the field, because these are not observed by the experimentalist [10] who only has access to the electronic state. Hence we compute, making use of the closure relation  $\sum_{\text{fin}} |\text{fin}\rangle\langle \text{fin}| = \hat{1}$ ,

$$\begin{aligned} \sum_{\text{fin}} \left| \langle e, \text{fin} | \hat{U}(t, t_0) | g, \text{init} \rangle \right|^2 &= \sum_{\text{fin}} \left( \frac{q}{\hbar m} \right)^2 \int_{t_0}^t du \int_{t_0}^t dv e^{-i(\omega_e - \omega_g)(u-v)} \langle g | \hat{p}_i(0) | e \rangle \langle e | \hat{p}_j(0) | g \rangle \\ &\quad \langle \text{init} | \hat{A}_i^-(\mathbf{x}_0, u) | \text{fin} \rangle \langle \text{fin} | \hat{A}_j^+(\mathbf{x}_0, u) | \text{init} \rangle \\ &\equiv \left( \frac{q}{\hbar m} \right)^2 \int_{t_0}^t du \int_{t_0}^t dv e^{-i(\omega_e - \omega_g)(u-v)} (p_i)_{\text{eg}} (p_j)_{\text{eg}}^* \langle \text{init} | \hat{A}_i^-(\mathbf{x}_0, u) \hat{A}_j^+(\mathbf{x}_0, v) | \text{init} \rangle. \end{aligned} \quad (4.1.6)$$

where Einstein's summation convention is implied. Hence a crucial quantity for photodetection is the expectation value  $\langle \text{init} | \hat{A}_i^-(\mathbf{x}_0, u) \hat{A}_j^+(\mathbf{x}_0, v) | \text{init} \rangle$ . Notice from Glauber's extraction rule (3.4.1) and from (3.4.11) that if  $|\text{init}\rangle$  is a single-photon state of the electromagnetic field, then  $\langle \text{init} | \hat{A}_i^-(\mathbf{x}_0, u) \hat{A}_j^+(\mathbf{x}_0, v) | \text{init} \rangle$  is simply expressed in terms of the Gross-Hawton wave function. We get back to this point in sect. 4.5.

In just about every reference we could find on photodetection, including [4] and [10] for instance, the light-matter interaction is not taken to be of the minimal  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  form but of the usual  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  form. Then the photodetection probability involves the expectation value  $\langle \text{init} | \hat{E}_i^-(\mathbf{x}_0, u) \hat{E}_j^+(\mathbf{x}_0, v) | \text{init} \rangle$  and hence the electric field, which usually considered to be more physical than the vector potential. The latter expectation value can be very easily obtained from  $\langle \text{init} | \hat{A}_i^-(\mathbf{x}_0, u) \hat{A}_j^+(\mathbf{x}_0, v) | \text{init} \rangle$ , namely by successive differentiations with respect to the two time variables  $u$  and  $v$ . Still in the case of the  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  interaction, another substitution to be made from (4.1.6) is to replace the matrix elements of the vector components of the linear momentum operator for the electron with these of the position operator. We will get back to the difference between the minimal  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  and usual  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  forms of the light-matter interaction Hamiltonian in chapters 6 and 7.

## 4.2 Single-mode quantum optics: physical modes

We saw in chapter 1 that the free electromagnetic field can be expanded over plane waves. Plane waves are just a possible choice of basis among many. They are particularly well adapted to formal investigations on relativistic invariance and quantisation. For more practical enquiries on specific problems, other choices of basis can be useful. For instance, when we no longer work in free space but rather within a metallic cavity, standing waves are the natural choice. For a thorough discussion with several examples, see sects. 2.1 and 2.3 of [15].

In many problems, we can go even further and simply focus on a single physically relevant electromagnetic mode. This is what is done in many textbooks on quantum optics [4, 5], where, after a rather terse treatment of the quantisation of the electromagnetic field, the focus is quickly shifted onto an expansive discussion of the “quantum states of radiation”. The caveat here is that the discussion is restricted from that point on to a single electromagnetic mode. Loudon [5] briefly but clearly mentions and motivates this point, while Scully and Zubairy rush through it within a single line of text.

We feel a proper, univocal definition of a physical single mode is necessary for the solidity and clarity of the mathematical framework of quantum optical phenomenology. This construction is neither original, nor difficult, but is absent from enough introductory texts (*e.g.*, [4]) to warrant a presentation here.

### 4.2.1 Physical modes from normalisable states

A simple way to introduce physical modes is to start from the single-photon state

$$|1_{\bar{f}}\rangle \equiv \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \bar{f}_{\lambda}(\mathbf{k}) \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}) |0\rangle \quad (4.2.1)$$

which we want to be of unit norm:

$$\langle 1_{\bar{f}} | 1_{\bar{f}} \rangle = \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} |\bar{f}_{\lambda}(\mathbf{k})|^2 \equiv 1. \quad (4.2.2)$$

We call such normalisable one-photon states **physical** one-photon states<sup>2</sup>. The spacetime dependence of the electromagnetic field corresponding to this state can be obtained through Glauber’s extraction rule (3.4.1). The function  $\bar{f}_{\lambda}(\cdot)$  describes how the single photon (4.2.1) is “spread” over polarisations and wave vectors. It thus defines a polychromatic mode (in other words, a wave packet).

If there is a good reason to only focus on this particular polychromatic mode, for instance, because it is useful to describe the field radiated by a known source, it will be very useful to introduce the mode creation operator

$$\hat{a}_{\bar{f}}^{\dagger} \equiv \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \bar{f}_{\lambda}(\mathbf{k}) \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}) \quad (4.2.3)$$

so that  $|1_{\bar{f}}\rangle = \hat{a}_{\bar{f}}^{\dagger} |0\rangle$ . This mode creation operator and its adjoint obey the usual harmonic oscillator algebra.

<sup>2</sup>Note that throughout the present chapter we work in the Coulomb gauge. The physical states defined by (4.2.1) and (4.2.2) have nothing to do with the physical states in the sense of Gupta and Bleuler (sect. 1.A.4.6).



Indeed, from (1.4.32), we write

$$\begin{aligned}
[\hat{a}_{\bar{f}}, \hat{a}_{\bar{f}}^\dagger] &= \sum_{\varkappa=\pm} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \int \frac{d\mathbf{q}}{2(2\pi)^3 \|\mathbf{q}\|} \bar{f}_{\varkappa}^*(\mathbf{k}) \bar{f}_{\lambda}(\mathbf{q}) [\hat{a}_{(\varkappa)}(\mathbf{k}), \hat{a}_{(\lambda)}^\dagger(\mathbf{q})] \\
&= \sum_{\varkappa=\pm} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \int \frac{d\mathbf{q}}{2(2\pi)^3 \|\mathbf{q}\|} \bar{f}_{\varkappa}^*(\mathbf{k}) \bar{f}_{\lambda}(\mathbf{q}) 2\|\mathbf{k}\| (2\pi)^3 \delta(\mathbf{k}-\mathbf{q}) \delta_{\varkappa\lambda} \\
&= \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} |\bar{f}_{\lambda}(\mathbf{k})|^2 \\
&= 1
\end{aligned} \tag{4.2.4}$$

from (4.2.2). We can then define  $\hat{N}_{\bar{f}} \equiv \hat{a}_{\bar{f}}^\dagger \hat{a}_{\bar{f}}$ . Following the usual Fock space rules, we then define  $n$ -photon states in the physical mode as

$$|n_{\bar{f}}\rangle = \frac{(\hat{a}_{\bar{f}}^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{4.2.5}$$

which obey  $\hat{N}_{\bar{f}} |n_{\bar{f}}\rangle = n |n_{\bar{f}}\rangle$  and

$$\langle n_{\bar{f}} | m_{\bar{f}} \rangle = \delta_{nm} \tag{4.2.6}$$

as can be shown from (4.2.4). Hence such physical modes are very easy to work with. We compute

$$\begin{aligned}
\langle 0 | \hat{\mathbf{A}}^+(\mathbf{x}, t) | 1_{\bar{f}} \rangle &= \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \frac{d\mathbf{q}}{2(2\pi)^3 \|\mathbf{q}\|} \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{q}) e^{-i(c\|\mathbf{q}\|t - \mathbf{q}\cdot\mathbf{x})} \sum_{\varkappa=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \bar{f}_{\varkappa}(\mathbf{k}) \langle 0 | \hat{a}_{(\lambda)}(\mathbf{q}) \hat{a}_{(\varkappa)}^\dagger(\mathbf{k}) | 0 \rangle \\
&= \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \bar{f}_{\lambda}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \\
&\equiv \mathbf{A}_{\bar{f}}(\mathbf{x}, t) \\
&= \mathbf{A}_{\bar{f}}(\mathbf{x}, t) \langle 0 | \hat{a}_{\bar{f}} | 1_{\bar{f}} \rangle.
\end{aligned} \tag{4.2.7}$$

where in the last step we introduced the Hermitian conjugate of the mode creation operator (4.2.3). When we know that all photons considered in our treatment will be excitations of this single physical mode, we can therefore introduce the single mode vector potential

$$\hat{\mathbf{A}}_{\bar{f}}(\mathbf{x}, t) \equiv \mathbf{A}_{\bar{f}}(\mathbf{x}, t) \hat{a}_{\bar{f}} + \mathbf{A}_{\bar{f}}^*(\mathbf{x}, t) \hat{a}_{\bar{f}}^\dagger. \tag{4.2.8}$$

Therefore in single-mode quantum optics the spacetime dependence of all objects which we can build will be governed by that of  $\mathbf{A}_{\bar{f}}$ .

## 4.2.2 Excursion: discrete basis for $L^2(\mathbb{R}^3)$

It is very noteworthy in our opinion that we can construct a discrete basis for the Lebesgue space  $L^2(\mathbb{R})$  of square-integrable functions, namely, the set of all Hermite functions  $h_n$ . Then the basis for  $L^2(\mathbb{R}^3)$  is just the tensor product basis:

$$\{h_l \otimes h_m \otimes h_n\}_{(l,m,n) \in \mathbb{N}^3}. \tag{4.2.9}$$

The Hermite functions are given by

$$h_n(k) \equiv \frac{(-1)^n}{\sqrt{2^n n! K_0 \sqrt{\pi}}} e^{\frac{1}{2} \left(\frac{k}{K_0}\right)^2} \frac{d^n}{d\left(\frac{k}{K_0}\right)^n} e^{-\left(\frac{k}{K_0}\right)^2} \tag{4.2.10}$$

where we introduced the constant  $K_0$  for the sake of dimensionality. It can come in handy to use the better known Hermite polynomials [6] which read

$$H_n(k) \equiv (-1)^n e^{\left(\frac{k}{K_0}\right)^2} \frac{d^n}{d\left(\frac{k}{K_0}\right)^n} e^{-\left(\frac{k}{K_0}\right)^2} \quad (4.2.11)$$

so that

$$h_n(k) = \frac{1}{\sqrt{2^n n! K_0 \sqrt{\pi}}} e^{-\frac{1}{2}\left(\frac{k}{K_0}\right)^2} H_n(k). \quad (4.2.12)$$

In sect. 6.1 of [6] the reader can find a very clear and accessible proof of the orthonormality

$$\int_{-\infty}^{+\infty} dk h_n(k) h_m(k) = \delta_{nm} \quad (4.2.13)$$

of the Hermite functions (4.2.10), which we do not reproduce here. It can also be shown that the Hermite functions form a complete set of functions for  $L^2(\mathbb{R})$ , namely

$$\sum_{n=0}^{+\infty} h_n(k) h_n(q) = \delta(k - q). \quad (4.2.14)$$

This is proved using an identity on Hermite polynomials known as Mehler's identity. See [16] for a very accessible proof.

With all this in mind we can assert that mode functions  $\bar{f}_\lambda$  which define normalised, and hence physical one-photon states (4.2.2) can be expanded over the basis of Hermite functions as

$$\bar{f}_\lambda(k_x, k_y, k_z) = (2\pi)^{\frac{3}{2}} \sqrt{2(k_x^2 + k_y^2 + k_z^2)} \sum_{l=0}^{+\infty} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} F_{lmn}^{(\lambda)} h_l(k_x) h_m(k_y) h_n(k_z) \quad (4.2.15)$$

with

$$\sum_{\lambda=\pm} \sum_{l=0}^{+\infty} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \left| F_{lmn}^{(\lambda)} \right|^2 = 1. \quad (4.2.16)$$

### 4.2.3 Excursion continued: discrete basis for the space of normalised electromagnetic states

In (4.2.15) we take  $F_{lmn}^{(\lambda)} = \delta_{ll_0} \delta_{mm_0} \delta_{nn_0} \delta_{\lambda\lambda_0}$ , which satisfies the normalisation condition (4.2.16). With this choice for  $\bar{f}_\lambda$  we introduce, from (4.2.3)

$$\begin{aligned} \hat{a}_{(\lambda_0)l_0m_0n_0}^\dagger &\equiv \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \bar{f}_\lambda(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \\ &= \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{\sqrt{2(2\pi)^3 \|\mathbf{k}\|}} \sum_{l=0}^{+\infty} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} F_{lmn}^{(\lambda)} h_l(k_x) h_m(k_y) h_n(k_z) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \\ &= \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{\sqrt{2(2\pi)^3 \|\mathbf{k}\|}} \sum_{l=0}^{+\infty} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \delta_{ll_0} \delta_{mm_0} \delta_{nn_0} \delta_{\lambda\lambda_0} h_l(k_x) h_m(k_y) h_n(k_z) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \\ &= \int \frac{d\mathbf{k}}{\sqrt{2(2\pi)^3 \|\mathbf{k}\|}} h_{l_0}(k_x) h_{m_0}(k_y) h_{n_0}(k_z) \hat{a}_{(\lambda_0)}^\dagger(\mathbf{k}). \end{aligned} \quad (4.2.17)$$

Since  $F_{lmn}^{(\lambda)} = \delta_{ll_0} \delta_{mm_0} \delta_{nn_0} \delta_{\lambda\lambda_0}$  is a solution of (4.2.16),  $\hat{a}_{(\lambda)l_0m_0n_0}^\dagger |0\rangle$  has unit norm.

We therefore give a discrete basis for the Hilbert space consisting of all the normalised states of the electromagnetic field:

$$\left\{ \left[ \prod_{\lambda=\pm} \prod_{l=0}^{+\infty} \prod_{m=0}^{+\infty} \prod_{n=0}^{+\infty} \frac{\left(\hat{a}_{(\lambda)lmn}^\dagger\right)^{P(\lambda)lmn}}{\sqrt{P(\lambda)lmn!}} \right] |0\rangle, \text{ with all possible combinations of } P(\lambda)lmn \right\}. \quad (4.2.18)$$

#### 4.2.4 A digression on Planck's $E = \hbar\omega$ and Einstein's $E = c\|\mathbf{p}\|$

Remember from chapter 1 the expression for the free field Hamiltonian:

$$\hat{H} = \hbar c \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}). \quad (4.2.19)$$

It is easy to see from (1.4.32) that the expectation value of the Hamiltonian in the physical one-photon state (4.2.1) is

$$E \equiv \langle 1_{\bar{f}} | \hat{H} | 1_{\bar{f}} \rangle = \hbar c \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| |\bar{f}_\lambda(\mathbf{k})|^2 \quad (4.2.20)$$

Notice in passing that this quantity can be infinite even if we require the state to be normalised through (4.2.2). In other words, a single-photon state with unit norm can have infinite energy. Let us restrict the rest of the discussion to states which have a finite energy. Now, if we want to know what the usual single-photon Planck relation  $E = \hbar\omega$  means in this context, we need to give a meaning to the frequency  $\omega$ . Of course, it cannot be the ‘‘frequency’’ of the photon in the usual naive sense, because for the single-photon state (4.2.1) to have a perfectly defined frequency  $\omega$ , we need  $\bar{f}_\lambda(\mathbf{k})$  to be proportional to  $\delta(\|\mathbf{k}\| - \omega/c)$ , in which case (4.2.2) does not hold. This is another way to state the well-known fact that plane waves are not normalisable and hence not physical. There is, however, a sense in which  $E = \hbar\omega$  is valid, namely, if we define

$$\omega \equiv \langle 1_{\bar{f}} | \frac{\hat{H}}{\hbar} | 1_{\bar{f}} \rangle = c \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| |\bar{f}_\lambda(\mathbf{k})|^2. \quad (4.2.21)$$

This is, of course, a bit of a tautology, but there is no way around it for physical states.

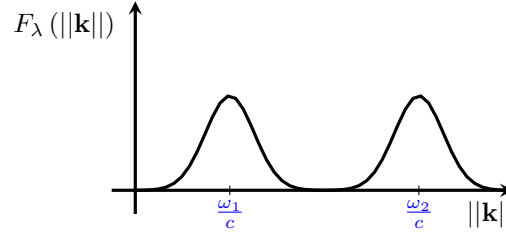
If, for instance, the spectral density quantity

$$F_\lambda(\|\mathbf{k}\|) \equiv \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta |\bar{f}_\lambda(\|\mathbf{k}\|, \theta, \varphi)|^2 \quad (4.2.22)$$

has two distinct peaks  $\omega_1$  and  $\omega_2$ , as in Fig. 4.2.1, then the frequency  $\omega$  of the single-photon as defined by (4.2.21) will have a very small weight in the spectral frequency of the single-photon state. Note that this is very different from a situation in which two photons of respective frequencies  $\omega_1$  and  $\omega_2$  would be present in the field. If, for instance, a photon detector measures (and thus, absorbs) and destroys a photon of frequency  $\omega_1$ , in the first case, there will be no photon left present in the field, while, in the second case, there will be a photon of frequency  $\omega_2$  left.

The usual single-photon Einstein relation  $E = c\|\mathbf{p}\|$  makes sense as an implicit eigenvalue equation obeyed by eigenstates of the free field linear momentum:

$$\hat{\mathbf{P}} = \hbar \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \mathbf{k} \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}). \quad (4.2.23)$$



**Fig. 4.2.1** – Spectral density  $F_\lambda (||\mathbf{k}||)$  with two peaks.

These states read

$$|\mathbf{p}_0\rangle \equiv \sum_{\lambda=\pm} g_\lambda \hat{a}_{(\lambda)}^\dagger \left( \frac{\mathbf{p}_0}{\hbar} \right) |0\rangle \quad (4.2.24)$$

and obey  $\hat{\mathbf{P}} |\mathbf{p}_0\rangle = \mathbf{p}_0 |\mathbf{p}_0\rangle$  and  $\hat{\mathbf{H}} |\mathbf{p}_0\rangle = c ||\mathbf{p}_0|| |\mathbf{p}_0\rangle$ . It is in this sense that Einstein's relation is verified for such states. But these eigenstates of the linear momentum are not normalisable and hence not physical.

It is easy to see from (1.4.32) that the expectation value of the linear momentum in the physical one-photon state (4.2.1) is

$$\mathbf{p} \equiv \langle 1_{\bar{f}} | \hat{\mathbf{P}} | 1_{\bar{f}} \rangle = \hbar \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 ||\mathbf{k}||} \mathbf{k} |\bar{f}_\lambda(\mathbf{k})|^2. \quad (4.2.25)$$

Comparing with (4.2.20), it is immediately seen that  $E > c ||\mathbf{p}||$ , except if  $\bar{f}_\lambda(\mathbf{k})$  is proportional to  $\delta(\varphi - \varphi_0) \delta(\theta - \theta_0)$ , where  $\varphi$  and  $\theta$  are the spherical angular coordinates of the wave vector  $\mathbf{k}$  (see Fig. 1.4.1), and  $\varphi_0$  and  $\theta_0$  label a particular direction in  $\mathbb{R}^3$ , in which case (4.2.2) does not hold. In other words, for physical single-photon states, we have

$$\langle 1_{\bar{f}} | \hat{\mathbf{H}} | 1_{\bar{f}} \rangle > c ||\langle 1_{\bar{f}} | \hat{\mathbf{P}} | 1_{\bar{f}} \rangle||. \quad (4.2.26)$$

## 4.3 Single-mode quantum optics: quantum optics

As already described at the start of the previous sect. 4.2, many textbooks discuss the quantum states of the electromagnetic field almost exclusively in a single-mode framework. Though it is a notable simplification of the general problem, single-mode quantum optics is a very rich topic dealing with how, even for a single physically relevant mode, the photon number statistics of the electromagnetic field can lead to many different field behaviours.

### 4.3.1 Phase operator—Quadrature space

Our discussion of sect. 4.2.1 is a solid basis for the formal grounding of single-mode quantum optics. We defined ladder operators  $\hat{a}_{\bar{f}}$  and  $\hat{a}_{\bar{f}}^\dagger$  which respectively destroy and create a polychromatic photon. The function  $\bar{f}_\lambda(\cdot)$  describes how the considered mode, and hence all its excitations (polychromatic photons), are “spread” over polarisations and wave vectors.

Remember that we established

$$[\hat{a}_{\bar{f}}, \hat{a}_{\bar{f}}^\dagger] = 1 \quad (4.3.1)$$

and defined  $n$ -photon states

$$|n_{\bar{f}}\rangle = \frac{(\hat{a}_{\bar{f}}^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (4.3.2)$$

which obey  $\hat{N}_{\bar{f}} |n_{\bar{f}}\rangle \equiv \hat{a}_{\bar{f}}^\dagger \hat{a}_{\bar{f}} |n_{\bar{f}}\rangle = n |n_{\bar{f}}\rangle$  and

$$\langle n_{\bar{f}} | m_{\bar{f}} \rangle = \delta_{nm} \quad (4.3.3)$$

We also introduced the single mode vector potential

$$\hat{\mathbf{A}}_{\bar{f}}(\mathbf{x}, t) \equiv \mathbf{A}_{\bar{f}}(\mathbf{x}, t) \hat{a}_{\bar{f}} + \mathbf{A}_{\bar{f}}^*(\mathbf{x}, t) \hat{a}_{\bar{f}}^\dagger. \quad (4.3.4)$$

with  $\mathbf{A}_{\bar{f}}(\mathbf{x}, t)$  given by (4.2.7).

We now introduce the mode quadrature operators [4]

$$\hat{X}_{1\bar{f}} \equiv \frac{1}{2} (\hat{a}_{\bar{f}} + \hat{a}_{\bar{f}}^\dagger), \quad (4.3.5a)$$

$$\hat{X}_{2\bar{f}} \equiv -\frac{i}{2} (\hat{a}_{\bar{f}} - \hat{a}_{\bar{f}}^\dagger). \quad (4.3.5b)$$

It will come in handy to represent the (single-mode) states of the electromagnetic field in the quadrature plane. The representation is built as follows. An arbitrary state  $|\psi\rangle$  is represented by a point in the  $(x_1, x_2)$  quadrature plane where

$$x_1 \equiv \langle \psi | \hat{X}_{1\bar{f}} | \psi \rangle, \quad (4.3.6a)$$

$$x_2 \equiv \langle \psi | \hat{X}_{2\bar{f}} | \psi \rangle \quad (4.3.6b)$$

and a “spot” of dimensions  $2\Delta x_1$  and  $2\Delta x_2$  along the  $x_1$  and  $x_2$  axes respectively, centred on  $(x_1, x_2)$ . The dimensions of the spot are the standard deviations

$$\Delta x_1 \equiv \sqrt{\langle \psi | \hat{X}_{1\bar{f}}^2 | \psi \rangle - \langle \psi | \hat{X}_{1\bar{f}} | \psi \rangle^2}, \quad (4.3.7a)$$

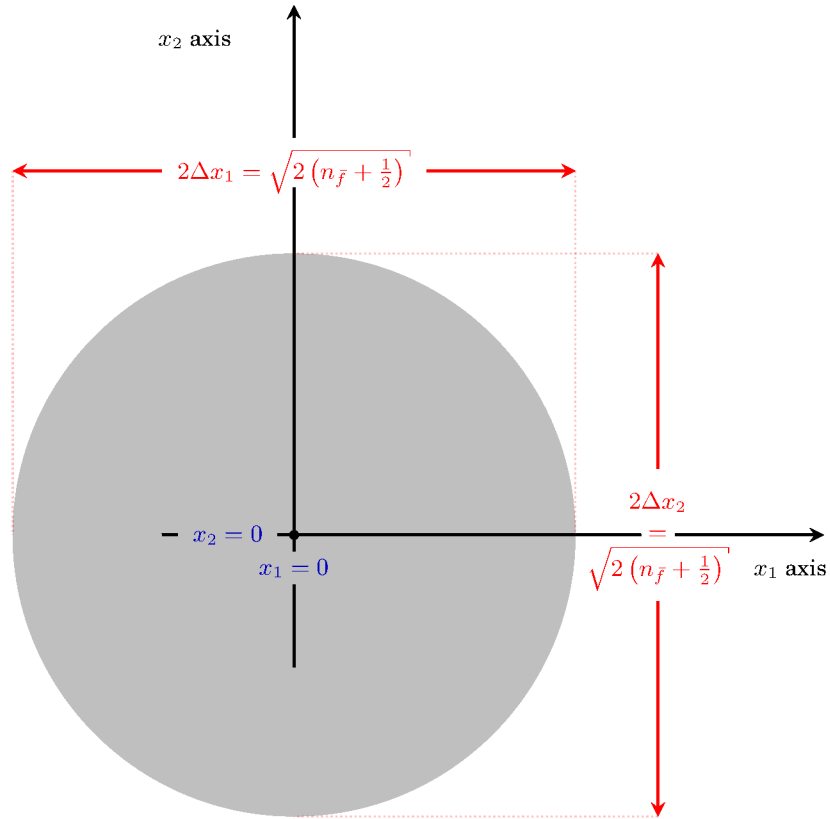
$$\Delta x_2 \equiv \sqrt{\langle \psi | \hat{X}_{2\bar{f}}^2 | \psi \rangle - \langle \psi | \hat{X}_{2\bar{f}} | \psi \rangle^2}. \quad (4.3.7b)$$

The physical meaning of quadrature space is understood from (4.2.8) and (4.3.5): the point and the spot which represent the quantum state in quadrature space give information on the expectation values and standard deviations for the vector potential and electric field in a given quantum state  $|\psi\rangle$ .

It is easily shown from (4.3.1) and (4.3.5) that  $[\hat{X}_{1\bar{f}}, \hat{X}_{2\bar{f}}] = i/2$ , whence, since  $\hat{X}_{1\bar{f}}$  and  $\hat{X}_{2\bar{f}}$  are Hermitian, the uncertainty relations

$$\Delta x_1 \Delta x_2 \geq \frac{1}{4}. \quad (4.3.8)$$

This means that regardless of the quantum state  $|\psi\rangle$ , the spot must have a minimal area equal to  $1/4$ . As usual, it is intuitive to consider that states with a very large uncertainty product  $\Delta x_1 \Delta x_2$  are highly nonclassical, while those which saturate the uncertainty relation (4.3.8) are the most classical. This intuition is vindicated by the study of the higher order correlation functions of the electromagnetic field, as seen in sect. 4.4.3.



**Fig. 4.3.1** – Quadrature space for a Fock state  $|n_f\rangle$ . Notice the large uncertainties, which grow as  $\sqrt{n_f}$  with increasing number  $n$  of photons.

## 4.3.2 Pure states

### 4.3.2.1 Fock states

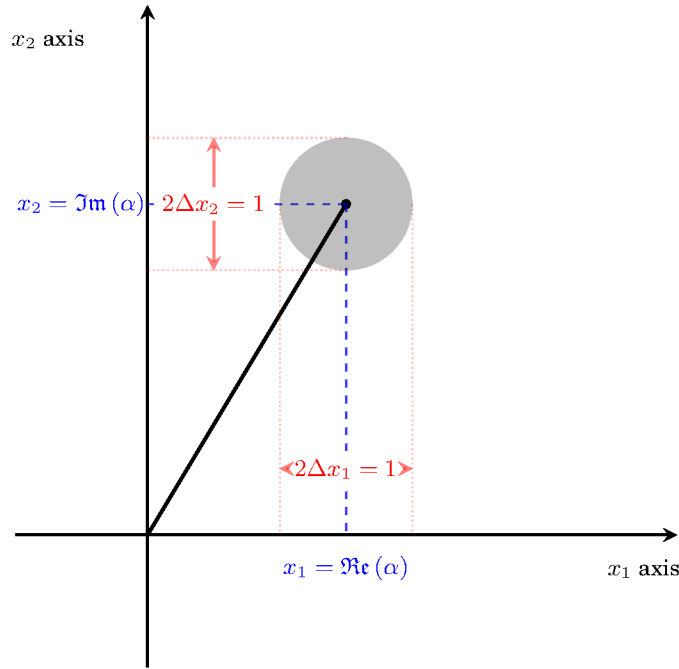
Fock states, of course, are simply defined by (4.3.2) and are eigenstates of the number operator. It is immediate to see that the expectation values of the quadrature operators (4.3.5) vanish for Fock states, while

$$\begin{aligned} \Delta x_1 = \Delta x_2 &= \frac{1}{2} \sqrt{\langle n_f | (\hat{a}_f \hat{a}_f^\dagger + \hat{a}_f^\dagger \hat{a}_f) | n_f \rangle} \\ &= \sqrt{\frac{1}{2} \left( n + \frac{1}{2} \right)}. \end{aligned} \quad (4.3.9)$$

Whence

$$\Delta x_1 \Delta x_2 = \frac{1}{4} + \frac{n}{2} \quad (4.3.10)$$

and the quadrature uncertainty product (4.3.10) for Fock states grows like the number  $n_f$  of photons (see Fig. 4.3.1). Note that the vacuum state  $0_f$  saturates the lower bound  $1/4$  of the inequality (4.3.8). In that sense, the vacuum state is “classical”, while all other Fock states are nonclassical. This is confirmed by an investigation of the properties of the Wigner distribution for Fock states [1].



**Fig. 4.3.2** – Quadrature space for a coherent state  $|\alpha_{\bar{f}}\rangle$ . Notice the “minimal” (in the sense that  $\Delta x_1 = \Delta x_2 = 1/2$ ) uncertainties, completely independent of the coherent state parameter  $\alpha$ .

### 4.3.2.2 Coherent states

Coherent states, the reader will remember, are the eigenstates of the photon annihilation operator  $\hat{a}_{\bar{f}}$ , which are easily shown to be expanded over the Fock basis as [4, 5]

$$|\alpha_{\bar{f}}\rangle = e^{-|\alpha|^2/2} \sum_{m=0}^{+\infty} \frac{\alpha^m}{\sqrt{m!}} |m_{\bar{f}}\rangle. \quad (4.3.11)$$

The eigenvalue equation reads  $\hat{a}_{\bar{f}} |\alpha_{\bar{f}}\rangle = \alpha |\alpha_{\bar{f}}\rangle$ . For a given mode, coherent states generate all possible states, as seen in appendix 4.A. It is shown in quantum optics textbooks [1, 4] that for coherent states

$$x_1 = \Re(\alpha), \quad (4.3.12a)$$

$$x_2 = \Im(\alpha) \quad (4.3.12b)$$

and

$$\Delta x_1 = \Delta x_2 = \frac{1}{2} \quad (4.3.13)$$

which means that all coherent states saturate the lower bound  $1/4$  of the inequality (4.3.8). This hints at the “classical” nature of coherent states, which will become apparent in sect. 4.4.3.

### 4.3.2.3 Squeezed coherent states

A more unusual family of electromagnetic states are the so-called squeezed coherent states. Squeezed coherent states, like coherent states, saturate the lower bound of the inequality (4.3.8), but, whereas the uncertainties  $\Delta x_{1/2}$  were equal (and equal to  $1/2$ ) for coherent states, we will see that, for squeezed states, one uncertainty is smaller than  $1/2$  while the other one is larger than  $1/2$ . Hence the spot corresponding to the quadrature space representation of squeezed coherent states has the same area  $1/4$  as the coherent state disk (see Fig. 4.3.2), but the shape of the spot is that of an ellipse, which can be seen as a “squeezed circle”, hence the name of these states.

Squeezed coherent states  $|\alpha_{\bar{f}} \mapsto \zeta_{\bar{f}}\rangle$  are obtained from coherent states  $|\alpha_{\bar{f}}\rangle$  by an application of the squeezing operator

$$\hat{S}_{\bar{f}}(\zeta) \equiv e^{\frac{1}{2}(\zeta \hat{a}_{\bar{f}}^{\dagger 2} - \zeta^* \hat{a}_{\bar{f}}^2)}, \quad (4.3.14)$$

namely

$$|\alpha_{\bar{f}} \mapsto \zeta_{\bar{f}}\rangle \equiv \hat{S}_{\bar{f}}(\zeta) |\alpha_{\bar{f}}\rangle. \quad (4.3.15)$$

Here the complex number  $\zeta$  has polar coordinates

$$\zeta \equiv r e^{2i\varphi}. \quad (4.3.16)$$

The best way to study the “squeezing” action of (4.3.14) on coherent states is to introduce the rotated quadrature operators

$$\hat{Y}_{1\bar{f}} \equiv \frac{1}{2} \left( e^{-i\varphi} \hat{a}_{\bar{f}} + e^{i\varphi} \hat{a}_{\bar{f}}^{\dagger} \right), \quad (4.3.17a)$$

$$\hat{Y}_{2\bar{f}} \equiv -\frac{i}{2} \left( e^{-i\varphi} \hat{a}_{\bar{f}} - e^{i\varphi} \hat{a}_{\bar{f}}^{\dagger} \right). \quad (4.3.17b)$$

It can then be shown [4] that the standard deviations for these rotated quadratures read

$$\Delta y_1 \equiv \sqrt{\langle \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} | \hat{Y}_{1\bar{f}}^2 | \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} \rangle - \langle \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} | \hat{Y}_{1\bar{f}} | \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} \rangle^2} = \frac{1}{2} e^{-r} \quad (4.3.18a)$$

$$\Delta y_2 \equiv \sqrt{\langle \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} | \hat{Y}_{2\bar{f}}^2 | \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} \rangle - \langle \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} | \hat{Y}_{2\bar{f}} | \alpha_{\bar{f}} \mapsto \zeta_{\bar{f}} \rangle^2} = \frac{1}{2} e^r. \quad (4.3.18b)$$

With the expectation values for the quadrature operators (4.3.5), which read [4]

$$x_1 = \Re(\alpha) \cosh r - \Re(\alpha e^{-2i\varphi}) \sinh r, \quad (4.3.19a)$$

$$x_2 = \Im(\alpha) \cosh r + \Im(\alpha e^{-2i\varphi}) \sinh r \quad (4.3.19b)$$

we can represent the squeezed coherent state (4.3.15) in quadrature space as done on Fig. 4.3.3, where the rotated axes correspond the rotated quadrature operators (4.3.17). As understood from Fig. 4.3.3,  $r$  is known as the squeezing factor.

## 4.3.3 Mixed states

### 4.3.3.1 General case

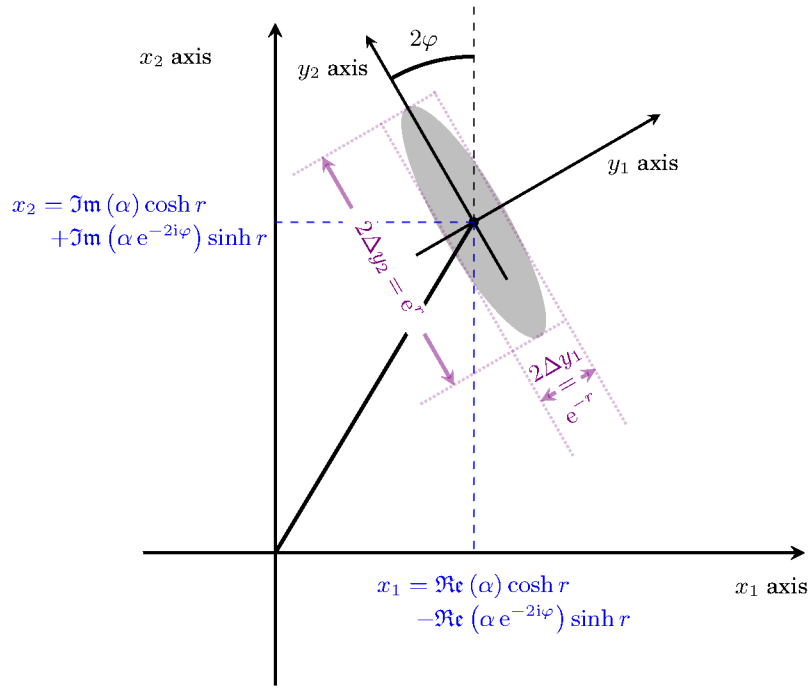
So far we only focused on pure quantum states, which constitute a rather idealised case. However, most quantum states of light “in the real world” are not pure, but rather entangled with other physical degrees of freedom. An important example of such mixed states is that of thermal fields, a class which “includes most fields commonly encountered in practice” [1]. Mixed states should be described not by state vectors but by the so-called statistical operator

$$\hat{\rho} \equiv \sum_i p_i |\psi_i\rangle \langle \psi_i| \quad (4.3.20)$$

where the set of states  $|\psi_i\rangle$  are normalised but need not be orthogonal [7]. All the probabilities  $p_i$  (of being in the state  $|\psi_i\rangle$ ) are real and positive and their sum is of course required to be  $\sum_i p_i = 1$ .

Note that here  $\hat{\rho}$  only carries information on the quantum state of light and not on the above-mentioned environment. The statistical operator arises precisely as a consequence of our renouncing to describe the environment. In that sense  $\hat{\rho}$  encodes the lack of information on the total (light+environment) system.





**Fig. 4.3.3** – Quadrature space for a squeezed coherent state  $|\alpha_{\bar{f}} \rightarrow \zeta_{\bar{f}}\rangle$ . Notice the squeezed and loosened uncertainties, respectively, along the axes of the rotated frame.

In the statistical operator formalism the expectation value of an operator  $\hat{A}$  is given [7] by the trace  $\text{Tr}(\hat{\rho}\hat{A})$ . Whence the expectation values

$$x_1 \equiv \text{Tr}(\hat{\rho}\hat{X}_{1\bar{f}}), \quad (4.3.21a)$$

$$x_2 \equiv \text{Tr}(\hat{\rho}\hat{X}_{2\bar{f}}) \quad (4.3.21b)$$

and the standard deviations

$$\Delta x_1 \equiv \sqrt{\text{Tr}(\hat{\rho}\hat{X}_{1\bar{f}}^2) - \text{Tr}^2(\hat{\rho}\hat{X}_{1\bar{f}})}, \quad (4.3.22a)$$

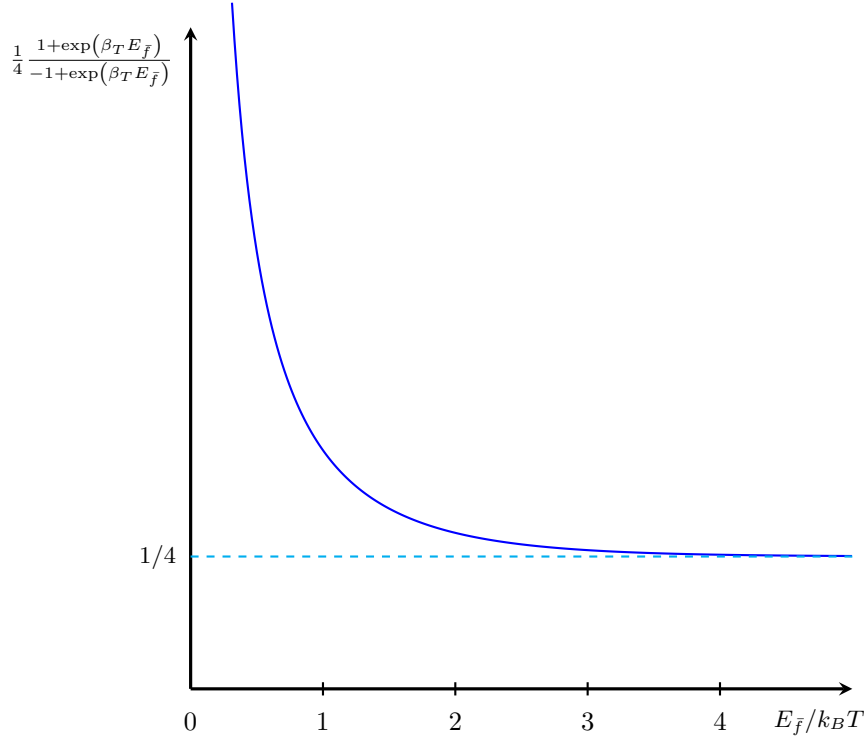
$$\Delta x_2 \equiv \sqrt{\text{Tr}(\hat{\rho}\hat{X}_{2\bar{f}}^2) - \text{Tr}^2(\hat{\rho}\hat{X}_{2\bar{f}})}. \quad (4.3.22b)$$

### 4.3.3.2 Blackbody radiation states

*“Monsieur, je ne puis absolument vous dire s’il a plu. Je vis si résolument en dehors des contingences physiques que mes sens ne prennent pas la peine de me les notifier.”*

Albert Bloch in À la recherche du temps perdu—Du côté de chez Swann, by Marcel Proust (Folio Gallimard, 1988)

The term “blackbody radiation” refers to an electromagnetic field in thermal equilibrium with a thermal reservoir at temperature  $T$ . For such a system it is easily proved [1] that any two electromagnetic modes are statistically independent, in other words, that the statistical operator for the field is a product of statistical operator over all the field modes. Accordingly, it is possible to learn quite a bit about this type of quantum state of light by restricting our study to a single-mode framework.



**Fig. 4.3.4** – Squared uncertainty  $\Delta x_1^2 = \Delta x_2^2$  for blackbody states as a function of the ratio between the electromagnetic mode energy  $E_{\bar{f}}$  and the thermal energy  $k_B T$ .

For a single mode  $\bar{f}$  of blackbody radiation the statistical operator reads [1]

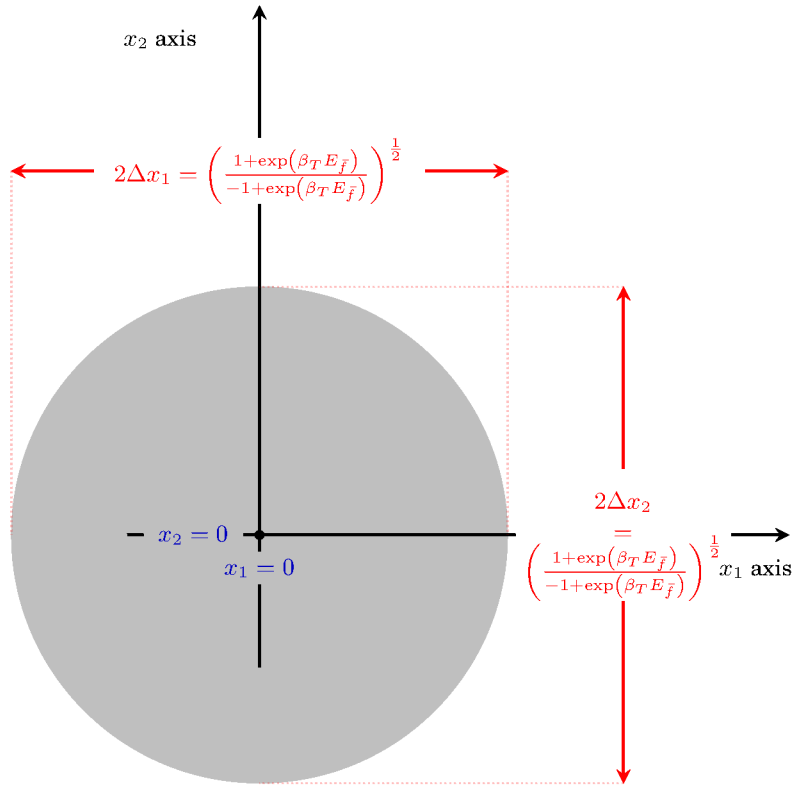
$$\hat{\rho}_{\bar{f}\text{bb}} = (1 - e^{-\beta_T E_{\bar{f}}}) \sum_{n=0}^{+\infty} e^{-n\beta_T E_{\bar{f}}} |n_{\bar{f}}\rangle \langle n_{\bar{f}}| \quad (4.3.23)$$

where we introduced<sup>3</sup> the inverse temperature  $\beta_T \equiv 1/(k_B T)$ . From this we can deduce the expectation values (4.3.21)  $x_1 = x_2 = 0$  and, in order to obtain the standard deviations (4.3.22), the quadratic errors

$$\begin{aligned} \text{Tr}(\hat{\rho}_{\bar{f}\text{bb}} \hat{X}_{1\bar{f}}^2) &= \text{Tr}(\hat{\rho}_{\bar{f}\text{bb}} \hat{X}_{2\bar{f}}^2) = \frac{(1 - e^{-\beta_T E_{\bar{f}}})}{4} \sum_{n=0}^{+\infty} e^{-n\beta_T E_{\bar{f}}} (2n + 1) \\ &= \frac{(1 - e^{-\beta_T E_{\bar{f}}})}{4} \left(1 - 2 \frac{\partial}{\partial \beta_T E_{\bar{f}}}\right) \frac{1}{1 - e^{-\beta_T E_{\bar{f}}}} \\ &= \frac{1}{4} \frac{1 + e^{\beta_T E_{\bar{f}}}}{-1 + e^{\beta_T E_{\bar{f}}}}. \end{aligned} \quad (4.3.24)$$

This quadratic error is plotted in Fig. 4.3.4 as a function of the ratio between the electromagnetic mode energy  $E_{\bar{f}}$  and the thermal energy  $k_B T$ . It is seen that when the energy of the electromagnetic mode is much smaller than the thermal energy, the quadratic errors become extremely large (with a  $\propto k_B T/E_{\bar{f}}$  behaviour for large values of that latter ratio), and can be made arbitrarily close to the saturation value  $1/4$  by increasing the field energy or decreasing the temperature. We can represent the blackbody state (4.3.23) in quadrature space as done on Fig. 4.3.5.

<sup>3</sup>The unusual  $T$  subscript stands for “temperature” or “thermodynamic” and is introduced to avoid any confusion with the  $\beta$  parameter in the photon wave function (see chapter 3).



**Fig. 4.3.5** – Quadrature space for the blackbody radiation state (4.3.23). Notice the uncertainties grow with decreasing electromagnetic energy or increasing temperature.

## 4.4 Interlude: $n$ -photon wave functions

For both and thermal states, it is easily seen that the expectation values of the electric and magnetic field operators vanish, leaving Maxwell's equations to read  $0 = 0$ . In other words, for such states, the expectation values carry little interesting information on the electromagnetic field. In this section we introduce more interesting quantities in the study of the quantum properties of light, that is, coherence functions. We also indicate the link between single-photon wave functions and photodetection probabilities, and, more generally, between  $n$ -photon wave functions and  $n$ -point joint photodetection probabilities.

### 4.4.1 Two-photon wave function

As was done in the single-photon case in chapter 3, we introduce a two-photon wave function. We will generalise the extraction rule (3.4.1). We first need to introduce two-photon states, which read

$$|2, \bar{f}\rangle = \sum_{\kappa=\pm} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \int \frac{d\mathbf{q}}{2(2\pi)^3 \|\mathbf{q}\|} \bar{f}_{(\kappa\lambda)}(\mathbf{k}, \mathbf{q}) \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}) \hat{a}_{(\mu)}^{\dagger}(\mathbf{q}) |0\rangle, \quad (4.4.1)$$

which yields a matrix wave function. For instance, if we focus on the Riemann-Silberstein ( $\beta = 1/2$ ) wave function, we can write

$$\psi_{\bar{f}}^{ij}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv -\frac{2\epsilon_0}{\hbar c} \langle 0 | \hat{E}^{+i}(\mathbf{x}_1, t_1) \hat{E}^{+j}(\mathbf{x}_2, t_2) | 2, \bar{f} \rangle. \quad (4.4.2)$$

Defining  $\hat{\mathbf{E}}^+(\mathbf{x}, t) = \hat{\mathbf{E}}^+_{(+)}(\mathbf{x}, t) + \hat{\mathbf{E}}^+_{(-)}(\mathbf{x}, t)$  with

$$\hat{\mathbf{E}}^+_{(+)}(\mathbf{x}, t) = i\sqrt{\frac{\hbar c}{\epsilon_0}} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ \hat{a}_{(+1)}(\mathbf{k}) \boldsymbol{\epsilon}_{(+1)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k}\cdot\mathbf{x})} \right], \quad (4.4.3a)$$

$$\hat{\mathbf{E}}_{(-)}^+(\mathbf{x}, t) = i\sqrt{\frac{\hbar c}{\epsilon_0}} \int \frac{d\mathbf{k}}{2(2\pi)^3 \|\mathbf{k}\|} \|\mathbf{k}\| \left[ \hat{a}_{(-)}(\mathbf{k}) \boldsymbol{\epsilon}_{(-)}(\mathbf{k}) e^{-i(c\|\mathbf{k}\|t - \mathbf{k} \cdot \mathbf{x})} \right] \quad (4.4.3b)$$

we introduce the definite-helicity two-photon wave function

$$\psi_{\bar{f}(\varkappa\lambda)}^{ij}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv -\frac{2\epsilon_0}{\hbar c} \langle 0 | \hat{E}_{(\varkappa)}^{+i}(\mathbf{x}_1, t_1) \hat{E}_{(\lambda)}^{+j}(\mathbf{x}_2, t_2) | 2, \bar{f} \rangle. \quad (4.4.4)$$

and write down the following wave equations for this object (which is a  $3 \times 3$  matrix), which are readily obtained from (4.4.4):

$$i\hbar \frac{\partial \psi_{\bar{f}(\varkappa\lambda)}^{ij}}{\partial t_1}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) = (c\hbar) \varkappa \left( \nabla_{\mathbf{x}_1} \times \psi_{\bar{f}(\varkappa\lambda)}^i \right)^j(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2), \quad (4.4.5a)$$

$$i\hbar \frac{\partial \psi_{\bar{f}(\varkappa\lambda)}^{ij}}{\partial t_2}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) = (c\hbar) \lambda \left( \nabla_{\mathbf{x}_2} \times \psi_{\bar{f}(\varkappa\lambda)}^j \right)^i(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2). \quad (4.4.5b)$$

In the case of arbitrary helicity, we can regroup helicity components in the same object. Defining

$$\overleftrightarrow{\psi}_{\bar{f}(\varkappa_0\lambda_0)}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \begin{bmatrix} \psi_{\bar{f}(+)}(\mathbf{x}_1, t_1) \\ \psi_{\bar{f}(-)}(\mathbf{x}_1, t_1) \end{bmatrix} \otimes \begin{bmatrix} \psi_{\bar{f}(+)}(\mathbf{x}_2, t_2) \\ \psi_{\bar{f}(-)}(\mathbf{x}_2, t_2) \end{bmatrix} \quad (4.4.6)$$

we can write [12]

$$i\hbar \frac{\partial \overleftrightarrow{\psi}_{\bar{f}}}{\partial t_i}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) = (c\hbar) \alpha_i \nabla_i \times \overleftrightarrow{\psi}_{\bar{f}}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \quad (4.4.7a)$$

with the matrices  $\alpha_i$  defined as

$$\alpha_1 \equiv \Sigma_z \otimes \Sigma_0, \quad \alpha_2 \equiv \Sigma_0 \otimes \Sigma_z, \quad (4.4.7b)$$

$$\Sigma_0 \equiv \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{bmatrix}, \quad \Sigma_z \equiv \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix} \quad (4.4.7c)$$

where  $\mathbb{1}$  is the  $(3 \times 3)$  identity matrix over the vector components of a wave function for a given helicity.

## 4.4.2 Two-photon Wolf equations

The two-time two-photon wave function (4.4.6) obeys the same equation as the second order coherence tensors for classical electromagnetic theory. These were defined by Wolf as correlation functions [1] (where the averages are ensemble averages, which means that averages are taken over uncontrolled and/or unknown parameters):

$$\overleftrightarrow{E}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \langle \mathbf{E}^-(\mathbf{x}_1, t_1) \otimes \mathbf{E}^+(\mathbf{x}_2, t_2) \rangle, \quad (4.4.8a)$$

$$\overleftrightarrow{H}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \langle \mathbf{B}^-(\mathbf{x}_1, t_1) \otimes \mathbf{B}^+(\mathbf{x}_2, t_2) \rangle, \quad (4.4.8b)$$

$$\overleftrightarrow{M}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \langle \mathbf{E}^-(\mathbf{x}_1, t_1) \otimes \mathbf{B}^+(\mathbf{x}_2, t_2) \rangle, \quad (4.4.8c)$$

$$\overleftrightarrow{N}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \langle \mathbf{B}^-(\mathbf{x}_1, t_1) \otimes \mathbf{E}^+(\mathbf{x}_2, t_2) \rangle \quad (4.4.8d)$$

where  $\mathbf{E}^\pm$  and  $\mathbf{B}^\pm$  are the analytic signal + for the corresponding fields and its complex conjugate (antianalytic signal) -. Remember that these are the classical equivalents of the positive and negative frequency parts of the corresponding fields and are defined through

$$\mathbf{G}^+(\mathbf{x}, t) = \int_0^{+\infty} d\omega e^{i\omega t} \int_{-\infty}^{+\infty} du e^{-i\omega u} \mathbf{G}(\mathbf{x}, u), \quad (4.4.9a)$$

$$\mathbf{G}^-(\mathbf{x}, t) = \int_{-\infty}^0 d\omega e^{i\omega t} \int_{-\infty}^{+\infty} du e^{-i\omega u} \mathbf{G}(\mathbf{x}, u). \quad (4.4.9b)$$

Define the second order coherence matrix as

$$\overleftrightarrow{\Gamma}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \begin{bmatrix} \overleftrightarrow{\gamma}_{+1+1}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) & \overleftrightarrow{\gamma}_{+1-1}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \\ \overleftrightarrow{\gamma}_{-1+1}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) & \overleftrightarrow{\gamma}_{-1-1}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \end{bmatrix} \quad (4.4.10a)$$

with

$$\overleftrightarrow{\gamma}_{\lambda_1 \lambda_2}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \equiv \frac{\epsilon_0}{2} \left[ \overleftrightarrow{E}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) + \frac{i}{c} \left( \lambda_1 \overleftrightarrow{N}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) + \lambda_2 \overleftrightarrow{M}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \right) - \mu_0 \lambda_1 \lambda_2 \overleftrightarrow{H}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) \right]. \quad (4.4.10b)$$

It can be shown from the Maxwell equations that the coherence matrix (4.4.10) satisfies the wave equations

$$i\hbar \frac{\partial \overleftrightarrow{\Gamma}_{(f,g)}}{\partial t_i}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) = (c\hbar) \alpha_i \nabla_i \times \overleftrightarrow{\Gamma}_{(f,g)}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2). \quad (4.4.11)$$

This equation is strictly identical to (4.4.7a). This means that second order classical electromagnetic coherence theory and two-photon two-time wave function theory are governed by the same equation, which is an important equivalence because classical coherence theory has been thoroughly studied (see [1] for a detailed presentation).

### 4.4.3 $n$ -photon wave function and $n$ -point correlation functions

The considerations of the previous sects. 4.4.1 and 4.4.2 can be extended to an arbitrary number of photons. Define an  $n$ -photon state

$$|n, \bar{f}\rangle = \sum_{\{\lambda_i\}} \int \prod_{q=1}^n \left( \frac{d\mathbf{k}_q}{2(2\pi)^3 \|\mathbf{k}_q\|} \hat{a}_{(\lambda_q)}^\dagger(\mathbf{k}_q) \right) \bar{f}_{(\{\lambda_a\})}(\{\mathbf{k}_a\}) |0\rangle. \quad (4.4.12)$$

The definite-helicity  $n$ -photon wave function, defined through the following generalisation of Glauber's extraction rule

$$\psi_{\bar{f}(\{\lambda_i\})}^{(\{j_i\})}(\{\mathbf{x}_i, t_i\}) \equiv (-i)^n \left( \frac{2\epsilon_0}{\hbar c} \right)^{\frac{n}{2}} \langle 0 | \prod_{q=1}^n \hat{E}_{(\lambda_q)}^{+j_q}(\mathbf{x}_q, t_q) |n, \bar{f}\rangle \quad (4.4.13)$$

with notations (4.4.3) obeys the wave equations

$$i\hbar \frac{\partial \psi_{\bar{f}(\{\lambda_i\})}^{(\{j_i\})}}{\partial t_a}(\{\mathbf{x}_i, t_i\}) = (c\hbar) \lambda_a \left( \nabla_{\mathbf{x}_a} \times \psi_{\bar{f}(\{\lambda_i\})}^{(\{j_i\})} \right)(\{\mathbf{x}_i, t_i\}). \quad (4.4.14)$$

More generally, for arbitrary states  $|\psi\rangle$  of the electromagnetic field, we introduce the  $2n^{\text{th}}$  order correlation functions as [1]

$$\Gamma_{(\{j_i\})}^{(2n)}(\{\mathbf{x}_i, t_i\}) \equiv \langle \psi | \left( \prod_{p=1}^n \hat{E}_{j_p}^-(\mathbf{x}_p, t_p) \right) \left( \prod_{q=n+1}^{2n} \hat{E}_{j_q}^+(\mathbf{x}_q, t_q) \right) | \psi \rangle. \quad (4.4.15)$$

Through a line of argument similar to the one we developed in sect. 4.1, the correlation functions (4.4.15) at spacetime points  $\Gamma_{(j_1 \dots j_n j_{n+1} \dots j_{2n})}^{(2n)}(\mathbf{x}_1, t_1, \dots, \mathbf{x}_n, t_n, \mathbf{x}_{n+1}, t_{n+1}, \dots, \mathbf{x}_{2n}, t_{2n})$  can be interpreted [15] as being, up to some dimensional factor, proportional to the joint probability, per unit (time) $^n$ , to detect a photon with electric field along  $j_1$  at  $\mathbf{x}_1$  and at time  $t_1, \dots$ , and a photon with electric field along  $j_n$  at  $\mathbf{x}_n$  and at time  $t_n$ .

Note for instance that if the state  $|\psi\rangle$  is a coherent state, then these correlation functions will be nonzero for all values of  $n$ . It is very easy to show that, if  $|\psi\rangle = |\alpha_{\bar{f}}\rangle$  is a coherent state, say of the mode  $\bar{f}$ , as discussed in

sect. 4.2.1, then the correlation functions (4.4.15) factorise:

$$\Gamma_{\{\{j_i\}\}}^{(2n)}(\{\{\mathbf{x}_i, t_i\}\}) = \left( \prod_{p=1}^n E_{j_p}^*(\mathbf{x}_p, t_p) \right) \left( \prod_{q=n+1}^{2n} E_{j_q}(\mathbf{x}_q, t_q) \right) |\alpha|^{2n}. \quad (4.4.16)$$

This illustrates the fact that, for coherent states, photon detection processes at different spacetime points are completely independent of one another.

On the other hand, if  $|\psi\rangle$  is a Fock state with occupation number  $n_0$ , all correlation functions (4.4.15) of order  $n > n_0$  will vanish identically everywhere in space and time. This illustrates the obvious fact that, if the electromagnetic field contains  $n_0$  photons, then there is no probability of detecting  $n > n_0$  photons.

Finally, we note the interesting fact that for (single-mode) blackbody radiation states, the  $2n^{\text{th}}$  order correlation functions (4.4.15) can be rewritten [1] in terms of second order correlation functions.

#### 4.4.4 Excursion: Hong-Ou-Mandel interferometry

Hong-Ou-Mandel interferometry [13] is usually presented in terms of annihilation and creation operators, but can also be understood in a first quantisation scheme, as we now discuss. When two indistinguishable photons are sent along two arms ( $A$  and  $B$ ) of a balanced beam-splitter, they interfere constructively so that both photons exit through the same outgoing arm. The beam-splitter sends the ingoing state  $|1_A^{\text{in}} 1_B^{\text{in}}\rangle$  where one photon is present in each ingoing arm to the outgoing state  $(|2_A^{\text{out}} 0_B^{\text{out}}\rangle + |0_A^{\text{out}} 2_B^{\text{out}}\rangle) / \sqrt{2}$ .

This phenomenon can be explained as is usually done [8] in a second-quantisation framework. But we can also propose the following first-quantised argument. We name the two photons  $\alpha$  and  $\beta$ . Since they are indistinguishable, the initial state of the system, where there is one photon in each ingoing arm, reads

$$\frac{1}{\sqrt{2}} (|A^{\text{in}}\rangle_\alpha |B^{\text{in}}\rangle_\beta + |B^{\text{in}}\rangle_\alpha |A^{\text{in}}\rangle_\beta). \quad (4.4.17)$$

As described in [8], the passage through a beam-splitter can be modeled by the coherent exchange of quanta between the two arms  $A$  and  $B$ . A balanced beamsplitter gives the transformation law

$$|A^{\text{in}}\rangle \rightarrow \frac{|A_A^{\text{out}}\rangle + |B^{\text{out}}\rangle}{\sqrt{2}} \quad (4.4.18a)$$

$$|B^{\text{in}}\rangle \rightarrow \frac{|A^{\text{out}}\rangle - |B^{\text{out}}\rangle}{\sqrt{2}}. \quad (4.4.18b)$$

Therefore for the initial state (4.4.17) the action of the beam-splitter is

$$\begin{aligned} \frac{1}{\sqrt{2}} (|A^{\text{in}}\rangle_\alpha |B^{\text{in}}\rangle_\beta + |B^{\text{in}}\rangle_\alpha |A^{\text{in}}\rangle_\beta) &\rightarrow \frac{1}{2\sqrt{2}} \left[ (|A^{\text{out}}\rangle + |B^{\text{out}}\rangle)_\alpha (|A^{\text{out}}\rangle - |B^{\text{out}}\rangle)_\beta \right. \\ &\quad \left. + (|A^{\text{out}}\rangle - |B^{\text{out}}\rangle)_\alpha (|A^{\text{out}}\rangle + |B^{\text{out}}\rangle)_\beta \right] \\ &= \frac{1}{\sqrt{2}} (|A^{\text{out}}\rangle_\alpha |A^{\text{out}}\rangle_\beta - |B^{\text{out}}\rangle_\alpha |B^{\text{out}}\rangle_\beta) \end{aligned} \quad (4.4.19)$$

as observed [13] and predicted in the second-quantised framework [8]. The initial and final states are both maximally entangled Bell states in this picture.

## 4.5 Single mode quantum optics: effective one-point wave function

Notice that in the single-photon case studied in chapter 3, the correlation function

$$\Gamma_{\mathbf{E}ij}^{(2)}(\mathbf{x}_0, u | \mathbf{x}_0, v) = \langle \text{init} | \hat{E}_i^-(\mathbf{x}_0, u) \hat{E}_j^+(\mathbf{x}_0, v) | \text{init} \rangle \quad (4.5.1)$$

can be easily obtained from the Riemann-Silberstein photon wave function<sup>4</sup>. Indeed

$$\begin{aligned} \langle 1_{\bar{f}} | \hat{E}_i^-(\mathbf{x}_0, u) \hat{E}_j^+(\mathbf{x}_0, v) | 1_{\bar{f}} \rangle &= \langle 1_{\bar{f}} | \hat{E}_i^-(\mathbf{x}_0, u) | 0 \rangle \langle 0 | \hat{E}_j^+(\mathbf{x}_0, v) | 1_{\bar{f}} \rangle \\ &= \frac{\hbar c}{2\epsilon_0} \left( \psi_i^{(1/2)} \right)^* (\mathbf{x}_0, u) \psi_j^{(1/2)} (\mathbf{x}_0, v) \end{aligned} \quad (4.5.2)$$

with  $|1_{\bar{f}}\rangle$  defined by (4.2.1), as seen from (3.4.12) and (3.4.14). This manipulation, valid in the framework of single-mode quantum optics as well as in the more general quantum field theoretical case, gives an interesting relevance to single-photon wave functions in the case of photodetection theory and can be extended to  $2n^{\text{th}}$  order correlation functions and  $n$ -photon states. The caveat being that the description of the field is made in terms of correlation functions of higher and higher order as the number of photons is increased. Moreover, this link between  $n$ -photon wave functions and correlation functions is only relevant for Fock states of the electromagnetic field. For these reasons we endeavour to focus on the second order coherence function which, in the degenerate case  $\mathbf{x}_1 = \mathbf{x}_2$ , reduces to the quantity featured in the detection probability (see (4.1.6) and below).

### 4.5.1 General case

We would like to find, for an arbitrary state of the electromagnetic field, a quantity which would play the part of the single-photon wave function as seen from (4.5.2). Namely, a quantity of which we could simply take the outer product with itself at two different times to obtain the correlation function (4.5.1). For this we turn back to (4.2.8), which we adapt to the electric field:

$$\begin{aligned} \hat{\mathbf{E}}_{\bar{f}}(\mathbf{x}, t) &\equiv \mathbf{E}_{\bar{f}}(\mathbf{x}, t) \hat{a}_{\bar{f}} + \mathbf{E}_{\bar{f}}^*(\mathbf{x}, t) \hat{a}_{\bar{f}}^\dagger \\ &\equiv \hat{\mathbf{E}}_{\bar{f}}^+(\mathbf{x}, t) + \hat{\mathbf{E}}_{\bar{f}}^-(\mathbf{x}, t). \end{aligned} \quad (4.5.3)$$

Say the initial state of the field, *i.e.*, at the start of the photodetection process, is such that there only are photons in mode  $\bar{f}$ . We start with the simpler case of pure states ( $|\text{init}\rangle \equiv |\psi_{\bar{f}}\rangle$ ) and compute the correlation function

$$\begin{aligned} \Gamma_{\mathbf{E}ij}^{(2)}(\mathbf{x}_0, u | \mathbf{x}_0, v) &= \langle \psi_{\bar{f}} | \hat{E}_{\bar{f}i}^-(\mathbf{x}_0, u) \hat{E}_{\bar{f}j}^+(\mathbf{x}_0, v) | \psi_{\bar{f}} \rangle \\ &= \sum_{n=0}^{+\infty} \langle \psi_{\bar{f}} | \hat{E}_{\bar{f}i}^-(\mathbf{x}_0, u) | n_{\bar{f}} \rangle \langle n_{\bar{f}} | \hat{E}_{\bar{f}j}^+(\mathbf{x}_0, v) | \psi_{\bar{f}} \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) \sum_{n=0}^{+\infty} \langle \psi_{\bar{f}} | \hat{a}_{\bar{f}}^\dagger | n_{\bar{f}} \rangle \langle n_{\bar{f}} | \hat{a}_{\bar{f}} | \psi_{\bar{f}} \rangle \quad (*) \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, v) E_{\bar{f}j}(\mathbf{x}_0, u) \sum_{n=0}^{+\infty} (n+1) |\langle \psi_{\bar{f}} | n+1, \bar{f} \rangle|^2 \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, v) E_{\bar{f}j}(\mathbf{x}_0, u) \sum_{n=0}^{+\infty} n |\langle \psi_{\bar{f}} | n, \bar{f} \rangle|^2 \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, v) E_{\bar{f}j}(\mathbf{x}_0, u) \langle \psi_{\bar{f}} | \hat{N}_{\bar{f}} | \psi_{\bar{f}} \rangle. \end{aligned} \quad (4.5.4)$$

<sup>4</sup>And, in the case of the correlation function  $\langle \text{init} | \hat{A}_i^-(\mathbf{x}_0, u) \hat{A}_j^+(\mathbf{x}_0, v) | \text{init} \rangle$ , from the Gross-Hawton photon wave function.

This means that as far as second order coherence functions are concerned, we can define the effective wave function for the arbitrary (single-mode) state  $|\psi_{\bar{f}}\rangle$  as

$$\psi_{\bar{f}}^{(\text{eff})}(\mathbf{x}, t) = \frac{2\epsilon_0}{\hbar c} \sqrt{\langle \psi_{\bar{f}} | \hat{N}_{\bar{f}} | \psi_{\bar{f}} \rangle} \mathbf{E}_{\bar{f}}(\mathbf{x}, t) \quad (4.5.5)$$

so that we can write a similar expression to (4.5.2) as

$$\Gamma_{\mathbf{E}_{ij}}^{(2)}(\mathbf{x}_0, u | \mathbf{x}_0, v) = \frac{\hbar c}{2\epsilon_0} \left( \psi_{\bar{f}i}^{(\text{eff})} \right)^*(\mathbf{x}_0, u) \psi_{\bar{f}j}^{(\text{eff})}(\mathbf{x}_0, v). \quad (4.5.6)$$

Now, we show that this prescription generalises to the case where the state of the (single-mode) electromagnetic field is described by a statistical operator:

$$\hat{\rho}_{\bar{f}} = \sum_{k=0}^{+\infty} \sum_{l=0}^{+\infty} b_{kl} |k_{\bar{f}}\rangle \langle l_{\bar{f}}|. \quad (4.5.7)$$

Then we compute the correlation function

$$\begin{aligned} \text{Tr} \left( \hat{\rho}_{\bar{f}} \hat{E}_{\bar{f}i}^{-}(\mathbf{x}_0, u) \hat{E}_{\bar{f}j}^{+}(\mathbf{x}_0, v) \right) &= \sum_{n=0}^{+\infty} \sum_{k=0}^{+\infty} \sum_{l=0}^{+\infty} b_{kl} \langle n_{\bar{f}} | k_{\bar{f}} \rangle \langle l_{\bar{f}} | \hat{E}_{\bar{f}i}^{-}(\mathbf{x}_0, u) \hat{E}_{\bar{f}j}^{+}(\mathbf{x}_0, v) | n_{\bar{f}} \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, v) E_{\bar{f}j}(\mathbf{x}_0, u) \sum_{k=0}^{+\infty} \sum_{l=0}^{+\infty} b_{kl} \langle l_{\bar{f}} | \hat{a}_{\bar{f}}^{\dagger} \hat{a}_{\bar{f}} | k \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, v) E_{\bar{f}j}(\mathbf{x}_0, u) \sum_{k=0}^{+\infty} k b_{kk} \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, v) E_{\bar{f}j}(\mathbf{x}_0, u) \text{Tr} \left( \hat{\rho}_{\bar{f}} \hat{N}_{\bar{f}} \right). \end{aligned} \quad (4.5.8)$$

This means that as far as second order coherence functions are concerned, we can define the effective wave function for the arbitrary (single-mode) statistical matrix  $\hat{\rho}_{\bar{f}}$  as

$$\psi_{\bar{f}}^{(\text{eff})}(\mathbf{x}, t) = \frac{2\epsilon_0}{\hbar c} \sqrt{\text{Tr} \left( \hat{\rho}_{\bar{f}} \hat{N}_{\bar{f}} \right)} \mathbf{E}_{\bar{f}}(\mathbf{x}, t). \quad (4.5.9)$$

We see that both for a pure state (4.5.5) and a statistical mixture (4.5.9), the effective wave function is proportional to the square root of the average number of photons in the mode  $\bar{f}$ . This prescription for an effective wave function is, we note, not unlike that giving the order parameter of a Bose-Einstein condensate (see, *e.g.*, sect. 2.2 of [9]). The analogy is more formal than it is profound, however, since it is due to the common focus of both approaches on second order coherence functions.

## 4.5.2 Fock and coherent states

The prescription we gave in the previous sect. 4.5.1 to obtain an effective wave function for an arbitrary single-mode state is, arguably, somewhat artificial, but we will now see that, for certain types of quantum states of the mode  $\bar{f}$ , namely, Fock and coherent states, we can introduce a wave function quite naturally. We turn back to computation that led to (4.5.4), but stop at the step labeled by an asterisk (\*).



For Fock states  $|\psi_{\bar{f}}\rangle = |n_{0\bar{f}}\rangle$  we have

$$\begin{aligned}\Gamma_{\mathbf{E}ij}^{(2)}(\mathbf{x}_0, u | \mathbf{x}_0, v) &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) \sum_{n=0}^{+\infty} \langle n_{0\bar{f}} | \hat{a}_{\bar{f}}^\dagger | n_{\bar{f}} \rangle \langle n_{\bar{f}} | \hat{a}_{\bar{f}} | n_{0\bar{f}} \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) n_0\end{aligned}\quad (4.5.10)$$

and (4.5.5) applies straightforwardly.

For coherent states  $|\psi_{\bar{f}}\rangle = |\alpha_{0\bar{f}}\rangle$  we have

$$\begin{aligned}\Gamma_{\mathbf{E}ij}^{(2)}(\mathbf{x}_0, u | \mathbf{x}_0, v) &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) \sum_{n=0}^{+\infty} \langle \alpha_{0\bar{f}} | \hat{a}_{\bar{f}}^\dagger | n_{\bar{f}} \rangle \langle n_{\bar{f}} | \hat{a}_{\bar{f}} | \alpha_{0\bar{f}} \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) |\alpha_0|^2 \sum_{n=0}^{+\infty} \langle \alpha_{0\bar{f}} | n_{\bar{f}} \rangle \langle n_{\bar{f}} | \alpha_{0\bar{f}} \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) |\alpha_0|^2 \langle \alpha_{0\bar{f}} | \alpha_{0\bar{f}} \rangle \\ &= E_{\bar{f}i}^*(\mathbf{x}_0, u) E_{\bar{f}j}(\mathbf{x}_0, v) |\alpha_0|^2\end{aligned}\quad (4.5.11)$$

and (4.5.5) applies straightforwardly as well.

## 4.6 Quantum optics and classical electrodynamics: an informal overview

A central question to quantum optics is that of how the behaviour of light as predicted by a quantum description departs from what is expected on the basis of classical electrodynamics. The postulates of quantum physics teach us that what we observe, on average, as, for instance, the electric field, is the expectation value of the electric field operator computed in the quantum state of the light. In that sense, the usual, classical picture of an electric field as oscillating in space and time is best reproduced by the coherent states of light as seen from (1.4.31) and (4.3.11). It is possible to confirm this paradigm experimentally [14]. It is very well-known (see, *e.g.*, [4]) that, on the other hand, the expectation value of the electric field operator in a Fock state is zero. It is, as far as we know, seldom mentioned that this is also the case for a blackbody radiation state, as can be seen from sect. 4.3.3.2.

Maxwell's equations, the cornerstone of classical electrodynamics, are valid in quantum electrodynamics as operator equations and hence in quantum optics as expectation value equations: for an arbitrary state  $\hat{\rho}$  of the electromagnetic field, the whole spacetime dependence of  $\text{Tr}(\hat{\rho} \hat{F}^{\mu\nu}(\mathbf{x}, t))$  is carried by the field operator  $\hat{F}^{\mu\nu}(\mathbf{x}, t)$ . But, as we just discussed, not only for the highly nonclassical Fock states of light, but also for the ubiquitous thermal states, do these expectation values vanish. This means that, taken as equations obeyed by expectation values of field operators, Maxwell's equations read, for Fock and thermal states,  $\mathbf{0} = \mathbf{0}$ , and thus carry no information at all. It is only by focusing on products of electric (and/or magnetic) field operators that we can gain more interesting insight on such quantum states of light. Hence the importance of the study of correlation functions of the electromagnetic field. As seen from (4.4.11), though, Maxwell's equations are still relevant to these correlation functions, but not as expectation value equations.

Two good approximations of blackbody thermal sources are [1] the surface of the Sun (with temperature  $T \sim 5 \times 10^3$  K) and incandescent lamps (with temperature  $T \sim 3 \times 10^3$  K). Mandel and Wolf give [1] the average

number of photons in electromagnetic modes of visible wavelength, which are of order  $10^{-2}$  for the Sun and  $10^{-3}$  for incandescent lamps. We saw in sect. 4.3.3.2 that the uncertainty in quadrature space, for blackbody states, is the product of a numerical factor by the quotient  $(1 + e^{\beta_T E_{\bar{f}}}) / (-1 + e^{\beta_T E_{\bar{f}}})$ , the behaviour of which is plotted in Fig. 4.3.4. For visible wavelengths and temperatures corresponding to the surface of the Sun or incandescent lamps, it is seen that the quotient  $(1 + e^{\beta_T E_{\bar{f}}}) / (-1 + e^{\beta_T E_{\bar{f}}})$  is very close to 2, the “most classical” value being 1. As far as quadrature uncertainties are concerned, therefore, visible wavelengths emitted by typical thermal sources have quantum states which are far less “classical” than coherent states.

## 4.A Completeness relation for coherent states

Our goal here is to show that we can build a completeness relation for coherent states:

$$\frac{1}{\pi} \int d(\Re\alpha) \int d(\Im\alpha) |\alpha\rangle\langle\alpha| = \hat{\mathbb{1}}, \quad (4.A.1)$$

where

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{m=0}^{+\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle. \quad (4.A.2)$$

This is proved by switching to polar coordinates for  $\alpha$ :

$$\begin{aligned} \frac{1}{\pi} \int d(\Re\alpha) \int d(\Im\alpha) |\alpha\rangle\langle\alpha| &= \frac{1}{\pi} \int d(\Re\alpha) \int d(\Im\alpha) e^{-|\alpha|^2} \sum_{m=0}^{+\infty} \sum_{k=0}^{+\infty} \frac{(\alpha)^m (\alpha^*)^k}{\sqrt{m!} \sqrt{k!}} |m\rangle\langle k| \\ &= \frac{1}{\pi} \int_0^{+\infty} dr r \int_0^{2\pi} d\theta e^{-r^2} \sum_{m=0}^{+\infty} \sum_{k=0}^{+\infty} r^{m+k} \frac{e^{i(m-k)\theta}}{\sqrt{m!} \sqrt{k!}} |m\rangle\langle k| \\ &= \frac{1}{\pi} (2\pi) \int_0^{+\infty} dr r e^{-r^2} \sum_{m=0}^{+\infty} \sum_{k=0}^{+\infty} r^{m+k} \frac{\delta_{mk}}{\sqrt{m!} \sqrt{k!}} |m\rangle\langle k| \\ &= 2 \int_0^{+\infty} dr r e^{-r^2} \sum_{m=0}^{+\infty} r^{2m} \frac{1}{m!} |m\rangle\langle m| \\ &= \int_0^{+\infty} du e^{-u} \sum_{m=0}^{+\infty} \frac{u^m}{m!} |m\rangle\langle m| \\ &= \sum_{m=0}^{+\infty} \frac{1}{m!} \Gamma(m+1) |m\rangle\langle m| \\ &= \sum_{m=0}^{+\infty} |m\rangle\langle m| \\ &= \hat{\mathbb{1}} \end{aligned}$$

and the proof of (4.A.1) is complete.

# REFERENCES

---

## Books

- [1] L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, 1995) (cit. on pp. 91, 101–105, 107–109, 112).
- [2] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, *Photons et atomes - Introduction à l'électrodynamique quantique*, 2nd ed. (EDP Sciences/CNRS Éditions, 2001) (cit. on p. 93).
- [3] A. Messiah, *Mécanique Quantique*, 1st ed., Vol. 1 (Dunod, Paris, 1965) (cit. on p. 93).
- [4] M.O. Scully and M.S. Zubairy, *Quantum Optics* (Cambridge University Press, 1997) (cit. on pp. 94, 95, 100, 102, 103, 112).
- [5] R. Loudon, *The Quantum Theory of Light*, 3rd ed. (Oxford University Press, 2000) (cit. on pp. 95, 102).
- [6] G.E. Andrews, R. Askey and R. Roy, *Special Functions* (Cambridge University Press, 1999) (cit. on p. 97).
- [7] M. Le Bellac, *Quantum Physics* (Cambridge University Press, 2006) (cit. on pp. 103, 104).
- [8] S. Haroche and J.M. Raimond, *Exploring the Quantum - Atoms, Cavities and Photons* (Oxford University Press, 2007) (cit. on p. 109).
- [9] L. Pitaevskii and S. Stringari, *Bose-Einstein condensation* (Clarendon Press, Oxford, 2003) (cit. on p. 111).

## Book Chapters

- [10] R.J. Glauber, 'Optical Coherence and Photon Statistics', in *Quantum Optics and Electronics - Les Houches 1964*, edited by C. DeWitt, A. Blandin and C. Cohen-Tannoudji (Gordon and Breach, 1964) (cit. on pp. 93, 94).

## Articles

- [11] M.I. Shirokov, 'Signal velocity in quantum electrodynamics', *Sov. Phys. Usp.* **21**, 345 (1978) (cit. on p. 93).
- [12] B.J. Smith and M.G. Raymer, 'Photon wave functions, wave-packet quantization of light, and coherence theory', *New J. Phys.* **9**, 414 (2007) (cit. on p. 107).
- [13] C.K. Hong, Z.Y. Ou and L. Mandel, 'Measurement of subpicosecond time intervals between two photons by interference', *Phys. Rev. Lett.* **59**, 2044 (1987) (cit. on p. 109).
- [14] G. Breitenbach, S. Schiller and J. Mlynek, 'Measurement of the quantum states of squeezed light', *Nature* **387**, 471 (1997) (cit. on p. 112).

## Theses

- [15] É. Brainis, Utilisation de l'optique fibrée pour l'ingénierie quantique : du support passif aux sources, PhD Thesis (Université Libre de Bruxelles, 2006) (cit. on pp. 95, 108).

## Unpublished Articles and Online Notes

- [16] F.W. Nijhoff, *Quantum Mechanics - App. D: Hermite Equation - Orthogonal Polynomials*, <http://www1.maths.leeds.ac.uk/~frank/math3383/AppD.pdf> (cit. on p. 97).



PART II

QUANTUM ELECTRODYNAMICS & LIGHT EMISSION



# INTRODUCTION TO PART II

---

Decay over time is one of the most ubiquitous behaviours exhibited by physical systems. In many instances the phenomenological law of exponential decay is a good approximation to the measured evolution. In quantum mechanics, the usual paradigm of decay is found in systems that consist of a few (usually, two) discrete states, and which interact with a very large environment (in terms of the dimension of the environmental Hilbert space). This paradigm is that of the Friedrichs model [2]. Under very general considerations, it is considered that if the system is initially placed in an excited state, then it is valid to assume that the survival probability of the system in that state follows an exponential time-decay law with some decay constant  $\Gamma$ . At times sufficiently shorter than  $1/\Gamma$ , that exponential behaviour is well approximated by a linear one, which is predicted by Fermi's golden rule, the most famous result of time-dependent perturbation theory (see Fig. II.1).

However, one can oppose [1] (sect. 19.1) the following argument to the paradigm of exponential decay: to derive the exponential decay law, one typically considers a situation where many identical unstable systems are present, *e.g.* atoms that are prone to decay. The key assumption is that the proportion of atoms that decay in a time interval  $dt$  around  $t$ —with respect to the total number of remaining atoms at time  $t$ —does not depend on  $t$ . This can only be true if the properties of the decaying system remain constant with time, but this clearly cannot be the case for decaying states. This shows that the exponential decay law, which is obtained heuristically, can at best give a very good approximation of the actual time-decay law, which it often does.

For very short times, however, the unitarity of the time-evolution operator strictly forbids exponential decay. This is true of all quantum systems and is known as the **Zeno behaviour**. To see this, let us focus on the so-called survival probability  $P_{\text{surv}}$  which is defined as the square modulus of the survival amplitude

$$A_{\text{surv}}(t) = \langle \psi(t=0) | e^{-\frac{i}{\hbar} \hat{H}t} | \psi(t=0) \rangle \quad (\text{II.1})$$

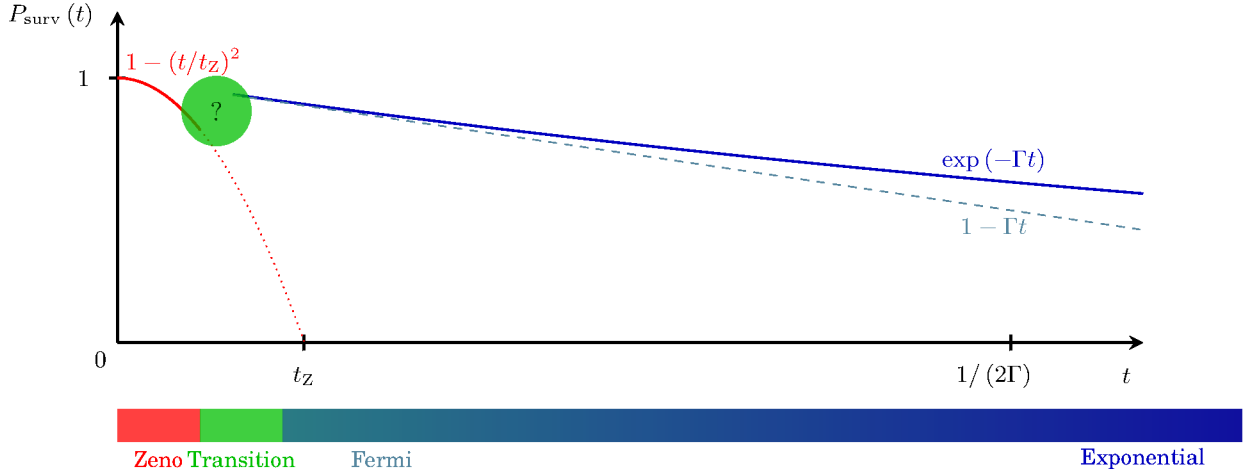
of the initial state  $|\psi(t=0)\rangle$  of the system. The spectral theorem allows us to rewrite (II.1) as an integral over the (in general, continuous and unbounded) spectrum  $\sigma(H)$  of  $\hat{H}$ :

$$A_{\text{surv}}(t) = \int_{\sigma(H)} d\epsilon |\langle \psi(t=0) | \epsilon \rangle|^2 e^{-\frac{i}{\hbar} \epsilon t} \quad (\text{II.2})$$

where  $|\epsilon\rangle$  is an eigenstate of the Hamiltonian. The differentiability of  $A_{\text{surv}}$  is then guaranteed [3], after using Lebesgue's dominated convergence theorem to differentiate (II.2), by the Cauchy-Schwarz inequality

$$\begin{aligned} \left| \frac{dA_{\text{surv}}}{dt} \right| &= \frac{1}{\hbar} \left| \langle \psi(t=0) | e^{-\frac{i}{\hbar} \hat{H}t} \hat{H} \psi(t=0) \rangle \right| \\ &\leq \frac{1}{\hbar} \| \psi(t=0) \| \| H \psi(t=0) \| \\ &< +\infty. \end{aligned} \quad (\text{II.3})$$





**Fig. II.1** – The different regimes in the time-decay of quantum systems, as seen from the time evolution of the survival probability  $P_{\text{surv}}(t)$  of the initial (excited) state, defined by (II.1) and (II.4). The decay is quadratic at very short times, in the so-called Zeno regime (solid crimson/red), and exponential at long times (solid midnight blue), the latter being well approximated at “intermediate” times by the linear prescription of Fermi’s golden rule (dashed teal). The transition (green spot) between the Zeno and Fermi regimes is *a priori* difficult to describe in the general case.

Note that for the last step in (II.3) to be valid, we need  $\|H\psi(t=0)\|$  to be finite. Now define the survival probability

$$P_{\text{surv}}(t) \equiv |A_{\text{surv}}(t)|^2. \quad (\text{II.4})$$

Since  $A_{\text{surv}}$  is differentiable, we write, following [4]

$$\begin{aligned} \frac{dP_{\text{surv}}}{dt} &= \frac{dA_{\text{surv}}}{dt} A_{\text{surv}}^*(t) + \frac{dA_{\text{surv}}^*}{dt} A_{\text{surv}}(t) \\ &= \frac{dA_{\text{surv}}}{dt} A_{\text{surv}}(-t) - \frac{dA_{\text{surv}}}{du} \Big|_{u=-t} A_{\text{surv}}(t) \end{aligned} \quad (\text{II.5})$$

where we made use of (II.2), whence  $(dP_{\text{surv}}/dt)(t=0) = 0$ . And the decay of the survival probability of any quantum system in an initial state with finite energy cannot be exactly exponential. It is indeed not linear around  $t=0$ , but, rather, in the general case, quadratic. This is easily seen from (II.1) and (II.4), under very general conditions. We then write

$$P_{\text{surv}}(t) \underset{t \rightarrow 0}{\sim} 1 - \left(\frac{t}{t_Z}\right)^2 \quad (\text{II.6})$$

where  $t_Z$  is the Zeno time. This short-time behaviour is shown in Fig. II.1. There even is a general method to obtain the Zeno time  $t_Z$ , which follows [4] from a series expansion of the survival probability

$$\begin{aligned} P_{\text{surv}}(t) &= \left| \langle \psi(t=0) | e^{-\frac{i}{\hbar} \hat{H} t} | \psi(t=0) \rangle \right|^2 \\ &= \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{(-1)^n}{k!n!} \left(\frac{t}{\hbar}\right)^{k+n} \langle \psi(t=0) | \hat{H}^k | \psi(t=0) \rangle \langle \psi(t=0) | \hat{H}^n | \psi(t=0) \rangle \\ &= \sum_{n=0}^{+\infty} (-1)^n \left(\frac{t}{\hbar}\right)^{2n} \sum_{k=0}^{2n} \frac{(-1)^k}{k!n!} \langle \psi(t=0) | \hat{H}^k | \psi(t=0) \rangle \langle \psi(t=0) | \hat{H}^{n-k} | \psi(t=0) \rangle \\ &\underset{t \rightarrow 0}{\sim} 1 - \left[ \langle \psi(t=0) | \hat{H}^2 | \psi(t=0) \rangle - \left( \langle \psi(t=0) | \hat{H} | \psi(t=0) \rangle \right)^2 \right] \left(\frac{t}{\hbar}\right)^2. \end{aligned} \quad (\text{II.7})$$

The Zeno time  $t_Z$  is then obtained by comparison of (II.6) with (II.7).

In quantum electrodynamics, theorists often focus on computing transition rates, for instance that of the decay of

an electron from an excited atomic level to a less energetic level. It is then implied that one considers the decay to be exponential (and, at intermediate times, linear). We endeavoured to examine, focusing on the problem of spontaneous emission, why this approach is so successful, in spite of its discrepancy with the short-time dynamics of quantum systems.

Chapter 5 gives a first impression of quantum decay through simple treatments of nuclear  $\alpha$  decay and cavity quantum electrodynamics. By studying such simple systems, we pave the way for ourselves in view of tackling the more involved quantum electrodynamic theory, which we understand here as the study of interactions between quantised light and atoms. Much of the complexity of quantum electrodynamics comes from the features of the quantised electromagnetic field, which we studied at length in chapters 1, 2 and 3. With both this and some of the key features of interacting and/or open systems discussed in chapter 5, we can hope that quantum electrodynamics will come somewhat naturally.

In chapter 6, we focus on the short-time aspects of the spontaneous emission of light by atomic hydrogen. Using the exact expression for the coupling between the decaying electron and the electromagnetic field, we discuss the relevance of the usual dipole approximation, which consists in considering that the electron emits light not from its own position, but rather from that of the nucleus to which it is bound. As announced above, we also inspect the relevance of Fermi's golden rule which predicts a linear time-decay but is known to be inaccurate for very short times.

We further investigate spontaneous emission in the final chapter 7 of this manuscript, where we shift the focus to the electromagnetic field emitted by the atomic transition studied in chapter 6. The photon wave function, introduced in chapter 3, is a particularly fitting quantity to consider in that framework. We refine the standard treatments of this problem of the propagation of spontaneously emitted light and keep the treatment as rigorous as possible.

# REFERENCES

---

## Books

- [1] R.G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, 1966) (cit. on p. 119).

## Articles

- [2] K.O. Friedrichs, 'On the Perturbation of Continuous Spectra', *Commun. Pure Appl. Math.* **1**, 361 (1948) (cit. on p. 119).

## Theses

- [3] R. Grummt, *On the Time-Dependent Analysis of Gamow Decay*, Diplomarbeit Thesis (Ludvig-Maximilians-Universität München, 2009) (cit. on p. 119).
- [4] P. Facchi, *Quantum Time Evolution: Free and Controlled Dynamics*, PhD Thesis (Università degli Studi di Bari, 2000) (cit. on p. 120).

## CHAPTER 5

---

# SIMPLE INTERACTING SYSTEMS

---

*“Physics: A very male kind of science, all mathematics-driven and cold, all about taking things apart and staring at the pieces. Haunt of rude abusive sarcastic people [...]”*

Part of the “Physics” entry in The Dictionary of Fashionable Nonsense—A Guide for Edgy People, by Ophelia Benson and Jeremy Stangroom (Souvenir Press, 2004)

Before proceeding on—or returning—to quantum electrodynamics, we present and study two simple but instructive models of interacting quantum systems. The first model (see sect. 5.1) is concerned with radioactive nuclear decay, especially  $\alpha$  decay. With simple analytical arguments and numerical investigations, we examine the relevance of the famous Gamow model for  $\alpha$  radioactivity. The second model, which is an illustration of the so-called two-level Friedrichs model studied in sect. 5.2, gives a simple description of cavity quantum electrodynamics [8], for example experiments carried out by Serge Haroche and his team at ÉNS in Paris [9]. With this simple model, we discuss in sect. 5.3 such issues as decoherence and light propagation from the cavity, the latter topic anticipating on chapter 7.

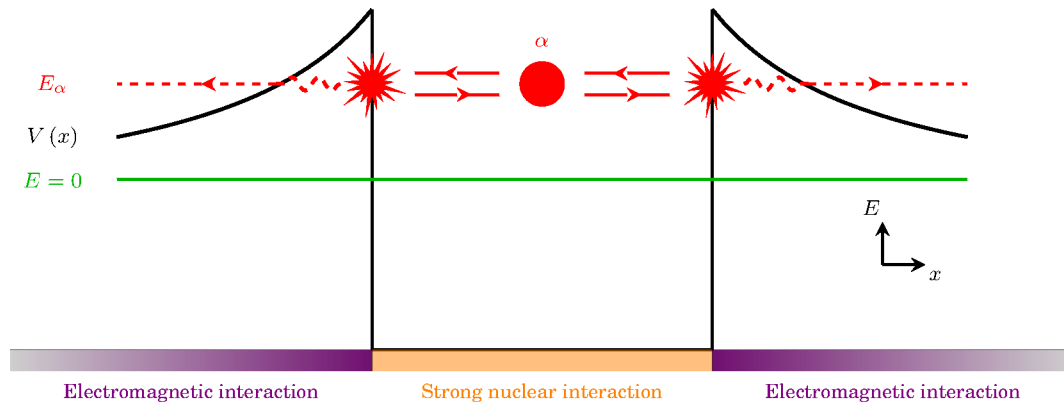
---

### Contents of the Chapter

5.1	Nuclear decay and Gamow states . . . . .	125
5.1.1	The Gamow model for $\alpha$ radioactivity . . . . .	125
5.1.2	Numerical simulations and the perfectly matched layer method . . . . .	126
5.1.3	On the validity of the Gamow model . . . . .	127
5.1.3.1	Numerical results . . . . .	127
5.1.3.2	Gamow vectors of the problem . . . . .	129
5.1.3.3	A simple argument in favour of Gamow’s expression for the decay constant . . . . .	129
5.2	On the two-level Friedrichs model . . . . .	130
5.2.1	From the Gamow model to the Friedrichs model . . . . .	130
5.2.2	Friedrichs coupling as a jump operator . . . . .	131
5.2.3	Time-dependent perturbation theory . . . . .	132
5.2.3.1	Equations of motion . . . . .	132
5.2.3.2	The Wigner-Weisskopf approximation . . . . .	132
5.3	A toy-model for the description of losses in cavity quantum electrodynamics . . . . .	134
5.3.1	Friedrichs model for cavity quantum electrodynamics . . . . .	134
5.3.2	Evolution of a single-photon cavity state . . . . .	135
5.3.3	Decoherence and pointer states of a quantum electrodynamical cavity . . . . .	136

5.3.3.1	Some elementary notions on decoherence . . . . .	136
5.3.3.2	Disentangled evolution for coherent states . . . . .	137
5.3.3.3	On the Lindblad master equation . . . . .	138
5.3.4	Photon propagation from the cavity . . . . .	139
5.A	Quantum scattering: complex poles and their eigenfunctions . . . . .	141

---



**Fig. 5.1.1** – Visualisation of the Gamow model. The potential is purely strong force-induced in the central zone, and purely electrostatic outside the strong force range.

## 5.1 Nuclear decay and Gamow states

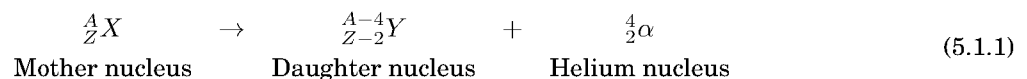
In this section we focus on radioactive nuclear  $\alpha$  decay, for which Gamow proposed a model [10–12] in the late 1920s. Gamow’s work was groundbreaking in the sense that he was the first to make use of the then-brand new quantum theory to study radioactive decay. Though approximate, his model yielded predictions reasonably close to experimental results, which constituted an important success for quantum theory.

### 5.1.1 The Gamow model for $\alpha$ radioactivity

*“Slow decay, I won’t stop fighting you!”*

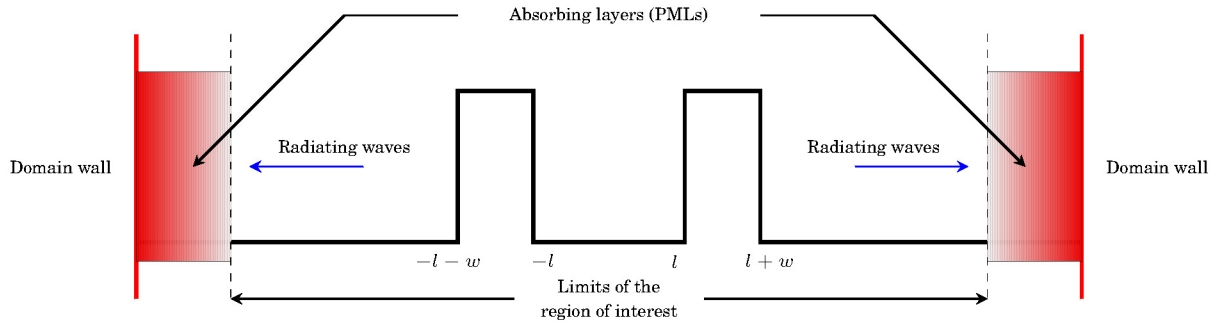
Interpol’s Paul Banks in “Who Do You Think”, **Our Love to Admire** (Capitol, 2007)

Nuclear disintegrations of the  $\alpha$  type



occur in heavy nuclei. At the nuclear scale, quantum mechanics must be used. Gamow [10–12] proposed a simple quantum model for  $\alpha$  radioactivity: within the mother nucleus, the  $\alpha$  particle is a quantum mechanical particle which “sees” the potential created by the other part of the mother nucleus, namely the daughter nucleus. Since all the objects featured in this process are charged, electromagnetic interactions are taken into account. Also, since the mother, daughter, and Helium nuclei are made of protons and neutrons, the strong nuclear interaction plays a major part here. The strong nuclear interaction is attractive but short-ranged, while the electromagnetic (Coulomb) interaction is repulsive—all the nuclei are positively charged—and long-ranged, but negligible with respect to the strong force at short distances. The total potential is assumed to have the profile drawn in Fig. 5.1.1. It is attractive at short distances and repulsive at long distances. Barriers separate these two regions of space. The energy  $E_\alpha$  of the  $\alpha$  particle is considered to be lower than the barrier height, so that it is in a “quasi-bound” state, but high enough so that it can tunnel through the Coulomb barrier towards the outside world. The situation is schematically represented in Fig. 5.1.1. Note that we will consider a one-dimensional system here.

In the framework of the Gamow model, one takes for granted that the time decay is exponential. That is to say, one considers that, for an  $\alpha$ -radioactive sample initially consisting of  $N(t=0)$  nuclei, the number of nuclei which are yet to decay at time  $t$  is  $N(t) = N(t=0) \exp(-\Gamma_G t)$ . The goal is then to find the decay constant  $\Gamma_G$ . To this end,



**Fig. 5.1.2** – Layout of the double potential barrier system within the PML framework. Near the domain walls, absorbing layers are artificially added into the program to avoid reflections.

one writes it [1] as a product of two factors

$$\Gamma_G = f T \quad (5.1.2)$$

where

- $f$  is the classical collision frequency between the  $\alpha$  particle and the potential barrier created by the daughter nucleus. If we denote by  $R_0$  the radius of the daughter nucleus and  $v_\alpha$  the velocity of the Helium nucleus ( $\alpha$  particle), then we make the approximation

$$f = \frac{v_\alpha}{2R_0}, \quad (5.1.3)$$

- $T$  is the tunneling probability through the potential barrier.

This can be summed up informally in the following way: the  $\alpha$  particle oscillates back and forth inside the potential well, every now and then it hits the barrier and a small part of the wave function is transmitted through the barrier (see Fig. 5.1.1). This seems reasonable at first sight, and even at second sight since it allows to derive [1] the empirical Geiger-Nuttall law

$$\log \Gamma_G = \text{cst} - \frac{Z-2}{\sqrt{E_\alpha}} \quad (5.1.4)$$

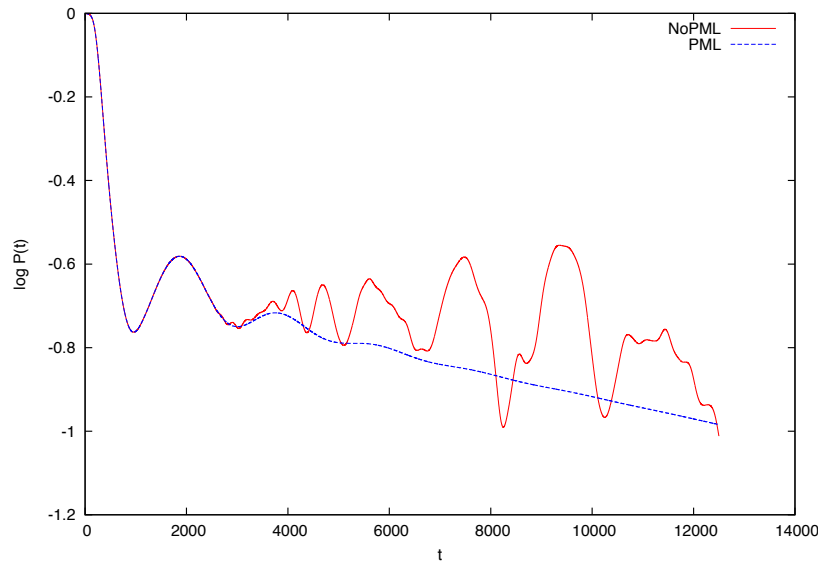
where  $E_\alpha$  is the energy of the  $\alpha$  particle and, as seen from (5.1.1),  $Z-2$  is the atomic number of the daughter nucleus. But we shall see in sect. 5.1.3 that the ansatz (5.1.2) is in fact highly questionable. In particular, the picture of a particle bouncing back and forth provided by (5.1.3) is at best misleading and eventually dispensable.

## 5.1.2 Numerical simulations and the perfectly matched layer method

The system that we studied as a simplified version of the Gamow potential of Fig. 5.1.1 is the so-called **double potential barrier**, sketched in Fig. 5.1.2. It features two potential barriers of height  $V_0$  situated between  $-l-w$  and  $-l$ , and  $l$  and  $l+w$  respectively. We were interested in the decay of a wave packet initially confined between the barriers. A natural quantity to consider in order to monitor the decay is the nonescape probability

$$P_{\text{nonesc}}(t) \equiv \int_{-l}^l dx |\psi(x, t)|^2. \quad (5.1.5)$$

To solve the Schrödinger equation numerically, space and time are discretised, keeping in mind the stability conditions of the finite-difference time-domain algorithm [29]. A problem in such numerical calculations is that one is condemned to work in limited space. Since we are interested in decaying states, that is, states for which the wave function spreads with time, this is particularly bothersome: sooner or later, the wave function is bound to be reflected off the domain walls and propagate its way back into the zone of interest. To tame these unphysical reflections, we use a well known method in computational electromagnetism, the perfectly matched layer (PML)



**Fig. 5.1.3** – Logarithm of the nonescape probability plotted against time without (red solid line) and with (blue dashed line) absorbing layers. We clearly see artifacts in the first case. These are due to reflections of the wave function off the domain limits. When we add the absorbing layer, these reflections disappear.

method. This method is based on complex coordinate stretching in the absorbing zone [13–16]. Radiating waves are oscillating in  $x$ , but if we analytically continue the wave equation and thus its solutions in the complex plane, the radiating waves will be exponentially decaying in the regions where the coordinate stretching was performed, that is, in the absorbing layers (see Fig. 5.1.2). This coordinate stretching can be written in the following way:

$$x \rightarrow \tilde{x} = (1 + i\eta(x))x$$

where  $\eta$  is a real function of the real argument  $x$ , and vanishes everywhere except in the absorbing layers. We then have to solve the Schrödinger equation for the stretched variable  $\tilde{x}$ . The Laplacian operator takes the form

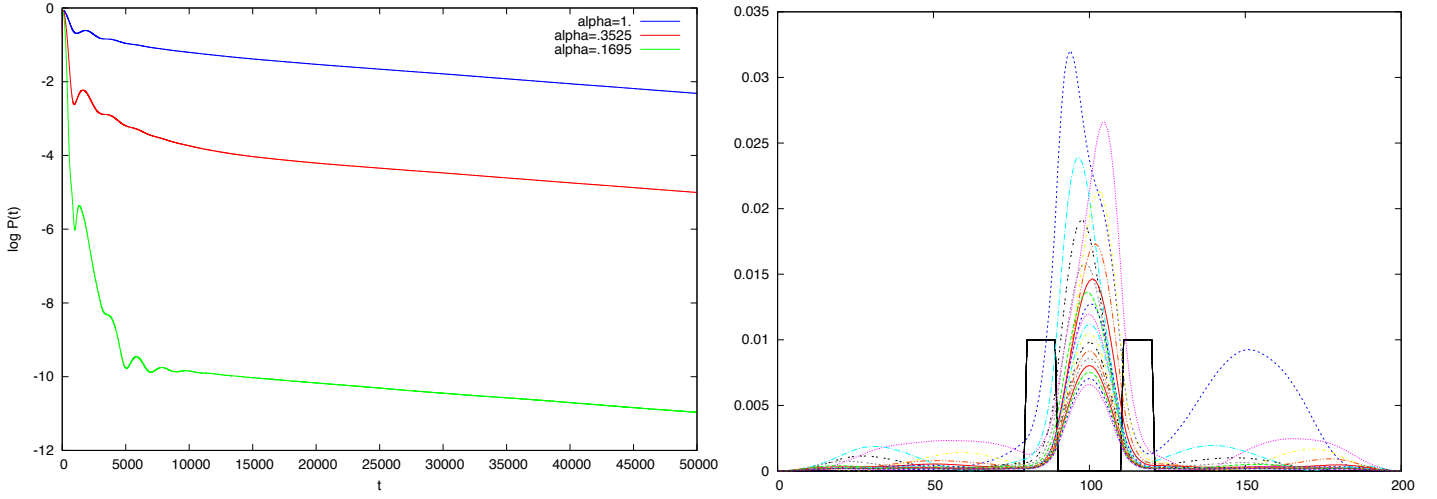
$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \rightarrow & -\frac{\hbar^2}{2m} \frac{1}{(1 + \eta^2(x))^2} \left[ (3 - \eta^2(x)) \left( -\frac{\eta(x)}{(1 + \eta^2(x))} \frac{d\eta}{dx} \frac{\partial}{\partial x} \right) \right. \\ & \left. + i(1 - 3\eta(x)) \left( -\frac{\eta(x)}{1 + \eta^2(x)} \frac{d\eta}{dx} \frac{\partial}{\partial x} \right) + (1 - \eta^2(x) - 2i\eta(x)) \frac{\partial^2}{\partial x^2} \right]. \end{aligned}$$

We can then discretise the Schrödinger equation written with this new, analytically continued Laplacian operator, and solve it numerically. To illustrate the efficiency of the PML method, we plotted the evolution of the logarithm of the nonescape probability (5.1.5) with time. Fig. 5.1.3 displays the results obtained without any treatment of the reflections and the results yielded by the PML method. In the absence of absorbing layers there is what could be called a “revival” of the wave after  $t \sim 2.5 \times 10^3$  timesteps. To make sure these large oscillations are indeed due to reflections, we performed a series of tests, including increasing the phase velocity of the Schrödinger wave, and increasing the size of the computation domain so that the walls are farther away from the double barrier. All these tests conclusively showed that, in the absence of PMLs, the wave function is indeed bouncing off the domain walls and reentering the well.

### 5.1.3 On the validity of the Gamow model

In this section we endeavour to test, through numerical simulations, the relevance of the “bouncing  $\alpha$  particle” picture provided by the Gamow model.





(a) Logarithm of the nonescape probability plotted against time for different values of the kinetic energy  $E_K$ . The initial states are given by  $k_0 = \pi/(2l)$  ( $\alpha = 1$ ),  $k_0 = 2\pi/(2l)$  ( $\alpha = 0.3525$ ),  $k_0 = 3\pi/(2l)$  ( $\alpha = 0.1695$ ), and  $\sigma = (2l)/2.5$  for all states (see (5.1.6)). Short-time behaviours are different but at longer times the decay is identical (and exponential).

(b) Time evolution of the square modulus of the wave function for  $k_0 = \pi/(2l)$  and  $\sigma = (2l)/2.5$  (see (5.1.6)). We see that Gamow's bouncing picture is valid at short times, but that the wave function rapidly becomes a "quasistationary" wave that leaks through the barriers.

Fig. 5.1.4

### 5.1.3.1 Numerical results

We start by taking the initial state of the particle to be described in configuration space by a Gaussian wave packet

$$\psi(x, t=0) = (\pi\sigma^2)^{-\frac{1}{4}} e^{-\frac{x^2}{2\sigma^2}} e^{ik_0x} \quad (5.1.6)$$

where the value of  $\sigma$  is taken so as to confine the initial state between the barriers. The kinetic energy  $E_K$  of such a Gaussian wave packet can be calculated by

$$\begin{aligned} E_K &= \langle \psi(t=0) | \frac{\hat{P}^2}{2m} | \psi(t=0) \rangle \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \frac{\hbar^2 k^2}{2m} |\bar{\psi}(k, t=0)|^2 \\ &= \frac{\hbar^2}{2m} \left( k_0^2 + \frac{1}{\sigma^2} \right). \end{aligned} \quad (5.1.7)$$

Let

$$\alpha \equiv \frac{V_0}{E_K}. \quad (5.1.8)$$

To test the validity of the Gamow model, we simulated the evolution of initially Gaussian states of various kinetic energies  $E_K$ . In Fig. 5.1.4a is plotted the logarithm of the nonescape probability (5.1.5) against time for three different kinetic energies. Though higher energy packets decay much faster at short times, it turns out that at long times, the decay is identical (and exponential) for all initial states. This means that the decay constant is independent of the kinetic energy, and solely depends on the potential profile which the particle evolves in. This seems to be a hard blow dealt at the Gamow model, since we expect the collision frequency, by way of the velocity of the particle, to depend on the "input" energy (see (5.1.3)).

However, it appears that the Gamow model remains accurate if we use it wisely, that is, if we focus on the specifications of the state at long times, the wave vector of which can be roughly taken to be equal to  $k_{\text{final}} = \pi/(2l)$ ,

as is motivated by the shape of the wave function at long times (see Fig. 5.1.4b). Let us for instance consider our system with an initial state given by  $k_0 = \pi/(2l)$  and  $\alpha = 1$ . The mass of the particle is taken to be equal to the electron mass<sup>1</sup>  $m_e = 9.109 \times 10^{-31}$  kg. From the numerical simulations, we obtain the decay rate  $\Gamma_{\text{num}} = 1.077 \times 10^{17} \text{ s}^{-1}$ . We can compare this with the results from the Gamow ansatz (5.1.2). In order to compute the collision frequency, we make use of the one-dimensional de Broglie identity  $p = \hbar k$  (with wave vector  $k_{\text{final}} = \pi/(2l)$ ). We use the expression [2]

$$T = \frac{1}{1 - \frac{\alpha^2}{4(1-\alpha)} \sinh^2(kw)} \quad (5.1.9)$$

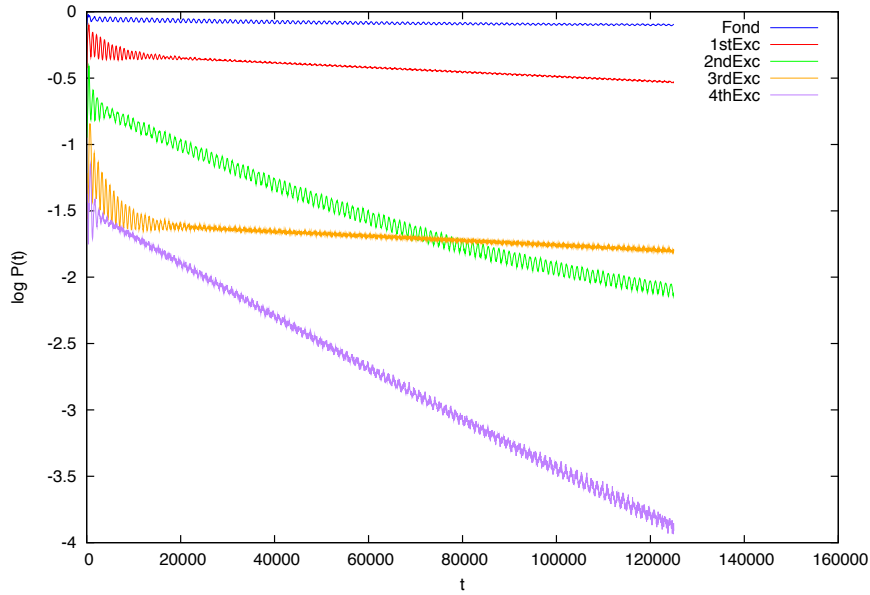
for the intensity transmission coefficient for a square potential barrier to finally obtain  $\Gamma_G = 1.868 \times 10^{17} \text{ s}^{-1}$ , which is fairly close to the direct numerical result. Another similar calculation, this time with  $\alpha = 5$ —that is, much higher barriers—gives us a Gamow decay constant of  $\Gamma_G = 3.145 \times 10^{14} \text{ s}^{-1}$  to compare to the direct numerical result  $\Gamma_{\text{num}} = 5.511 \times 10^{14} \text{ s}^{-1}$ . This good agreement shows that, when carefully used, the Gamow model can give a fair approximation of the decay constant. The key step is to forget about the specifications of the initial state, and especially about its energy, and to focus on the final, exponentially decaying state (which is the state the characteristics of which are accessible to the experimentalist who verifies the Geiger-Nuttal law). As a matter of fact, for fixed barrier height, we at first always observed the same final state, *i.e.* the same decay constant. This leads us to the more formal topic of Gamow functions and complex poles.

### 5.1.3.2 Gamow vectors of the problem

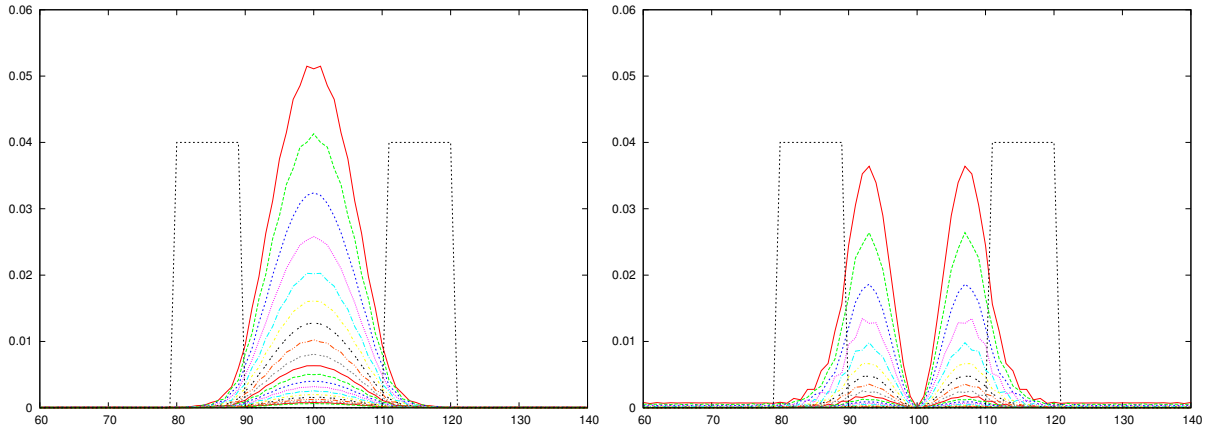
The complex pole approach—which we present in the appendix 5.A to this chapter—consists in finding the normalised generalised eigenfunctions of the system, which have poles in the complex  $k$ -plane. Denoting such a pole as  $k_n$ , we obtain, through the dispersion relation  $E_n = (\hbar k_n)^2 / (2m)$ , a complex energy. The real part of  $E_n$  corresponds, as usual, to an angular frequency, while the imaginary part corresponds to the inverse of the lifetime of the corresponding eigenfunction. This approach explains why we always observed the same decay rate for our system when entering naive initial states: since the normalised generalised eigenfunctions form a basis, our Gaussian wave packets (5.1.6) were superpositions of Gamow states corresponding to various poles, and only the component of our initial state “along” the longest-lived Gamow state survived at long times. Using the tetrachotomy algorithm [27] to find poles in the complex  $k$ -plane, we were able to find other Gamow states and thus to observe other decay constants. This is shown in Fig. 5.1.5. We see that as announced in [17], the complex pole approach only gives accurate results for long-lived states, that is, for poles associated to eigenenergies with small imaginary part. Subsequent (shorter-lived) Gamow states are less accurately described, that is, they do not necessarily behave differently from the first two Gamow states at long times. In Fig. 5.1.6 we plot the time evolution of the two longest-lived Gamow states. We find that, accordingly to what is inferred in [17], their space-dependence inside and between the barriers is time-invariant and that they simply “melt” with time. These Gamow states can thus be seen as leaky eigenmodes of the system for which the time-dependence can be factored out of a time-independent spatial envelope (see (5.1.10)). Note that they resemble the modes of an infinite potential well.

The complex pole approach of [17] (see appendix 5.A) gives the lifetime of radioactive uranium 234 (for which the mass of the moving particle, a Helium nucleus, is  $m = 6.69 \times 10^{-27}$  kg, the distance  $2l$  between the two barriers is twice the radius  $l = 7.2 \times 10^{-15}$  m of the uranium nucleus, and the width of the barriers is taken [17] to be  $w = 1.44 \times 10^{-14}$  m) with good accuracy: the experimental decay rate is  $\Gamma_{\text{exp}} = 2.5872 \times 10^{-13} \text{ s}^{-1}$ ,

<sup>1</sup>See the next sect. 5.1.3.2 for a discussion of radioactive decay in uranium 234, a system closer to the spirit of Gamow’s investigations.



**Fig. 5.1.5** – Plots of the logarithm of the nonescape probability against time for the first five Gamow states.



**Fig. 5.1.6** – Time evolution of the square modulus of the wave function for the longest-lived (left) and next-to-longest-lived (right) Gamow states. We see that the space-dependence of the wave function in the central region is stationary and that the wave leaks through the barriers.

while the fitted theoretical value is  $\Gamma_{\text{pole}} = 2.6722 \times 10^{-13} \text{ s}^{-1}$ . Using the same pole to compute the decay rate in the Gamow approach (5.1.2) yields a bouncing frequency of  $f = 1.138 \times 10^{21} \text{ s}^{-1}$  and a tunneling probability of  $T = 2.751 \times 10^{-34}$ , which means that  $\Gamma_G = 3.130 \times 10^{-13} \text{ s}^{-1}$ , a fairly good approximation to the experimental value. We were unable to conduct numerical simulations for this system, since the stability requirements [29] of the finite-difference time-domain algorithm forbade us to increase the numerical time step as needed.

### 5.1.3.3 A simple argument in favour of Gamow’s expression for the decay constant

Since the picture of a particle that bounces back and forth between the barriers proved rather irrelevant—the “final state” tends to be an (almost) standing wave which leaks through the barriers—one might wonder why it yields such “accurate” results. In order to explain this, we propose the following argument: at sufficiently long times, and in the central region ( $x \in [-l - w, l + w]$ ), we can write the wave function as

$$\psi(x, t) = \varphi(x) e^{(i\omega - \frac{\Gamma}{2})t}. \quad (5.1.10)$$

It is then easily checked that

$$\Gamma = \frac{\frac{d}{dt} \int_{-l-w}^{l+w} dx |\psi(x, t)|^2}{\int_{-l-w}^{l+w} dx |\psi(x, t)|^2}.$$

Making use of the probability conservation equation yields

$$\Gamma = \frac{j(l+w, t) - j(-l-w, t)}{\int_{-l-w}^{l+w} dx |\psi(x, t)|^2}$$

where the probability current is given by

$$j(x, t) = \frac{\hbar}{2mi} \left[ \psi^*(x, t) \frac{\partial \psi}{\partial x}(x, t) - \psi(x, t) \frac{\partial \psi^*}{\partial x}(x, t) \right]. \quad (5.1.11)$$

The wave function is purely outgoing at the interface between the potential barrier and the outside world, that is, at  $x = \pm(l+w)$ , which allows us to write

$$\psi(-l-w, t) = A_- e^{ik(l+w)} e^{(i\omega - \frac{\Gamma}{2})t} \quad (5.1.12a)$$

$$\psi(l+w, t) = A_+ e^{ik(l+w)} e^{(i\omega - \frac{\Gamma}{2})t} \quad (5.1.12b)$$

and finally yields

$$\Gamma = \frac{\hbar k}{2m(l+w)} \frac{|A_+|^2 + |A_-|^2}{\langle |\varphi|^2 \rangle_{\text{within}}} \quad (5.1.13)$$

where  $\langle \cdot \rangle_{\text{within}}$  is the average taken over the  $[-l-w, l+w]$  region (see Fig. 5.1.2). The first factor on the right-hand side of (5.1.13) is of particular interest, since it strongly resembles the bouncing frequency of the “semiclassical” Gamow model (see (5.1.3)). As for the second factor, it is reminiscent of a tunneling coefficient, which links the intensity of the wave function at the outer end of the barrier to the intensity of the wave function at its inner end.

## 5.2 On the two-level Friedrichs model

### 5.2.1 From the Gamow model to the Friedrichs model

The strong prevalence of a single Gamow state—as far as the lifetime of the system is concerned—suggests a simple rewriting of the problem: we can consider that the state of the Gamow particle belongs to a Hilbert space  $\mathcal{H}$  that has a tensor product structure:  $\mathcal{H} = \mathcal{H}_{\text{in}} \otimes \mathcal{H}_{\text{out}}$  where  $\mathcal{H}_{\text{in}}$  is two-dimensional and allows to describe the presence or the absence of the Gamow particle in the longest-lived Gamow state, while  $\mathcal{H}_{\text{out}}$  is infinite-dimensional (and allows to describe which modes of free space the Gamow particle occupies). In the Gamow model the natural structure of the Hilbert space  $\mathcal{H}$  is given by  $\mathcal{H} = \mathcal{H}_{\text{in}} \oplus \mathcal{H}_{\text{out}}$ , but this is not a problem. Indeed, for the direct sum structure we write

$$\langle x | \psi^{(i)} \rangle = \psi_{\text{in}}^{(i)}(x) \mathbb{1}_{\text{in}}(x) + \psi_{\text{out}}^{(i)}(x) \mathbb{1}_{\text{out}}(x) \quad (5.2.1)$$

where  $\mathbb{1}_{\text{in}}$  and  $\mathbb{1}_{\text{out}}$  are indicator functions for the in and out regions respectively, and the dot product is given by

$$\langle \psi^{(1)} | \psi^{(2)} \rangle = \langle \psi_{\text{in}}^{(1)} \mathbb{1}_{\text{in}} | \psi_{\text{in}}^{(2)} \mathbb{1}_{\text{in}} \rangle + \langle \psi_{\text{out}}^{(1)} \mathbb{1}_{\text{out}} | \psi_{\text{out}}^{(2)} \mathbb{1}_{\text{out}} \rangle. \quad (5.2.2)$$

For the tensor product structure, we write

$$|\psi^{(i)}\rangle = |\psi_{\text{in}}^{(i)}\rangle \otimes |0_{\text{out}}\rangle + |0_{\text{in}}\rangle \otimes |\psi_{\text{out}}^{(i)}\rangle \quad (5.2.3)$$

where the vacuum states  $|0_{\text{in/out}}\rangle$  are normalised states. It is then readily found that we get the same expression as (5.2.2) for the dot product. We thus adopt this tensor product structure, which constitutes the basis for the Friedrichs model [18]. Notice that our system is now a two-level quantum well coupled with the infinitely many modes of the outside world. To some extent, it is similar to the model for atom-field interaction presented and studied in chapter 6.

In the rest of the present section we adopt this more general framework, corresponding to the two-level Friedrichs model, which describes a two-level system coupled to a large number of environmental degrees of freedom. For such systems we write the quantum state as

$$|\psi(t)\rangle = \alpha(t) |1_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle + \int d\omega(k) \beta(k,t) |0_{\text{in}}\rangle \otimes |\omega(k)_{\text{out}}\rangle. \quad (5.2.4)$$

## 5.2.2 Friedrichs coupling as a jump operator

We write the following Hamiltonian for the system:

$$\begin{aligned} \hat{H} = & \hbar\omega_0 |1_{\text{in}}\rangle\langle 1_{\text{in}}| \otimes \hat{\mathbb{1}}_{\text{out}} + \hat{\mathbb{1}}_{\text{in}} \otimes \int d\omega(k) \hbar |\omega(k)_{\text{out}}\rangle\langle \omega(k)_{\text{out}}| \\ & + \int d\omega(k) [\lambda(\omega(k)) |0_{\text{in}}\rangle\langle 1_{\text{in}}| \otimes |\omega(k)_{\text{out}}\rangle\langle 0_{\text{out}}| + \lambda^*(\omega(k)) |1_{\text{in}}\rangle\langle 0_{\text{in}}| \otimes |0_{\text{out}}\rangle\langle \omega(k)_{\text{out}}|]. \end{aligned} \quad (5.2.5)$$

The first summand on the right-hand side of (5.2.5) is sometimes called the self-Hamiltonian of the system and describes the dynamics of the two-level system in the absence of any environment, while the second summand mirrors that paradigm for environmental degrees of freedom. The last integral on the right-hand side describes the coupling between the system and its environment. Notice that it features jumps: the operator  $|0_{\text{in}}\rangle\langle 1_{\text{in}}| \otimes |\omega(k)_{\text{out}}\rangle\langle 0_{\text{out}}|$  takes the two-level system from its excited state to its ground state and creates an excitation in the environment, while the action of  $|1_{\text{in}}\rangle\langle 0_{\text{in}}| \otimes |0_{\text{out}}\rangle\langle \omega(k)_{\text{out}}|$  is converse.

Schrödinger infamously declared “If we have to go on with these damned quantum jumps, then I’m sorry that I ever got involved”. The main problem regarding quantum jumps is that—like other collapse processes—they violate unitarity. On the other side, the quantum “jumps” described by our coupling operator

$$\hat{H}_{\text{jump}} = \int d\omega(k) [\lambda(\omega(k)) |0_{\text{in}}\rangle\langle 1_{\text{in}}| \otimes |\omega(k)_{\text{out}}\rangle\langle 0_{\text{out}}| + \lambda^*(\omega(k)) |1_{\text{in}}\rangle\langle 0_{\text{in}}| \otimes |0_{\text{out}}\rangle\langle \omega(k)_{\text{out}}|], \quad (5.2.6)$$

obviously arise in the course of the unitary evolution of the system, since  $\hat{H}_{\text{jump}}$  is part of the (self-adjoint) Hamiltonian of the system. The price we pay for constructing this simple, unitary model, is veering farther from the Gamow model. Indeed, our jump operator (5.2.6) has intrinsically non-local features, since it describes instantaneous jumps through the potential barriers.

At this level we do not make any specifications on the coupling function  $\lambda$ , but it will be useful in the following to ask that it be sufficiently regular in the vicinity of  $\omega_0$ , and also that  $|\lambda(\omega_0)|^2/\hbar^2$  is much smaller than  $\omega_0$ . As we shall see, the latter condition is typical of the regime of Fermi’s golden rule (the so-called weak coupling regime), which is valid when the decay constant  $\Gamma$  is much smaller than the transition frequency  $\omega_0$  of the system. We shall also see that, essentially on energy conservation grounds,  $|\lambda(\omega_0)|^2$  is the important parameter here. For now, we do not take explicit values for the bounds of integrals of the type  $\int d\omega(k)$ . The relevance of those bounds will be commented upon in sect. 5.3.4.

## 5.2.3 Time-dependent perturbation theory

### 5.2.3.1 Equations of motion

Problems defined by (5.2.4) and (5.2.5) are studied through time-dependent perturbation theory. Since our interest is still focused on initially confined states, we choose the initial conditions

$$\begin{cases} \alpha(t=0) &= 1, \\ \forall k \quad \beta(k, t=0) &= 0. \end{cases} \quad (5.2.7)$$

From (5.2.4) and (5.2.5) notice that

$$\begin{aligned} i\hbar \frac{d\alpha}{dt} &= (\langle 1_{\text{in}} | \otimes \langle 0_{\text{out}} |) \hat{H} | \psi(t) \rangle, \\ i\hbar \frac{\partial \beta}{\partial t}(k, t) &= (\langle 0_{\text{in}} | \otimes \langle \omega(k)_{\text{out}} |) \hat{H} | \psi(t) \rangle \end{aligned}$$

to write coupled equations for the coefficients:

$$\begin{aligned} i\hbar \frac{d\alpha}{dt} &= \hbar\omega_0 \alpha(t) + \int d\omega(k) \lambda^*(\omega(k)) \beta(k, t), \\ i\hbar \frac{\partial \beta}{\partial t}(k, t) &= \lambda(\omega(k)) \alpha(t) + \hbar\omega(k) \beta(k, t). \end{aligned}$$

Making use of the initial conditions (5.2.7) yields the following equations [3]

$$\beta(k, t) = -\frac{i}{\hbar} \lambda(\omega(k)) \int_0^t dt' e^{-i\omega(k)(t-t')} \alpha(t'), \quad (5.2.8a)$$

$$\frac{d}{dt} (e^{i\omega_0 t} \alpha(t)) = - \int d\omega(k) \left| \frac{\lambda(\omega(k))}{\hbar} \right|^2 \int_0^t dt' e^{i(\omega_0 - \omega(k))(t-t')} (e^{i\omega_0 t'} \alpha(t')). \quad (5.2.8b)$$

These equations have no known exact solution [4] and must be solved through an approximation technique.

### 5.2.3.2 The Wigner-Weisskopf approximation

Since the self-Hamiltonian of the inside region reads  $\hat{H}_{\text{in}} = \hbar\omega_0 |1_{\text{in}}\rangle\langle 1_{\text{in}}|$ , we assume that  $\alpha$  is the product of an oscillating exponential of frequency  $\omega_0$  with a function  $f$  the variations of which are negligible on a timescale of  $\omega_0^{-1}$ :

$$\alpha(t) = e^{-i\omega_0 t} f(t). \quad (5.2.9)$$

With this ansatz we rewrite (5.2.8b) as

$$\frac{d}{dt} f(t) = - \int d\omega(k) \left| \frac{\lambda(\omega(k))}{\hbar} \right|^2 \int_0^t dt' e^{i(\omega_0 - \omega(k))(t-t')} f(t'). \quad (5.2.10)$$

Notice that for values of  $\omega(k)$  far from  $\omega_0$ , destructive interference between different values of  $t'$  will make the second integral on the right-hand side (5.2.10) approximately vanish, because of the slow variations of  $f$  on timescales of order  $\omega_0^{-1}$ . Accordingly, if  $\lambda(\omega(k))$  is sufficiently regular around  $\lambda(\omega_0)$ , then we can approximate (5.2.10) by

$$\begin{aligned} \frac{d}{dt} f(t) &\simeq - \left| \frac{\lambda(\omega_0)}{\hbar} \right|^2 \int_0^t dt' \int d\omega(k) e^{i(\omega_0 - \omega(k))(t-t')} f(t') \\ &= - \left| \frac{\lambda(\omega_0)}{\hbar} \right|^2 \int_0^t dt' 2\pi \delta(t-t') f(t') \\ &= -\pi \left| \frac{\lambda(\omega_0)}{\hbar} \right|^2 f(t) \end{aligned} \quad (5.2.11)$$

where in the second step we made the approximation that the spectrum of  $\omega(k)$  is the whole real axis, and the last step can be proved to be valid through distribution theory [19]. This refines our ansatz (5.2.9) into the Wigner-Weisskopf exponential approximation

$$\alpha(t) = e^{-i\omega_0 t} e^{-\frac{1}{2}\Lambda t}. \quad (5.2.12)$$

with  $\Lambda \equiv \Gamma + 2i\omega_{\text{LS}}$  a complex-valued number. For (5.2.12) to be compatible with our requirement that the variations of  $f$  be negligible on a time-scale of  $\omega_0^{-1}$ , we should ask that  $|\Lambda| \ll \omega_0$ . Starting again from (5.2.8b) we get the following relation for  $\Lambda$

$$\frac{1}{2}\Lambda = i \int d\omega(k) \left| \frac{\lambda(\omega(k))}{\hbar} \right|^2 \frac{1 - e^{-i(\omega(k) - \omega_0)t} e^{\frac{1}{2}\Lambda t}}{\omega_0 - \omega(k) - \frac{i}{2}\Lambda}. \quad (5.2.13)$$

Clearly, this is not a very satisfactory result at that point, since a time-dependence persists on the right-hand side of (5.2.13) while we have taken  $\Lambda$  to be time-independent. In the weak coupling  $\Lambda/\omega_0 \rightarrow 0$  limit we can use the Plemelj-Sochocki theorem (see appendix 6.A.1, especially the identity (6.A.6)) to write

$$\frac{1}{2}\Lambda = i \int d\omega(k) \left| \frac{\lambda(\omega(k))}{\hbar} \right|^2 \left\{ \text{vp} \left[ \frac{1 - e^{-i(\omega(k) - \omega_0)t}}{\omega_0 - \omega(k)} \right] + i\pi \left( 1 - e^{-i(\omega(k) - \omega_0)t} \right) \delta(\omega_0 - \omega(k)) \right\}. \quad (5.2.14)$$

The second term on the right-hand side of (5.2.14) vanishes. Now, use Euler's expansion of the complex exponential and remember that the cardinal sine is equal to its principal value to write

$$\frac{1}{2}\Lambda = i \int d\omega(k) \left| \frac{\lambda(\omega(k))}{\hbar} \right|^2 \left\{ \text{vp} \left[ \frac{1 - \cos[(\omega(k) - \omega_0)t]}{\omega_0 - \omega(k)} \right] + i \frac{\sin[(\omega(k) - \omega_0)t]}{\omega_0 - \omega(k)} \right\}. \quad (5.2.15)$$

Since the cosine term oscillates rapidly for values of  $\omega(k)$  far from  $\omega_0$ , its contribution to the integral on the right-hand side of (5.2.15) is negligible for these values of  $\omega(k)$ . When  $\omega(k)$  is close to  $\omega_0$  the cosine cancels the 1, but this makes little difference since the principal value already ensures that we forget what happens around  $\omega_0$ . Accordingly we can discard the cosine term altogether [3]. For large times we can use the identity [5]

$$\lim_{a \rightarrow +\infty} \frac{\sin(ax)}{x} = \pi \delta(x). \quad (5.2.16)$$

to define the transition rate

$$\Gamma \equiv 2\pi \frac{|\lambda(\omega_0)|^2}{\hbar^2} \quad (5.2.17)$$

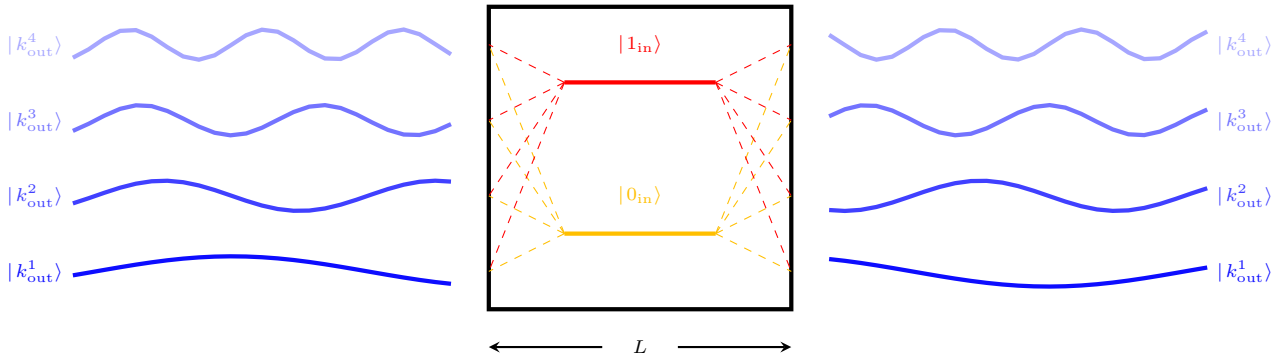
and the Lamb shift

$$\omega_{\text{LS}} \equiv -\frac{1}{\hbar^2} \text{vp} \int d\omega(k) \frac{|\lambda(\omega(k))|^2}{\omega(k) - \omega_0}, \quad (5.2.18)$$

and rewrite (5.2.15) as  $\Lambda = \Gamma + 2i\omega_{\text{LS}}$ . We finally have the following expressions [3] for  $\alpha$  (compare with (5.2.12)) and  $\beta(k, \cdot)$ , the latter being obtained via (5.2.8a):

$$\alpha(t) = e^{-i(\omega_0 + \omega_{\text{LS}})t} e^{-\frac{1}{2}\Gamma t}, \quad (5.2.19a)$$

$$\beta(k, t) = e^{-i\omega(k)t} \frac{\lambda(\omega(k))}{\hbar} \frac{1 - e^{-i(\omega_0 + \omega_{\text{LS}} - \omega(k))t} e^{-\frac{1}{2}\Gamma t}}{\omega(k) - (\omega_0 + \omega_{\text{LS}}) + \frac{i}{2}\Gamma}. \quad (5.2.19b)$$



**Fig. 5.3.1** – Toy-model for cavity quantum electrodynamics. A two-state field inside the box is coupled to the continuum of free space modes that exists outside.

## 5.3 A toy-model for the description of losses in cavity quantum electrodynamics

In cavity quantum electrodynamics experiments, photons are “trapped” in a superconducting cavity. Atoms are injected in that cavity in order to measure the state of the electromagnetic field. The high quality superconducting mirrors which span the inside of the cavity allow for the photons to survive for  $1.3 \times 10^{-1}$  s [9] before they are absorbed by the cavity walls and/or escape the cavity through its openings<sup>2</sup>. The long lifespan of the photons allows experimentalists to accurately—and repeatedly—measure the number of photons that are present inside the cavity. One can thus monitor the time decay of the photon number.

### 5.3.1 Friedrichs model for cavity quantum electrodynamics

In the case of the cavity used by Haroche and his collaborators at ÉNS, the cavity has an open geometry [21]. Such structures have leaky eigenmodes similar to that of the double potential barrier of sect. 5.1. The most important leaky eigenmodes are those that have the longest lifetimes. In the case of [21], two modes have a lifetime of the order of  $1.3 \times 10^{-1}$  s. We propose a very simple, one-dimensional model for this type of cavity, considering that only one cavity mode is relevant, and accounting for its finite lifetime by coupling it to the infinitely many electromagnetic modes of the vacuum (see Fig. 5.3.1).

The electromagnetic field inside the cavity is considered to have states  $|0_{\text{in}}\rangle$  and  $|1_{\text{in}}\rangle$ , and the coupling to the outside will be formally identical to the one defined in sect. 5.2.2, so that the results derived within the framework of the Wigner-Weisskopf approach are immediately relevant here. For the language to be closer to that of quantum electrodynamics, however, we shall make use of ladder operators. We take  $\hat{a}$  and  $\hat{a}^\dagger$  to respectively destroy and create a photon in the longest-lived leaky eigenmode of the cavity, and  $\hat{b}(k)$  and  $\hat{b}^\dagger(k)$  to respectively destroy and create a photon with wave vector  $k$  outside the cavity. In the Schrödinger picture, the equivalent Hamiltonian to (5.2.5) is (introducing the linear dispersion  $\omega(k) = c|k|$  for photons)

$$\hat{H}_S = \hbar\omega_0 \hat{a}_S^\dagger \hat{a}_S \otimes \hat{\mathbb{1}}_{\text{out}} + \hat{\mathbb{1}}_{\text{in}} \otimes \int dk |k| \hbar c \hat{b}_S^\dagger(k) \hat{b}_S(k) + \int dk \left[ \lambda(|k|) \hat{a}_S \hat{b}_S^\dagger(k) + \lambda^*(|k|) \hat{a}_S^\dagger \hat{b}_S(k) \right] \quad (5.3.1)$$

where the Schrödinger picture ladder operators for the cavity ( $\hat{a}_S$  and  $\hat{a}_S^\dagger$ ) and external world ( $\hat{b}_S(k)$  and  $\hat{b}_S^\dagger(k)$ )

<sup>2</sup>It is still, to some extent, an open question, whether absorption by the cavity walls or radiative losses (“escape through the cavity openings”) sets the more stringent limit on that photon lifetime. This was explored through the numerical search for the (leaky) electromagnetic eigenmodes of the Haroche group cavity in [20] and is still under investigation [28].



obey the following commutation relations:

$$\left[ \hat{a}_S, \hat{a}_S^\dagger \right] = \hat{\mathbb{1}}, \quad (5.3.2a)$$

$$\left[ \hat{b}_S(k), \hat{b}_S^\dagger(q) \right] = \delta(k - q) \hat{\mathbb{1}} \quad (5.3.2b)$$

with all other commutators being zero. The positive (negative) wavelength modes propagate in the right (left) outside region and are associated to plane waves  $\mathbb{1}_{\text{rg}} e^{-ikx}$  ( $\mathbb{1}_{\text{lf}} e^{+ikx}$ ), where  $\mathbb{1}_{\text{rg}}$  and  $\mathbb{1}_{\text{lf}}$  are indicator functions for the right and left regions respectively. Introducing the size  $L$  of the cavity, they are simply given by

$$\mathbb{1}_{\text{rg/lf}}(x) = \Theta\left(\pm x - \frac{L}{2}\right). \quad (5.3.3)$$

### 5.3.2 Evolution of a single-photon cavity state

We now switch to the Heisenberg picture. Since the Hamiltonian in the Schrödinger picture has no explicit time dependence, the evolution operator has the standard form  $\hat{U}(t) = \exp\left[-(i/\hbar)\hat{H}_S t\right]$ . The operators in the Heisenberg picture are defined by  $\hat{A}_H(t) \equiv \hat{U}^\dagger(t) \hat{A}_S(t) \hat{U}(t)$  and obey the Heisenberg equations

$$\frac{d\hat{A}_H}{dt} = \frac{i}{\hbar} \left[ \hat{H}_S, \hat{A}_H(t) \right] + \hat{U}^\dagger(t) \frac{d\hat{A}_S}{dt} \hat{U}(t). \quad (5.3.4a)$$

In the case of the ladder operators which are time-independent in the Schrödinger picture, the right-hand side of (5.3.4a) is reduced to the commutator:

$$\frac{d\hat{A}_H}{dt} = \frac{i}{\hbar} \left[ \hat{H}_S, \hat{A}_H(t) \right]. \quad (5.3.4b)$$

From the readily shown equality

$$\left[ \hat{H}_S, \hat{A}_H(t) \right] = \hat{U}^\dagger(t) \left[ \hat{H}_S, \hat{A}_S(t) \right] \hat{U}(t) \quad (5.3.5)$$

one gets the following Heisenberg equations for the ladder operators:

$$\frac{d\hat{a}_H}{dt} = -i\omega_0 \hat{a}_H(t) - \frac{i}{\hbar} \int dk \lambda^*(|k|) \hat{b}_H(k, t), \quad (5.3.6a)$$

$$\frac{\partial \hat{b}_H}{\partial t}(k, t) = -\frac{i}{\hbar} \lambda(|k|) \hat{a}_H(t) - ic|k| \hat{b}_H(k, t) \quad (5.3.6b)$$

and the adjoint evolution equations for the respective adjoint operators. Since  $\hat{a}_H(t=0) = \hat{a}_S$  the Heisenberg equation (5.3.6a) ensures that

$$\hat{a}_H(t) = \alpha(t) \hat{a}_S + \int dk \beta(k, t) \hat{b}_S(k) \quad (5.3.7)$$

is correct at all times. This allows us to rewrite (5.3.6) as

$$\frac{d\alpha}{dt} = -i\omega_0 \alpha(t) - \frac{i}{\hbar} \int dk c \lambda^*(|k|) \beta(k, t), \quad (5.3.8a)$$

$$\frac{\partial \beta}{\partial t}(k, t) = -\frac{i}{\hbar} \lambda(|k|) \alpha(t) - ic|k| \beta(k, t). \quad (5.3.8b)$$

As is clear from  $\hat{a}_H(t) = \hat{U}^\dagger(t) \hat{a}_S \hat{U}(t)$ , the initial conditions are

$$\begin{cases} \alpha(t=0) & = 1, \\ \forall k \quad \beta(k, t=0) & = 0. \end{cases} \quad (5.3.9)$$

When taken into account in the system (5.3.8), these initial conditions yield the following evolution equations:

$$\frac{d}{dt} (e^{i\omega_0 t} \alpha(t)) = - \int dk \left| \frac{\lambda(|k|)}{\hbar} \right|^2 \int_0^t dt' e^{i(\omega_0 - c|k|)(t-t')} (e^{i\omega_0 t'} \alpha(t')), \quad (5.3.10a)$$

$$\beta(k, t) = -\frac{i}{\hbar} \lambda(|k|) \int_0^t dt' e^{-ic|k|(t-t')} \alpha(t'). \quad (5.3.10b)$$

We see that they are strictly equivalent to the Friedrichs evolution equations (5.2.8). We know from sect. 5.2.3.2 an approximate solution to this system. Define the transition rate

$$\Gamma \equiv \frac{2\pi}{c} \frac{|\lambda(\frac{\omega_0}{c})|^2}{\hbar^2} \quad (5.3.11)$$

and the Lamb shift

$$\omega_{\text{LS}} \equiv -\frac{1}{c\hbar^2} \text{vp} \int dk \frac{|\lambda(|k|)|^2}{c|k| - \omega_0}, \quad (5.3.12)$$

to write the following expressions for  $\alpha$  and  $\beta(k, \cdot)$ :

$$\alpha(t) = e^{-i(\omega_0 + \omega_{\text{LS}})t} e^{-\frac{1}{2}\Gamma t}, \quad (5.3.13a)$$

$$\beta(k, t) = e^{-ic|k|t} \frac{\lambda(|k|)}{\hbar} \frac{1 - e^{-i(\omega_0 + \omega_{\text{LS}} - c|k|)t} e^{-\frac{1}{2}\Gamma t}}{c|k| - (\omega_0 + \omega_{\text{LS}}) + \frac{i}{2}\Gamma}. \quad (5.3.13b)$$

From (5.3.7) and (5.3.13) we can directly read the time-evolution of an initially confined photon. In sect. 5.3.3.2 we will extend this to multi-photon states and eventually coherent states.

## 5.3.3 Decoherence and pointer states of a quantum electrodynamical cavity

### 5.3.3.1 Some elementary notions on decoherence

Though its building blocks are quantum and thus obey the superposition principle—a linear combination of solutions to the Schrödinger equation constitutes another valid solution to the Schrödinger equation—the macroscopic world clearly displays a departure from such superpositions. The reason why the macroscopic world does not (directly) obey quantum mechanical laws has been a subject of ongoing debate. The decoherence program is based on the insight that a quantum systems is never isolated [22]: its evolution is at least partly monitored by its environment with which it continuously interacts. The goal of the decoherence program is to build on this insight to explain how the “classical” properties of the macroscopic world can be retrieved from a purely quantum mechanical paradigm at the microscopic level. In this approach, one can show [23, 24] how the interaction between a quantum system and its environment destroys the coherence between a particular set of quantum states, the so-called “pointer states”, which correspond to the “pointer” positions of the macroscopic measurement apparatus, that is, the different outcomes of a macroscopic measurement performed on the system [22].

As is indicated by the fact that they are associated to the outcomes of macroscopic measurements on a system, the so-called quantum pointer states are quasi-classical states of a quantum system. In a nutshell, they are singled out by their robustness to the interaction between the system and its environment, which explains why considerations on pointer states are referred to as “quantum darwinism”. It is well known that, since decoherence is a corollary of entanglement, pointer states of the system can be defined as the states which become minimally entangled with the environment in the course of their evolution [25]. In our model, the inside region plays the part of the system while the outside region is the environment.

### 5.3.3.2 Disentangled evolution for coherent states

Let us write symbolically

$$\beta^*(t) |1_{\text{out}}\rangle \equiv \int d\omega(k) \beta^*(k, t) |\omega(k)_{\text{out}}\rangle. \quad (5.3.14)$$

We know from sect. 5.3.2 that a one-photon cavity state  $|1_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle$  evolves into the linear superposition  $\alpha^*(t) |1_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle + \beta^*(t) |0_{\text{in}}\rangle \otimes |1_{\text{out}}\rangle$ . Thus, we can write the following time-evolution for  $n$  (indistinguishable) photons which we label with the index  $k$ :

$$\begin{aligned} \bigotimes_{k=1}^n (|1_{\text{in}}\rangle_k \otimes |0_{\text{out}}\rangle_k) &\xrightarrow{t} \bigotimes_{k=1}^n (\alpha^*(t) |1_{\text{in}}\rangle_k \otimes |0_{\text{out}}\rangle_k + \beta^*(t) |0_{\text{in}}\rangle_k \otimes |1_{\text{out}}\rangle_k) \\ &= \sum_{j=0}^n (\alpha^*)^j(t) (\beta^*)^{n-j}(t) \sqrt{\frac{n!}{j!(n-j)!}} |j_{\text{in}}\rangle \otimes |(n-j)_{\text{out}}\rangle. \end{aligned} \quad (5.3.15)$$

Indeed the normalised states  $|j_{\text{in}}\rangle \otimes |(n-j)_{\text{out}}\rangle$  are defined by symmetrization over all possible states having  $j$  particles in and  $(n-j)$  particles out. The corresponding nonnormalised states read

$$\begin{aligned} [|j_{\text{in}}\rangle \otimes |(n-j)_{\text{out}}\rangle]_{\text{non}} &\equiv [(|1_{\text{in}}\rangle_1 \otimes |0_{\text{out}}\rangle_1) \otimes \dots \otimes (|1_{\text{in}}\rangle_j \otimes |0_{\text{out}}\rangle_j)] \otimes [(|0_{\text{in}}\rangle_{j+1} \otimes |1_{\text{out}}\rangle_{j+1}) \otimes \dots \otimes (|0_{\text{in}}\rangle_n \otimes |1_{\text{out}}\rangle_n)] \\ &\quad + \text{all other combinations with } j \text{ photons in and } (n-j) \text{ photons out.} \end{aligned}$$

There are  $(n!) / (j!(n-j)!)$  such combinations, which means that

$$|j_{\text{in}}\rangle \otimes |(n-j)_{\text{out}}\rangle = \sqrt{\frac{j!(n-j)!}{n!}} [|j_{\text{in}}\rangle \otimes |(n-j)_{\text{out}}\rangle]_{\text{non}}. \quad (5.3.16)$$

It is straightforward to see that

$$\bigotimes_{k=1}^n (\alpha^*(t) |1_{\text{in}}\rangle_k \otimes |0_{\text{out}}\rangle_k + \beta^*(t) |0_{\text{in}}\rangle_k \otimes |1_{\text{out}}\rangle_k) = \sum_{j=0}^n (\alpha^*)^j(t) (\beta^*)^{n-j}(t) [|j_{\text{in}}\rangle \otimes |(n-j)_{\text{out}}\rangle]_{\text{non}}$$

which along with (5.3.16) proves (5.3.15). In particular, if at time  $t = 0$  the cavity is prepared in a coherent state and the outside world is in its vacuum state, then the evolution (5.3.15) yields coherent states for the outside world. Indeed

$$\begin{aligned} |\psi(t=0)\rangle &= e^{-\frac{|\xi|^2}{2}} \sum_{n=0}^{+\infty} \frac{\xi^n}{\sqrt{n!}} |n_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle \\ \rightarrow |\psi(t)\rangle &= e^{-\frac{|\xi|^2}{2} |\alpha(t)|^2} \sum_{n=0}^{+\infty} \sum_{m=0}^n \frac{(\xi \alpha^*(t))^m}{\sqrt{m!}} |m_{\text{in}}\rangle \otimes e^{-\frac{|\xi|^2}{2} |\beta(t)|^2} \frac{(\xi \beta^*(t))^{n-m}}{\sqrt{(n-m)!}} |(n-m)_{\text{out}}\rangle \end{aligned}$$

where we used the identity  $|\alpha(t)|^2 + |\beta(t)|^2 = 1$ . The state at time  $t$  can be rewritten as

$$|\psi(t)\rangle = e^{-\frac{|\xi|^2}{2} |\alpha(t)|^2} \sum_{k=0}^{+\infty} \frac{(\xi \alpha^*(t))^k}{\sqrt{k!}} |k_{\text{in}}\rangle \otimes e^{-\frac{|\xi|^2}{2} |\beta(t)|^2} \sum_{m=0}^{+\infty} \frac{(\xi \beta^*(t))^m}{\sqrt{m!}} |m_{\text{out}}\rangle. \quad (5.3.17)$$

This establishes that coherent states of the cavity interact with the environment without getting entangled with it. They can thus be considered as ‘‘classical pointers’’ according to the criterion for classicality derived by Zurek in the framework of the quantum darwinist approach.

### 5.3.3.3 On the Lindblad master equation

The Lindblad master equation is a widely used dissipative (*i.e.* nonunitary) equation which models the coherence loss which a quantum system undergoes when it interacts with its environment. It governs the evolution of the reduced density matrix of the system, and, in the case of a quantum electrodynamical cavity (at zero temperature), it reads [6]

$$\frac{d}{dt} \hat{\rho}_{\text{in}}(t) = \frac{1}{i\hbar} \left[ \hat{H}_{\text{eff}}, \hat{\rho}_{\text{in}}(t) \right] + \frac{\Gamma}{2} \left[ 2\hat{a}\hat{\rho}_{\text{in}}(t)\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho}_{\text{in}}(t) - \hat{\rho}_{\text{in}}(t)\hat{a}^\dagger\hat{a} \right] \quad (5.3.18)$$

where  $\hat{H}_{\text{eff}} = \hbar(\omega_0 + \omega_{\text{LS}})\hat{a}^\dagger\hat{a}$  is the renormalised self-Hamiltonian of the system where energy shifts are included. The reduced density matrix reads

$$\hat{\rho}_{\text{in}}(t) \equiv \text{Tr}_{\text{out}}(|\psi(t)\rangle\langle\psi(t)|) \quad (5.3.19)$$

where  $|\psi(t)\rangle$  is simply the state of the full system—that is, the system and its environment—at time  $t$  and the partial trace is taken over the environmental degrees of freedom. A common way to derive the Lindblad master equation is to introduce the so-called quantum Monte-Carlo trajectories. In this framework the derivation can be sketched out as follows: we assume that at time  $t$  the cavity is in a  $n$  photon-Fock state. During the time interval  $[t, t + dt]$ , one elementary excitation of the system is dissipated in the environment with probability  $\Gamma n dt$ , in which case the cavity state at time  $t$  should be replaced by the properly normalised  $(n - 1)$  photon Fock state at time  $t + dt$ . Otherwise (and this happens with probability  $(1 - \Gamma n dt)$ ), no excitation is released, and the state is simply appropriately normalised. The master equation (5.3.18) is then obtained.

We propose here an alternate derivation of the Lindblad master equation. Our proof is based on the well known fact that any damped coherent state of the form

$$|\xi_{\text{in}}(t)\rangle = e^{-\frac{|\xi|^2}{2}|\alpha(t)|^2} \sum_{m=0}^{+\infty} \frac{(\xi\alpha^*(t))^m}{\sqrt{m!}} |m_{\text{in}}\rangle, \quad (5.3.20)$$

with  $\alpha$  given by (5.3.13a), obeys the Lindblad equation (5.3.18). To prove this we write the reduced density matrix when the system is in a coherent state of the form (5.3.17). It is straightforward to see that it reads

$$\hat{\rho}_{\text{in}}(t) = e^{-|\xi\alpha(t)|^2} \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{(\xi\alpha^*(t))^k}{\sqrt{k!}} \frac{(\xi^*\alpha(t))^n}{\sqrt{n!}} |k_{\text{in}}\rangle\langle n_{\text{in}}|. \quad (5.3.21)$$

Compute

$$\frac{d}{dt} \hat{\rho}_{\text{in}}(t) = e^{-|\xi\alpha(t)|^2} \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \left[ -|\xi|^2 \frac{d}{dt} |\alpha(t)|^2 + \left( \frac{k}{\alpha^*(t)} \frac{d\alpha}{dt} + \frac{n}{\alpha(t)} \frac{d\alpha}{dt} \right) \right] \frac{(\xi\alpha^*(t))^k}{\sqrt{k!}} \frac{(\xi^*\alpha(t))^n}{\sqrt{n!}} |k_{\text{in}}\rangle\langle n_{\text{in}}|$$

and use the Wigner-Weisskopf expression (5.3.13a) to get

$$\frac{d}{dt} \hat{\rho}_{\text{in}}(t) = e^{-|\xi\alpha(t)|^2} \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \left[ \Gamma \left( |\xi|^2 |\alpha(t)|^2 - \frac{1}{2}(k+n) \right) - i(\omega_0 + \omega_{\text{LS}})(k-n) \right] \frac{(\xi\alpha^*(t))^k}{\sqrt{k!}} \frac{(\xi^*\alpha(t))^n}{\sqrt{n!}} |k_{\text{in}}\rangle\langle n_{\text{in}}|.$$

We now compare this to the right-hand side of (5.3.18). Recall that  $\hat{H}_{\text{eff}} = \hbar(\omega_0 + \omega_{\text{LS}})\hat{a}^\dagger\hat{a}$  to write

$$\frac{1}{i\hbar} \left[ \hat{H}_{\text{eff}}, \hat{\rho}_{\text{in}}(t) \right] = -i e^{-|\xi\alpha(t)|^2} \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{(\xi\alpha^*(t))^k}{\sqrt{k!}} \frac{(\xi^*\alpha(t))^n}{\sqrt{n!}} (\omega_0 + \omega_{\text{LS}})(k-n) |k_{\text{in}}\rangle\langle n_{\text{in}}|,$$

while

$$\begin{aligned}
2a\hat{\rho}_{\text{in}}(t)\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho}_{\text{in}}(t) - \hat{\rho}_{\text{in}}(t)\hat{a}^\dagger\hat{a} &= e^{-|\xi\alpha(t)|^2} \left[ 2 \sum_{k=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{(\xi\alpha^*(t))^k (\xi^*\alpha(t))^n}{\sqrt{k!} \sqrt{n!}} \sqrt{kn} |(k-1)_{\text{in}}\rangle \langle (n-1)_{\text{in}}| \right. \\
&\quad \left. - \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \left[ \frac{(\xi\alpha^*(t))^k (\xi^*\alpha(t))^n}{\sqrt{k!} \sqrt{n!}} k - \frac{(\xi\alpha^*(t))^k (\xi^*\alpha(t))^n}{\sqrt{k!} \sqrt{n!}} n \right] |k_{\text{in}}\rangle \langle n_{\text{in}}| \right] \\
&= e^{-|\xi\alpha(t)|^2} \sum_{k=0}^{+\infty} \sum_{n=0}^{+\infty} \left[ 2|\xi|^2 |\alpha(t)|^2 - (k+n) \right] \frac{(\xi\alpha^*(t))^k (\xi^*\alpha(t))^n}{\sqrt{k!} \sqrt{n!}} |k_{\text{in}}\rangle \langle n_{\text{in}}|.
\end{aligned}$$

Putting everything together, we see that (5.3.18) is verified for coherent states. An accessible, if slightly qualitative derivation of the Lindblad master equation, is given in terms of Kraus maps in sects. 4.2 and 4.3 of [6]. It is explained that for a master equation to be derived with the help of Kraus maps, the system and environment have to be uncorrelated, or, at least have to have short-lived correlations. This is precisely the case for coherent states of the cavity, since we saw in the previous sect. 5.3.3.2 that they do not entangle with the environment of the cavity. Consequently, they are the states to be used if one is to derive a master equation for this system. Since they solve the Lindblad master equation (5.3.18), it shows that this equation is the valid master equation for our simple model of an electro-dynamical cavity.

### 5.3.4 Photon propagation from the cavity

To present a final result on this model, we get back to the situation in which a single photon is initially present inside the cavity, with no photon outside. The quantum jump operator commutes with the total photon number operator

$$\hat{N} \equiv \hbar\omega_0 \hat{a}_S^\dagger \hat{a}_S \otimes \hat{\mathbb{1}}_{\text{out}} + \hat{\mathbb{1}}_{\text{in}} \otimes \int dk \hat{b}_S^\dagger(k) \hat{b}_S(k) \quad (5.3.22)$$

so that the total photon number is conserved. In particular, if at time  $t = 0$ , the initial state is located inside the cavity

$$|\psi(t=0)\rangle = |1_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle = \hat{a}_S^\dagger |0_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle \quad (5.3.23)$$

then at time  $t$  it will still be a coherent superposition of single-photon states in the in and out regions:

$$\begin{aligned}
|\psi(t)\rangle &= \hat{a}_H^\dagger(t) |0_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle \\
&= \alpha^*(t) \hat{a}_S^\dagger |0_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle + |0_{\text{in}}\rangle \otimes \int dk \beta^*(k, t) \hat{b}_S^\dagger(k) |0_{\text{out}}\rangle \\
&= \alpha^*(t) |1_{\text{in}}\rangle \otimes |0_{\text{out}}\rangle + \beta^*(t) |0_{\text{in}}\rangle \otimes |1_{\text{out}}\rangle
\end{aligned}$$

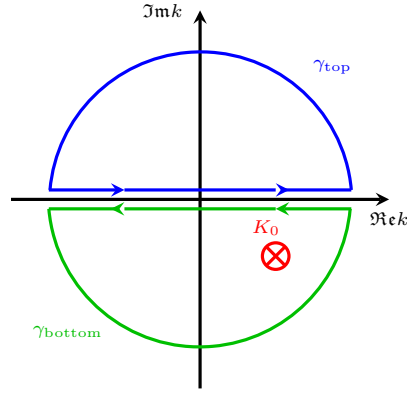
where we wrote, symbolically,

$$\beta^*(t) \hat{b}_S \equiv \int dk \beta^*(k, t) \hat{b}_S^\dagger(k). \quad (5.3.24)$$

Introduce the one-dimensional photon wave function outside the cavity through Glauber's extraction rule (see sect. 3.4)

$$\begin{aligned}
\psi(x, t) &\equiv \mathbb{1}_{\text{rg/lf}}(x) \langle 0_{\text{out}} | \int_a^b dq \hat{b}_S(q) e^{iqx} \int dk \beta^*(k, t) \hat{b}_S^\dagger(k) |0_{\text{out}}\rangle \\
&= \mathbb{1}_{\text{rg/lf}}(x) \int_a^b dk \beta^*(k, t) e^{ikx}.
\end{aligned} \quad (5.3.25)$$

Remember that  $\mathbb{1}_{\text{rg}}$  and  $\mathbb{1}_{\text{lf}}$  are indicator functions for the right and left regions respectively (see (5.3.3)). In these integrals we have  $a = 0$  and  $b = +\infty$  for right-outgoing waves, and  $a = -\infty$  and  $b = 0$  for left-outgoing waves.



**Fig. 5.3.2** – Jordan loops in the complex  $k$ -plane used to compute the integrals (5.3.26). The (isolated) simple pole  $K_0$  (5.3.27) of the integrands is represented by the red circled cross.

Let us introduce the notation  $\bar{\omega}_0 \equiv \omega_0 + \omega_{\text{LS}}$ . From the expression (5.3.13b) of  $\beta(k, \cdot)$  we get, making the usual [7, 26] approximation of extending the integration domain to the whole real line because the main contribution is centred around the pole (which lies close to the positive real axis and far from the origin)

$$\begin{aligned} \psi_{\text{rg/lf}}(x, t) &= \mathbb{1}_{\text{rg/lf}}(x) \int dk \frac{\lambda^*(|k|)}{ck - \bar{\omega}_0 + \frac{i}{2}\Gamma} \left[ e^{ik(x \mp ct)} - e^{i(\bar{\omega}_0 t + kx)} e^{-\frac{1}{2}\Gamma t} \right] \\ &\equiv \mathbb{1}_{\text{rg/lf}}(x) \frac{1}{\sqrt{2\pi}} \left[ I_{\text{rg/lf}}(x \mp ct) - J_{\text{rg/lf}}(x) \right] \end{aligned} \quad (5.3.26)$$

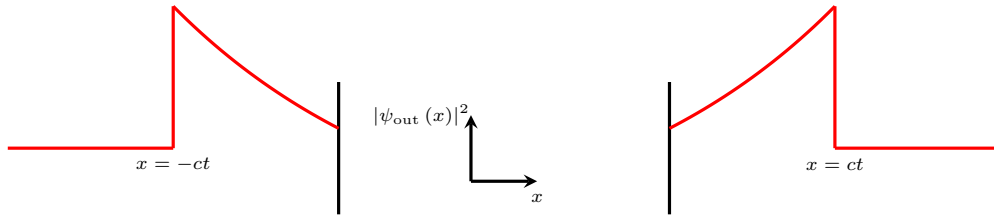
To compute these integrals, we use the Cauchy residue theorem along the Jordan loops drawn on Fig. 5.3.2. We see that the pole  $K_0$  of the integrands is always

$$K_0 = \frac{1}{c} \left[ \bar{\omega}_0 - \frac{i}{2}\Gamma \right]. \quad (5.3.27)$$

Let us first deal with the  $J$ s. We are only interested in  $J_{\text{rg}}(x)$  when  $\mathbb{1}_{\text{rg}}(x)$  does not vanish, that is, when  $x > 0$ . In this case, we use the Jordan loop  $\gamma_{\text{top}}$  and see that  $J_{\text{rg}}(x) = 0$ , which means that this integral never contributes to (5.3.26). With a similar reasoning, we see that  $J_{\text{lf}}(x)$  does not contribute. We now turn to the  $I$ s, and focus on  $I_{\text{rg}}$ . For  $x - ct > 0$ , we use the Jordan loop  $\gamma_{\text{top}}$ , and thus  $I_{\text{rg}}(x - ct)$  vanishes. For  $x - ct < 0$ , we use the Jordan loop  $\gamma_{\text{bottom}}$ . A similar reasoning is valid for  $I_{\text{lf}}$  and we finally get

$$\psi_{\text{rg/lf}}(x, t) = \pm \frac{2i\pi}{\hbar} \mathbb{1}_{\text{rg/lf}}(x) \Theta(ct \mp x) \lambda^* \left( \frac{\bar{\omega}_0}{c} \right) e^{-\frac{i}{c}(\bar{\omega}_0 - \frac{1}{2}\Gamma)(ct \mp x)} \quad (5.3.28)$$

where the value of  $\lambda$  is taken at  $\bar{\omega}_0$  since this function has meaning for real values of the argument only. Thus we see that the wave function is nonvanishing inside the lightcone only. At a fixed time, it increases exponentially—within the lightcone—with increasing  $x$  or  $-x$ , depending on whether we look at what happens on the right or on the left of the cavity (see Fig. 5.3.3). As we see from (5.3.28) photons are mainly localised on a space interval of the order of  $c/\Gamma$ , in agreement with time-energy uncertainties. The propagation of emitted photons is studied in depth in chapter 7. We will learn more about the importance of the approximation we made between (5.3.25) and (5.3.26), namely, the extension of the integration interval. In order to evaluate the strength of the violation of causality when the integration is not extended to the whole real axis, it comes in handy to use the properties of the Breit-Wigner distribution [20]. In the Wigner-Weisskopf framework this distribution is asymptotically reached as an emission spectrum after a time of the order of the lifetime  $1/\Gamma$  of the cavity. Straightforward computations show that the weight of the negative frequencies in this spectrum is equal to the ratio between  $\Gamma$  and  $\omega_0$ . In Haroche's cavity this ratio is of the order of  $10^{-10}$ , which means that causality is very weakly violated.



**Fig. 5.3.3** – Profile of the square modulus of the photon wave function in the outside region at fixed time. It increases exponentially with increasing  $\pm x$  and vanishes outside the lightcone.

## 5.A Quantum scattering: complex poles and their eigenfunctions

Our discussion here follows [17]. We are considering the double barrier system (see sect. 5.1.2 and Figure 5.1.2), for which we want to write the normalised generalised eigenfunctions  $u_{\pm}(k, \cdot)$  (there are two such functions because the Schrödinger equation is a second-order equation with respect to space coordinates). These functions form a basis on which to expand the solutions to the Schrödinger equation:

$$\varphi(x) = \int_0^{+\infty} dk [\bar{\psi}_+(k) u_+(k, x) + \bar{\psi}_-(k) u_-(k, x)] \quad (5.A.1a)$$

$$\text{where } \bar{\psi}_{\pm}(k) \equiv \int_{-\infty}^{+\infty} dx \psi(x) u_{\pm}^*(k, x). \quad (5.A.1b)$$

First, we look for the (nonnormalised) generalised eigenfunctions  $f_{\pm}$ . Since the potential has finite range and is an even function of  $x$ , the ansatz is [17]

$$f_+(k, x) = \begin{cases} a_+(k) e^{ikx} + b_+(k) e^{-ikx} & \forall x \leq -l - w, \\ c_+(k) e^{ikx} & \forall x \geq l + w \end{cases} \quad (5.A.2a)$$

$$f_-(k, x) = \begin{cases} c_-(k) e^{-ikx} & \forall x \leq -l - w, \\ a_-(k) e^{-ikx} + b_-(k) e^{ikx} & \forall x \geq l + w. \end{cases} \quad (5.A.2b)$$

It is natural in order to normalise these eigenfunctions to take  $a_{\pm}(k) = 1$ , however it is not the choice that is made. Instead, we set  $c_{\pm}(k) = 1$  and the normalisation, which has to ensure that

$$\delta(k - q) = \int dx u_{\pm}(k, x) u_{\pm}^*(q, x), \quad (5.A.3)$$

is yielded by the choice

$$u_{\pm}(k, x) = \frac{1}{\sqrt{2\pi}} \frac{f_{\pm}(k, x)}{a(k)} \quad (5.A.4)$$

where  $a_+(k) = a_-(k) \equiv a(k)$  [17]. It is then clear that any zero of  $a$  is a pole of  $u_{\pm}(\cdot, x)$ . As it turns out, the corresponding residue is precisely a Gamow function, *i.e.* a function that satisfies the Schrödinger equation for complex eigenvalue  $\hbar^2 k^2 / (2m)$  as well as plane-wave-like conditions

$$\lim_{x \rightarrow \pm\infty} (G(x) - e^{\pm ikx}) = 0. \quad (5.A.5)$$

This can be shown by the following argument: defining the Wronskian  $W(g, h)$  of two functions  $g$  and  $h$  to be

$$W(g, h)(x) = g(x) \frac{dh}{dx} - \frac{dg}{dx} h(x), \quad (5.A.6)$$

one can readily show from (5.A.2) that  $W_x(f_+, f_-)(k, x) = -2ika(k)$ , so that when  $a$  vanishes (let us call  $\omega$  such a point), so does the Wronskian, which, according to (5.A.6), means that  $f_+(\omega, \cdot)$  and  $f_-(\omega, \cdot)$  are proportional to each other. Taking a look at (5.A.2) and remembering that  $a_+(k) = a_-(k) \equiv a(k)$ , this yields  $b_{\pm}(\omega) = 1$  (remember that we set  $c_{\pm}(k) = 1$ ). Putting everything together, we find that  $f_{\pm}(\omega, \cdot)$  satisfies the plane-wave-like conditions (5.A.5). Since  $f_{\pm}(\omega, \cdot)$  also solves the Schrödinger equation, it is clear that

$$f_{\pm}(\omega, x) = G(x),$$

that is,

$$\text{Res}(u_{\pm}(\cdot, x), \omega) = \eta G(x) \quad (5.A.7)$$

where  $\eta$  is simply a constant. This shows that the search for the complex eigenenergies of the Gamow functions is simply a search for the zeroes of  $a$ . For the double potential barrier system of sect. 5.1,  $a$  can be calculated explicitly using continuity conditions for the wave function [17]: defining

$$q \equiv \sqrt{k^2 - \frac{2m}{\hbar^2} V_0}$$

and

$$A(k) = \cos(qw) - \frac{i}{2} \left( \frac{k}{q} + \frac{q}{k} \right) \sin(qw), \quad (5.A.8)$$

it is given by

$$a(k) = a_1(k) a_2(k) \quad (5.A.9a)$$

$$\text{where } a_{1/2}(k) = e^{ikw} \left( A(k) \mp \frac{i}{2} e^{2ikl} \left( \frac{k}{q} - \frac{q}{k} \right) \sin(qw) \right). \quad (5.A.9b)$$



# REFERENCES

---

## Books

- [1] W.S.C. Williams, *Nuclear and Particle Physics* (Clarendon Press, 1991) (cit. on p. 126).
- [2] A. Messiah, *Mécanique Quantique*, 1st ed., Vol. 1 (Dunod, Paris, 1965) (cit. on p. 128).
- [3] B.G. Englert, *Lectures On Quantum Mechanics*, Vol. 3 (World Scientific, 2006) (cit. on pp. 132, 133).
- [4] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Mécanique Quantique*, 2nd ed., Vol. 2 (Hermann, 1996) (cit. on p. 132).
- [5] W. Appel, *Mathematics for Physics & Physicists*, 1st ed. (Princeton University Press, 2007) (cit. on p. 133).
- [6] S. Haroche and J.M. Raimond, *Exploring the Quantum - Atoms, Cavities and Photons* (Oxford University Press, 2007) (cit. on pp. 138, 139).
- [7] M.O. Scully and M.S. Zubairy, *Quantum Optics* (Cambridge University Press, 1997) (cit. on p. 140).

## Articles

- [8] S. Haroche and D. Kleppner, 'Cavity Quantum Electrodynamics', *Phys. Today* **42**, 24 (1989) (cit. on p. 123).
- [9] S. Gleyzes, S. Kuhr, C. Guerlin, J. Bernu, S. Deléglise, U.B. Hoff, M. Brune, J.M. Raimond and S. Haroche, 'Quantum jumps of light recording the birth and death of a photon in a cavity', *Nature* **446**, 297 (2007) (cit. on pp. 123, 134).
- [10] G. Gamow, 'Zur Quantentheorie des Atomkernes', *Z. Phys.* **51**, 204 (1928) (cit. on p. 125).
- [11] G. Gamow, 'Zur Quantentheorie des radioaktiven Kerns', *Z. Phys.* **52**, 496 (1929) (cit. on p. 125).
- [12] G. Gamow, 'Zur Quantentheorie der Atomzertrümmerung', *Z. Phys.* **52**, 510 (1929) (cit. on p. 125).
- [13] E. Balslev and J.M. Combes, 'Spectral properties of many-body Schrödinger operators with dilatation-analytic interactions', *Comm. Math. Phys.* **22**, 280 (1971) (cit. on p. 127).
- [14] B. Simon, 'Resonances in  $n$ -Body Quantum Systems With Dilatation Analytic Potentials and the Foundations of Time-Dependent Perturbation Theory', *Ann. Math.* **97**, 247 (1973) (cit. on p. 127).
- [15] X. Antoine, A. Arnold, C. Besse, M. Ehrhardt and A. Schädle, 'A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations', *Commun. Comput. Phys.* **4**, 729 (2008) (cit. on p. 127).
- [16] Y. Ould Agha, F. Zolla, A. Nicolet and S. Guenneau, 'On the use of the PML for the computation of leaky modes: an application to gradient index MOF', *COMPEL* **27**, 95 (2008) (cit. on p. 127).
- [17] D. Dürr, R. Grummt and M. Kolb, 'On the time-dependent analysis of Gamow decay', *Eur. J. Phys.* **32**, 1311 (2011) (cit. on pp. 129, 141, 142).

- [18] K.O. Friedrichs, ‘On the Perturbation of Continuous Spectra’, *Commun. Pure Appl. Math.* **1**, 361 (1948) (cit. on p. 131).
- [19] M. Courbage, T. Durt and S.M. Saberi Fathi, ‘Two-level Friedrichs model and kaonic phenomenology’, *Phys. Lett. A* **362**, 100 (2007) (cit. on p. 133).
- [20] V. Debierre, G. Demésy, T. Durt, A. Nicolet, B. Vial and F. Zolla, ‘Absorption in quantum electrodynamic cavities in terms of a quantum jump operator’, *Phys. Rev. A* **90**, 033806 (2014) (cit. on pp. 134, 140).
- [21] S. Kuhr, S. Gleyzes, C. Guerlin, J. Bernu, U.B. Hoff, S. Deléglise, S. Osnaghi, M. Brune, J.M. Raimond, S. Haroche, E. Jacques, P. Bosland and B. Visentin, ‘Ultrahigh finesse Fabry-Pérot superconducting resonator’, *Appl. Phys. Lett.* **90**, 164101 (2007) (cit. on p. 134).
- [22] M. Schlosshauer, ‘Decoherence, the measurement problem, and interpretations of quantum mechanics’, *Rev. Mod. Phys.* **76**, 1267 (2004) (cit. on p. 136).
- [23] W.H. Zurek, ‘Pointer basis of quantum apparatus: Into what mixture does the wave packet collapse?’, *Phys. Rev. D* **24**, 1516 (1981) (cit. on p. 136).
- [24] W.H. Zurek, ‘Decoherence and the Transition from Quantum to Classical’, *Phys. Today* **44**, 36 (1991) (cit. on p. 136).
- [25] J.P. Paz and W.H. Zurek, ‘Quantum Limit of Decoherence: Environment Induced Superselection of Energy Eigenstates’, *Phys. Rev. Lett.* **82**, 5181 (1999) (cit. on p. 137).
- [26] E. Fermi, ‘Quantum Theory of Radiation’, *Rev. Mod. Phys.* **4**, 87 (1932) (cit. on p. 140).

## Theses

- [27] B. Vial, Étude de résonateurs électromagnétiques ouverts par approche modale - Application au filtrage multispectral dans l’infrarouge, PhD Thesis (École Centrale de Marseille, 2013) (cit. on p. 129).
- [28] N. Marsic, Solveurs électromagnétiques éléments finis massivement parallèles, PhD Thesis (Université de Liège, ongoing) (cit. on p. 134).

## Unpublished Articles and Online Notes

- [29] J.R. Nagel, *The One-Dimensional Finite-Difference Time-Domain Algorithm Applied to the Schrödinger Equation*, [http://www.scipy.org/Cookbook/SchrodingerFDTD?action=AttachFile&do=get&target=Schrodinger\\_FDTD\\_new.pdf](http://www.scipy.org/Cookbook/SchrodingerFDTD?action=AttachFile&do=get&target=Schrodinger_FDTD_new.pdf) (cit. on pp. 126, 129).



## CHAPTER 6

---

# TRANSIENT REGIME IN THE ATOM-LIGHT INTERACTION

---

*“Be gone, be gone, be gone your olden ways, be gone!*

*Don’t be afraid of anyone*

*Like seasons, just move on.”*

British Sea Power’s Jan Scott Wilkinson in “Be Gone”, **Open Season** (Rough Trade, 2005)

The description of spontaneous light emission by atomic electrons is a standard topic in quantum electrodynamics and atomic physics. Two main approximations are often made in the treatment. The first one, Fermi’s golden rule, was already briefly discussed in the introduction to the present Part II of this work, as well as in the previous chapter 5. The second one is the dipole approximation which consists [9] in considering that the decaying electron does not emit light from its own position but rather from the position of the nucleus to which it is bound. In this chapter we investigate the validity of the Fermi and dipole approximations in the case of the  $2p - 1s$  transition in atomic Hydrogen. Sect. 6.1 is a quick introduction to nonrelativistic quantum electrodynamics. In sect. 6.2 we examine the pitfalls of the dipole approximation. In sect. 6.3 we show how Fermi’s golden rule emerges from rigorous first order time-dependent perturbation theory. In sect. 6.4 we return to the dipole approximation, and show that when applied learnedly it can be made to be relevant. We conclude in sect. 6.5, and in app. 6.A we briefly derive some results from distribution theory, which we use not only in the present chapter 6 but throughout this work.

---

### Contents of the Chapter

6.1	Interaction of light with nonrelativistic matter . . . . .	147
6.1.1	Electromagnetic fields in the presence of sources . . . . .	147
6.1.2	Standard Hamiltonian for nonrelativistic quantum electrodynamics . . . . .	148
6.1.3	Restriction to the $1s$ and $2p$ levels in atomic Hydrogen . . . . .	149
6.1.4	Matrix element of the interaction Hamiltonian . . . . .	149
6.1.5	Time-dependent perturbation theory at short times and the rotating wave approximation . . . . .	151
6.2	The dipole approximation and its shortcomings . . . . .	154
6.2.1	The approximation and a discussion . . . . .	154
6.2.2	A cutoff-independent regularisation . . . . .	156
6.3	Improving on the dipole approximation: exact atom-field coupling . . . . .	158

6.4	Bonus: the ideal cutoff frequency for the dipole approximation . . . . .	163
6.5	Discussion . . . . .	164
6.A	Some useful results of distribution theory . . . . .	166
6.A.1	The Plemelj-Sochocki theorem . . . . .	166
6.A.2	Fourier transform of the Heaviside step distribution . . . . .	168

---

## 6.1 Interaction of light with nonrelativistic matter

In nonrelativistic quantum electrodynamics, which purports to describe the interaction of light with matter at sufficiently low energies, it is adequate to describe matter by the means of standard, nonrelativistic quantum mechanics. Light, of course, is described by quantum field theory, as discussed at length in chapter 1. The interaction between light and matter then arises as a simple consequence of a request: that the physics of the system be invariant under local gauge transformations, which affect both the scalar and vector potentials of electrodynamics and the wave functions of the charged, massive particles that constitute matter.

### 6.1.1 Electromagnetic fields in the presence of sources

It is well known [1] that in the presence of matter, Maxwell's equations (1.2.17) become

$$\boxed{\partial^\nu \partial_\nu A_\mu - \partial^\nu \partial_\mu A_\nu = \mu_0 J_\mu}. \quad (6.1.1)$$

where  $J^\mu = (c\rho, \mathbf{j})$  is the electric charge density-current four-vector. As was the case in the absence of charges and currents (sources), (6.1.1) is not sufficient to determine  $A_\mu$ : for a solution  $A_\mu$  and an arbitrary function  $\Xi$  of spacetime coordinates we can make the transformation

$$A_\mu \rightarrow A_\mu + \partial_\mu \Xi \equiv \check{A}_\mu \quad (6.1.2)$$

and  $\check{A}_\mu$  is a new solution to (6.1.1). As was the case in chapter 1, this allows us to make a gauge choice. While, in the absence of sources, the Coulomb gauge condition  $A^0 = 0$ ,  $\nabla \cdot \mathbf{A} = 0$  was a valid choice, it is no longer possible here. Indeed, if one made that choice, we would have

$$\begin{aligned} \partial^\nu \partial_\nu A_0 - \partial^\nu \partial_0 A_\nu &= \partial^\nu \partial_\nu A_0 - \partial_0 (\partial^0 A_0 + \nabla \cdot \mathbf{A}) \\ &= 0 \end{aligned} \quad (6.1.3)$$

which is not compatible with Maxwell's equations (6.1.1). Thus the Coulomb gauge condition must be relaxed. Following [2], we waive  $A^0 = 0$  and retain  $\nabla \cdot \mathbf{A} = 0$ . It is then seen from (6.1.1) and (6.1.3) that the scalar potential  $A^0$  obeys the Poisson equation

$$\nabla^2 A^0 + \mu_0 c \rho = 0. \quad (6.1.4)$$

The equation for the vector potential, as also seen from (6.1.1), is

$$\square \mathbf{A} - \nabla \partial_0 A^0 = \mu_0 \mathbf{j}. \quad (6.1.5)$$

It follows from  $\nabla \cdot \mathbf{A} = 0$  that in Fourier space  $\mathbf{k} \cdot \bar{\mathbf{A}} = 0$ . Writing, for a general vector field  $\bar{\mathbf{F}}$  in Fourier space

$$\bar{\mathbf{F}}_{\parallel}(\mathbf{k}) = (\bar{\mathbf{F}}(\mathbf{k}) \cdot \mathbf{k}) \frac{\mathbf{k}}{k^2}, \quad (6.1.6a)$$

$$\bar{\mathbf{F}}_{\perp} = \bar{\mathbf{F}}(\mathbf{k}) - (\bar{\mathbf{F}}(\mathbf{k}) \cdot \mathbf{k}) \frac{\mathbf{k}}{k^2} \quad (6.1.6b)$$

and  $\mathbf{F}_{\parallel}$  (the so-called longitudinal part of  $\mathbf{F}$ ) and  $\mathbf{F}_{\perp}$  (the so-called transverse part of  $\mathbf{F}$ ) their respective inverse Fourier transforms, we immediately see that  $\mathbf{A} = \mathbf{A}_{\perp}$  and hence that (6.1.5) can be decomposed in a longitudinal and a transverse part as follows:

$$-\nabla \partial_0 A^0 = \mu_0 \mathbf{j}_{\parallel}, \quad (6.1.7a)$$

$$\square \mathbf{A}_{\perp} = \mu_0 \mathbf{j}_{\perp}. \quad (6.1.7b)$$

It is easily seen, upon taking its divergence, that (6.1.7a) expresses the conservation of charge when compared with (6.1.4).

## 6.1.2 Standard Hamiltonian for nonrelativistic quantum electrodynamics

In nonrelativistic quantum electrodynamics the Hamiltonian  $\hat{H} = \hat{H}_A + \hat{H}_R + \hat{H}_I$  is a sum of three terms. We write them in Schrödinger's picture here.

- The Hamiltonian  $\hat{H}_A$  of charged matter. Summing over charged particles, it reads

$$\hat{H}_A = \sum_{\alpha} \frac{\hat{\mathbf{p}}_{\alpha}^2}{2m_{\alpha}} + \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha}q_{\beta}}{\|\hat{\mathbf{x}}_{\alpha} - \hat{\mathbf{x}}_{\beta}\|} \quad (6.1.8)$$

where  $\hat{\mathbf{x}}_{\alpha}$  is the position operator for charge  $\alpha$  and  $\hat{\mathbf{p}}_{\alpha}$  is its linear momentum operator. It is the sum of the kinetic energy of the charged particles with their Coulombian interaction energy. If the only two charged particles present in the system are a proton and an electron, then exact solutions exist for the dynamics of this system: these are the wave functions of the Hydrogen atom [3], and it is that case which we will consider in the following.

- The electromagnetic field Hamiltonian  $\hat{H}_R$  which has the same form as in the case of free electrodynamics:

$$\hat{H}_R = \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \hbar c \|\mathbf{k}\| \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}). \quad (6.1.9)$$

- The interaction Hamiltonian  $\hat{H}_I$  which is derived from gauge invariance considerations reads

$$\hat{H}_I = \sum_{\alpha} \left[ -\frac{q_{\alpha}}{m} \hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{A}}(\hat{\mathbf{x}}_{\alpha}, t=0) + \frac{1}{2} \frac{q_{\alpha}^2}{m_{\alpha}} \hat{\mathbf{A}}^2(\hat{\mathbf{x}}_{\alpha}, t=0) \right]. \quad (6.1.10)$$

The Coulomb gauge condition  $\nabla \cdot \mathbf{A} = 0$  implies the usual identity  $\mathbf{k} \cdot \epsilon_{(\lambda)}(\mathbf{k}) = 0$ , which allows us to write  $\hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{A}}(\hat{\mathbf{x}}_{\alpha}, t=0) = \hat{\mathbf{A}}(\hat{\mathbf{x}}_{\alpha}, t=0) \cdot \hat{\mathbf{p}}_{\alpha}$ , hence (6.1.10). The second summand<sup>1</sup> on the right-hand side of (6.1.10) is often neglected because it only comes into play in very strong field situations [2]. We do neglect it ourselves in the following.

The vector potential  $\hat{\mathbf{A}}(\hat{\mathbf{x}}, t)$  is expanded over plane waves as

$$\hat{\mathbf{A}}(\mathbf{x}, t) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \left[ \hat{a}_{(\lambda)}(\mathbf{k}, t) \epsilon_{(\lambda)}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} + \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}, t) \epsilon_{(\lambda)}^*(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}} \right]. \quad (6.1.11)$$

Notice that the time dependence is not known here. This is because the dynamics of interacting systems is generally not solvable, in stark contrast to the free case (see (1.4.30)) where every electromagnetic mode oscillates at its own eigenfrequency. The commutation relation between the photon ladder operators is given in the Schrödinger picture by

$$\left[ \hat{a}_{(\lambda)}(\mathbf{k}, t=0), \hat{a}_{(\lambda)}^{\dagger}(\mathbf{q}, t=0) \right] = 2 \|\mathbf{k}\| (2\pi)^3 \delta(\mathbf{k} - \mathbf{q}) \delta_{\lambda\lambda}. \quad (6.1.12)$$

The electric field operator is given as usual by

$$\hat{\mathbf{E}}(\mathbf{x}, t) = -\nabla \hat{\varphi}(\mathbf{x}, t) - \frac{\partial \hat{\mathbf{A}}(\mathbf{x}, t)}{\partial t} \quad (6.1.13)$$

<sup>1</sup>Which goes under the name of "seagull term".

with

$$\hat{\varphi}(\mathbf{x}, t) = \frac{1}{4\pi\epsilon_0} \int d\mathbf{x}' \frac{\hat{\rho}(\mathbf{x}', t)}{|\mathbf{x} - \mathbf{x}'|} \quad (6.1.14)$$

where we introduced the charge density

$$\hat{\rho}(\mathbf{x}, t) = \sum_{\alpha} q_{\alpha} \delta(\mathbf{x} - \hat{\mathbf{x}}_{\alpha}(t)). \quad (6.1.15)$$

It is easily checked from (6.1.13) and  $\nabla \cdot \hat{\mathbf{A}} = 0$  that

$$\bar{\mathbf{E}}_{\parallel}(\mathbf{x}, t) = -\nabla \hat{\varphi}(\mathbf{x}, t), \quad (6.1.16a)$$

$$\bar{\mathbf{E}}_{\perp}(\mathbf{x}, t) = -\frac{\partial \hat{\mathbf{A}}(\mathbf{x}, t)}{\partial t}. \quad (6.1.16b)$$

As seen from (6.1.11), (6.1.14), (6.1.15) and (6.1.16), the longitudinal part of the electric field operator is expressed in terms of matter degrees of freedom (essentially, the position operators for the various electric charges), while the transverse part of the electric field operator is similar to the electric field operator in the free (interactionless) case (see (1.4.31)).

### 6.1.3 Restriction to the 1s and 2p levels in atomic Hydrogen

We consider the 1s and 2p levels in atomic Hydrogen, and for brevity we will use interchangeably, for the corresponding eigenstates of  $\hat{H}_A$ , the notations  $|g\rangle$  and  $|1s\rangle$  for what we will call the ground state (which has angular frequency  $\omega_g$ ), that is, the 1s level, and  $|e\rangle$  and  $|2pm_2\rangle$  for what we will call the excited state (which has angular frequency  $\omega_e$ ), that is, the 2p $m_2$  (sub)level (with  $m_2$  the magnetic quantum number). We call  $e$  the (positive) elementary electric charge,  $m_e$  is the electron mass. In the approximation where the ratio  $m_e/m_p$  of the electronic mass over the protonic mass is considered to be zero, the proton (Hydrogen nucleus) is sitting at all times at  $\mathbf{x} = 0$  in the centre-of-mass frame of the system. Hence we can simplify the notations and call  $\hat{\mathbf{x}}$  the position operator and  $\hat{\mathbf{p}}$  the linear momentum operator for the electron. The atom is considered to be in free space.

The restriction of the atomic Hamiltonian to the Hilbert subspace of interest reads

$$\hat{H}_A = \hbar\omega_g |g\rangle\langle g| + \hbar\omega_e |e\rangle\langle e| \quad (6.1.17)$$

while, in the weak-field approximation where we neglect the “seagull term” proportional to  $\hat{\mathbf{A}}^2$ , the interaction Hamiltonian is given by

$$\hat{H}_I = \frac{e}{m_e} \hat{\mathbf{A}}(\hat{\mathbf{x}}, t=0) \cdot \hat{\mathbf{p}} \quad (6.1.18)$$

### 6.1.4 Matrix element of the interaction Hamiltonian

The nontrivial features of the problem are encompassed by the matrix elements of the interaction Hamiltonian in the Hilbert (sub)space spanned by  $|e, 0\rangle$  and  $|g, 1_{\lambda, \mathbf{k}}\rangle$ . The state  $|e, 0\rangle$  corresponds to the electron on the excited atomic level and the field containing no photons while  $|g, 1_{\lambda, \mathbf{k}}\rangle = \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}, t=0) |g, 0\rangle$  corresponds to the electron on the ground atomic level and the field containing a photon of wave vector  $\mathbf{k}$  and polarisation  $\lambda$ . We have the following expressions for the electronic wave functions of the 1s and 2p  $m_2$  sublevels:

$$\psi_{1s}(\mathbf{x}) = \frac{\exp\left(-\frac{|\mathbf{x}|}{a_0}\right)}{\sqrt{\pi a_0^3}}, \quad (6.1.19a)$$



$$\psi_{2p m_2}(\mathbf{x}) = \frac{\exp\left(-\frac{||\mathbf{x}||}{2a_0}\right) \sqrt{2}}{8\sqrt{\pi a_0^3}} \frac{1}{a_0} \mathbf{x} \cdot \boldsymbol{\xi}_{m_2}. \quad (6.1.19b)$$

with  $a_0$  the Bohr radius. The vectors  $\boldsymbol{\xi}_{m_2}$  give the preferred directionality of the wave function of the 2p substates, the angular dependence of which is given by the usual spherical harmonics [3]. They are given by

$$\boldsymbol{\xi}_0 = \mathbf{e}_z, \quad (6.1.20a)$$

$$\boldsymbol{\xi}_{\pm 1} = \mp \frac{\mathbf{e}_x \pm i\mathbf{e}_y}{\sqrt{2}}. \quad (6.1.20b)$$

From (6.1.11) we see that

$$\hat{\mathbf{A}}(\mathbf{x}, t=0) = \sqrt{\frac{\hbar}{\epsilon_0 c}} \sum_{\lambda=\pm} \int \tilde{d}k \left[ \hat{a}_{(\lambda)}(\mathbf{k}, t=0) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{a}_{(\lambda)}^\dagger(\mathbf{k}, t=0) \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \quad (6.1.21)$$

whence, from (6.1.12), the matrix element of the interaction Hamiltonian:

$$\begin{aligned} \langle 1s, 1_{\lambda, \mathbf{q}} | \hat{H}_I | 2p m_2, 0 \rangle &= \sqrt{\frac{\hbar}{\epsilon_0 c}} \frac{e}{m_e} \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \langle 1s | e^{-i\mathbf{q}\cdot\hat{\mathbf{x}}} \hat{\mathbf{p}} | 2p m_2 \rangle \\ &\equiv \sqrt{\frac{\hbar}{\epsilon_0 c}} \frac{e}{m_e} \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \mathbf{C}_{m_2}(\mathbf{q}). \end{aligned} \quad (6.1.22)$$

Now use  $e^{-i\mathbf{q}\cdot\hat{\mathbf{x}}} |\mathbf{p}\rangle = |\mathbf{p} - \mathbf{q}\rangle$  to write

$$\begin{aligned} \mathbf{C}_{m_2}(\mathbf{q}) &= \int d\mathbf{k} \int d\mathbf{p} \langle 1s | e^{-i\mathbf{q}\cdot\hat{\mathbf{x}}} |\mathbf{k}\rangle \langle \mathbf{k} | \hat{\mathbf{p}} | \mathbf{p} \rangle \langle \mathbf{p} | 2p m_2, 0 \rangle \\ &= \hbar \int d\mathbf{k} \langle 1s | e^{-i\mathbf{q}\cdot\hat{\mathbf{x}}} |\mathbf{k}\rangle \langle \mathbf{k} | 2p m_2, 0 \rangle \mathbf{k} \\ &= \hbar \int d\mathbf{k} \mathbf{k} \bar{\psi}_{1s}^*(\mathbf{k} - \mathbf{q}) \bar{\psi}_{2p m_2}(\mathbf{k}) \end{aligned} \quad (6.1.23)$$

The reader can check via straightforward, if somewhat lengthy, calculations that the Fourier transforms of the wave functions for the 1s and 2p  $m_2$  states read

$$\begin{aligned} \bar{\psi}_{1s}(\mathbf{k}) &\equiv \int \frac{d\mathbf{x}}{(2\pi)^{\frac{3}{2}}} e^{-i\mathbf{k}\cdot\mathbf{x}} \psi_{1s}(\mathbf{x}) \\ &= \frac{4}{\pi\sqrt{2}} \frac{1}{a_0^{\frac{5}{2}}} \frac{1}{\left[\frac{1}{a_0^2} + \mathbf{k}^2\right]^2} \end{aligned} \quad (6.1.24a)$$

and

$$\begin{aligned} \bar{\psi}_{2p m_2}(\mathbf{k}) &\equiv \int \frac{d\mathbf{x}}{(2\pi)^{\frac{3}{2}}} e^{-i\mathbf{k}\cdot\mathbf{x}} \psi_{2p m_2}(\mathbf{x}) \\ &= -\frac{i}{\pi} \frac{1}{a_0^{\frac{7}{2}}} \frac{\boldsymbol{\xi}_{m_2} \cdot \mathbf{k}}{\left[\frac{1}{a_0^2} + \mathbf{k}^2\right]^3}. \end{aligned} \quad (6.1.24b)$$

Choosing a coordinate system for which  $\mathbf{q}$  points along the third axis (in other words, such that  $\mathbf{q} = ||\mathbf{q}|| \mathbf{e}_3$ ) and writing, in such a reference frame,

$$\boldsymbol{\xi}_{m_2} = \sum_{i=1}^3 \xi_{m_2}^{(i)} \mathbf{e}_i \quad (6.1.25)$$

we compute (6.1.23):

$$\begin{aligned}
\mathbf{C}_{m_2}(\mathbf{q}) &= -\frac{i}{\pi^2} \frac{4}{\sqrt{2}} \frac{\hbar}{a_0^6} \int d\mathbf{k} \mathbf{k} (\boldsymbol{\xi}_{m_2} \cdot \mathbf{k}) \frac{1}{\left[\frac{1}{a_0^2} + \|\mathbf{k} - \mathbf{q}\|^2\right]^2} \frac{1}{\left[\frac{1}{a_0^2} + k^2\right]^3} \\
&= -\frac{i}{\pi^2} \frac{4}{\sqrt{2}} \frac{\hbar}{a_0^6} \int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\varphi \begin{bmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{bmatrix} \left( \xi_{m_2}^{(1)} \sin \theta \cos \varphi + \xi_{m_2}^{(2)} \sin \theta \sin \varphi + \xi_{m_2}^{(3)} \cos \theta \right) \\
&\quad \int_0^{+\infty} dk k^4 \frac{1}{\left[\frac{1}{a_0^2} + k^2 + \mathbf{q}^2 - 2k \|\mathbf{q}\| \cos \theta\right]^2} \frac{1}{\left[\frac{1}{a_0^2} + k^2\right]^3} \\
&= -\frac{i}{\pi} \frac{4}{\sqrt{2}} \frac{\hbar}{a_0^6} \int_0^\pi d\theta \sin \theta \begin{bmatrix} \xi_{m_2}^{(1)} \sin^2 \theta \\ \xi_{m_2}^{(2)} \sin^2 \theta \\ 2\xi_{m_2}^{(3)} \cos^2 \theta \end{bmatrix} \int_0^{+\infty} dk k^4 \frac{1}{\left[\frac{1}{a_0^2} + k^2 + \mathbf{q}^2 - 2k \|\mathbf{q}\| \cos \theta\right]^2} \frac{1}{\left[\frac{1}{a_0^2} + k^2\right]^3} \\
&= -\frac{i}{\pi} \sqrt{2} \frac{\hbar}{a_0^6} \int_{-1}^1 d\eta \begin{bmatrix} \xi_{m_2}^{(1)} (1 - \eta^2) \\ \xi_{m_2}^{(2)} (1 - \eta^2) \\ 2\xi_{m_2}^{(3)} \eta^2 \end{bmatrix} \int_{-\infty}^{+\infty} dk k^4 \frac{1}{\left[\frac{1}{a_0^2} + k^2 + \mathbf{q}^2 - 2k \|\mathbf{q}\| \eta\right]^2} \frac{1}{\left[\frac{1}{a_0^2} + k^2\right]^3}.
\end{aligned} \tag{6.1.26}$$

Now notice from (6.1.22) that we are interested in the dot product  $\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \mathbf{C}_{m_2}(\mathbf{q})$ . With our choice of basis, with the third axis along  $\mathbf{q}$ , the polarisation vector  $\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q})$  has no third component and hence we have

$$\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \mathbf{C}_{m_2}(\mathbf{q}) = -\frac{i}{\pi} \sqrt{2} \frac{\hbar}{a_0^6} \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \boldsymbol{\xi}_{m_2} \int_{-1}^1 d\eta (1 - \eta^2) \int_{-\infty}^{+\infty} dk k^4 \frac{1}{\left[\frac{1}{a_0^2} + k^2 + \mathbf{q}^2 - 2k \|\mathbf{q}\| \eta\right]^2} \frac{1}{\left[\frac{1}{a_0^2} + k^2\right]^3}. \tag{6.1.27}$$

We then use the identity

$$\int_{-1}^1 d\eta \frac{1 - \eta^2}{(A - B\eta)^2} = -\frac{2}{B^2} \left[ 2 + \frac{A}{B} \log \left( \frac{A - B}{A + B} \right) \right] \tag{6.1.28}$$

to conclude<sup>2</sup> that

$$\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \mathbf{C}_{m_2}(\mathbf{q}) = -i \frac{2^{\frac{9}{2}}}{3^4} \frac{\hbar}{a_0} \frac{\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{q}) \cdot \boldsymbol{\xi}_{m_2}}{\left[1 + \left(\frac{2}{3} a_0 \|\mathbf{q}\|\right)^2\right]^2}. \tag{6.1.29}$$

The exact matrix element [13] thus reads

$$G_\lambda(\mathbf{k}) \equiv \langle 1s, 1_{\lambda, \mathbf{k}} | \hat{H}_I | 2p m_2, 0 \rangle = -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \frac{\hbar e}{m_e a_0} \frac{2^{\frac{9}{2}}}{3^4} \frac{\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{k}) \cdot \boldsymbol{\xi}_{m_2}}{\left[1 + \left(\frac{2}{3} a_0 \|\mathbf{k}\|\right)^2\right]^2}. \tag{6.1.30}$$

## 6.1.5 Time-dependent perturbation theory at short times and the rotating wave approximation

Since we are interested in spontaneous emission, we set the initial state of the system to be  $|\psi(t=0)\rangle = |e, 0\rangle$ . We want to compute emission probabilities such as

$$P_{\text{emiss.} \rightarrow \lambda, \mathbf{k}}(t) = \left| \langle g, 1_{\lambda, \mathbf{k}} | \hat{U}(t) | \psi(t=0) \rangle \right|^2 = \left| \langle g, 1_{\lambda, \mathbf{k}} | \hat{U}(t) | e, 0 \rangle \right|^2 \tag{6.1.31a}$$

<sup>2</sup>By way of a delicate final integration.

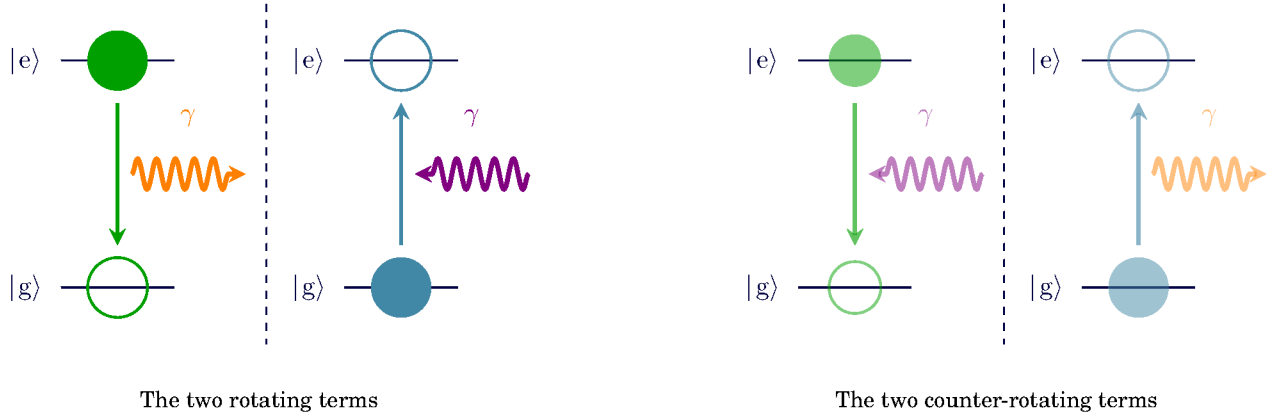


Fig. 6.1.1 – The interaction Hamiltonian  $\hat{H}_I$  features four terms.

where  $\hat{U}(t) = \exp\left[(-i/\hbar)\hat{H}t\right]$  is the evolution operator for the system. It is well-known [4, 5] that a time-dependent perturbative treatment of such a problem yields, to first order in time,

$$P_{\text{emiss.} \rightarrow \lambda, \mathbf{k}}(t) = \frac{t^2}{\hbar^2} \left| \langle g, 1_{\lambda, \mathbf{k}} | \hat{H}_I | e, 0 \rangle \right|^2 \text{sinc}^2 \left[ (\omega_0 - c \|\mathbf{k}\|) \frac{t}{2} \right] \quad (6.1.31b)$$

where we introduced the notation

$$\boxed{\omega_0 \equiv \omega_e - \omega_g}. \quad (6.1.32)$$

We give the value for the transition frequency  $\omega_0$

$$\omega_0 = \frac{3}{8} \frac{\hbar}{m_e a_0^2} \quad (6.1.33)$$

where the Bohr radius  $a_0$  is

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}. \quad (6.1.34)$$

The restriction of the interaction Hamiltonian to the Hilbert subspace of interest (1s and 2p Hydrogen levels, and zero- and one-photon states) reads

$$\begin{aligned} \hat{H}_I = & \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{(2\pi)^3 2 \|\mathbf{k}\|} \left( G_\lambda(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |g\rangle \langle e| + G_\lambda^*(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) |e\rangle \langle g| \right) \\ & + \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{(2\pi)^3 2 \|\mathbf{k}\|} \left( F_\lambda(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) |g\rangle \langle e| + F_\lambda^*(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |e\rangle \langle g| \right) \end{aligned} \quad (6.1.35)$$

with atom-field couplings  $G_\lambda(\mathbf{k})$  given by (6.1.30) and  $F_\lambda(\mathbf{k})$  by

$$F_\lambda(\mathbf{k}) \equiv \langle 1s, 0 | \hat{H}_I | 2p m_2, 1_{\lambda, \mathbf{k}} \rangle = -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \frac{\hbar e}{m_e a_0} \frac{2^{\frac{9}{2}}}{3^4} \frac{\boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) \cdot \boldsymbol{\xi}_{m_2}}{\left[ 1 + \left( \frac{2}{3} a_0 \|\mathbf{k}\| \right)^2 \right]^2}. \quad (6.1.36)$$

The two terms on the first line on the right-hand side of (6.1.35) are known as the rotating terms, while the two terms on the second line on the right-hand side are known as the counter-rotating terms. They are represented schematically on Fig. 6.1.1, with colour correspondences with (6.1.35).

Similarly to (6.1.31b) to first order, time-dependent perturbation theory gives us the probability

$$|\langle \varphi | \psi(t) \rangle|^2 = \frac{t^2}{\hbar^2} \left| \langle \varphi | \hat{H}_I | e, 0 \rangle \right|^2 \text{sinc}^2 \left[ (\omega_0 - \omega_\lambda) \frac{t}{2} \right] \quad (6.1.37)$$

that the state of the system evolves to an **arbitrary eigenstate**  $|\varphi\rangle$  of the free Hamiltonian  $\hat{H}_A + \hat{H}_R$ .

It is readily seen from (6.1.35) that

$$\langle e, 0 | \hat{H}_I | e, 0 \rangle = 0, \quad (6.1.38a)$$

$$\langle e, 1_{\lambda, \mathbf{k}} | \hat{H}_I | e, 0 \rangle = 0, \quad (6.1.38b)$$

$$\langle g, 0 | \hat{H}_I | e, 0 \rangle = 0, \quad (6.1.38c)$$

$$\langle g, 1_{\lambda, \mathbf{k}} | \hat{H}_I | e, 0 \rangle = G_\lambda(\mathbf{k}) \quad (6.1.38d)$$

while all quantum states of the system with more than one photon present are orthogonal to  $\hat{H}_I | e, 0 \rangle$ . We see from (6.1.37) and (6.1.38) that the counter-rotating part of the interaction Hamiltonian does not contribute to the short-time dynamics of the system. This is only true for the initial state we chose. For different initial states, counter-rotating terms must be taken into account. The rotating wave approximation consists in dropping the counter-rotating terms from the interaction Hamiltonian (6.1.35). We showed that in the framework of spontaneous emission into an initially empty electromagnetic field (that is, with  $|e, 0\rangle$  as the initial state), this approximation is valid at short times, which are the focus of our investigations here. Hence we consider in the following that

$$\hat{H}_I = \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{(2\pi)^3 2|\mathbf{k}|} \left( G_\lambda(\mathbf{k}) \hat{a}_{(\lambda)}^\dagger(\mathbf{k}) |g\rangle \langle e| + G_\lambda^*(\mathbf{k}) \hat{a}_{(\lambda)}(\mathbf{k}) |e\rangle \langle g| \right). \quad (6.1.39)$$

With our initial state, and in the framework of the rotating wave approximation, the state of the system at time  $t$  reads

$$|\psi(t)\rangle = c_e(t) e^{-i\omega_e t} |e, 0\rangle + \sum_{\lambda=\pm} \int d\tilde{k} c_{g,\lambda}(\mathbf{k}, t) e^{-i(\omega_g + c|\mathbf{k}|)t} |g, 1_{\lambda, \mathbf{k}}\rangle. \quad (6.1.40)$$

With (6.1.9), (6.1.17), (6.1.39) and (6.1.40), we obtain Schrödinger's equations of motion for the probability amplitudes:

$$\dot{c}_e(t) = \frac{i}{\hbar} \sum_{\lambda=\pm} \int \frac{d\mathbf{k}}{(2\pi)^3 2|\mathbf{k}|} G_\lambda^*(\mathbf{k}) c_{g,\lambda}(\mathbf{k}, t) e^{-i(c|\mathbf{k}| - \omega_e + \omega_g)t}, \quad (6.1.41a)$$

$$\dot{c}_{g,\lambda}(\mathbf{k}, t) = -\frac{i}{\hbar} G_\lambda(\mathbf{k}) c_e(t) e^{i(c|\mathbf{k}| - \omega_e + \omega_g)t}. \quad (6.1.41b)$$

From (6.1.40) we deduce that the probability that, at time  $t$ , the electron is still in the excited state, the so-called **survival probability**, is given by

$$\begin{aligned} P_{\text{surv}}(t) &\equiv |c_e(t)|^2 = 1 - \sum_{\lambda=\pm} \int d\tilde{k} |c_{g,\lambda}(\mathbf{k}, t)|^2 \\ &= 1 - \frac{t^2}{\hbar^2} \sum_{\lambda=\pm} \int d\tilde{k} \left| \langle g, 1_{\lambda, \mathbf{k}} | \hat{H}_I | e, 0 \rangle \right|^2 \text{sinc}^2 \left[ (\omega_0 - c|\mathbf{k}|) \frac{t}{2} \right]. \end{aligned} \quad (6.1.42)$$

where we used (6.1.31b). What is usually done [4–6] at this point is to use the distributional limit

$$\lim_{a \rightarrow +\infty} \frac{\sin^2(ax)}{a^2 x} = \pi \delta(x) \quad (6.1.43)$$

of the square cardinal sine, to conclude that the only single-photon states available by spontaneous emission have a

frequency equal to the atomic transition frequency  $\omega_0$ . Indeed the use of (6.1.43) in (6.1.31b) yields Fermi's golden rule

$$P_{\text{emiss.} \rightarrow \lambda, \mathbf{k}}(t) \underset{t \rightarrow +\infty}{\sim} 2\pi \frac{t}{\hbar^2} \left| \langle g, 1_{\lambda, \mathbf{k}} | \hat{H}_I | e, 0 \rangle \right|^2 \delta(\omega_0 - c||\mathbf{k}||). \quad (6.1.44)$$

In making use of (6.1.43) in (6.1.42), we take the limit  $t \rightarrow +\infty$ , a strange manipulation in the framework of time-dependent perturbation theory around  $t = 0$ . Fermi's golden rule is thus valid at what is known as intermediate times: times large enough to guarantee that we can approximate the square cardinal sine by its limit (6.1.43), but small enough to ensure that first-order perturbation theory still applies.

## 6.2 The dipole approximation and its shortcomings

*“When you get down, down to the subatomic part of it  
That's when it breaks, you know, that's when it falls apart.”*

British Sea Power's Jan Scott Wilkinson in “Atom”, **Do You Like Rock Music?** (Rough Trade, 2008)

### 6.2.1 The approximation and a discussion

Fermi's golden rule (6.1.44) tells us that, at sufficiently large times, the only relevant modes of the electromagnetic field are the ones which have a frequency very close to  $\omega_0$ . They are, in other words, resonant with the atomic transition. The corresponding electromagnetic wavelengths are much larger than the uncertainty on the position of the atomic electron. In that view the electromagnetic field does not “see” the details of matter configuration at the atomic scale, and hence the precise location of the point of light emission is irrelevant. This is best illustrated by Shirokov [9] who described the dipole approximation as assuming that “the electron [...] emits [...] a photon, not at its own position, but at the center of the potential which binds [it]”. In other words, one can simply set  $\hat{\mathbf{x}} = \mathbf{0}$  in the interaction Hamiltonian, and this yields the following dipole-approximated coupling:

$$\langle 1s, 1_{\lambda, \mathbf{k}} | \hat{H}_I | 2p m_2, 0 \rangle = -i \sqrt{\frac{\hbar}{\epsilon_0 c}} \frac{\hbar e}{m_e a_0} \frac{2^{\frac{3}{2}}}{3^4} \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{k}) \cdot \boldsymbol{\xi}_{m_2}. \quad (6.2.1)$$

On the other hand, there is no good argument in favour of the dipole approximation at very short times, for which it may not be justified by Fermi's golden rule.

In the framework of the dipole approximation, it is necessary to introduce a cutoff over electromagnetic field frequencies. To see this, write the survival probability of the electron in the excited state at time  $t$  as given by (6.1.42) and (6.2.1). We perform the angular integrations, using (1.4.23), (6.1.20) and (6.1.34). We use an arbitrary

basis where the spherical coordinates of  $\mathbf{k}$  are  $(k, \theta, \varphi)$  (see Fig. 1.4.18) and where we have (6.1.25). This yields

$$\begin{aligned}
P_{\text{surv}}(t) &= 1 - \frac{2^9 t^2 \hbar}{3^8 \hbar^2 \epsilon_0 c} \left( \frac{\hbar e}{m_e a_0} \right)^2 \sum_{\lambda=\pm} \int d\tilde{\mathbf{k}} \left( \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{k}) \cdot \boldsymbol{\xi}_{m_2} \right) \left( \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) \cdot \boldsymbol{\xi}_{m_2}^* \right) \text{sinc}^2 \left[ (\omega_0 - c \|\mathbf{k}\|) \frac{t}{2} \right] \\
&= 1 - \left( \frac{2}{3} \right)^8 t^2 \frac{\hbar}{\epsilon_0 c} \left( \frac{e}{m_e a_0} \right)^2 \int \frac{d\mathbf{k}}{(2\pi)^3 \|\mathbf{k}\|} \left[ \boldsymbol{\xi}_{m_2} \cdot \boldsymbol{\xi}_{m_2}^* - \frac{1}{\mathbf{k}^2} (\mathbf{k} \cdot \boldsymbol{\xi}_{m_2}) (\mathbf{k} \cdot \boldsymbol{\xi}_{m_2}^*) \right] \text{sinc}^2 \left[ (\omega_0 - c \|\mathbf{k}\|) \frac{t}{2} \right] \\
&= 1 - \frac{1}{(2\pi)^3} \left( \frac{2}{3} \right)^8 t^2 \frac{\hbar}{\epsilon_0 c} \left( \frac{e^3}{4\pi\epsilon_0 \hbar^2} \right)^2 \int_0^{+\infty} dk k \text{sinc}^2 \left[ (\omega_0 - ck) \frac{t}{2} \right] \int_0^\pi d\theta \sin \theta \\
&\quad \int_0^{2\pi} d\varphi \left[ 1 - \left[ \xi_{m_2}^{(1)} \sin(\theta) \cos(\varphi) + \xi_{m_2}^{(2)} \sin(\theta) \sin(\varphi) + \xi_{m_2}^{(3)} \cos(\theta) \right] \right. \\
&\quad \quad \left. \left[ \xi_{m_2}^{(1)*} \sin(\theta) \cos(\varphi) + \xi_{m_2}^{(2)*} \sin(\theta) \sin(\varphi) + \xi_{m_2}^{(3)*} \cos(\theta) \right] \right] \\
&= 1 - \frac{1}{2(2\pi)^2} \left( \frac{2}{3} \right)^8 t^2 \frac{\hbar}{\epsilon_0 c} \left( \frac{e^3}{4\pi\epsilon_0 \hbar^2} \right)^2 \int_0^{+\infty} dk k \text{sinc}^2 \left[ (\omega_0 - ck) \frac{t}{2} \right] \\
&\quad \int_0^\pi d\theta \sin \theta \left[ 2 - \left[ \left| \xi_{m_2}^{(1)} \right|^2 \sin^2(\theta) + \left| \xi_{m_2}^{(2)} \right|^2 \sin^2(\theta) + 2 \left| \xi_{m_2}^{(3)} \right|^2 \cos^2(\theta) \right] \right] \\
&= 1 - \frac{1}{2(2\pi)^2} \left( \frac{2}{3} \right)^8 t^2 \frac{e^6}{(4\pi)^2 \epsilon_0^3 \hbar^3 c} \int_0^{+\infty} dk k \text{sinc}^2 \left[ (\omega_0 - ck) \frac{t}{2} \right] \left[ 4 - \frac{4}{3} \left( \left| \xi_{m_2}^{(1)} \right|^2 + \left| \xi_{m_2}^{(2)} \right|^2 + \left| \xi_{m_2}^{(3)} \right|^2 \right) \right] \\
&= 1 - \frac{4}{3(2\pi)^2} \left( \frac{2}{3} \right)^8 t^2 \frac{e^6}{(4\pi)^2 \epsilon_0^3 \hbar^3 c^3} \int_0^{+\infty} d\omega \omega \text{sinc}^2 \left[ (\omega_0 - \omega) \frac{t}{2} \right] \\
&= 1 - \frac{2^{10}}{3^9 \pi} \alpha^3 t^2 \int_0^{+\infty} d\omega \omega \text{sinc}^2 \left( (\omega_0 - \omega) \frac{t}{2} \right).
\end{aligned} \tag{6.2.2}$$

Here

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \tag{6.2.3}$$

is the fine structure constant of electrodynamics. The integral on the right-hand side of (6.2.2) diverges at all times. In this situation, taking the limit  $t \rightarrow +\infty$  under the integral to obtain Fermi's golden rule is simply not a valid option. We must introduce a cutoff frequency corresponding to an upper bound on the validity domain of the dipole approximation for the atom-field coupling. A natural frequency in that framework is  $\omega_C = c/a_0$ : electromagnetic waves with higher frequencies than  $\omega_C$  are not "indifferent" to the detailed configuration of sources on the atomic scale  $a_0$ , and for these frequencies the dipole approximation breaks down. This argument, of course, only gives a qualitative prescription for the cutoff frequency. We will see that this is especially problematic when investigating the very short-time dynamics of the system. Also, for lack of a better solution, we must consider that electromagnetic field modes with frequency larger than this cutoff frequency  $\omega_C$  are uncoupled to the atom. Several objections can be raised with regard to this ubiquitous procedure. We discuss them along with their more or less satisfying rebuttals:

- In order to introduce a cutoff, one must assume that high-frequency electromagnetic modes do not interact with the atom. This is justified by a quick look at the exact coupling. The matrix elements are proportional to  $\langle 1s | \hat{\mathbf{p}} \exp(i\mathbf{k} \cdot \hat{\mathbf{x}}) | 2p m_2 \rangle$ . When the wave number  $\|\mathbf{k}\|$  becomes higher than the inverse of the Bohr radius  $a_0$ , such matrix elements are *de facto* negligibly small because the oscillating exponential  $\exp(i\mathbf{k} \cdot \hat{\mathbf{x}})$  averages out during the integration, as seen from (6.1.19).
- The approximation yields cutoff-dependent results. Since the qualitative argument above only provides an order of magnitude (the ratio  $c/a_0$ ) for the cutoff frequency  $\omega_C$ , this is especially problematic. Indeed, one can check that the truncated integral

$$\int_0^{\omega_C} d\omega \omega \text{sinc}^2 \left( (\omega_0 - \omega) \frac{t}{2} \right) = \frac{2}{t^2} \left[ \log \left( -1 + \frac{\omega_C}{\omega_0} \right) - [\text{Ci}((\omega_C - \omega_0)t) - \text{Ci}(\omega_0 t)] \right]$$

$$+ \frac{\omega_0}{\omega_C - \omega_0} (-1 + \cos((\omega_C - \omega_0)t)) + (-1 + \cos(\omega_0 t)) + t (\text{Si}((\omega_C - \omega_0)t) + \text{Si}(\omega_0 t)) \Big] \quad (6.2.4)$$

is strongly dependent on the value of the cutoff frequency  $\omega_C$ . Here Ci and Si stand for the cosine integral and the sine integral respectively, defined by

$$\text{Ci}(x) \equiv - \int_x^{+\infty} du \frac{\cos(u)}{u}, \quad (6.2.5a)$$

$$\text{Si}(x) \equiv \int_0^x du \frac{\sin(u)}{u}. \quad (6.2.5b)$$

- When a cutoff is implemented, the distinction between electromagnetic modes which are considered to be coupled to the atom and those who are excluded from the treatment is binary: the coupling function is taken to be exactly zero beyond the cutoff frequency. One could envision to introduce a smoother cutoff procedure along the lines of the cutting off of ultrarelativistic frequencies presented in [2], but we feel this would do nothing but introduce further arbitrariness in the model.

## 6.2.2 A cutoff-independent regularisation

We now investigate what happens if, understandably unconvinced by the above arguments in favour of the implementation of a cutoff on electromagnetic frequencies, we refrain from introducing such a cutoff and instead retain the result (6.2.2) from the dipole approximation without cutoff, but try and regularise the divergence in the integral.

We focus our interest on the integral featured in (6.2.2), that is

$$\int_{-\infty}^{+\infty} d\omega f(\omega, t) \quad \text{where} \quad f(\omega, t) = \theta(\omega) \omega \text{sinc}^2\left((\omega_0 - \omega) \frac{t}{2}\right) \equiv \theta(\omega) g(\omega, t). \quad (6.2.6)$$

Though the function  $f(\cdot, t)$  does not belong to the vector space  $L^1(\mathbb{R})$  of summable functions, it is a slowly growing function, and, as such, a tempered distribution. It therefore admits a Fourier transform in the sense of distributions  $\bar{f}(\cdot, t)$ .

We thus compute the Fourier transform

$$\bar{f}(\tau, t) = \int_{-\infty}^{+\infty} d\omega f(\omega, t) e^{-i\omega\tau} \quad (6.2.7)$$

and then shall take the limit  $\tau \rightarrow 0$  at the end to retrieve the desired integral (6.2.6). In this limit, some terms in  $\bar{f}(\tau, t)$  become ill-defined, a consequence of the fact that  $f(\cdot, t)$  is not summable. We will simply discard these terms at the end of our treatment, and focus on the well-defined terms in the limit  $\tau \rightarrow 0$ .

From (6.2.6), (6.2.7) and (6.A.15), we write

$$\bar{f}(\tau, t) = \frac{1}{2} \left[ \left( \delta(\cdot) - \frac{i}{\pi} \text{vp} \frac{1}{\cdot} \right) * \bar{g}(\cdot, t) \right] (\tau) \quad (6.2.8)$$

where

$$\bar{g}(\tau, t) = \int_{-\infty}^{+\infty} d\omega g(\omega, t) e^{-i\omega\tau}. \quad (6.2.9)$$

From (6.2.6) we get

$$\bar{g}(\tau, t) = -\frac{1}{t^2} \int_{-\infty}^{+\infty} d\omega \frac{\omega}{(\omega - \omega_0)^2} \left( e^{i\omega(t-\tau)} e^{-i\omega_0 t} + e^{-i\omega(t+\tau)} e^{i\omega_0 t} - 2e^{-i\omega\tau} \right). \quad (6.2.10)$$

We would like to compute this as a sum of three integrals corresponding to the three summands on the right-hand side of (6.2.10), but, taken individually, these integrals will diverge because of the singularity at  $\omega = \omega_0$ . The full integrand in (6.2.10), however, has no singularity at  $\omega = \omega_0$ . Accordingly we introduce a small positive imaginary part  $\epsilon > 0$  in the denominator, which enables us to compute (6.2.10) as a sum of three integrals. Introduce

$$G_\epsilon(\tau) \equiv \int_{-\infty}^{+\infty} d\omega \frac{\omega}{(\omega - \omega_0 + i\epsilon)^2} e^{-i\omega\tau} \quad (6.2.11)$$

to rewrite

$$\bar{g}(\tau, t) = -\frac{1}{t^2} \lim_{\epsilon \rightarrow 0^+} (e^{-i\omega_0 t} G_\epsilon(\tau - t) + e^{i\omega_0 t} G_\epsilon(\tau + t) - 2G_\epsilon(\tau)). \quad (6.2.12)$$

Thus to compute  $\bar{g}(\cdot, t)$  we need only compute  $G_\epsilon$ , which we do now. Notice first that

$$\frac{\omega}{(\omega - \omega_0 + i\epsilon)^2} = \frac{1}{\omega - \omega_0 + i\epsilon} + \frac{\omega_0 + i\epsilon}{(\omega - \omega_0 + i\epsilon)^2}. \quad (6.2.13)$$

Since  $\epsilon > 0$ , an application of Cauchy's residue theorem therefore yields

$$\lim_{\epsilon \rightarrow 0^+} G_\epsilon(\tau) = 2\pi e^{-i\omega_0 \tau} (i + \omega_0 \tau) \theta(\tau). \quad (6.2.14)$$

Plugging this back in (6.2.12), we get

$$\bar{g}(\tau, t) = 2\pi \frac{1}{t^2} e^{-i\omega_0 \tau} [\theta(\tau - t) (i + \omega_0(\tau - t)) + \theta(\tau + t) (i + \omega_0(\tau + t)) - 2\theta(\tau) (i + \omega_0 \tau)]. \quad (6.2.15)$$

Then we further plug this in (6.2.8) to get

$$\bar{f}(\tau, t) = \frac{1}{2} \bar{g}(\tau, t) - \frac{i}{t^2} \text{vp} \int_{-\infty}^{+\infty} d\sigma \frac{e^{-i\omega_0 \sigma}}{\tau - \sigma} [\theta(\sigma - t) (i + \omega_0(\sigma - t)) + \theta(\sigma + t) (i + \omega_0(\sigma + t)) - 2\theta(\sigma) (i + \omega_0 \sigma)]. \quad (6.2.16)$$

After some algebra we obtain

$$\begin{aligned} \bar{f}(\tau, t) = & \frac{1}{t^2} \left\{ \pi [\theta(\tau - t) (i + \omega_0(\tau - t)) + \theta(\tau + t) (i + \omega_0(\tau + t)) - 2\theta(\tau) (i + \omega_0 \tau)] \right. \\ & \left. - i \text{vp} \left[ i \left( \int_{-t}^0 d\sigma \frac{e^{-i\omega_0 \sigma}}{\tau - \sigma} - \int_0^t d\sigma \frac{e^{-i\omega_0 \sigma}}{\tau - \sigma} \right) + \omega_0 \left( t \int_{-t}^t d\sigma \frac{e^{-i\omega_0 \sigma}}{\tau - \sigma} + \int_{-t}^0 d\sigma \frac{e^{-i\omega_0 \sigma}}{\tau - \sigma} \sigma - \int_0^t d\sigma \frac{e^{-i\omega_0 \sigma}}{\tau - \sigma} \sigma \right) \right] \right\}. \end{aligned} \quad (6.2.17)$$

Hence we can finally write

$$\begin{aligned} \bar{f}(\tau = 0, t) = & \frac{1}{t^2} \left\{ \pi [\theta(-t) (i - \omega_0 t) + \theta(t) (i + \omega_0 t) - 2i\theta(0)] \right. \\ & \left. - i \text{vp} \left[ i \left( \int_{-t}^0 d\sigma \frac{e^{-i\omega_0 \sigma}}{-\sigma} - \int_0^t d\sigma \frac{e^{-i\omega_0 \sigma}}{-\sigma} \right) + \omega_0 \left( t \int_{-t}^t d\sigma \frac{e^{-i\omega_0 \sigma}}{-\sigma} - \int_{-t}^0 d\sigma e^{-i\omega_0 \sigma} + \int_0^t d\sigma e^{-i\omega_0 \sigma} \right) \right] \right\}. \end{aligned} \quad (6.2.18)$$

Now we want to identify and discard the singular terms in (6.2.18). Making use of  $\theta(-t) + \theta(t) = 1$ , we can rewrite  $2\theta(0) = 1 + \theta(0) - \theta(-0)$ . The difference  $\theta(0) - \theta(-0)$ , which is equal to  $\text{sgn}(0)$ , is ill-defined, and we drop it from our treatment. We identify another singular term by writing

$$\begin{aligned} \int_{-t}^0 d\sigma \frac{e^{-i\omega_0 \sigma}}{-\sigma} - \int_0^t d\sigma \frac{e^{-i\omega_0 \sigma}}{-\sigma} &= 2 \int_0^t d\sigma \frac{\cos(\omega_0 \sigma)}{\sigma} \\ &= 2 \sum_{n=0}^{+\infty} \frac{(-1)^n}{(2n)!} \omega_0^{2n} \int_0^t d\sigma \sigma^{2n-1}. \end{aligned} \quad (6.2.19)$$



For  $n = 0$ , this last integral diverges, and taking its principal value will not change that fact. Accordingly, we simply discard the  $n = 0$  term in the sum (6.2.19). We write the remainder of the series in closed form:

$$\begin{aligned} \sum_{n=1}^{+\infty} \frac{(-1)^n}{(2n)!} \omega_0^{2n} \int_0^t d\sigma \sigma^{2n-1} &= \sum_{n=1}^{+\infty} \frac{(-1)^n}{2n(2n)!} (\omega_0 t)^{2n} \\ &= \text{Ci}(\omega_0 t) - \log(\omega_0 t) - \gamma \end{aligned} \quad (6.2.20)$$

where  $\gamma$  is the Euler-Mascheroni constant. Computing the other integrals on the second line on the right-hand side of (6.2.18), we can rewrite the regular part of (6.2.18) as

$$\bar{f}(\tau = 0, t) \stackrel{\text{r.p.}}{\equiv} \frac{1}{t^2} \left[ -4 \sin^2 \left( \frac{\omega_0 t}{2} \right) + 2 (\text{Ci}(\omega_0 t) - \log(\omega_0 t) - \gamma) + \pi \omega_0 t \left( \text{sgn}(t) + \frac{2}{\pi} \text{Si}(\omega_0 t) \right) \right] \quad (6.2.21)$$

where r.p. stands for “regular part”. The term

$$\pi \frac{\omega_0}{t} \left( \text{sgn}(t) + \frac{2}{\pi} \text{Si}(\omega_0 t) \right) \quad (6.2.22)$$

on the right-hand side of (6.2.21) is particularly interesting, and can be directly linked to Fermi’s golden rule. Indeed, remember from (6.2.2) that the decay probability (that is,  $1 - P_{\text{surv}}(t)$ ) features the product of (6.2.21) by  $t^2$ . Further, notice that  $\text{Si}(\omega_0 t)$  quickly converges to the Dirichlet value  $\pi/2$  as  $t$  becomes substantially larger than  $1/\omega_0$ . For such times the leading term in (6.2.21) is clearly  $2\pi\omega_0/t$  (*i.e.*, the limit of (6.2.22) as  $t \rightarrow +\infty$ ) which is equal to the result obtained from illegally “sneaking” the limit  $t \rightarrow +\infty$  into the divergent integral on the right-hand side of (6.2.2). Hence, we have shown how the golden rule can be retrieved from a formal, cutoff-independent regularisation of the integral featured in the expression for the survival probability. We refrain from claiming that the other terms on the right-hand side of (6.2.21) are relevant descriptions of short-time deviations from the golden rule, as it is clear that using a more exact expression for the atom-field coupling will give better results<sup>3</sup>. This is examined in the upcoming sect. 6.3. Nevertheless, we can notice that decay probability  $1 - P_{\text{surv}}(t)$  which features the product of (6.2.21) by  $t^2$  tends to zero as  $t \rightarrow 0$ , which we feel is an important validation of our regularisation procedure.

## 6.3 Improving on the dipole approximation: exact atom-field coupling

In the present section we will start from the same integral (6.1.42), and investigate the short-time dynamics yielded by the exact matrix element (6.1.30). This treatment features no infinities and thus does not call for any regularisation procedure. This is so because (6.1.30) already features a “natural cutoff”

$$\omega_X \equiv \frac{3}{2} \frac{c}{a_0}. \quad (6.3.1)$$

For electromagnetic frequencies larger than the natural cutoff  $\omega_X$ , it is readily seen from (6.1.30) that the coupling becomes smaller and smaller as the frequency increases: without the dipole approximation, everything is well-defined and there are no ambiguities in the model.

Going beyond the dipole approximation allows us to investigate short-time deviations from Fermi’s golden rule in a

<sup>3</sup>For the sake of exhaustiveness, the regularised dipole-approximated result (6.2.21) is plotted in Figs. 6.3.3 and 6.3.4, where it is shown that it does not provide an accurate description of the very short-time behaviour of the system.

direct and reliable way. To do this we start from the survival probability of the electron in the excited state

$$P_{\text{surv}}(t) = 1 - \frac{2^{10}}{3^9 \pi} \alpha^3 t^2 \int_0^{+\infty} d\omega \frac{\omega}{\left[1 + \left(\frac{\omega}{\omega_X}\right)^2\right]^4} \text{sinc}^2\left(\left(\omega_0 - \omega\right) \frac{t}{2}\right) \quad (6.3.2)$$

The integral in (6.3.2) is finite at all times and we can compute it numerically or, as we now do, analytically.

Define

$$I_F(t) = \int_{-\infty}^{+\infty} d\omega d(\omega, t) \quad \text{where} \quad d(\omega, t) = \theta(\omega) \frac{\omega}{\left[1 + \left(\frac{\omega}{\omega_X}\right)^2\right]^4} \text{sinc}^2\left(\left(\omega_0 - \omega\right) \frac{t}{2}\right). \quad (6.3.3)$$

It can be rewritten

$$I_F(t) = -\frac{1}{t^2} \int_0^{+\infty} d\omega \frac{\omega}{(\omega - \omega_0)^2} \frac{1}{\left[1 + \left(\frac{\omega}{\omega_X}\right)^2\right]^4} (e^{i\omega t} e^{-i\omega_0 t} + e^{-i\omega t} e^{i\omega_0 t} - 2). \quad (6.3.4)$$

We would like to compute this as a sum of three integrals corresponding to the three summands on the right-hand side of (6.3.4), but, taken individually, these integrals will diverge because of the singularity at  $\omega = \omega_0$ . The full integrand in (6.3.4), however, has no singularity at  $\omega = \omega_0$ . Accordingly we introduce a small positive imaginary part  $\epsilon > 0$  in the denominator. Introduce

$$H_\epsilon(t) \equiv \int_{-\infty}^{+\infty} d\omega \frac{\omega}{(\omega - \omega_0 + i\epsilon)^2} \frac{\theta(\omega)}{\left[1 + \left(\frac{\omega}{\omega_X}\right)^2\right]^4} e^{-i\omega t} \quad (6.3.5a)$$

$$\equiv \int_{-\infty}^{+\infty} d\omega h_\epsilon(\omega) \theta(\omega) e^{-i\omega t} \quad (6.3.5b)$$

to rewrite

$$I_F(t) = -\frac{1}{t^2} \lim_{\epsilon \rightarrow 0^+} (e^{-i\omega_0 t} H_\epsilon(-t) + e^{i\omega_0 t} H_\epsilon(t) - 2H_\epsilon(0)). \quad (6.3.6)$$

Thus to compute  $I_F$  we need only compute  $H_\epsilon$ , which we do now. From (6.3.5) and (6.A.15) we have

$$H_\epsilon(t) = \frac{1}{2} \left[ \left( \delta(\cdot) - \frac{i}{\pi} \text{vp} \frac{1}{\cdot} \right) * \bar{h}_\epsilon(\cdot) \right](t). \quad (6.3.7)$$

We therefore need to compute the Fourier transform

$$\bar{h}_\epsilon(t) = \int_{-\infty}^{+\infty} d\omega h_\epsilon(\omega) e^{-i\omega t} \quad (6.3.8)$$

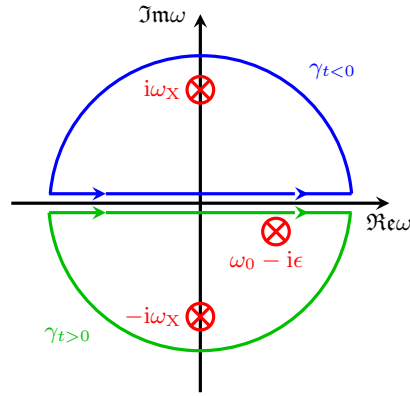
of  $h_\epsilon$ . We use Cauchy's residue theorem. We know from (6.3.5) that  $h_\epsilon$  has a second order pole at  $\omega_0 - i\epsilon$  and two fourth order poles at  $\pm i\omega_X$ , pictured on Fig. 6.3.1. From (6.3.8) we see that we have to close the integration path (Jordan loop) in the lower half of the complex plane for  $t > 0$ , and in the upper half of the plane for  $t < 0$ .

It can be checked that the residues of  $h_\epsilon(\omega) e^{-i\omega t}$  read

$$\text{Res}(h_\epsilon(\cdot) e^{-i\cdot t}, \omega_0 - i\epsilon) = e^{-i(\omega_0 - i\epsilon)t} (a_0 + a_1 t), \quad (6.3.9a)$$

$$\text{Res}(h_\epsilon(\cdot) e^{-i\cdot t}, i\omega_X) = e^{\omega_X t} (b_0^+ + b_1^+ t + b_2^+ t^2 + b_3^+ t^3), \quad (6.3.9b)$$

$$\text{Res}(h_\epsilon(\cdot) e^{-i\cdot t}, -i\omega_X) = e^{-\omega_X t} (b_0^- + b_1^- t + b_2^- t^2 + b_3^- t^3) \quad (6.3.9c)$$



**Fig. 6.3.1** – Jordan loops in the complex  $\omega$ -plane used to compute the Fourier transform (6.3.8). The poles  $\omega_0 - i\epsilon$  and  $\pm i\omega_X$  of the integrand are represented by red circled crosses.

where the  $a_i$  and  $b_i^\pm$  coefficients depend on  $\epsilon$ . Whence the Fourier transform (6.3.8)

$$\bar{h}_\epsilon(t) = -2i\pi \left[ \theta(t) e^{-i(\omega_0 - i\epsilon)t} (a_0 + a_1 t) + \theta(t) e^{-\omega_X t} (b_0^+ + b_1^+ t + b_2^+ t^2 + b_3^+ t^3) - \theta(-t) e^{\omega_X t} (b_0^- + b_1^- t + b_2^- t^2 + b_3^- t^3) \right]. \quad (6.3.10)$$

One can then deduce  $H_\epsilon(t)$  and its limit as  $\epsilon \rightarrow 0^+$ . Setting

$$a_i \xrightarrow{\epsilon \rightarrow 0^+} A_i, \quad (6.3.11a)$$

$$b_i^\pm \xrightarrow{\epsilon \rightarrow 0^+} B_i^\pm, \quad (6.3.11b)$$

one can see that

$$\begin{aligned} B_0^+ &= B_0^{-*} \equiv B_0, \\ B_1^+ &= -B_1^{-*} \equiv B_1, \\ B_2^+ &= B_2^{-*} \equiv B_2, \\ B_3^+ &= -B_3^{-*} \equiv B_3. \end{aligned}$$

The coefficients in the residues read

$$A_0 = \frac{\omega_X^8 (\omega_X^2 - 7\omega_0^2)}{(\omega_0^2 + \omega_X^2)^5}, \quad (6.3.12a)$$

$$A_1 = -i \frac{\omega_0}{\left[ 1 + \left( \frac{\omega_0}{\omega_X} \right)^2 \right]^4} \quad (6.3.12b)$$

and

$$B_0 = -\frac{\omega_X^3 (-6\omega_0^2 + 30i\omega_0\omega_X + 48\omega_X^2)}{96(\omega_X + i\omega_0)^5}, \quad (6.3.13a)$$

$$B_1 = \frac{\omega_X^3 (-3i\omega_0^3 - 21\omega_0^2\omega_X + 51i\omega_0\omega_X^2 + 33\omega_X^3)}{96(\omega_X + i\omega_0)^5}, \quad (6.3.13b)$$

$$B_2 = -\frac{\omega_X^3 (-3i\omega_0^3\omega_X - 15\omega_0^2\omega_X^2 + 21i\omega_0\omega_X^3 + 9\omega_X^4)}{96(\omega_X + i\omega_0)^5}, \quad (6.3.13c)$$

$$B_3 = \frac{\omega_X^3 (-i\omega_0^3\omega_X^2 - 3\omega_0^2\omega_X^3 + 3i\omega_0\omega_X^4 + \omega_X^5)}{96(\omega_X + i\omega_0)^5}. \quad (6.3.13d)$$

The computation of  $H_{0+}(t)$  from (6.3.7) and (6.3.10) features no notable conceptual or technical difficulty, but is quite tedious. We only give the result, which reads

$$\begin{aligned}
H_{0+}(t) = & -i\pi \left[ \theta(t) e^{-i\omega_0 t} (A_0 + A_1 t) + \theta(t) e^{-\omega_X t} (B_0^+ + B_1^+ t + B_2^+ t^2 + B_3^+ t^3) \right. \\
& \left. - \theta(-t) e^{\omega_X t} (B_0^- + B_1^- t + B_2^- t^2 + B_3^- t^3) \right] \\
& + e^{-i\omega_0 t} \left[ -i(A_0 + A_1 t) \text{Si}(\omega_0 t) + \frac{2}{\omega_0} A_1 \sin(\omega_0 t) - (A_0 + A_1 t) \left( \text{Ci}(\omega_0 t) + i\frac{\pi}{2} \right) - \frac{i}{\omega_0} A_1 e^{i\omega_0 t} \right] \\
& - \left[ (B_0^* - B_1^* t + B_2^* t^2 - B_3^* t^3) e^{-\omega_X t} \text{Ei}(\omega_X t) + (B_0 + B_1 t + B_2 t^2 + B_3 t^3) e^{\omega_X t} \text{Ei}(-\omega_X t) \right] \\
& - \frac{1}{\omega_X} \left[ (B_1 + B_1^*) - (B_2 + B_2^*) t + 2(B_3 + B_3^*) t^2 \right] - \frac{1}{\omega_X^2} \left[ (B_2 - B_2^*) \omega_X t + 2(B_3 - B_3^*) t \right] - \frac{1}{\omega_X^3} (B_3 + B_3^*) \omega_X^2 t^2.
\end{aligned} \tag{6.3.14}$$

Here Ei stands for the exponential integral

$$\text{Ei}(x) \equiv - \int_{-x}^{+\infty} du \frac{e^{-u}}{u}. \tag{6.3.15}$$

We then have to add three such terms as prescribed by (6.3.6), so as to obtain the exact expression for the survival probability as given by first-order time-dependent perturbation theory. It is noteworthy that the identity

$$A_0 + B_0 + B_0^* = 0 \tag{6.3.16}$$

results in the cancellation of all singular terms. As seen from (6.3.9), the quantity  $A_0 + B_0 + B_0^*$  is, up to a factor of  $\pm 2i\pi$ , equal to the integral of  $h_{0+}$  over any closed curve  $\Gamma$  circling around the three poles of  $h_{0+}$  (see Fig. 6.3.1). We can take  $\Gamma$  to be a circle of radius  $R$  centred around  $z = 0$ . Since for large  $\omega$ ,  $h_{0+}$  behaves as  $\omega^{-9}$ , we see from Jordan's *lemmata* that the integral of  $h_{0+}$  over such a curve vanishes when  $R \rightarrow +\infty$  (and hence for any  $R$  large enough that the circle will still enclose the three poles), whence (6.3.16).

With the help of (6.3.16) we can finally write, from (6.3.6) and (6.3.14),

$$\begin{aligned}
I_F(t) = & \frac{1}{t^2} \left\{ -2A_0 \left( \log \left( \frac{\omega_0}{\omega_X} \right) - \text{Ci}(\omega_0 |t|) \right) + i\pi (B_0 - B_0^*) + A_1 \left[ -4 \frac{i}{\omega_0} \sin^2 \left( \frac{\omega_0 t}{2} \right) + i\pi t \left( \text{sgn}(t) + \frac{2}{\pi} \text{Si}(\omega_0 t) \right) \right] \right. \\
& + i\pi \left[ e^{-\omega_X t} \theta(t) \left[ (B_0^* e^{i\omega_0 t} - B_0 e^{-i\omega_0 t}) + (-B_1^* e^{i\omega_0 t} + B_1 e^{-i\omega_0 t}) t \right. \right. \\
& \quad \left. \left. + (B_2^* e^{i\omega_0 t} - B_2 e^{-i\omega_0 t}) t^2 + (-B_3^* e^{i\omega_0 t} + B_3 e^{-i\omega_0 t}) t^3 \right] \right. \\
& \left. + e^{\omega_X t} \theta(-t) \left[ (B_0^* e^{-i\omega_0 t} - B_0 e^{i\omega_0 t}) - (-B_1^* e^{-i\omega_0 t} + B_1 e^{i\omega_0 t}) t \right. \right. \\
& \quad \left. \left. + (B_2^* e^{-i\omega_0 t} - B_2 e^{i\omega_0 t}) t^2 - (-B_3^* e^{-i\omega_0 t} + B_3 e^{i\omega_0 t}) t^3 \right] \right] \\
& + e^{-\omega_X t} \text{Ei}(\omega_X t) \left[ (B_0^* - B_1^* t + B_2^* t^2 - B_3^* t^3) e^{i\omega_0 t} + (B_0 - B_1 t + B_2 t^2 - B_3 t^3) e^{-i\omega_0 t} \right] \\
& + e^{\omega_X t} \text{Ei}(-\omega_X t) \left[ (B_0^* + B_1^* t + B_2^* t^2 + B_3^* t^3) e^{-i\omega_0 t} + (B_0 + B_1 t + B_2 t^2 + B_3 t^3) e^{i\omega_0 t} \right] \\
& + \frac{2}{\omega_X^3} \left[ -2 \left( (B_1 + B_1^*) \omega_X^2 - (B_2 + B_2^*) \omega_X + 2(B_3 + B_3^*) \right) \sin^2 \left( \frac{\omega_0 t}{2} \right) \right. \\
& \quad \left. + i \left( (B_2 - B_2^*) \omega_X - (B_3 - B_3^*) \right) \omega_X t \sin(\omega_0 t) + (B_3 + B_3^*) \omega_X^2 t^2 \cos(\omega_0 t) \right] \left. \right\}.
\end{aligned} \tag{6.3.17}$$

In spite of its formidable appearance, (6.3.17) features the now familiar ‘‘seed’’ of Fermi's golden rule, namely, the quantity

$$\frac{1}{t} i\pi A_1 \left( \text{sgn}(t) + \frac{2}{\pi} \text{Si}(\omega_0 t) \right), \tag{6.3.18}$$

found on the first line on the right-hand side of (6.3.17). Notice from (6.3.12) that in the dipole limit  $\omega_0/\omega_X \rightarrow 0$ , one has  $A_1 = -i\omega_0$ , and one retrieves, from (6.3.2), the decay constant given by Fermi's golden rule in the dipole approximation. Keeping  $\omega_X$  to its actual value, we find a relative error  $|iA_1 - \omega_0|/\omega_0 = 1.33 \times 10^{-5}$ . With  $\omega_X$  and

thus  $A_1$  kept to their actual value, our decay constant

$$\Gamma = 2 \frac{i}{\pi} \left( \frac{2}{3} \right)^9 \alpha^3 A_1 \quad (6.3.19)$$

matches that found by Facchi and Pascazio [10], who treated the problem nonperturbatively, by finding the resolvent for the Hamiltonian of the system in the Laplace domain and then getting back to the time domain. All the other terms in (6.3.17) are short-time deviations from Fermi's golden rule.

It is not too hard, but very tedious to show from (6.3.17), making use, of course, of (6.3.12) as well as (6.3.13), that the leading term in the Taylor series of  $t^2 I_F(t)$  at  $t = 0$  takes the very simple form  $(\omega_X t)^2 / 6$ . Whence the survival probability at very short times:

$$P_{\text{surv}}(t) \underset{t \rightarrow 0}{\sim} 1 - \frac{2^{10}}{3^9 \pi} \frac{\alpha^3}{6} (\omega_X t)^2 \quad (6.3.20)$$

as deduced from (6.3.2). This short-time expansion matches that obtained by Facchi and Pascazio [10].

Facchi and Pascazio used nonperturbative techniques to find the exact expression for the survival amplitude at all times:

$$c_e(t) = Z e^{i\zeta} e^{i(\omega_{\text{LS}} + \frac{1}{2}\Gamma)t} + y_e(t). \quad (6.3.21)$$

This expression is intimately linked to the analytical properties of the so-called self-energy in the energy plane. This self-energy function is a multivalued function of the energy, as illustrated by its having a branch cut in the energy plane. It also has a pole in the second Riemann sheet, from which the first summand on the right-hand side of (6.3.21) originates. Here  $\omega_{\text{LS}}$  is the partial Lamb shift [10] of the excited 2p level due to the 1s level and  $\Gamma$  is the decay rate (6.3.19). The numerical factor  $Z e^{i\zeta}$  is very close to unity. The second summand reads

$$y_e(t) = \left( \frac{\lambda}{\omega_X t} \right)^2 \int_0^{+\infty} du \frac{u e^{-u}}{\left[ 1 - \left( \frac{u}{\omega_X t} \right)^2 \right]^4} \frac{1}{\left[ \frac{\lambda^2}{\omega_X t} - i \frac{\omega_0}{\omega_X} - \lambda^2 Q \left( -\frac{u}{\omega_X t} \right) \right]} \frac{1}{\left[ \frac{\lambda^2}{\omega_X t} - i \frac{\omega_0}{\omega_X} - \lambda^2 Q_{\text{R2}} \left( -\frac{u}{\omega_X t} \right) \right]} \quad (6.3.22)$$

where

$$\lambda^2 = \frac{2}{\pi} \left( \frac{2}{3} \right)^9 \alpha^3 \simeq 6.4 \times 10^{-9} \quad (6.3.23)$$

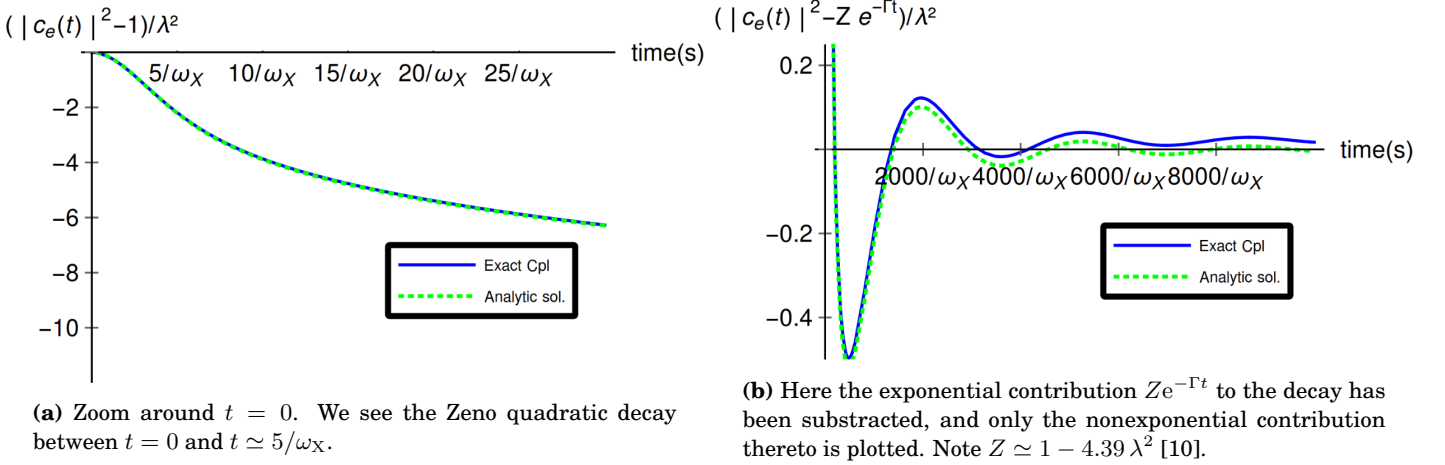
and

$$Q(s) = \frac{15i\pi(-1 + s^4) - 8((11 - 6i\pi) + 9s^4)s - 3i\pi(15 + s^4)s^2 + 16(9 + s^4)s^3 - 96s \log(s)}{96(1 - s^2)^4}, \quad (6.3.24a)$$

$$Q_{\text{R2}} = Q(s) + 2i\pi \frac{s}{(1 - s^2)^4}. \quad (6.3.24b)$$

The second summand on the right-hand side of (6.3.21) can thus be written explicitly but the integral on the right-hand side of (6.3.22) must be computed numerically. This second summand, which comes from the branch cut in the energy plane, is relevant both at very short times, which are of interest to us here, as well as at very long times ( $t \gg 1/\Gamma$ ) which we will not consider here. In both these time regimes,  $y_e$  becomes non-negligible and the decay is therefore nonexponential.

As shown on Figs. 6.3.2a and 6.3.2b, the agreement between our perturbative treatment and the exact solution (6.3.21) is very good. We can therefore use our method to investigate the short-time behaviour of this system in more detail.



**Fig. 6.3.2** – Behaviour of the survival probability  $|c_e(t)|^2$  with the exact coupling as given by the perturbative solution (6.3.17) (solid blue), and Facchi and Pascazio’s exact solution [10] (dashed green). Facchi and Pascazio define the dimensionless constant  $\lambda^2$  as given by (6.3.23). The time axis is graduated in terms of  $1/\omega_X = 1.18 \times 10^{-19}$  s.

The survival probability (6.3.2) is plotted in Fig. 6.3.3. We see that the maximal deviation from Fermi’s golden rule is of order  $10^{-8}/10^{-7}$ . For the system under study here, the golden rule is thus valid to an excellent approximation.

To illustrate the transition between the Zeno regime (6.3.20) and Fermi’s golden rule as predicted by our treatment, we plot in Fig. 6.3.4 the decay probability as given by (6.3.17) as well as the short-time expansion (6.3.20) and the linear prediction of the golden rule. Note that the transition between the Zeno and Fermi regimes takes place around  $10^{-17}$  s after the start of the decay and that after  $10^{-15}$  s, the behaviour of the system is completely indistinguishable from that predicted by the golden rule.

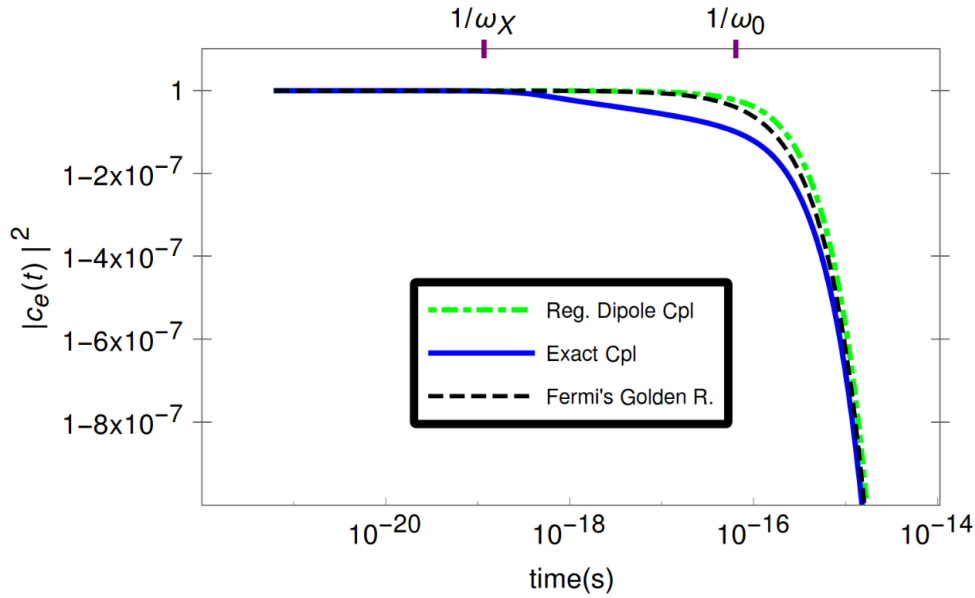
## 6.4 Bonus: the ideal cutoff frequency for the dipole approximation

While the regularisation procedure of sect. 6.2.2 provides a nicely cutoff-independent treatment of the problem in the framework of the dipole approximation, and yields a result which is in agreement with Fermi’s golden rule at “long times”, the predictions it yields on the very short time dynamics of the system are inadequate. Namely, it does not provide the correct dynamics in the Zeno regime, as seen on Fig. 6.3.4. We might ask, however, how the predictions of the dipole approximation fare when the regularisation is performed more directly—and, arguably, less elegantly—via the introduction of a cutoff, as presented in sect. 6.2.1. The very short time behaviour yielded by the truncated integral (6.2.4) follows

$$1 - \frac{2^{10}}{3^9 \pi} \alpha^3 t^2 \int_0^{\omega_C} d\omega \omega \operatorname{sinc}^2 \left[ (\omega_0 - \omega) \frac{t}{2} \right] \underset{t \rightarrow 0}{\sim} 1 - \frac{2^{10}}{3^9 \pi} c^2 \frac{\alpha^3}{2} (\omega_C t)^2. \quad (6.4.1)$$

Remember that in the case of the exact coupling, the Zeno behaviour is given by (6.3.20). We can then choose the cutoff frequency of the dipole approximation so that the very short time predictions of the dipole approximation, with cutoff, match the exact short-time dynamics of the system. Comparison of (6.3.20) with (6.4.1) shows that a perfect match is reached if we choose

$$\omega_C \equiv \frac{\omega_X}{\sqrt{3}} = \frac{\sqrt{3}}{2} \frac{c}{a_0} \simeq .866 \frac{c}{a_0}. \quad (6.4.2)$$



**Fig. 6.3.3** – Decay of the survival probability  $|c_e(t)|^2$  with the regularised dipole-approximated coupling (plotted for exhaustiveness) as given by expression (6.2.21) (dot-dashed green), the exact coupling as given by expression (6.3.17) (solid blue) and Fermi’s golden rule (dashed black). The time axis is logarithmic.

In Fig. 6.4.1 we compare the predictions of the dipole approximation, with the carefully picked cutoff frequency (6.4.2), with the predictions obtained with the exact atom-field coupling. It is interesting, and quite impressive, that while the dipole approximation here was made to fit, by a simple choice of the cutoff frequency, the exact Zeno dynamics of the system, we see that with our choice for the cutoff, we obtain an excellent agreement during the transition between the Zeno and Fermi regimes<sup>4</sup>. Hence we can conclude that for the  $2p - 1s$  transition in atomic Hydrogen, the dynamics of the electronic decay is very well described at all times within the framework of the dipole approximation, if one makes the “correct” choice (6.4.2) for the cutoff.

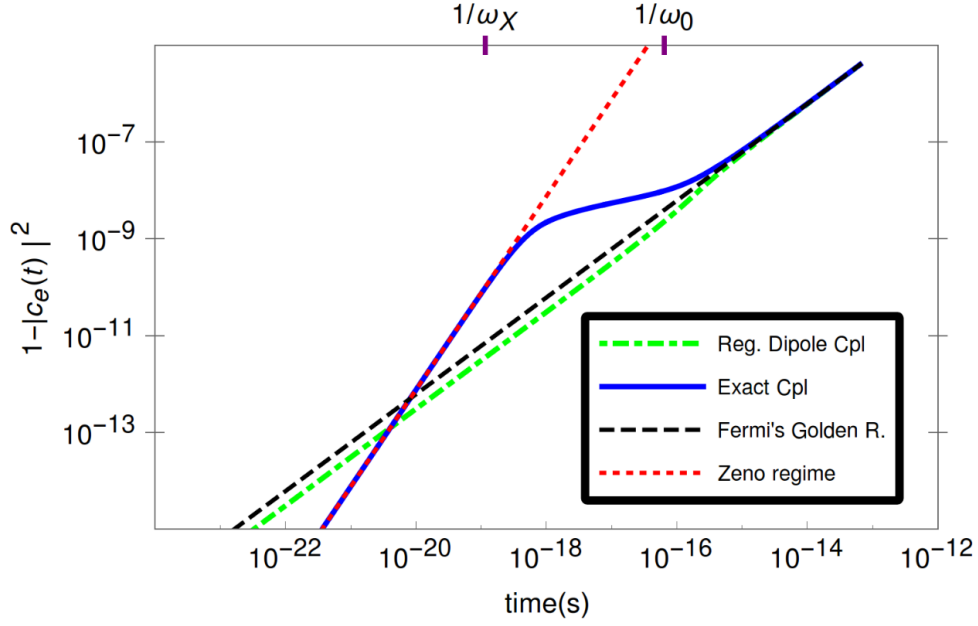
## 6.5 Discussion

For the  $2p - 1s$  transition in atomic Hydrogen, Fermi’s rule that predicts a linear decay of the survival probability can, indeed, be called “golden”. The maximal deviation from the golden rule is of order  $10^{-8}/10^{-7}$ , as seen on Figs. 6.3.3 and 6.3.4. This shows that Fermi’s golden rule is more solid than its rather delicate derivation, which, as argued in sect. 6.1.5, requires a discussion of time regimes.

There is no reason to think that much larger deviations from the golden rule could not be found in other physical systems. The square cardinal sine integral in (6.1.42) tells us that with an enhanced coupling between a two-level system and (electromagnetic) modes which are off-resonant with the transition frequency of the two-level system, one would witness more important deviations from the golden rule.

In [10] Facchi and Pascazio considered the ratio between the Zeno time  $t_Z$  defined by (II.6) and the lifetime  $1/\Gamma$  of the excited level as the relevant parameter for the observability of Zeno deviations from Fermi’s golden rule. We argue that the relevant ratio is that between the “cutoff time”  $t_X$  and the Zeno time  $t_Z$ . The cutoff time is understood to be defined so that after  $t_X$ , the system exits the Zeno regime in which the survival probability decays quadratically. Therefore, at  $t = t_X$ , we have  $P_{\text{surv}}(t) = 1 - (t_X/t_Z)^2$ , and the strength of the Zeno decay is

<sup>4</sup>We also obtain an excellent agreement in the Fermi regime, but that was to be expected. The agreement is not perfect, though, as the decay constant in the exact and dipole coupling are slightly different. See the discussion below (6.3.18).



**Fig. 6.3.4** – Behaviour of the decay probability  $1 - |c_e(t)|^2$  with the regularised dipole-approximated coupling (plotted for exhaustiveness) as given by expression (6.2.21) (dot-dashed green), the exact coupling as given by expression (6.3.17) (solid blue), Fermi's golden rule (dashed black), and the Zeno behaviour (6.3.20) (dotted red). Both axes are logarithmic.

given by  $t_X/t_Z$ . This is confirmed by looking at Fig. 6.3.4, which shows that the maximal discrepancy between the predictions of the golden rule and the actual dynamics of the system is reached approximately at the moment when the system exits the Zeno regime. The general method to obtain the Zeno time  $t_Z$  is given in the introduction to the present Part II of this work. Another discussion of the Zeno regime can be found in [11], where it is also noted that the duration of the Zeno regime is much shorter than the Zeno time  $t_Z$ , and the possibility of anti-Zeno behaviour is discussed.

For hydrogen-like atoms with  $Z$  protons, the Zeno time scales, as noted in [10], like  $Z^{-2}$ . For such systems, since the Bohr radius scales like  $Z^{-1}$ , the cutoff frequency scales like  $Z$ , and the cutoff time like  $Z^{-1}$ , so that the ratio  $t_X/t_Z$  scales like  $Z$ , while Facchi and Pascasio's parameter ( $t_Z/t_E$ ) scales like  $Z^2$ .

A very convincing method to define the relevant parameter in the observability in the Zeno region is given in [12]. The authors use time-dependent perturbation theory up to fourth order in time. The survival probability of the initial state is written as

$$\begin{aligned}
 P_{\text{surv}}(t) &= \left| \langle \psi(t=0) | e^{-\frac{i}{\hbar} \hat{H} t} | \psi(t=0) \rangle \right|^2 \\
 &= \left| \langle \psi(t=0) | 1 - \frac{i}{\hbar} \hat{H} t - \frac{1}{2\hbar^2} \hat{H}^2 t^2 + \frac{i}{\hbar} \hat{H}^3 t^3 + \frac{1}{24\hbar^2} \hat{H}^4 t^4 | \psi(t=0) \rangle \right|^2 + O(t^6) \\
 &= 1 - \left( \frac{t}{\hbar} \right)^2 \left( \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 \right) + \left( \frac{t}{\hbar} \right)^4 \left( \frac{1}{12} \langle \hat{H}^4 \rangle - \frac{1}{3} \langle \hat{H}^3 \rangle \langle \hat{H} \rangle + \frac{1}{4} \langle \hat{H}^2 \rangle^2 \right) + O(t^6) \quad (6.5.1)
 \end{aligned}$$

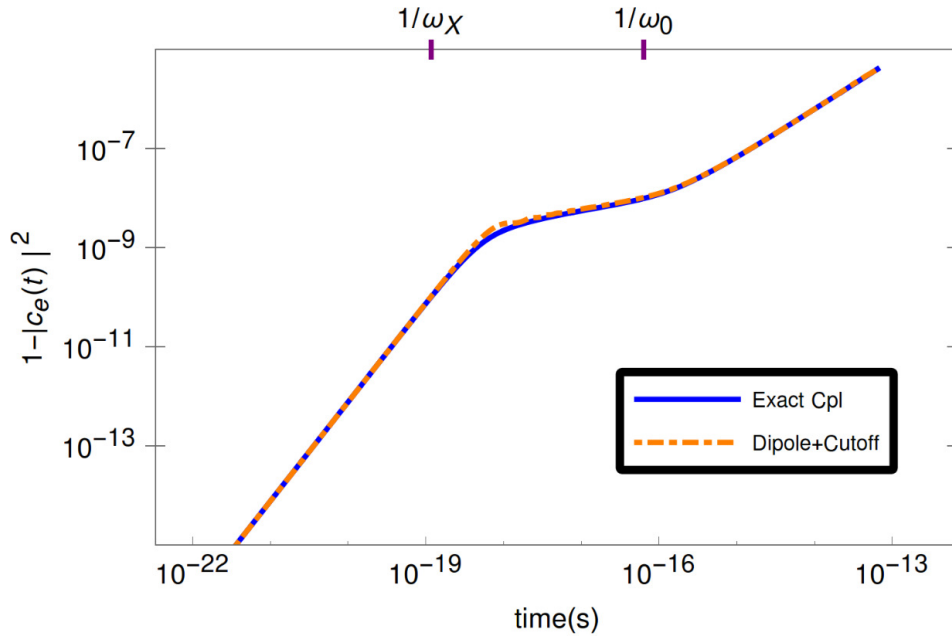
where the expectation values  $\langle \cdot \rangle$  are taken in the initial state  $|\psi(t=0)\rangle$ . In the weak-coupling limit they were able to find [12] that

$$P_{\text{surv}}(t) = 1 - \lambda^2 I_0 (\omega_X t)^2 + \lambda^2 \frac{I_2}{12} (\omega_X t)^4 + O(t^6) \quad (6.5.2)$$

with the integrals

$$I_j \equiv \frac{1}{(\lambda \hbar)^2} \sum_{\lambda=\pm} \int d\tilde{k} \left( \frac{c \|\mathbf{k}\|}{\omega_X} \right)^j |G_\lambda(\mathbf{k})|^2 \quad (6.5.3)$$





**Fig. 6.4.1** – Behaviour of the decay probability  $1 - |c_e(t)|^2$  with the exact coupling as given by expression (6.3.17) (solid blue) and the dipole-approximated coupling with cutoff frequency  $\omega_C = \omega_X/\sqrt{3}$  as given by expression (6.2.4) (dot-dashed orange). Both axes are logarithmic.

with the coupling constant  $\lambda$  defined at (6.3.23). Then it is easily seen when the system exits the Zeno regime, namely, as soon as the quartic in term in (6.5.2) becomes comparable to the quadratic term. It is then possible to give an expression for the cutoff time  $t_X$  (which the authors of [12] call the Zeno time, but we stick to our convention here): inspection of (6.5.2) yields

$$t_X = \frac{2}{\omega_X} \sqrt{3 \frac{I_0}{I_2}}. \quad (6.5.4)$$

With this analysis one finds [12]  $t_X = 5.8 \times 10^{-19}$  s for the  $2p - 1s$  transition in atomic Hydrogen, very much in accordance with our own results (see Fig. 6.3.4). Then we use (6.5.4) to assess the strength of the Zeno decay: when the system exits the parabolic Zeno regime, the excited state of the system has been depleted—in terms of expectation value—of

$$\left( \frac{t_X}{t_Z} \right)^2 = 12\lambda^2 \frac{J_0^2}{I_2}. \quad (6.5.5)$$

This means that for the Zeno decay to be strong—and hopefully observable—we must find a system with “high” coupling constant  $\lambda^2$  (but not too high, as  $\lambda^2$  must be much smaller than 1 in order for the weak-coupling limit to be relevant) and, according to (6.5.3), enhanced coupling to the environmental modes which are smaller than the cutoff frequency. Both these requirements are rather tautological in a sense, but the analysis of [12] gives quantitative indications as to their importance. The cutoff time (6.5.4) after which the system exits the Zeno regime of quadratic decay, and the strength (6.5.5) of the Zeno regime are, we argue, the two key quantities as far as the experimental observability of the Zeno regime is concerned. A “large” cutoff time is favourable for obvious reasons pertaining to the time resolution of observations, while a strong decay is also favourable for no less obvious reasons.

In atomic physics the interaction Hamiltonian is often taken to be of the usual  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  form instead of the minimal  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  form. This usual interaction Hamiltonian is obtained [2] from the minimal one by a unitary transformation. For the physical predictions of the theory to remain unchanged, this unitary transformation should also be made to act on the quantum states of the system, which it usually is not [2]. It is then argued [7] that this is not a problem since for electromagnetic frequencies which are resonant with atomic transitions, the results remain

the same. This argument is only relevant at long enough times though, when Fermi's golden rule selects the relevant electromagnetic frequencies to be these resonant frequencies. At very short times, on the other hand, the predictions of the  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  interaction Hamiltonian are completely different from that of  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$ . In the case of the Hydrogen  $2p - 1s$  transition at hand, the difference is the following: in the dipole approximation<sup>5</sup>, the integrand in the integral corresponding to (6.2.2) in the  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  case is equal to  $(\omega/\omega_0)^2$  times the integrand in (6.2.2). The divergence of the integral is therefore quadratic instead of logarithmic as a function of the cutoff frequency of the dipole approximation. When we try and regularise this divergence in the  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  case using the same procedure as that presented in sect. 6.2.2 for the  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  case, several extra singular terms appear in the sister expression to (6.2.18). When we extracted the regular terms, we obtained an expression very similar to (6.2.21), with two extra terms that feature, respectively, the Cauchy principal value of  $1/t$  and the Hadamard principal part of  $1/t^2$ .

## 6.A Some useful results of distribution theory

In this appendix we provide proofs for two interesting results of distribution theory. In sect. 6.A.1 we prove the Plemelj-Sochocki theorem, which is used in sects. 3.A and 5.2.3.2. In sect. 6.A.2 we compute the Fourier transform of the Heaviside step distribution.

### 6.A.1 The Plemelj-Sochocki theorem

Remember the definition of the Cauchy principal value of the integral of a function of the type  $x \mapsto f(x)/(x-x_0)$ : for  $a < x_0 < b$ , the principal value integral is

$$\text{vp} \int_a^b dx \frac{f(x)}{x-x_0} \equiv \lim_{\epsilon \rightarrow 0^+} \left( \int_a^{x_0-\epsilon} dx \frac{f(x)}{x-x_0} + \int_{x_0+\epsilon}^b dx \frac{f(x)}{x-x_0} \right). \quad (6.A.1)$$

Principal value integration is a means to make sense of an undefined integral of the type

$$\int_a^b dx \frac{f(x)}{x-x_0} \quad (6.A.2)$$

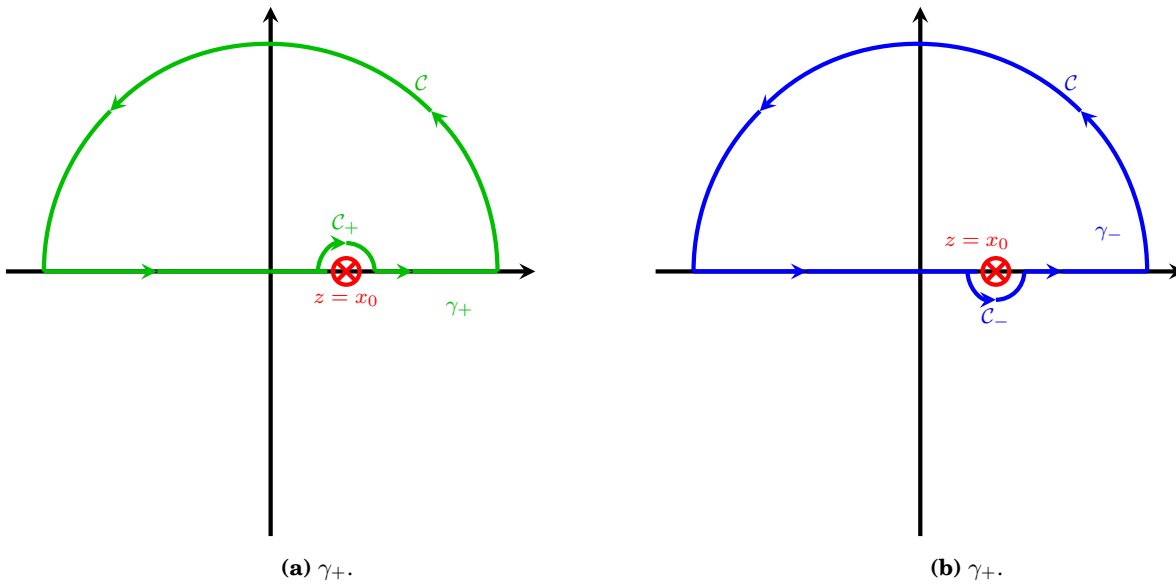
which diverges unless  $f(x_0) = 0$ . Another way to make sense of (6.A.2) consists in introducing a real parameter  $\eta > 0$  to compute

$$\int_a^b dx \frac{f(x)}{x-x_0 \pm i\eta} \quad (6.A.3)$$

and taking the limit  $\eta \rightarrow 0^+$  at the end. The fact that the results yielded by these two different regularisation methods are linked through a simple relation is the nontrivial content of the Sochocki-Plemelj theorem. To see this, consider [8] two integration paths, drawn on Fig.6.A.1. Assume that, as a function of the complex variable  $z$ ,  $f$  decays quickly enough as  $|z| \rightarrow +\infty$  so that the integral of  $f(z)/(z-x_0)$  over the large half-circle  $\mathcal{C}$  (see Fig. 6.A.1) vanishes at the radius of that half-circle increases. We are then left with

$$\begin{aligned} \int_{\gamma_{\pm}} dz \frac{f(z)}{z-x_0} &= \int_{-\infty}^{x_0-\epsilon} dx \frac{f(x)}{x-x_0} + \int_{x_0+\epsilon}^{+\infty} dx \frac{f(x)}{x-x_0} + \int_{\mathcal{C}_{\pm}} dz \frac{f(z)}{z-x_0} \\ &= \int_{-\infty}^{x_0-\epsilon} dz \frac{f(x)}{x-x_0} + \int_{x_0+\epsilon}^{+\infty} dx \frac{f(x)}{x-x_0} + \int_{\pi}^{\pi(1 \mp 1)} d\theta \frac{f(x_0 + \epsilon e^{i\theta})}{\epsilon e^{i\theta}} i\epsilon e^{i\theta} \\ &= \int_{-\infty}^{x_0-\epsilon} dx \frac{f(x)}{x-x_0} + \int_{x_0+\epsilon}^{+\infty} dx \frac{f(x)}{x-x_0} + i \int_{\pi}^{\pi(1 \mp 1)} d\theta f(x_0 + i\epsilon e^{i\theta}) \\ &\xrightarrow{\epsilon \rightarrow 0^+} \text{vp} \int_{-\infty}^{+\infty} dx \frac{f(x)}{x-x_0} \mp i\pi f(x_0) \end{aligned} \quad (6.A.4)$$

<sup>5</sup>The dipole approximation is already included in the  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  form, the exact expression being much more complicated.



**Fig. 6.A.1** – Integration contours in the complex plane used for the proof of the Sochocki-Plemelj theorem. The small half-circles  $C_{\pm}$  have the same radius  $\epsilon$ .

where we made use of definition (6.A.1). Now notice that

$$\begin{aligned}
 \int_{\gamma_{\pm}} dz \frac{f(z)}{z - x_0} &= \lim_{\eta \rightarrow 0^+} \int_{\gamma_{\pm}} dz \frac{f(z)}{z - x_0 \pm i\eta} \\
 &= \lim_{\eta \rightarrow 0^+} \left[ \int_{-\infty}^{+\infty} dx \frac{f(x)}{x - x_0 \pm i\eta} + \int_C dz \frac{f(z)}{z - x_0 \pm i\eta} \right] \\
 &= \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{+\infty} dx \frac{f(x)}{x - x_0 \pm i\eta}.
 \end{aligned} \tag{6.A.5}$$

Indeed when the pole at  $x_0$  is shifted by  $\pm i\eta$ , the contour  $\gamma_{\pm}$  can be freely deformed, according to Cauchy's integral theorem (the deformation does not affect which poles are enclosed by the contour). By equating (6.A.4) and (6.A.5), the Sochocki-Plemelj theorem is established:

$$\lim_{\eta \rightarrow 0^+} \frac{1}{x - x_0 \pm i\eta} = \text{vp} \frac{1}{x - x_0} \mp i\pi \delta(x - x_0). \tag{6.A.6}$$

This is the link between the two regularisations of the ill-defined integral (6.A.2), namely, the principal value integration (6.A.1) and the parametrisation (6.A.3).

## 6.A.2 Fourier transform of the Heaviside step distribution

In this manuscript we compute several quantities of the type

$$F(\omega) \equiv \int_0^{+\infty} dt e^{-i\omega t} f(\omega, t). \tag{6.A.7}$$

Such integrals are often troublesome because the integration runs only from 0 to  $+\infty$ . Hence complex integration techniques are generally not directly useful. But rewriting (6.A.7) as

$$F(\omega) = \int_{-\infty}^{+\infty} dt e^{-i\omega t} \theta(t) f(\omega, t) \tag{6.A.8}$$

comes in very handy, as we can make use of the folding theorem which states that

$$F(\omega) = \frac{1}{2\pi} \left[ \int_{-\infty}^{+\infty} dt e^{-i\omega t} \theta(t) * \int_{-\infty}^{+\infty} du e^{-i\omega u} f(\cdot, u) \right] (\omega) \quad (6.A.9)$$

where the convolution is made on the “dot variable”. In general

$$\bar{f}(\omega) = \int_{-\infty}^{+\infty} dt e^{-i\omega t} f(\omega, t)$$

which appears in (6.A.9), is easier to compute than (6.A.8)—it is usually computed through Cauchy’s residue theorem—and can then be convoluted with the Fourier transform of the Heaviside step distribution, which can be found by the use of two simple theorems of distribution theory, which we will use as *lemmata*:

1. The solutions to the distributional equation  $xT(x) = 0$  are all the distributions proportional to the Dirac delta distribution. Indeed

$$\int_{-\infty}^{+\infty} dx x \delta(x) \varphi(x) = 0. \quad (6.A.10)$$

2. The nonhomogeneous solution to the distributional equation  $xT(x) = 1$  is the Cauchy principal value of  $1/x$ . Indeed

$$\text{vp} \int_{-\infty}^{+\infty} dx x \frac{\varphi(x)}{x} = \int_{-\infty}^{+\infty} dx \varphi(x). \quad (6.A.11)$$

Then remember that the Fourier transform of the Dirac delta distribution is the constant function 1. Since the Dirac delta distribution is the derivative of the Heaviside step distribution, the properties of the Fourier transform under differentiation tell us that

$$i\omega \bar{\theta}(\omega) = 1, \quad (6.A.12)$$

whence, from our two *lemmata* above

$$\bar{\theta}(\omega) = \alpha \delta(\omega) - i \text{vp} \frac{1}{\omega}. \quad (6.A.13)$$

Here  $\alpha$  is a complex number to be determined. This is done [8] by noticing that, since  $\theta - 1/2$  is an odd function, its Fourier transform  $\bar{\theta} - 2\pi\delta/2$  should be an odd function too, whence  $\alpha = \pi$  (since  $\delta$  is even and the principal value is odd). Finally

$$\boxed{\bar{\theta}(\omega) = \pi \delta(\omega) - i \text{vp} \frac{1}{\omega}}. \quad (6.A.14)$$

And thus, according to the folding theorem (6.A.9)

$$\begin{aligned} F(\omega) &= \frac{1}{2} \left[ \left( \delta(\cdot) - \frac{i}{\pi} \text{vp} \frac{1}{\cdot} \right) * \bar{f}(\cdot) \right] (\omega) \\ &= \frac{1}{2} \bar{f}(\omega) - \frac{i}{2\pi} \text{vp} \int_{-\infty}^{+\infty} \frac{d\sigma}{\omega - \sigma} \bar{f}(\sigma). \end{aligned} \quad (6.A.15)$$

# REFERENCES

---

## Books

- [1] J.D. Jackson, *Classical Electrodynamics*, 2nd ed. (John Wiley & Sons, 1975) (cit. on p. 147).
- [2] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, *Photons et atomes - Introduction à l'électrodynamique quantique*, 2nd ed. (EDP Sciences/CNRS Éditions, 2001) (cit. on pp. 147, 148, 156, 165, 166).
- [3] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Mécanique Quantique*, 2nd ed., Vol. 1 (Hermann, 1996) (cit. on pp. 148, 150).
- [4] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Mécanique Quantique*, 2nd ed., Vol. 2 (Hermann, 1996) (cit. on pp. 152, 153).
- [5] B.G. Englert, *Lectures On Quantum Mechanics*, Vol. 3 (World Scientific, 2006) (cit. on pp. 152, 153).
- [6] M. Le Bellac, *Quantum Physics* (Cambridge University Press, 2006) (cit. on p. 153).
- [7] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, *Processus d'interaction entre photons et atomes*, 2nd ed. (EDP Sciences/CNRS Éditions, 2001) (cit. on p. 166).
- [8] W. Appel, *Mathematics for Physics & Physicists*, 1st ed. (Princeton University Press, 2007) (cit. on pp. 166, 168).

## Articles

- [9] M.I. Shirokov, 'Signal velocity in quantum electrodynamics', *Sov. Phys. Usp.* **21**, 345 (1978) (cit. on pp. 145, 154).
- [10] P. Facchi and S. Pascazio, 'Temporal behavior and quantum Zeno time of an excited state of the hydrogen atom', *Phys. Lett. A* **241**, 139 (1998) (cit. on pp. 162–165).
- [11] P. Facchi, H. Nakazato and S. Pascazio, 'From the Quantum Zeno to the Inverse Quantum Zeno Effect', *Phys. Rev. Lett.* **86**, 2699 (2001) (cit. on p. 164).
- [12] I. Antoniou, E. Karpov, G. Pronko and E. Yarevsky, 'Quantum Zeno and anti-Zeno effects in the Friedrichs model', *Phys. Rev. A* **63**, 062110 (2001) (cit. on p. 165).

## Theses

- [13] P. Facchi, *Quantum Time Evolution: Free and Controlled Dynamics*, PhD Thesis (Università degli Studi di Bari, 2000) (cit. on p. 151).

## CHAPTER 7

---

# CAUSALITY IN SPONTANEOUS EMISSION AND HEGERFELDT'S THEOREM

---

*“But I don’t mind losing you this time  
I’ll meet you coming backwards, I’ll meet you coming back  
When the universe has expanded, time will contract, you’ll come back  
And I’ll meet you coming backwards.”*

Franz Ferdinand’s Alex Kapranos in “The Universe Expanded”, **Right Thoughts, Right Words, Right Action**  
(Domino, 2013)

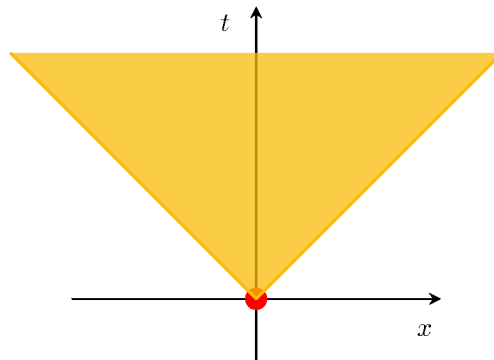
In this final chapter we turn to the other aspect of spontaneous emission: the dynamics of the emitted electromagnetic field. Focusing on the spacetime dependence of a relevant matrix element of the electric field operator, which we compute very carefully, we find a noncausal result. We identify three distinct sources for this noncausality, one of which is well known in the literature: Hegerfeldt’s theorem, which we introduce in sect. 7.1. Sect. 7.2 features the derivation of the emitted electric field, and sect. 7.3 is a discussion of our findings. In sect. 7.A we introduce the Paley-Wiener theorem, which is the background for Hegerfeldt’s theorem.

---

### Contents of the Chapter

7.1	Hegerfeldt’s theorem as a Paley-Wiener theorem . . . . .	172
7.1.1	The free case: propagation of a single-particle state . . . . .	172
7.1.2	The interacting case: the Fermi problem . . . . .	174
7.2	Photon propagation in spontaneous emission . . . . .	175
7.2.1	Wave function of the emitted photon . . . . .	175
7.2.2	Formal computation . . . . .	177
7.2.2.1	Transverse field . . . . .	178
7.2.2.2	Longitudinal field . . . . .	183
7.3	Discussion . . . . .	184
7.A	The Paley-Wiener theorem . . . . .	185

---



**Fig. 7.0.1** – Lightcone around the spacetime point  $(0, 0)$  corresponding to the time  $t = 0$  at which the decay starts, and the position  $\mathbf{x} = \mathbf{0}$  of the Hydrogen nucleus (proton).

In the previous chapter 6 we focused on the fate of the decaying atomic electron in the process of spontaneous emission. In the present chapter we switch our interest to the emitted electromagnetic field. We shall focus on a particular matrix element of the electric field operator. This operator, we remember from sect. 6.1, has a transverse and a longitudinal part. The transverse part corresponds to the familiar Riemann-Silberstein (*i.e.*,  $\beta = 1/2$ ) single-photon wave function introduced in chapter 3 (see sec. 3.4). The longitudinal part is expressed in terms of electronic wave functions and corresponds to the gradient of the Coulombian potential.

In computing the emitted electric field, we expect it to be vanishing outside of the lightcone centred on the spacetime point  $(0, 0)$  which labels the time at which the decay starts and the position of the Hydrogen nucleus, which also is the expectation value of the electron's position in its initial excited state  $|e\rangle$ . There are several (three, to be precise) reasons why this is not the case. The first one is the well-known Hegerfeldt theorem, which we present in the upcoming sect. 7.1. The Hegerfeldt theorem links the boundedness by below of the Hamiltonian of a system to the impossibility of causal propagation for that system. Remember that in sect. 5.3.4 we extended the integration domain over wave vectors to obtain a causal propagation for photons exiting a one-dimensional cavity. Hegerfeldt's theorem makes the link between this extension of the integration domain and causality explicit.

## 7.1 Hegerfeldt's theorem as a Paley-Wiener theorem

In a series of papers published in the 1970s, 1980s and 1990s, Hegerfeldt used an important result of Fourier analysis, known as the Paley-Wiener theorem, to point to the surprising inconsistency of relativistic quantum field theory with Einstein causality.

### 7.1.1 The free case: propagation of a single-particle state

Let us consider a free relativistic particle, initially localised in a volume  $V$ . By that we mean [6] that at  $t = 0$  the probability of finding the particle in  $V$  is equal to unity. For this initial condition to be possibly true is an assumption in and of itself, but this assumption is, in the case of massive particles, motivated by the existence of pointwise localised states, namely, the Newton-Wigner localised states [7]. Indeed we can use these pointwise localised states  $|\mathbf{x}_{0(s)}\rangle$ , where  $s$  stands for the spin of the massive particle, to build operators such as

$$\hat{N}(V) = \sum_s \int_V d\mathbf{x}_0 |\mathbf{x}_{0(s)}\rangle \langle \mathbf{x}_{0(s)}| \quad (7.1.1)$$

As discussed in chapter 2, Newton and Wigner found that no (pointwise) localised state exists for relativistic fields with zero mass and helicity larger equal (in absolute value) to 1 or larger. But, as presented in detail in that

same chapter 2, such pointwise localised states do in fact exist for photons. Indeed, Hawton built [8, 9] a position operator for photons with commuting components. The common eigenvectors of the three vector components are the pointwise localised states. We think that there is no reason to think that Hawton's procedure could not be extended to massless particles of higher (in absolute value) helicity, thus pointing to the—at least, formal—existence of pointwise localised states for all particles.

One-particle states localised in  $V$  (at  $t = 0$ ) then verify, by definition

$$\hat{N}(V) |\varphi(t=0)\rangle = |\varphi(t=0)\rangle. \quad (7.1.2)$$

Now let us turn to the requirement for causality as formulated by Hegerfeldt [6]. We reword it as follows: if the single-particle state is initially localised in a volume as given by (7.1.2), then at time  $t > 0$  it is **not everywhere**. As a consequence, for each  $t > 0$  one can find a distance  $r(t)$  such that, for all vectors  $\mathbf{a}$  which verify  $\|\mathbf{a}\| \geq r(t)$  a translation with vector  $\mathbf{a}$  of the system will take the single-particle state entirely out of  $V$ , making the probability of finding the particle in  $V$  equal to zero.

This requirement can seem strange at first sight, but it is simply a consequence of requiring finite propagation speed. Mathematically, it is written as

$$\hat{N}(V) \hat{U}(-\mathbf{a}) \hat{U}(t) |\varphi(t=0)\rangle = 0 \quad (7.1.3)$$

for  $\|\mathbf{a}\| \geq r(t)$  where  $\hat{U}(-\mathbf{a})$  is the translation operator of vector  $\mathbf{a}$ .

We write the initial state as

$$|\varphi(t=0)\rangle = \sum_{\sigma} \int \tilde{d}k \bar{\varphi}_{(\sigma)}(\mathbf{k}) \hat{a}_{(\sigma)}^{\dagger}(\mathbf{k}) |0\rangle \quad (7.1.4)$$

where

$$\sum_{\sigma} \int \tilde{d}k |\bar{\varphi}_{(\sigma)}(\mathbf{k})|^2 = 1. \quad (7.1.5)$$

In the general case the invariant volume  $\tilde{d}k$  on the so-called mass hyperboloid reads

$$\tilde{d}k \equiv \frac{d\mathbf{k}}{2(2\pi)^3 2\sqrt{\left(\frac{mc}{\hbar}\right)^2 + \mathbf{k}^2}}. \quad (7.1.6)$$

Computing the scalar product of (7.1.3) with the dual space state  $\langle\varphi(t=0)|$  (remember that (7.1.2) ensures  $\langle\varphi(t=0)| \hat{N}(V) = \langle\varphi(t=0)|$ ), we get the requirement that for each  $t > 0$  one can find a distance  $r(t)$  such that

$$\sum_{\sigma} \int \tilde{d}k |\bar{\varphi}_{(\sigma)}(\mathbf{k})|^2 e^{-ic\sqrt{\left(\frac{mc}{\hbar}\right)^2 + \mathbf{k}^2}t} e^{-i\mathbf{k}\cdot\mathbf{a}} = 0 \quad (7.1.7)$$

for  $\|\mathbf{a}\| \geq r(t)$ . As noted by Hegerfeldt [6], the Paley-Wiener theorem (see the appendix 7.A to the present chapter) gives a necessary condition for (7.1.7) to hold:

$$\frac{1}{\sqrt{\left(\frac{mc}{\hbar}\right)^2 + .2}} \sum_{\sigma} |\bar{\varphi}_{(\sigma)}(\cdot)|^2 e^{-ic\sqrt{\left(\frac{mc}{\hbar}\right)^2 + .2}t}$$

must be<sup>1</sup> an entire function on  $\mathbb{C}^3$ . The square roots make that impossible for more than a single value of  $t$ . As a consequence, there is no  $r(t)$  for which, for all vectors  $\mathbf{a}$  which verify  $\|\mathbf{a}\| \geq r(t)$ , (7.1.7) holds. And therefore there

<sup>1</sup>The version of the theorem presented in the appendix is a one-dimensional version of the Paley-Wiener theorem which does not apply directly here, but the theorem can be extended to higher dimensions. See [1].



is a nonzero probability to find the single-particle state everywhere for all  $t > 0$ .

## 7.1.2 The interacting case: the Fermi problem

The Paley-Wiener theorem is also relevant to interacting systems. We shall focus on the case which is of interest to us: the spontaneous emission of light by an atomic electron. The question of causality in that problem has been a recurring theme in atomic physics and quantum electrodynamics. Fermi was the first to study the electromagnetic field emitted during an atomic transition [10]. The situation he considered was the following: two atoms sit in space separated by some distance  $R$ . For the sake of simplicity they are treated as two-level atoms. One atom is initially in its excited state and the other one initially in its ground state. Fermi found that, if the survival probability of the electron of the first atom in the excited state is assumed to decay exponentially in time (that is, to follow the Wigner-Weisskopf decay law discussed in sect. 5.2.3.2), then the probability that the second atom be excited is only nonzero for times  $t > R/c$  (the instant at which the emission starts is taken to be  $t = 0$ ). This problem consisting in examining causality in spontaneous emission has thenceforth been known in the literature as the ‘‘Fermi problem’’.

It was then noticed by Shirokov [11] that Fermi’s causal result rested on an unmentioned approximation, which consisted in extending the range of integration over electromagnetic frequencies from the positive real semi-axis to the whole real axis, thereby including nonphysical electromagnetic negative frequency modes in the treatment. Notice that this is the same approximation as that we made in sect. 5.3.4 to obtain a causal result in the one-dimensional propagation of light out of a cavity (also see [12]). Hegerfeldt later [13] generalised Shirokov’s remark, linking the absence of negative electromagnetic frequencies with the noncausal field propagation via arguments similar to those of Paley and Wiener.

As mentioned above, in [10, 11, 13] the authors consider two atoms and they focus on the probability of excitation of the second atom as a function of time. We will focus on a single atom in free space, initially in its excited state, and obtain as rigorously as possible the spacetime dependence of the spontaneously emitted electromagnetic field. We now adapt Hegerfeldt’s arguments, developed to address the (two-atom) Fermi problem, to our somewhat different interrogation.

As implied just above, our investigation of causality concerns the situation studied in the previous chapter 6. We therefore use the same notations. We shall focus on the following matrix element of the electric field operator:

$$\psi(\mathbf{x}, t) \equiv \langle g, 0(t) | \hat{\mathbf{E}}(\mathbf{x}, 0) | \psi(t) \rangle \quad (7.1.8)$$

where  $|\psi(t)\rangle$  is the (Schrödinger picture) state of the system at time  $t$  and

$$\langle g, 0(t) | = e^{i\omega_g t} \langle g, 0 |. \quad (7.1.9)$$

This trivial time evolution is due to the rotating wave approximation, discussed in some detail in sec. 6.1.5. Our focusing on this particular matrix element is motivated in sect. 7.2.1. With (7.1.9) in mind we rewrite (7.1.8) as

$$\psi(\mathbf{x}, z) \equiv e^{i\omega_g z} \langle g, 0 | \hat{\mathbf{E}}(\mathbf{x}, 0) \hat{U}(z) | \psi(t=0) \rangle \quad (7.1.10)$$

We now follow Hegerfeldt’s line of argument [13]. Consider  $\psi(\mathbf{x}, \cdot)$  as a (vector-valued) function of a complex variable. Now, since

$$\hat{U}(z) = e^{-\frac{i}{\hbar} \hat{H} z} \quad (7.1.11)$$

it is clear that for  $z$  with negative imaginary part,  $\psi(\mathbf{x}, \cdot)$  is holomorphic. On the other hand, for  $z$  with positive

imaginary part, there are subtleties because the total Hamiltonian  $\hat{H}$  of the system is not bounded from above. That last point, however, is unimportant to the present discussion. The function  $\psi(\mathbf{x}, \cdot)$  being holomorphic in the (open) lower complex half plane, it is straightforward to see that Schwarz's reflected function, defined through  $\psi_{\text{Schwarz}}(\mathbf{x}, z) = \psi^*(\mathbf{x}, z^*)$ , is a holomorphic function of  $z$  in the upper complex half plane.

Now, the expectation of causality would require that  $\psi(\mathbf{x}, \cdot)$  be zero on an interval  $I$  on the real line (namely, the interval between the time  $t = 0$  when the emission starts and the time  $t = \|\mathbf{x}\|/c$  when the point  $(t, \mathbf{x})$  enters the lightcone centred on the spacetime point  $(0, \mathbf{0})$  where  $\mathbf{x} = \mathbf{0}$  is the position of the Hydrogen nucleus, but the particular boundaries of that interval are not relevant to the argument). The function  $\psi(\mathbf{x}, \cdot)$  being holomorphic in the (open) lower complex half plane and  $\psi_{\text{Schwarz}}(\mathbf{x}, \cdot)$  being holomorphic in the (open) upper complex half plane, it is a matter of a few complex analysis arguments, centred on an application of Morera's theorem, to conclude that  $\psi(\mathbf{x}, \cdot)$  is holomorphic on the interval  $I$ .

But since we required  $\psi(\mathbf{x}, \cdot)$  to be identically zero on  $I$ , its being holomorphic on that same interval means that it will be zero for all values of  $z$ , including the whole real axis. And then the matrix element (7.1.8) of the electric field operator is always zero. This is very counter-intuitive, and there is a way around it: one can waive the requirement that  $\psi(\mathbf{x}, \cdot)$  vanish on any interval  $I$ . But that means that the propagation is noncausal, as the matrix element (7.1.8) of the electric field operator is then nonzero everywhere in space for all  $t > 0$ . We now show that this second alternative is the relevant one in the framework of spontaneous emission.

## 7.2 Photon propagation in spontaneous emission

In the rest of the chapter, we will use (a variation on) the Riemann-Silberstein photon wave function (see chapter 3) to investigate the spontaneous emission of light during the  $2p - 1s$  transition in atomic Hydrogen. We will focus on the question of causality.

It is interesting to note that in [14], Sipe used the problem of spontaneous decay and light emission to discriminate, through considerations on causality, between different candidates for the photon wave function. Our investigation here will flow along similar lines, but in the opposite direction. We will indeed use the photon wave function as a tool to investigate the spontaneous emission of light during the atomic transition at hand.

### 7.2.1 Wave function of the emitted photon

The photon wave function is obtained through Glauber's extraction rule which, when states and operators are defined in the Schrödinger picture, reads

$$\psi_{\perp}(\mathbf{x}, t) = \langle 0(t) | \hat{\mathbf{E}}_{\perp}(\mathbf{x}, 0) | 1_f(t) \rangle \quad (7.2.1)$$

where the one-photon state  $|1_f\rangle$  is defined as usual through

$$|1_f(t)\rangle \equiv \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \tilde{f}(\mathbf{k}, t) \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}) |0\rangle. \quad (7.2.2)$$

The transverse electric field operator is given by (6.1.11) and (6.1.16b)

$$\hat{\mathbf{E}}_{\perp}(\mathbf{x}, 0) = i\sqrt{\frac{\hbar c}{\epsilon_0}} \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \|\mathbf{k}\| \left[ \hat{a}_{(\lambda)}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} - \hat{a}_{(\lambda)}^{\dagger}(\mathbf{k}) \boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \quad (7.2.3)$$

Note that (7.2.1) only applies to (pure) one-photon Fock states of the electromagnetic field. In the present case, it is seen from (6.1.40) that the state of the electromagnetic field is entangled with that of the atom. Hence, we define the single-photon wave function as the matrix element

$$\begin{aligned}\psi_{\perp}(\mathbf{x}, t) &\equiv \langle g, 0(t) | \hat{\mathbf{E}}_{\perp}(\mathbf{x}, 0) | \psi(t) \rangle \\ &= \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \langle 0 | \hat{\mathbf{E}}_{\perp}(\mathbf{x}, 0) c_{g,\lambda}(\mathbf{k}, t) e^{-ic\|\mathbf{k}\|t} | 1_{\lambda,\mathbf{k}} \rangle \\ &= i\sqrt{\frac{\hbar c}{\epsilon_0}} \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \|\mathbf{k}\| e^{i(\mathbf{k}\cdot\mathbf{x}-c\|\mathbf{k}\|t)} c_{g,\lambda}(\mathbf{k}, t) \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k})\end{aligned}\quad (7.2.4)$$

where again we used  $|g, 0(t)\rangle = e^{-i\omega_g t} |g, 0\rangle$  (see (7.1.9) and below). Note that  $\psi_{\perp}$  only gives information on the spacetime dependence of the transverse electric field.

Also note that in (7.2.4) we no longer restrict the extraction rule to the positive frequency part of the electric field. This is due to very practical reasons: in the interacting case at hand, there is no easy way to extract the positive frequency part of field operators because, as discussed in the previous chapter 6, their time-dependence is no longer trivial.

At this point, it comes in handy to notice that Schrödinger's equation (6.1.41b) for the probability amplitude  $c_{g,\lambda}(\mathbf{k}, \cdot)$  of the plane-wave mode  $(\lambda, \mathbf{k})$  can be formally integrated, yielding

$$c_{g,\lambda}(\mathbf{k}, t) = -\frac{i}{\hbar} G_{\lambda}(\mathbf{k}) \int_0^t dt' c_e(t') e^{i(c\|\mathbf{k}\|-\omega_e+\omega_g)t'} \quad (7.2.5)$$

so that the single-photon wave function reads

$$\begin{aligned}\psi_{\perp}(\mathbf{x}, t) &= \sqrt{\frac{c}{\hbar\epsilon_0}} \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \|\mathbf{k}\| e^{i(\mathbf{k}\cdot\mathbf{x}-c\|\mathbf{k}\|t)} \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) G_{\lambda}(\mathbf{k}) \int_0^t dt' c_e(t') e^{i(c\|\mathbf{k}\|-\omega_e+\omega_g)t'} \\ &= -i\frac{2^{\frac{9}{2}}}{3^4} \frac{\hbar e}{\epsilon_0 m_e a_0} \sum_{\lambda=\pm} \int \tilde{d}\mathbf{k} \|\mathbf{k}\| e^{i(\mathbf{k}\cdot\mathbf{x}-c\|\mathbf{k}\|t)} \boldsymbol{\epsilon}_{(\lambda)}(\mathbf{k}) \frac{\boldsymbol{\epsilon}_{(\lambda)}^*(\mathbf{k}) \cdot \boldsymbol{\xi}_{m_2}}{\left[1 + \left(\frac{\|\mathbf{k}\|}{k_X}\right)^2\right]^2} \int_0^t dt' c_e(t') e^{i(c\|\mathbf{k}\|-\omega_0)t'}\end{aligned}\quad (7.2.6)$$

with the notations  $\omega_0 \equiv \omega_e - \omega_g$  and  $k_X \equiv 3/(2a_0)$  introduced in the previous chapter 6. The closure relation (1.4.22) obeyed by the polarisation vectors allows us to rewrite

$$\psi_{\perp}(\mathbf{x}, t) = -i\frac{2^{\frac{9}{2}}}{3^4} \frac{\hbar e}{\epsilon_0 m_e a_0} \int \tilde{d}\mathbf{k} \|\mathbf{k}\| \frac{e^{i(\mathbf{k}\cdot\mathbf{x}-c\|\mathbf{k}\|t)}}{\left[1 + \left(\frac{\|\mathbf{k}\|}{k_X}\right)^2\right]^2} \left( \boldsymbol{\xi}_{m_2} - \frac{\boldsymbol{\xi}_{m_2} \cdot \mathbf{k}}{k^2} \mathbf{k} \right) \int_0^t dt' c_e(t') e^{i(c\|\mathbf{k}\|-\omega_0)t'}. \quad (7.2.7)$$

Choosing a coordinate system for which  $\mathbf{x}$  points along the third axis (in other words, such that  $\mathbf{x} = \|\mathbf{x}\| \mathbf{e}_3$ ) and writing, in such a reference frame,

$$\boldsymbol{\xi}_{m_2} = \sum_{i=1}^3 \xi_{m_2}^{(i)} \mathbf{e}_i \quad (7.2.8)$$

we can compute the angular integrals:

$$\mathbf{F}(k, \|\mathbf{x}\|) \equiv \int_0^{\pi} d\theta \sin \theta \int_0^{2\pi} d\varphi \left[ \boldsymbol{\xi}_{m_2} - \left( \boldsymbol{\xi}_{m_2} \cdot \frac{\mathbf{k}}{\|\mathbf{k}\|} \right) \frac{\mathbf{k}}{\|\mathbf{k}\|} \right] e^{ik\|\mathbf{x}\| \cos \theta}$$

$$\begin{aligned}
&= \int_0^\pi d\theta \sin \theta e^{ik||\mathbf{x}|| \cos \theta} \int_0^{2\pi} d\varphi \left\{ \begin{bmatrix} \xi_{m_2}^{(1)} \\ \xi_{m_2}^{(2)} \\ \xi_{m_2}^{(3)} \end{bmatrix} - \begin{bmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{bmatrix} \left( \xi_{m_2}^{(1)} \sin \theta \cos \varphi + \xi_{m_2}^{(2)} \sin \theta \sin \varphi + \xi_{m_2}^{(3)} \cos \theta \right) \right\} \\
&= 2\pi \int_0^\pi d\theta \sin \theta e^{ik||\mathbf{x}|| \cos \theta} \begin{bmatrix} \xi_{m_2}^{(1)} \left(1 - \frac{1}{2} \sin^2 \theta\right) \\ \xi_{m_2}^{(2)} \left(1 - \frac{1}{2} \sin^2 \theta\right) \\ \xi_{m_2}^{(3)} \sin^2 \theta \end{bmatrix} \\
&\equiv 2\pi \mathbf{I}(k, ||\mathbf{x}||).
\end{aligned}$$

The integrals over  $\theta$  give

$$I^{(1,2)}(k, ||\mathbf{x}||) = i \frac{\xi_{m_2}^{(1,2)}}{k ||\mathbf{x}||} \left[ \left( e^{-ik||\mathbf{x}||} - e^{ik||\mathbf{x}||} \right) - \frac{i}{k ||\mathbf{x}||} \left( e^{-ik||\mathbf{x}||} + e^{ik||\mathbf{x}||} \right) - \frac{1}{(k ||\mathbf{x}||)^2} \left( e^{-ik||\mathbf{x}||} - e^{ik||\mathbf{x}||} \right) \right], \quad (7.2.9)$$

$$I^{(3)}(k, ||\mathbf{x}||) = -2i \frac{\xi_{m_2}^{(3)}}{k ||\mathbf{x}||} \left[ -\frac{i}{k ||\mathbf{x}||} \left( e^{-ik||\mathbf{x}||} + e^{ik||\mathbf{x}||} \right) - \frac{1}{(k ||\mathbf{x}||)^2} \left( e^{-ik||\mathbf{x}||} - e^{ik||\mathbf{x}||} \right) \right] \quad (7.2.10)$$

where  $I^{(3)}(k, ||\mathbf{x}||)$  is the component of  $\mathbf{I}(k, ||\mathbf{x}||)$  pointing in the direction of  $\mathbf{x}$  and  $I^{(1,2)}(k, ||\mathbf{x}||)$  are the components of the same vector along two arbitrary axes in the plane orthogonal to  $\mathbf{x}$ .

As we can see, the photon wave function contains contributions proportional to  $1/||\mathbf{x}||$ ,  $1/||\mathbf{x}||^2$  and  $1/||\mathbf{x}||^3$ , which are respectively known as the far-field, mid-field and near-field contributions, an intuitive enough convention. We then have

$$\psi_\perp(\mathbf{x}, t) = -i \frac{2^{\frac{7}{2}} \hbar e}{3^4 \epsilon_0 m_e a_0} \int_0^{+\infty} \frac{dk}{(2\pi)^2} k^2 \frac{e^{-ickt}}{\left[1 + \left(\frac{k}{k_x}\right)^2\right]^2} \mathbf{I}(k, ||\mathbf{x}||) \int_0^t dt' c_e(t') e^{i(ck - \omega_0)t'}. \quad (7.2.11)$$

## 7.2.2 Formal computation

*"It's all computational! It's all educational!"*

British Sea Power's Jan Scott Wilkinson in "Monsters of Sunderland", **Machineries of Joy** (Rough Trade, 2013)

### 7.2.2.1 Transverse field

To first order in perturbation theory around  $t = 0$ , we have  $c_e(t) = 1$ , whence

$$\begin{aligned}
\int_0^t dt' c_e(t') e^{i(ck - \omega_0)t'} &= \int_0^t dt' e^{i(ck - \omega_0)t'} \\
&= \left[ \frac{e^{i(ck - \omega_0)t'}}{i(ck - \omega_0)} \right]_0^t \\
&= i \frac{1 - e^{i(ck - \omega_0)t}}{ck - \omega_0}.
\end{aligned} \quad (7.2.12)$$

This yields

$$\psi_{\perp}(\mathbf{x}, t) = -\frac{2^{\frac{7}{2}}}{3^4} \frac{\hbar e}{\epsilon_0 m_e a_0} \int_0^{+\infty} \frac{dk}{(2\pi)^2} k^2 \frac{e^{-i\omega_0 t}}{\left[1 + \left(\frac{k}{k_X}\right)^2\right]^2} \mathbf{I}(k, \|\mathbf{x}\|) \frac{1 - e^{-i(ck - \omega_0)t}}{ck - \omega_0}. \quad (7.2.13)$$

The usual trick [10, 2] is then to extend the range of integration from the positive real semi-axis to the whole real axis in order to retrieve a causal result. We want to improve on this usual approximate treatment and hence find ourselves computing integrals of the type

$$K_n^{(\pm)}(\|\mathbf{x}\|, t) \equiv \int_0^{+\infty} dk \frac{k^{2-n}}{\left[1 + \left(\frac{k}{k_X}\right)^2\right]^2} e^{\pm ik\|\mathbf{x}\|} \frac{1 - e^{-i(ck - \omega_0)t}}{ck - \omega_0} \quad (7.2.14)$$

with  $n \in \{1, 2, 3\}$ , and where the label  $+(-)$  is assigned to outgoing (ingoing) radial waves.

Just like the integral we computed in sect. 6.3, the integrand features two extra poles at  $k = \pm ik_X$  on top of the Wigner-Weisskopf pole at  $k = \omega_0/c$ , which sits on the real axis. This latter singularity at  $k = \omega_0/c$  is artificial. To compute the integral (7.2.14), we want to split the integrand in two summands as per (5.3.26), and both these summands have a first order pole at  $k = \omega_0/c$ . Since we integrate over the real axis, this could be a serious problem, but, since the singularity is artificial, we can shift it away from the real axis  $\omega_0 \rightarrow \omega_0/c - i\epsilon$  to compute the integral (see Fig. 7.2.1), before taking the limit  $\epsilon \rightarrow 0$  at the end. For  $n = 3$  the integrand has a singularity at  $k = 0$ , which we are allowed to shift to  $k = -i\alpha$  since we will be interested in computing the difference  $(K_3^{(+)} - K_3^{(-)})(\|\mathbf{x}\|, t)$ , which is an integral over a function which, as seen from (7.2.14), has only an artificial singularity at  $k = 0$ . We can rewrite (7.2.14) as

$$\begin{aligned} K_n^{(\pm)}(\|\mathbf{x}\|, t) &\equiv \int_{-\infty}^{+\infty} dk \frac{\theta(k) (k + i\alpha)^{2-n}}{\left[1 + \left(\frac{k}{k_X}\right)^2\right]^2} e^{\pm ik\|\mathbf{x}\|} \frac{1 - e^{-i(ck - \omega_0)t}}{ck - (\omega_0 - ic\epsilon)} \\ &\equiv \int_{-\infty}^{+\infty} dk \theta(k) f_n(k, t) e^{\pm ik\|\mathbf{x}\|} \\ &\equiv \int_{-\infty}^{+\infty} dk \theta(k) (g_n(k) - h_n(k, t)) e^{\pm ik\|\mathbf{x}\|} \end{aligned} \quad (7.2.15)$$

where it is implied that the limit  $\alpha \rightarrow 0^+$ ,  $\epsilon \rightarrow 0^+$  should be taken outside the integral. Here the functions  $g_n$  and  $h_n$  are defined as

$$g_n(k) \equiv \frac{(k + i\alpha)^{2-n}}{\left[1 + \left(\frac{k}{k_X}\right)^2\right]^2} \frac{1}{ck - (\omega_0 - ic\epsilon)}, \quad (7.2.16a)$$

$$h_n(k, t) \equiv \frac{(k + i\alpha)^{2-n}}{\left[1 + \left(\frac{k}{k_X}\right)^2\right]^2} \frac{e^{-i(ck - \omega_0)t}}{ck - (\omega_0 - ic\epsilon)}. \quad (7.2.16b)$$

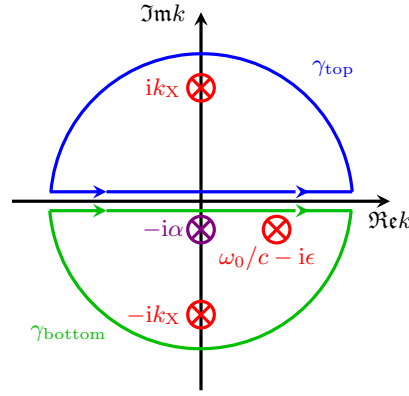
From (6.A.15) we have

$$K_n^{(\pm)}(\|\mathbf{x}\|, t) = \frac{1}{2} \left[ \left( \delta(\cdot) - \frac{i}{\pi} \text{vp} \frac{1}{\cdot} \right) * \bar{f}_n(\cdot, t) \right] (\mp \|\mathbf{x}\|) \quad (7.2.17)$$

where

$$\bar{f}_n(x, t) = \int_{-\infty}^{+\infty} dk f_n(k, t) e^{-ikx} \quad (7.2.18)$$

We use Cauchy's residue theorem to compute (7.2.18). We know from (7.2.14) that  $f_n$  has a first order pole at  $\omega_0/c - i\epsilon$  and two second order poles at  $\pm ik_X$ , pictured on Fig. 7.2.1. From (7.2.15) and (7.2.18) we see that we have to close the integration path (Jordan loop) in the lower half of the complex plane for  $x > 0$  and  $x + ct > 0$  for  $g_n$  and  $h_n$  respectively, and in the upper half of the plane for  $x < 0$  or  $x + ct < 0$  for  $g_n$  and  $h_n$  respectively.



**Fig. 7.2.1** – Jordan loops in the complex  $k$ -plane used to compute the Fourier transform (7.2.18). The (isolated) poles  $\omega_0/c - i\epsilon$  and  $\pm ik_X$  are represented by red circled crosses while the (isolated) simple pole  $-i\alpha$  is represented by a purple circled cross.

It can be checked that the residues of  $g_n(\omega) e^{-ikx}$  and  $h_n(\omega) e^{-ikx}$  read

$$\text{Res} \left( g_n(\cdot) e^{-i\cdot x}, \frac{\omega_0}{c} - i\epsilon \right) \xrightarrow{\epsilon \rightarrow 0^+} e^{-i\frac{\omega_0}{c}x} G_0^{(n)}, \quad (7.2.19a)$$

$$\text{Res} \left( g_n(\cdot) e^{-i\cdot x}, ik_X \right) \xrightarrow{\epsilon \rightarrow 0^+} e^{k_X x} \left( \gamma_0^{+(n)} + \gamma_1^{+(n)} x \right), \quad (7.2.19b)$$

$$\text{Res} \left( g_n(\cdot) e^{-i\cdot x}, -ik_X \right) \xrightarrow{\epsilon \rightarrow 0^+} e^{-k_X x} \left( \gamma_0^{-(n)} + \gamma_1^{-(n)} x \right) \quad (7.2.19c)$$

and

$$\text{Res} \left( h_n(\cdot, t) e^{-i\cdot x}, \frac{\omega_0}{c} - i\epsilon \right) \xrightarrow{\epsilon \rightarrow 0^+} e^{-i\frac{\omega_0}{c}x} G_0^{(n)}, \quad (7.2.20a)$$

$$\text{Res} \left( h_n(\cdot, t) e^{-i\cdot x}, ik_X \right) \xrightarrow{\epsilon \rightarrow 0^+} e^{k_X x} \left( \gamma_0^{+(n)} + \gamma_1^{+(n)} (x + ct) \right), \quad (7.2.20b)$$

$$\text{Res} \left( h_n(\cdot, t) e^{-i\cdot x}, -ik_X \right) \xrightarrow{\epsilon \rightarrow 0^+} e^{-k_X x} \left( \gamma_0^{-(n)} + \gamma_1^{-(n)} (x + ct) \right) \quad (7.2.20c)$$

where the  $G_0^{(n)}$  and  $\gamma_i^{\pm(n)}$  depend on  $n$ , as suggested by the notation. We can see that

$$\begin{aligned} \gamma_0^{+(n)} &= \gamma_0^{-*(n)} \equiv \gamma_0^{(n)}, \\ \gamma_1^{+(n)} &= -\gamma_1^{-*(n)} \equiv \gamma_1^{(n)}. \end{aligned}$$

We give

$$G_0^{(n)} = \frac{\left(\frac{\omega_0}{c}\right)^{2-n} (ck_X)^4}{(\omega_0^2 + c^2 k_X^2)^2}, \quad (7.2.21a)$$

$$\gamma_0^{(n)} = \frac{ck_X (ik_X)^{2-n} [-i(-3+n)\omega_0 - (n-2)ck_X]}{4(i\omega_0 + ck_X)^2}, \quad (7.2.21b)$$

$$\gamma_1^{(n)} = \frac{ck_X^2 (ik_X)^{2-n}}{4(i\omega_0 + ck_X)}. \quad (7.2.21c)$$

The Fourier transform (7.2.18) is thus given for  $n \in \{1, 2\}$  by

$$\begin{aligned} \frac{\bar{f}_n(x, t)}{2i\pi} &= -\theta(x) \left[ e^{-k_X x} \left( \gamma_0^{*(n)} - \gamma_1^{*(n)} x \right) + e^{-i\frac{\omega_0}{c}x} G_0^{(n)} \right] + \theta(-x) \left[ e^{-k_X x} \left( \gamma_0^{(n)} + \gamma_1^{(n)} x \right) \right] \\ &+ \theta(x + ct) \left[ e^{i\omega_0 t} e^{-k_X(x+ct)} \left( \gamma_0^{*(n)} - \gamma_1^{*(n)} (x + ct) \right) + e^{-i\frac{\omega_0}{c}x} G_0^{(n)} \right] \\ &- \theta(-(x + ct)) \left[ e^{i\omega_0 t} e^{k_X(x+ct)} \left( \gamma_0^{(n)} + \gamma_1^{(n)} (x + ct) \right) \right]. \end{aligned} \quad (7.2.22)$$

We can then compute the convolution—which we call  $C_n(x, t)$ —with the principal value as prescribed by (7.2.17). It yields, still for  $n \in \{1, 2\}$ ,

$$\begin{aligned}
C_n(x, t) &\equiv -\frac{i}{2\pi} \left[ \text{vp} \frac{1}{\cdot} * \bar{f}_n(\cdot, t) \right] (x) \\
&= -\frac{i}{2\pi} \text{vp} \int_{-\infty}^{+\infty} \frac{du}{x-u} \bar{f}_n(u, t) \\
&= e^{-k_X x} \left[ \left( \gamma_0^{*(n)} - \gamma_1^{*(n)} x \right) \left[ -\text{Ei}(k_X x) + e^{(i\omega_0 - ck_X)t} \text{Ei}(k_X(x+ct)) \right] \right. \\
&\quad \left. + \frac{\gamma_1^{*(n)}}{k_X} \left( -e^{k_X x} + e^{(i\omega_0 - ck_X)t} e^{k_X(x+ct)} \right) - c\gamma_1^{*(n)} t e^{(i\omega_0 - ck_X)t} \text{Ei}(k_X(x+ct)) \right] \\
&+ e^{k_X x} \left[ \left( \gamma_0^{(n)} + \gamma_1^{(n)} x \right) \left[ -\text{Ei}(-k_X x) + e^{(i\omega_0 + ck_X)t} \text{Ei}(k_X(-x-ct)) \right] \right. \\
&\quad \left. + \frac{\gamma_1^{(n)}}{k_X} \left( -e^{-k_X x} + e^{(i\omega_0 + ck_X)t} e^{k_X(-x-ct)} \right) + c\gamma_1^{(n)} t e^{(i\omega_0 + ck_X)t} \text{Ei}(k_X(-x-ct)) \right] \\
&+ e^{-i\frac{\omega_0}{c}x} G_0^{(n)} \left[ -\text{Ei}\left(i\frac{\omega_0}{c}x\right) + \text{Ei}\left(i\frac{\omega_0}{c}(x+ct)\right) \right]. \tag{7.2.23}
\end{aligned}$$

Now, remember that for  $n = 3$ , the integrand in (7.2.14) has a (simple) pole at  $k = 0$ . As argued above (7.2.15), we can shift this singularity away from the real axis  $0 \rightarrow -i\alpha$  to compute the integral (see Fig. 7.2.1), before taking the limit  $\alpha \rightarrow 0$  at the end. This yields

$$\begin{aligned}
\frac{\bar{f}_3(x, t)}{2i\pi} &= -\theta(x) \left[ e^{-k_X x} \left( \gamma_0^{*(3)} - \gamma_1^{*(3)} x \right) + e^{-i\frac{\omega_0}{c}x} G_0^{(3)} \right] + \theta(-x) \left[ e^{-k_X x} \left( \gamma_0^{(3)} + \gamma_1^{(3)} x \right) \right] \\
&+ \theta(x+ct) \left[ e^{i\omega_0 t} e^{-k_X(x+ct)} \left( \gamma_0^{*(3)} - \gamma_1^{*(3)}(x+ct) \right) + e^{-i\frac{\omega_0}{c}x} G_0^{(3)} \right] \\
&- \theta(-(x+ct)) \left[ e^{i\omega_0 t} e^{k_X(x+ct)} \left( \gamma_0^{(3)} + \gamma_1^{(3)}(x+ct) \right) \right] + \frac{1}{\omega_0} \left[ \theta(x) - \theta(x+ct) e^{i\omega_0 t} \right] \tag{7.2.24}
\end{aligned}$$

and

$$\begin{aligned}
C_3(x, t) &= e^{-k_X x} \left[ \left( \gamma_0^{*(3)} - \gamma_1^{*(3)} x \right) \left[ -\text{Ei}(k_X x) + e^{(i\omega_0 - ck_X)t} \text{Ei}(k_X(x+ct)) \right] \right. \\
&\quad \left. + \frac{\gamma_1^{*(3)}}{k_X} \left( -e^{k_X x} + e^{(i\omega_0 - ck_X)t} e^{k_X(x+ct)} \right) - c\gamma_1^{*(3)} t e^{(i\omega_0 - ck_X)t} \text{Ei}(k_X(x+ct)) \right] \\
&+ e^{k_X x} \left[ \left( \gamma_0^{(3)} + \gamma_1^{(3)} x \right) \left[ -\text{Ei}(-k_X x) + e^{(i\omega_0 + ck_X)t} \text{Ei}(k_X(-x-ct)) \right] \right. \\
&\quad \left. + \frac{\gamma_1^{(3)}}{k_X} \left( -e^{-k_X x} + e^{(i\omega_0 + ck_X)t} e^{k_X(-x-ct)} \right) + c\gamma_1^{(3)} t e^{(i\omega_0 + ck_X)t} \text{Ei}(k_X(-x-ct)) \right] \\
&+ e^{-i\frac{\omega_0}{c}x} G_0^{(3)} \left[ -\text{Ei}\left(i\frac{\omega_0}{c}x\right) + \text{Ei}\left(i\frac{\omega_0}{c}(x+ct)\right) \right] - \frac{1}{\omega_0} \text{vp} \left[ \int_{-x}^{+\infty} \frac{dv}{v} - e^{i\omega_0 t} \int_{-x-ct}^{+\infty} \frac{du}{u} \right] \tag{7.2.25}
\end{aligned}$$

which is an infinite quantity (because of the principal value integrals on the right-hand side), but this is not a problem as we are interested in  $C_3(-x, t) - C_3(x, t)$ , which, as we shall see, is finite. Keeping in mind that  $x$  and  $t$  are both positive we compute, for  $n \in \{1, 2\}$

$$\begin{aligned}
\bar{f}_n(-x, t) \mp \bar{f}_n(x, t) &= 2i\pi \left\{ G_0^{(n)} \theta(-x+ct) e^{i\frac{\omega_0}{c}x} \right. \\
&\quad \left. + \theta(-x+ct) e^{i\omega_0 t} \left[ e^{-k_X(ct-x)} \left( \gamma_0^{*(n)} + \gamma_1^{*(n)}(x-ct) \right) + e^{k_X(ct-x)} \left( \gamma_0^{(n)} - \gamma_1^{(n)}(x-ct) \right) \right] \right. \\
&\quad \left. + e^{-k_X x} \left[ \left( \gamma_0^{(n)} \mp \gamma_0^{*(n)} \right) - \left( \gamma_1^{(n)} \mp \gamma_1^{*(n)} \right) x \right] \right. \\
&\quad \left. e^{i\omega_0 t} \left[ \mp e^{-k_X(ct+x)} \left( \gamma_0^{*(n)} - \gamma_1^{*(n)}(x+ct) \right) + e^{k_X(ct-x)} \left( \gamma_0^{(n)} - \gamma_1^{(n)}(x-ct) \right) \right] \right\} \tag{7.2.26}
\end{aligned}$$

and, for  $n = 3$ , the difference

$$\begin{aligned} \bar{f}_3(-x, t) - \bar{f}_3(x, t) = 2i\pi \left\{ G_0^{(3)} \theta(-x + ct) e^{i\frac{\omega_0}{c}x} \right. \\ + \theta(-x + ct) e^{i\omega_0 t} \left[ e^{-k_X(ct-x)} \left( \gamma_0^{*(3)} + \gamma_1^{*(3)}(x - ct) \right) + e^{k_X(ct-x)} \left( \gamma_0^{(3)} - \gamma_1^{(3)}(x - ct) \right) \right] \\ + e^{-k_X x} \left[ \left( \gamma_0^{(3)} \mp \gamma_0^{*(3)} \right) - \left( \gamma_1^{(3)} \mp \gamma_1^{*(3)} \right) x \right] \\ e^{i\omega_0 t} \left[ \mp e^{-k_X(ct+x)} \left( \gamma_0^{*(3)} - \gamma_1^{*(3)}(x + ct) \right) + e^{k_X(ct-x)} \left( \gamma_0^{(3)} - \gamma_1^{(3)}(x - ct) \right) \right] \\ \left. - \frac{1}{\omega_0} \left[ 1 - (1 - \theta(ct - x)) e^{i\omega_0 t} \right] \right\}. \end{aligned} \quad (7.2.27)$$

The quantities  $C_n(-x, t) \mp C_n(x, t)$  are not illuminating enough to warrant their explicit writing out here, but their expression follows immediately from (7.2.23) and (7.2.25). It is noteworthy, though, that the contribution to  $C_3(-x, t) \mp C_3(x, t)$  from the last summand on the right-hand side of (7.2.25) (the summand featuring the two principal value integrals) reads

$$- \frac{1}{\omega_0} e^{i\omega_0 t} \log \left( \frac{x + ct}{|-x + ct|} \right). \quad (7.2.28)$$

Also, note that (7.2.17) can be rewritten

$$K_n^{(\pm)}(\|\mathbf{x}\|, t) = \frac{1}{2} \bar{f}_n(\mp \|\mathbf{x}\|, t) - C_n(\mp \|\mathbf{x}\|, t), \quad (7.2.29)$$

while the Riemann-Silberstein photon wave function is given, according to (7.2.9), (7.2.13) and (7.2.14), by

$$\begin{aligned} \psi_{\perp}(\mathbf{x}, t) = -i \frac{2^{\frac{7}{2}} \hbar e}{3^4 \epsilon_0 m_e a_0} \\ \left[ \begin{array}{l} \frac{\xi_{m_2}^{(1,2)}}{\|\mathbf{x}\|} \left[ \left[ K_1^{(-)} - K_1^{(+)} \right](\|\mathbf{x}\|, t) - \frac{i}{\|\mathbf{x}\|} \left[ K_2^{(-)} + K_2^{(+)} \right](\|\mathbf{x}\|, t) - \frac{1}{x^2} \left[ K_3^{(-)} - K_3^{(+)} \right](\|\mathbf{x}\|, t) \right] \\ 2 \frac{\xi_{m_2}^{(3)}}{\|\mathbf{x}\|} \left[ \left[ K_1^{(-)} - K_1^{(+)} \right](\|\mathbf{x}\|, t) + \frac{i}{\|\mathbf{x}\|} \left[ K_2^{(-)} + K_2^{(+)} \right](\|\mathbf{x}\|, t) + \frac{1}{x^2} \left[ K_3^{(-)} - K_3^{(+)} \right](\|\mathbf{x}\|, t) \right] \end{array} \right] \end{aligned} \quad (7.2.30)$$

where it is of course understood that the values of all functions  $K_i^{(\pm)}$  are taken at  $(\|\mathbf{x}\|, t)$ . Remember that  $\xi_{m_2}^{(1,2)}$  are the components of  $\xi_{m_2}$  in the plane perpendicular to the vector between the position of the atom (that is, the origin of space) and the position of observation  $\mathbf{x}$ , that is, perpendicular to  $\mathbf{x}$  itself, while  $\xi_{m_2}^{(3)}$  is the component of  $\xi_{m_2}$  in the direction of  $\mathbf{x}$ .

The dipole approximation for the atom-field coupling (see sect. 6.2.1) consists in forgetting the denominator  $\left[ 1 + (k/k_X)^2 \right]^2$  as one lets  $k_X \rightarrow +\infty$  in (7.2.13). In this approximation, therefore, the integrand in (7.2.15) has no poles at  $k = \pm i k_X$ . Extending the integration domain over wave numbers from the positive real semi-axis to the whole real axis, as done for instance in [10, 2, 3], simply yields  $K_n^{(-)}(x, t) = \bar{f}_n(x, t)$ . And then for  $n = 1, 2$ , the wave function of the outgoing photon is causal in the dipole approximation—that is, for  $\gamma_0^{(n)} = 0$  and  $\gamma_1^{(n)} = 0$ , which is seen from (7.2.21) to follow from  $k_X \rightarrow +\infty$ —as seen on (7.2.26). On the other hand, this is not the case for  $n = 3$ , since (7.2.27) features a clearly noncausal term even in the dipole approximation  $\gamma_0^{(n)} = 0$ ,  $\gamma_1^{(n)} = 0$ . Comparison of (7.2.27) with (7.2.26) shows that the result for  $n = 3$  features not only an extra noncausal contribution (the one given by the 1 in the square brackets on the last line of the right-hand side of (7.2.27)), but also a strange “anticausal” term (the one given by  $(-1 + \theta(ct - x)) e^{i\omega_0 t} = -\theta(x - ct) e^{i\omega_0 t}$ , which is **only nonvanishing outside the lightcone**). The presence of these two terms (we shall reuse the labels “noncausal” and “anticausal” to refer to them in the following) is a consequence of the slow dependence of the  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  atom-field coupling on the norm of the electromagnetic wave vector  $\mathbf{k}$ . As far as we know, similar calculations [10, 14, 2, 15] of the outgoing field—or the excitation probability of a second atom—have mostly been carried out in the



Power-Zineau-Woolley picture [4] of quantum electrodynamics where the interaction Hamiltonian is of the form  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$ . In this case the integrand in (7.2.15) features no singularity at  $k = 0$  and one retrieves a causal result, with the dipole approximation, if we extend the range of integration as described just above.

Whatever the choice of the interaction Hamiltonian, however, we see that if the range of integration is not extended to include the negative real semi-axis, we do not retrieve a causal propagation, even in the dipole approximation, as first noted by Shirokov [11]. This is an illustration of the Hegerfeldt theorem (see sect. 7.1), which states that non-causalities will always arise for Hamiltonians bounded by below. The relevant Hamiltonian here for the Hegerfeldt theorem is the Hamiltonian  $\hat{H}_R$  (6.1.9) of the free field, which has  $\mathbb{R}_+$  as its spectrum and is hence bounded. The noncausal terms which come from the boundedness of the field Hamiltonian are seen in (7.2.23) for the mid- and far-fields and (7.2.25) for the near-field. Similar noncausal corrections were first obtained by Shirokov in [16].

When we go beyond the dipole approximation as we did here, another source of noncausality arises: as seen from (7.2.23), (7.2.25), (7.2.26) and (7.2.27): the contributions from the poles of the integrand in (7.2.15) at  $k = \pm ik_X$  are (in part) nonvanishing outside the lightcone centred at  $t = 0$  (the instant when the decay starts) and  $\mathbf{x} = \mathbf{0}$  (the position of the Hydrogen nucleus). This is in fact to be expected because, as opposed to the dipole approximation where it is assumed that the emission of light takes place at the position of the atomic nucleus, in the exact treatment the uncertainty on the position of the electron makes the lightcone “fuzzy”, as illustrated in Fig. 7.3.1. This particular feature of the emission was predicted by Shirokov in [11], but, despite our efforts which included translating an article [16] from Russian<sup>2</sup>, we could not find evidence that he performed the actual calculation. As such, our detailed description of how going beyond the dipole approximation results in finding tails outside of the lightcone is a first.

The non-causality seen in (7.2.27) is of a different kind—it is not a manifestation of the Hegerfeldt theorem—and is, as far as we know, obtained for the first time here in the theory of spontaneous decay. Notice that the  $n = 3$  case at hand corresponds, as can be seen from (7.2.9), to the near-field part of the emitted photon wave function. We will see in the next sect. 7.2.2.2 that the noncausal (the one given by the 1 in the square brackets on the right-hand side of (7.2.27)) contribution to the electric field is cancelled by the longitudinal part of the field, which comes from the Coulomb interaction between the electron and the nucleus.

### 7.2.2.2 Longitudinal field

Remember that the starting point of the computation of the photon wave function was

$$\psi_{\perp}(\mathbf{x}, t) = \langle g, 0(t) | \hat{\mathbf{E}}_{\perp}(\mathbf{x}, 0) | \psi(t) \rangle. \quad (7.2.31)$$

We now compute the corresponding matrix element for the longitudinal electric field. It is given by

$$\psi_{\parallel}(\mathbf{x}, t) = \langle g, 0(t) | \hat{\mathbf{E}}_{\parallel}(\mathbf{x}, 0) | \psi(t) \rangle. \quad (7.2.32)$$

The longitudinal part of the electric field is given by (6.1.14) and (6.1.16a). Since the ground  $|g\rangle$  and excited  $|e\rangle$  states are orthogonal, and the electric field operator is taken at  $t = 0$ , we have

$$\begin{aligned} \langle g | \hat{\rho}(\mathbf{x}, 0) | e \rangle &= -e \langle g | \delta(\mathbf{x} - \hat{\mathbf{x}}) | e \rangle \\ &= -e \psi_{1s}^*(\mathbf{x}) \psi_{2p m_2}(\mathbf{x}) \end{aligned} \quad (7.2.33)$$

<sup>2</sup>Once again, many thanks to Vladyslav Atavin for taking so much of his time to do that.

Now compute, with the help of (6.1.19), and keeping the convention that  $\mathbf{x}$  points along the third axis of our basis:

$$\begin{aligned}
\int d\mathbf{x}' \frac{\psi_{1s}^*(\mathbf{x}') \psi_{2p m_2}(\mathbf{x}')}{\|\mathbf{x} - \mathbf{x}'\|} &= \int d\mathbf{x}' \frac{e^{-\frac{3}{2} \frac{\|\mathbf{x}'\|}{a_0}}}{\|\mathbf{x} - \mathbf{x}'\|} \frac{1}{2^{\frac{3}{2}} \pi a_0^4} (\mathbf{x}' \cdot \boldsymbol{\xi}_{m_2}) \\
&= \frac{\xi_{m_2}^{(3)}}{2^{\frac{3}{2}} a_0^4} \int_0^{+\infty} dr r^3 e^{-\frac{3}{2} \frac{r}{a_0}} \int_{-1}^1 d\eta \frac{\eta}{\sqrt{r^2 + \mathbf{x}^2 - 2\eta r \|\mathbf{x}\|}} \\
&= -\frac{\xi_{m_2}^{(3)}}{2^{\frac{3}{2}} 3 a_0^4} \int_0^{+\infty} dr r e^{-\frac{3}{2} \frac{r}{a_0}} [(r + \|\mathbf{x}\|) (-r^2 - \mathbf{x}^2 + r \|\mathbf{x}\|) + |r - \|\mathbf{x}\|| (r^2 + \mathbf{x}^2 + r \|\mathbf{x}\|)] \\
&= -\frac{2^{\frac{3}{2}}}{3^5} \xi_{m_2}^{(3)} \frac{e^{-\frac{3}{2} \frac{\|\mathbf{x}\|}{a_0}}}{a_0} \left[ 27 \frac{\|\mathbf{x}\|}{a_0} + 72 + 96 \frac{a_0}{\|\mathbf{x}\|} + 64 \frac{a_0^2}{\mathbf{x}^2} - 64 e^{\frac{3}{2} \frac{\|\mathbf{x}\|}{a_0}} \frac{a_0^2}{\mathbf{x}^2} \right].
\end{aligned} \tag{7.2.34}$$

Four of the five summands in (7.2.34) are exponentially decaying with increasing distance from the Hydrogen nucleus. Remember that  $k_X \equiv 3/(2a_0)$  is the natural cutoff wave vector of the atom-field interaction, which is brought to infinity in the dipole approximation. Hence, in the framework of the dipole approximation, the first four summands in (7.2.34) would vanish, and we would just retain the last summand and compute its gradient. Remembering that

$$\xi_{m_2}^{(3)} \equiv \frac{\boldsymbol{\xi}_{m_2} \cdot \mathbf{x}}{\|\mathbf{x}\|} \tag{7.2.35}$$

we get

$$\nabla \left( \frac{\xi_{m_2}^{(3)}}{\mathbf{x}^2} \right) = \frac{1}{\|\mathbf{x}\|^3} \begin{bmatrix} \xi_{m_2}^{(1,2)} \\ -2\xi_{m_2}^{(3)} \end{bmatrix} \tag{7.2.36}$$

It is thus seen from (7.2.9) that the (non-exponentially decaying part of the) longitudinal electric field is colinear to the transverse electric field, and depends on  $\|\mathbf{x}\|$  in the way the near-field part of the latter does. We thus have

$$\begin{aligned}
\psi_{\parallel}(\mathbf{x}, t) &= \frac{2^{\frac{15}{2}} e a_0}{3^5 4\pi\epsilon_0} \frac{e^{-i\omega_0 t}}{\|\mathbf{x}\|^3} \begin{bmatrix} \xi_{m_2}^{(1,2)} \\ -2\xi_{m_2}^{(3)} \end{bmatrix} + \text{exponentially decaying (in space) terms} \\
&\equiv \psi_{\parallel}^{(\text{nonatt})}(\mathbf{x}, t) + \text{exponentially decaying (in space) terms.}
\end{aligned} \tag{7.2.37}$$

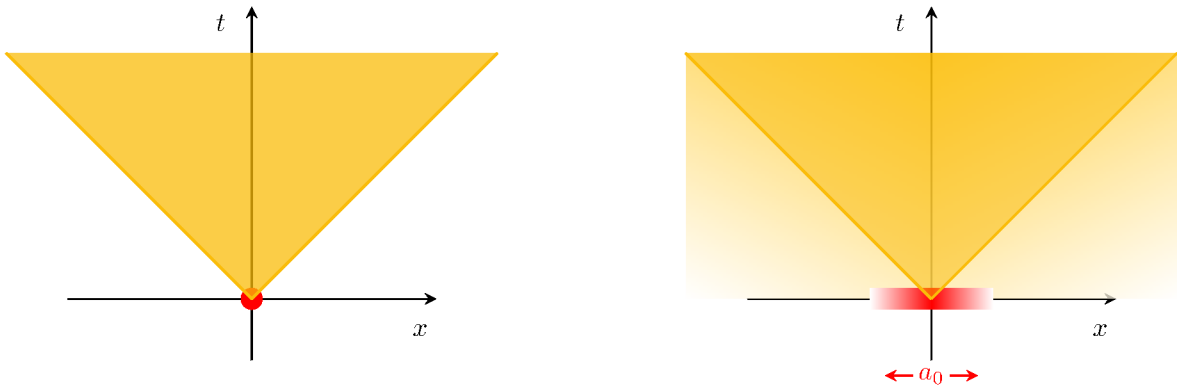
We could say that the contributions to the longitudinal electric field (or, as they stand in (7.2.34), to the scalar potential) which are exponentially decaying with increasing distance  $\|\mathbf{x}\|$  are attached to the sources. This is why we choose to refer to the fifth contribution (the one which is explicitly written in (7.2.37)) to the longitudinal field as non-attached, hence the superscript.

## 7.3 Discussion

It can be checked with the help of the expression (6.1.33) for the atomic transition frequency that the contribution to the photon wave function given by the 1 in the square brackets on the last line of the right-hand side of (7.2.27) (what we called the noncausal term) is exactly the opposite of  $\psi_{\parallel}^{(\text{nonatt})}(\mathbf{x}, t)$  given in (7.2.37), so that this noncausal term is not present in the matrix element of the total electric field

$$\langle g, 0(t) | \hat{\mathbf{E}}(\mathbf{x}, 0) | \psi(t) \rangle = \langle g, 0(t) | \hat{\mathbf{E}}_{\perp}(\mathbf{x}, 0) | \psi(t) \rangle + \langle g, 0(t) | \hat{\mathbf{E}}_{\parallel}(\mathbf{x}, 0) | \psi(t) \rangle. \tag{7.3.1}$$

This compensation is a very nice feature of the  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  atom-field coupling. As we discussed in sect. 7.2.2.1, the contribution to the photon wave function (transverse field) which is equal to the opposite of (7.2.37) is not present if the more common choice of the  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  coupling. In that case, the total electric field features the completely noncausal term (7.2.37) in the near-field, which is not cancelled by any contribution to the transverse electric field. To us this is a strong argument against the standard  $\hat{\mathbf{E}} \cdot \hat{\mathbf{x}}$  choice for the coupling.



(a) Standard “binary” lightcone. This simple picture is relevant in the dipole approximation where the emission is assumed to take place from  $\mathbf{x} = \mathbf{0}$ .

(b) “Fuzzy” lightcone due to the uncertainty on the position of the atomic electron when the dipole approximation is **not** performed.

**Fig. 7.3.1** – Lightcone (a) and fuzzy lightcone (b) around the spacetime point  $(0, \mathbf{0})$  corresponding to the time  $t = 0$  at which the decay starts, and the position  $\mathbf{x} = \mathbf{0}$  of the Hydrogen nucleus (proton).

Our treatment, however, features the apparition of a strange term, which only vanishes inside the lightcone. Understanding this term is the subject of ongoing work.

Finally, we note that though our computations were carried at the first order in time-dependent perturbation theory, it can be shown [17] that the exact short-time dynamics of the system is very well reproduced by such a simple approximation. Moreover, it has been shown [18, 19] that the exact expression for the survival amplitude  $c_e(t)$  is the sum of a decaying exponential and a nonexponential contribution, the latter being negligible except at very short and very long times (also see sect. 6.3). At intermediate times, the survival amplitude is very well approximated by the exponentially decaying term, and as a consequence, up to very small corrections, our results for the matrix elements of the electric field hold, with a grain of salt:  $\omega_0$  should be replaced by  $\omega_0 + \omega_{\text{LS}} - (i/2)\Gamma$  where  $\omega_{\text{LS}}$  is the partial Lamb shift [18] of the excited  $2p$  level due to the  $1s$  level and  $\Gamma$  is the decay rate given by (6.3.19). Therefore, our perturbative treatment works directly at short times and indirectly (through the substitution which we just specified) at intermediate times. It only fails at very long times, where the decay becomes nonexponential [18].

## 7.A The Paley-Wiener theorem

Several important results on Fourier analysis in the complex plane are known as the Paley-Wiener theorem, but for our purposes we can limit ourselves to the following type of functions:

$$\bar{f}(z) = \int_{-A}^A dt e^{-izt} f(t) = \int_{-\infty}^{+\infty} dt e^{-izt} f(t), \quad (7.A.1)$$

in other words, to Fourier transforms of functions which vanish outside a (symmetric) interval of  $\mathbb{R}$ . Here  $A > 0$  for convenience and it is an important requirement [5] that  $f \in L^2[-A, A]$ . Compute the integral of  $\bar{f}(z)$  as defined

in (7.A.1) along a closed contour  $\gamma$  in the complex plane:

$$\begin{aligned} \int_{\gamma} dz \bar{f}(z) &= \int_{\gamma} dz \int_{-A}^A dt e^{-izt} f(t) \\ &= \int_{-A}^A dt f(t) \int_{\gamma} dz e^{-izt} \\ &= 0 \end{aligned} \tag{7.A.2}$$

where we made use of Fubini's theorem. By Morera's theorem,  $\bar{f}$  is an entire function (that is, it is holomorphic in the whole complex plane  $\mathbb{C}$ ). Now, writing  $z = x + iy$ , we find an upper bound on the modulus of the Fourier transform  $\bar{f}$  through the simple manipulation

$$\begin{aligned} |\bar{f}(z)| &\leq \int_{-A}^A dt e^{-ty} |f(t)| \\ &\leq e^{A|y|} \int_{-A}^A dt |f(t)|. \end{aligned} \tag{7.A.3}$$

Since the last integral on the right-hand side of (7.A.3) is simply a real number, we write it  $C$  and obtain

$$|\bar{f}(z)| \leq C e^{A|z|}. \tag{7.A.4}$$

This is all we want as far as Paley-Wiener theorems are concerned. We proved that a function of the type (7.A.1) with  $f \in L^2[-A, A]$  is an entire function which verifies (7.A.4) (it is then to be said an entire function of exponential type). A converse of this result exists [5], but we do not need it.

# REFERENCES

---

## Books

- [1] E.M. Stein and G. Weiss, *Introduction to Fourier Analysis on Euclidean Spaces* (Princeton University Press, 1971) (cit. on p. 174).
- [2] M.O. Scully and M.S. Zubairy, *Quantum Optics* (Cambridge University Press, 1997) (cit. on pp. 178, 182).
- [3] P. Meystre and M. Sargent, III, *Elements of Quantum Optics*, 3rd ed. (Springer-Verlag, 1999) (cit. on p. 182).
- [4] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, *Photons et atomes - Introduction à l'électrodynamique quantique*, 2nd ed. (EDP Sciences/CNRS Éditions, 2001) (cit. on p. 182).
- [5] W. Rudin, *Real and Complex Analysis*, 3rd ed. (McGraw-Hill, 1987) (cit. on pp. 185, 186).

## Articles

- [6] G. Hegerfeldt, 'Remark on causality and particle localization', *Phys. Rev. D* **10**, 3320 (1974) (cit. on pp. 172, 173).
- [7] T.D. Newton and E.P. Wigner, 'Localized States for Elementary Systems', *Rev. Mod. Phys.* **21**, 400 (1949) (cit. on p. 172).
- [8] M. Hawton, 'Photon position operator with commuting components', *Phys. Rev. A* **59**, 954 (1999) (cit. on p. 173).
- [9] M. Hawton and W.E. Baylis, 'Photon position operators and localized bases', *Phys. Rev. A* **64**, 012101 (2001) (cit. on p. 173).
- [10] E. Fermi, 'Quantum Theory of Radiation', *Rev. Mod. Phys.* **4**, 87 (1932) (cit. on pp. 174, 178, 182).
- [11] M.I. Shirokov, 'Signal velocity in quantum electrodynamics', *Sov. Phys. Usp.* **21**, 345 (1978) (cit. on pp. 174, 182).
- [12] V. Debievre, G. Demésy, T. Durt, A. Nicolet, B. Vial and F. Zolla, 'Absorption in quantum electrodynamic cavities in terms of a quantum jump operator', *Phys. Rev. A* **90**, 033806 (2014) (cit. on p. 174).
- [13] G. Hegerfeldt, 'Causality Problems for Fermi's Two-Atom System', *Phys. Rev. Lett.* **72**, 596 (1994) (cit. on p. 174).
- [14] J.E. Sipe, 'Photon Wave Functions', *Phys. Rev. A* **52**, 1875 (1995) (cit. on pp. 175, 182).
- [15] A.K. Biswas, G. Compagno, G.M. Palma, R. Passante and F. Persico, 'Virtual photons and causality in the dynamics of a pair of two-level atoms', *Phys. Rev. A* **42**, 4291 (1990) (cit. on p. 182).
- [16] M.I. Shirokov, 'The Velocity of the Excitation Exchange in Quantum Electrodynamics', *JINR Preprint*, 1719 (1964) (cit. on p. 182).

- [17] V. Debierre, T. Durt, A. Nicolet and F. Zolla, ‘Spontaneous light emission by atomic Hydrogen: Fermi’s golden rule without cheating’, accepted by Phys. Lett. A (cit. on p. 184).
- [18] P. Facchi and S. Pascazio, ‘Temporal behavior and quantum Zeno time of an excited state of the hydrogen atom’, Phys. Lett. A **241**, 139 (1998) (cit. on p. 184).

## **Theses**

- [19] P. Facchi, Quantum Time Evolution: Free and Controlled Dynamics, PhD Thesis (Università degli Studi di Bari, 2000) (cit. on p. 184).



# CONCLUSION

---

*“You only know me like the shoreline knows the sea.”*

Paul Banks in “Over My Shoulder”, **Banks** (Matador, 2012)

We begin this conclusion by recalling what we learned in the various chapters of this Thesis.

In chapter 1 we saw how photons are defined by relativistic quantum field theory as objects of definite helicity and wave vector. We discussed how the idea of “photons” is based on the invariance of helicity and masslessness under all transformations of the Poincaré group [2, 3]. In the process, we obtained the expression of the representatives  $\hat{P}^\mu$  and  $\hat{J}^{\mu\nu}$  of the generators of Poincaré transformations on the Hilbert space of the quantum states of the electromagnetic field. The expressions we derived for these generators in the Lorenz gauge (see sect. 1.A.4.9) were obtained here for the first time as far as we know.

In chapter 2 we showed, following Hawton’s procedure [4, 5], how it is possible to define a position operator for photons with commuting vector components, thereby allowing for the formal existence of single-photon states which are perfectly localised in all three directions of space.

The definite momentum (wave vector) photon states of chapter 1 and definite position photon states of chapter 2 are both mathematically useful objects, but are of dubious physical relevance. In chapter 3 we showed how more physical wave functions (*i.e.* wave packets) for photons can be built. We discussed in detail how different possible momentum space normalisations for these wave functions are possible, as determined by a parameter [6, 7] we called  $\beta$ , leading to different physical meanings for the wave functions. We saw that two choices in particular for that normalisation result in the wave function carrying direct physical meaning, namely, the vector potential ( $\beta = -1/2$ , Gross-Hawton wave function [6, 8, 9]) and the electric field ( $\beta = +1/2$ , Riemann-Silberstein wave function [10–14]). We highlighted the similarity between the usual Schrödinger equation and the wave equation (3.2.3) for photon wave functions. We showed the relevance of Glauber’s extraction rule [14, 15] as a straightforward prescription to link single-photon states of the electromagnetic field with single photon wave functions. We discussed the difficulties that arise in defining a positive-definite number density for photons and the related difficulties in defining Bohmian trajectories. A quick summary of these points is given in Tab. 3.1.

In chapter 4 we briefly discussed how Glauber’s extraction rule can be extended from single-photon states to arbitrary states of the electromagnetic field, in order to investigate the coherence properties of light, and, with the help of the correlation functions of the electromagnetic field, assess [1] how much the behaviour of the field corresponding to quantum states of light departs from that of classical electromagnetic fields.

In chapter 5 we gave results on simple interacting systems (toy-models for nuclear  $\alpha$  decay and the description of losses in cavity quantum electrodynamics) which exhibit time decay of the initial (excited) quantum state.



We explained how the relevance of Gamow’s simple model for nuclear  $\alpha$  decay overcomes the specificities of the initial state of the decaying particle and examined the propagation of single photons away from a quantum electro-dynamical cavity, anticipating on the more involved version on the problem treated in chapter 7.

We showed in chapter 6 that for the  $2p - 1s$  transition in atomic Hydrogen, Fermi’s golden rule is an excellent approximation to the exact dynamics of the electronic decay. The maximal deviation from the golden rule is of order  $10^{-8}/10^{-7}$ , as seen on Figs. 6.3.2 and 6.3.3. Moreover, just  $10^{-15}$  s after the start of the decay, the behaviour of the decaying electron is completely indistinguishable from that predicted by Fermi’s golden rule. We also showed that for the same transition, the dynamics of the decay is very well described at all times within the framework of the dipole approximation for the atom-field interaction, if we make the “correct” choice (6.4.2) for the cutoff frequency. The fact that this prescription for the cutoff yields such good results, however, can only be known by comparison with the dynamics yielded by the exact atom-field coupling.

Finally, chapter 7 was devoted to an investigation of the electromagnetic field emitted during the same Hydrogen atomic  $2p - 1s$  transition. We asked whether this field vanishes outside the lightcone centred on the spacetime point  $(0, 0)$  which labels the time at which the decay starts and the position of the Hydrogen nucleus. We found that for the transition under study, the well-known Hegerfeldt theorem is not the only source of noncausality. We detailed Shirokov’s qualitative description [16] of the out-of-lightcone terms that appear in the field when the dipole approximation is not performed. We emphasised the relevance of the contribution of the longitudinal electric field, which we argued shows that the minimal  $\hat{\mathbf{A}} \cdot \hat{\mathbf{p}}$  atom-field coupling is the correct choice for the interaction Hamiltonian.

Further investigations based on the expression obtained for the emitted electromagnetic field are natural extensions of the present work. Arguments based on the asymptotic behaviour of the exponential integral function  $Ei$ —ubiquitous in our expressions—could come in handy to assess the behaviour of the field at large distances from the source (or at long times). Beyond that, numerical investigations seem in order, and are already ongoing. Since our result was derived as rigorously as possible in the framework of perturbation theory at short times, and, as we argued in sect. 7.3, can be adapted to longer times via a very simple substitution, we think that it is a fruitful basis on which to investigate the question of causality in spontaneous emission in detail. As we hope chapter 7 made clear, the physics of the emitted field is very rich, several distinct points—the Hegerfeldt problem of negative frequencies, the delocalisation of the emitting electron, the causal propagation of the Coulomb field with anticausal support—come into play. They are as many sources of departure from the naive expectation of causality, and, as we see it, as many sources of curiosity and wonder.

On a different note, it would also be interesting to try and find systems for which the quantum Zeno regime is experimentally accessible. Relying on the analysis of chapter 6, informed by the works of Facchi and Pascazio [17, 18] and Antoniou, Karpov, Pronko and Yarevsky [19], and especially on the discussion of sect. 6.5, we conclude that both what we called the cutoff time  $t_X$ —defined so that after  $t_X$ , the system exits the Zeno regime in which the survival probability decays quadratically—and the strength of the Zeno decay—the quantity by which the survival probability of the initial, excited state has decayed when the dynamics exits the Zeno regime—are relevant parameters to the experimental observation of the Zeno regime. A long cutoff time  $t_X$  and a strong Zeno decay are desirable for the experimentalist. As established, notably on the basis of [19], searches for systems with an observable Zeno regime should turn towards systems which are rather strongly coupled to their (electromagnetic) environment, especially at low frequencies with respect to the cutoff frequency of the coupling<sup>3</sup>.

---

<sup>3</sup>Here “cutoff frequency” is to be understood as a quantity similar to the  $\omega_X$  of the exact Hydrogen atom-field coupling (see sect. 6.1.4) rather than as in the usual sense of the frequency beyond which the coupling is taken to be exactly zero.

Another line of enquiry is the generalisation of Hawton's photon position operator—which was derived in [4, 5] in the Coulomb gauge (see chapter 2)—to a covariant framework. The most direct path is to use the Lorenz gauge instead. Beyond the formal appeal of such a result, this could make the position operator more directly relevant to physical problems which lack a privileged frame of reference. First steps have already been taken in that direction, and the careful investigation of the algebra of polarisation four-vectors, undertaken in sect. 1.A.4.9 provides helpful results in our efforts, but work is still to be done to shed some light on the rather complicated expressions obtained so far.

# REFERENCES

---

## Books

- [1] L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, 1995) (cit. on p. 189).

## Articles

- [2] E.P. Wigner, ‘On Unitary Representations of the Inhomogeneous Lorentz Group’, *Ann. Math* **40**, 149 (1939) (cit. on p. 189).
- [3] V. Bargmann and E.P. Wigner, ‘Group Theoretical Discussion of Relativistic Wave Equations’, *Proc. Natl. Acad. Sci. USA* **34**, 211 (1948) (cit. on p. 189).
- [4] M. Hawton, ‘Photon position operator with commuting components’, *Phys. Rev. A* **59**, 954 (1999) (cit. on pp. 189, 191).
- [5] M. Hawton and W.E. Baylis, ‘Photon position operators and localized bases’, *Phys. Rev. A* **64**, 012101 (2001) (cit. on pp. 189, 191).
- [6] M. Hawton, ‘Photon wave mechanics and position eigenvectors’, *Phys. Rev. A* **75**, 062107 (2007) (cit. on p. 189).
- [7] M. Hawton, ‘Lorentz-invariant photon number density’, *Phys. Rev. A* **78**, 012111 (2008) (cit. on p. 189).
- [8] M. Hawton, ‘Photon wave functions in a localized coordinate space basis’, *Phys. Rev. A* **59**, 3223 (1999) (cit. on p. 189).
- [9] L. Gross, ‘Norm Invariance of Mass-Zero Equations under the Conformal Group’, *J. Math. Phys.* **5**, 687 (1964) (cit. on p. 189).
- [10] L. Silberstein, ‘Elektromagnetische Grundgleichungen in bivectorieller Behandlung’, *Ann. Phys. (Leipzig)* **327**, (the link points to an English version of the article), 579 (1907) (cit. on p. 189).
- [11] L. Silberstein, ‘Nachtrag zur Abhandlung über ‘Elektromagnetische Grundgleichungen in bivectorieller Behandlung’’, *Ann. Phys. (Leipzig)* **329**, (the link points to an English version of the article), 783 (1907) (cit. on p. 189).
- [12] J.E. Sipe, ‘Photon Wave Functions’, *Phys. Rev. A* **52**, 1875 (1995) (cit. on p. 189).
- [13] I. Białynicki-Birula, ‘Photon Wave Function’, *Prog. Opt.* **36**, 245 (1996) (cit. on p. 189).
- [14] B.J. Smith and M.G. Raymer, ‘Photon wave functions, wave-packet quantization of light, and coherence theory’, *New J. Phys.* **9**, 414 (2007) (cit. on p. 189).
- [15] U.M. Titulaer and R.J. Glauber, ‘Density Operators for Coherent Fields’, *Phys. Rev.* **145**, 1041 (1966) (cit. on p. 189).

- [16] M.I. Shirokov, 'Signal velocity in quantum electrodynamics', *Sov. Phys. Usp.* **21**, 345 (1978) (cit. on p. 190).
- [17] P. Facchi and S. Pascazio, 'Temporal behavior and quantum Zeno time of an excited state of the hydrogen atom', *Phys. Lett. A* **241**, 139 (1998) (cit. on p. 190).
- [18] P. Facchi, H. Nakazato and S. Pascazio, 'From the Quantum Zeno to the Inverse Quantum Zeno Effect', *Phys. Rev. Lett.* **86**, 2699 (2001) (cit. on p. 190).
- [19] I. Antoniou, E. Karpov, G. Pronko and E. Yarevsky, 'Quantum Zeno and anti-Zeno effects in the Friedrichs model', *Phys. Rev. A* **63**, 062110 (2001) (cit. on p. 190).