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Université Paris Diderot - Paris 7
UFR de Physique

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THESE DE DOCTORAT
DE L'UNIVERSITE PARIS DIDEROT - PARIS 7

Spécialité

Physique Théorique

présentée par

Seyed Majid Saberi Fathi

Chaos, entropie et durée de vie dans les systèmes classiques et quantiques

Soutenue le 19 juillet 2007
devant le jury composé de Messieurs:

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Résumé

Dans cette thèse, nous étudions un modèle de désintégration (decay) d'un système quantique à plusieurs niveaux appelé le modèle de Friedrichs. Dans un premier travail, nous considérons un couplage d'un kaon avec un environnement décrit par un continuum d'énergie. On montre que les oscillations du kaon entre les états $\mathrm{K}_1, \mathrm{K}_2$, leur decay et la violation CP sont bien décrits par ce type de modèle. Ensuite, nous appliquons à ce modèle le formalisme de l'opérateur de temps qui décrit la résonance, c'est-à-dire la probabilité de survie des états instables. Enfin, nous considérons un gaz de Lorentz comme un ensemble de boules de billard avec des collisions élastiques contre des obstacles et un système de sphères dures en dimension 2. Nous étudions la simulation numérique de la dynamique du système et calculons l'augmentation de l'entropie de non-équilibre au cours du temps sous l'effet des collisions et sa relation avec les exposants de Lyapounov positifs.

Abstract

In this thesis, we first study Lorentz gas as a billiard ball with elastic collision with the obstacles and a system of hard spheres in 2-dimensions. We study a numerical simulation of the dynamical system and we investigate the entropy increasing in non-equilibrium with time under the effect of collisions and its relation to positive Lyapounov exponents. Then, we study a decay model in a quantum system called Friedrichs model. We consider coupling of the kaons and environment with continuous energies. Then, we show that this model is well adapted to describe oscillation, regeneration, decay and CP violation of a kaonic system. In addition, we apply in the Friedrichs model, the time super-operator formalism that predicts the resonance, i.e. the survival probability of the instable states.

Acknowledgements

I wish to express my sincere gratitude to Maurice Courbage, my supervisor, for his guidance and support throughout my thesis. I am extremely grateful to members of the thesis committee. Arno Bohm accepted to be the president of the jury and he changed his travel schedule to participate in the defense session. Tuong T. Truong accepted to be reader of my thesis and expressed his helpful comments and suggestions. George Zaslavsky accepted to be reader of my thesis and he let me collaborate in another research work with him and I benefited his useful remarks. Thomas Durt accepted to be a member of jury and collaborated on a part of my thesis.

I would specially like to thank Tuong T. Truong for offering me a Post-Doc in 2007-2008.

I wish to thank Pascal Monceau for his technical discussions in the numerical computation and Ilyes Kamoun for the grammatical editing of this thesis. I give my thanks to the members of the old LPTMC and MSC specially: Jean-Claude Lévy, Jean-Marc Di Meglio, Eric Huguet, Michel Pereau, Mohamed Hebache, Stéphane Metens, Nöelle Pottier, Ardishir Rabeie, Mabrouk Zemzemi, Pedro Garcia de Leon, Tarik Garidi, Julien Queva, Avi Elkharrat, Sebastien Villain, Evelyne Authier, Carole Barache, Claudine Héneaux, Danielle Champeau, and Nadine Beyer.

Of course, I am grateful to my wife Maryam, my parents Tayyebeh and Morteza Saberi Fathi, my brothers Mohamad Reza and Mohamad Nasser, my sister Marzieh and my family in-law for their patience and *love*.

Paris,

Seyed Majid Saberi Fathi

June 20, 2007.

Introduction (En Français)

0.1 Première partie: Systèmes chaotiques classiques

Le théorème-H pour les systèmes dynamiques décrit l'approche à l'équilibre, l'irréversibilité et l'augmentation d'entropie pour des évolutions déterministes. L'existence de telles fonctionnelles dans les systèmes dynamiques conservatifs a été l'objet de plusieurs investigations pendant les dernières décennies, voir [20]- [23], [25], [28, 29, 32]). Dans ce travail, nous étudions ce problème pour le gaz de Lorentz et les disques durs.

Le gaz de Lorentz à deux dimensions est un système de particules sans interactions se déplaçant avec une vitesse constante et étant élastiquement refléchis par des diffuseurs périodiquement distribués. Les diffuseurs sont des disques fixes. A cause de l'absence des interactions entre les particules la distribution statistique du système est réduit au mouvement d'une boule de billard. Nous étudierons l'augmentation d'entropie sous l'effet des collisions des particules avec les obstacles.

Dans la première partie de cette thèse, nous calculerons d'abord l'augmentation d'entropie pour quelques distributions remarquables de non-équilibre au-dessus de l'espace de phase du billard de Sinaï. Le système de billard est un système hyperbolique (avec beaucoup de lignes de singularité) et, afin d'avoir un mélange rapide, nous considérerons des distributions initiales portées par les fibres dilatantes. De telles mesures initiales ont été utilisées dans [20, 23, 32]. Pour le billard, les fibres dilatantes sont des ensembles de particules avec des vitesses parallèles. Nous appelons cette classe des ensembles initiaux un "faisceau de particules". Nous calculons d'abord l'augmentation d'entropie en fonction des collisions pour ces dernières distributions initiales. Nous considérerons les obstacles uniformes finies dans l'espace de phase. Le calcul prouve que quel que soit le coarsening de ces partitions, l'entropie a

la propriété monotone dans les premières collisions. Il est clair que, le long du processus de mélange, la distribution initiale se répartira dans toutes les cellules jusqu'à atteindre la valeur d'équilibre. Physiquement, ce processus est dirigé par l'instabilité forte, elle est exprimée par l'exposant positif de Lyapounov.

Nous considérons également la relation du taux d'augmentation des fonctionnelles d'entropie aux exposants de Lyapounov du gaz de Lorentz. Notre calcul prouve que cette relation est exprimée par une inégalité

$$\max(\mathcal{S}(n+1) - \mathcal{S}(n)) \equiv \triangle\mathcal{S} \leq \sum_{\lambda_i \geq 0} \lambda_i = h_{K-S}$$

Autrement dit l'entropie de Kolmogorov-Sinaï $(K - S)$ est une limite supérieure du taux d'augmentation de cette fonctionnelle.

Nous considérerons les systèmes de disques durs et calculerons une fonctionnelle de l'entropie comme l'entropie spatiale sur le tore avec plusieurs cellules. Les probabilités sont définies comme à l'entropie de l'espace dans le gaz de Lorentz. Nous ferons également quelques comparaisons entre le thèorem-H et la somme des exposants de Lyapounov positifs.

0.2 Deuxième partie: "Systèmes instables quantiques"

Les systèmes quantiques instables font l'objet de la deuxième partie de cette thèse. Nous avons employé le modèle de Friedrichs pour décrire les phénomènes de désintégration (decay) dans l'espace de Hilbert et également dans l'espace de Liouville en utilisant l'opérateur de temps.

"Phénoménologie du Kaon"

Généralement la mécanique quantique est décrite par les lois unitaires d'évolution réversible (par l'intermédiaire de l'équation de Schrödinger). Cette description contredit notre expérience journalière où le vieillissement, la dissipation et l'irréversibilité sont omniprésentes. Dans ce contexte, il est intéressant d'étudier les systèmes quantiques hybrides, qui suffisamment complexes, sont en tout unitaires et dissipatifs dans des évolutions de temps. Ce but peut être atteint dans le cadre du modèle de Friedrichs.

Le modèle d’un niveau de Friedrichs est bien compris [57, 58, 59]: il prévoit que l’état excité disparaît et “fond” dans le continuum. Sa probabilité de survie se désintégre exponentiellement dans le temps. La durée de vie est proportionnelle au couplage entre le mode discret et le continuum. Les systèmes à decroissance exponentielle sont très communs dans la physique classique et quantique. Ils sont relativement insignifiants quand nous les considérons du point de vue de l’irréversibilité temporelle parce que, bien que la loi de décroissance ne soit pas réversible au temps, de tels systèmes se comportent comme si ils n’ont pas possédé une horloge ou une mémoire interne : le taux de décroissance est constant dans le temps, et l’état du système non-désintégré reste le même à tout moment. En général, les systèmes à décroissance exponentielle montrent un comportement irréversible mais ignorent le vieillissement.

Nous prouverons que le système de deux niveaux de Friedrichs [48] permet à décrire une classe de systèmes qui montrent des comportements riches et complexes : les oscillations, régénérations, etc, et décrit un modèle phénoménologique relativement exact de la physique de kaons. Il y a eu plusieurs approches à la violation de CP dans les kaons en utilisant la théorie de jauge (Gauge Theory) [91] ou la théorie de renormalisation [50]. Nous ne considérons pas ces aspects ici, également parce que la question est toujours partiellement ouverte aujourd’hui. Notre traitement est basé sur la description des systèmes à désintégration similaires à la généralisation de l’approche de Weisskopf-Wigner, formulée par Lee, Oehme et Yang (LOY) [51] dans le cas de la désintégration de kaon. Plus tard, Chiu et Sudarshan [52] ont employé un modèle de Lee afin d’obtenir une correction de la théorie de LOY pendant des durées courtes.

Résolvant l’équation du Schrödinger pour le hamiltonien, nous montrons une équation maîtresse pour la désintégration des états à deux niveaux. Notre nouvelle approche est basée sur l’obtention d’une équation maîtresse d’un hamiltonien décrivant des modes à décroissance de (K_1, K_2) et non pas pour des modes de $(\mathrm{K}^0, \overline{\mathrm{K}}^0)$ comme est montré dans la théorie de LOY. En supposant un faible couplage, nous obtenons une équation markovienne maîtresse qui nous permet de simuler la durée de vies des kaons, aussi bien que leurs oscillations et leurs régénérations. Il adapte même plus étroitement le paramètre de la destruction de la symétrie de CP. Dans un premier exemple, par le spectre non-borné dans l’énergie, nous obtenons l’angle exact tandis que le module est 14 fois au résultat expérimental. Cependant, nous montrons qu’en utilisant les différentes fonctions de coupure des degrés continus de liberté, nous pouvons améliorer l’évaluation ci-dessus.

Nous montrons aussi, qu'il est possible d'obtenir tous les dispositifs intéressants du modèle quand le hamiltonien possède un spectre seulement borné de l'inférieur. Dans ce cas-là, avec la coupure gaussienne, l'évaluation précédente est améliorée et nous obtenons la valeur de paramètre de violation de CP qui est seulement 3 fois du résultat expérimental. Notre étude confirme qu'il est possible de calculer quelques dispositifs essentiels de la phénoménologie très riche de kaon avec un modèle très simple tel que le modèle à deux niveaux de Friedrichs. Elle confirme également que l'ingrédient essentiel pour obtenir une dynamique de temps irréversible des sous-ensembles est la présence des degrés continus de liberté d'environnement.

“Opérateur de temps ”

Le temps apparaît dans la physique principalement dans la description de mouvement. Mais, ce temps n'est pas celui qui correspond au changement d'état du temps d'un corps ou d'un système complexe. D'une part, la transformation de temps-orienté des états de systèmes complexes est déterminé comme le dispositif le plus fondamental de la thermodynamique. La deuxième loi est le premier rapport faisant une distinction entre le passé et le futur dans les processus physiques. En parlant de l'état d'un corps ou d'un système, nous comprenons évidemment un état macroscopique. Néanmoins, dans la mécanique quantique, la découverte des durées de temps des particules élémentaires instables a présenté une nouvelle distinction entre le passé et le futur au niveau microscopique.

Dans l'autre part, nous étudierons les propriétés de la probabilité de survie des systèmes quantiques instables en utilisant les projections spectrales d'opérateur de temps établies dans le cadre de la description de Liouville-von Neumann [92, 93]. Nous examinerons ces propriétés dans le modèle de Friedrichs [48]. La probabilité de survie devrait être une fonction de temps monotone décroissante et cette propriété ne pourrait pas exister dans le cadre de l'approche mécanique quantique habituelle [94, 95, 96]. Elle peut seulement être correctement traitée par un opérateur observable de temps T dont les projections propres décrivent la distribution de probabilité de la durée de décroissance.

0.3 Présentation

Cette thèse contient quatre articles. Avant chaque article, un ou plusieurs chapitres sont consacrés à l'explication des théories appropriées contenue dans l'article qui suit. Dans ces chapitres, l'idéa principale est une bréve étude des théories. A cette fin, parfois, j'ai évoqué briévement une partie des références qui sont mentionnés à la fin de la section.

Dans le premier chapitre nous avons présenté quelques concepts dans les systèmes dynamiques comme la dynamique différentielle, les exposants de Lyapunov, le gaz de Lorentz et les sphères dures. Nous avons également fait quelques discussions sur le théorem de H, la théorie ergodique, l'entropie de Shanonn et entropie de Kolmogorov-Sinaï ($K - S$) dans le premier article "**Computation of entropy increase for Lorentz gas and hard disks**", dans le chapitre 2. Dans celui-ci, nous avons d'abord présenté nos systèmes dynamiques. Ensuite, nous avons calculé l'entropie pour la map de collision pour le gaz de Lorentz, et l'entropie d'espace pour le gaz de Lorentz et les disques durs.

Dans le chapitre 3, nous avons discuté au sujet de certains préliminaires mathématiques comme des processus de Markov, définition de quelques espaces et transformations. Puis, dans le quatrième chapitre nous avons présenté quelques concepts de mécanique statistique quantique comme la matrice de densité, l'opérateur de projection, l'enchevêtrement quantique (quantum entanglement), la décohérence et l'entropie de von Neumann. La théorie de Wiesskopf-Wigner et la théorie de la Lie-Oehme-Yang (LOY) ont été discutées dans le chapitre 5. Le sixième chapitre contient le deuxième article, "**Two-Level Friedrichs model and kaonic phenomenology**". Dans cet article nous avons utilisé le modèle de Friedrichs sans fonction de coupure et avec l'énergie entre $-\infty$ et $+\infty$, pour expliquer la phénoménologie de kaon et également une évaluation de paramètre de violation de CP. Dans le troisième article, "**Quantum-mechanical decay laws in the neutral kaons**",(chapitre 7), nous avons utilisé le modèle de Friedrichs avec quelques fonctions de coupure, et nos résultats sont très proches des résultats expérimentaux.

L'effet quantique de Zeno, l'opérateur de temps et l'asymétrie de temps sont les autres modèles quantiques de H qui ont été discutés dans le huitième chapitre. A la fin, dans le dernier chapitre nous avons présenté le quatrième article, "**Decay of quantum-mechanical unstable systems and spectral projections of time operator in Friedrichs model**", pour obtenir la probabilité de survie d'un système

instable en employant le modèle à un niveau de Friedrichs. Nos résultats ont été présentés pour des durées courtes qui ne correspondent pas à un effet quantique de Zeno.

Publications[1]

- M. Courbage, S.M. Saberi Fathi; "Computation of entropy increase for Lorentz gas and hard disks", Communications in nonlinear science and numerical simulation, **13** Issue 2 (2008) 444-455.

- M. Courbage, T. Durt, S.M. Saberi Fathi; "Two-Level Friedrichs model and kaonic phenomenology," Physics Letters A **362** (2007) 100-104.

- M. Courbage, T. Durt, S.M. Saberi Fathi; "Quantum-mechanical decay laws in the neutral kaons," Journal of Physics A : Math. Theor. **40** (2007) 2773-2785.

- M. Courbage, S.M. Saberi Fathi; "Decay of quantum-mechanical unstable systems and spectral projections of time operator in Friedrichs model", soumis.

- M. Courbage, S.M. Saberi Fathi; "A formula for the spectral projection of time operator", Sera publié dans le *proceeding of XXV Workshop on Geometric Methods in Physics.*

Conférences

- "Quantum Hamiltonian dynamics of the kaons phenomenology", Chaos, Complexity and Transport: Theory and Applications , Marsielle June 4-8, 2007.

- "Computation of entropy increase for Lorentz gas and hard disks", 27ème Journées de Physique Statistique, Paris, 25-26 Janvier 2007.

- "A formula for the spectral projection of time operator," XXV Workshop on Geometric Methods in Physics, Bialowieza, Pologne, 2-8 Juillet 2006.

[1]Les noms des auteurs sont classés dans l'ordre alphabétique.

Introduction

0.4 First part: Classical chaotic systems

The H-theorem for dynamical systems describes the approach to equilibrium, the irreversibility and entropy increase for deterministic evolutions. The existence of such functional in measure-theoretical dynamical systems has been the object of several investigations during last decades. see [20]- [23], [25], [28, 29, 32]). Here we study this problem for the Lorentz gas and hard disks.

The Lorentz gas in two dimensions is a system of non-interacting particles moving with constant velocity and being elastically reflected from periodically distributed scatterers. The scatterers are fixed disks. On account of the absence of interactions between particles, the system is reduced to the motion of one billiard ball. We shall investigate the entropy increase under the effect of collisions of the particles with the obstacles.

In the first part of this thesis, we will first compute the entropy increase for some remarkable non-equilibrium distributions over the phase space of the Sinaï billiard. The billiard system is a hyperbolic system (with many singularity lines) and, in order to have a rapid mixing, we will consider initial distributions supported by the expanding fibers. Such initial measures have been used in [20, 23, 32]. For the billiard the expanding fibers are well approximated by particles with parallel arrows velocity. We call this class initial beams of particles. We first compute the entropy increase under the collision map for these initial distributions. For this, we will consider finite uniform partitions of the phase space. The computation shows that whatever the coarsening of these partitions, the entropy has the monotonic property in the initial stage. It is clear that, along mixing process, the initial distribution will spread over all cells almost reaching the equilibrium value. Physically, this process is directed by the strong instability, that is expressed by the positive Lyapounov exponent.

We also consider the relation of the rate of increase of the entropy functionals and Lyapounov exponents of the Lorentz gas. Our computation shows that this relation is expressed by an inequality

$$\max(\mathcal{S}(n+1) - \mathcal{S}(n)) \equiv \triangle\mathcal{S} \leq \sum_{\lambda_i \geq 0} \lambda_i = h_{K-S}$$

where the "max" is taken over n, which means that Kolmogorov-Sinaï $(K-S)$ entropy is an upper bound of the rate of increase of this functional.

We shall consider the hard disks systems. We shall compute an entropy functional similar to the space entropy on extended torus with several cells. The probabilities are defined for the space entropy in the Lorentz gas. We shall also do some comparisons of the H-theorem with the sum of normalized positive Lyapounov exponents.

0.5 Second part: Unstable quantum systems

Unstable quantum systems is the second part of this thesis. We have used the Friedrichs model to describe the decay phenomena in Hilbert space and also in Liouville space by using the time super operator.

"Kaon phenomenology"

In general, Quantum Mechanics provides a continuous, reversible in time and unitary evolution law (via the Schrödinger equation). This description contradicts our everyday experience in which ageing, dissipation and irreversibility are omnipresent. In this context, it is interesting to study hybrid quantum systems, sufficiently complex, that exhibit altogether unitary and dissipative time evolutions. This goal can be achieved in the framework of the Friedrichs model.

One-level Friedrichs model is well understood [57, 58, 59]: it predicts that the excited state disappears and "fuses" into the continuum. Its survival probability decays exponentially in time. The lifetime is proportional to the coupling between the discrete mode and the continuum. Exponentially decaying systems are very common in classical and quantum physics. They are relatively trivial when we consider them from the point of view of temporal irreversibility because, although the decay law is not reversible in time, such systems behave as if they did not possess an internal clock or memory: the decay rate is constant throughout time, and the non-decayed

system is in the same state at all times. Roughly speaking, exponentially decaying systems exhibit an irreversible behavior but ignore ageing.

We shall show that the two-level Friedrichs system [48] makes it possible to describe a class of systems that exhibit rich and complex behaviors: oscillations, regenerations and so on, and provides a relatively exact phenomenological model of kaons physics. There have been several approaches to CP-violations in kaons using Gauge Theory [91] or Renormalization Theory [50]. We do not consider these aspects here, also because the question is still partially open today. Our treatment is based on the description of decaying systems similarly to the generalization of the Weisskopf-Wigner approach, formulated by Lee, Oehme and Yang (LOY) [51] in the case of kaonic decay. Later on, Chiu and Sudarshan [52] used a Lee model in order to obtain a correction to the LOY theory for short times.

Solving the Schrödinger equation for the Hamiltonian, we derive a master equation for the decaying two-level states. Our new approach is based on the derivation of a master equation from a Hamiltonian describing (K_1, K_2) decaying modes and not for $(\mathrm{K}^0, \overline{\mathrm{K}}^0)$ modes as done in LOY theory. Under weak coupling hypothesis this leads to a Markovian master equation which allows us to simulate the kaonic lifetimes as well as kaonic oscillations and regeneration. It even fits closer the CP symmetry breaking parameter. In a first example with non-bounded spectrum in energy, we obtain the exact angle while the modulus is 14 times the experimental data. However, we show that using different cut-off functions of the continuous degrees of freedom we can improve the above estimate.

We prove that it is possible to obtain all the interesting features of the model when the Hamiltonian possesses a spectrum only bounded from below. In this case, with Gaussian cut-off the previous estimate is improved and we obtain a CP violation parameter value only 3 times the experimental data. Our treatment confirms that it is possible with a very simple model such as the two-level Friedrichs model to compute some essential features of the very rich kaon phenomenology. It also confirms that the essential ingredient for deriving an irreversible in time dynamics of subsystems is the presence of a continuous degrees of freedom of environment.

"Time operator"

Time appears in physics mainly in the description of motion. But this time is not the one that corresponds to the alteration of time state of a body or a complex system. On the other hand, the time-oriented transformation of the states of complex systems is recognized as the most fundamental feature of thermodynamics. The second law

is the first statement making a distinction between past and future in the physical processes. In speaking of the state of a body or a system, we obviously understand a macroscopic state. Nevertheless, in quantum mechanics, the discovery of lifetimes of unstable elementary particles has introduced a new distinction between past and future on the microscopic level.

In other hand, we shall study the properties of the survival probability of unstable quantum systems using the spectral projections of time operator built in the framework of the Liouville-von Neumann description [92, 93]. We shall test these properties in the Friedrichs model [48]. The survival probability should be a monotonically decreasing time function and this property could not exist in the framework of the usual quantum-mechanical approach [94, 95, 96]. It can only be properly treated through an observable time operator T whose eigenprojections provide the probability distribution of the time of decay.

0.6 Presentation

This thesis contains four articles. Before each article, one or some chapters exist to explain the relevant theories. The main idea in these chapters is a short study of the theories. For this purpose, sometimes, I stated briefly a part of the references which are maintained in the end of the section.

In the first chapter we introduce some concepts in dynamical systems like, differential dynamics, Lyapunov exponents, Lorentz gas and hard spheres. We also discuss about H-theorem, ergodic theory, shannon entropy and $K-S$ entropy to introduce the first article, "**Computation of entropy increase for Lorentz gas and hard disks**" in the chapter 2. In this chapter, we introduce our dynamical systems. Then, we compute entropy for collision map for Lorentz gas and spatially extended Lorentz gas and hard disks entropy.

In the chapter 3, we discuss about some mathematical preliminaries like, Markov process, definition of some space and transformations. Then, in the Fourth chapter we present some concepts in the quantum statistical mechanics like density matrix, projection operator, quantum entanglement, decoherence and von Neumann entropy. The Wiesskopf-Wigner theory and Lee-Oehme-Yang (LOY) theory are discussed in chapter 5. The Sixth chapter is the second article, "**Two-Level Friedrichs model**

and kaonic phenomenology". In this paper we use the Friedrichs model without cutoff function and unbounded energy to explain kaon phenomenology and also an estimation of CP violation parameter. In the third paper, "**Quantum-mechanical decay laws in the neutral kaons**" (chapter 7), we use the Friedrichs model with many cutoff functions, and our results are very near to experimental results.

The quantum Zeno effect, time operator and time asymmetry are the other quantum decay models which are discussed in the eighth chapter. Finally, in the last chapter we present the fourth article, " **Decay of quantum-mechanical unstable systems and spectral projections of time operator in Friedrichs model**" to obtain the survival probability of an unstable system by using the one-level Friedrichs model. Our results present for short-time limit it is not correspond to a quantum Zeno effect.

Publications[2]

- M. Courbage, S.M. Saberi Fathi; "Computation of entropy increase for Lorentz gas and hard disks", Communications in nonlinear science and numerical simulation, **13** Issue 2 (2008) 444-455.

- M. Courbage, T. Durt, S.M. Saberi Fathi; "Two-Level Friedrichs model and kaonic phenomenology," Physics Letters A **362** (2007) 100-104.

- M. Courbage, T. Durt, S.M. Saberi Fathi; "Quantum-mechanical decay laws in the neutral kaons," Journal of Physics A : Math. Theor. **40** (2007) 2773-2785.

- M. Courbage, S.M. Saberi Fathi; " Decay of quantum-mechanical unstable systems and spectral projections of time operator in Friedrichs model", Submitted.

- M. Courbage, S.M. Saberi Fathi; "A formula for the spectral projection of time operator", in proceeding of XXV Workshop on Geometric Methods in Physics, In press.

Conferences and Talks

- "Quantum Hamiltonian dynamics of the kaons phenomenology", Chaos, Complexity and Transport: Theory and Applications , Marsilles June 4-8, 2007.

- "Computation of entropy increase for Lorentz gas and hard disks", 27ème Journées de Physique Statistique, Paris, Jan. 25-26, 2007.

- "A formula for the spectral projection of time operator," XXV Workshop on Geometric Methods in Physics, Bialowieza, Poland, July 2-8, 2006.

[2]The authors names appear in alphabetical order.

Part I

Classical Chaotic Systems

Chapter 1

Dynamical systems and statistical mechanics

1.1 Differential dynamics

It is a rarity that a dynamical system can be described by mapping. The far more common case is that differential equations are required, perhaps even partial differential equations. In this section, we focus on dynamical systems whose evolution is modeled by ordinary differential equations. The differential dynamical equations is of the general type

$$\dot{\mathbf{r}} = \mathbf{f}_\mu(\mathbf{r}) \tag{1.1}$$

where μ is a map parameter and $\mathbf{r} \equiv \{x_1, \ldots, x_n\} \in \mathbb{R}^n$. For example, a simple pendulum driven by a periodic force and subject to damping proportional to velocity, has the following Newtonian dynamics

$$\ddot{x} + \Omega^2 \sin x = \epsilon(-\alpha\dot{x} + f\cos\omega t), \tag{1.2}$$

where ϵ, ω and f are the parameters of the system. The above equation can be written under the form of (1.1) in the usual way by defining a new variable $y = \dot{x}$. To obtain the autonomous[1] form, we let $t \to \theta$ and then add $d\theta/dt = 1$ to the differential system[1].

We refer to a solution of (1.1) as a trajectory depending on the given initial conditions. We also refer to the trajectories resulting from a neighborhood of initial

[1] A differential equation is called an autonomous differential equation if it is not dependent explicitly on time.

conditions as a flow.

1.1.1 Linearization

The dynamics determined by the vector field $\mathbf{f}_\mu(\mathbf{r})$ on the right-hand side of (1.1) can be highly nonlinear and complicated. However, as with maps, attracting sets and fixed points are of special interest. The fixed points are readily recognized as just those values of $\mathbf{r}$ for which $\mathbf{f}_\mu(\mathbf{r})$ is equal to zero. Fixed points can be stable or unstable, and so the behavior of fixed points is significant. To study this behavior we must linearize (1.1) in the neighborhood of such a fixed point.

Suppose $\mathbf{r}_e$ to be a fixed point of (1.1) (i.e. $\mathbf{r}_e$ is the solution of $\mathbf{f}_\mu(\mathbf{r}) = 0$), where for the moment we suppress the map parameter μ. We now make a Taylor expansion of $\mathbf{f}(\mathbf{r})$ around $\mathbf{r}_e$, assuming of course that $\mathbf{f}$ has adequate differentiability properties.

$$\mathbf{f}(\mathbf{r}) = \mathbf{f}(\mathbf{r}_e) + \mathbf{Df}(\mathbf{r}_e)(\mathbf{r} - \mathbf{r}_e) + \cdots \tag{1.3}$$

where $\mathbf{Df}(\mathbf{r}_e)$ is the matrix of functions $\partial f_i/\partial x_j$ evaluated at the fixed point $\mathbf{r}_e$. Since $\mathbf{f}(\mathbf{r}_e) = 0$, for small $(\mathbf{r} - \mathbf{r}_e)$ the dynamics is determined solely by the linear term.

By letting $\mathbf{y} = \mathbf{r} - \mathbf{r}_e$, $\mathbf{Df}(\mathbf{r}_e) = A$, we have

$$\dot{\mathbf{y}} = A\mathbf{y}. \tag{1.4}$$

We see that we can always expand the system to make it autonomous. The above equation is a valid approximation of (1.1) if only in a sufficiently small neighborhood of the fixed point $\mathbf{r}_e$. A specific solution of (1.4) with initial condition $\mathbf{y}_0$ is given by

$$\mathbf{y}(t) = e^{tA}\mathbf{y}_0 \tag{1.5}$$

and the general solution of (1.4) is obtained as linear superposition of n linearly independent solutions of $\mathbf{y}_i(t), \quad i = 1, \cdots, n$.

$$\mathbf{y}(t) = \sum_{i=1}^{n} c_i \mathbf{y}_i(t) \tag{1.6}$$

where the n unknown constants are determined by the initial conditions. If the system is not degenerate we have

$$\mathbf{y}_i(t) = e^{t\lambda_i}\mathbf{v}_i \tag{1.7}$$

where λ_i, and $\mathbf{v}_i$, $i = 1, \cdots, n$ are the (possible complex) eigenvalues and the eigenvectors of the matrix A, respectively. If the system has degeneracies so that λ is an eigenvalue of A with multiplicity k, then we must compute the generalized eigenvectors. For $k = 2$ solve for $\mathbf{u}$ and $\mathbf{v}$, where

$$A\mathbf{v} = \lambda\mathbf{v}, \qquad (a - \lambda I)\mathbf{u} \neq 0, \qquad (a - \lambda I)^2\mathbf{u} = 0, \tag{1.8}$$

giving the independent solution vectors [1]

$$\begin{aligned} \mathbf{y}_1(t) &= e^{\lambda t}\mathbf{v} \\ \mathbf{y}_2(t) &= e^{\lambda t}[\mathbf{u} + t(A - \lambda I)\mathbf{u}]. \end{aligned} \tag{1.9}$$

1.2 Lyapounov Exponents

The Lyapounov exponent or Lyapounov characteristic exponent (LCE) of a dynamical system is a quantity that characterizes the rate of separation of infinitesimally close trajectories. Quantitatively, two trajectories in phase space with initial separation δx_0 diverge

$$|\delta x(t)| \approx e^{\lambda t}|\delta x_0| \tag{1.10}$$

The rate of separation can be different for different orientations of initial separation vectors. Thus, there is a whole spectrum of Lyapounov exponents corresponding to the number of dimensions of the phase space. It is common to just refer to the largest one, because it determines the predictability of a dynamical system [35].

1.2.1 The Lyapounov Exponent for a map in one dimension

Consider two point x_0 and $x_0 + \epsilon$ mapped by the function $f : I \to I$, where $I \subset \mathbb{R}$ is some bounded interval on the real line $\mathbb{R}$. For n iterations of this map the Lyapounov exponent λ approximately satisfies the equation

$$\epsilon e^{n\lambda} = f^n(x_0 + \epsilon) - f^n(x_0). \tag{1.11}$$

where $f^n(x_0) = f(f(\cdots(f(x_0))\cdots))$. Dividing by ϵ and taking $\epsilon \to 0$ gives

$$e^{n\lambda} = \frac{df^n}{dx}\Big|_{x_0}. \tag{1.12}$$

By taking $n \to \infty$, then we have the definition for the Lyapounov exponent:

$$\lambda \equiv \lim_{n\to\infty} \frac{1}{n} \ln \left| \frac{df^n}{dx}\Big|_{x_0} \right| \tag{1.13}$$

where

$$\frac{df^n}{dx}\Big|_{x_0} = \frac{df}{dx}\Big|_{x_{n-1}} \frac{df}{dx}\Big|_{x_{n-2}} \cdots \frac{df}{dx}\Big|_{x_0} = f'(x_{n-1}) f'(x_{n-2}) \cdots f'(x_0) \tag{1.14}$$

Thus, equation (1.13) can be rewritten as [1]:

$$\lambda \equiv \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln \left| f'(x_i) \right|. \tag{1.15}$$

1.2.2 Lyapounov Characteristic Exponents

In the last subsection, we introduced the concept of a Lyapounov Characteristic Exponent (LCE). In this subsection we expand the result of the previous subsection to more than one dimension. To state the problem in a more quantitative way, we consider a general smooth dynamical system

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}) \tag{1.16}$$

where $\mathbf{z} \equiv (\mathbf{r}, \mathbf{v})$ is a phase space of the system. Note that the dynamical system represented by a differential equation the trajectories are referred to as flows. Let M denote the phase space manifold of an arbitrary system and denote a flow in M as

$$\phi^t : M \to M. \tag{1.17}$$

If one takes an initial point $\mathbf{z}_0 \in M$, then ϕ^t maps this initial point to $\phi^t(\mathbf{z}_0) \equiv \mathbf{z}(t)$. A flow is a one-parameter group of diffeomorphisms[2] with the composition law

$$\phi^{t_2+t_1} = \phi^{t_2} \circ \phi^{t_1}. \tag{1.18}$$

Let $\mathbf{z}(t)$ denote the reference trajectory, and $\mathbf{z}_s(t)$ a perturbed trajectory connected to $\mathbf{z}(t)$ by a parametrized path with parameter s such that $\lim_{s\to 0} \mathbf{z}_s(t) = \mathbf{z}(t)$. The associated tangent vector is defined by

$$\delta\mathbf{z}(t) = \lim_{s\to 0} \frac{\mathbf{z}_s(t) - \mathbf{z}(t)}{s} \tag{1.19}$$

[2] A diffeomorphism is an invertible function that maps one differentiable manifold to another, such that both the function and its inverse are smooth [35].

Its equation of motion is obtained by linearizing (1.16),

$$\delta\dot{\mathbf{z}}(t) = \mathbf{D}(\mathbf{z}(t)).\delta\mathbf{z}(t) \tag{1.20}$$

where $\mathbf{D}(\mathbf{z}(t)) = \partial\mathbf{f}/\partial\mathbf{z}$ is the Jacobi matrix of the system [2]. Then, its solution according to (1.5) is equal to:

$$\delta\mathbf{z}(t) = \mathbf{D}\phi^t_{\mathbf{z}}.\delta\mathbf{z}_0 \tag{1.21}$$

where

$$\mathbf{D}\phi^t_{\mathbf{z}} = e^{\int_{t_0}^{t} dt' \mathbf{D}(\mathbf{z}(t'))}, \tag{1.22}$$

is a derivative map on the tangent vectors, i.e. it is a map in $T_{\mathbf{z}}M$ (space tangent of M at $\mathbf{z}$) onto $T_{\phi^t(\mathbf{z})}M$ (space tangent of M at $\phi^t(\mathbf{z})$). In the particular case of a periodic orbit of period t_p, $\mathbf{D}\phi^{t_p}_{\mathbf{z}}$ is a mapping of $T_{\mathbf{z}}M$ onto itself [4].

The composition rule (1.18) implies for $\mathbf{D}\phi^t_{\mathbf{z}}$ that [1]

$$\mathbf{D}\phi^{t_1+t_2}_{\mathbf{z}} = \mathbf{D}\phi^{t_2}_{\phi^{t_1}(\mathbf{z})} \circ \mathbf{D}\phi^{t_2}_{\mathbf{z}} \tag{1.23}$$

Now, we define the LCE of $\delta\mathbf{z}_0 \in T_{\mathbf{z}_0}M$ as:

$$\lambda(\mathbf{z}_0, \delta\mathbf{z}_0) = \lim_{t\to\infty} \frac{1}{t} \ln \frac{\|\delta\mathbf{z}(t)\|}{\|\delta\mathbf{z}_0\|} \tag{1.24}$$

where $\|.\|$ denotes the Euclidean norm on $T_{\mathbf{z}}M$.

Oseledec's multiplicative ergodic theorem [3] states that for ergodic systems under very general assumptions, λ exists and that in L-dimensional phase space there are L orthonormal initial vectors $\delta\mathbf{z}_0$ yielding a set of n exponents $\{\lambda_l\}$, which is referred to as the Lyapounov spectrum of the system. The exponents are taken to be ordered, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_L$. Since, according to Oseledec, the λ_l are independent of the metric and the initial condition, we can drop the argument $\mathbf{z}_0$ [2]. By using (1.21), the equation (1.24) can be written as:

$$\lambda(\mathbf{z}_0, \delta\mathbf{z}_0) = \lim_{t\to\infty} \frac{1}{t} \ln \|\mathbf{D}\phi^t_{\mathbf{z}}\| \tag{1.25}$$

Geometrically the Lyapounov exponents can be interpreted as the mean exponential growth rates of the principal axes of an infinitesimal ellipsoid surrounding a phase point and evolving according to (1.11). Thus the Lyapounov spectrum describes the stretching and contraction characteristics of the phase flow .

The Lyapounov exponents of the class of symplectic systems[3], to which our hard particles belong if in equilibrium, exhibit a Smale-pair symmetry, $\lambda_l + \lambda_{L+1-l} = 0$, for $l = 1, ..., L$. Furthermore, for each quantity conserved by the equations of motion one Lyapounov exponent vanishes. In a d-dimensional equilibrium system of N hard particles and phase space dimension $L = 2dN$ the total momentum, the total (kinetic) energy, and the center of mass coordinates are conserved. Since also one exponent associated with a displacement in the flow direction equals zero, altogether $2d + 2$ Lyapounov exponents vanish in this case.

Nonequilibrium steady-state systems cease to be symplectic and become dissipative. Nevertheless, the Smale-pairing symmetry is not totally lost for homogeneous systems for which conjugate pairs of exponents add up to a constant negative value. Negative total sum of all Lyapounov exponents corresponds to irreversible entropy production. Furthermore, it can be shown that the sum of all Lyapounov exponents can be related to the respective macroscopic transport coefficients. The number of vanishing exponents due to the conserved quantities-center of mass, momentum, and kinetic energy-in the nonequilibrium case is a more subtle question [2].

Let $\delta\mathbf{z}_0^1, \ldots, \delta\mathbf{z}_0^k$, $1 \leq k \leq L$, be the parallelepiped generated by the linearly independent vectors $\delta\mathbf{z}_0^1, \ldots, \delta\mathbf{z}_0^k$ belonging to $T_\mathbf{z}M$. We denote the corresponding k-dimensional volume by $V^k(\delta\mathbf{z}_0^1, \ldots, \delta\mathbf{z}_0^k)$. The limit

$$\lambda^k(\mathbf{z}_0, \delta\mathbf{z}_0^1, \ldots, \delta\mathbf{z}_0^k) = \lim_{t\to\infty} \frac{1}{t} \ln V^k(\mathbf{D}\phi_\mathbf{z}^t(\delta\mathbf{z}_0^1), \ldots, \mathbf{D}\phi_\mathbf{z}^t\delta\mathbf{z}_0^k) \tag{1.26}$$

where λ^k are LCE's of order k.

For almost all vectors $\delta\mathbf{z}_0^1, \ldots, \delta\mathbf{z}_0^k$, $1 \leq k \leq L$ belonging to $T_\mathbf{z}M$, one has [4]

$$\lambda^k(\mathbf{z}_0, \delta\mathbf{z}_0^1, \ldots, \delta\mathbf{z}_0^k) = \sum_{i=1}^{k} \lambda_i(\mathbf{z}_0), \qquad k = 1, \ldots, L \tag{1.27}$$

1.2.3 Numerical computation of Lyapounov spectra

The practical computation of Lyapounov spectra according to the classic algorithm of Benettin et al. [4] proceeds by simultaneously solving the original equations of motion (1.11) for the reference trajectory $\mathbf{z}(t)$ and the linear variational equations (1.20) for a complete set of offset vectors $\delta\mathbf{z}(t)$, The difficulties associated with the choice of the generally unknown initial vectors $\delta\mathbf{z}_0$ and the rounding-error off effects of the

[3] A symplectic system is a nondegenerate closed bilinear system, like a Hamiltonian system.

computer are overcome by periodic reorthonormalization of the set of offset vectors, such that the Lyapounov exponents are obtained from the time averaged logarithms of the respective normalizing factors. The classical method of Benettin *et al.* [16] can be straightforwardly applied to differentiable dynamical systems. In principle the LCE's of any order k could be obtained by choosing randomly k vectors in $T_{\mathbf{z}}M$ and applying definition (1.25). Practically, naive application of the definition is not possible, because in general, in the stochastic region, the vectors become too large and the angles between their directions too small to allow a numerical computation of volumes. The procedure which follows overcomes these difficulties.

Choose $\delta\mathbf{z}_0^1, ..., \delta\mathbf{z}_0^k$ orthonormal and fix at not-too-large time τ. The idea is to replace, at regular time intervals τ, the evolved vectors by new orthonormal vectors, using, the Gram-Smith procedure. Precisely, denoting $v_0^i = \delta\mathbf{z}_0^i, i = 1, ..., k$, one defines and computes recursively

$$\begin{aligned} \tilde{v}_l^i &= D\phi^{\tau}_{\phi^{(l-1)\tau}(z)}(v_{l-1}^i) \\ \alpha_l^i &= \|(\tilde{v}_l^i)_\perp\| \\ v_l^i &= \frac{\|(\tilde{v}_l^i)_\perp\|}{\alpha_l^i} \end{aligned} \tag{1.28}$$

where $(\tilde{v}_l^i)_\perp$ stands for the component of $\tilde{v}_l^i$ orthogonal to all the (already orthonormal) v_l^j with $j < i$, i.e.,

$$\begin{aligned} (\tilde{v}_l^i)_\perp &= \tilde{v}_l^i, \quad i = 1 \\ (\tilde{v}_l^i)_\perp &= \tilde{v}_l^i - \sum_{j=1}^{i-1} \langle v_l^j . \tilde{v}_l^i \rangle v_l^j, \quad i > 1, \end{aligned} \tag{1.29}$$

where $\langle . \rangle$ is the Euclidean scalar product on T_zM. It is then not to difficult to prove, using the linearity of $D\phi_z^t$ and relation (1.27), that one has [4]

$$\lambda_i(\mathbf{z}_0) = \lim_{L\to\infty} \frac{1}{n\tau} \sum_{l=1}^{n} \ln \alpha_l^i. \tag{1.30}$$

1.3 Hard spheres model

Hard spheres are the hard balls of radii $\{a_1, a_2, \ldots, a_N\}$ and of masses $\{m_1, m_2, \ldots, m_N\}$, where N is the total number of hard balls. The motion of hard ball is composed of

free flights between binary collisions which are elastic and instantaneous. Energy and the total linear momenta are conserved [26], i.e.

$$m_i\mathbf{v}_i + m_j\mathbf{v}_j = m_i\mathbf{v}'_i + m_j\mathbf{v}'_j \tag{1.31}$$

$$\frac{1}{2}m_i v_i^2 + \frac{1}{2}m_j v_j^2 = \frac{1}{2}m_i v_i'^2 + \frac{1}{2}m_j v_j'^2. \tag{1.32}$$

where $\mathbf{v}_i \equiv \mathbf{v}_i(t_n)$ and $\mathbf{v}'_i \equiv \mathbf{v}'_i(t_n)$ are the velocity of ith hard balls before and after n^{th} collision in time t_n respectively. Now, we rewrite the above equations as:

$$\begin{cases} v'_{i\|} = v_{i\|}, \\ v'_{j\|} = v_{j\|}, \\ m_i v_{in} + m_j v_{jn} = m_i v'_{in} + m_j v'_{jn}, \end{cases} \tag{1.33}$$

and

$$\frac{1}{2}m_i v_{in}^2 + \frac{1}{2}m_j v_{jn}^2 = \frac{1}{2}m_i v_{in}'^2 + \frac{1}{2}m_j v_{jn}'^2 \tag{1.34}$$

where the indices "$\|$" and "n" are indicates to the velocities components parallel to and perpendicular on surface at the collision point. Then, the above equations yield

$$\begin{cases} v'_{i\|} = v_{i\|}, \\ v'_{j\|} = v_{j\|}, \\ v'_{in} = \frac{2m_j}{m_i+m_j}v_{jn} + \frac{m_i-m_j}{m_i+m_j}v_{in} = v_{in} - \frac{2m_j}{m_i+m_j}(v_{in} - v_{jn}), \\ v'_{jn} = \frac{2m_i}{m_i+m_j}v_{in} + \frac{m_j-m_i}{m_i+m_j}v_{jn} = v_{jn} + \frac{2m_i}{m_i+m_j}(v_{in} - v_{jn}). \end{cases} \tag{1.35}$$

Finally, in the vectorial form they can be written as

$$\begin{cases} \mathbf{v}'_i = \mathbf{v}_i - \frac{2m_j}{m_i+m_j}(\mathbf{n}.\mathbf{v}_{ij})\mathbf{n} \\ \mathbf{v}'_j = \mathbf{v}_j + \frac{2m_i}{m_i+m_j}(\mathbf{n}.\mathbf{v}_{ij})\mathbf{n} \end{cases} \tag{1.36}$$

where $\mathbf{v}_{ij} = (\mathbf{v}_i - \mathbf{v}_j)$ and $\mathbf{n} = \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}$, the unit vector perpendicular to surface at the collision point (in the collision point $|\mathbf{r}_i - \mathbf{r}_j| = a_i + a_j$).

The free flight between binary collisions are obtained as:

$$\mathbf{r}_i(t_n) = \mathbf{r}'_i(t_{n-1}) + (t_n - t_{n-1})\mathbf{v}'_i(t_{n-1}) \tag{1.37}$$

where the indice " $'$ " is indicated after collision. Noting that:

$$\mathbf{r}_i(t_n) = \mathbf{r}'_i(t_n) \tag{1.38}$$

and

$$\mathbf{v}_i(t_n) = \mathbf{v}'_i(t_{n-1}) \tag{1.39}$$

Now, for obtaining the LCE we must calculate the offset vector before and after collision. Thus, we take the differential from equations (1.36)-(1.39), for position we have,

$$\delta\mathbf{r}_i(t_n) = \delta\mathbf{r}'_i(t_{n-1}) + (t_n - t_{n-1})\delta\mathbf{v}'_i(t_{n-1}) \tag{1.40}$$

where $\delta\mathbf{r}'_i$ on time t_n can be defined as $\mathbf{v}_i\triangle t$ by multiply equation (1.36) on $\triangle t$ we obtain,

$$\begin{cases} \delta\mathbf{r}'_i(t_n) = \delta\mathbf{r}_i(t_n) - \frac{2m_j}{m_i+m_j}(\mathbf{n}.\delta\mathbf{r}_{ij}(t_n))\mathbf{n} \\ \delta\mathbf{r}'_j(t_n) = \delta\mathbf{r}_j(t_n) + \frac{2m_i}{m_i+m_j}(\mathbf{n}.\delta\mathbf{r}_{ij}(t_n))\mathbf{n}. \end{cases} \tag{1.41}$$

where $\delta\mathbf{r}_{ij} = (\delta\mathbf{r}_i - \delta\mathbf{r}_j)$. For the velocities we also have,

$$\begin{cases} \delta\mathbf{v}'_i(t_n) = \delta\mathbf{v}_i(t_n) - \frac{2m_j}{m_i+m_j}[(\delta\mathbf{n}.\mathbf{v}_{ij}(t_n))\mathbf{n} + (\mathbf{n}.\delta\mathbf{v}_{ij}(t_n))\mathbf{n} + (\mathbf{n}.\mathbf{v}_{ij}(t_n))\delta\mathbf{n}] \\ \delta\mathbf{v}'_j(t_n) = \delta\mathbf{v}_j(t_n) - \frac{2m_i}{m_i+m_j}[(\delta\mathbf{n}.\mathbf{v}_{ij}(t_n))\mathbf{n} + (\mathbf{n}.\delta\mathbf{v}_{ij}(t_n))\mathbf{n} + (\mathbf{n}.\mathbf{v}_{ij}(t_n))\delta\mathbf{n}] \end{cases} \tag{1.42}$$

and

$$\delta\mathbf{v}_i(t_n) = \delta\mathbf{v}'_i(t_{n-1}). \tag{1.43}$$

where $\delta\mathbf{v}_{ij} = (\delta\mathbf{v}_i - \delta\mathbf{v}_j)$, and

$$\delta\mathbf{n} = \frac{1}{a_1 + a_2}(\delta\mathbf{r}_{ij}(t_n) + \mathbf{v}_{ij}(t_n)\delta t_c). \tag{1.44}$$

Here δt_c is the delating time respect to the reference trajectory by [2]

$$\delta t_c = -\frac{\mathbf{n}.\delta\mathbf{r}_{ij}(t_n).}{\mathbf{n}.\mathbf{v}_{ij}(t_n)} \tag{1.45}$$

The next chapter will consider the hard spheres in two dimensions (hard disks) with the same masses.

1.4 Lorentz gas

By considering the following assumptions for the hard balls described in the last section, we can define the Lorentz gas

$$\begin{cases} m_i \to \infty, \\ a_i \to a, \\ m_j \to m, \\ a_j \to 0. \end{cases} \tag{1.46}$$

These assumptions are that the ith hard ball (with infinite mass and radius $a_i = a$) is fixed and the j hard ball (with mass $m_j = m$ and radius $a_j = 0$) is a punctual. In our simulation in the next chapter we consider all fixed hard balls (for this reason we have chosen $m_i = \infty$) in two dimensions that are distributed periodically.

1.5 *H*-theorem

First, we start by the Boltzmann transport equation:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1.\nabla_r + \frac{\mathbf{F}}{m}.\nabla_{\mathbf{v}_1}\right) f_1 = \int d\Omega \int d^3 v_2 \sigma(\Omega) |\mathbf{v}_1 - \mathbf{v}_2| (f_2' f_1' - f_2 f_1) \tag{1.47}$$

where $\sigma(\Omega)$ is the differential cross section for the collision $\{\mathbf{v}_1, \mathbf{v}_2\} \to \{\mathbf{v}_1', \mathbf{v}_2'\}$, Ω is the angle between $(\mathbf{v}_2 - \mathbf{v}_1)$ and $(\mathbf{v}_2' - \mathbf{v}_1')$, the prim index is indicated after collision, and

$$\begin{aligned} f_1 &\equiv f_1(\mathbf{r}, \mathbf{v}_1, t) \\ f_2 &\equiv f_1(\mathbf{r}, \mathbf{v}_2, t) \\ f_1' &\equiv f_1'(\mathbf{r}, \mathbf{v}_1', t) \\ f_2' &\equiv f_1(\mathbf{r}, \mathbf{v}_2', t), \end{aligned} \tag{1.48}$$

are the distributions functions. The equation (1.47) is a nonlinear integro-differential equation for f. The equilibrium distribution function of the equation (1.47) is a time independent function $f_0(\mathbf{v})$ that is the limit of distribution function as time goes to infinity. Assume that there is no external force. Thus, the distribution function is independent of $\mathbf{r}$, i.e. $f(\mathbf{v}, t)$. The equilibrium distribution function,denoted by $f_0(\mathbf{v})$,

is the solution of the equation $\partial f_0(\mathbf{v})/\partial t = 0$. The Boltzmann transport equation (1.47) for $f_0(\mathbf{v})$ satisfies the following integral equation

$$0 = \int d\Omega \int d^3v_2 \sigma(\Omega)|\mathbf{v}_1 - \mathbf{v}_2|(f_0(\mathbf{v}_2')f_0(\mathbf{v}_1') - f_0(\mathbf{v}_2)f_0(\mathbf{v}_1)) \tag{1.49}$$

where $\mathbf{v}_1$ is a given velocity. The above equation yields:

$$f_0(\mathbf{v}_2')f_0(\mathbf{v}_1') - f_0(\mathbf{v}_2)f_0(\mathbf{v}_1) = 0. \tag{1.50}$$

To show that the necessity of (1.50), we define the following functional:

$$H(t) \equiv \int d^3v f(\mathbf{v}, t) \log f(\mathbf{v}, t) \tag{1.51}$$

where $f(\mathbf{v}, t)$ is the distribution at time, satisfying

$$\frac{\partial f(\mathbf{v}_1, t)}{\partial t} = \int d\Omega \int d^3v_2 \sigma(\Omega)|\mathbf{v}_1 - \mathbf{v}_2|(f_2'f_1' - f_2f_1) \tag{1.52}$$

Differentiation of (1.51) yields

$$\frac{dH(t)}{dt} = \int d^3v \frac{\partial f(\mathbf{v}, t)}{\partial t}[1 + \log f(\mathbf{v}, t)] \tag{1.53}$$

Therefore, the condition $\partial f/\partial t = 0$ is necessary for $dH/dt = 0$. Now, we see that the statement $dH/dt = 0$ is the same as (1.50). It would then follow that (1.50) is also a necessary condition of (1.49).

Boltzmann's H-Theorem: If f satisfies the Boltzmann transport equation, then

$$\frac{dH(t)}{dt} \leq 0. \tag{1.54}$$

Proof: By substituting (1.47) in (1.53) we obtain

$$\frac{dH(t)}{dt} = \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\Omega)|\mathbf{v}_1 - \mathbf{v}_2|(f_2'f_1' - f_2f_1)[1 + \log f_1]. \tag{1.55}$$

The above integral is invariant under changing $\mathbf{v}_1$ and $\mathbf{v}_2$ because $\sigma(\Omega)$ is invariant under this interchanging. We now write the above formula as follows

$$\frac{dH(t)}{dt} = \frac{1}{2}\int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\Omega)|\mathbf{v}_1 - \mathbf{v}_2|(f_2'f_1' - f_2f_1)[2 + \log(f_1f_2)]. \tag{1.56}$$

This integral is invariant under interchanging $\{\mathbf{v}_1, \mathbf{v}_2\}$ and $\{\mathbf{v}'_1, \mathbf{v}'_2\}$ because for each collision there is an inverse collision with the same cross section. Hence

$$\frac{dH(t)}{dt} = \frac{1}{2}\int d^3v'_1 \int d^3v'_2 \int d\Omega\sigma'(\Omega)|\mathbf{v}'_1 - \mathbf{v}'_2|(f_2 f_1 - f'_2 f'_1)[2 + \log(f'_1 f'_2)]. \quad (1.57)$$

By noting $d^3v'_1 d^3v'_2 = d^3v_1 d^3v_2$, $|\mathbf{v}'_1 - \mathbf{v}'_2| = |\mathbf{v}_1 - \mathbf{v}_2|$, $\sigma'(\Omega) = \sigma(\Omega)$ and taking the sum of two last equation we obtain

$$\frac{dH(t)}{dt} = \frac{1}{4}\int d^3v_1 \int d^3v_2 \int d\Omega\sigma(\Omega)|\mathbf{v}_1 - \mathbf{v}_2|(f'_2 f'_1 - f_2 f_1)[\log(f_1 f_2) - \log(f'_1 f'_2)]. \quad (1.58)$$

The integrand is always negative. $dH(t)/dt = 0$ only if integrand becomes zero i.e. $(f'_2 f'_1 - f_2 f_1) = 0$, or under an arbitrary initial condition $f(\mathbf{v}, t) \to f_0(\mathbf{v})$ as $t \to \infty$[5].

H-theorem asserts that, if at any instant the value of a certain function H, a property of a system or of an ensemble associated with the system, is much greater than the minimum value of H, this value is very likely to decrease, although fluctuations away from the minimum value may occur; the minimum value of H is that which possessed a stationary ensemble of systems, and thus is the equilibrium value. Thus, the H-theorem is a statistical theorem that gives an expression of the irreversibility characteristic of macroscopic system in terms of a quantity which is a microscopic analogue of the negative generalized entropy of a system in nonequilibrium thermodynamics[6].

1.6 Ergodic Theory

Why are election polls often inaccurate? Why is racism wrong? Why are your assumptions often mistaken? The answers to all these questions and to many others have a lot to do with the non-ergodicity of human ensembles. Many scientists agree that ergodicity is one of the most important concepts in statistics. So, what is it?

Ergodicity is usually described in terms of objective properties of an ensemble of objects, and the discussion often gets lost in mathematical subtleties and thus it is often difficult to understand. Nonetheless, it will be described in bayesian, subjectivist terms; hopefully this will make the concept very accessible.

Suppose you are concerned with determining what the most visited parks in a city are. One idea is to take a momentary snapshot to see how many people are at this moment in park A, how many are in park B and so on. Another idea is to look at one individual (or few of them) and to follow him for a certain period of time, e.g. a

year. Then, you observe how often the individual is going to park A, how often he is going to park B and so on.

Thus, you obtain two different results: one statistical analysis over the entire ensemble of people at a certain moment in time, and one statistical analysis for one person over a certain period of time. The first one may not be representative for a longer period of time, while the second one may not be representative for all the people. The idea is that an ensemble is ergodic if the two types of statistics give the same result. Many ensembles, like the human populations, are not ergodic [7].

1.6.1 Introduction

The first aim of ergodic theory in statistical mechanics is to determine the conditions in which the methods of statistical mechanics can be used to describe dynamical systems.

In the exact dynamical description, a single macroscopic state corresponds to many microscopic states. Thus, with exactly solving the simultaneous equations of motion of, 10^{24} particles could be handled. Also, if the experimental measurements could be carried out with accuracy sufficient to yield a complete set of initial conditions for this equations, the solution gives a purely dynamical description of the system. But the thermodynamical description of a macroscopic system is characterized by the comparatively small number of parameters (which normally are the averages of the microscopic dynamical parameters) needed to specify completely the thermodynamic state of the system. Statistical mechanics uses ensembles, in order to calculate thermodynamical properties of a single system. The corresponding properties at one instant of each ensemble of systems are averaged over this ensemble; these ensemble averages represent the properties of the single system. It is clear that is not exact calculation; not only it neglects the weak interaction between particles and but also it uses some form of approximation. But, the importance of statistical elements is in the calculation of various thermodynamical properties. As regards these properties of statistical mechanics is far from being a mere substitute for exact mechanics. But, in fact, it has a much more positive significance.

Introducing some form of statistical technique is required in passing from a dynamical to thermodynamical description of a macroscopic system. Ergodic theory accepts the dynamical description as basic, and it seeks conditions for the dynamical system to exhibit those thermodynamical properties that may be represented by

ensemble averages.

The general procedure of statistical mechanics is the Boltzmann method which it is concerned with a single dynamical system and uses statistical methods to make calculation pertaining to such a system. On the other treatment introduced by Gibbs, consider a collection of similar systems, together with an appropriate distribution function, and calculates averages over such ensembles of systems; the statistical considerations are thus much more fundamental in this approach. Gibbs, however, refrained on the whole from attributing physical significance to his concept of an ensemble, and regarded the behavior of an ensemble of systems as being but formally analogous to that of a single physical system. Ergodic theory, or at any rate, the main body of ergodic theory, is grounded firmly on the microscopic dynamical description of a single macroscopic system; it is from this that the statistical description has to be deduced. It is carried out therefore, for the most part, within the Boltzmann framework in which the entire theory is based on a priori statistical postulates [6].

1.6.2 Statement of Ergodic Theorem

We turn now to the principal consequence of ergodicity. A function $g(\omega)$ (assumed to be measurable μ) is said to be invariant if $g(T\omega) = g(\omega)$. If $g(\omega)$ is an invariant function which is not trivial in the sense of begin a.e. constant, then for some α the invariant set $\{\omega : g(\omega) \leq \alpha\}$ has a measure strictly between 0 and 1. Thus, T is ergodic if and only if each invariant function is a.e. constant. Now, we can state the ergodic theorem as:

Theorem: If f is integrable, then there exists an integrable, invariant function $\hat{f}$ which is defined as:

$$\hat{f}(\omega) = \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f(T^k\omega) \tag{1.59}$$

and such that $\langle \hat{f} \rangle = \int \hat{f} dP = \int f dP = \langle f \rangle$. If T is ergodic then $\hat{f} = \int f dP = \langle f \rangle$ [8].

To explain the above ergodic theorem we consider that $\hat{f}$ represents a time average, and that $\langle f \rangle$ an averaging process, then

$$\langle f \rangle = \widehat{\langle f \rangle} = \langle \hat{f} \rangle = \hat{f}.$$

the first equality is obviously true for stationary ensembles, and the second follows from the resumption that one can interchange averaging processes. But the last

equality follows only if $\hat{f}$ is the same for all systems in the ensemble, and this is true only if the system is ergodic [9].

To pure mathematicians it is the existence of the time averages, subject to certain conditions, that constitutes the ergodic theorem; to physicists, on the other hand the ergodic theorem expresses the equivalence of time averages and ensemble averages. The difference in terminology may perhaps have arisen from the fact that in the classical theory, which has been developed the more by mathematicians, it is the proof of the existence of the time averages that is the most difficult part of the above program, whereas in the quantum theory the existence of the time averages is a trivial problem, and it is determining the conditions under which these may be replaced by ensemble averages. Here the term the ergodic theorem will be used in the second sense with respect to both the classical and the quantal treatments. It should be recognized, however that this is a generic term, referring to any theorem expressing the equivalence of time and ensemble averages rather than to one specific set of conditions under which this equivalence holds. In the other words, the ergodic theorem embraces many ergodic theorems [6].

1.7 Coarse-graining

A measurement which is made on a macroscopic system, but which, although necessarily of limited accuracy, is thought of as being carried out instantaneously, may be referred to conveniently as an instantaneous macroscopic measurement. Groups of dynamical states indistinguishable by means of any set of instantaneous macroscopic measurements may be termed *phase cells*, the number of dynamical states within each phase cell being dependent on the degree of accuracy of the instantaneous macroscopic measurements. A set of instantaneous macroscopic measurements thus yields a description of the system which is much coarser than the microscopic, dynamical description; it approximates to the dynamical state by means of the phase cell which includes the dynamical state and to dynamical properties of the system by means of values characterizing ranges of values of the dynamical properties. This approximate determination of the microstate of the system may be thought of as an accurate determination of the instantaneous macro-state of the system, the instantaneous macro-state being defined by the appropriate phase cell, and the approximate

values of the microscopic parameters may be regarded as accurate values of instantaneous macroscopic observables, which, whether quantum or classical, possess discrete spectra. These instantaneous macro-observables are thus coarse-grained forms of the microscopic observables. It is by way of this coarse-graining that statistical concepts enter the route leading from the dynamical to the thermodynamical description of a system, since coarse-graining is equivalent to a statistical averaging over the various microscopic states in the phase cells. However, the statistical concepts enter in a very general form namely that there is no requirement anything like as strong as that of equal probabilities for all microscopic states within each phase cell. Nevertheless, unlike the time averaging, in which the averaging is carried out over states actually occupied by the system, there is here a definite introduction of ideas extraneous to the dynamical description, since in this coarse-grained description there are involved dynamical states additional to those which the system occupies at the time.

Coarse-graining, in fact, plays so large a part in the transition from dynamical to thermodynamical treatments that coarse-grained microscopic variables are very often regarded as being sufficiently close representations of macroscopic observables for the time averaging over a finite time interval to be used in characterizing the macroscopic observables; thus macroscopic observables are identified with what have been termed instantaneous macroscopic observables. As is remarked upon shortly, this permits a different interpretation of the significance of the time averaging over an infinite period with which the ergodic theorem deals.

The procedure of coarse-graining brings about a reduction in the number of parameters used to handle the system theoretically, and such a reduction is necessary in passing to a thermodynamical description which uses only a small number of independent macroscopic variables [6].

One it be admitted that it is with coarse-grained quantities that thermodynamical properties are to be associated, it follows that the fine-grained classical ergodic theorem is $\hat{f} = \langle f \rangle$, where accuracy of measurement is completely unlimited. What is of interest for thermodynamics is the coarse-grained ergodic theorem

$$\widehat{\overline{f}} = \langle \overline{f} \rangle \tag{1.60}$$

where $\overline{f}$ represents value of instantaneous coarse-grained quantities. But even if this coarse-grained theorem can be proved, there remain certain general problems. Does the time average over an infinite period have any physical significance? Is it permissible to regard a macroscopic physical system as isolated? And how many

instantaneous macroscopic observables must be measured in order to determine the site of the phase cells? Although several attacks have been made on ergodic theory on the grounds that the proper response to both the first and the second questions is negative, it seems to be a solution of the third problem, that of defining phase cells, that ergodic theory needs most. Before such discussions are entered upon, however, one further feature may be mentioned, namely, that it is with only one type of thermodynamical variable that ergodic theory deals.

In ergodic theory external parameters of a system, such as the volume of the system and the intensifies of any fields external to the system, are assumed to have constant values, and so when the temporal behavior of the system is studied, no specific account need be taken of the dependence of the properties of the system on these external parameters. Apart from these external parameters thermodynamical observables are of one of two types. The first consists of properties that have dynamical, no less than thermodynamical, import; such are, for example, the energy of the system and the pressure exerted by the system. These thermodynamical properties may be regarded as coarse-grained, and time-smoothed, forms of the corresponding fine-grained dynamical variables, and it is with such observables alone that ergodic theory deals; these are the variables the values of which are evaluated as ensemble averages in the usual practice of statistical mechanics.

The other kind of thermodynamical variable is of a specifically statistical nature, and chose variables - temperature, entropy, chemical potentials, and derivative quantities, such as free energy have no significance with respect to a single microscopic state, and cannot be expressed in the form of ensemble averages of corresponding dynamical properties. Moreover, ergodic theory, or at any rate the main body thereof, is concerned with isolated systems, and for such systems neither temperature nor chemical potentials can be defined in the usual thermodynamical manner; it is when systems in mutual interaction are discussed that these concepts appear in thermodynamics. Although statistical mechanics, as distinct from thermodynamics, can provide formal definitions of temperature and of chemical potentials for an isolated system, entropy is the only one of these specifically statistical properties to have immediate thermodynamical significance for an isolated system. This is not to say, however, that these specifically statistical quantities do not appear in the development of statistical mechanics based on ergodic theory. A statistical-mechanical entropy, identifiable under appropriate conditions with thermodynamical entropy, can be defined easily in terms of the ergodic distribution, which pertains to equilibrium situations, and

can be generalized to nonequilibrium situations as well. Unlike the method of the H-theorem, however, ergodic theory makes no use of this entropy in obtaining the equilibrium distribution. As regards temperature, chemical potentials and other statistical quantifies, these, too, although not considered in ergodic theory itself, appear when systems in mutual interaction are discussed. And in order to relate dynamical and thermodynamical descriptions of a system it is important to consider such interacting systems; ergodic theory alone, insofar as it deals with an isolated system, cannot yield the required relationship, but constitutes merely the first albeit the fundamental step towards obtaining results of thermodynamical significance from a dynamical description of a system [6].

1.8 Entropy

1.8.1 Shannon entropy

There exists a quantity that measures the non-predictability degree of a deterministic and conservative dynamical system, it is called Kolmogorov-Sinaï entropy. This concept is not confused with thermodynamical entropy in nonequilibrium which is defined by information theory of Shannon. More precisely, it is a global character and uncertainly in the results of cross-graining observation in spite of it is known all precedent results. Moreover, the observation is smooth. It is depended on the instability of motion so that in some conditions $K - S$ entropy is equal to the sum of the positive Lyapounov exponents. Instability creates the unpredictability. We memorize some concepts of information theory.

In the information theory, the information is obtained by transmission of a message. It is measured by the logarithm of the number of messages possible. For example, the message of N letters by k alphabet letters $(a_1, \ldots, a_k) = \alpha$ is obtained as: If in each message of N letters each letter a_i is repeated p_i-times, then this letter is produced in the message with $N_i = p_i N$ frequency. Now, P is

$$P = \frac{N!}{N_1! \cdots N_k!} \tag{1.61}$$

and information is obtained by the transmission of a letter is:

$$I = \frac{\log P}{N} \tag{1.62}$$

by using Stirling formula for I we have

$$I(\alpha) = -\sum_i p_i \log p_i. \tag{1.63}$$

If we transmit many letters we must also consider the correlations between successive letters. We call $I(\alpha), I(\alpha_1, \alpha_2), \ldots$ as the information of one letter, two letters, etc. For example, to calculate $I(\alpha_1, \alpha_2)$ the probability $p(\alpha_1, \alpha_2)$ must be known in a message of the letter $\alpha_{1,i}$, then the letter $\alpha_{2,j}$, successively.

$$I(\alpha_1, \alpha_2) = -\sum_{i,j} p(\alpha_{1,i}, \alpha_{2,j}) \log p(\alpha_{1,i}, \alpha_{2,j}). \tag{1.64}$$

One can obtain

$$I(\alpha_1, \alpha_2) \leq I(\alpha_1) + I(\alpha_2) \tag{1.65}$$

the equal sing is possible when the letters successive are independent. Effectively, we can first measure the average correlation between two successive letters with conditional information $I(\alpha_2|\alpha_{1,i})$, averaging on the $\alpha_{1,i}$ values:

$$I(\alpha_2|\alpha_1) = -\sum_i p(\alpha_{1,i}) I(\alpha_2|\alpha_{1,i}) \tag{1.66}$$

where

$$I(\alpha_2|\alpha_{1,i}) = -\sum_j p(\alpha_{2,j}|\alpha_{1,i}) \log p(\alpha_{2,j}|\alpha_{1,i}) \tag{1.67}$$

and

$$p(\alpha_{2,j}|\alpha_{1,i}) = \frac{p(\alpha_{2,j}, \alpha_{1,i})}{p(\alpha_{1,i})}. \tag{1.68}$$

Then, we have

$$I(\alpha_2|\alpha_1) \leq I(\alpha_2) \tag{1.69}$$

the equal is valid only if α_1 and α_2 are independents. We see that the correlation between α_1 and α_2 is reduced the information. Shannon considered the correlation between a letter and the n precedent letters when n is very large as:

$$i(\alpha) = \lim_{n\to\infty} I(\alpha_n|\alpha_1, \ldots, \alpha_{n-1}) \tag{1.70}$$

where we used the definitions on the (1.66)-(1.68) and it is defined by information of a stochastic process. We see that for a determinist system, i.e. a letter determines the following letters, the equation (1.70) is zero. This quantity is undefinable with intrinsic uncertainly of the message before its transmission [10].

1.8.2 $K - S$ entropy

Kolmogorov used the spirit of the Shannon theory to introduce the entropy of a determinist conservative dynamical system. The essential idea is consisted by making the partitions in phase space M, the partition with reversible transformation S that is a conserved measure, μ, for an initial point x, the cells is appeared as $x, Sx, S^2x, \ldots, S^{-1}x, S^{-2}, \ldots$. It is used a partition of M : $(P_0, P_1, \ldots, P_n)$ and to associate with all x double continuation $u_i,\ i = 0, \pm 1, \pm 2, \ldots$ where each u_i is the cell number of the partition which appears $S^i x$. That is

$$x \to \{u_i(x)\} : \quad S^i x \in P_{u_i(x)} \tag{1.71}$$

in each point of x is associated a doubly infinite message and Sx is associated with the shifted message:

$$u_i(Sx) = u_{i+1}(x). \tag{1.72}$$

the stochastic process (u_i) is determined by the probability μ from (1.71):

$$P(u_n = i_0, u_[n+1 = i_1, \ldots, un+k = i_k) = \mu(S^{-n}P_{i_0} \cap S^{-(n+1)}P_{i_1} \cap \ldots \cap S^{-(n+k)}P_{i_k}). \tag{1.73}$$

This new representation of the transformation S is called a symbolic dynamics. We can measure the predictability of a dynamical system by predictability of the different symbolics dynamics associated with different partitions. For a partition $\mathcal{P}$ uncertainly of a future observation (if the ensemble of last observations is known), is defined by:

$$h(\mathcal{P}, S) = \lim_{n \to \infty} I(u_n | u_1, \ldots, u_{n-1}). \tag{1.74}$$

The $K - S$ entropy is the upper limit of $h(\mathcal{P}, S)$ for all the finite partitions [10]:

$$h(S) = \sup_{\mathcal{P}} h(\mathcal{P}, S) \tag{1.75}$$

1.8.3 Entropy functional under coarse-graining

The explanation of the irreversible approach to equilibrium in conservative systems by a coarse-graining procedure goes back to Gibbs [11, 12]. This is a summary of his main ideas.

The macroscopic level of description of a system of N molecules differs from the microscopic level by the fact that it is concerned with a small number (compared to

N) of macroscopic observables $(y_l, ..., y_k)$. Maintaining these observables to definite values (up to small fluctuations) still allows the system to be found into a wide range of possible microscopic states of the phase space M of the N molecules, the set of which defines a certain region of M. Thus, to a distinct k-tuple of fixed values these observables correspond to disjoint regions of the phase space forming a finite partition $\mathcal{P} \equiv (P_0, P_1, \ldots, P_n)$ of this space. A statistical description of the system corresponding to the above macroscopic observation does not distinguish between different microstates into each region and is therefore represented by a probability distribution which is uniform in each P_i. We shall refer to this type of distribution as coarse-grained with respect to the observables $\{y_i\}$ or to the partition $\mathcal{P}$.

Let us turn to the quantitive description of a coarse-grained state. The system being isolated, its state of equilibrium will be described by the microcanonical ensemble denoted by $d\mu(x)$. Let $\rho_t(x)$ be the probability density (relative to μ) out of equilibrium. We assume that initially this distribution is coarse-grained. By definition, this means that [22, 13]

$$\rho_0(x) = \sum_i \alpha_i \chi_{P_i}(x) \tag{1.76}$$

where $\chi_{P_i}(x)$ denotes the characteristic function of the P_i. Integrating (1.76) over the set P_j, we obtain the coefficient α_j:

$$\alpha_j = \frac{1}{\mu(P_j)} \int_{P_j} \rho_0(x) d\mu(x) \tag{1.77}$$

where $\mu(E)$ denotes the (equilibrium) probability of the set E.

The Liouvillian time evolution of the initial density under the dynamical flow ϕ^t is given by

$$(U_t \rho_0)(x) = \rho_t(x) = \rho_0(\phi^{-t} x) \tag{1.78}$$

where the operators U_t define a group.

It is clear that $\rho_t(x), t > 0$ is not necessarily coarse-grained with respect to $\mathcal{P}$, but, as we are interested in the macroscopic description, we consider its coarse-grained projection along $\mathcal{P}$, that is, a new density $P\rho_t$, which is constant onto each region P_i. Following equations (1.76) and (1.77) this density is given by

$$P\rho_t = \sum_i \left[\frac{1}{\mu(P_i)} \int_{P_i} \rho_t(y) d\mu(y) \right] \chi_{P_i}(x) \tag{1.79}$$

In what follows, we shall denote $\mu(P_i)$ by μ_i.

According to the general arguments of Gibbs, a coarse-grained density will approach monotonically the microcanonical density $\rho_e(=1)$. Here monotonicity is expressed as the decrease of the following functional:

$$\mathcal{S}(P\rho_t) = \int_M P\rho_t(x) \log P\rho_t(x) d\mu(x) = -\mathcal{H}(P\rho_t) \tag{1.80}$$

This is the so-called H-theorem and $\mathcal{H}(P\rho_t)$ is interpreted as the nonequilibrium entropy.

Now, it is well known that the Liouville theorem implies that the functional $\mathcal{S}(P\rho_t)$ remains constant in time. On the other hand, owing to the convexity of 0, the following inequality holds:

$$\int_M P\rho_t(x) \log P\rho_t(x) d\mu(x) \leq \int_M \rho_t(x) \log \rho_t(x) d\mu(x) \tag{1.81}$$

Unfortunately this does not entail that $\mathcal{S}(P\rho_t)$ decreases monotonically, nor that it converges to its equilibrium value unless PU_tP is a semi-group for $t \geq 0$. To secure an H-theorem one must therefore repeat the coarse-graining operation at regular time intervals, which is rather artificial.

Our principal objective is to examine the possibility of obtaining an exact H-theorem for coarse-grained probability distributions. To this end, we will identify the class of conservative dynamical systems for which $P\rho_t$ evolves under an irreversible Markov process, that is a Markov process for which $\mathcal{S}(P\rho_t)$ converges monotonically to its equilibrium value for any coarse-grained initial state[22].

We shall limit ourselves to discrete time conservative dynamical systems. We see from (1.79) that the coarse-graining density has a simple representation in the orthogonal basis $(1/\mu_i)\chi_{P_i}$ involving the row probability vector

$$\Pi_t = \{\nu_t(P_i)\}, \qquad i = 0, 1, \ldots, k, \tag{1.82}$$

where $\nu_t(E)$ denotes the time-dependent probability of the set E:

$$\nu_t(E) = \int_E \rho_t(x) d\mu(x). \tag{1.83}$$

Let us now formulate the H-theorem in terms of Π_t. We have

$$\mathcal{S}(P\rho_t) = \int_M P\rho_t(x) \log P\rho_t(x) d\mu(x) = \sum_i \int_{P_i} P\rho_t(x) \log P\rho_t(x) d\mu(x). \tag{1.84}$$

But, for any $x \in P_i$, $P\rho_t(x)$ takes the constant value $\nu_t(P_i)/\mu_i$ (see (1.79)), thus

$$\mathcal{S}(P\rho_t) = \sum_i \mu_i \left(\frac{\nu_t(P_i)}{\mu_i} \right) \log \left(\frac{\nu_t(P_i)}{\mu_i} \right), \tag{1.85}$$

or

$$\mathcal{S}(P\rho_t) = \sum_i \nu_t(P_i) \log \left(\frac{\nu_t(P_i)}{\mu_i} \right). \tag{1.86}$$

It is well known that this is a positive functional which vanishes only if $\nu_t(P_i) = \mu_i$ and decreases monotonically. Thus, $K - S$ entropy, $\mathcal{H}(P\rho_t) = -\mathcal{S}(P\rho_t)$ increases monotonically [22, 14]. In the next chapter, we will use equation (1.86) to compute entropy in our simulations.

Chapter 2

Computation of entropy increase for Lorentz gas and hard disks

Abstract: Entropy functionals are computed for non-stationary distributions of particles of Lorentz gas and hard disks. The distributions consisting of beams of particles are found to have the largest amount of entropy and entropy increase. The computations show exponentially monotonic increase during initial time of rapid approach to equilibrium. The rate of entropy increase is bounded by sums of positive Lyapounov exponents[1].

[1]This paper will be published in Communications in nonlinear science and numerical simulation, **13**, Issue 2 (2008) 444-455.

2.1 Introduction

The H-theorem for dynamical systems describes the approach to equilibrium, the irreversibility and entropy increase for deterministic evolutions. Suppose that a dynamical transformation T on a phase space X has some "equilibrium" measure μ, invariant under T, i.e. $\mu(T^{-1}E) = \mu(E)$ for all measurable subsets E of X. Suppose also that there is some mixing type mechanism of the approach to equilibrium for T, i.e. there is a sufficiently large family of non-equilibrium measures ν such that $\nu_t(E) =: \nu(T^{-t}E)) \underset{t\to\infty}{\longrightarrow} \mu(E)$ for all E. Then, the H-theorem means the existence of a

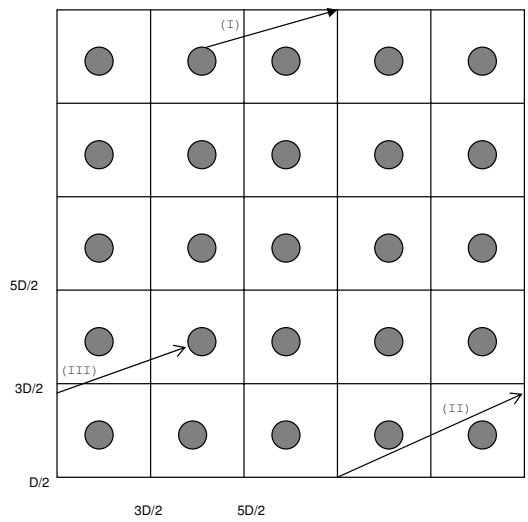

Figure 2.1: The motion of the particle on a toric billiard.

negative entropy functional $S(\nu_t)$ which increases monotonically with t to zero, being attained only for $\nu = \mu$. The existence of such functional in measure-theoretical dynamical systems has been the object of several investigations during last decades see [20]-[23][25, 28, 29, 32]). Here we study this problem for the Lorentz gas and hard disks. The dynamical and stochastic properties of the Lorentz gas in two dimensions which we consider here was investigated by Sinaï and Bunimovich as an ergodic dynamical system [30, 18, 19]. Other transport properties have been also studied numerically (see [26, 33]). This is a system of non interacting particles moving with

constant velocity and being elastically reflected from periodically distributed scatterers. The scatterers are fixed disks. On account of the absence of interactions between particles the system is reduced to the motion of one billiard ball. We shall investigate the entropy increase under the effect of collisions of the particles with the obstacles. For this purpose, we consider the map T which associates to an ingoing state of a colliding particle the next ingoing colliding state. The particle moves on an infinite plane, periodically divided into squares of side D called "cells", on the center of which are fixed the scatterers of radius a (Fig. 2.1). The ingoing colliding state is described by an ingoing unitary velocity arrow at some point of the disk. To a colliding arrow $\mathbf{V}_1(P_1)$ at point P_1 on the boundary of the disk the map associates the next colliding arrow $\mathbf{V}_2(P_2)$ according to elastic reflection law. Thus, the collision map does not take into account the free evolution between successive collisions.

Let ν be a non-equilibrium measure, which means that ν is a non invariant measure approaching the equilibrium μ in the future. It is mathematically possible to define a non-equilibrium entropy for a family of such measures, using conditional expectations (i.e. a generalized averaging) relatively to the some remarkable partitions, namely the contracting fibers of the hyperbolic dynamics [20]. However, in our numerical simulations some given finite precision is needed, so that we consider partitions into cells with positive μ-measure. Here, we use slightly similar entropy functionals. Starting from the non-equilibrium initial distribution ν, and denoting by $\mathcal{P}$ such partition formed by cells ($\mathcal{P}_1$,$\mathcal{P}_2$, ..., $\mathcal{P}_n$) and by $\nu_t(\mathcal{P}_i) = \nu \circ T^{-t}(\mathcal{P}_i)$, the probability at time t for the system to be in the cell $\mathcal{P}_i$ and such that $\nu(\mathcal{P}_i) \neq \mu(\mathcal{P}_i)$ for some i, the approach to equilibrium implies that $\nu_t(\mathcal{P}_i) \to \mu(\mathcal{P}_i)$ as $t \to \infty$ for any i. The entropy functional will be defined by:

$$\mathcal{S}(t, \nu, \mathcal{P}) = -\sum_{i=1}^{N} \nu_t(\mathcal{P}_i) \ln(\frac{\nu_t(\mathcal{P}_i)}{\mu(\mathcal{P}_i)}) := -\mathcal{H}(t, \nu, \mathcal{P}) \tag{2.1}$$

which we simply denote here after $\mathcal{S}(t)$. The H-functional (2.1) is maximal when the initial distribution is concentrated on only one cell and minimal if and only if $\nu_t(\mathcal{P}_i) = \mu(\mathcal{P}_i), \forall i$. These properties are shown straightforwardly. This formula describes the relative entropy of the non-equilibrium measure ν_t with respect to μ for the observation associated to $\mathcal{P}$. It coincides with the information theoretical concept of relative entropy of a probability vector (p_i) with respect to another probability vector (q_i) defined as follows: $-\ln p_i$ being the information of the ith issue under the first distribution, $-\sum_i p_i \ln(\frac{p_i}{q_i})$, is equal to the average uncertainty gain of the

experience (p_i) relatively to (q_i).

A condition under which formula (2.1) shows a monotonic increase with respect to t is that the process $\nu_t(\mathcal{P}_i) = \nu \circ T^{-t}(\mathcal{P}_i)$ verifies the Chapman-Kolmogorov equation valid for Markov chains and other infinite memory chains. For a dynamical system, this condition is hardly verified for given partition $\mathcal{P}$. However, the very rapid mixing leads to a monotonic increase of the above entropy, at least during some initial stage, which can be compared with the relaxation stage in gas theory.

In this paper, we will first compute the entropy increase for some remarkable non-equilibrium distributions over the phase space of the Sinaï billiard. The billiard system is a hyperbolic system (with many singularity lines) and, in order to have a rapid mixing, we will consider initial distributions supported by the expanding fibers. Such initial measures have been used in [20, 23, 32]. For the billiard the expanding fibers are well approximated by particles with parallel arrows velocity. We call this class of initial ensemble beams of particles. We first compute the entropy increase under the collision map for these initial distributions. We will consider finite uniform partitions of the phase space as explained below. The entropy functional will be defined through (2.1). For this purpose, the phase space of the collision map is described using two angles (β, ψ), where β is the angle between the outer normal at P and the incoming arrows $\mathbf{V}(P)$, $\beta \in [0, \frac{\pi}{2}[$, and $\psi \in [0, \pi]$ is the angle between x-axis and the outer normal at P. Thus, the collision map induces a map: $(\beta_1, \psi_1) \to (\beta_2, \psi_2)$ (see Fig. 2.14) and we shall first use a uniform partition of the (β, ψ) space. The computation shows that whatever is the coarsening of these partitions the entropy has the monotonic property in the initial stage. It is clear that, along mixing process, the initial distribution will spread over all cells almost reaching the equilibrium value. Physically, this process is directed by the strong instability, that is expressed by the positive Lyapounov exponent.

We also consider the relation of the rate of increase of the entropy functionals and Lyapounov exponents of the Lorentz gas. Our computation shows that this relation is expressed by an inequality

$$\max(\mathcal{S}(n+1) - \mathcal{S}(n)) \equiv \triangle\mathcal{S} \leq \sum_{\lambda_i \geq 0} \lambda_i \tag{2.2}$$

where the "max" is taken over n, which means that the K-S entropy is an upper bound of the rate of increase of this functional.

In section 3, we shall consider another phase space and another partitions associated to spatial extension of the motion of the Lorentz gas. Here the space in which

moves a particle is a large torus divided into rectangular cells, in the center of each cell there is one disk. Denoting the total number of cells by n and the number of particles initially distributed in only one region, by N, and following them until each executes t collisions with obstacles, we compute the probability that a particle is located in the ith cell as given by:

$$\rho_i(t) = \frac{\text{Number of particles in cell } i \text{ having made } t \text{ collisions}}{N}$$

The equi-distribution of the cells leads to take, as equilibrium measure, $\mu_i = \frac{1}{n}$, so that this "space entropy" is defined by:

$$\mathcal{S}_{sp}(t) = -\sum_{i=1}^{n} \rho_i(t) \ln(\rho_i(t)n) \tag{2.3}$$

The maximum of absolute value of this entropy is equal to $-\ln n$. So we normalize as follows:

$$\mathbf{s}_{sp}(t) = \frac{\mathcal{S}_{sp}(t)}{\ln n} \tag{2.4}$$

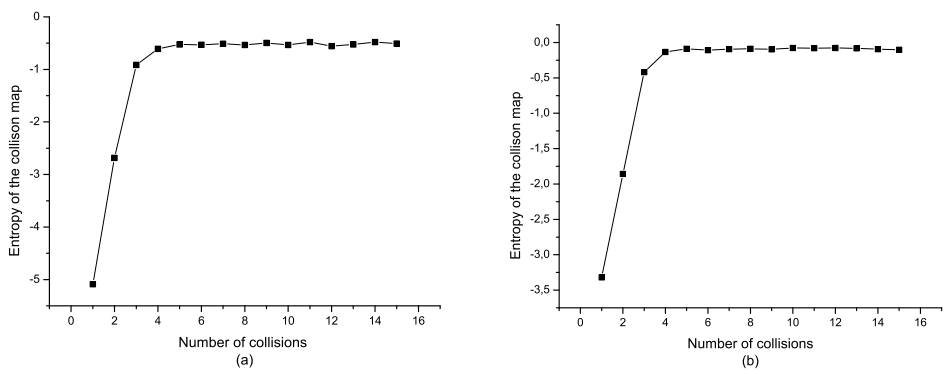

Figure 2.2: Entropy of the collision map versus number of collisions for (a) a beam of 640 particles for a radius a=0.2, neighboring disks centers distance 1 and a partition of (β, ψ) space into 25×25 cells, (b) a beam of 512 particles for the obstacles of radius 0.2, neighboring disks centers distance 1 and a partition of (β, ψ) space into 9×9 cells.

In section 2.4 we shall consider the hard disks systems. We shall compute an entropy functional similar to the space-entropy on extended torus with several cells.

The probabilities are defined as for the space entropy in the Lorentz gas. We shall also do some comparisons of the H-theorem with the sum of normalized positive Lyapounov exponents.

2.2 Entropy for collision map

The entropy for the collision map is computed for a beam of N particles on a toric checkerboard with n cells. We start to calculate the entropy, just after all particles have executed the first collision. In this computation, all particles have the same initial velocity and are distributed in a small part of one cell. For each particle we determine the first obstacle and the angles (β_1, ψ_1) of the velocity incoming vector $\mathbf{V}_1(P_1)$ (see the figures given in the Appendix). For a uniform partition $\mathcal{P}$ of the space of the variables (β, ψ), the entropy $\mathcal{S}(t)$is computed iteratively just after all particles have executed the tth collision. We use the formula (2.1) where

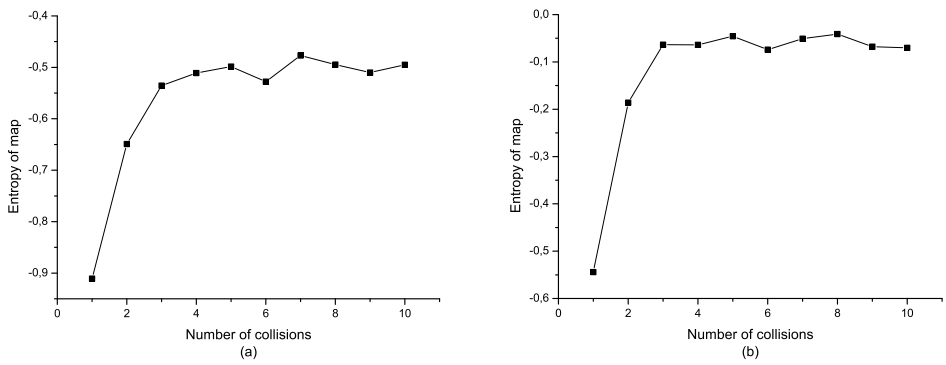

Figure 2.3: (a) and (b) are the entropy of the collision map with random initial conditions versus number of collisions for the system of particles of the Fig. 2.2, respectively.

$$\mu(\mathcal{P}_i) = \int_{\beta_i}^{\beta_{i+1}} \int_{\psi_i}^{\psi_{i+1}} \cos\beta d\beta d\psi \tag{2.5}$$

is the invariant measure [30] of the cell $\mathcal{P}_i = [\beta_i, \beta_{i+1}[\times[\psi_i, \psi_{i+1}[$ and $\nu_t(\mathcal{P}_i)$ is the probability that a particle is located after t collisions in $\mathcal{P}_i$ computed as

$$\frac{\text{Number of particles in } \mathcal{P}_\text{i} \text{ having made } t \text{ collisions}}{\text{N}}.$$

The velocity after the collision is computed from the following equation:

$$\mathbf{V}(P_2) = \mathbf{V}(P_1) - 2(\mathbf{V}(P_1).\mathbf{n})\mathbf{n} \tag{2.6}$$

where $\mathbf{n}$ is the normal vector at the collision point. We explain in the Appendix the

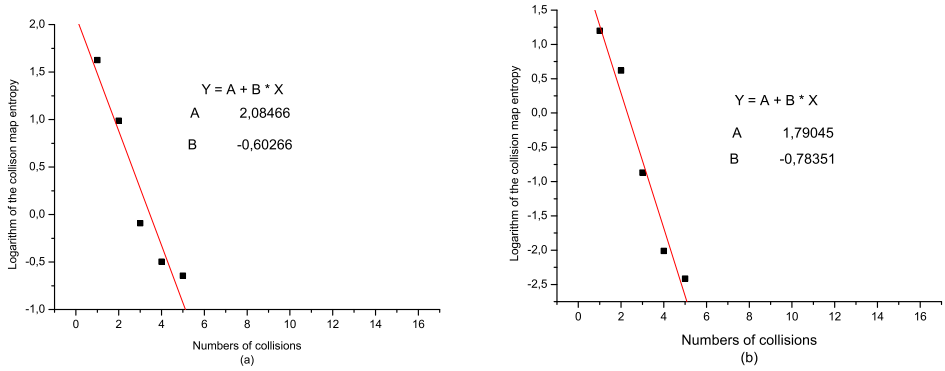

Figure 2.4: Logarithm of the collision map entropy versus number of collisions for the system of particles of Fig. 2.2.

main geometric formula used for this computation. This entropy increase is shown in the Fig. 2.2 for various partitions and various initial distributions. The absolute value of the entropy of a distribution of particles, that we call its amount of entropy, represents in fact its distance to equilibrium. This is illustrated in the examples of randomly distributed initial velocity of particles having small amount of entropy (see Fig. 2.3) comparatively with beams of particles. It is to be noted that the amount of entropy increase under one collision is remarkably greater for the few first ones (more or less 2-4 collisions) which corresponds to an exponential type increase (Fig. 2.4).

In order to calculate Lyapounov exponents by using the method of Benettin et al [16], first we calculate the Jacobian matrix in the tangent space of the collision map:

$$\begin{pmatrix} \frac{\partial \beta_2}{\partial \beta_1} & \frac{\partial \beta_2}{\partial \alpha_1} \\ \\ \frac{\partial \alpha_2}{\partial \beta_1} & \frac{\partial \alpha_2}{\partial \alpha_1} \end{pmatrix}.$$

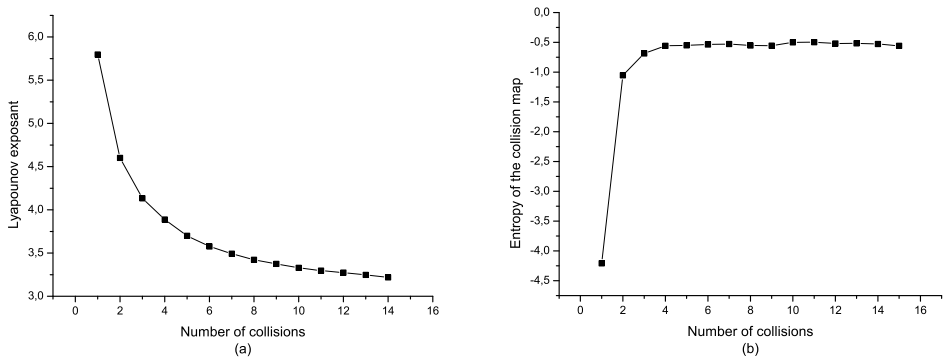

Figure 2.5: (a) Lyapounov exponent and (b) entropy of the collision map, versus of number of collisions for each particle. We see that the maximum of the entropy increase between two collisions is less than of the value of the Lyapounov exponent.

Now, comparing $\triangle\, \mathcal{S} = \max(\mathcal{S}(t+1) - \mathcal{S}(t))$ (where the "max" is taken over t) with the positive Lyapounov exponent, λ, of the collision map we verify the inequality:

$$\triangle\, \mathcal{S} < \lambda \tag{2.7}$$

as shown in Fig. 2.5, where this exponent is ~ 3.2. The maximal entropy increase by collision for the distribution computed in this figure is not far from this value. So it could be conjectured that in some suitable refinement limit, the entropy increase of a beam tends to the positive Lyapounov exponent. The rate of the approach to equilibrium is thus related to the positive Lyapounov exponent. Furthermore, the value of Lyapounov exponent is only dependent of $\frac{D}{a}$, i.e. the ratio of the distance between two successive obstacles over the radius of the obstacle, and its variation is exponential as shown in Fig. 2.6.

Collision number	1	2	3	4	5	6	7
Mean free time	1.966	26.174	5.801	3.820	3.611	4.452	4.177
Collision number	8	9	10	11	12	13	14
Mean free time	4.162	4.208	4.212	3.863	4.272	4.051	4.397

Table 2.1: Mean free time obtained for a beam of 640 particles for a radius a=0.2, neighboring disks centers distance 1 and a partition of (β, ψ) space 25×25 cells.

In order to compare the entropy increase as a function of the collisions with the entropy increase as a function of time, we compute the distribution of mean free time

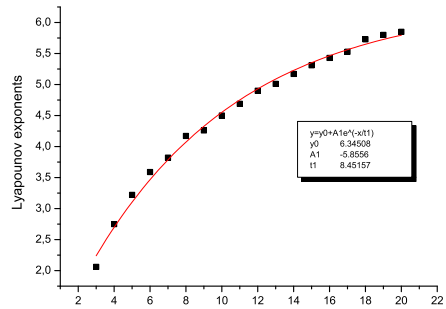

Figure 2.6: Lyapounov exponent versus D/a.

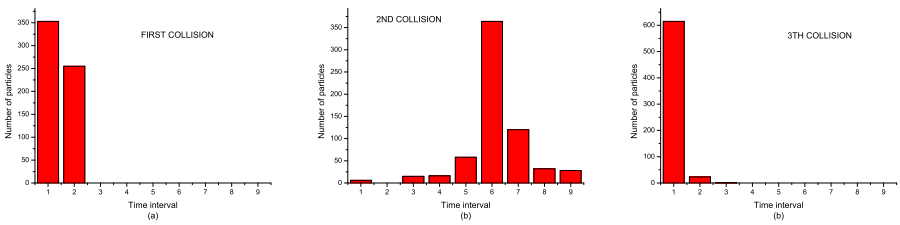

Figure 2.7: Free time histogram for (a) first, (b) second and (c) third collision.

for the first 3 collisions. From time histogram for the first three collisions of this system (Fig. 2.7), we see that a great number of particles have the same mean free time. As shown in the table 2.1, the mean free time vary during the first three or four collisions but after those, for the following collisions, rapidly the system comes near the equilibrium, where we have a constant mean free time approximately.

2.3 Spatially extended Lorentz gas entropy

The computation of the normalized space entropy equation by using (2.4) versus the number of collisions shows a remarkable exponential increase both for beams and for random initial distributions (Fig. 2.8). The computation of sum of the two positive Lyapounov exponents of the flow of one particle is equal to 1.046. Thus, we observe

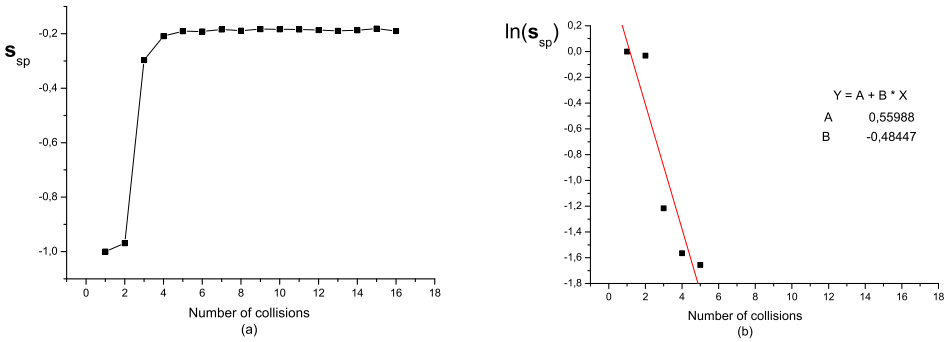

Figure 2.8: (a) Normalized space entropy of the Lorentz gas versus number of collisions for a beam of 640 particles for obstacles of radius a=0.2, neighboring disks centers distance 1 and a partition of (x, y) space into 25×25 cells, (b) Logarithm of the space entropy versus number of collisions for this system.

that the inequality between the normalized increase of the density of the space entropy and this sum is verified.

2.4 Hard disks

Considering a uniform space partition of a large toric space we compute the particles densities, ρ_i, and the normalized space entropy as a function of time by using the equation (2.4). Starting with a distribution of disks with localized positions in some cell and random velocities, we compute binary collisions instants and the trajectories of the hard disks. These instants are determined by checking the distance between particles, after a time interval is passed. The Lyapounov exponents of the flow are calculated by using the Benettin et al. algorithm. The result is shown in the Figs. 2.9 and 2.10. These figures show the entropy and logarithm of monotonic part of entropy versus time of the same gas with two distinct densities. The system in the Fig. 2.10 is more dense than the system in Fig. 2.9, and its entropy increases more rapidly. Fig. 2.11 is a histogram of the number of collisions, so we see that the number of collisions in a fixed time interval is reduced for large time. From Figs. 2.9 and 2.10 we see that the monotonic part of the non-equilibrium entropy is also

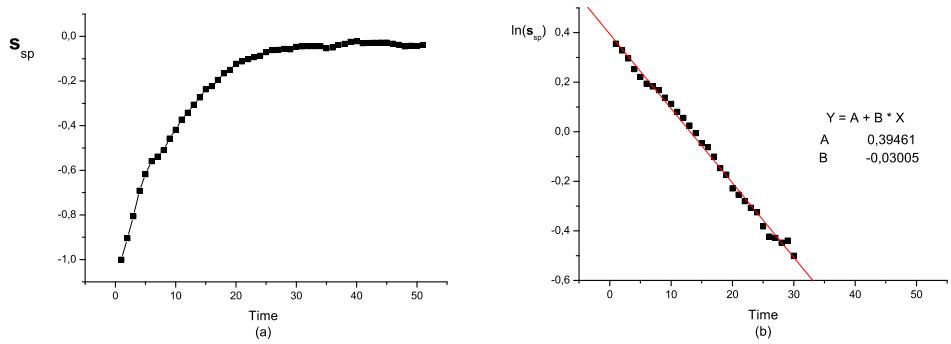

Figure 2.9: (a) Normalized space entropy and (b) its monotonic part logarithm versus time, for 128 hard disks with radius a=0.05 which are initially localized in the first cell of (x, y) space with 6×6 cells and a density $\sigma_1 = 0.889$ disks per unit area.

varying exponentially with respect to time. This shows that the collision is the main ingredient responsible of the entropy increase as described in the Boltzmann equation theory.

Density	$\frac{1}{N}\sum_{\lambda_i>0}(\frac{\lambda_i}{\lambda_{max}})$	$\triangle \mathbf{s}_{sp}$
3.555	0.367	0.139
0.889	0.294	0.115
0.222	0.239	0.144

Table 2.2: The data for the hard disks systems of radius, $a = 0.05$ and the same initial conditions, with cells 6×6, in terms of the density.

We shall now vary the density $\sigma = \frac{N}{V}$ and compute the characteristic quantities. The graph of the normalized positive Lyapounov exponents spectrum per particle for the same system as in Fig. 2.9 is shown in Fig. 2.12. The computation of the normalized sums of the positive Lyapounov exponent, $\frac{1}{N}\sum_{\lambda_i>0}(\frac{\lambda_i}{\lambda_{max}})$, shows that the inequality between maximum entropy increase and the sum of normalized of positive Lyapounov exponents is verified (Table 2.2).

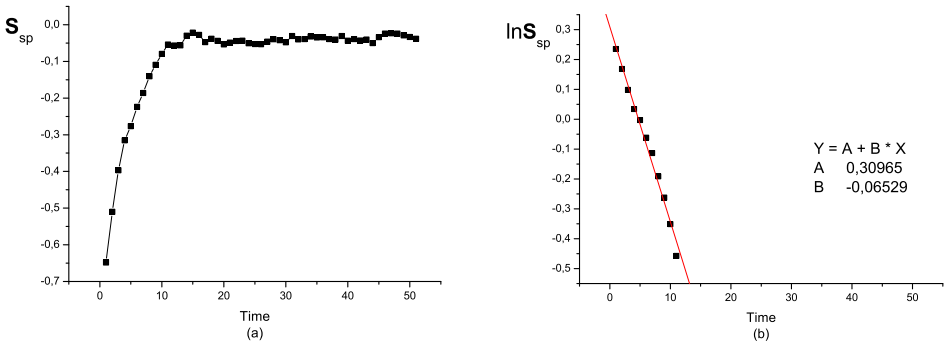

Figure 2.10: Normalized space entropy and its and its monotonic part logarithm for the same system as Fig. 2.9, with a density $\sigma_2 = 3.555$ disks per unit area.

2.5 Concluding remarks

The computations of the entropy amount of some given non-equilibrium initial distributions relatively to the equilibrium measure show an exponential type increase for all considered partitions and distributions during initial stage after which the entropy increases slowly and fluctuates near its maximal value. These computations confirm the existence of a relaxation time generally assumed in the derivation of kinetic equations [15] and the origin of the rapid increase of the entropy due to the number of collisions. The dispersive nature of the obstacles is responsible of the exponential mixing type increase. This exponential type increase has been demonstrated for the Sinaï entropy functional [32] in hyperbolic automorphisms of the torus. On the other hand, the relation of the entropy increase to Lyapounov exponents can be understood through Pesin relation and Ruelle inequality. In fact, the rate of entropy increase should be bounded by the Kolmogorov-Sinaï entropy and such bound have been found by Goldstein and Penrose for measure-theoretical dynamical systems under some assumptions [28]. An open question is to characterize the measures reaching the upper bound.

Any entropy functional is not a completely monotonic function of time for any dynamical system. In order to define a completely monotonic entropy functional for a dynamical system some conditions on the dynamics should be imposed. We can

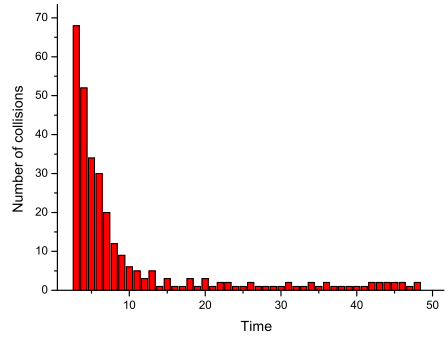

Figure 2.11: Number of collisions histogram system versus time in Fig. 2.9.

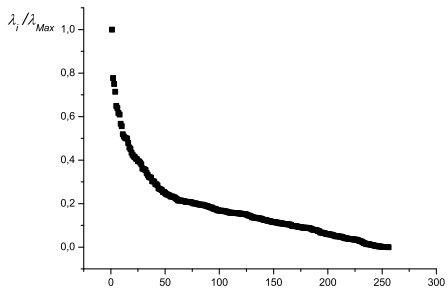

Figure 2.12: Normalized spectrum Lyapounov of exponent of system in Fig. 2.9.

first suppose the map T on a phase space X to be a Bernoulli system or, slightly more generally, a K-system. This means that there is an invariant measure μ and some partition ξ_0 of X such that $T\xi_0$ becomes finer than ξ_0 (we denote it: $T\xi_0 \geq \xi_0$). Using the notation: $T^n\xi_0 = \xi_n$, we obtain a family of increasingly refined partitions, in the sense of the above order of the partitions. Moreover, ξ_n tends, as $n \to \infty$, to the finest partition of X into points, and ξ_n tends, as $n \to -\infty$, to the most coarse partition, into one set of measure 1 and another set of measure zero. A physical prototype of a Bernoulli and a K-system is the above billiard [30, 24]. A geometric prototype of a Bernoulli and a K-system is uniformly hyperbolic system with Sinaï invariant measure [31]. A non-equilibrium entropy for a family of initial measures,

using conditional expectations relatively to the ξ_n partitions was first obtained as an equivalence between the unitary group evolution and a semi-group of contraction operators in the space of square integrable functions $L^2(\mu)$ successively for the baker transformation [29], for Bernoulli systems [21] and for K-systems [27]. Its extension to the space of measures in K-systems has been realized in [20]. In differentiable hyperbolic dynamical systems where the fibers of the ξ_n partitions are pieces of contracting fibers, the construction of such entropy functional results from a generalized coarse-graining with respect to these contracting fibers, each fiber being a piece of manifold of zero measure.

2.6 Appendix

2.6.1 Collision Map

We shall give the formula of the *collision map*. We consider a particle which undergoes the first collision with the disk of center O_1 with velocity $\mathbf{V}_1(p_1)$ and the second collision with the disk of center O_2 with velocity $\mathbf{V}_1(p_2)$. Two cases are possible. First, we consider non-crossing of the centers line as in the Fig. 2.13. In this figure the angle $\widehat{\mathrm{P}_1\mathrm{P}_2M}$ is $\alpha_2 - \beta_2 = -(\alpha_1 - \beta_1)$, where M is such that MP_2 is parallel to $\mathrm{O}_1\mathrm{O}_2$. We can write

$$\mathrm{P}_1\mathrm{M} = \mathrm{P}_1\mathrm{P}_2 \cos(\beta_1 - \alpha_1) = d - a\cos\alpha_1 - a\cos\alpha_2. \tag{2.8}$$

and

$$\mathrm{P}_2\mathrm{M} = \mathrm{P}_1\mathrm{P}_2 \sin(\beta_1 - \alpha_1) = a\sin\alpha_1 - a\sin\alpha_2, \tag{2.9}$$

if we eliminate α_2 between these equations we arrive at

$$\beta_2 = \arcsin[\frac{d}{a}\sin(\beta_1 - \alpha_1) + \sin\beta_1]. \tag{2.10}$$

In crossing case which we present in Fig. 2.14 we see that the angle $\widehat{\mathrm{P}_2\mathrm{P}_1\mathrm{M}}$ is equal to $\alpha_2 - \beta_2 = \alpha_1 - \beta_1$, and the length of $\mathrm{P}_2\mathrm{M}$ is changed to:

$$\mathrm{P}_2\mathrm{M} = \mathrm{P}_1\mathrm{P}_2 \sin(\beta_1 - \alpha_1) = a\sin\alpha_1 + a\sin\alpha_2, \tag{2.11}$$

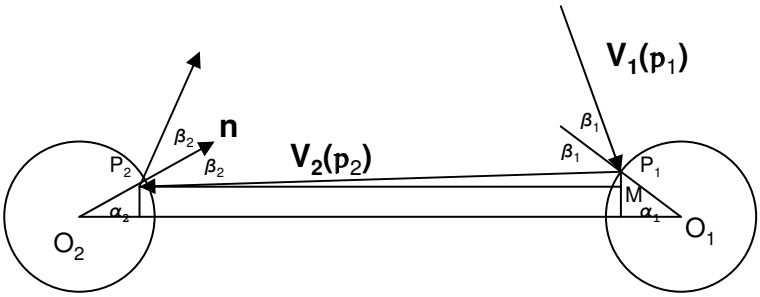

Figure 2.13: non-crossing Collision.

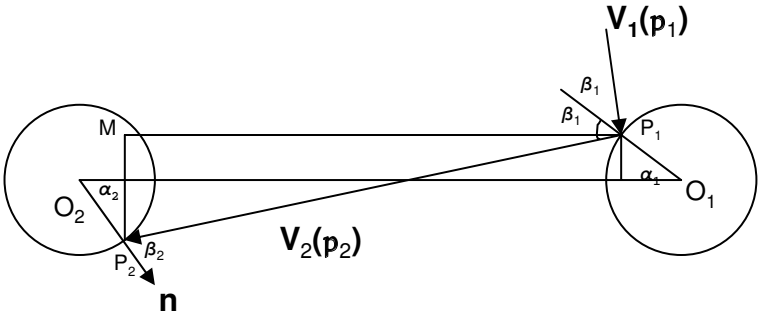

Figure 2.14: crossing Collision.

then, we have

$$\beta_2 = \arcsin[\frac{d}{a}\sin(\beta_1 - \alpha_1) - \sin\beta_1]. \tag{2.12}$$

To obtain β_2 in the first collision between particle and obstacle Fig. 2.15 , we take $d = \mathrm{OP}_1$, $\beta_1 = 0$ and $\alpha_1 = \vartheta$ in the collision map.

2.6.2 Algorithm description

In this section we describe the algorithm which we used in our program for Lorentz gas. We first define in the *main* of our program the initial conditions for the particles and the obstacles positions. In the second step, we compute with which obstacle, a particle will collide: we measure the angle between velocity of particle and the line between this particle and the center of obstacle, OP_1 in Fig. 2.16, if this angle is less than or equal to the angle between this line, OP_1, and the tangent line on the circle, i.e. $\mathrm{P}_1\mathrm{N}$, in brief if $\vartheta \leq \varphi$ in Fig. 2.16, we have a collision. Now, we use the collision

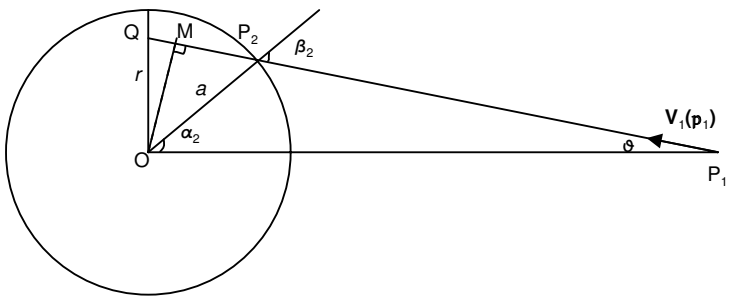

Figure 2.15: Particle obstacle Collision.

map equation (2.10) or (2.12) to obtain the collision angles, β_2, and α_2 (see Fig. 2.15). In this step, we can also obtain the length of arrow of our induced collision map, i.e. $\mathrm{P}_1\mathrm{P}_2$ (see Fig. 2.15), easily as:

$$\mathrm{P}_1\mathrm{P}_2 = \frac{\mathrm{OP}_1 - a\cos\alpha_2}{\cos\vartheta} \tag{2.13}$$

where $\alpha_2 = \beta_2 - \vartheta$. Then, we can calculate the time of flight of particle between two

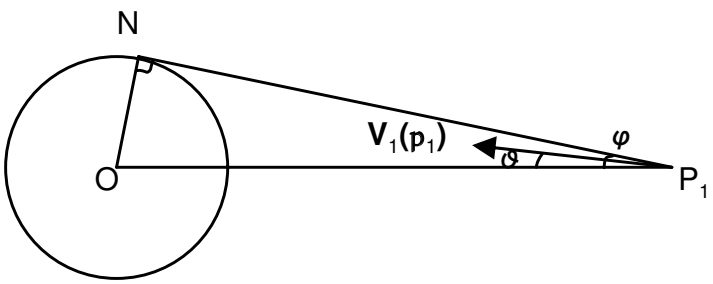

Figure 2.16: Particle obstacle Collision.

collisions, respectively, as $t = \mathrm{P}_1\mathrm{P}_2/v$. This provides the trajectory of a particles.
Let us turn the computation of space entropy. When a particle arrives at a wall of the big torus, before it does a collision with an obstacle (see on the Fig. 2.1) trajectories are pursued until it undergoes a collision on the torus. We have to compute the position of the obstacle that the particle will hit (see Fig. 2.17) and the angle α_1

in the collision map, and to determine which type of collision, i.e. crossing or non-crossing case, will occur. We first find the angle of collision

$$\beta_2 = \vartheta + \varphi = \arcsin[\frac{\mathrm{MO}_2}{a}\sin\vartheta], \tag{2.14}$$

then we arrive at α_1 and α_1 as

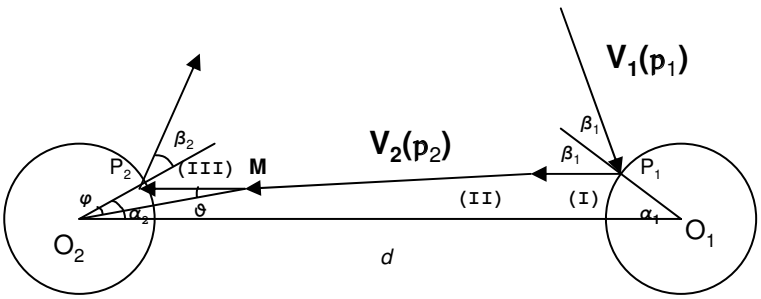

Figure 2.17: The motion of the particle take place on a tours.

$$\begin{cases} \alpha_1^n = \beta_1 + \arcsin[\frac{a}{d}(\sin\beta_2 - \sin\beta_1)], & \alpha_2^n = \beta_2 + (\beta_1 - \alpha_1) \\ \alpha_1^c = \beta_1 - \arcsin[\frac{a}{d}(\sin\beta_2 + \sin\beta_1)], & \alpha_2^c = \beta_2 - (\beta_1 - \alpha_1) \end{cases} \tag{2.15}$$

where the superscript "c" corresponds to crossing case and "n" corresponds to non-crossing case see equations (2.10) and (2.12), respectively. In the above equations, the d parameter is unknown, and will be recognized it in the end of this Appendix. If we subtract the above equations we obtain

$$\alpha_1^c - \alpha_1^n = -\arcsin[\frac{a}{d}(\sin\beta_2 + \sin\beta_1)] - \ arcsin[\frac{a}{d}(\sin\beta_2 - \sin\beta_1)] \tag{2.16}$$

We can see the above equation yields $\alpha_1^c - \alpha_1^n \leq 0$. It means that in the same conditions the angle α_1 in the non-crossing is greater than crossing case. Also, we can get the same conclusion for α_2, i.e. $\alpha_2^c \leq \alpha_2^n$. Now, we initiate the algorithm in the non-crossing case and we find α_1^c and α_2^n. If $\vartheta \leq \alpha_2$, thus, we had a correct supposition, otherwise, we must consider the crossing case, and we re-calculate these angles. In order to find in this case the parameter $d = |\mathrm{O}_1\mathrm{O}_2|$, we calculate it by approximation method. The equation that recognize d is:

$$d = vdt\cos(\beta_1 - \alpha_1) + a(\cos\alpha_1 + \cos\alpha_2) \tag{2.17}$$

where dt is the time of free flight of particle between two collisions, see Figs. (2.1 and 2.17). In the above equation we have two unknown variables, α_1 and α_2. We use the *zeroth approximation* as

$$d \approx vdt \tag{2.18}$$

where we used $a \ll vdt$. Now, we calculate the angles, α_1 and α_2, as mentioned in above of this Appendix. Then, we re-calculate d with the *first approximation*, and we can repeat this procedure. However, the convergence is very rapid.

Part II

Unstable Quantum Systems

Chapter 3

Mathematical Preliminaries

3.1 Markov process

3.1.1 Stochastic process

By stochastic processes we mean, in a loose sense, systems which evolve probabilistically in time or more precisely, systems in which a certain time-dependent random variable $X(t)$ exists. We can measure values $x_1, x_2, x_3, \ldots$, etc., of $X(t)$ at times $t_l, t_2, t^3, \ldots$ and we assume that a set of joint probability densities exists

$$P(x_1, t_1; x_2, t_2; \ldots) \tag{3.1}$$

which describe the system completely.

In terms of these joint probability density functions, one can also define conditional probability densities:

$$P(x_1, t_1; x_2, t_2; \ldots | y_1, \tau_1; y_2, \tau_2; \ldots) = \frac{P(x_1, t_1; x_2, t_2; \ldots; y_1, \tau_1; y_2, \tau_2; \ldots)}{P(y_1, \tau_1; y_2, \tau_2; \ldots)} \tag{3.2}$$

These definitions are valid independently of the ordering of the times, although it is customary to consider only times which increase from right to left i.e.,

$$t_1 \geq t_2 \geq \cdots \geq \tau_1 \geq \tau_2 \geq \cdots . \tag{3.3}$$

The concept of an evolution equation leads us to consider the conditional probabilities as predictions of the future values of $X(t)$ (i.e., $x_1, x_2, \ldots$ at times $t_l, t_2, \ldots$), given the knowledge of the past (values $y_l, y_2, \ldots$, at times $\tau_1, \tau_2, \ldots$).

The concept of a general stochastic process is very loose. To define the process we need to know at least all possible joint probabilities of the kind in (3.1). If such knowledge does define the process, it is known as a separable stochastic process. All the processes considered here will be assumed to be separable.

The most simple kind of stochastic process is that of complete independence:

$$P(x_1, t_1; x_2, t_2; \ldots) = \prod_i P(x_i, t_i) \tag{3.4}$$

which means that the value of X at time t is completely independent of its values in the past (or future). An even more special case occurs when the $P(x_i, t_i)$ are independent of t so that the same probability law governs the process at all times. We then have the Bernoulli trials, in which a probabilistic process is repeated at successive times [34].

The next most simple idea is that of the Markov process in which knowledge of only the present determines the future.

3.1.2 Markov process

The Markov assumption is formulated in terms of the conditional probabilities. We emphasize that if the times satisfy the ordering (3.3), the conditional probability is determined entirely by the knowledge of the most recent condition, i.e.,

$$P(x_1, t_1; x_2, t_2; \ldots | y_1, \tau_1; y_2, \tau_2; \ldots) = P(x_1, t_1; x_2, t_2; \ldots | y_1, \tau_1) \tag{3.5}$$

This is simply a more precise statement of the assumptions made by Einstein, Smoluchowski and others. It is, even by itself, extremely powerful. For it means that we can define everything in terms of the simple conditional probabilities $P(x_1, t_1|y_1, \tau_1)$. For example, by definition of the conditional probability density $P(x_1, t_1; x_2, t_2|y_1, \tau_1) = P(x_1, t_1|x_2, t_2; y_1, \tau_1)P(x_2, t_2|y_1, \tau_1)$ and using the Markov assumption (3.5), we find

$$P(x_1, t_1; x_2, t_2; y_1, \tau_1) = P(x_1, t_1|x_2, t_2)P(x_2, t_2|y_1, \tau_1) \tag{3.6}$$

and it is not difficult to see that an arbitrary joint probability can be expressed simply as

$$\begin{aligned} P(x_1, t_1; x_2, t_2; \ldots; x_n, t_n) &= \\ P(x_1, t_1|x_2, t_2)P(x_2, t_2|x_3, t_3)P(x_3, t_3|x_4, t_4) &\cdots P(x_{n-1}, t_{n-1}|x_n, t_n) \end{aligned} \tag{3.7}$$

provided [34]

$$t_1 \geq t_2 \geq \cdots \geq t_{n-1} \geq t_n. \tag{3.8}$$

3.2 Support

A support of a real-valued function F (e.g. continuous function) on a set X (e.g. topological space as a real line) is the subset of X on which F is nonzero, i.e. the support of F is the smallest closed subset of X outside of which F is zero.

Compact support: Compact support is a closed and bounded subset of X. Function with compact support in X is the function with compact support, that is a compact subset of X. For example, if X is the real line, they are examples of functions that vanish at infinity. Indeed, they are special cases of such functions that must vanish at finite bounds. Note that every function on a compact space has a compact support since every closed subset of a compact space is compact.

We can talk about *support of a distribution*, e.g. Dirac delta function $\delta(x)$ on the real line, with a smooth test function F, with support not including the point 0. Thus, if $\delta(F)$ (the distribution δ applied as linear functional to F) is 0, we can say that the support of δ is $\{0\}$ only.

A distribution has a *singular support*, such that the set X has a subset which a distribution fails to be a function. For example, the Fourier transform of the Heaviside step function[1] is equal to $\sim \frac{1}{x}$ except at $x = 0$. Now, we say this transform distribution has a singular support at $\{0\}$. It cannot accurately be expressed as a function in relation to test functions with support including 0. It can be expressed as an application of a Cauchy principal value improper integral [35].

3.3 $\mathbb{L}^p$ space

$\mathbb{L}^p$ space is a space of the p-power integrable function. For example, for any $p \geq 1$, the Euclidean space $\mathbb{R}^n$ together with the p-norm (i.e. $\|x\|_p = (|x_1|^p + ... + |x_n|^p)^{\frac{1}{p}}$) becomes an $\mathbb{L}^p$ space. In $\mathbb{L}^p$, if we have a vectors with infinite number of components,

[1]Heaviside step function: $F(x) = \begin{cases} 0 & x < 0, \\ 1 & x > 0. \end{cases}$

real or complex, we can define the vector sum as

$$(x_1, x_2, ..., x_n, ...) + (y_1, y_2, ..., y_n, ...) = (x_1 + y_1, x_2 + y_2, ..., x_n + y_n, ...), \tag{3.9}$$

and the scalar action is given by

$$\alpha(x_1, x_2, ..., x_n, ...) = (\alpha x_1, \alpha x_2, ..., \alpha x_n, ...), \tag{3.10}$$

then, p-norm is

$$\|x\|_p = (|x_1|^p + ... + |x_n|^p + ...)^{\frac{1}{p}}. \tag{3.11}$$

Here instead of using a sum for this definition we can use an integral. Now, the series in the right hand side of the above is not always convergence, for example $(1, 1, ...)$, and we have an infinite $p - norm$, for $p \geq 1$. Now, we define L^p as the set of all infinite sequences of real numbers such that the p-norm is finite. We can also define ∞-norm as

$$\|x\|_\infty = \lim_{p\to\infty} \|x\|_p. \tag{3.12}$$

The L^p together with its p-norm is a *Banach space*. Banach space is studied in functional analysis, and it defined as a vector space over real or complex numbers with a norm complete.

The some properties of L^p space are [35]:

i) L^2 is the Hilbert space.

ii)L^p, $1 < p < \infty$ is reflexive, i.e. $(L^p)^* = L^q$, where $\frac{1}{p} + \frac{1}{p} = 1$. For example, L^1 is a dual of L^∞, and we know that L^1 is a dual of $\mathbb{C}^0$ which is the space of all sequence converging to zero, with identical to $\|x\|_\infty$.

3.4 Hardy space

Hardy space $\mathbb{H}^p(D)$, for $0 < p < \infty$, is the class of functions holomorphic on the open unit disk D which is satisfy the following condition

$$\sup_{0<r<1} \left(\frac{1}{2\pi} \int_0^{2\pi} \left| f(re^{i\theta}) \right|^p d\theta \right)^{\frac{1}{p}} < \infty. \tag{3.13}$$

Here, p refers to the Hardy space of p-norm which is denoted by $\|f\|_{\mathbb{H}^p}$. In fact, in the complex analysis Hardy space is an analogue of the $\mathbb{L}^p$ space of functional analysis [35, 36].

3.5 Fock space

The Hilbert space in the quantum-mechanical describes a single Schrödinger particle. The Fock space is an algebraic system (Hilbert space) used in quantum mechanics to describe quantum states with a variable or unknown number of particles.

For defining the Fock spaces, let be a Hilbert space and denote by $\mathcal{H}^n$ the n-fold tensor product $\mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}$. Set $\mathcal{H}^0 = \mathbb{C}$ and

$$\mathfrak{F}(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{H}^n \tag{3.14}$$

$\mathfrak{F}(\mathcal{H})$ is called the Fock space over $\mathcal{H}$; it will be separable if $\mathcal{H}$ is separable. For example, if $\mathcal{H} = L^2(\mathbb{R})$, then an element $\psi \in \mathfrak{F}(\mathcal{H})$ is a sequence of functions

$$\psi = \{\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \psi_3(x_1, x_2, x_3), \ldots\} \tag{3.15}$$

so that

$$|\psi_0|^2 + \sum_{n=0}^{\infty} \int_{\mathbb{R}^n} |\psi_n(x_1, \ldots, x_n)|^2 dx_1 \cdots dx_n < \infty \tag{3.16}$$

Actually, it is not $\mathfrak{F}(\mathcal{H})$ itself, but two of its subspaces which are used most frequently in quantum field theory. These two subspaces are defined as follows: let us consider the S_n as an orthogonal projection with an n-fold symmetric tensor product of $\mathcal{H}$ range. In the case where $\mathcal{H} = L^2(\mathbb{R}^n)$ and $\mathcal{H}^n = L^2(\mathbb{R}) \otimes \cdots \otimes L^2(\mathbb{R})$, $S_n\mathcal{H}^n$ is just the subspace of $L^2(\mathbb{R}^n)$ of all functions left invariant under any permutation of the variables. We now define

$$\mathfrak{F}_s(\mathcal{H}) = \bigoplus_{n=0}^{\infty} S_n\mathcal{H}^n \tag{3.17}$$

$\mathfrak{F}_s(\mathcal{H})$ is called the symmetric Fock space over $\mathcal{H}$ or the Boson Fock space.

Let us define A as an orthogonal projection on $\mathcal{H}$. $A_n\mathcal{H}^n$ is just the subspace of $L^2(\mathbb{R}^n)$ consisting of those functions odd under interchange of two coordinates. The subspace

$$\mathfrak{F}_a(\mathcal{H}) = \bigoplus_{n=0}^{\infty} A_n\mathcal{H}^n \tag{3.18}$$

is called the antisymmetric Fock space [40] over $\mathcal{H}$ or the Fermion Fock space over $\mathcal{H}$.

3.6 Hilbert-Schmidt operators

Let $\mathcal{H}$ is the Hilbert space and $\{\mathbf{e}_i : i \in I\}$ is an orthonormal basis of $\mathcal{H}$. A bounded operator, T, in $\mathcal{H}$ with the following property

$$\sum_{i \in I} \|T\mathbf{e}_i\| < \infty, \tag{3.19}$$

is called an Hilbert-Schmidt operator. If the above relation is true for one orthonormal basis it is true for any other orthonormal basis.
Let T_1 and T_2 are the Hilbert-Schmidt operators, the Hilbert-Schmidt inner product is defined by

$$\langle T_1, T_2 \rangle_{HS} = \sum_{i \in I} \langle T_1\mathbf{e}_i, T_2\mathbf{e}_i \rangle. \tag{3.20}$$

This definition is independent of an orthonormal basis [37, 38].

3.7 Convolution

The convolution is a mathematical operator which takes two functions f and g and produces a third function that in a sense represents the amount of overlap between f and a reversed and translated version of g. A convolution is a kind of very general moving average, as one can see by taking one of the functions to be an indicator function of an interval.

Definition: The convolution of f and g is written $f * g$. It is defined as the integral of the product of the two functions after one is reversed and shifted. As such, it is a particular kind of integral transform:

$$(f * g)(t) = \int_0^t f(\tau)g(t-\tau)d\tau \tag{3.21}$$

By change of variables, replacing τ by $(t - \tau)$, it is sometimes written as:

$$(f * g)(t) = \int_0^t f(t-\tau)g(\tau)d\tau \tag{3.22}$$

The integration range depends on the domain on which the functions are defined. While the symbol t is used above, it need not represent the time domain. In the case of a finite integration range, f and g are often considered to extend periodically in

both directions, so that the term $g(t-\tau)$ does not imply a range violation. This use of periodic domains is sometimes called a cyclic, circular or periodic convolution. Of course, extension with zeros is also possible. Using zero-extended or infinite domains is sometimes called a linear convolution[35, 39].

3.8 Fourier Transforms

3.8.1 Definition

we introduce the Fourier transforms as:

$$\hat{f}(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{\mathrm{i}ux} dx \tag{3.23}$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(u).e^{-\mathrm{i}ux} du \tag{3.24}$$

We shall call such functions simply Fourier transforms of each other. For example

$$f(x) = e^{-|x|}, \qquad \hat{f}(u) = \sqrt{\frac{2}{\pi}} \frac{1}{1+x^2} \tag{3.25}$$

are the Fourier transforms of each other.

If $f(x)$ is even, $\hat{f}(u) = \hat{f}_c(x)$ which is defined as:

$$\hat{f}_c(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_c(x) \cos ux \; dx \tag{3.26}$$

$$f_c(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}_c(u) \cos ux \; du. \tag{3.27}$$

We shall call functions so related is the *Fourier cosine transforms* of each other.

If $f(x)$ is odd, $\hat{f}(u) = \hat{f}_s(x)$ which is defined as:

$$\hat{f}_s(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_s(x) \sin ux \; dx \tag{3.28}$$

$$f_s(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}_s(u) \sin ux \; du. \tag{3.29}$$

We shall call functions so related is the *Fourier sine transforms* of each other [98].

3.8.2 Generalized Fourier transforms

The existence of the integral defining $\hat{f}(u)$ implies a certain restriction on $f(x)$ at infinity. Even if $\hat{f}(u)$ does not exist, the functions

$$\hat{f}_+(w) = \frac{1}{\sqrt{2\pi}} \int_0^\infty f(x) e^{\mathrm{i}wx} dx \tag{3.30}$$

$$\hat{f}_-(w) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^0 f(x) e^{\mathrm{i}wx} dx \tag{3.31}$$

where $w = u + \mathrm{i}v$, may exist, the former for sufficiently large positive v, the latter for sufficiently large negative v. For

$$\hat{f}_+(w) = \frac{1}{\sqrt{2\pi}} \int_0^\infty f(x) e^{-vx} e^{\mathrm{i}ux} dx, \tag{3.32}$$

so that $\hat{f}_+(w)$ is the transformation of the function equal to $f(x)e^{-vx}$ for $t > 0$, and to 0 for $t < 0$. The formula reciprocal to (3.32) is

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \hat{f}_+(u + iv) e^{-\mathrm{i}ux} du = \begin{cases} f(x)e^{-vx}, & x > 0 \\ 0, & x < 0 \end{cases} \tag{3.33}$$

or

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \hat{f}_+(u + iv) e^{-\mathrm{i}(u+\mathrm{i}v)x} du = \begin{cases} f(x), & x > 0 \\ 0, & x < 0. \end{cases} \tag{3.34}$$

There is a similar formula for $\hat{f}_-$. Adding we may write

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathrm{i}a-\infty}^{\mathrm{i}a+\infty} \hat{f}_+(w) e^{-\mathrm{i}wx} dw + \frac{1}{\sqrt{2\pi}} \int_{\mathrm{i}b-\infty}^{\mathrm{i}b+\infty} \hat{f}_-(w) e^{-\mathrm{i}wx} dw \tag{3.35}$$

where a is a sufficiently large positive number, b a sufficiently large negative number.

For example, if $f(x) = e^x$, the we have

$$\begin{aligned} \hat{f}_+(w) &= -\sqrt{\frac{1}{2\pi}} \frac{1}{1 + \mathrm{i}w} \\ \hat{f}_-(w) &= \sqrt{\frac{1}{2\pi}} \frac{1}{1 + \mathrm{i}w} \end{aligned} \tag{3.36}$$

By replacing the above equations in the (3.35)

$$f(x) = -\frac{1}{2\pi} \int_{\mathrm{i}a-\infty}^{\mathrm{i}a+\infty} \frac{e^{-\mathrm{i}wx}}{1 + \mathrm{i}w} dw + \frac{1}{2\pi} \int_{\mathrm{i}b-\infty}^{\mathrm{i}b+\infty} \frac{e^{-\mathrm{i}wx}}{1 + \mathrm{i}w} dw. \tag{3.37}$$

Taking the first integral by considering a semi-circle contour in the half-plane superior we see that this integral is equal to e^x, because there is a pole at "$w = \mathrm{i}$" in this contour. The second integral is equal to 0, since in the half-plane inferior is no pole [98].

3.9 Laplace transforms

The formula

$$F(s) = \int_0^\infty f(t)e^{-st}dx \tag{3.38}$$

is known as Laplace's integral. If $f(t)$ is given function, $F(s)$ is in general analytic for Re$s > 0$. The reciprocal formula is [98]

$$\frac{1}{2\pi\mathrm{i}}\int_{k-\mathrm{i}\infty}^{k+\mathrm{i}\infty} F(s)e^{sx}ds = \begin{cases} f(x), & x > 0 \\ 0, & x < 0. \end{cases} \tag{3.39}$$

From the formal point of view the formulae are a particular case of those of Subsection 3.8.1, as is seen on putting $s = \sigma + \mathrm{i}t$.

3.10 Hilbert transforms

The Hilbert transforms formula are defined as:

$$g(x) = \frac{1}{\pi}\mathsf{P}\int_{-\infty}^{\infty}\frac{f(t)}{t-x}dt \tag{3.40}$$

$$f(x) = -\frac{1}{\pi}\mathsf{P}\int_{-\infty}^{\infty}\frac{g(t)}{t-x}dt \tag{3.41}$$

where P denote principal value and g and f are reciprocity Hilbert transforms of each other.

Now we introduce a theorem which we admit to do analytical continuation in Hilbert transforms [98, 36].

Theorem: Let $\Phi(z)$ be an analytical function, regular for $y > 0$, and let

$$\frac{1}{\pi\mathrm{i}}\int_{-\infty}^{\infty}|\Phi(x+\mathrm{i}y)|^2dx \tag{3.42}$$

exist for every positive y, and be bounded. Then, as $y \to 0$, $\Phi(x+\mathrm{i}y)$ converge in mean to a function $\Phi(x)$, also $\Phi(x+\mathrm{i}y) \to \Phi(x)$ for almost all x. For $y > 0$

$$\Phi(x) = \frac{1}{\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\Phi(u)}{u-z} du, \qquad (u \text{ real}). \tag{3.43}$$

If $\Phi(z) = U(x,y) + \mathrm{i}V(x,y)$, $\Phi(x) = f(x) + \mathrm{i}g(x)$, the functions f and g are conjugate[2] and the functions U and V are connected by the following formulae:

$$U(x,y) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{t-x}{(t-x)^2+y^2}\, g(t)dt \tag{3.44}$$

$$V(x,y) = -\frac{y}{\pi} \int_{-\infty}^{\infty} \frac{g(t)}{(t-x)^2+y^2}\, g(t)dt. \tag{3.45}$$

3.11 Paley-Wiener theorem

The Paley-Wiener theorem relates growth properties of entire functions[3], $F(z)$ and Fourier-Laplace transformation of distributions of compact support, $\psi(\lambda)$, which is defined as follows:

$$F(z) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int e^{-\mathrm{i}\lambda z} \psi(\lambda) d\lambda, \tag{3.46}$$

where z is an element in the complex space $\mathbb{C}^n$.

Paley-Wiener theorem: An entire function F on a complex space, $\mathbb{C}^n$, is the Fourier-Laplace transform of distribution $\psi(\lambda)$ of compact support if and only if for all $z \in \mathbb{C}^n$,

$$|F(z)| \leq C(1+|z|)^N e^{B|\mathrm{Im} z|}, \tag{3.47}$$

for some constants C, B, and N. Additional growth conditions on the entire function F impose regularity properties on the distribution $\psi(\lambda)$. For example, if for every positive N there is a constant C_N such that for all $z \in \mathbb{C}^n$,

$$|F(z)| \leq C_N(1+|z|)^{-N} e^{B|\mathrm{Im} z|}, \tag{3.48}$$

[2]They are connected by Hilbert transforms (3.40) and (3.41)

[3]An entire function is a function that is analytic everywhere on the whole complex plane. Typical examples of entire functions are the polynomials, the exponential function, and sums, products and compositions of these. Every entire function can be represented as a power series which converges everywhere. Neither the natural logarithm nor the square root function is entire. Note that an entire function may have a singularity or even an essential singularity at the complex point at infinity. In the latter case, it is called a *transcendental entire function*.

then $\psi(\lambda)$ is infinitely differentiable and conversely. In other words, the Paley-Wiener theorem explicitly describes the Hardy space $\mathbb{H}^2(\mathbb{R})$ by using the unitary Fourier transform $\mathcal{F}$. The theorem states that

$$\mathcal{F}\mathbb{H}^2(\mathbb{R}) = \mathbb{L}^2(\mathbb{R}^+). \tag{3.49}$$

This is a very useful result as it enables one pass to the Fourier transform of a function in the Hardy space and perform calculations in the easily understood space of square-integrable functions supported on the positive axis [98, 35].

Chapter 4

Some Quantum Statistical Mechanical Concepts

4.1 Density matrix

Before we define the density matrix let us note that an operator is defined when all its matrix elements with respect to a complete set of states are defined. Its matrix elements with respect to any other complete set of states can be found by the well-known rules of transformation theory in quantum mechanics. Therefore, if all the matrix elements of an operator are defined in one representation, the operator is thereby defined in any representation.

Defining the mean of a dynamical operator, B, in a system in a mixed state $|\phi\rangle = \sum_a P(a)|\phi_a\rangle$ is

$$\langle B\rangle = \sum_a P(a)\langle\phi_a|B|\phi_a\rangle, \tag{4.1}$$

where $P(a)$ is the probability that each state occurs, this probability is not depending in quantum effects but simply depending in the randomness of state preparation. Now, we introduce the density matrix (or operator) ρ by

$$\rho = \sum_a P(a)|\phi_a\rangle\langle\phi_a|. \tag{4.2}$$

Defining trace operation, Tr:

$$\mathrm{Tr}(A) = \sum_n \langle\phi_n|A|\phi_n\rangle, \tag{4.3}$$

where $\sum_n |\phi_n\rangle\langle\phi_n| = 1$, we can rewrite equation (4.1) as:

$$\begin{aligned}\langle B\rangle &= \sum_a P(a)\langle\phi_a|B|\phi_a\rangle \\ &= \sum_{a,n} P(a)\langle\phi_a|B|\phi_n\rangle\langle\phi_n|\phi_a\rangle \\ &= \sum_{a,n} P(a)\langle\phi_n|\phi_a\rangle\langle\phi_a|B|\phi_n\rangle \\ &= \mathrm{Tr}(\rho B) \end{aligned} \tag{4.4}$$

The important properties of density matrix are:

i) $\mathrm{Tr}(\rho) = \sum_{a,n} P(a)\langle\phi_n|\phi_a\rangle\langle\phi_a|\phi_n\rangle = \sum_a P(a) = 1$.

ii) For any state $|A\rangle$, ρ is always positive, i.e. $\langle A|\rho|A\rangle = \sum_a P(a)|\langle A|\phi_a\rangle|^2 \geq 0$.

iii) For pure state we have $P(a) = \delta(a, a')$, for some a'. Here $\delta(a, a')$ is Dirac delta-function for continuous spectrum and delta Kronecker for discret state. Thus, yielding $\rho^2 = \rho$ and conversely.

iv) $\mathrm{Tr}(\rho^2) \leq \mathrm{Tr}(\rho)$, equal is only for pure state.

v) ρ is self-adjoint: $\rho^\dagger = \rho$.

The introduction of the density matrix merely introduces a notation. It does not introduce new physical content. The usefulness of the density matrix lies solely in the fact that with its help (4.4) is presented in a form that is manifestly independent of the choice of the basis ϕ_a, although this independence is a property that the expectation value always possesses [34, 38, 35].

4.2 Quantum Liouville equation

The density operator ρ defined by (4.2) contains all the information about an ensemble. It is independent of time if it commutes with the Hamiltonian of the system and if the Hamiltonian is independent of time.

This statement is an immediate consequence of the equation of the motion of ρ is obtained from Schrödinger equation, $H|\psi\rangle = \mathrm{i}\frac{\partial|\psi\rangle}{\partial t}(\hbar = 1)$, for any state. We can

obtain corresponding equation for density matrix as

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \sum_a P(a)[(\partial_t|\phi_a\rangle)\langle\phi_a| + |\phi_a\rangle(\partial_t\langle\phi_a|)] \\ &= -\mathrm{i}(H\rho - \rho H). \end{aligned} \tag{4.5}$$

That is,

$$\mathrm{i}\frac{\partial\rho}{\partial t} = [H, \rho] \tag{4.6}$$

which is *quantum Liouville equation* [34].

4.3 Projection operator

In linear algebra and functional analysis, a projection is a linear transformation $\mathcal{P}_a$ from a vector space to itself such that $\mathcal{P}_a^2 = \mathcal{P}_a$. Projections map the whole vector space to a subspace and leave the points in that subspace unchanged . Thus, we use the *projection operator*,

$$\mathcal{P}_a = |\phi_a\rangle\langle\phi_a|, \tag{4.7}$$

for a system in a pure state instead of density matrix. Only 0 and 1 can be an eigenvalue of a projection.

The subspaces $\mathbb{U}$ and $\mathbb{V}$ are complementary, i.e. the underlying vector space is the direct sum $\mathbb{X} \equiv \mathbb{U} \oplus \mathbb{V}$. This means that any vector $|\phi\rangle$ in the domain can uniquely be written as $|\phi\rangle = |\phi_a\rangle + \sum_{b\neq a}|\phi_b\rangle$ with $|\phi_a\rangle \in \mathbb{U}$ and $\{|\phi_b\rangle\} \in \mathbb{V}$. The vector $|\phi_a\rangle$ in this decomposition is given by $|\phi_a\rangle = \mathcal{P}_a|\phi\rangle$, where $\mathcal{P}_a$ is the projection along $\mathbb{V}$ onto $\mathbb{X}$. The vector $\sum_{b\neq a}|\phi_b\rangle$ is given by $\sum_{b\neq a}|\phi_b\rangle = (1-\mathcal{P}_a)|\phi\rangle$. The operator $1-\mathcal{P}_a$ is called the *complementary projection*[35].

The projection operator has the following proprieties [41]:

i) $\langle B\rangle = \mathrm{Tr}(\mathcal{P}_a B) = \mathrm{Tr}(B\mathcal{P}_a)$,

ii) $\mathcal{P}_a^2 = \mathcal{P}_a$,

iii) $\mathrm{Tr}(\mathcal{P}_a) = 1$,

iv) $\mathrm{i}\frac{d}{dt}\mathcal{P}_a = [H, \mathcal{P}_a]$.

4.4 Density matrix of bipartite system

If we have two systems A and B in the Hilbert space with states $|\phi_a\rangle_A \in \mathcal{H}_A$ and $|\phi_a\rangle_B \in \mathcal{H}_B$, those interactions give

$$\sqrt{\mathrm{P}_a}|\phi_a\rangle_A \otimes |\phi_a\rangle_B \equiv |\psi_a\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B, \tag{4.8}$$

where "$\otimes$" is the tensor product. Then, the density matrix of this bipartite quantum system is written as:

$$\rho_{AB} = \sum_a \mathrm{P}_a |\psi_a\rangle_{AB}\ {}_{AB}\langle\psi_a|. \tag{4.9}$$

We also have

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}), \tag{4.10}$$

where Tr_B is partial trace relative to the system B, an ρ_A is called reduced density matrix (operator) . we can prove the above equation as follows [34, 38, 35]:

$$\begin{aligned}
\mathrm{Tr}_B(\rho_{AB}) &= \sum_{a,a'} \mathrm{P}_a\ {}_B\langle\phi_{a'}|\psi_a\rangle_A\ {}_B\langle\psi_a|\phi_{a'}\rangle_B \\
&= \sum_{a,a'} \mathrm{P}_a\ {}_B\langle\phi_{a'}|\phi_a\rangle_B \otimes |\phi_a\rangle_A\ {}_A\langle\phi_a| \otimes\ {}_A\langle\phi_a|\phi_{a'}\rangle_B \\
&= \sum_a \mathrm{P}_a |\phi_a\rangle_A\ {}_A\langle\phi_a| \\
&= \rho_A,
\end{aligned} \tag{4.11}$$

where ${}_B\langle\phi_{a'}|\phi_a\rangle_B = \delta_{aa'}$.

4.5 Quantum entanglement

4.5.1 Introduction

Quantum entanglement is a quantum mechanical phenomenon in which the quantum states of two or more objects have to be described with reference to each other, even though the individual objects may be spatially separated. This leads to correlations between observable physical properties of the system. For example, it is possible to prepare two particles in a single quantum state such that when one is observed to be spin-up, the other one will always be observed to be spin-down and vice versa, despite

the fact that it is impossible to predict, according to quantum mechanics, which set of measurements will be observed. As a result, measurements performed on one system seem to be instantaneously influencing other systems entangled with it. But quantum entanglement does not enable the transmission of classical information faster than the speed of light. It prompts some of the more philosophically oriented discussions concerning quantum theory. The correlations predicted by quantum mechanics, and observed in experiment, reject the principle of local realism, which is that information about the state of a system should only be mediated by interactions in its immediate surroundings. Different views of what is actually occurring in the process of quantum entanglement can be related to different interpretations of quantum mechanics.

Entanglement is one of the properties of quantum mechanics which caused Einstein and others [78] to dislike the theory. In 1935, Einstein, Podolsky, and Rosen formulated the EPR paradox, a quantum-mechanical thought experiment with a highly counterintuitive and apparently nonlocal outcome. Einstein famously derided entanglement as "spooky action at a distance".

On the other hand, quantum mechanics has been highly successful in producing correct experimental predictions, and the strong correlations associated with the phenomenon of quantum entanglement have in fact been observed [35]. One apparent way to explain quantum entanglement is an approach known as *hidden variable theory*, in which unknown, shared, local parameters would cause the correlations. However, in 1964 Bell derived an upper limit, known as Bell's inequality, on the strength of correlations for any theory obeying *local realism*. Quantum entanglement can lead to stronger correlations that violate this limit, so that quantum entanglement is experimentally distinguishable from a broad class of local hidden-variable theories. Results of subsequent experiments have overwhelmingly supported quantum mechanics. Although there are a number of known loopholes in these experiments, high-efficiency and high-visibility experiments are now in progress which should confirm or disaffirm the influence of those loopholes.

Observations on entangled states naively appear to conflict with the property of relativity that information cannot be transferred faster than the speed of light. Although two entangled systems appear to interact across large spatial separations, no useful information can be transmitted in this way, so causality cannot be violated through entanglement. This is the statement of no communication theorem.

Although no information can be transmitted through entanglement alone, it is possible to transmit information using a set of entangled states used in conjunction with

a classical information channel. This process is known as quantum teleportation[35].

4.5.2 Entanglement States

Now, we introduce the mathematical form of the entanglement. If we can write a state, $|\psi\rangle_{AB}$, in $\mathcal{H}_A \otimes \mathcal{H}_B$ as product of two states in $\mathcal{H}_A$ and $\mathcal{H}_B$, i.e. $|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\phi\rangle_B$, we say that $|\psi\rangle_{AB}$ is separable, else it is an *entangled state* or nonseparable state. For example, we consider two following systems:

$$|\phi\rangle_A = \alpha_0|0\rangle_A + \alpha_1|1\rangle_A \quad \text{and} \quad |\phi\rangle_B = \alpha_0|0\rangle_B + \alpha_1|1\rangle_B, \tag{4.12}$$

and we writing $|\psi\rangle_{AB}$, as

$$|\psi\rangle_{AB} = \alpha_{00}|0\rangle_A \otimes |0\rangle_B + \alpha_{01}|0\rangle_A \otimes |1\rangle_B + \alpha_{10}|1\rangle_A \otimes |0\rangle_B + \alpha_{11}|1\rangle_A \otimes |1\rangle_B, \tag{4.13}$$

thus, $|\psi\rangle_{AB}$ is a separable state if

$$\alpha_{00} = \alpha_0\alpha_0, \quad \alpha_{01} = \alpha_0\alpha_1, \quad \alpha_{10} = \alpha_1\alpha_0 \text{ and } \alpha_{11} = \alpha_1\alpha_1, \tag{4.14}$$

else $|\psi\rangle_{AB}$ is an entangled state [38, 42].

4.6 Schmidt decomposition theorem

All state $|\psi\rangle_{AB}$ in $\mathcal{H}_A \otimes \mathcal{H}_B$ can be written as the following form

$$|\psi\rangle_{AB} = \sum_a \sqrt{\mathrm{P}_a}|\phi_a\rangle_A \otimes |\phi_a\rangle_B, \tag{4.15}$$

with ${}_A\langle\phi_a|\phi_{a'}\rangle_A = \delta_{aa'}$ and ${}_B\langle\phi_a|\phi_{a'}\rangle_B = \delta_{aa'}0$. Equation (4.15) is called the Schmidt decomposition of $|\psi\rangle_{AB}$. In a bipartite pure state, subsystems A and B separately are described by density operators ρ_A and ρ_B, it follows from equation (4.15) that ρ_A and ρ_B have the same nonvanishing eigenvalues (the P_a's). The number of nonvanishing eigenvalues is called the *Schmidt number* of $|\psi\rangle_{AB}$. A bipartite pure state is said to be entangled if its Schmidt number is greater than one. From expression (4.15) we can obtain reduced density matrix ρ_A and ρ_B as [38, 42]

$$\rho_A = \sum_a \mathrm{P}_a|\phi_a\rangle_A \, {}_A\langle\phi_a| \quad \text{and} \quad \rho_B = \sum_a \mathrm{P}_a|\phi_a\rangle_B \, {}_B\langle\phi_a|. \tag{4.16}$$

4.7 von Neumann entropy

The density matrix was introduced, with different motivations, by von Neumann and by Lev Landau. The motivation that inspired Landau was the impossibility of describing a subsystem of a composite quantum system by a state vector. On the other hand, von Neumann introduced the density matrix in order to develop both quantum statistical mechanics and a theory of quantum measurements. Given the density matrix ρ, von Neumann defined the entropy as

$$\mathcal{S}_{vn}(\rho) = -\mathrm{Tr}(\rho \log \rho) \tag{4.17}$$

which is a proper extension of Shannon's entropy to the quantum case. To compute (4.17) one has to find a basis in which ρ possesses a diagonal representation. We note that the entropy $\mathcal{S}_{vn}(\rho)$ times the Boltzmann constant k_B equals the thermodynamical or physical entropy. If the system is finite (finite dimensional matrix representation) the entropy (4.17) describes the departure of our system from a pure state. In other words, it measures the degree of mixture of our state describing a given finite system. Properties of the von Neumann entropy:

i) *Purity:* A pure state $\rho = |\phi\rangle\langle\phi|$ has $\mathcal{S}_{vn}(\rho) = 0$

ii) *Maximum:* If ρ has N nonvanishing eigenvalues N-dimensional Hilbert space, then

$$\mathcal{S}_{vn}(\rho) \leq \log N. \tag{4.18}$$

The maximum reaches for a maximally mixed state.

iii) *Invariance:* $\mathcal{S}_{vn}(\rho)$ is invariant under unitary changes in the basis of ρ, that is,

$$\mathcal{S}_{vn}(U\rho U^{-1}) = \mathcal{S}_{vn}(\rho) \tag{4.19}$$

This is obvious, since $\mathcal{S}_{vn}(\rho)$ depends only on the eigenvalues of ρ.

iv) *Concavity:* For $\lambda_1, \lambda_2, \ldots, \lambda_n \geq 0$ and $\lambda_1 + \lambda_2 + \cdots + \lambda_n = 1$, $\mathcal{S}_{vn}(\rho)$ is concave, that is,

$$\mathcal{S}_{vn}(\sum_i^n \lambda_i \rho_i) \geq \sum_i^n \lambda_i \mathcal{S}_{vn}(\rho_i) \tag{4.20}$$

that is, von Neumann entropy is larger if we are more ignorant about how the state was prepared. This property is a consequence of the convexity of the log function.

v)*Subadditivity:* Consider a bipartite system AB in the state ρ_{AB}. Then

$$\mathcal{S}_{vn}(\rho_{AB}) \leq \mathcal{S}_{vn}(\rho_A) + \mathcal{S}_{vn}(\rho_B) \tag{4.21}$$

where $\rho_A = \mathrm{Tr}_B \rho_{AB}$ and $\rho_B = \mathrm{Tr}_A \rho_{AB}$, with equality for $\rho_{AB} = \rho_A \otimes \rho_B$. Thus, entropy is additive for uncorrelated systems, but otherwise the entropy of the whole is less than the sum of the entropy of the parts.

vi) *Strong subadditivity:* For any state ρ_{ABC} of a tripartite system,

$$\mathcal{S}_{vn}(\rho_{ABC}) + \mathcal{S}_{vn}(\rho_B) \leq \mathcal{S}_{vn}(\rho_{AB}) + \mathcal{S}_{vn}(\rho_{BC}) \tag{4.22}$$

This property is called "strong" subadditivity in that it reduces to subadditivity in the event that B is one-dimensional. The proof of the corresponding property of Shannon entropy is quite simple, but the proof for von Neumann entropy turns out to be surprisingly difficult. You may find the strong subadditivity property easier to remember by thinking about it this way: AB and BC can be regarded as two overlapping subsystems. The entropy of their union (ABC) plus the entropy of their intersection (B) does not exceed the sum of the entropies of the subsystems (AB and BC). We will see that strong subadditivity has deep and important consequences.

vii) *Triangle inequality:*(1) For a bipartite system [35, 38]

$$\mathcal{S}_{vn}(\rho_{AB}) \geq |\mathcal{S}_{vn}(\rho_A) - \mathcal{S}_{vn}(\rho_B)|. \tag{4.23}$$

4.8 Decoherence

4.8.1 Definition

Unitary evolution condemns every closed quantum system to "purity". Yet if the outcome of a measurement are to become independent, with consequences that can be explored separately, a way must be found to dispose of the excess information. This disposal can be caused by interaction with the degrees of freedom external to the system, which we shall summarily refer to as "the environment".

If the phase relative between two wave function ($|\phi_1\rangle$ and $|\phi_2\rangle$), is constant or it does not fluctuate randomly with time, these wave function are *coherent*. Now, the superposition of two coherent wave functions, i.e.

$$|\phi\rangle = (\alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle), \tag{4.24}$$

gives the interference effect in the probability density $|\phi|^2 = \langle\phi|\phi\rangle$, that is equal to

$$|\phi|^2 = |\alpha_1|^2\langle\phi_1|\phi_1\rangle + \alpha_1^*\alpha_2\langle\phi_1|\phi_2\rangle + \alpha_2^*\alpha_1\langle\phi_2|\phi_1\rangle + |\alpha_2|^2\langle\phi_2|\phi_2\rangle \tag{4.25}$$

The diagonals terms, i.e. the first and forth terms, in the above equation are the corresponding to classical probability densities, whereas, the off-diagonals terms, i.e. the second and third terms, are called interference terms which are the quantum effect. If this system, ϕ, is coupled to an environment, the relative phase between $|\phi_1\rangle$ and $|\psi_2\rangle$ will typically fluctuate with time, and the interference terms will rapidly average to zero. Their vanishing is called *decoherence*, i.e. the different components of wave function lose their ability to interfere.

We can also use the density matrix to describe the probability distribution for the alternative outcome, by taking the pure state density matrix

$$\rho = |\alpha_1|^2|\phi_1\rangle\langle\phi_1| + \alpha_1^*\alpha_2|\phi_2\rangle\langle\phi_1| + \alpha_2^*\alpha_1|\phi_1\rangle\langle\phi_2| + |\alpha_2|^2|\phi_2\rangle\langle\phi_2|. \tag{4.26}$$

Thus, the decay of off-diagonal elements in the density matrix gives the reduced density matrix as:

$$\rho_{red} = |\alpha_1|^2|\phi_1\rangle\langle\phi_1| + |\alpha_2|^2|\phi_2\rangle\langle\phi_2|. \tag{4.27}$$

Reduction of the state from ρ to ρ_{red} decreases the information available to the observer about the composite system (system+detector). Thus its entropy $\mathcal{S}_{vn}$ increases as it must,

$$\triangle\mathcal{S}_{vn} = \mathcal{S}_{vn}(\rho_{red}) - \mathcal{S}_{vn}(\rho) = |\alpha_1|^2 \log|\alpha_1|^2 + |\alpha_2|^2 \log|\alpha_2|^2. \tag{4.28}$$

The initial state described by ρ was pure, and the reduced state, ρ_{red} is mixed. Information gain-the objective of measurement-is accomplished only when the observer interacts and becomes correlated with the detector in the already precollapsed state ρ_{red}. This must be preceded by an increase in entropy if the outcomes are to become classical, so that they can used as initial conditions to predict the future [43, 44].

4.8.2 Decoherence free subspace

It might appear as if accelerated decoherence is an inevitable fact, a fundamental natural law. This is, however, not the case. It is well known by now that certain subspaces of Hilbert space might be completely decoherence free. Such a situation arises if the coupling to the environment has a certain symmetry, in the sense that the interaction Hamiltonian his degenerate eigenvalues. If $|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle$ are eigenstates of H_{int} with the same eigenvalue, then there is no accelerated decoherence in the subspace they span.

The physical principle behind this is very simple. If the system Hamiltonian can be neglected, the states of the system are propagated by $e^{-\mathrm{i}H_{\mathrm{int}}t/\hbar}$. States that are eigenstates of H_{int} with the same eigenvalue acquire exactly the same phase factors as a function of time. Therefore the phase coherence between such states remains intact.

The benefits of symmetric couplings have been known for a long time. For example, it is well known that rotational tunneling of small molecular groups attached to large molecules can be observed up to temperatures much higher than what would correspond to the tunneling frequency. The reason is that the coupling to the environment has exactly the same symmetry as the hindering potential. This is very much in contrast to the ordinary tunnel effect in a linear coordinate x, where decoherence sets in at temperatures comparable to the tunneling frequency. Another way of phrasing the robustness against decoherence in rotational tunneling is to say that single-phonon transitions in the tunneling-split ground state are forbidden owing to selection rules originating from the symmetry of the coupling to the environment. Here the latter consists basically of normal vibration modes of the carrier molecule or of the crystal in which it is embedded.

Recently, decoherence-free subspaces have attracted renewed attention in quantum computing. It has been shown that general Markovian master equations of the Lindblad form

$$\frac{\partial \rho}{\partial t} = -\frac{\mathrm{i}}{\hbar}[H_s, \rho] + L_D[\rho], \tag{4.29}$$

$$L_D[\rho] = \frac{1}{2}\sum_{\alpha,\beta}^{M} \alpha_{\alpha\beta} L_{\alpha\beta}[\rho], \tag{4.30}$$

$$L_{\alpha\beta}[\rho] = [F_\alpha, \rho F_\beta^\dagger] + [F_\alpha \rho, F_\beta^\dagger] \tag{4.31}$$

where the coefficients $\alpha_{\alpha,\beta}$ form a Hermitian matrix. The system operators F_α are known as "coupling agents" or, in the context of quantum computing, as "error generators". They span an M-dimensional Lie algebra. A decoherence-free subspace is defined as all states ρ with $L_D[\rho] = 0$, since then only the unitary evolution according to the first terms in (4.29) remains [43].

Chapter 5

Quantum Decay Models (I)

5.1 Weisskopf-Wigner theory

Weisskopf-Wigner Theory is used in the atomic decay. In this treatment first we consider an exponential time dependence for states and then the integrating over continuum energy where we are neglecting the variation of the matrix elements with energy of the original state. Also, we change the interval of integration over continuum energy to $]-\infty,\ \infty[$. Now, we consider two-level atom Hamiltonian as:

$$H = H_0 + H_I \tag{5.1}$$

where

$$H_0 = \omega_1|1\rangle\langle 1| + \omega_2|2\rangle\langle 2| + \sum_k \omega_k|k\rangle\langle k| \tag{5.2}$$

and

$$H_I = \sum_{i=1}^{2}\sum_k [V_i^*(\omega_k)|i\rangle\langle k| + V_i(\omega_k)|k\rangle\langle i|] \tag{5.3}$$

where we consider $\hbar = c = 1$ and $V_i(\omega_k)$ a factor form. Now, we write time dependence Schrödinger equation as:

$$\mathrm{i}\partial\psi(t)/\partial t = H\psi(t) \tag{5.4}$$

where $\psi(t) \equiv \{a_1(t)|1\rangle, a_2(t)|2\rangle, b(\omega_k, t)|k\rangle\}$. Thus, we have

$$\mathrm{i}\frac{\partial a_1(t)}{\partial t} = \omega_1 a_1(t) + \sum_k V_1^*(\omega_k) b(\omega_k, t), \tag{5.5}$$

$$\mathrm{i}\frac{\partial a_2(t)}{\partial t} = \omega_2 a_2(t) + \sum_k V_2^*(\omega_k) b(\omega_k, t) \tag{5.6}$$

and

$$\mathrm{i}\frac{\partial b(\omega_k, t)}{\partial t} = \omega_k b(\omega_k, t) + [V_1(\omega_k) a_1(t) + V_2(\omega_k) a_2(t)]. \tag{5.7}$$

Now, we make some approximations [45, 46]. First, replacing summation with integration as:

$$\sum_k V_i(\omega_k) \to \int_0^\infty d\omega v_i(\omega) \tag{5.8}$$

where we assume that the modes of fields are closely spaced. By solving equation(5.7) we obtain

$$b(\omega, t) = -\mathrm{i}e^{-\mathrm{i}\omega t} \int_0^t d\tau [v_1(\omega) a_1(\tau) + v_2(\omega) a_2(\tau)] e^{\mathrm{i}\omega\tau} \tag{5.9}$$

Subsisting the above equation in equation (5.5) yields

$$\mathrm{i}\frac{\partial a_1(t)}{\partial t} = \omega_1 a_1(t) - \mathrm{i}\int_0^t d\tau \int_0^\infty d\omega v_1^*(\omega) e^{-\mathrm{i}\omega t} [v_1(\omega) a_1(\tau) + v_2(\omega) a_2(\tau)] e^{\mathrm{i}\omega\tau} \tag{5.10}$$

where we have assumed the variations of $v_1(\omega)$ and $v_2(\omega)$ over ω are negligible with $|\omega| \lesssim$ "uncertainty of the original state energy", i.e. $v_i(\omega) \approx v_i$ $(i = 1, 2)$. Also the other assumption is: the lower limit of integration over ω is replaced by $-\infty$. Now, the above equation is written as:

$$\mathrm{i}\frac{\partial a_1(t)}{\partial t} = \omega_1 a_1(t) - \mathrm{i}2\pi \int_0^t [|v_1|^2 a_1(\tau) + v_1^* v_2 a_2(\tau)] \delta(\tau - t) d\tau \tag{5.11}$$

where we used

$$\int_{-\infty}^\infty e^{-\mathrm{i}\omega(\tau - t)} d\omega = 2\pi\delta(\tau - t) \tag{5.12}$$

Finally, (5.11) can be written as the following Markovian form

$$\mathrm{i}\frac{\partial a_1(t)}{\partial t} = \omega_1 a_1(t) - \mathrm{i}2\pi [|v_1|^2 a_1(t) + v_1^* v_2 a_2(t)]. \tag{5.13}$$

Similarly $a_2(t)$ is obtained as:

$$\mathrm{i}\frac{\partial a_2(t)}{\partial t} = -\mathrm{i}2\pi [v_1 v_2^* a_1(t) + |v_2|^2 a_2(t)] + \omega_2 a_2(t). \tag{5.14}$$

Thus, the reduced Schrödinger is written as follows:

$$\mathrm{i}\frac{\partial}{\partial t} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = (M - \mathrm{i}\Gamma) \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} \tag{5.15}$$

where

$$M - \mathrm{i}\Gamma = \begin{pmatrix} \omega_1 - \mathrm{i}2\pi|v_1|^2 & -\mathrm{i}2\pi v_1^* v_2 \\ -\mathrm{i}2\pi v_1 v_2^* & \omega_2 - \mathrm{i}2\pi|v_2|^2 \end{pmatrix}. \tag{5.16}$$

Weisskopf-Wigner treatment also assumes that [45, 46]

$$\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = \psi e^{-\nu t}, \tag{5.17}$$

then it gives

$$(M - \mathrm{i}\Gamma)\psi = \nu\psi. \tag{5.18}$$

5.2 Lee-Oehme-Yang theory (LOY)

5.2.1 Mass-Decay Matrix

By using Weisskopf-Wigner Theory one can write the schrödinger equation as

$$\mathrm{i}\frac{d\psi(t)}{dt} = H\psi(t) = (M - \mathrm{i}\Gamma)\psi(t) \tag{5.19}$$

where M and Γ are both 2×2 Hermitian matrices. We consider weak interaction as a perturbation in the total Hamiltonian, i.e. $H = H_{\mathrm{st}} + H_{\mathrm{el}} + H_{\mathrm{wk}}$, where $H_{\mathrm{st}}, H_{\mathrm{el}}$ and H_{wk} are the Strong, Electromagnetic and Weak interactions Hamiltonian, respectively. Since $H_{\mathrm{st}} + H_{\mathrm{el}}$ commute with CPT, then $|\mathrm{K}^0\rangle$ and $|\overline{\mathrm{K}}^0\rangle$ are the eigenstates of $H_{\mathrm{st}} + H_{\mathrm{el}}$ with degenerate m_k eigenvalue. Then, weak interaction connects K^0 and $\overline{\mathrm{K}}^0$ with the other continuum states such as $2\pi, 3\pi, \pi e\nu$ etc. Thus, various decay modes removes their degeneracy [55]. Now, by using perturbation formula, one obtains

$$(M - \mathrm{i}\Gamma)_{mn} = \langle m|H|n\rangle + \sum_{l \neq m,n} \frac{\langle m|H_{\mathrm{wk}}|l\rangle\langle l|H_{\mathrm{wk}}|n\rangle}{m_k - (m_l + \mathrm{i}\epsilon)} + O(H_{\mathrm{wk}}^3) \tag{5.20}$$

where m, n can be K^0 or $\overline{\mathrm{K}}^0$ and ϵ is the positive infinitesimal real number. Then, easily, by eliminating the order $O(H_{\mathrm{wk}}^3)$ one obtains,

$$M_{mn} = \langle m|H|n\rangle + \sum_{l \neq m,n} \mathsf{P}\frac{\langle m|H_{\mathrm{wk}}|l\rangle\langle l|H_{\mathrm{wk}}|n\rangle}{m_k - m_l} \tag{5.21}$$

and

$$\Gamma_{mn} = \pi \sum_{l \neq m,n} \langle m|H_{\rm wk}|l\rangle\langle l|H_{\rm wk}|n\rangle \delta(m_k - m_l). \tag{5.22}$$

where P indicates the "principal value" and we used the following identity in equation (5.20)

$$\frac{1}{x - x_0 + \mathrm{i}\epsilon} = \mathsf{P}\frac{1}{x - x_0} - \delta(x - x_0). \tag{5.23}$$

Theorem 1: $i)\Gamma$ is a positive matrix, i.e.

$$\Gamma_{11} \geq 0, \quad \Gamma_{22} \geq 0, \quad \text{and} \quad \Gamma \geq 0. \tag{5.24}$$

$ii)$ If CPT invariance holds, then independently of T symmetry

$$\Gamma_{11} = \Gamma_{22}, \quad M_{11} = M_{22}. \tag{5.25}$$

$iii)$ If T invariance holds, then independently of CPT symmetry [55]

$$\frac{\Gamma_{12}^*}{\Gamma_{12}} = \frac{M_{12}^*}{M_{12}}. \tag{5.26}$$

Theorem 2: $i)$ if CPT invariance holds, then independently of T invariance [55],

$$|\mathrm{K}_S\rangle = [2(1 + |\epsilon|^2)]^{-\frac{1}{2}} \begin{pmatrix} 1 + \epsilon \\ 1 - \epsilon \end{pmatrix}, \ |\mathrm{K}_L\rangle = [2(1 + |\epsilon|^2)]^{-\frac{1}{2}} \begin{pmatrix} 1 + \epsilon \\ -(1 - \epsilon) \end{pmatrix} \tag{5.27}$$

$\mathcal{E} = \langle \mathrm{K}_S|\mathrm{K}_L\rangle$ is real number.
$ii)$ if T invariance holds, then independently of CPT invariance,

$$|\mathrm{K}_S\rangle = [2(1 + |\delta|^2)]^{-\frac{1}{2}} \begin{pmatrix} 1 + \delta \\ 1 - \delta \end{pmatrix}, \ |\mathrm{K}_L\rangle = [2(1 + \delta^2)]^{-\frac{1}{2}} \begin{pmatrix} 1 - \delta \\ -(1 + \delta) \end{pmatrix} \tag{5.28}$$

$\mathcal{E}$ is real imaginary.

5.2.2 *CP* violation

If both CPT and T were exact symmetries, then CP must be conserved and then $\mathcal{E} = 0$. Thus, $\mathcal{E}$ can be a good CP-violation parameter.

Now, the eigenvalue equation of equation (5.19) is written as

$$(M - \mathrm{i}\Gamma)\psi_{\pm} = \omega_{\pm}\psi_{\pm} \tag{5.29}$$

where $\psi_{-} = |\mathrm{K}_S\rangle$ and $\psi_{+} = |\mathrm{K}_L\rangle$ are the eigenstates which are defined in equation (5.27). By taking $p = 1 + \epsilon$ and $q = -(1 - \epsilon)$ in (5.27) we have

$$\psi_{\pm} = (|p|^2 + |q|^2)^{-\frac{1}{2}} \begin{pmatrix} p \\ \pm q \end{pmatrix} \tag{5.30}$$

and corresponding eigenvalues are:

$$\omega_{\pm} = M_{11} - \mathrm{i}\Gamma_{11} \pm pq; \tag{5.31}$$

where p and q are two complex numbers given by

$$p^2 = M_{12} - \mathrm{i}\Gamma_{12}, \quad q^2 = M_{21} - \mathrm{i}\Gamma_{21} = M_{12}^{*} - \mathrm{i}\Gamma_{12}^{*}. \tag{5.32}$$

If at the $t = 0$ a K^0 particle is produced, i.e. we have in state $|\mathrm{K}^0\rangle = \binom{1}{0}$, then

$$\psi(t) = \frac{1}{2p}(|p|^2 + |q|^2)^{\frac{1}{2}}[\psi_{+}e^{-\frac{1}{2}\omega_{+}t} + \psi_{-}e^{-\frac{1}{2}\omega_{-}t}]. \tag{5.33}$$

We can write

$$\omega_{+} = \Gamma_S, \quad \text{and} \quad \omega_{-} = \Gamma_L + 2\mathrm{i}\Delta m, \tag{5.34}$$

where Γ_S and Γ_L are the real numbers which are representing short and long lifetimes, respectively and Δm is the mass difference between these two eigenstates.

Now, the fractional number of kaon that decay at time t after production is given by

$$N(t)dt = -d[\psi^{\dagger}\psi]. \tag{5.35}$$

Using equation (5.19) one obtain

$$N(t) = -\frac{d}{dt}[\psi^{\dagger}\psi] = \psi^{\dagger}\Gamma\psi. \tag{5.36}$$

By using equation (5.30)-(5.33), the above equation becomes

$$\begin{aligned} N(t) \quad = \quad & \frac{1}{2}(1 + \mathcal{E})^{-1}\{\gamma_{+}e^{-\Gamma_S t} + \Gamma_L e^{-\Gamma_L t} + \mathcal{E}e^{-\frac{1}{2}(\Gamma_S + \Gamma_S)t} \\ & \times[(\Gamma_S + \Gamma_L)\cos\Delta m t - 2\Delta m \sin\Delta m t]\}, \end{aligned} \tag{5.37}$$

where

$$\mathcal{E} = \psi_+^\dagger \psi_- = \frac{|p|^2 - |q|^2}{|p|^2 + |q|^2}, \tag{5.38}$$

is a real number that represents the nonorthogonalities of these two eigenstates. The four real numbers $\Gamma_S, \Gamma_L, \Delta m, \mathcal{E}$ characterize the decay of the kaon and satisfy the inequalities [51]

$$\Gamma_{S,L} \geq 0, \quad |\mathcal{E}|^2 \leq \frac{4\Gamma_S\Gamma_L}{(\Gamma_S + \Gamma_L)^2 + 4(\Delta m)^2} \tag{5.39}$$

which follow from Γ is positive Hermitian matrix. The experimental values of Γ_S and Γ_L indicate that $\Gamma_L/\Gamma_S = 1.8 \times 10^{-3}$ then, $|\mathcal{E}|^2 < 4\Gamma_S/\Gamma_L < 7.2 \times 10^{-3}$.

Chapter 6

Two-level Friedrichs model and kaonic phenomenology

Abstract: In the present paper, we study in the framework of the Friedrichs model the evolution of a two-level system coupled to a continuum. This unitary evolution possesses a non-unitary component with a non-Hermitian effective Hamiltonian. We show that this model is well adapted in order to describe kaon phenomenology (oscillation, regeneration) and leads to a CP violation, although in this case the prediction is not quantitatively quite satisfying[1].

PACS number: 03.65.Ud, 03.67.Dd, 89.70.+c

[1]This paper was published in Physics Letters A, 2007, **362**, p. 100-104

6.1 Introduction

We shall show that the two-level Friedrichs system [48] makes it possible to describe a class of systems that exhibit rich and complex behaviors: oscillations, regenerations and so on, and provides a relatively exact phenomenological model of kaons physics. There have been several approaches to CP-violations in kaons using Gauge Theory [91] or Renormalization Theory [50]. We do not consider these aspects here, also because the question is still partially open today. Our treatment is based on the description of decaying systems similarly to the generalization of the Weisskopf-Wigner approach, formulated by Lee, Oehme and Yang (LOY) [51] in the case of kaonic decay. Later on, Chiu and Sudarshan [52] used a Lee model in order to obtain a correction to the LOY theory for short times (Zeno effect). Our new approach is based on the derivation of a master equation from a Hamiltonian description for K_1 and K_2 decaying modes weakly coupled to the decay product and not for $(\mathrm{K}^0, \overline{\mathrm{K}}^0)$ modes as done in LOY theory. In this letter, we use a simple version of the model with a constant factor form. This leads to a Markovian master equation which allows us to simulate the kaonic lifetimes as well as kaonic oscillations and regeneration. It even predicts a CP symmetry breaking. Unfortunately this last prediction is not very accurate quantitatively, which, in a sense, is not astonishing for such a simplified approach. In any case, our computations show that it is possible with a very simple model such as the two-level Friedrichs model to capture essential features of the very rich kaon phenomenology, and of their non-trivial temporal survival distributions.

In the second section, we recall the main features of kaon phenomenology. In the third section we show how to simulate them thanks to the Friedrichs model. We show that the fit with phenomenological data about CP violation is satisfying since we recover the experimental data for the phase, but not quantitatively (our estimation of the modulus effect is fourteen times too strong in comparison to experimental data). At the end of the paper, we make some remarks on an improvement of the model.

6.2 Main features of kaon phenomenology.

Kaons are bosons that were discovered in the forties during the study of cosmic rays. They are produced by collision processes in nuclear reactions during which the strong interactions dominate. They appear in pairs K^0, $\overline{\mathrm{K}}^0$ [53, 54]. It is possible to

produce preferentially the K^0 particle essentially due to the fact that the $\overline{K}^0$ kaon is less probable kinematically and that the threshold pion energy for its production is higher.

The K mesons are eigenstates of the parity operator P: $P|K^0\rangle = -|K^0\rangle$, and $P|\overline{K}^0\rangle = -|\overline{K}^0\rangle$. K^0 and $\overline{K}^0$ are charge conjugate to each other $C|K^0\rangle = |\overline{K}^0\rangle$, and $C|\overline{K}^0\rangle = |K^0\rangle$. We get thus

$$CP|K^0\rangle = -|\overline{K}^0\rangle, \qquad CP|\overline{K}^0\rangle = -|K^0\rangle. \tag{6.1}$$

Clearly $|K^0\rangle$ and $|\overline{K}^0\rangle$ are not CP-eigenstates, but the following combinations

$$|K_1\rangle = \frac{1}{\sqrt{2}}\big(|K^0\rangle + |\overline{K}^0\rangle\big), \qquad |K_2\rangle = \frac{1}{\sqrt{2}}\big(|K^0\rangle - |\overline{K}^0\rangle\big), \tag{6.2}$$

are CP-eigenstates.

$$CP|K_1\rangle = -|K_1\rangle, \qquad CP|K_2\rangle = +|K_2\rangle. \tag{6.3}$$

In the absence of matter, kaons disintegrate through weak interactions [54]. Actually, K^0 and $\overline{K}^0$ are distinguished by their mode of *production*, K_1 and K_2 are distinguished by their mode of *decay*. In first approximation we can neglect CP violation so that the weak Hamiltonian commutes with CP. In this regime, the weak disintegration process distinguishes the K_1 states which decay only into "2π" while the K_2 states decay into "$3\pi, \pi e\nu, ...$" [55]. The lifetime of the K_1 kaon is short ($\tau_S \approx 8.92 \times 10^{-11}$ s), while the lifetime of the K_2 kaon is quite longer ($\tau_L \approx 5.17 \times 10^{-8}$ s). The difference of mass of the 1 and 2 kaons is quite small in comparison to their mass ($\frac{m_L - m_S}{m_S + m_L} \approx 0.35 \times 10^{-14}$, with $(m_L - m_S)c^2 \approx 3.52 \times 10^{-6}$eV). The amplitude of the mode K_1 at time t can be written as

$$a_1(t) = a_1(0)e^{-\frac{iE_S}{\hbar}t}e^{-\frac{\Gamma_S}{2\hbar}t}, \tag{6.4}$$

where E_S is the total energy of particle and $\Gamma_S = \frac{\hbar}{\tau_S}$ is the width of the state. We can write the amplitude of the mode K_2 in a similar fashion for the long lifetime. The intensity is

$$\begin{aligned} I_1(t) &= a_1(t)a_1^*(t) = a_1(0)a_1^*(0)e^{-\frac{\Gamma_S}{\hbar}t} \\ &= I_1(0)e^{-\frac{t}{\tau_S}}. \end{aligned} \tag{6.5}$$

Setting $\hbar = c = 1$ and considering a situation during which kaons are at rest we get that τ_S is the proper lifetime and $E_S = m_S$, the rest mass of the K_1 particle. Its amplitude is then

$$a_1(t) = a_1(0)e^{-(im_S + \frac{\Gamma_S}{2})t}. \tag{6.6}$$

Similarly, for K_2,

$$a_2(t) = a_2(0)e^{-(\mathrm{i}m_L + \frac{\Gamma_L}{2})t}. \tag{6.7}$$

From equation (7.14) we can write [53] the corresponding amplitudes of K^0 and $\overline{K}^0$ as

$$a_0(t) = \frac{1}{\sqrt{2}}\big(a_1(t) + a_2(t)\big), \qquad \overline{a}_0(t) = \frac{1}{\sqrt{2}}\big(a_1(t) - a_2(t)\big) \tag{6.8}$$

and the intensities are equal to

$$I_0(t) = \frac{I_0(0)}{4}\big(e^{-\Gamma_S t} + e^{-\Gamma_L t} + 2e^{-\frac{\Gamma_S+\Gamma_L}{2}t}\cos(\triangle m t)\big) \tag{6.9}$$

and

$$\overline{I}_0(t) = \frac{\overline{I}_0(0)}{4}\big(e^{-\Gamma_S t} + e^{-\Gamma_L t} - 2e^{-\frac{\Gamma_S+\Gamma_L}{2}t}\cos(\triangle m t)\big). \tag{6.10}$$

Here $\triangle m = |m_L - m_S| = 3.52\times10^{-6}$ and $\triangle m \tau_S \approx 0.47$, so that K^0- and $\overline{K}^0-$intensities *oscillate* with the frequency $|\triangle m|$.

This corresponds to the process called kaonic *oscillation*. We can explain it intuitively as follows: in the vacuum the disintegration of kaons is due to weak interactions, and the weak Hamiltonian controls and dominates the evolution. Therefore, the eigenstates of the "free" (weak) Hamiltonian in vacuum are (in first approximation) the K_1 and K_2 kaons. In the presence of matter, strong interactions are present during the collisions between kaons and nuclei. They dominate the decay process and therefore K^0 and $\overline{K}^0$ kaons are observed, and it is also possible to distinguish them experimentally because they possess different disintegration channels. Because the preparation and measurement bases differ from the eigenbasis of the Hamiltonian that controls the free evolution, interference effects are likely to occur. This is the essence of kaonic oscillations. What is interesting is that if we compare their difference of mass (in convenient units) to the inverse of the lifetime of the K_1 kaon, we get a comparable result: $(m_L - m_S)\tau_S \approx 0,47$. Thanks to this relation and due to the fact that it was possible experimentally to carry out observations occurring during a time comparable to the lifetime of the K_1 kaon, which is relatively long in comparison to other elementary particles, it was possible to observe kaonic oscillations experimentally.

Generation and *regeneration* are similar phenomena. If we produce (in matter, in the strong regime) K^0 particles, no $\overline{K}^0$ particle is present, but if we wait (in absence of matter) during a time long relatively to τ_S the lifetime of the K_1 kaon, the K_2

particle only has survived and the probability to find a $\overline{\mathrm{K}}^0$ particle is 0.5, so that $\overline{\mathrm{K}}^0$ particles were *generated*.

Regeneration is due to the fact that in the presence of matter, the $\overline{\mathrm{K}}^0$ particle disintegrates more quickly than the K^0 one. Henceforth their respective amplitudes are not equal in modulus with as a consequence that $a_1(t) = \frac{1}{\sqrt{2}}(a_0(t) + \overline{a}_0(t))$ differs from zero. Consequently, even if we wait (in the absence of matter, in the weak regime) a time longer than the lifetime of the K_1 kaon, and that only the K_2 particle is present, the K_1 component is re-generated in the presence of matter.

CP-violation is another interesting feature of the kaons phenomenology. It was discovered by Christenson et al. [56]. CP violation means that the long-lived kaon can also decay to "2π" then, the CP symmetry is slightly violated (by a factor of 10^{-3}) by weak interactions so that the CP eigenstates K_1 and K_2 are not exact eigenstates of the decay interaction. Let us consider that $\mathrm{K}_S(S =$ short-lived) and $\mathrm{K}_L(L =$ long-lived) are the eigenstates of the decay interaction; they can be expressed as a superpositions of the K_1 and K_2 eigenstates. Then

$$\begin{aligned} |\mathrm{K}_L\rangle &= \frac{1}{\sqrt{1+|\epsilon|^2}}\big[\epsilon\ |\mathrm{K}_1\rangle + |\mathrm{K}_2\rangle\big] \\ &= \frac{1}{\sqrt{2(1+|\epsilon|^2)}}\big[(1+\epsilon)|\mathrm{K}^0\rangle - (1-\epsilon)|\overline{\mathrm{K}}^0\rangle\big], \end{aligned} \tag{6.11}$$

and

$$\begin{aligned} |\mathrm{K}_S\rangle &= \frac{1}{\sqrt{1+|\epsilon|^2}}\big[|\mathrm{K}_1\rangle + \epsilon\ |\mathrm{K}_2\rangle\big] \\ &= \frac{1}{\sqrt{2(1+|\epsilon|^2)}}\big[(1+\epsilon)|\mathrm{K}^0\rangle + (1-\epsilon)|\overline{\mathrm{K}}^0\rangle\big], \end{aligned} \tag{6.12}$$

where ϵ is a CP violation parameter, $|\epsilon| \ll 1$ where ϵ does not have to be real. K_L and K_S are the eigenstates of the Hamiltonian for the mass-decay matrix [54, 55], i.e.

$$H = M - \frac{\mathrm{i}}{2}\Gamma \equiv \begin{pmatrix} M_{11} - \frac{\mathrm{i}}{2}\Gamma_{11} & M_{12} - \frac{\mathrm{i}}{2}\Gamma_{12} \\ M_{21} - \frac{\mathrm{i}}{2}\Gamma_{21} & M_{22} - \frac{\mathrm{i}}{2}\Gamma_{22} \end{pmatrix} \tag{6.13}$$

where M and Γ are individually hermitian since they correspond to observable (mass and lifetime). The corresponding eigenvalues of the mass-decay matrix are equal to

$$m_L - \frac{\mathrm{i}}{2}\Gamma_L, \qquad m_S - \frac{\mathrm{i}}{2}\Gamma_S \tag{6.14}$$

The CP violation was established by the observation that K_L decays not only via three-pion, which has natural CP parity, but also via the two-pion mode with a $|\epsilon|$ of order 10^{-3}, which is truly unexpected. The experimental value of ϵ is

$$|\epsilon| = (2.27 \pm 0.02) \times 10^{-3}, \quad \arg(\epsilon) = 43.37 \tag{6.15}$$

6.3 Friedrichs's model and kaon phenomenology

6.3.1 The two-levels Friedrichs model

The Friedrichs interaction Hamiltonian between the two modes and the continuous degree of freedom is the following [48, 57, 58, 59]:

$$H_{\text{Friedrichs}} = \begin{pmatrix} \omega_1 & 0 & \lambda_1 \\ 0 & \omega_2 & \lambda_2 \\ \lambda_1 & \lambda_2 & \omega \end{pmatrix} \tag{6.16}$$

The masses $\omega_{1,2}$ represent the energies of the discrete levels, and the factors $\lambda_{1,2}$ represent the couplings to the continuum of decay product. In this model, the energies ω of the different modes of the continuum range from $-\infty$ to $+\infty$. The two-level Friedrichs model Schrödinger equation is

$$\begin{pmatrix} \omega_1 & 0 & \lambda_1 \\ 0 & \omega_2 & \lambda_2 \\ \lambda_1 & \lambda_2 & \omega \end{pmatrix} \begin{pmatrix} f_1(t) \\ f_2(t) \\ g(\omega, t) \end{pmatrix} = \mathrm{i}\frac{\partial}{\partial t} \begin{pmatrix} f_1(t) \\ f_2(t) \\ g(\omega, t) \end{pmatrix}. \tag{6.17}$$

which means:

$$\omega_1 f_1(t) + \lambda_1 \int_{-\infty}^{\infty} d\omega g(\omega, t) = \mathrm{i}\frac{\partial f_1(t)}{\partial t}, \tag{6.18}$$

$$\omega_2 f_2(t) + \lambda_2 \int_{-\infty}^{\infty} d\omega g(\omega, t) = \mathrm{i}\frac{\partial f_2(t)}{\partial t}, \tag{6.19}$$

and

$$\lambda_1 f_1(t) + \lambda_2 f_2(t) + \omega g(\omega, t) = \mathrm{i}\frac{\partial g(\omega, t)}{\partial t}. \tag{6.20}$$

ω is coupled here through uniform factor forms (λ_1, λ_2); this constitutes a very rough approximation which allows an integration of the equation of motion and an illustration of the application to CP violation in kaons. More physical cutoffs that can

improve our estimation will be studied in a future publication, as well as the analogy between our model and models used in quantum optics in order to simulate certain spontaneous radiative processes. Let us now solve the Schrödinger equation and trace out the continuum in order to derive the master equation for the two-level system. From the equation (6.20) we can obtain $g(\omega, t)$, taking $g(\omega, 0) = 0$, as

$$g(\omega, t) = -\mathrm{i}e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] e^{\mathrm{i}\omega\tau}, \tag{6.21}$$

where $t > 0$. Then, we substitute $g(\omega, t)$ in the equation (6.18) we obtain

$$\mathrm{i}\frac{\partial f_1(t)}{\partial t} = \omega_1 f_1(t) - \mathrm{i}\lambda_1 \int_{-\infty}^{\infty} d\omega e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] e^{\mathrm{i}\omega\tau}, \tag{6.22}$$

we also obtain the same relation for $f_2(t)$ from equation(6.19):

$$\mathrm{i}\frac{\partial f_2(t)}{\partial t} = \omega_2 f_2(t) - \mathrm{i}\lambda_2 \int_{-\infty}^{\infty} d\omega e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] e^{\mathrm{i}\omega\tau}, \tag{6.23}$$

6.3.2 The two-levels Friedrichs model and kaonic behavior

In this subsection, we shall make use of the Friedrichs model in order to simulate interesting properties of the kaonic systems. In order to do so, we shall identify the discrete modes of the Friedrichs model with the K_1 and K_2 states and ω_1 and ω_2 with their masses, respectively. This is our basic postulate according to which we can now make use of the Friedrichs model in order to establish a phenomenology for the kaonic behavior. More precisely, we shall assume that

$$|\mathrm{K}_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\mathrm{K}_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{6.24}$$

The continuum mode aims at representing the decay products as explained in Section 2. Let us consider the solution of two-level Friedrichs model Schrödinger equation (6.17). According to this equation, the state is at time t superposition of two components that correspond to the two (complex) eigenvalues of the effective Hamiltonian. In order to avoid confusion, we shall use different parameters when we deal with the "real" kaons that are associated with experimental data and when we deal with the "theoretic" ones in the framework of the Friedrichs model.

It is worth noting that the use of simple two-level models to explain kaon oscillations goes back to Gell-Man and Pais (see Feynman lectures vol III, p.11-16). What is new in our paper is that we introduce a continuous degree of freedom (a scalar field) in a simple and exactly solvable model to describe kaon decay, in which $|\mathrm{K}_1\rangle$ and $|\mathrm{K}_2\rangle$ particles communicate via the decay channel (and not $|\mathrm{K}^0\rangle$ and $|\overline{\mathrm{K}}^0\rangle$ as in the LOY theory).

-The masses m_S and m_L and the lifetimes τ_S and τ_L will remain attributed to the real objects.

-The parameters ω_1, ω_2, λ_1, λ_2, ω_+ and ω_- will refer to the theoretic quantities.

To solve equations (6.22) and (6.23) we shall compute the integral part of equation (6.22) f_1 and f_2 being supposed integrable functions on $[0, \infty[$. We consider a test function as $e^{-\alpha^2\omega^2}$, then we can rewrite it as follows

$$\int_0^t d\tau(\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)) \int_{-\infty}^{\infty} d\omega e^{-\mathrm{i}\omega(t-\tau)} e^{-\alpha^2\omega^2}, \tag{6.25}$$

with the limit $\alpha \to 0$. After integration on ω of in the above equation we obtain

$$\frac{\sqrt{\pi}}{\alpha} \int_0^t d\tau[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)] e^{-\frac{(t-\tau)^2}{4\alpha^2}} \tag{6.26}$$

or

$$\frac{\sqrt{\pi}}{\alpha}[\lambda_1 f_1(t) + \lambda_2 f_2(t)] * e^{-\frac{t^2}{4\alpha^2}} \tag{6.27}$$

where we used the convolution definition, i.e.

$$\int_0^t k(t-u)y(u)du = k(t) * y(t). \tag{6.28}$$

Laplace transformation of the equation (6.27) yields,

$$\pi[\lambda_1 F_1(s) + \lambda_2 F_2(s)]\ e^{\alpha^2 s^2} \mathrm{Erfc}(\alpha s), \tag{6.29}$$

where

$$\mathrm{Erfc}(x) = 1 - \mathrm{Erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy. \tag{6.30}$$

Taking the limit $\alpha \to 0$ we obtain

$$\pi[\lambda_1 F_1(s) + \lambda_2 F_2(s)], \tag{6.31}$$

and taking and the inverse Laplace transformation yields $\pi[\lambda_1 f_1(t) + \lambda_2 f_2(t)]$. So we proved

$$\int_{-\infty}^{\infty} d\omega e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] e^{\mathrm{i}\omega\tau} = \pi[\lambda_1 f_1(t) + \lambda_2 f_2(t)]. \tag{6.32}$$

Now, we substitute the above result in the equations (6.22) and (6.23). Thus, we obtain

$$\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} = \begin{pmatrix} \omega_1 - \mathrm{i}\pi\lambda_1^2 & -\mathrm{i}\pi\lambda_1\lambda_2 \\ -\mathrm{i}\pi\lambda_1\lambda_2 & \omega_2 - \mathrm{i}\pi\lambda_2^2 \end{pmatrix}\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix}. \tag{6.33}$$

Thus, we obtain an effective non-Hermitian Hamiltonian evolution, $H_{eff} = M - \mathrm{i}\frac{\Gamma}{2}$. The eigenvalues of the system are

$$\begin{aligned} \omega_\pm \;=\; & \frac{1}{2}\Big\{(\omega_1+\omega_2) - \mathrm{i}\pi(\lambda_1^2+\lambda_2^2) \pm \Big[\big((\omega_1+\omega_2) - \mathrm{i}\pi(\lambda_1^2+\lambda_2^2)\big)^2 \\ & -4(\omega_1\omega_2 - \mathrm{i}\pi(\lambda_1^2\omega_2 + \lambda_2^2\omega_1))\Big]^{\frac{1}{2}}\Big\}, \end{aligned} \tag{6.34}$$

and under the weak coupling constant approximation, they become :

$$\omega_+ = \omega_1 - \mathrm{i}\pi\lambda_1^2 + O(\lambda^4), \quad \omega_- = \omega_2 - \mathrm{i}\pi\lambda_2^2 + O(\lambda^4), \tag{6.35}$$

In a first and very rough approximation, the eigenvectors of the effective Hamiltonian are the same as the postulated kaons states.

$$|f_+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |K_1\rangle \quad \text{and} \quad |f_-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |K_2\rangle, \tag{6.36}$$

and the solutions of Schrödinger equations are superpositions of these two states with amplitudes

$$f_1(t) = e^{-\mathrm{i}\omega_+ t}, \quad f_2(t) = e^{-\mathrm{i}\omega_- t}. \tag{6.37}$$

Phenomenology imposes that the complex Friedrichs energies $\omega_\pm$ coincide with the observed complex energies. The Friedrichs energies depend on the choice of the four parameters ω_1, ω_2, λ_1 and λ_2 and the observed complex energies are directly derived from the experimental determination of four other parameters, the masses m_S and m_L and the lifetimes τ_S and τ_L. We must thus adjust the theoretical parameters in order that they fit the experimental data. This can be done by comparing the normalized

intensities $\frac{4I_0(t)}{I_0(0)}$ and $\frac{4\bar{I}_0(t)}{\bar{I}_0(0)}$ of equations (6.9) and (6.10) with the theoretical prediction for the K^0 and $\overline{\mathrm{K}}^0$ intensities:

$$|f_1(t) \pm f_2(t)|^2 = (e^{-2\pi\lambda_1^2 t} + e^{-2\pi\lambda_2^2 t} \pm 2e^{-\pi(\lambda_1^2+\lambda_2^2)t}\cos(\triangle\omega t)), \tag{6.38}$$

where $\triangle\omega = |\omega_1 - \omega_2|$. From this comparison of experimental and theoretical results we obtain (see equations (6.9) and (6.10)).

$$\begin{aligned} \omega_1 &= m_S, \quad 2\pi\lambda_1^2 = \Gamma_S, \\ \omega_2 &= m_L, \quad 2\pi\lambda_2^2 = \Gamma_L. \end{aligned} \tag{6.39}$$

CP **violation:** Let us study in this case the CP violation. The Friedrichs model allows us to estimate the value of ϵ. For this purpose, the effective Hamiltonian (equation (6.33)) acts on the $|\mathrm{K}_S\rangle$ vector states (equation (6.11)) as an eigenstate corresponding to the eigenvalue $\omega_+ = \omega_1 - \mathrm{i}\pi\lambda_1^2 = m_S - \mathrm{i}\frac{\Gamma_S}{2}$, so that we must impose that $H_{\text{eff}}\binom{1}{\epsilon} = \omega_-\binom{1}{\epsilon}$, from which we obtain after straightforward calculations that

$$\epsilon = \frac{\mathrm{i}\pi\lambda_1\lambda_2}{(\omega_2 - \omega_1) - \mathrm{i}\pi(\lambda_2^2 - \lambda_1^2)} \tag{6.40}$$

and if we replace λ's and ω's by corresponding values in equation (6.39) we have,

$$\epsilon = \frac{\frac{\mathrm{i}}{2}\sqrt{\Gamma_L\Gamma_S}}{(m_L - m_S) - \frac{\mathrm{i}}{2}(\Gamma_L - \Gamma_S)}. \tag{6.41}$$

By using the above experimental values of Γ_L, Γ_S, m_L, m_S and the ratio $\frac{(m_L - m_S)}{-(\Gamma_L - \Gamma_S)} \approx \triangle m\tau_S \approx 0.47$ we obtain the following estimated value for ϵ:

$$\epsilon = \sqrt{(1.82 \times 10^{-3})/2}\ \ e^{\mathrm{i}(43.37)^\circ} \tag{6.42}$$

which shows that our estimation of the modulus of ϵ is ~ 14 times greater than its experimental modulous value while the estimated phase is correct.

Although this last prediction is not very accurate quantitatively, which in a sense is not astonishing for such a simplified approach, we think that a better fit is possible provided we finely tune the cut off between the discrete levels and the continuous modes, especially when negative energy modes are decoupled from the two-level system. In any case, our computations show that it is possible with a very simple model such as the two level Friedrichs model to capture essential features of the very rich kaon phenomenology, and of their non-trivial temporal survival distributions.

6.4 Conclusions.

We have shown that the framework of the Friedrichs model is relevant in order to grasp , despite of its simplicity, essential features of kaons decay. This model allows us to describe complex temporal evolutions (such as kaonic oscillations, generation and regeneration) and to simulate at least qualitatively CP violation. We also recover the experimental value of the phase, 43.37^o, as a result of the equations (6.41)-(6.42).

We have to notice that ever since LOY paper, new problems and effects have been studied in CP violation among then we notice the paper of L.A. Khalfin [60] which could not be considered in the scope of this letter.

It is also out of the scope of the present paper but it would be very interesting to study the properties of the Friedrichs model and of kaonic oscillations in terms of the Time Operator approach. This can be done for the one-level Friedrichs model [61, 62] but higher level systems present more subtle and involved temporal behavior [63] so that it is worth studying the Time-Operator in this context.

One should consider situations during which the spectrum of the continuous degree of freedom is cut off, because an unbounded spectrum in energy is not very sound from a physical point of view. This will be studied in a future publication as well as the analogy between our model and models used in quantum optics in order to simulate certain spontaneous radiative processes.

Finally, it is worth comparing our results with those obtained in Refs.[64, 65] where it is shown that in the framework of the rigged Hilbert space approach another effect of CP violation is also predicted despite of the fact that the Hamiltonian respects the CP symmetry. In our case the Friedrichs Hamiltonian does not respect this symmetry, that is, if we consider all the degrees of freedom of the system, the commutator between the Hamiltonian and the CP operator is different from zero. The commutator is equal to zero when we consider the free Hamiltonian (corresponding to $\lambda_1 = \lambda_2 = 0$) . As we noted before, this result can be understood as follows: in our approach, the continuous degree of freedom mediates an effective weak-like interaction of order two in the coupling constants, which "explains" why the CP violation is small.

Chapter 7

Quantum-mechanical decay laws in the neutral kaons

Abstract: The Hamiltonian Friedrichs model [48] describing the evolution of a two-level system coupled to a continuum is used in order to model the decay of the kaon states K_1, K_2. Using different cut-off functions of the continuous degrees of freedom, we show that this model leads to a CP violation that qualitatively fits with experimental data improving previous numerical estimates. We also discuss the relation of our model to other models of open systems[1].

PACS number: 03.65.Ud, 03.67.Dd, 89.70.+c

[1]This paper published in Journal of Physics A : Math. Theor., 2007, **40**, p. 2773-2785

7.1 Introduction

There have been several theoretical approaches to CP violation in Kaons (see e.g, the collection of papers edited in [66]) and the question is partially open today. In this paper, we use a Hamiltonian model, describing a two-level states coupled to a continuum of degrees of freedom, that makes is possible to obtain the phenomenology of neutral kaons and provides new numerical estimate of the parameters of CP violation. Solving the Schrödinger equation for the Hamiltonian, we derive a master equation for the decaying two-level states similarly to the generalization of the Weisskopf-Wigner approach formulated by Lee, Oehme and Yang [51](LOY) in the case of kaonic decay. Later on, Chiu and Sudarshan [52] used a Lee model in order to obtain a correction to the LOY theory for short times, departing from the exponential decay. Their Hamiltonian describes $(\mathrm{K}^0, \overline{\mathrm{K}}^0)$ modes as done in the LOY theory. In this paper the authors point out to a numerical Khalfin estimate of the CP violation parameter $\epsilon \sim 0.06 \times e^{\mathrm{i}\pi/4}$. That is 30 times the experimental data. Our new approach is based on the derivation of a master equation from a Hamiltonian describing $(\mathrm{K}_1, \mathrm{K}_2)$ decaying modes and not for $(\mathrm{K}^0, \overline{\mathrm{K}}^0)$ modes as done in LOY theory. Under weak coupling hypothesis this leads to a Markovian master equation which allows us to simulate the kaonic lifetimes as well as kaonic oscillations and regeneration. It even fits closer the CP symmetry breaking parameter. Unfortunately this last prediction is not very quite accurate quantitatively, which, in a sense, is not astonishing for such a simplified approach. In a first example with non-bounded spectrum in energy, we obtain the exact angle while the modulus is 14 times the experimental data. However, we show that using different cut-off functions of the continuous degrees of freedom we can improve the above estimate.

We prove that it is possible to obtain all the interesting features of the model when the Hamiltonian possesses a spectrum only bounded from below. In this case, with Gaussian cut-off the previous estimate is improved and we obtain a CP violation parameter value only 3 times the experimental data. Our treatment confirms that it is possible with a very simple model such as the two-level Friedrichs model to compute some essential features of the very rich kaon phenomenology. It also confirms that the essential ingredient for deriving an irreversible in time dynamics of subsystems is the presence of a continuous degrees of freedom of environment.

In general, Quantum Mechanics provides a continuous, reversible in time and unitary evolution law (via the Schrödinger equation). This description contradicts our

everyday experience in which ageing, dissipation and irreversibility are omnipresent. In this context, it is interesting to study hybrid quantum systems, sufficiently complex, that exhibit altogether unitary and dissipative in time evolutions. This goal can be achieved in the framework of the Friedrichs model.

One-level Friedrichs model is well understood [57, 58, 59]: it predicts that the excited state disappears and "fuses" into the continuum. Its survival probability decays exponentially in time. The lifetime is proportional to the coupling between the discrete mode and the continuum. Exponentially decaying systems are very common in classical and quantum physics. They are relatively trivial when we consider them from the point of view of temporal irreversibility because, although the decay law is not reversible in time, such systems behave as if they did not possess an internal clock or memory: the decay rate is constant throughout time, and the non-decayed system is in the same state at all times. Roughly speaking, exponentially decaying systems exhibit an irreversible behavior but ignore ageing.

The two-level Friedrichs system makes it possible to describe a class of systems that exhibit richer behaviors: oscillations, regenerations and so on. If we accept a general definition [67, 63] according to which each departure from the pure exponential decay law can be labeled as a Zeno behavior (or anti-Zeno, depending of the sign of the departure), then, as we shall show the two-level Friedrichs model is rich enough in order to describe Zeno and anti-Zeno behaviors (for N-levels generalizations see[63]), and provides a relatively exact phenomenological model of kaons physics.

In the second section we define the two-level Friedrichs model. In the third section, we recall the main features of kaon phenomenology. In the fourth section we show how to simulate them thanks to the Friedrichs model when (a) the spectrum of the continuous mode is unbounded, in the presence of a Gaussian cut-off and (b) in the presence of a Gaussian cut-off when negative energy levels of the continuum are decoupled from the two-level system.

In the fifth section, we compare our approach with other recent approaches [68]-[75] where an open system interacts with its environment having a Lindblad form of evolution and we also discuss the question of decoherence.

7.2 The two-level Friedrichs model.

The Friedrichs interaction Hamiltonian between the two discrete modes and the continuous degree of freedom is given by the operator H on the Hilbert space of the wave functions of the form $\mid \psi >= \{f_1, f_2, g(\omega, t)\}, f_1, f_2 \in \mathbb{C}, g \in L^2(\mathbb{R}^+)$

$$H = H_0 + \lambda_1 V_1 + \lambda_2 V_2, \tag{7.1}$$

where λ_1 and λ_2 are the positive coupling constants, and

$$H_0 \mid \psi >= \{\omega_1 f_1, \omega_2 f_2, \omega g(\omega, t)\}, (\omega_1 \text{ and } \omega_2 > 0). \tag{7.2}$$

The operators V_i $(i = 1, 2)$ are given by:

$$\begin{aligned} V_1\{f_1, f_2, g(\omega, t)\} &= \{< v(\omega), g(\omega, t) >, 0, f_1.v(\omega)\} \\ V_2\{f_1, f_2, g(\omega, t)\} &= \{0, < v(\omega), g(\omega, t) >, f_2.v(\omega)\} \end{aligned} \tag{7.3}$$

where

$$< v(\omega), g(\omega, t) >= \int d\omega v^*(\omega) g(\omega, t), \tag{7.4}$$

is the inner product. Thus H can be represented as a matrix :

$$H_{\text{Friedrichs}} = \begin{pmatrix} \omega_1 & 0 & \lambda_1 v^*(\omega) \\ 0 & \omega_2 & \lambda_2 v^*(\omega) \\ \lambda_1 v(\omega) & \lambda_2 v(\omega) & \omega \end{pmatrix} \tag{7.5}$$

$\omega_{1,2}$ represent the energies of the discrete levels, and the factors $\lambda_i v(\omega)$ $(i = 1, 2)$ represent the couplings to the continuous degree of freedom. The energies ω of the different modes of the continuum range from $-\infty$ to $+\infty$ when $v(\omega) = 1$, but we are free to tune the coupling $v(\omega)$ in order to introduce a selective cut off to extreme energy modes. Let us now solve the Schrödinger equation and trace out the continuum in order to derive the master equation for the two-level system. The two-level Friedrichs model Schrödinger equation with $\hbar = 1$ is formally written as

$$\begin{pmatrix} \omega_1 & 0 & \lambda_1 v^*(\omega) \\ 0 & \omega_2 & \lambda_2 v^*(\omega) \\ \lambda_1 v(\omega) & \lambda_2 v(\omega) & \omega \end{pmatrix} \begin{pmatrix} f_1(t) \\ f_2(t) \\ g(\omega, t) \end{pmatrix} = \mathrm{i}\frac{\partial}{\partial t} \begin{pmatrix} f_1(t) \\ f_2(t) \\ g(\omega, t) \end{pmatrix}. \tag{7.6}$$

Easily, we obtain

$$\omega_1 f_1(t) + \lambda_1 \int d\omega v^*(\omega) g(\omega, t) = \mathrm{i}\frac{\partial f_1(t)}{\partial t}, \tag{7.7}$$

$$\omega_2 f_2(t) + \lambda_2 \int d\omega v^*(\omega) g(\omega, t) = \mathrm{i}\frac{\partial f_2(t)}{\partial t}, \tag{7.8}$$

and

$$\lambda_1 v(\omega) f_1(t) + \lambda_2 v(\omega) f_2(t) + \omega g(\omega, t) = \mathrm{i}\frac{\partial g(\omega, t)}{\partial t}. \tag{7.9}$$

integrating the last equation we obtain $g(\omega, t)$ assuming $g(\omega, t = 0) = 0$:

$$g(\omega, t) = -\mathrm{i}e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] v(\omega) e^{\mathrm{i}\omega\tau}, \tag{7.10}$$

then, we substitute $g(\omega, t)$ in the above equation (7.7) we obtain

$$\mathrm{i}\frac{\partial f_1(t)}{\partial t} = \omega_1 f_1(t) - \mathrm{i}\lambda_1 \int d\omega |v(\omega)|^2 e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] e^{\mathrm{i}\omega\tau}, \tag{7.11}$$

we also obtain the same relation for $f_2(t)$ as:

$$\mathrm{i}\frac{\partial f_2(t)}{\partial t} = \omega_2 f_2(t) - \mathrm{i}\lambda_2 \int d\omega |v(\omega)|^2 e^{-\mathrm{i}\omega t} \int_0^t d\tau \big[\lambda_1 f_1(\tau) + \lambda_2 f_2(\tau)\big] e^{\mathrm{i}\omega\tau}. \tag{7.12}$$

In a next section, we shall make use of the Friedrichs model in order to simulate interesting properties of the kaonic systems. Before we do so, it is useful to recall certain of them.

7.3 Main features of kaon phenomenology.

Kaons are bosons that were discovered in the forties during the study of cosmic rays. They are produced by collision processes in nuclear reactions during which the strong interactions dominate. They appear [53, 54] in pairs K^0, $\overline{\mathrm{K}}^0$. It is possible to produce preferentially the K^0 particle essentially due to the fact that the $\overline{\mathrm{K}}^0$ kaon is less probable kinematically and that the threshold pion energy for its production is higher.

The K mesons are eigenstates of the parity operator P: $P|\mathrm{K}^0\rangle = -|\mathrm{K}^0\rangle$, and $P|\overline{\mathrm{K}}^0\rangle = -|\overline{\mathrm{K}}^0\rangle$. K^0 and $\overline{\mathrm{K}}^0$ are charge conjugate to each other $C|\mathrm{K}^0\rangle = |\overline{\mathrm{K}}^0\rangle$, and $C|\overline{\mathrm{K}}^0\rangle = |\mathrm{K}^0\rangle$. We get thus

$$CP|\mathrm{K}^0\rangle = -|\overline{\mathrm{K}}^0\rangle, \qquad CP|\overline{\mathrm{K}}^0\rangle = -|\mathrm{K}^0\rangle. \tag{7.13}$$

Clearly $|\mathrm{K}^0\rangle$ and $|\overline{\mathrm{K}}^0\rangle$ are not CP-eigenstates, but the following combinations

$$|\mathrm{K}_1\rangle = \frac{1}{\sqrt{2}}\big(|\mathrm{K}^0\rangle + |\overline{\mathrm{K}}^0\rangle\big), \qquad |\mathrm{K}_2\rangle = \frac{1}{\sqrt{2}}\big(|\mathrm{K}^0\rangle - |\overline{\mathrm{K}}^0\rangle\big), \tag{7.14}$$

are CP-eigenstates.

$$CP|\mathrm{K}_1\rangle = -|\mathrm{K}_1\rangle, \qquad CP|\mathrm{K}_2\rangle = +|\mathrm{K}_2\rangle. \tag{7.15}$$

In the absence of matter, kaons disintegrate through weak interactions. Actually, K^0 and $\overline{\mathrm{K}}^0$ are distinguished by their mode of *production*, K_1 and K_2 are distinguished by their mode of *decay* [53]. In first approximation we can neglect CP violation so that the weak Hamiltonian commutes with CP. In this regime, the weak disintegration process distinguishes the K_1 and the K_2 states. The lifetime of the K_1 kaon is short ($\tau_S = \frac{1}{\Gamma_S} \approx 8.92 \times 10^{-11}$ s), while the lifetime of the K_2 kaon is quite longer ($\tau_L \approx 5.17 \times 10^{-8}$ s). The difference of mass of the 1 and 2 kaons is quite small in comparison to their mass ($\frac{m_L - m_S}{m_S + m_L} \approx 0.35 \times 10^{-14}$, with $(m_L - m_S)c^2 \approx 3.52 \times 10^{-6}$eV). The amplitudes of state K_1 at time t can be written as

$$a_1(t) = a_1(0)e^{-\frac{\mathrm{i}E_S}{\hbar}t}e^{-\frac{\Gamma_S}{2\hbar}t}, \tag{7.16}$$

where E_S is the total energy of particle; so $\omega_S = \frac{E_S}{\hbar}$ is the angular frequency, and $\Gamma_S = \frac{\hbar}{\tau_S}$ is the width of the state. We can write the amplitude of state K_2 in a similar fashion for the long lifetime. The intensity is

$$\begin{aligned} I_1(t) &= a_1(t)a_1^*(t) = a_1(0)a_1^*(0)e^{-\frac{\Gamma_S}{\hbar}t} \\ &= I_1(0)e^{-\frac{t}{\tau_S}}. \end{aligned} \tag{7.17}$$

Setting $\hbar = c = 1$ and considering a situation during which kaons are at rest we get that τ_S is the proper lifetime and $E_S = m_S$, the rest mass of the K_1 particle. Its amplitude is then

$$a_1(t) = a_1(0)e^{-(\mathrm{i}m_S + \frac{\Gamma_S}{2})t}. \tag{7.18}$$

Similarly, for K_2,

$$a_2(t) = a_2(0)e^{-(\mathrm{i}m_L + \frac{\Gamma_L}{2})t}. \tag{7.19}$$

From equation (7.14) we can write [53] the corresponding amplitudes of K_0 and $\overline{\mathrm{K}}_0$ as

$$a_0(t) = \frac{1}{\sqrt{2}}\big(a_1(t) + a_2(t)\big), \qquad \overline{a}_0(t) = \frac{1}{\sqrt{2}}\big(a_1(t) - a_2(t)\big) \tag{7.20}$$

and the intensities are equal to

$$I_0(t) = \frac{I_0(0)}{4}\big(e^{-\Gamma_S t} + e^{-\Gamma_L t} + 2e^{-\frac{\Gamma_S+\Gamma_L}{2}t}\cos(\triangle m t)\big) \tag{7.21}$$

and

$$\overline{I}_0(t) = \frac{\overline{I}_0(0)}{4}\big(e^{-\Gamma_S t} + e^{-\Gamma_L t} - 2e^{-\frac{\Gamma_S+\Gamma_L}{2}t}\cos(\triangle m t)\big). \tag{7.22}$$

Here $\triangle m = |m_L - m_S| \approx 3.52\times10^{-6}$ and $\triangle m \tau_S \approx 0.47$, so that K^0- and $\overline{\mathrm{K}}^0-$intensities *oscillate* with the frequency $|\triangle m|$.

This corresponds to the process called strangeness oscillation. We can explain it intuitively as follows: in the vacuum the disintegration of kaons is due to weak interactions, and the weak Hamiltonian controls and dominates the evolution. Therefore, the eigenstates of the "free" (weak) Hamiltonian in vacuum are (in first approximation) the K_1 and K_2 kaons. In the presence of matter, strong interactions are present during the collisions between kaons and nuclei. They dominate the decay process and therefore K^0 and $\overline{\mathrm{K}}^0$ kaons are observed, and it is also possible to distinguish them experimentally because they possess different disintegration channels. This can be compared, if we develop the analogy with spin 1/2 systems, to situations in which the spin is measured along the Z direction while it undergoes a precession due to a magnetic field along the X direction between preparation and measurement. This is also analog to what occurs when polarized light propagates in birefringent supports[2]. Because the preparation and measurement bases differ from the eigenbasis of the Hamiltonian that controls the free evolution, interference effects are likely to occur. This is the essence of strangeness oscillations. What is interesting is that if we compare their difference of mass (in convenient units) to the inverse of the lifetime of the K_1 kaon, we get a comparable result: $(m_S - m_L)\tau_S \approx 0,47$. Thanks to this relation and due to the fact that it was possible experimentally to carry out observations during a time comparable to the lifetime of the K_1 kaon, which is relatively long in comparison to other elementary particles, it was possible to observe strangeness oscillations experimentally.

Generation and regeneration are similar phenomena. If we produce (in matter, in the strong regime) K^0 particles, no $\overline{\mathrm{K}}^0$ particle is present, but if we wait (in absence of matter) during a time long relatively to τ_S the lifetime of the K_1 kaon, the K_2 particle only has survived and the probability to find a $\overline{\mathrm{K}}^0$ particle is 0.5, so that $\overline{\mathrm{K}}^0$ particles were *generated*.

[2]This analogy is carefully developed in ref.[68]

Regeneration is due to the fact that in the presence of matter, the $\overline{\mathrm{K}}^0$ particle disintegrates more quickly than the K^0 one. Henceforth their respective amplitudes are not equal in modulus with as a consequence that $a_1(t) = \frac{1}{\sqrt{2}}(a_0(t) + \overline{a}_0(t))$ differs from zero. Consequently, even if we wait (in the absence of matter, in the weak regime) a time longer than the lifetime of the K_1 kaon, and that only the K_2 particle is present, the K_1 component is re-generated in the presence of matter.

CP violation is another interesting feature of the kaons phenomenology. It was discovered by Christenson et al. [56]. CP violation means that CP symmetry is slightly violated (by a factor of 10^{-3}) by weak interactions so that the CP eigenstates K_1 and K_2 are not exact eigenstates of the decay interaction. Let us consider that $\mathrm{K}_S(S = \text{short-lived })$ and $\mathrm{K}_L(L = \text{long-lived })$ are the eigenstates of the decay interaction; they can be expressed as a superpositions of the K_1 and K_2 eigenstates. Then

$$\begin{aligned} |\mathrm{K}_L\rangle &= \frac{1}{\sqrt{1+|\epsilon|^2}}\big[\epsilon\ |\mathrm{K}_1\rangle + |\mathrm{K}_2\rangle\big] \\ &= \frac{1}{\sqrt{2(1+|\epsilon|^2)}}\big[(1+\epsilon)|\mathrm{K}^0\rangle - (1-\epsilon)|\overline{\mathrm{K}}^0\rangle\big], \end{aligned} \tag{7.23}$$

and

$$\begin{aligned} |\mathrm{K}_S\rangle &= \frac{1}{\sqrt{1+|\epsilon|^2}}\big[|\mathrm{K}_1\rangle + \epsilon\ |\mathrm{K}_2\rangle\big] \\ &= \frac{1}{\sqrt{2(1+|\epsilon|^2)}}\big[(1+\epsilon)|\mathrm{K}^0\rangle + (1-\epsilon)|\overline{\mathrm{K}}^0\rangle\big], \end{aligned} \tag{7.24}$$

where $|\epsilon| \ll 1$ and ϵ does not have to be real. K_L and K_S are the eigenstates of the Hamiltonian for mass-decay matrix [53, 54], i.e.

$$H = M - \frac{\mathrm{i}}{2}\Gamma \equiv \begin{pmatrix} M_{11} - \frac{\mathrm{i}}{2}\Gamma_{11} & M_{12} - \frac{\mathrm{i}}{2}\Gamma_{12} \\ M_{21} - \frac{\mathrm{i}}{2}\Gamma_{21} & M_{22} - \frac{\mathrm{i}}{2}\Gamma_{22} \end{pmatrix} \tag{7.25}$$

where M and Γ are individually Hermitian since they correspond to observables (mass and lifetime). The corresponding eigenvalues of the mass-decay matrix are equal to

$$m_L - \frac{\mathrm{i}}{2}\Gamma_L, \qquad m_S - \frac{\mathrm{i}}{2}\Gamma_S \tag{7.26}$$

The CP violation was established by the observation that K_L decays not only via three-pion, which has natural CP parity, but also via the two-pion mode with a $|\epsilon|$ of order 10^{-3}, which is truly unexpected. The experimental value of ϵ is [76]:

$$|\epsilon| = (28.1 \pm 4.1) \times 10^{-4}, \quad \arg(\epsilon) = 43.37 \tag{7.27}$$

7.4 Friedrichs's model and kaon phenomenology.

In what follows, we shall identify the discrete modes of the Friedrichs model with the K_1 and K_2 states. This is our basic postulate according to which we can now make use of the Friedrichs model in order to establish a phenomenology for the kaonic behavior. More precisely, we shall assume that

$$|K_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |K_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{7.28}$$

Let us consider the solution of the two-level Friedrichs model Schrödinger equation (7.6). According to this equation, the state is at time t superposition of two components that correspond to the two (complex) eigenvalues of the effective Hamiltonian. In order to avoid confusion, we shall use different parameters when we deal with the "real" kaons that are associated with experimental data and when we deal with the "theoretic" ones in the framework of the Friedrichs model.

-The masses m_S and m_L and the lifetime τ_S and τ_S will remain attributed to the real objects.

-The parameters ω_1, ω_2, λ_1, λ_2, ω_+ and ω_- will refer to the theoretic quantities.

7.4.1 Solutions for $v(\omega) = e^{-\alpha\omega^2/2}, \alpha > 0, \alpha \to 0$

Case $\omega \in]-\infty, +\infty[$

If we substitute $v(\omega) = e^{-\alpha\omega^2/2}$ in the equations (7.11) and integrate from $-\infty$ to ∞ we obtain

$$\mathrm{i}\frac{\partial f_1(t)}{\partial t} = \omega_1 f_1(t) - \mathrm{i}\lambda_1\sqrt{\frac{\pi}{\alpha}}[\lambda_1 f_1(t) + \lambda_2 f_2(t)] * e^{-\frac{t^2}{4\alpha}}, \tag{7.29}$$

where we used the convolution relation, i.e.

$$\begin{aligned} \frac{\partial y(t)}{\partial t} &= f(t) + \int_0^t k(t-u)y(u)du \\ &= f(t) + k(t) * y(t). \end{aligned} \tag{7.30}$$

Then the Laplace transformation of the above equation is

$$sY(s) - y(0) = F(s) + K(s)Y(s). \tag{7.31}$$

Thus we write the Laplace transformation of the equation (7.29) as

$$\mathrm{i}(sF_1(s) - f_1(0)) = \omega_1 F_1(s) - \mathrm{i}\pi\lambda_1[\lambda_1 F_1(s) + \lambda_2 F_2(s)]\; e^{\alpha s^2}\mathrm{Erfc}(\sqrt{\alpha}\; s), \tag{7.32}$$

where

$$\mathrm{Erfc}(x) = 1 - \mathrm{Erf}(x) = 1 - \frac{2}{\sqrt{\pi}}\int_0^x e^{-y^2}dy. \tag{7.33}$$

Expanding Erfc and exponential functions (this corresponds to the Markovian or Wigner-Weisskopf regime) we obtain

$$\mathrm{i}(sF_1(s) - f_1(0)) = \omega_1 F_1(s) - \mathrm{i}\pi\lambda_1[\lambda_1 F_1(s) + \lambda_2 F_2(s)](1 - 2\sqrt{\frac{\alpha}{\pi}}\; s) + O(\alpha). \tag{7.34}$$

Now, the inverse Laplace transformation yields,

$$\mathrm{i}(1 - 2\sqrt{\pi\alpha}\lambda_1^2)\frac{\partial f_1(t)}{\partial t} = \omega_1 f_1(t) - \mathrm{i}\pi\lambda_1[\lambda_1 f_1(t) + \lambda_2 f_2(t)] + 2\mathrm{i}\lambda_1\lambda_2\sqrt{\pi\alpha}\frac{\partial f_2(t)}{\partial t}. \tag{7.35}$$

We can obtain the same relation for f_2. Then we can easily obtain

$$\begin{aligned}
&\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} \\
&= \begin{pmatrix} \frac{\omega_1 - \mathrm{i}\pi\lambda_1^2}{1-2\sqrt{\pi\alpha}\lambda_1^2} & \lambda_1\lambda_2(-\frac{\mathrm{i}\pi}{(1-2\sqrt{\pi\alpha}\lambda_1^2)} + \frac{2\sqrt{\pi\alpha}\omega_2}{1-2\sqrt{\pi\alpha}(\lambda_1^2+\lambda_2^2)}) \\ \lambda_1\lambda_2(-\frac{\mathrm{i}\pi}{(1-2\sqrt{\pi\alpha}\lambda_2^2)} + \frac{2\sqrt{\pi\alpha}\omega_1}{1-2\sqrt{\pi\alpha}(\lambda_1^2+\lambda_2^2)} & \frac{\omega_2 - \mathrm{i}\pi\lambda_2^2}{1-2\sqrt{\pi\alpha}\lambda_2^2}) \end{pmatrix} \\
&\times \begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix},
\end{aligned} \tag{7.36}$$

in which we neglect the $O(\lambda^4)$ contributions. The eigenvalues of the above effective Hamiltonian, here denoted H_{eff}, are

$$\omega_+ = \frac{\omega_1 - \mathrm{i}\pi\lambda_1^2}{1 - 2\sqrt{\pi\alpha}\lambda_1^2} + O(\lambda^4) \approx (\omega_1 - \mathrm{i}\pi\lambda_1^2)(1 + 2\sqrt{\pi\alpha}\lambda_1^2 + ...) \approx (1 + 2\sqrt{\pi\alpha}\lambda_1^2)\omega_1 - \mathrm{i}\pi\lambda_1^2, \tag{7.37}$$

and

$$\omega_- \approx (1 + 2\sqrt{\pi\alpha}\lambda_2^2)\omega_2 - \mathrm{i}\pi\lambda_2^2. \tag{7.38}$$

In this approximation the eigenvectors of the effective Hamiltonian are obtained as follows,

$$|f_+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |f_-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{7.39}$$

Comparing the eigenvalues in equations (7.37) and (7.38) with the equations in (7.26) we obtain

$$\begin{aligned} 2\pi\lambda_1^2 = \Gamma_S, \quad \omega_1 &= \frac{m_S}{1+2\sqrt{\pi\alpha}\,\Gamma_S} \approx m_S(1-2\sqrt{\pi\alpha}\,\Gamma_S), \\ 2\pi\lambda_2^2 = \Gamma_L, \quad \omega_2 &= \frac{m_L}{1+2\sqrt{\pi\alpha}\,\Gamma_L} \approx m_L(1-2\sqrt{\pi\alpha}\,\Gamma_L). \end{aligned} \tag{7.40}$$

CP **violation:** Let us study in this case the CP violation. The Friedrichs model allows us to estimate the value of ϵ. If the effective Hamiltonian (equation (7.36)) acts on $|\mathrm{K}_L\rangle$ vector states (equation (7.23)) as an eigenstate corresponding to the eigenvalue $\omega_- = (1+2\sqrt{\pi\alpha}\lambda_2^2)\omega_2 - \mathrm{i}\pi\lambda_2^2$ we must impose (as the sign of ϵ is arbitrary), that $H_{\text{eff}}\binom{-\epsilon}{1} = \omega_-\binom{-\epsilon}{1}$, from which we obtain straightforwardly that, at the dominating order,

$$\epsilon = \frac{-\lambda_1\lambda_2(-\frac{\mathrm{i}\pi}{(1-2\sqrt{\pi\alpha}\lambda_1^2)} + \frac{2\sqrt{\pi\alpha}\omega_2}{1-2\sqrt{\pi\alpha}(\lambda_1^2+\lambda_2^2)})}{[(1+2\sqrt{\pi\alpha}\lambda_2^2)\omega_2 - \mathrm{i}\pi\lambda_2^2] - [(1+2\sqrt{\pi\alpha}\lambda_1^2)\omega_1 - \mathrm{i}\pi\lambda_1^2]}, \tag{7.41}$$

and if we expand and neglect the $O(\lambda^4)$ we obtain

$$\epsilon \approx \frac{-\lambda_1\lambda_2(-\mathrm{i}\pi + 2\sqrt{\pi\alpha}\;\omega_2)}{(1+2\sqrt{\pi\alpha}\lambda_1^2)\omega_2 - (1+2\sqrt{\pi\alpha}\lambda_2^2)\omega_1 - \mathrm{i}\pi(\lambda_2^2-\lambda_1^2)}. \tag{7.42}$$

If we replace λ's and ω's by their corresponding values from equation (7.40) we have,

$$\epsilon \approx \frac{\frac{\mathrm{i}}{2}\sqrt{\Gamma_L\Gamma_S}(1+2\mathrm{i}\sqrt{\frac{\alpha}{\pi}}m_S)}{(m_L-m_S) - \frac{\mathrm{i}}{2}(\Gamma_L-\Gamma_S)}, \tag{7.43}$$

In the zeroth approximation of α we obtain thus

$$\epsilon \approx \sqrt{(1.82\times 10^{-3})/2}\;\; e^{\mathrm{i}(43.37)^\circ} \tag{7.44}$$

which shows that our estimation of the modulus of ϵ is ~ 14 times greater than its experimental value while the estimated phase is correct. Now, in the case $\alpha \neq 0$, ϵ is given as

$$\epsilon \approx \sqrt{(1.82\times 10^{-3})/2}\;\; e^{\mathrm{i}(43.37)^\circ}(1+2\mathrm{i}\sqrt{\frac{\alpha}{\pi}}m_S) \tag{7.45}$$

we see that $\alpha > 0$ both changes the argument of ϵ and increases its modulus. Henceforth, a Gaussian test function in $]-\infty,\infty[$ is not a good choice if we aim at improving the fit with the experimental CP violation.

Case $\omega \in [0, +\infty[$

If we substitute $v(\omega) = e^{-\alpha\omega^2/2}$ in the equations (7.11) and integrate from 0 to ∞ we obtain

$$\mathrm{i}\frac{\partial f_1(t)}{\partial t} = \omega_1 f_1(t) - \mathrm{i}\frac{\lambda_1}{2}\sqrt{\frac{\pi}{\alpha}}[\lambda_1 f_1(t) + \lambda_2 f_2(t)] * e^{-\frac{t^2}{4\alpha}}\mathrm{Erfc}(\frac{\mathrm{i}t}{2\sqrt{\alpha}}). \tag{7.46}$$

The Laplace transformation and the expansion in α of the above equation (7.46) lead to

$$\mathrm{i}(sF_1(s) - f_1(0)) = \omega_1 F_1(s) - \frac{\mathrm{i}\pi\lambda_1}{2}[\lambda_1 F_1(s) + \lambda_2 F_2(s)][(1 - \frac{2\mathrm{i}}{\pi}) + 2(-1+\mathrm{i})\sqrt{\frac{\alpha}{\pi}}\ s] + O(\alpha). \tag{7.47}$$

Now, the inverse Laplace transformation yields,

$$\mathrm{i}(1-(1-\mathrm{i})\sqrt{\pi\alpha}\lambda_1^2)\frac{\partial f_1(t)}{\partial t} = \omega_1 f_1(t) - \frac{(\mathrm{i}\pi+2)\lambda_1}{2}[\lambda_1 f_1(t) + \lambda_2 f_2(t)] + (1+\mathrm{i})\lambda_1\lambda_2\sqrt{\pi\alpha}\frac{\partial f_2(t)}{\partial t}. \tag{7.48}$$

We can obtain the same relation for f_2. Then we can easily obtain

$$\begin{aligned} &\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} \\ = &\begin{pmatrix} \frac{\omega_1 - (\frac{\mathrm{i}\pi}{2}+1)\lambda_1^2}{1-(1-\mathrm{i})\sqrt{\pi\alpha}\lambda_1^2} & \lambda_1\lambda_2(-\frac{(\mathrm{i}\pi+2)}{2(1-(1-\mathrm{i})\sqrt{\pi\alpha}\lambda_1^2)} + \frac{(1+\mathrm{i})\sqrt{\pi\alpha}\omega_2}{1-(1-\mathrm{i})\sqrt{\pi\alpha}(\lambda_1^2+\lambda_2^2)}) \\ \lambda_1\lambda_2(-\frac{(\mathrm{i}\pi+2)}{2(1-(1-\mathrm{i})\sqrt{\pi\alpha}\lambda_2^2)} + \frac{(1+\mathrm{i})\sqrt{\pi\alpha}\omega_1}{1-(1-\mathrm{i})\sqrt{\pi\alpha}(\lambda_1^2+\lambda_2^2)} & \frac{\omega_2 - (\frac{\mathrm{i}\pi}{2}+1)\lambda_2^2}{1-(1-\mathrm{i})\sqrt{\pi\alpha}\lambda_2^2}) \end{pmatrix} \\ \times &\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix}, \end{aligned} \tag{7.49}$$

in which we neglected the $O(\lambda^4)$ contributions. Obtaining the eigenvalues of the above effective Hamiltonian and comparing with the equations in (7.26) we get

$$\begin{aligned} \lambda_1^2 &\approx \frac{\Gamma_S}{\pi}(1 - 2m_S\sqrt{\frac{\alpha}{\pi}}), \quad \omega_1 \approx m_S + \Gamma_S - 6m_S\Gamma_S\sqrt{\frac{\alpha}{\pi}}, \\ \lambda_2^2 &\approx \frac{\Gamma_L}{\pi}(1 - 2m_L\sqrt{\frac{\alpha}{\pi}}), \quad \omega_2 \approx m_L + \Gamma_L - 6m_L\Gamma_L\sqrt{\frac{\alpha}{\pi}}. \end{aligned} \tag{7.50}$$

CP **violation:** Once again, let us estimate the value of ϵ. We obtain,

$$\begin{aligned}\epsilon &\approx \frac{\mathrm{i}\sqrt{\Gamma_L\Gamma_S}[(\frac{1}{2}-\mathrm{i}\frac{1}{\pi})+(-2+\mathrm{i}\frac{\pi+2}{\pi})m_S\sqrt{\frac{\alpha}{\pi}}]}{(m_L-m_S)-\frac{\mathrm{i}}{2}(\Gamma_L-\Gamma_S)}\\ &\approx \sqrt{2(1.82\times10^{-3})}e^{\mathrm{i}(43.37)^\circ}[(\frac{1}{2}-\mathrm{i}\frac{1}{\pi})+(-2+\mathrm{i}\frac{\pi+2}{\pi})m_S\sqrt{\frac{\alpha}{\pi}}].\end{aligned} \tag{7.51}$$

We see that if $m_S\sqrt{\frac{\alpha}{\pi}}=\frac{1}{2+\pi}$ the imaginary part in the bracket of above equation is zero and the real part is equal to 0.111, which corresponds to the estimation

$$\epsilon = 6.69\times10^{-3}e^{\mathrm{i}(43.37)^\circ} \tag{7.52}$$

So, in this case, $|\epsilon| = 6.69\times10^{-3}$ which is only ~ 3 times greater than the experimental value while the estimated phase is correct.

7.5 Discussion of other approaches.

We present here a heuristic discussion of other recent approaches to the decay phenomena in Quantum Mechanics and a comparison with the Friedrichs model. Our approach in the above sections considers the decay, oscillation, regeneration, and CP violation of kaons in the Hilbert space. On the other hand the open systems approach aims, briefly speaking, to study some basic questions namely decoherence, Bell inequality, nonlocality, etc [68, 77, 78, 75, 71, 72].

The key ingredient for deriving irreversible in time evolution laws from the unitary Schrödinger evolution is indeed, in open systems approach, to focus on subsystems of a very large system (system plus environment). The role of the environment is played in the Friedrichs model by continuous degree of freedom, while the subsystem is a discrete (two-level in our case) system. As we have shown, these ingredients (discrete system coupled to a continuum) suffice in order to be able to derive a non-unitary master equation for the two-level system. It is worth noting that this approach in which the environment is coupled to the subsystem is very general in quantum physics. It is for instance the approach followed in order to derive master equations [72, 71], or to solve the measurement problem in the so-called decoherence approach [79] and it led to interesting treatments of the general Zeno paradox in the sense of [67, 63].

In the usual formulation of the Friedrichs model, the border line between system and environment is ill defined because the Hilbert spaces associated to those degrees of freedom is not the tensorial product of their respective Hilbert spaces but is rather their direct sum. Nevertheless it is possible, as we shall see below, to imbed the direct sum of the Hilbert spaces associated to the discrete and continuous degrees of freedom into a larger space in which those subspaces (tensorially) factorize, and to formulate an equivalent Hamiltonian dynamics that contains as a special subset of solutions all the solutions of the original model. Such a framework is also useful and necessary, as we shall show, in order to compare our model with other approaches of open, dissipative, noisy dynamics that have recently been proposed to describe kaon phenomenology and possible new experimental tests on entangled kaonic pairs.

This modified Friedrichs model can be explained heuristically as follows. Instead of representing the state of the system at time t by a direct sum of the Hilbert spaces associated to the discrete and continuous degrees of freedom, we imbed it into the tensorial products of a three-dimensional Hilbert space $\mathbb{C}^3$ (that corresponds to the two discrete levels plus their decay product) and of a Fock space; $\mathbb{C}^3 \bigotimes \mathcal{H}_{\text{photon}}$,

$$\psi_{\text{kaon}} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \end{pmatrix} \text{ and } \psi_{\text{photon}} = \begin{pmatrix} f^0 \\ f^1(\omega') \\ f^2(\omega', \omega'') \\ \dots \end{pmatrix} \text{ and the state is given by:}$$

$$\Psi_{0,1,2,\omega^i} = \begin{pmatrix} f_0 \\ 0 \\ 0 \end{pmatrix} \bigotimes \begin{pmatrix} 0 \\ f^1(\omega') \\ f^2(\omega', \omega'') \\ \vdots \\ f^2(\omega', \omega'', \dots, \omega^{(n)}) \\ \dots \end{pmatrix} + \begin{pmatrix} 0 \\ f_1 \\ f_2 \end{pmatrix} \bigotimes \begin{pmatrix} f^0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{7.53}$$

where f_0 represents the amplitude of a new discrete state $|0\rangle$ that is assumed to contain the "decay products" resulting from the disintegration of the two discrete kaonic states $|1\rangle$ and $|2\rangle$; besides, $f^n(\omega', \omega'', ..., \omega^{(n)})$ $(n = 1, 2...)$ represents the amplitude of the n environment particles.

Now that we defined our representation of the state of the system, we can define

the free Hamiltonian:

$$H_{\text{free}} = \begin{pmatrix} \omega_0 & 0 & 0 \\ 0 & \omega_1 & 0 \\ 0 & 0 & \omega_2 \end{pmatrix} \otimes Id.^{\omega} + Id.^{0,1,2} \otimes \omega a^{\dagger}.a \tag{7.54}$$

The first part of it represents the energies of the discrete modes, while the second one contains the energies of the excited modes. Here the operators $a^{\dagger}.a$ count the number of excitations in the mode ω.

The interaction Hamiltonian, H_{int}, is equal to

$$H_{\text{int}} = \begin{pmatrix} 0 & \lambda_1 v(\omega) & \lambda_2 v(\omega) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \otimes a^{\dagger} + \begin{pmatrix} 0 & 0 & 0 \\ \lambda_1 v^*(\omega) & 0 & 0 \\ \lambda_2 v^*(\omega) & 0 & 0 \end{pmatrix} \otimes a. \tag{7.55}$$

In analogy with quantum optics, this interaction represents the decay of the kaonic "excited" states (1 and 2) to the "ground" state (0), with excitation of a mode of energy (ω) while by unitarity the inverse process is also possible (diminution of the energy of a continuous mode by one quantum of energy ω (here $\hbar = 1$), and repopulation of the discrete states $|1\rangle$ and $|2\rangle$). If the initial state is such that no continuous mode is excited ($f^i(\omega', \omega'', ..., \omega^{(i)}, t = 0) = 0 \forall i > 0$), then, the dynamics of the state $\Psi_{0,1,2,\omega}(t)$ is considerably simplified because there will never occur more than one excitation.

In that case $f_1(t)$, $f_2(t)$ and $f^1(\omega, t)$) obey a closed system of three equations:

$$\omega_1 f_1(t) + \lambda_1 \int d\omega v^*(\omega) f^1(\omega, t) = \mathrm{i}\frac{\partial f_1(t)}{\partial t}, \tag{7.56}$$

$$\omega_2 f_2(t) + \lambda_2 \int d\omega v^*(\omega) f^1(\omega, t) = \mathrm{i}\frac{\partial f_2(t)}{\partial t}, \tag{7.57}$$

and

$$\lambda_1 v(\omega) f_1(t) + \lambda_2 v(\omega) f_2(t) + \omega f^1(\omega, t) = \mathrm{i}\frac{\partial f^1(\omega, t)}{\partial t}. \tag{7.58}$$

where we used $\langle v(\omega), f^1(\omega)\rangle = \int d\omega v^*(\omega) f^1(\omega)$, and the components f_0 and f^0 remain unaffected on the evolution so we take them equal to 1, all the other modes are zero.

After identification of $f^1(\omega, t)$ and our previous $g(\omega, t)$ we recover a system of equations of evolution that is rigorously identical to the system of equations (7.7), (9.1) and (7.9) derived in the framework of the Friedrichs model.

At this level, we can compare the Friedrichs model with other models where a system interacts with its environment, which leads to a non-unitary evolution for the reduced system. Quite an amount of recent literature [69, 72, 68], theoretical and phenomenological, deals precisely with the possibility to treat Kaon properties by making them an open system. In those dissipative models, the evolution law can be brought to the Lindblad form (this form is standard provided we assume that the evolution law is completely positive, not merely positive, an hypothesis which can be justified, to some extent, on physical grounds [72]). The markovian Lindblad evolution has the following form:

$$\frac{\partial}{\partial t}\rho = -\mathrm{i}H_{\mathrm{eff}}\rho + \mathrm{i}\rho H_{\mathrm{eff}}^{\dagger} - D(\rho), \tag{7.59}$$

where H_{eff} is a non-necessary Hermitian Hamiltonian, while $D(\rho)$ is the so-called dissipator (see e.g. Refs. [71, 69] for its precise description) of which the main effect is that it induces a loss of coherence of the reduced system. This is not the case with the Hamiltonian part H_{eff} of the evolution operator as shown by direct computation: the von Neumann entropy of the reduced system $\rho_N = \rho/(\mathrm{Tr}(\rho))$, which is by definition equal to $S(\rho_N(t)) = -\mathrm{Tr}(\rho_N(t)\log_2\rho_N(t))$ is constant in time whenever the dissipator $D(\rho)$ is identically equal to zero throughout time. This means among others that in this case pure states remain pure states (up to a global decay), which is effectively the case in our model where the dissipator is identically equal to zero throughout time as can be seen from the Markovian limits (7.36) and (7.49)(the Wigner-Weisskopf regime) of equations (7.11) and (7.12). However, another result may be obtained if we consider a weak coupling limit of the evolution of a kaon system state tensorized with an equilibrium state of an infinite environment [80]. This is quite different from our approach and out of the scope of this paper which makes the weak coupling limit in the frame of the Hilbert space. Here we considered only the process of emission and absorption of one particle of the environment.

It is worth noting that properties that make kaonic phenomenology so interesting and attractive such as oscillations, generation and regeneration are a manifestation of the superposition principle, which is of application precisely because pure states remain pure throughout time.

Remark: The coherence between the decay products $|0\rangle$ at one side and the space spanned by the kaonic modes $|1\rangle$ and $|2\rangle$ at the other side is not preserved under the partial trace. In fact, this comes out from the computation of the partial trace over

the biorthogonal decomposition of the full state:

$$\Psi_{0,1,2,\omega^i}(t) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \bigotimes \begin{pmatrix} 0 \\ f^1(\omega_1, t) \\ 0 \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ f_1(t) \\ f_2(t) \end{pmatrix} \bigotimes \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{7.60}$$

Recall that if $|\Psi\rangle^{AB} = \sum_{i,j} \alpha_{ij} |i\rangle^A \otimes |j\rangle^B$ then

$$\mathrm{Tr}_A(|\Psi\rangle^{AB}\ {}^{AB}\langle\Psi|) = \sum_{i,j,j'} \alpha_{ij}\alpha_{ij'} |j\rangle^B \otimes\ {}^B\langle j'| \tag{7.61}$$

and

$$\mathrm{Tr}_B(|\Psi\rangle^{AB}\ {}^{AB}\langle\Psi|) = \sum_{i,i',j} \alpha_{ij}\alpha_{ij'} |i\rangle^A \otimes\ {}^A\langle i'| \tag{7.62}$$

Then, taking a partial trace of this state over continuous degrees of freedom it is easy to check that the reduced density matrix of the discrete (tripartite) degrees of freedom is equal to:

$$\rho^{\text{kaons}} = \begin{pmatrix} \|f^1\|^2 & 0 & 0 \\ 0 & |f_1|^2 & f_1 f_2^* \\ 0 & f_1^* f_2 & |f_2|^2 \end{pmatrix} \tag{7.63}$$

where $\|f^1\|^2 = \int |f^1(\omega)|^2 d\omega$ and $\|f^1\|^2 + |f_1|^2 + |f_2|^2 = 1$. This is clearly the incoherent sum of the decay-products and a pure state that is coherent superposition of the K_1 and K_2 modes.

7.6 Concluding remarks

We have shown that the framework of the Friedrichs model is relevant in order to grasp , despite of its simplicity, essential features of kaons decay. This model allows us to describe complex temporal evolutions (such as kaonic oscillations, generation and regeneration) and to simulate at least qualitatively CP violation. We also recover the experimental value of the phase, 43.37^o as a results of equations (7.43), (7.44) and (7.52).

The measurement problem suggests that two regimes characterize the temporal evolution of a quantum system: a continuous, unitary evolution in the absence of measurement, and a sudden, irreversible in time evolution during the measurement process (quantum jump). In the present paper, we studied an approach in which the evolution of a two-level system coupled to a continuum is continuous in time but possesses both a unitary and non-unitary component.

We showed that in the framework of the Friedrichs model the main feature that is responsible for the derivation of an irreversible in time master equation for the discrete system is the energy continuum. We also showed that the Friedrichs model is relevant in order to describe complex temporal evolutions (such as kaonic oscillations, generation and regeneration) and to simulate at least qualitatively CP violation.

In section 9.4 we discussed the lindbladian approach to decay problem using a Fock space formulation for the Friedrichs model.

It is out of the scope of the present paper but it would be very interesting to study the properties of the Friedrichs model and of kaonic oscillations in terms of the Time Operator approach. This can be done for the one-level Friedrichs model [61, 62] but higher level systems present more subtle and involved temporal behavior [63] so that it is worth studying the time-operator in this context.

Chapter 8

Quantum Decay Models (II)

8.1 One-level Friedrichs model

Hamiltonian for one-level Friedrichs model is written as $H = H_0 + V$ where H_0 is equal as

$$\begin{pmatrix} \omega_1 & 0 \\ 0 & \omega \end{pmatrix}, \tag{8.1}$$

and its eigenstates are $\{f_0, g_0\} = \{1, \delta(\omega - \nu)\}$. Now, we write the time independent Schrödinger equation for H, i.e. $H|\psi\rangle = \nu|\psi\rangle$, we have,

$$\begin{pmatrix} \omega_1 & \lambda v^*(\omega) \\ \lambda v(\omega) & \omega \end{pmatrix} \begin{pmatrix} f \\ g(\omega) \end{pmatrix} = \nu \begin{pmatrix} f \\ g(\omega) \end{pmatrix}. \tag{8.2}$$

The continuous spectrum of H is the same as that of H_0. Moreover, H may have one (even two) point eigenvalues[58].

From the definition of H we see that if $\{f, g(\omega)\}$ is an eigenfunction of this operator corresponding to the eigenvalue ν, then the following equations must be satisfied

$$\omega_1 f + \lambda \int d\omega' v^*(\omega') g(\omega') = \nu f, \tag{8.3}$$

and

$$\lambda v(\omega) f + \omega g(\omega) = \nu g(\omega). \tag{8.4}$$

If ν is a point eigenvalue then $g(\omega)$ must be square integrable. Thus, from the last equation we arrive at

$$g(\omega) = \frac{\lambda v(\omega) f}{\nu - \omega}. \tag{8.5}$$

If we assume that

$$v(\omega) \neq 0, \qquad \omega \in [0, \infty[, \tag{8.6}$$

the eigenvalue ν must lie outside the continuous spectrum of H_0. Introducing equation (8.5) into equation (8.3) we get

$$\left(\nu - \omega_1 + \lambda^2 \int_0^\infty d\omega' \frac{|v(\omega')|^2}{\omega' - \nu}\right) = 0, \tag{8.7}$$

Therefore ν is a zero of the function

$$\eta(z) = z - \omega_1 + \lambda^2 \int_0^\infty d\omega' \frac{|v(\omega')|^2}{\omega' - z}, \tag{8.8}$$

and because $\eta(z)$ is analytic except for a cut along $[0, \infty[$ its zeros are isolated. It is easy to verify that $\eta(z)$ has only real simple zeros (H is self-adjoint!). Moreover, if $0 \leq \omega_1 < \infty$, $v(\omega)$ vanishes at the end points and λ is sufficiently small, $\eta(z)$ has no zeros and thus H has no point eigenvalue. In the other words, the absence of zeros in $\eta(z)$ on the negative axis depends essentially on the absence of H-bound states with negative energy.

We consider now the continuous spectrum of H, i.e. containing no bound state, thus the $\eta(z)$ is a regular analytic function in the z-plane except for a cut along $[0, \infty[$. If $0 \leq \nu < \infty$ the expression given by equation (8.5) is a solution of equation (8.3) provided we interpret $(\omega - \nu)^{-1}$, as a principal part. The general solution of equation (8.3) is obtained by "*key formulae of scattering theory*", which is introduced by Jean-Paul Marchand [57] as:

$$g(\omega) = g_0 - \lim_{\epsilon \to 0} g(\omega \mp \mathrm{i}\epsilon) \tag{8.9}$$

where "+" is indicated for "incoming" and "−" for "outgoing" wave. Thus, we have

$$g(\omega) = \delta(\omega - \omega') - \lim_{\epsilon \to 0} \frac{\lambda v(\omega) f}{\nu - \omega - \mathrm{i}\epsilon}. \tag{8.10}$$

Inserting $g(\omega)$ in equation(8.3), obtains,

$$f(\nu) = \frac{\lambda v(\nu)}{\eta^+(\nu)}, \tag{8.11}$$

where $\eta^+(z) =: \eta(z + \mathrm{i}\epsilon)$ defined as:

$$\eta^+(z) = z - \omega_1 + \lambda^2 \lim_{\epsilon \to 0} \int_0^\infty d\omega' \frac{|v(\omega')|^2}{\omega' - (z + \mathrm{i}\epsilon)}. \tag{8.12}$$

$\eta^+(z)$ is an analytic continuation of $\eta(z)$ that was permitted by existence of the interaction function ($|v(\omega)|^2$) [57], so it has a zero in lower half plane at

$$z_1 = \widetilde{\omega}_1 - \mathrm{i}\frac{\gamma}{2} \tag{8.13}$$

where z_1^{-1} is called the the resonance with energy $\widetilde{\omega}_1$ and a lifetime $1/\gamma$, ($\hbar = 1$). The proof will be given in the next chapter.

8.2 Two-level Friedrichs model

Now, we write the two-level Friedrichs model Schrödinger equation as

$$\begin{pmatrix} \omega_1 & 0 & \lambda_1 v^*(\omega) \\ 0 & \omega_2 & \lambda_2 v^*(\omega) \\ \lambda_1 v(\omega) & \lambda_2 v(\omega) & \omega \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ g(\omega) \end{pmatrix} = \nu \begin{pmatrix} f_1 \\ f_2 \\ g(\omega) \end{pmatrix}. \tag{8.14}$$

Easily, we obtain

$$\omega_1 f_1 + \lambda_1 \int d\omega' v^*(\omega') g(\omega') = \nu f_1, \tag{8.15}$$

$$\omega_2 f_2 + \lambda_2 \int d\omega' v^*(\omega') g(\omega') = \nu f_2, \tag{8.16}$$

and

$$\lambda_1 v(\omega) f_1 + \lambda_2 v(\omega) f_2 + \omega g(\omega) = \nu g(\omega). \tag{8.17}$$

from the last equation we have

$$g(\omega) = \frac{\lambda_1 v(\omega) f_1 + \lambda_2 v(\omega) f_2}{\nu - \omega}. \tag{8.18}$$

Using the "*key formulae of scattering theory*", one obtains

$$g(\omega) = \delta(\omega - \omega') - \lim_{\epsilon \to 0} \frac{\lambda_1 v(\omega) f_1 + \lambda_2 v(\omega) f_2}{\nu - \omega - \mathrm{i}\epsilon}. \tag{8.19}$$

Putting the above equation in the equations(8.15) yields

$$f_1 = \frac{\lambda_1 v(\nu)}{\eta_1^+(\nu)} - \left(\lambda_1 \lambda_2 \lim_{\epsilon \to 0} \int d\omega \frac{|v(\omega)|^2}{\omega - \nu - \mathrm{i}\epsilon} \right) f_2, \tag{8.20}$$

where

$$\eta_1^+(z) = z - \omega_1 + \lambda_1^2 \lim_{\epsilon \to 0} \int d\omega \frac{|v(\omega)|^2}{\omega - (z + \mathrm{i}\epsilon)}. \tag{8.21}$$

We can also obtain the similar relations for f_2 by changing the indices 1 with 2 and vis versa, and by replacing f_2 in equation(8.20) we obtain

$$f_1(\nu) = \frac{1}{1 - O(\lambda^4)} \left(\frac{\lambda_1 v(\nu)}{\eta_1^+(\nu)} - O(\lambda^3) \right) \tag{8.22}$$

$$\simeq \frac{\lambda_1 v(\nu)}{\eta_1^+(\nu)}. \tag{8.23}$$

In this approximation, the above equation for f_1 is the same equation as we obtained for f in the one-level Friedrichs model (equation (8.5)), i.e. we can write two-level Friedrichs model as two one-level Friedrichs models, and so on.

8.3 Quantum Zeno effect (QZE)

Zeno's paradox is a sped arrow which never reaches its target, because at every instant of time, if we look at the arrow, we see that it occupies a portion of space equal to its own size. At any given moment the arrow is therefore immobile, and by summing up may such immobilities it is clearly impossible, according to Zeno, to obtain motion. It is amusing that some quantum-mechanical states, under particular conditions, behave in a way that is reminiscent to this paradox.

The main features of the so-called quantum Zeno effect is that the evolution of a quantum-mechanical state can be slowed down (or even halted in some limit) when very frequent measurements are performed on the system. In order to check whether is still in its initial state (if it is being continuously observed), then Zeno's quantum arrow (the wave function) does not move.

The very nature of quantum physics is counterintuitive to conventional thinking. Among the many bizarre quantum characteristics is the quantum Zeno paradox, an odd mathematical result that is being debated to this day. Assuming an unstable quantum state, intuition would dictate that eventually, the system will irreversibly decay in certain amount of time, defined as the Zeno time. However, if the system is measured in a period shorter than the Zeno time, then the wave function of the system will repeatedly collapse before decay. In effect, constant measurements of the

system will actually prevent its collapse! Even more mysterious, if the time interval between measurements is longer than the Zeno time, the decay rate of the system will increase, leading to what is termed the inverse Zeno effect [81].

The temporal decay of an unstable system is classically represented as an exponential function. However, for the very short or very long time domain, exponential decay is not applicable. For the very short time region the decay behavior is Gaussian and for the very long time region the decay behavior is power tail. It is in the very short time regime that certain unusual quantum properties can be found.

Let H be the total Hamiltonian of a quantum system and $|\psi\rangle$ its initial state at t=0. The survival probability in state $|\psi\rangle$ is

$$p(t) = |\langle\psi|e^{-\mathrm{i}Ht}|\psi\rangle|^2 \tag{8.24}$$

and a short time expansion yields a quadratic behavior

$$p(t) \sim 1 - \frac{t^2}{\tau_z^2} \tag{8.25}$$

where τ_z is the Zeno time. It is defined as:

$$\tau_z^{-2} = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \tag{8.26}$$

If we write Hamiltonian as $H = H_0 + H_{\text{int}}$ where H_0 is a free and H_{int} is an (off-diagonal) interaction Hamiltonian, we have

$$\tau_z^{-2} = \langle\psi|H_{\text{int}}^2|\psi\rangle. \tag{8.27}$$

Perform N (instantaneous) measurements at time $\tau = t/N$, in order to check whether the system is still in state $|\psi\rangle$. The survival probability after measurements ($t = N\tau$) reads

$$p^{(N)}(t) = p(\tau)^N = p(t/N)^N \sim \big(1 - \frac{t^2}{N^2\tau_z^2}\big)^N \xrightarrow{N\text{large}} e^{-\frac{t^2}{N\tau_z^2}} \xrightarrow{N\to\infty} 1. \tag{8.28}$$

If $N = \infty$ the evolution is completely hindered. For very large N (but finite) the evolution is slowed down: indeed, the survival probability after N pulsed measurements ($t = N\tau$) is interpolated by an exponential law [67]

$$p^{(N)}(t) = p(\tau)^N = e^{-\gamma_{\text{eff}}(\tau)t} \tag{8.29}$$

where $\gamma_{\text{eff}}(\tau)$ is an effective decay rate which it was defined by:

$$\gamma_{\text{eff}}(\tau) = -\frac{1}{\tau}\log p(\tau) \geq 0 \tag{8.30}$$

For $\tau \to 0$ (i.e. $N \to \infty$), hence we have:

$$p(\tau) = e^{-\frac{\tau^2}{\tau_z^2}}, \qquad \gamma_{\text{eff}}(\tau) \sim \frac{\tau}{\tau_z^2} \tag{8.31}$$

Note that $\gamma_{\text{eff}}(\tau)$ in equation (8.30) represents the effective decay rate of a system that evolves freely up to time τ and it is measured at time τ. One expects to recover the natural decay rate γ (if it exists), in agreement with the fermi "golden" rule, for sufficiently long times, i.e., after initial quadratic region is over

$$\gamma_{\text{eff}}(\tau) \xrightarrow{\text{long } \tau} \gamma \tag{8.32}$$

The meaning of "long" is that τ_z is not the right time scale.

We now concentrate our attention on truly unstable systems, with decay rate γ. We ask whether it is possible to find a finite time τ^* such that

$$\gamma_{\text{eff}}(\tau^*) = \gamma. \tag{8.33}$$

If such a time exists, then by performing measurements at time intervals τ^* the system decays according to its natural lifetime, as if no measurements were performed. By equations (8.30) and (8.33) one gets

$$p(\tau^*) = e^{-\gamma\tau^*}, \tag{8.34}$$

i.e. τ^* is the intersection between the curves $p(t)$ and $e^{-\gamma t}$. Fig.8.1 illustrates an example in which such a time τ^* exists. By looking at this figure, it is evident that if $\tau = \tau_1 < \tau^*$ one obtains a QZE. Vice versa, if $\tau = \tau_2 > \tau^*$, one obtains an inverse Zeno effect (IZE). In this sense, τ^* can be viewed as a transition time from a quantum Zeno to an inverse Zeno effect. In general, it is not always possible to determine τ^*: equation (8.33) may have no finite solutions. This will be thoroughly discussed in the following, but it is interesting to anticipate some general conclusions. For an unstable system and for sufficiently "long" times (the definition of "long" times will be sharpened later) the survival probability reads with very good approximation

$$p(t) \sim Ze^{-\gamma t}, \tag{8.35}$$

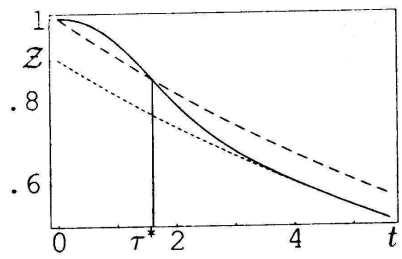

Figure 8.1: Determination of τ^*. The solid line is the survival probability, the dashed line is the exponential $e^{-\gamma t}$, and the dotted line is the asymptotic exponential ,$Ze^{-\gamma t}$ in equation (8.35)[81].

where Z, the intersection of the asymptotic exponential with the $t = 0$ axis, is the wave function renormalization and is given by the square modulus of the residue of the pole of the propagator. We claim that a sufficient condition for the existence of a solution τ^* of equation (8.33) is that $Z < 1$. This is easily proved by graphical inspection. The case $Z < 1$ is shown in Fig.8.1 : $p(t)$ and $e^{-\gamma t}$ must intersect, since according to (8.35) $p(t) \sim Ze^{-\gamma t}$ for large t, and a finite solution τ^* can always be found. The other case, $Z > 1$, is shown in Fig.8.2 A solution may or may not exist, depending on the features of the model investigated [81].

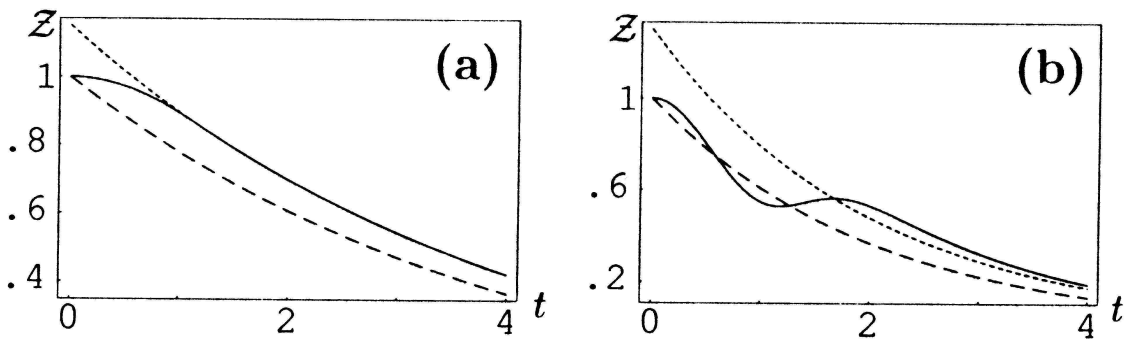

Figure 8.2: Study of the case $Z > 1$. The solid line is the survival probability, the dashed line is the renormalized exponential $e^{-\gamma t}$, and the dotted line is the asymptotic exponential $Ze^{-\gamma t}$. (a) If $p(t)$ and $e^{-\gamma t}$ do not intersect, then no finite solution τ^* exists. (b) If $p(t)$ and $e^{-\gamma t}$ intersect, then a finite solution τ^* exists[81].

8.4 Time operator in quantum mechanics

Time appears in physics mainly in the description of motion. But this time is not the one that corresponds to the alteration of the time state of a body or a complex system. On the other hand, the time-oriented transformation of the states of complex systems is recognized as the most fundamental feature of thermodynamics. The second law is the first statement making a distinction between past and future in the physical processes. In speaking of the state of a body or a system, we obviously understand a macroscopic state. Nevertheless, in quantum mechanics, the discovery of lifetimes of unstable elementary particles has introduced a new distinction between past and future on the microscopic level.

The mathematical theory of the macroscopic irreversible phenomena follows one of two directions. The first one, based on empirical observations is the theory of stochastic processes, which succeeded since the work of Einstein on the Browian motion to explain basic macroscopic properties like diffusion, viscosity, etc. The second one strives to derive the irreversible approach to equilibrium from the first principles. This is the nonequilibrium statistical mechanics. The aspect of driven return to equilibrium of open systems coupled to "reservoirs" is of secondary importance here. We are mainly interested in the time evolution of states of autonomous systems under their own dynamics.

As is well known in classical mechanics, any microscopic system of particles is well described by its trajectory. But one knows from the early arguments of Maxwell and Boltzmann that no effective information on the long term motion of a macroscopic system can be obtained from the Newton equations. This fact is well understood today by the modern theory of dynamical systems. The trajectories of most complex dynamical, systems are all unstable and have positive Lyapounov exponents. Therefore, no available information on the long term motion can be derived from the knowledge of a microscopic state. For these systems, one needs more global information. We follow the Gibbs point of view which stipulates that the information on the system is of a statistical nature and the nonequilibrium state is, therefore, given by a probability distribution on the phase space.

Time operator T is based on the concept of a lifetime of a dynamical system. It is impossible to associate such a concept to a trajectory of a system, however complex it is. It is associated to the statistical states. Consider first, a system in the idealization of a classical dynamical systems with discrete time $t = -\infty, \ldots, -1, 0, 1, \ldots, \infty$. One

thinks of the iterative action of some more or less chaotic mapping or some Poincaré section of a flow. The time operator defines a family of subspaces of nonequilibrium statistical state labeled by t such that the dynamics propagates an initial state along these spaces. Moreover, it gives a definition of a lifetime and the description of the approach to the equilibrium state. In fact, the dynamical action transports the system from one eigenspace of T to an older one in the future. The eigenfunctions of the time operator are the probability distributions that correspond to states of the system at different moments of its evolution. These ideas have been developed in early papers [82, 83, 84]. Here we shall show that the concept of time operator is suitable to describe the irreversible processes of physics and an even more general class of irreversible dynamical processes [93].

8.4.1 Definition

We first consider the quantum mechanical time operator. Let the quantum system be described by the Hamiltonian H acting in the Hilbert space $\mathcal{H}$ of wave functions. The quantum statistical states of the system are density matrices. The time evolution of any density matrix ρ is generated by:

$$\rho(t) = e^{-\mathrm{i}Ht}\rho e^{\mathrm{i}Ht} = e^{-\mathrm{i}Lt}\rho \tag{8.36}$$

where L is the Liouville operator defined on the Liouville space, to which belong all the quantum statistical states by

$$L\rho = [H, \rho]. \tag{8.37}$$

In what follows, $U_t = e^{-\mathrm{i}Lt}$ is denoted. Pauli has already noted the impossibility of defining a time operator T in the space of wave functions, since by definition, it should be canonically conjugated to the time evolution generator H:

$$[H, T] = \mathrm{i}I. \tag{8.38}$$

The impossibility follows from the semiboundedness of the spectrum of the Hamiltonian. The Liouville operator does not suffer from this inconvenience. A sufficient condition is that the Hamiltonian has a semiunbounded continuous spectrum [84]. In this case, it is possible to find a family of subspaces of the space of states corresponding to the continuous spectrum of the Liouville space[1] $\mathfrak{L}_\tau$, $-\infty < \tau < \infty$, such that

[1] A Liouville space is defined as a direct product of two Hilbert space: $\mathfrak{L} = \mathcal{H} \otimes \mathcal{H}$.

$(i)\mathfrak{L}_\tau \subseteq \mathfrak{L}_{\tau+t}$ for$t \geq 0$

$(ii)U_t\mathfrak{L}_\tau = \mathfrak{L}_{\tau+t}$.

Denote now by $\mathcal{P}_\tau$ the orthogonal projection operator onto $\mathfrak{L}_\tau$. The properties (i) and (ii) then translate respectively into

(i) $\mathcal{P}_\tau\mathcal{P}_{\tau'} = \mathcal{P}_\tau$, if $\tau < \tau'$ and $\mathcal{P}_\tau$; is a family of spectral projection operators of T defined by:

$$T = \int \tau d\mathcal{P}_\tau \tag{8.39}$$

and (ii)

$$U_t\mathcal{P}_\tau U_{-t} = \mathcal{P}_{\tau+t} \tag{8.40}$$

This implies the Weyl relation

$$U_{-t}TU_t = T + tI \tag{8.41}$$

and T is the canonical conjugate of the Liouville operator. This commutation relation justifies calls T a time operator. It should be noted that in quantum mechanics, time operator can only have a continuous spectrum and there is no density matrix that can be an eigenfuction of T. It is also necessary that H is unbounded continuous spectrum. In other words, the infinite volume limit is a necessary condition for the existence of a time operator.

From the above Weyl relation, a new rigorous proof of the fourth uncertainty relation between time (as an operator) and energy is derived. Thus, the time operator is also an observable, like spatial position and energy, with the main difference that it acts only on the space of the statistical states and not on the space of wave functions. On this level of generality, it also describes the time occurrence of specified events such as time of arrival of a beam of particles to screen or time of decay of unstable particle. Since the time of occurrence of such events fluctuates, the spectral projection operator $\mathcal{P}_\tau$ gives the probability of occurrence of such an event during any time interval.

The projection of the density matrix ρ on the subspace, $\mathfrak{L}_0$ corresponds to undecayed states or prepared initial states (also called a coarse-grained projection in the context of the projection technique theory). This projection obeys a closed equation (i.e., the projection of $\rho(t)$ depends only on the projection of $\rho(0)$) which is called the Master equation, since this evolution is a semigroup for $t > 0$. In fact, applying the property (i): $U_t\mathcal{P}_0U_{-t} = \mathcal{P}_t$, one obtains

$$U_t\mathcal{P}_0 = \mathcal{P}_tU_t. \tag{8.42}$$

Multiplying the above equation by $\mathcal{P}_0$ and using (ii) one obtains

$$\mathcal{P}_0 U_t \mathcal{P}_0 = \mathcal{P}_0 \mathcal{P}_t U_t = \mathcal{P}_0 U_t, \quad t > 0. \tag{8.43}$$

This implies that any initial density matrix ρ satisfies to the equation

$$\mathcal{P}_0 U_t \rho = \mathcal{P}_0 U_t \mathcal{P}_0 \rho, \quad t > 0. \tag{8.44}$$

which means that the complementary part $(1-\mathcal{P}_0)\rho_0$ does not contribute to the evolution of the projection part $\mathcal{P}_0 U_t \rho$, which has, therefore, a closed evolution. Moreover, the family of evolution operators for the diagonal part $W_t = \mathcal{P}_0 U_t \mathcal{P}_0$ verifies, owing to the above relations, the semigroup property for $t,\ t' > 0$:

$$\begin{aligned} W_t W_{t'} &= \mathcal{P}_0 U_t \mathcal{P}_0 \mathcal{P}_0 U_t' \mathcal{P}_0 \\ &= \mathcal{P}_0 U_t U_t' \mathcal{P}_0 \\ &= \mathcal{P}_0 U_{t+t'} \mathcal{P}_0 \\ &= W_{t+t'} \end{aligned} \tag{8.45}$$

Finally, this decays to zero monotonically. In fact, using the Hilbert-Schmidt norm on the family of density matrices,

$$\langle \rho_1 | \rho_2 \rangle = \mathrm{Tr}(\rho_1 \rho_2) \tag{8.46}$$

and the unitarity of U_t, one obtains

$$\|\mathcal{P}_0 U_t \rho\| = \|U_{-t} \mathcal{P}_0 U_t \rho\| = \|\mathcal{P}_{-t} \rho\|. \tag{8.47}$$

Since $\bigcap_\tau \mathfrak{L}_\tau = 0$, this quantity decays to zero as t goes to $+\infty$. Unstable statistical states with finite lifetime are those for which the above decay has an exponential rate [93].

In fact, two important properties are fullfilled by this subspace which enable it to be described this way.

First, it was proved that the time operator satisfies the fourth uncertainty relation between time and energy with the following sense. Considering that a time operator should be a quantum observable, like spatial position and energy, which describes the time occurrence of specified events such as the time of arrival of a beam of particles to a screen or time of decay of unstable particles and extending the von-Neumann

formulation of quantum mechanics to Liouville space, it is possible to define the states of a quantum system by normalized elements $\rho \in \mathfrak{L}$ with respect to the scalar product. The expectation of T in the state ρ is given by:

$$\langle T \rangle_\rho = \langle \rho | T | \rho \rangle_\rho \tag{8.48}$$

and the "uncertainty" of the observable T as its fluctuation in the state ρ:

$$(\triangle T)_\rho = \sqrt{\langle T^2 \rangle_\rho - (\langle T \rangle_\rho)^2} \tag{8.49}$$

Embedding the normalized elements $\psi \in \mathcal{H}$ as elements $\rho = |\psi\rangle\langle\psi| \in \mathfrak{L}$, and the observables A operating on $\mathcal{H}$ as observables $\hat{A}$ operating on $\mathfrak{L}$ as a multiplication by A: $\hat{A}\rho = A.\rho$, the above definition coincides with the usual quantum rule giving the expectation of an observable A, operating on $\mathcal{H}$, in the state $\psi \in \mathcal{H}$:

$$\langle A \rangle_\rho = \langle \rho | \hat{A} | \rho \rangle = \langle \psi | \hat{A} \psi \rangle. \tag{8.50}$$

A density matrix state M (i.e. a positive operator on with $\mathrm{Tr}(M) = 1$), is embedded in $\mathfrak{L}$ as element $\rho = M^{1/2}$. Then, the expectation of the observable A operating on $\mathcal{H}$ in the mixture state M usually given by $\mathrm{Tr}(M.A)$ is also preserved, for :

$$\langle A \rangle_\rho = \langle \rho | \hat{A} | \rho \rangle = \mathrm{Tr}(M.A). \tag{8.51}$$

Let $\triangle E$ be the usual energy uncertainty in the state M given by:

$$\triangle E = \sqrt{\mathrm{Tr}(M.H^2) - (\mathrm{Tr}(M.H))^2} \tag{8.52}$$

and $\triangle T = (\triangle T)_{M^{1/2}}$ be the uncertainty of T in the state M defined as in (9.6). It has been shown that:

$$\triangle E \triangle T \geq \frac{1}{2\sqrt{2}} \tag{8.53}$$

This uncertainty relation leads to the interpretation of T as the time occurrence of specified random events. The time of occurrence of such events fluctuates and we speak of the probability of its occurrence in a time interval $I =]t_1, t_2]$. The observable T' associated to such event in the initial state ρ_0 has to be related to the time parameter t by:

$$\langle T' \rangle_{\rho_t} = \langle T' \rangle_{\rho_0} - t \tag{8.54}$$

where $\rho_t = e^{-itL}\rho_0$. Comparing this condition with the above Weyl relation we see that we have to define T' as: $T' = -T$. Let $\mathcal{Q}_\tau$ be the family of spectral projections

of T', then, in the state ρ, the probability of occurrence of the event in a time interval I is given, as in the usual von Neumann formulation by:

$$\mathcal{P}(I,\rho) = \|\mathcal{Q}_{t_2}\rho\|^2 - \|\mathcal{Q}_{t_1}\rho\|^2 = \|(\mathcal{Q}_{t_2} - \mathcal{Q}_{t_1})\rho\|^2 := \|\mathcal{Q}(I)\rho\|^2 \tag{8.55}$$

The unstable "undecayed" states prepared at $t_0 = 0$ are the states ρ such that $\mathcal{P}(I,\rho) = 0$ for any negative time interval I, that is:

$$\|\mathcal{Q}_\tau\rho\|^2 = 0, \quad \forall\tau \leq 0 \tag{8.56}$$

In other words, these are the states verifying $\mathcal{Q}_0\rho = 0$. It is straightforwardly checked that the spectral projections $\mathcal{Q}_\tau$ are related to the spectral projections $\mathcal{P}_\tau$ by the following relation:

$$\mathcal{Q}_\tau = 1 - \mathcal{P}_{-\tau} \tag{8.57}$$

Thus, the unstable states are those states verifying, $\rho = \mathcal{P}_0\rho$ and they coincide with our subspace $\mathfrak{F}_0$[2]. For these states, the probability that a system prepared in the undecayed state ρ is found to decay sometime during the interval $I =]0,t]$ is $\|\mathcal{Q}_t\rho\|^2 = 1 - \|\mathcal{P}_{-t}\rho\|^2$ a monotonically nondecreasing quantity which converges to 1 as $t \to \infty$ for $\|\mathcal{P}_{-t}\rho\|^2$ tends monotonically to zero. As noticed by [94], such quantity could not exist in the usual quantum mechanical treatment of the decay processes and could not be related to the "survival probability" ($p_\phi(t) = \|\mathcal{P}_0 e^{\mathrm{i}tH}\phi\|$) for it is not a monotonically decreasing quantity in the Hilbert space formulation. In the Liouville space, given any initial state ρ, its survival probability in the unstable space is given by:

$$p_\rho(t) = \|\mathcal{P}_0 e^{-\mathrm{i}Lt}\rho\|^2 \tag{8.58}$$

This survival probability and the probability of finding the system to decay sometime during the interval $I =]0,t]$, $q_\rho(t) = \|\mathcal{Q}_t\rho\|^2$ are related by:

$$\begin{aligned} q_\rho(t) &= 1 - \|\mathcal{P}_{-t}\rho\|^2 \\ &= 1 - \|U_{-t}\mathcal{P}_{-t}U_t\rho\|^2 \\ &= 1 - \|\mathcal{P}_0 e^{-\mathrm{i}Lt}\rho\|^2 \\ &= 1 - p_\rho(t) \end{aligned} \tag{8.59}$$

The survival probability is monotonically decreasing to 0 as $t \to \infty$. This is true for for any general initial state as can be seen from the equation (8.59). It should noted that the projection operator $\mathcal{P}_0$ is not a "factorizable" operator, that is, not of the form $\mathcal{P}_0\rho = E\rho E$ where E is a projection operator [92].

[2] We define the subspace $\mathfrak{F}_{t_0}$ as the set of decaying states prepared at time t_0

8.5 Time asymmetry in quantum mechanics

8.5.1 Rigged Hilbert Space (RHS)

In quantum mechanics, observable quantities are represented by linear operators. The eigenvalues of an operator represent the possible values of the measurement of the corresponding observable. These eigenvalues, which mathematically correspond to the spectrum of the operator, can be discrete (as the energies of a particle in a box), continuous (as the energies of a free, unconstrained particle), resonant (as in a decay), or a combination thereof.

The Hilbert space includes only the bound and scattering spectra because the Hilbert space spectrum of an observable is real, thereby discarding the resonance spectrum as unphysical. However, radioactive nuclei and unstable elementary particles are physical objects that ought to have a place in the quantum mechanical formalism. This is why we need to extend the Hilbert space to a rigged Hilbert space, within which the resonance spectrum has a place.

When the spectrum of an observable A is discrete and A is bounded, then A is defined on the whole of the Hilbert space $\mathcal{H}$ and the eigenvectors of A belong to $\mathcal{H}$. In this case, A can be essentially seen as a matrix. This means that, as far as discrete spectrum is concerned, there is no need to extend A. However, quantum mechanical observables are in general unbounded and their spectrum has in general a continuous part. In order to deal with continuous spectrum, we use Dirac's bra-ket formalism. This formalism does not fit within the Hilbert space alone, but within the rigged Hilbert space.

Loosely speaking, a rigged Hilbert space (also called a Gelfand triplet) is a triad of spaces

$$\Phi \subset \mathcal{H} \subset \Phi^{\times} \tag{8.60}$$

such that $\mathcal{H}$ is a Hilbert space, Φ is a dense subspace of $\mathcal{H}$, and $\Phi^{\times}$ is the space of antilinear functionals over Φ. Mathematically, Φ is the space of test functions, and $\Phi^{\times}$ is the space of distributions. The space $\Phi^{\times}$ is called the antidual space of Φ. Associated with the rigged Hilbert space (8.60), there is always another rigged Hilbert space,

$$\Phi \subset \mathcal{H} \subset \Phi' \tag{8.61}$$

where Φ' is called the dual space of Φ and contains the linear functionals over Φ.

The basic reason why we need the space Φ is that unbounded operators are not defined on the whole of $\mathcal{H}$ but only on dense subdomains of $\mathcal{H}$ that are not invariant under the action of the observables. Such non-invariance makes expectation values, uncertainties and commutation relations not well defined on the whole of $\mathcal{H}$. The space Φ is the largest subspace of the Hilbert space on which such expectation values, uncertainties and commutation relations are well defined.

Besides accommodating resonances and Dirac's bra-ket formalism, the rigged Hilbert space seems to capture the physical principles of quantum mechanics better than the Hilbert space. For example, assuming that the Hilbert space provides the whole mathematical framework for quantum mechanics may lead one to the conclude that Heisenberg's uncertainty relations are not physical, since they cannot be defined on the whole of the Hilbert space. Using the rigged Hilbert space, one overcomes this difficulty after realizing that the commutation relations are well defined on Φ.

The completeness relation is a good place to appreciate the added value of the rigged Hilbert space. Consider, for example, the Hamiltonian H of a system. In the Hilbert space, one writes the completeness relation as

$$\int_{\mathcal{E}} d\mathcal{P}_E = 1 \tag{8.62}$$

where $\mathcal{P}_E$ are the spectral projections of H and $\mathcal{E}$ is its spectrum. However, within the rigged Hilbert space one can write

$$\int_0^\infty dE|E\rangle\langle E| + \sum_k |E_n\rangle\langle E_n| = 1 \tag{8.63}$$

where $|E_k\rangle$ and $|E\rangle$ are the bound and scattering states of H, respectively [85].

Though not part of the traditional axioms these basic hypotheses are usually augmented by the Dirac kets, e.g., of the Hamiltonian $|E\rangle$, and Dirac's basis vector expansion [86]

$$\phi = \int |E\rangle\langle E|\phi\rangle dE. \tag{8.64}$$

8.5.2 Breit-Wigner energy distributions

The phenomenological Breit-Wigner i.e.

$$a^{BW} = \frac{1}{E - (E_R - \mathrm{i}\Gamma/2)}, \quad 0 \leq E < \infty, \tag{8.65}$$

for which the energy extends over the "physical" values $0 \leq E < \infty$ that cannot be related to an exponential are

$$\frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-\mathrm{i}Et}}{E-(E_R-\mathrm{i}\Gamma/2)}\,dE = \theta(t)e^{\mathrm{i}(E_R-\mathrm{i}\Gamma/2)t} \tag{8.66}$$

where $\theta(t)$ is a step function and defined as:

$$\theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases} \tag{8.67}$$

and

$$\frac{\mathrm{i}}{E-(E_R-\mathrm{i}\Gamma/2)} = \int_0^{\infty} e^{\mathrm{i}(E_R-\mathrm{i}\Gamma/2)t}e^{\mathrm{i}Et}\,dt, \qquad -\infty < E < \infty. \tag{8.68}$$

Mathematics requires that the energy E range over the entire real axis $-\infty < E < \infty$ and the values of time range only from $0 < t < \infty$. In contrast, in the traditional quantum theory in Hilbert space the time evolves over $-\infty < t < \infty$ and energy (spectrum of the Hamiltonian H) is bounded from below $0 \leq E < \infty$. The usual textbook derivation of the exponential time evolution for vectors with the Breit-Wigner energy distributions is one example of the "approximate" character of quantum mechanical derivations for scattering and decay phenomena [86].

The mathematical results (8.66) and (8.68) show us which way we have to go to obtain a mathematical theory of quantum mechanical scattering and decay: the energy must be continued from the "physical" values $0 \leq E < \infty$ of (8.65) into the complex energy plane, in particular to the negative values of (8.68) and the exponential time evolution (8.66) is asymmetric, it starts at a "beginning" $t = t_0 = 0$. Thus using the simple but exact mathematical relations (8.66) and (8.68), not the usual approximations of textbooks, show already what many have felt about decay processes namely that the time evolution is asymmetric $t > t_0$ and the decay is an irreversible process.

The reason for this concern with deviations from the exponential is a mathematical theorem [87, 88] which states that there is no vector in Hilbert space that has an exact exponential time evolution. It means if one wants the exponential law cannot take for a Hilbert space vector, ϕ^D. One has to take a vector $\phi^D \to \psi^G$ with the properties

$$H\psi^G = z\psi^G, \quad z = E - \frac{\mathrm{i}}{2}\Gamma \tag{8.69}$$

and

$$\psi^G(t) = e^{-\mathrm{i}Ht/\hbar}\psi^G(0) = e^{-\mathrm{i}zt/\hbar}\psi^G(0) \tag{8.70}$$

This vector ψ^G, which needs to be properly defined, is called a Gamow vector [86].

In addition to (8.63), the rigged Hilbert space gives you an additional completeness relation in which the resonance states participate:

$$\int_{-\infty}^{0} dE|E\rangle\langle E| + \sum_R |z_R\rangle\langle z_R| + \sum_k |E_k\rangle\langle E_k| = 1 \tag{8.71}$$

where $|z_R\rangle$ are the Gamow (resonance) states of H and the last integral, called the background, is performed in the complex plane right below the negative real axis of the second sheet. Thus, the completeness relation (8.71) substitutes the scattering states contribution by the resonance contribution plus a background, thereby putting the resonance spectrum on the same footing as the bound and scattering spectra.

It is important to note that the integrals in (8.63) and (8.71) are different, and that the resonance contribution does not appear in (8.63), because resonances are not asymptotic states. Also it is important to note that the resonance states, and therefore expansion (8.71), need a different rigged Hilbert space from that needed by the scattering states and expansion (8.63) [85].

8.5.3 Lippmann-Schwinger kets representations in Hardy space

The Lippmann-Schwinger equation is one of the cornerstones of scattering theory. It is written as

$$|E^{\pm}\rangle = |E\rangle + \frac{1}{E - H_0 \pm \mathrm{i}\epsilon} V|E^{\pm}\rangle, \tag{8.72}$$

where $|E^{\pm}\rangle$ are the "in" and "out" Lippmann-Schwinger kets, $|E\rangle$ is an eigenket of the free Hamiltonian H_0,

$$H_0|E\rangle = E|E\rangle \tag{8.73}$$

and V is the potential. The Lippmann-Schwinger kets are, in particular, eigenvectors of H:

$$H|E^{\pm}\rangle = E|E^{\pm}\rangle. \tag{8.74}$$

To the kets $|E^{\pm}\rangle$, there correspond the bras $\langle\, {}^{\pm}E|$, which satisfy

$$\langle\, {}^{\pm}E| = \langle E| + \langle\, {}^{\pm}E|V\frac{1}{E - H_0 \mp \mathrm{i}\epsilon}, \tag{8.75}$$

The bras $\langle\, {}^{\pm}E|$ are left eigenvectors of H,

$$\langle\, {}^{\pm}E|H = E\langle\, {}^{\pm}E|, \tag{8.76}$$

and the bras $\langle E|$ are left eigenvectors of H_0,

$$\langle E|H_0 = E\langle E|. \tag{8.77}$$

The Lippmann-Schwinger equation (8.72) for the "in" $|E^+\rangle$ and "out" $|E^-\rangle$ kets has the scattering "in" and "out" boundary conditions built into the $\pm i\epsilon$, since equation (8.72) is equivalent to the time-independent Schrtödinger equation (8.74) subject to those "in" $(+i\epsilon)$ and "out" $(-i\epsilon)$ boundary conditions. Like any bra and ket, the Lippmann-Schwinger bras and kets do not have a place in the Hilbert space [85].

We define the Gamow vector ψ^G as energy eigenkets of a self-adjoint Hamiltonian H, but with complex generalized eigenvalue $z = E - \frac{i}{2}\Gamma$. As a guide to find the space of analytic wave functions we use the well-known empirical concepts of quantum scattering. The Lippmann-Schwinger kets $|E^+\rangle$ and $|E^-\rangle$ are the eigenvectors of the (self adjoint) Hamiltonian H which fulfill the boundary conditions given by the Lippmann-Schwinger (integral) equation. They have already energy values with "infitesimal imaginary part" $|E^{\mp}\rangle = |E_{\mp i\epsilon}\rangle$, $\epsilon > 0$, this means the complex conjugate of the energy wave functions $\langle f|E^{\mp}\rangle = \langle f|E_{\mp i\epsilon}\rangle \equiv \overline{f^{\mp}(E)}$ can be continued into the lower (for -) and upper (for +) complex energy plane, or $f^{\mp}(E) = \overline{\overline{f^{\mp}(E)}} = \langle\, {}^{\mp}E|f\rangle$ can be continued into the upper (for -) and lower (for +) energy plane. From this we conjecture that the energy wave functions for the outgoing particles $\langle\, {}^{-}E|\psi^-\rangle$ and the energy wave functions of the prepared in-states $\langle\, {}^{+}E|\psi^+\rangle$ form two distinct spaces of Schwartz functions which can be analytically continued into the upper and lower complex energy plane, respectively. To make this into a precise hypothesis, we postulate

(i)The set of prepared in-state wave functions on the positive real semi-axis $E \in \mathbb{R}^+\{\langle\, {}^{+}E|\psi^+\rangle\} = \mathbb{S} \cap \mathbb{H}^-(\mathbb{R}^+)$ are smooth Hardy functions of the lower energy plane.

(ii)The set of observed (detector defined) out-particles wave functions $\{\langle\, {}^{-}E|\psi^-\rangle\} = \mathbb{S} \cap \mathbb{H}^+(\mathbb{R}^+)$ are smooth Hardy function of the upper complex energy plane.

Thus the set of the outparticle "state" vector ψ^- is given ψ^- by [bohm]

$$\psi^- = \int_0^\infty |E^-\rangle\langle\, {}^{-}E|\psi^-\rangle dE \tag{8.78}$$

The set of these vectors ψ^- form an abstract linear space which we call Φ^+. This is the abstract Hardy space of vectors $\psi_1^-, \psi_2^-, \cdots$ which is mathematically (algebraically and topologically (has the same meaning of convergence)) equivalent to the function space (i). $\mathbb{S} \cap \mathbb{H}^+(\mathbb{R}^+)$ is called a realization of the abstract space Φ_+ in the same way

as $L^2(\mathbb{R}^+)$ is the realization of the abstract Hilbert space $\mathcal{H}$ by the space of Lebesgue square integrable functions.

Equivalently, the set of the vectors ϕ^+ given by

$$\phi^+ = \int_0^\infty |E^+\rangle\langle\, {}^+E|\phi^+\rangle dE \tag{8.79}$$

using the set of energy wave functions $\langle\, {}^+E|\phi^+\rangle \in \mathbb{S}\cap\mathbb{H}^-(\mathbb{R}^+)$ form an abstract linear topological space which we call Φ_-. Therewith one has a pair of RHSs of Hardy type

$$\Phi_\mp \subset \mathcal{H} \subset \Phi_\mp^\times. \tag{8.80}$$

The same Hilbert space is equipped with two different Hardy spaces and their duals $\Phi_\mp^\times$ (space of antilinear continuous fuctionals). The Lippmann-Schwinger kets are then mathematically defined as functionals [86].

Now, we need two RHSs, one for prepared in-states ϕ^+:

$$\{\phi^+\} \in \Phi_- \subset \mathcal{H} \subset \Phi_-^\times \tag{8.81}$$

and the other for the registered observables $|\psi^-\rangle\langle\psi^-|$ or detected out-states ψ^-:

$$\{\psi^-\} \in \Phi_+ \subset \mathcal{H} \subset \Phi_+^\times \tag{8.82}$$

where $\mathcal{H}$ is the same Hilbert space in (8.81) and (8.81). Thus, with the new Hardy space boundary conditions (8.81) for $\phi^+ \in \Phi_-$ we have

$$\phi^+(t) = e^{-\mathrm{i}Ht}\phi^+ \equiv U_-^\dagger(t)\phi^+; \quad 0 \le t < \infty. \tag{8.83}$$

And boundary conditions (8.82) for $\psi^- \in \Phi_+$ we have

$$\psi^-(t) = e^{\mathrm{i}Ht}\psi^- \equiv U_+(t)\psi^-; \quad 0 \le t < \infty. \tag{8.84}$$

Herein we obtain under the new Hardy space boundary conditions (8.81) and (8.81) the semigroup solution (8.83) and (8.84).

8.5.4 Time evolution of Gamow vector

The Born probability for measuring the observable ψ^- in the state ϕ^+,

$$P_{\psi^-}(\phi^+(t)) = |(\psi^-|\phi^+(t))|^2 = |(\psi^-(t)|\phi^+)|^2 \tag{8.85}$$

are predicted for $t \geq t_0 = 0$ only.

The Born probability amplitude $(\psi^-|\phi^+(t))$ to register the observable $A^- = |\psi^-\rangle\langle\psi^-|$, $\psi^- \in \Phi_+$, in the state $\phi^+ \in \Phi_-$ is expressed using the standard notions of scattering theory as the matrix element of the S-operator:

$$(\psi^-|\phi^+) = (\Omega^-\psi^{\text{out}}|\Omega^+\phi^{\text{in}}) = (\psi^{\text{out}}|S\phi^{\text{in}}) = (\psi^{\text{out}}|\phi^{\text{out}}) \tag{8.86}$$

This is essentially the statement of standard scattering theory [100, 90, 91] except that is that case one speaks of out-states ϕ^- instead of outobservables $\psi^- \equiv \Omega^-\psi^{\text{out}}$. But Born probabilities correlate observables and states, not states and other states, and the detector in scattering experiments is not built to the specifications of prepared states, but to the specification of the particles to be registered in the outregion, which are therefore observables. The matrix element $(\psi^-|\phi^+)$ can now be expressed using (8.78) and (8.79), and with the use of symmetries (angular momentum, energy conservation) one obtains

$$(\psi^-|\phi^+) = \int_0^\infty \langle\psi^-|E^-\rangle S\langle\,^+E|\phi^+\rangle \tag{8.87}$$

where $S \equiv \langle\,^-E|E^+\rangle$ is the S-matrix element. Under the new hypothesis (ii) the energy wave functions are not only smooth square integrable functions but also analytic in such a way that the integral in the S-matrix element (8.87) can be continued into the lower half plane of the second sheet. The contour integration can therefore be deformed from the continuous spectrum of H ($0 \leq E < \infty$, the scattering energies) into a contour around the resonance pole and some background integral that corresponds to (8.65) [89].

In the integrals along the circles around each resonance pole at $Z_{R_i} = E_{R_i} - \mathrm{i}\Gamma_i/2$ of (8.87) one uses the expansion

$$S = \frac{R_{(i}}{z - z_{R_i}} + R_0 + R_1(z - z_{R_i}) + \cdots \tag{8.88}$$

Now, we define the Gamow vectors $|z^-_{R_i}\rangle$ as functionals over all $\psi^- \in \Phi_+$:

$$\langle\psi^-|z^-_{R_i}\rangle = \frac{\mathrm{i}}{2\pi}\oint_{C_i} \frac{\langle\psi^-|z^-\rangle}{z - z_{R_i}}dz = \frac{\mathrm{i}}{2\pi}\int_{-\infty_{II}}^{+\infty} \frac{\langle\psi^-|E^-\rangle}{E - z_{R_i}}dE \tag{8.89}$$

The integral along the energy axis extends from $-\infty$ in the second sheet along the upper rim of the second sheet to $+\infty$ and the values along the cut $0 \leq E < \infty$ are

the physical scattering energies. Since the values of $\langle\psi^-|E^-\rangle$ for negative E of Hardy functions are already determined by their values for $0 \leq E < \infty$, the values in (8.89) are determined from the scattering energies.

This means we have the following result (as a consequence of the Hardy space axiom): if we replace the phenomenological Breit-Wigner in (8.65) which is measured only for $0 \leq E < \infty$ by the "exact" Breit-Wigner of (8.66) for which the energy extend from $-\infty \leq E < \infty$, then one can associate to an ideal Gamow vector ψ^G , defined as the continuous superposition of the Lippmann-Schwinger kets $|E^-\rangle$ with the "exact" Breit-Wigner as the wave function of $\langle\ ^-E|\psi^G\rangle$

$$\begin{aligned} a^{BW} = \frac{1}{E-(E_R-\mathrm{i}\Gamma/2)} \Longleftrightarrow \psi^G &= |z_R^-\rangle \\ &= \frac{\mathrm{i}\sqrt{2\pi\Gamma}}{2\pi}\int_{-\infty_{II}}^{+\infty}\frac{|E^-\rangle}{E-z_R}dE \end{aligned} \tag{8.90}$$

where $z_R = E_R - \mathrm{i}\frac{\Gamma}{2}$ and $-\infty_{II} \leq E < \infty$. And we have

$$\langle H\psi^-|\psi^G\rangle \equiv \langle\psi^-|H^\times|\psi^G\rangle = (E_R - \mathrm{i}\frac{\Gamma}{2})\langle\psi^-|\psi^G\rangle \quad \text{for all } psi^- \in \Phi_+. \tag{8.91}$$

The Gamow vector represents the resonance pole without the background. For this state vector the exponential time evolution is given as:

$$\psi^G(t) \equiv e^{-\mathrm{i}H^\times t}\psi^G = e^{-\mathrm{i}E_R t}e^{-\mathrm{i}\frac{\Gamma}{2}t}\psi^G, \quad \text{for } t \geq 0. \tag{8.92}$$

Finally, considering the background, the prepared state vector ϕ^+ is given as:

$$\phi^+ = \phi^{\mathrm{bg}} + \sum_i c_{R_i}|z_{R_i}^-\rangle \tag{8.93}$$

where the sum is over all resonances, and ϕ^{bg} is the functional on $\Phi_+^\times = \{\psi^-\}$ given by

$$\begin{aligned} \langle\psi^-|\phi^{bg}\rangle &= \int_0^{-\infty_{II}}\langle\psi^-|E^-\rangle\langle\ ^+E|\phi^+\rangle S_{II}(E)dE \\ &= \int_0^{+\infty}\langle\psi^-|E^-\rangle\langle\ ^+E|\phi^+\rangle b(E)dE \end{aligned} \tag{8.94}$$

where $b(E)$ is background amplitude.

8.5.5 Summary

To obtain a meaningful theory of resonance and decay phenomena, one needs a vector with the following properties:

1. It must have a Breit-Wigner energy distribution.
2. It must have an exponential time evolution.
3. The parameter of the Lorentzian Γ and the parameter of the exponential t must be related by $\tau = \hbar/\Gamma$.

The vectors which have these properties are the Gamow vectors of (8.90) defined by (8.89) as a functional over the Hardy space Φ_+. Such vectors cannot exist in Hilbert space. They cannot even exist as generalized eigenvector defined as functional over the Schwartz space, like the usual Dirac ket $|E\rangle \in \Phi^\times$ of (8.60).

The kets that one needs are suggested by the Lippmann-Schwinger equations. The Lippmann-Schwinger kets (of which there are two kinds $|E^\mp\rangle$, require some analyticity properties. We give them a mathematical meaning by defining them as functional over the Hardy spaces of (8.80):

$$|E^\mp\rangle \in \Phi^\times_\pm \tag{8.95}$$

They can be analytically continued to $|Z^\mp\rangle \in \Phi^\times_\pm$ for $z \in \mathbb{C}^R_\mp$.

The Gamow state vectors are associated with the singular point of the analytically continued Lippmann-Schwinger kets $|z^-$. The Gamow vector (8.90) represents a first-order resonance [86].

Chapter 9

Decay of quantum-mechanical unstable systems and spectral projections of time operator in Friedrichs model

Abstract: We give a formula of the projection operators of self-adjoint time super-operator in terms of the spectral representation of the Hamiltonian. We apply this formula to the quantum mechanical Friedrichs model to compute the excited state decay inside the continuum in term of time super-operator. Then we show that this formula eliminates the Zeno effect for short-time decay. We also show that the long-time asymptotics of the survival probability is a sum of an algebraically decaying term and an exponentially decaying one.

PACS number: 0.3.65-w

9.1 Introduction

In this paper we shall study the properties of the survival probability of unstable quantum systems using the spectral projections of time operator built in the framework of the Liouville-von Neumann description [92, 93]. We shall test these properties in the Friedrichs model [48]. The survival probability should be a monotonically decreasing time function and this property could not exist in the framework of the usual quantum-mechanical approach [94, 95, 96]. It can only be properly treated through an observable time operator T whose eigenprojections provide the probability distribution of the time of decay. The equation defining time operator is the following:

$$U_{-t}TU_t = T + tI \tag{9.1}$$

where U_t is the unitary group of states evolution. It is known that such an operator cannot exist when the evolution is governed by the Schrödinger equation, since the Hamiltonian has a bounded spectrum from below, and this contradicts the equation:

$$[H, T] = iI \tag{9.2}$$

in the Hilbert space of pure states $\mathcal{H}$. However, a time operator can exist under some conditions, for mixed states. They can be embedded [92, 97] in the "Liouville space", denoted $\mathcal{L}$, that is the space of Hilbert-Schmidt operators ρ on $\mathcal{H}$ such that $Tr(\rho^*\rho) < \infty$, equipped with the scalar product: $< \rho, \rho' >= Tr(\rho^*\rho')$. The time evolution of these operators is given by the group of operators:

$$U_t\rho = e^{-itH}\rho e^{itH} \tag{9.3}$$

The infinitesimal self-adjoint generator of this group is the Liouville von-Neumann operator L given by:

$$L\rho = H\rho - \rho H \tag{9.4}$$

That is, $U_t = e^{-itL}$. The states of a quantum system are defined by normalized elements $\rho \in \mathcal{L}$ with respect to the scalar product, the expectation of T in the state ρ is given by:

$$\langle T \rangle_\rho = \langle \rho, T\rho \rangle \tag{9.5}$$

and the"uncertainty" of the observable T as its fluctuation in the state ρ:

$$(\Delta T)_\rho = \sqrt{\langle T^2 \rangle_\rho - (\langle T \rangle_\rho)^2} \tag{9.6}$$

It is shown that [92] the unstable states are those states verifying $\rho = \mathcal{P}_0\rho$. In fact, let M be a density matrix states and $\rho = M^{1/2}$, let $\triangle E$ be the usual energy uncertainty in the state M given by:

$$\triangle E = \sqrt{\mathrm{Tr}(M.H^2) - (\mathrm{Tr}(M.H))^2} \tag{9.7}$$

and $\triangle T = (\triangle T)_{M^{1/2}}$ be the uncertainty of T in the state M defined as in (9.6). It has been shown that:

$$\triangle E \triangle T \geq \frac{1}{2\sqrt{2}} \tag{9.8}$$

This uncertainty relation leads to the interpretation of T as the time occurrence of specified random events. The time of occurrence of such events fluctuates and we speak of the probability of its occurrence in a time interval $I =]t_1, t_2]$. The observable T' associated to such event in the initial state ρ_0 has to be related to the time parameter t by:

$$\langle T' \rangle_{\rho_t} = \langle T' \rangle_{\rho_0} - t \tag{9.9}$$

where $\rho_t = e^{-\mathrm{i}tL}\rho_0$. Comparing this condition with the above Weyl relation we see that we have to define T' as: $T' = -T$. Let $\mathcal{P}_\tau$ denote the family of spectral projection operators of T:

$$T = \int_{\mathbb{R}} \tau d\mathcal{P}_\tau \tag{9.10}$$

and let $\mathcal{Q}_\tau$ be the family of spectral projections of T', then, in the state ρ, the probability of occurrence of the event in a time interval I is given, as in the usual von Neumann formulation, by:

$$\mathcal{P}(I, \rho) = \|\mathcal{Q}_{t_2}\rho\|^2 - \|\mathcal{Q}_{t_1}\rho\|^2 = \|(\mathcal{Q}_{t_2} - \mathcal{Q}_{t_1})\rho\|^2 := \|\mathcal{Q}(I)\rho\|^2 \tag{9.11}$$

The unstable "undecayed" states prepared at $t_0 = 0$ are the states ρ such that $\mathcal{P}(I, \rho) = 0$ for any negative time interval I, that is:

$$\|\mathcal{Q}_\tau\rho\|^2 = 0, \quad \forall \tau \leq 0 \tag{9.12}$$

In other words, these are the states verifying $\mathcal{Q}_0\rho = 0$. It is straightforwardly checked that the spectral projections $\mathcal{Q}_\tau$ are related to the spectral projections $\mathcal{P}_\tau$ by the following relation:

$$\mathcal{Q}_\tau = 1 - \mathcal{P}_{-\tau} \tag{9.13}$$

The subspaces $\mathfrak{F}_\tau$ on which project $\mathcal{P}_\tau$ verify: $i)\mathfrak{F}_\tau \subseteq \mathfrak{F}_{\tau+t}$ and $ii)U_t\mathfrak{F}_\tau \subseteq \mathfrak{F}_{\tau+t}$ for $t \geq 0$. Thus, the unstable states are those states verifying: $\rho = \mathcal{P}_0\rho$ and they coincide

with our subspace $\mathfrak{F}_0$[1]. For these states, the probability that a system prepared in the undecayed state ρ is found to decay sometime during the interval $I =]0, t]$ is $\|\mathcal{Q}_t\rho\|^2 = 1 - \|\mathcal{P}_{-t}\rho\|^2$ a monotonically nondecreasing quantity which converges to 1 as $t \to \infty$ for $\|\mathcal{P}_{-t}\rho\|^2$ tends monotonically to zero. As noticed by Misra and Sudarshan [94], such quantity could not exist in the usual quantum mechanical treatment of the decay processes and could not be related to the "survival probability" for it is not a monotonically decreasing quantity in the Hilbert space formulation. In the Liouville space, given any initial state ρ, its survival probability in the unstable space is given by:

$$p_\rho(t) = \|\mathcal{P}_0 e^{-\mathrm{i}tL}\rho\|^2 \tag{9.14}$$

Then using a standard definition [96] of the survival probability adapted to the Liouville space, given any initial state ρ, its survival probability in the unstable space is given by:

$$\begin{aligned} p_\rho(t) &= \|\mathcal{P}_0 e^{-\mathrm{i}tL}\rho\|^2 \\ &= \|U_{-t}\mathcal{P}_0 U_t\rho\|^2 \\ &= \|\mathcal{P}_{-t}\rho\|^2 \end{aligned} \tag{9.15}$$

Here we used the following relation: $\mathcal{P}_{-t} = U - t\mathcal{P}_0 U_t$. Then, the survival probability is monotonically decreasing to 0 as $t \to \infty$. As $\mathcal{P}_t$ is a spectral family of projections $p_\rho(t) \to 1$ when $t \to -\infty$. This survival probability and the probability of finding the system to decay sometime during the interval $I =]0, t]$, $q_\rho(t) = \|\mathcal{Q}_\rho(t)\|^2$ are related by:

$$q_\rho(t) = 1 - p_\rho(t) \tag{9.16}$$

on account of its monotonicity, $q_\rho(t)$ represents an entropy content of $\rho(t)$. For any given ρ it is shown that [92] $\mathcal{P}_0 U_t\rho = W_t\rho$ where W_t is a semi-group of contracting operators on $\mathcal{L}$.

The paper is organized as follows: Section 9.2 gives a formula (9.32) for the projection operator of T in terms of the spectrum of H. Section 9.3 and Appendix A present the Friedrichs model and its spectral representation of the free Hamiltonian excited state and Section 9.4 gives its projection on the unstable state space. Sections 9.5 and 9.6 study the short-time and long-time asymptotic of the survival probability.

[1] We define the subspace $\mathfrak{F}_{t_0}$ to the set of decaying states prepared at time t_0

9.2 A formula for the spectral projection of time operator

The expression of time operator is given in a spectral representation of H. As shown in [97], H should have an unbounded absolutely continuous spectrum. In the simplest case, we shall suppose that H is represented as the multiplication operator on $\mathcal{H} = L^2(\mathbb{R}^+)$:

$$H\psi(\omega) = \omega\psi(\omega). \tag{9.17}$$

The Hilbert-Schmidt operators on $L^2(\mathbb{R}^+)$ correspond to the square-integrable functions $\rho(\omega, \omega^{'}) \in L^2(\mathbb{R}^+ \times \mathbb{R}^+)$ and the Liouville-von Neumann operator L is given by :

$$L\rho(\omega, \omega^{'}) = (\omega - \omega^{'})\rho(\omega, \omega^{'}) \tag{9.18}$$

Then we obtain a spectral representation of L via the change of variables:

$$\nu = \omega - \omega^{'} \tag{9.19}$$

and

$$E = \min(\omega, \omega^{'}) \tag{9.20}$$

This gives a spectral representation of L:

$$L\rho(\nu, E) = \nu\rho(\nu, E), \tag{9.21}$$

where $\rho(\nu, E) \in L^2(\mathbb{R} \times \mathbb{R}^+)$. In this representation $T\rho(\nu, E) = \mathrm{i}\frac{d}{d\nu}\rho(\nu, E)$ so that the spectral representation of T is obtained by the inverse Fourier Transform:

$$\hat{\rho}(\tau, E) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{\mathrm{i}\tau\nu}\rho(\nu, E)d\nu = (\mathcal{F}^*\rho)(\tau, E) \tag{9.22}$$

and

$$T\hat{\rho}(\tau, E) = \tau\hat{\rho}(\tau, E). \tag{9.23}$$

The spectral projection operators $\mathcal{P}_s$ of T are given in the (τ, E)-representation by:

$$\mathcal{P}_s\hat{\rho}(\tau, E) = \chi_{]-\infty,s]}(\tau)\hat{\rho}(\tau, E) \tag{9.24}$$

where $\chi_{]-\infty,s]}$ is the characteristic function of $]-\infty, s]$. So that we obtain in the (ν, E)-representation the following expression of these spectral projection operators:

$$\begin{aligned}\mathcal{P}_s\rho(\nu,E) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{s} e^{-\mathrm{i}\nu\tau}\hat{\rho}(\tau,E)\,d\tau \\ &= e^{-\mathrm{i}\nu s}\int_{-\infty}^{0} e^{-i\nu\tau}\hat{\rho}(\tau+s,E)\,d\tau. \end{aligned} \tag{9.25}$$

Let us denote the Fourier transform $\mathcal{F}g(\nu) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\mathrm{i}\nu\tau}\hat{g}(\tau)\,d\tau$ and remind of the Paley-Wiener theorem which says that a function $g(\nu)$ belongs to the Hardy class $\mathbb{H}^+$(i.e. the limit as $y \to 0^+$ of an analytic function $\Phi(\nu + \mathrm{i}y)$ such that $\int_{-\infty}^{\infty} \mid \Phi(\nu+\mathrm{i}y) \mid^2\ dy < \infty$) if and only if it is of the form $g(\nu) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty} e^{-\mathrm{i}\nu\tau}\hat{g}(\tau)\,d\tau$ where $\hat{g} \in L^2(\mathbb{R}^+)$ [98]. Using the Hilbert transformation:

$$\mathbf{H}g(x) = \frac{1}{\pi}\mathsf{P}\int_{-\infty}^{\infty}\frac{g(t)}{t-x}\,dt \tag{9.26}$$

for only $g \in L^2(\mathbb{R})$, we can write the decomposition:

$$\begin{aligned} g(x) &= \frac{1}{2}[g(x) - \mathrm{i}\mathbf{H}g(x)] + \frac{1}{2}[g(x) + \mathrm{i}\mathbf{H}g(x)] \\ &:= g_+(x) + g_-(x) \end{aligned} \tag{9.27}$$

Also according to the Paley-Wiener theorem, $g_+(x)$ (resp.$g_-(x)$) belongs to the Hardy class $\mathbb{H}^+$(resp.$\mathbb{H}^-$) and this decomposition is unique. Thus taking the Fourier transformation of g we obtain :

$$\begin{aligned}\mathcal{F}(g)(\nu) &= \frac{1}{2}[\mathcal{F}(g)(\nu) - \mathrm{i}\mathbf{H}\mathcal{F}(g)(\nu)] + \frac{1}{2}[\mathcal{F}(g)(\nu) + \mathrm{i}\mathbf{H}\mathcal{F}(g)(\nu)] \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0} e^{-\mathrm{i}\nu\tau}\hat{g}(\tau)\,d\tau + \frac{1}{\sqrt{2\pi}}\int_{0}^{\infty} e^{-\mathrm{i}\nu\tau}\hat{g}(\tau)\,d\tau. \end{aligned} \tag{9.28}$$

It follows that:

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0} e^{-\mathrm{i}\nu\tau}\hat{g}(\tau)\,d\tau = \frac{1}{2}(\mathcal{F}(g) - \mathrm{i}\mathbf{H}\mathcal{F}(g)). \tag{9.29}$$

Now, using the well known property of the translated Fourier transformation $\sigma_s\hat{g}(\tau) = \hat{g}(\tau + s)$ we have :

$$\mathcal{F}(\sigma_s\hat{g})(\nu) = e^{\mathrm{i}\nu s}\mathcal{F}.\hat{g}(\nu) = e^{\mathrm{i}\nu s}g(\nu), \tag{9.30}$$

then (9.25) and (9.29) yield:

$$\mathcal{P}_s\rho(\nu,E) = \frac{1}{2}e^{-\mathrm{i}\nu s}[e^{i\nu s}\rho(\nu,E) - \mathrm{i}\mathbf{H}(e^{\mathrm{i}\nu s}\rho(\nu,E))]. \tag{9.31}$$

Thus:

$$\mathcal{P}_s\rho(\nu, E) = \frac{1}{2}[\rho(\nu, E) - \mathrm{i}e^{-\mathrm{i}\nu s}\mathbf{H}(e^{\mathrm{i}\nu s}\rho(\nu, E))]. \tag{9.32}$$

It is clear from (9.32) that $\mathcal{P}_s\rho(\nu, E)$ is in the Hardy class $\mathbb{H}^+$.

9.3 One-level Friedrichs model

The one-level Friedrichs model (see Appendix A) is a simple model of Hamiltonian in which a discrete eigenvalue of the free Hamiltonian H_0 disappears under coupling with the continuum. It has been often used as a simple model of decay of unstable states illustrating the Weisskopf-Wigner theory of decaying quantum systems. The Hamilton operator H is an operator on the Hilbert space of the wave functions of the form $\mid \psi >= \{f_0, g(\mu)\}, f_0 \in \mathbb{C}, g \in L^2(\mathbb{R}^+)$,

$$H = H_0 + \lambda V, \tag{9.33}$$

where λ is a positive coupling constant, and

$$H_0 \mid \psi\rangle = \{\omega_1 f_0, \mu g(\mu)\}, (\omega_1 > 0). \tag{9.34}$$

We shall denote the eigenfunction of H_0 by $\chi = \{1, 0\}$. The operator V is given by:

$$V\{f, g(\mu)\} = \{\langle v(\mu), g(\mu)\rangle, f_0.v(\mu)\}. \tag{9.35}$$

where

$$\langle v(\mu), g(\mu, t)\rangle = \int d\mu v^*(\mu)g(\mu, t), \tag{9.36}$$

is the inner product. Thus, H can be represented as a matrix :

$$H = \begin{pmatrix} \omega_1 & \lambda v^*(\mu) \\ \lambda v(\mu) & \mu \end{pmatrix} \tag{9.37}$$

where ω_1 represents the energy of the discrete level and $v(\mu) \in L^2(\mathbb{R}^+)$, it is called a factor form. The $\lambda v(\mu)$ represents the coupling to the continuous degree of freedom. The energies μ of the different modes of the continuum range from $-\infty$ to $+\infty$ when $v(\mu) = 1$, but we are free to tune the coupling $v(\mu)$ in order to introduce a selective cut off to extreme energy modes. It has been shown than for λ small enough, H has

no eigenvalues and that the spectrum of H is continuous extending over $\mathbb{R}^+$. The outgoing spectral representation of the vector χ given in [57] is:

$$f_1(\omega) = \frac{\lambda v^*(\omega)}{\eta^+(\omega)}, \tag{9.38}$$

where

$$\eta^+(\omega) = \eta(\omega + \mathrm{i}\epsilon) := \omega - \omega_1 + \lambda^2 \lim_{\epsilon \to 0} \int_0^\infty \frac{|v(\omega')|^2}{\omega' - (\omega + \mathrm{i}\epsilon)} d\omega' \tag{9.39}$$

$f_1(\omega)$ is the spectral representation of χ and $H\chi$ is represented by $\omega f_1(\omega)$. In what follows, we shall also denote $\eta^-(\omega) = \eta(\omega - \mathrm{i}\epsilon)$. $\eta^\pm(\omega)$ are complex conjugate of each other, we can see that

$$\eta^\pm(\omega) = \omega - \omega_1 + \lambda^2 \ \mathsf{P} \int_0^\infty \frac{|v(\omega')|^2}{\omega' - \omega} \ d\omega' \pm \mathrm{i}\pi\lambda^2 |v(\omega)|^2, \tag{9.40}$$

where P indicates the "principal value" and we used the following identity in equation (9.40)

$$\frac{1}{x - x_0 \pm \mathrm{i}\epsilon} = \mathsf{P}\frac{1}{x - x_0} \mp \mathrm{i}\pi\delta(x - x_0). \tag{9.41}$$

By choosing a cutoff $v(\omega)$ as $(\alpha\omega/\pi)^{1/4} e^{-\alpha\omega/2}$, we see that the principal value integral can be written as:

$$\mathsf{P} \int_0^\infty \frac{|v(\omega')|^2}{\omega' - \omega} \ d\omega' = (1 - \mathrm{i}e^{-\alpha\omega}\sqrt{\alpha\pi\omega} \ \mathrm{erf}(\mathrm{i}\sqrt{\alpha\omega}\ )) \tag{9.42}$$

where error function is defined as $\mathrm{erf}(z) = \int_0^z e^{-x^2} dx$, and "i $\mathrm{erf}(\mathrm{i}\sqrt{\alpha\omega}\ )$" is a real function (see (9.45)). By replacing the above equation in the equation(9.40) we have

$$\eta^+(\omega) = \omega - \omega_1 + \lambda^2 \ [1 + \mathrm{i}\sqrt{\alpha\pi\omega} e^{-\alpha\omega}(1 - \mathrm{erf}(\mathrm{i}\sqrt{\alpha\omega}\ ))]. \tag{9.43}$$

Then,

$$\frac{d\eta^+(\omega)}{d\omega} = 1 + \lambda^2 \ [2\alpha\sqrt{\omega} + \mathrm{i}\sqrt{\alpha\pi}(\frac{1}{2\sqrt{\omega}} - \alpha\sqrt{\omega})e^{-\alpha\omega}(1 - \mathrm{erf}(\mathrm{i}\sqrt{\alpha\omega}\ ))], \tag{9.44}$$

is never equal to zero for small λ, that means $\eta^+(\omega)$ has a simple pole in the inferior complex plan. By using the expansion of error function and exponential function as $x \to 0$

$$\mathrm{erf}(x) = \frac{1}{\sqrt{\pi}}(2x - \frac{2x^3}{3} + \frac{x^5}{5} - \frac{x^7}{21} + ...) \tag{9.45}$$

and

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + ... \tag{9.46}$$

we can write equation (9.43) for $\alpha \to 0$ as follows:

$$\begin{aligned} \eta^+(\omega) = \omega - \omega_1 \quad &+ \quad \lambda^2 \, [(1 + 2\alpha\omega + \frac{2(\alpha\omega)^2}{3} + \frac{(\alpha\omega)^3}{5} + ...) \\ &+ \quad \mathrm{i}\sqrt{\alpha\pi\omega}(1 - \alpha\omega + \frac{(\alpha\omega)^2}{2!} - \frac{(\alpha\omega)^3}{3!} + ...)]. \end{aligned} \tag{9.47}$$

Thus, we rewrite the above equation with approximation as

$$\begin{aligned} \eta^+(\omega) \quad &\approx \quad \omega - \omega_1 + \lambda^2 \, [(1 + O(\alpha)) + \mathrm{i}\sqrt{\alpha\pi\omega}(1 - O(\alpha))] \\ &= \quad \omega - z_I. \end{aligned} \tag{9.48}$$

where $z_I = \widetilde{\omega}_1 - \mathrm{i}\frac{\gamma}{2}$ and

$$\widetilde{\omega}_1 \approx \omega_1 - \lambda^2 \approx \omega_1 \quad \text{and} \quad \frac{\gamma}{2} \approx \lambda^2\sqrt{\alpha\pi\omega_1}. \tag{9.49}$$

Thus, z_I is the resonance with energy $\widetilde{\omega}_1$ and a lifetime $1/\gamma$, $(\hbar = 1)$. According to the above calculation, we obtain,

$$\eta^+(\omega) - \eta^-(\omega) = \mathrm{i}\gamma. \tag{9.50}$$

From (9.39), we have

$$\frac{\mathrm{i}}{2}[\frac{1}{\eta^+(\omega)} - \frac{1}{\eta^-(\omega)}] = \frac{\pi\lambda^2|v(\omega)|^2}{|\eta^+(\omega)|^2}. \tag{9.51}$$

Consequently, the two above equations yield

$$\frac{\pi\lambda^2|v(\omega)|^2}{|\eta^+(\omega)|^2} = \frac{\frac{\gamma}{2}}{|\eta^+(\omega)|^2}. \tag{9.52}$$

This equation will be used in the next section.

The quantity $| < \chi, e^{-\mathrm{i}Ht}\chi > |^2 = \int_0^\infty |f_1(\omega)|^2 e^{-\mathrm{i}\omega t} d\omega$ is usually called the survival probability at time t. It is however clear that this is not a true probability, since it is not a monotonically decreasing quantity, although it tends to zero as a result of the Riemann-Lebesgue lemma.

Let us now identify the state χ with element $\rho = |\chi >< \chi|$ of the Liouville space, that is the kernel operator:

$$\rho_{11}(\omega, \omega^{'}) = f_1(\omega)\overline{f_1(\omega^{'})}. \tag{9.53}$$

We shall compute first the unstable component $\mathcal{P}_0\rho_{11}$ and show that $\mathcal{P}_0\rho_{11} \neq \rho_{11}$ that is, ρ_{11} is not in the unstable subspace of T. Then we shall compute the survival probability of the state ρ and $\|\mathcal{P}_{-s}\rho\|^2$ and show how is reached the following limit:

$$\lim_{s\to\infty} \|\mathcal{P}_{-s}\rho\|^2 \to 0. \tag{9.54}$$

9.4 Computation of spectral projections of T in a Friedrichs model

As explained above the Liouville operator is given by:

$$L\rho(\omega, \omega^{'}) = (\omega - \omega^{'})\rho(\omega, \omega^{'}) \tag{9.55}$$

and the spectral representation of L is given by the change of variables:

$$\nu = \omega - \omega^{'} \tag{9.56}$$

and

$$E = \min(\omega, \omega^{'}). \tag{9.57}$$

Thus we obtain for $\rho_{11}(\nu, E)$:

$$\rho_{11}(\nu, E) = \begin{cases} \lambda^2 \frac{v(E)}{\eta^-(E)} \frac{v^*(E+\nu)}{\eta^+(E+\nu)} & \nu > 0 \\ \\ \lambda^2 \frac{v^*(E)}{\eta^+(E)} \frac{v(E-\nu)}{\eta^-(E-\nu)} & \nu < 0. \end{cases} \tag{9.58}$$

By considering $v(\omega)$ a real test function and using the equation (9.52) we obtain $\rho_{11}(\nu, E)$ in the following form:

$$\rho_{11}(\nu, E) = Af(\nu, E), \tag{9.59}$$

where

$$f(\nu, E) = \begin{cases} \frac{1}{\nu_0^*(\nu+\nu_0)} & \nu > 0 \\ \\ \frac{1}{\nu_0(\nu_0^*-\nu)} & \nu < 0. \end{cases} \tag{9.60}$$

where $\nu_0 = a + \mathrm{i}b = (E - \widetilde{\omega}_1) + \mathrm{i}\frac{\gamma}{2}$ and A is the normalization constant which is obtained as:

$$|A|^2 = \left(\int_0^\infty dE \int_{-\infty}^\infty d\nu |f(\nu, E)|^2 \right)^{-1} = \frac{\gamma^2}{4} \left(\frac{\pi}{2} + \arctan(\frac{2\widetilde{\omega}_1}{\gamma}) \right)^{-2} \tag{9.61}$$

For obtaining $\mathcal{P}_s f(\nu, E)$ $(s < 0)$, we shall use the formula (9.32). First we compute:

$$G_s(\nu, E) = \mathbf{H}(e^{\mathrm{i}s\nu} f)(\nu) = \frac{1}{\pi} \mathsf{P} \int_{-\infty}^\infty \frac{e^{\mathrm{i}sx} f(x)}{x - \nu} dx \tag{9.62}$$

Now, we substitute (9.60) in (9.62), so we have,

$$G_s(\nu, E) \;=\; \frac{1}{\pi} \mathsf{P}[\int_{-\infty}^0 \frac{e^{\mathrm{i}sx}}{\nu_0(x-\nu)(\nu_0^* - x)} dx + \int_0^{+\infty} \frac{e^{\mathrm{i}sx}}{\nu_0^*(x-\nu)(\nu_0 + x)} dx], \tag{9.63}$$

which for the $\nu > 0$ has the following form:

$$G_s(\nu, E) = \frac{1}{\pi} [\int_{-\infty}^0 \frac{e^{\mathrm{i}sx}}{\nu_0(x-\nu)(\nu_0^* - x)} dx + \mathsf{P} \int_0^{+\infty} \frac{e^{\mathrm{i}sx}}{\nu_0^*(x-\nu)(\nu_0 + x)} dx]. \tag{9.64}$$

In the Appendix B we will calculate $G_s(\nu, E)$. Finally, $\mathcal{P}_s f(\nu, E)$ is obtained as:

$$\begin{aligned} \mathcal{P}_s f(\nu, E) = \mathrm{i}e^{-\mathrm{i}s\nu} \Bigg[& \frac{-1}{2\pi\nu_0(\nu_0^* - \nu)} \left(\int_{-\infty}^0 \frac{e^{-sy}}{y + \mathrm{i}\nu_0^*} dy - \int_{-\infty}^0 \frac{e^{-sy}}{y + \mathrm{i}\nu} dy \right) \\ & + \frac{1}{2\pi\nu_0^*(\nu + \nu_0)} \left(\int_{-\infty}^0 \frac{e^{-sy}}{y - \mathrm{i}\nu_0} dy - \int_{-\infty}^0 \frac{e^{-sy}}{y + \mathrm{i}\nu} dy \right) \Bigg] \\ & + \begin{cases} e^{-\mathrm{i}s\nu} [\frac{e^{\mathrm{i}s\nu_0^*}}{\nu_0(\nu_0^* - \nu)} - \frac{e^{-\mathrm{i}s\nu_0}}{\nu_0^*(\nu_0 + \nu)}], & E < \widetilde{\omega}_1 \\ \\ 0, & E > \widetilde{\omega}_1. \end{cases} \end{aligned} \tag{9.65}$$

In this equation the non integral terms yield the poles and lead to the resonance shown in equation (9.81), and the integral terms yield an algebraical term analog to

the background in the Hamiltonian theories [99, 100, 101]. We can also compute the same result for the case $\nu < 0$.

The above expression is well defined for $\nu = 0$. In fact, for $\nu \to 0$ the sum of the two integrals which are dependent of ν goes to zero as $\nu \log(\mathrm{i}s\nu) \to 0$ and the of above equation is written as:

$$\lim_{\nu\to 0} \mathcal{P}_s f(\nu, E) = \frac{\mathrm{i}}{2\pi|\nu_0|^2}\Big(-\int_{-\infty}^{0} \frac{e^{-sy}}{y+\mathrm{i}\nu_0^*}dy + \int_{-\infty}^{0} \frac{e^{-sy}}{y-\mathrm{i}\nu_0}dy\Big) + \begin{cases} \frac{1}{|\nu_0|^2}[e^{\mathrm{i}s\nu_0^*} - e^{-\mathrm{i}s\nu_0}], & E < \widetilde{\omega}_1 \\ 0, & E > \widetilde{\omega}_1. \end{cases} \tag{9.66}$$

9.4.1 The case $s = 0$

Now, we would calculate an analytic expression of $\mathcal{P}_0 f(\nu, E)$. For $s = 0$ equation (9.65) becomes:

$$\begin{aligned}\mathcal{P}_0 f(\nu, E) = \lim_{R\to\infty} \frac{1}{2\pi}\Bigg[&\frac{-\mathrm{i}}{\nu_0(\nu_0^* - \nu)}\Big(\int_{-R}^{0} \frac{1}{y+\mathrm{i}\nu_0^*}dy - \int_{-\mathbb{R}}^{0} \frac{1}{y+\mathrm{i}\nu}dy\Big) \\ &+ \frac{\mathrm{i}}{\nu_0^*(\nu+\nu_0)}\Big(\int_{-R}^{0} \frac{1}{y-\mathrm{i}\nu_0}dy - \int_{-R}^{0} \frac{1}{y+\mathrm{i}\nu}dy\Big)\Bigg] \\ &+ \begin{cases} [\frac{1}{\nu_0(\nu_0^*-\nu)} - \frac{1}{\nu_0^*(\nu_0+\nu)}], & E < \widetilde{\omega}_1 \\ 0, & E > \widetilde{\omega}_1. \end{cases}\end{aligned} \tag{9.67}$$

Here the two first integrals in the above equation are equal to

$$\lim_{R\to\infty} \{[\log^+(\mathrm{i}\nu_0^*) - \log^+(\mathrm{i}\nu_0^* - R)] - [\log^+(\mathrm{i}\nu) - \log^+(\mathrm{i}\nu - R)]\} = -\log^+(\frac{\nu}{\nu_0^*}), \tag{9.68}$$

where $\log^+ z$ is the analytic function with a cut along the negative y-axis Fig.9.1:

$$\log^+ z = \log|z| + \mathrm{i}\arg(z), \quad \arg(z) \in]-\tfrac{\pi}{2}, \tfrac{3\pi}{2}[\ . \tag{9.69}$$

Also, we used $\lim_{R\to\infty} \log^+(\frac{\mathrm{i}\nu - R}{\mathrm{i}\nu_0^* - R}) \to 0$. Similarly, the two last integrals in the equation (9.67) can be calculated as:

$$\lim_{R\to\infty} \{[\log^+(-\mathrm{i}\nu_0) - \log^+(-\mathrm{i}\nu_0 - R)] - [\log^+(\mathrm{i}\nu) - \log^+(\mathrm{i}\nu - R)]\} = -\log^+(-\frac{\nu}{\nu_0}) \tag{9.70}$$

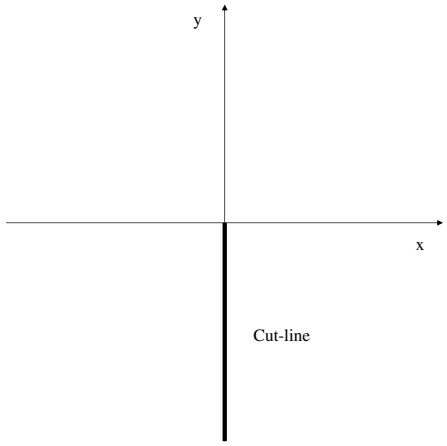

Figure 9.1: The definition of $\log^+ z$.

where we used $\lim_{R\to\infty} \log^+(\frac{\mathrm{i}\nu - R}{-\mathrm{i}\nu_0 - R}) \to 0$.

Finally, the equation (9.67) is obtained as:

$$\mathcal{P}_0 f(\nu, E) = \frac{\mathrm{i}}{2\pi\nu_0(\nu_0^* - \nu)} \log^+(\frac{\nu}{\nu_0^*}) - \frac{\mathrm{i}}{2\pi\nu_0^*(\nu + \nu_0)} \log^+(-\frac{\nu}{\nu_0}) + \begin{cases} [\frac{1}{\nu_0(\nu_0^* - \nu)} - \frac{1}{\nu_0^*(\nu_0 + \nu)}], & E < \widetilde{\omega}_1 \\ 0, & E > \widetilde{\omega}_1. \end{cases} \tag{9.71}$$

Thus, we have shown that at time equal to zero the projection of $f(\nu, E)$, i.e. $\mathcal{P}_0 f(\nu, E)$, is a Hardy class function in the upper plane. This verifies the general theorem about the properties of the unstable states associated to time operator, as being in the upper Hardy class[92].

By the above result we can calculate the survival probability at time equal to zero. It is obtained as:

$$\begin{aligned} \|\mathcal{P}_0 f\|^2 &= \int_0^\infty dE \int_{-\infty}^{+\infty} |\mathcal{P}_0 f(\nu, E)|^2 d\nu \\ &= \frac{2\pi(2\widetilde{\omega}_1/\gamma)}{\widetilde{\omega}_1^2 + (\gamma/2)^2} \end{aligned} \tag{9.72}$$

and

$$p_\rho(0) = |A|^2 \|\mathcal{P}_0 f\|^2 = \frac{\pi}{2(\frac{\pi}{2} + \arctan(2\widetilde{\omega}_1/\gamma))^2} \frac{2\widetilde{\omega}_1/\gamma}{(2\widetilde{\omega}_1/\gamma)^2 + 1} \tag{9.73}$$

which shows that $\mathcal{P}_0 f \neq f$. Since the equality would imply that $p_\rho(0) = 1$.

9.5 Short time behavior of survival probability

To study the Zeno effect for short times we shall obtain the behavior of the survival probability $p_\rho(-s)$, $(s < 0)$ in the short time, using the following approximation [102]

$$\begin{aligned}
\lim_{s\to 0}\int_{-\infty}^{0}\frac{e^{-st}}{t+z}dt &= -\lim_{s\to 0} e^{sz}\int_{-sz}^{\infty}\frac{e^{t}}{t}dt \\
&= -\lim_{s\to 0} e^{sz}[\gamma_e + \log(sz) + \sum_{k=1}^{\infty}\frac{(-sz)^k}{k!k}], \quad |\arg(-sz)| < \pi, \text{and } |z| < \infty. \\
&\sim -e^{sz}[\gamma_e + \log(sz) - sz + \cdots] \qquad (9.74)
\end{aligned}$$

which is valid in the plane cut along the positive real axis. Here $\gamma_e = 0.577215\ldots$ is Euler's constant, since it is not important in our computation for simplicity we take $\gamma_e \approx \frac{1}{2}$.

Now, using (9.75) for the evaluation of (9.65) we can write this equation as $s \to 0$ as,

$$\mathcal{P}_s f(\nu, E) \sim e^{\mathrm{i}s\nu}[\mathcal{P}_0 f(\nu, E) + sg(\nu, \nu_0) + \cdots] \qquad (9.75)$$

where the first order of s is sufficient for our computation (see after equation (9.80)), $\mathcal{P}_0 f(\nu, E)$ is defined by (9.71) and

$$g(\nu, \nu_0) = \frac{3(1 + 2a - 4\mathrm{i}ab)\nu + 2a|\nu_0|^2}{4\pi|\nu_0|^2(\nu_0^* - \nu)(\nu_0 + \nu)} + \begin{cases} \frac{2a(\mathrm{i}|\nu_0|^2 + 2b\nu)}{|\nu_0|^2(\nu_0^* - \nu)(\nu_0 + \nu)}, & E < \widetilde{\omega}_1 \\ \\ 0, & E > \widetilde{\omega}_1. \end{cases} \qquad (9.76)$$

is a square integrable function. Now, the survival probability can be obtained by computation of

$$\begin{aligned}
p_\rho(-s) &= |A|^2\|\mathcal{P}_s f\|^2 \\
&\simeq |A|^2\Big[\|\mathcal{P}_0 f(\nu, E)\|^2 + sg_1(\widetilde{\omega}_1, \gamma) + s^2 g_2(\widetilde{\omega}_1, \gamma) + \cdots\Big]
\end{aligned} \qquad (9.77)$$

where

$$g_1(\widetilde{\omega}_1, \gamma) = \int_0^\infty dE \int_{-\infty}^\infty (g^*(\nu, \nu_0)\mathcal{P}_0 f(\nu, E) + \text{C.C.})d\nu \tag{9.78}$$

and

$$g_2(\widetilde{\omega}_1, \gamma) = \int_0^\infty dE \int_{-\infty}^\infty |g(\nu, \nu_0)|^2 d\nu \tag{9.79}$$

where $g_1(\widetilde{\omega}_1, \gamma)$ and $g_2(\widetilde{\omega}_1, \gamma)$ are the finite nonzero functions. Thus,

$$\frac{\partial}{\partial s} q_\rho(-s)\Big]_{s=0} = |A|^2 g_1(\widetilde{\omega}_1, \gamma). \tag{9.80}$$

where $q_\rho(-s)$ is the decay probability which is defined in the (9.16). In fact, in the equation (9.75) we do not need the higher order of s, because the differentials relative to s of order greater than of s in equation at $s = 0$ are zero. The above result coincides with the result of the case $s = 0$ (9.73).

The above equation shows that for short time limit $\frac{\partial}{\partial s} p_\rho(-s)]_{s=0} \neq 0$ which means that at sufficiently small time the survival probability behaves as would be expected on the basis of exponential decay law[2], i.e. this case does not correspond to quantum mechanical Zeno effect.

9.6 Asymptotical behavior of the survival probability for $t = -s \to \infty$

We shall study the asymptotical behavior of quantity $p_\rho(-s)$. By using equations (9.65) and (9.59) and the approximations for $s \to -\infty$ which is shown in Appendix C, we obtain the decay of the probability as:

$$\begin{aligned} p_{\rho_{11}}(-s) &= \|\mathcal{P}_s \rho_{11}\|^2 = \int_0^\infty dE \int_{-\infty}^{+\infty} |\mathcal{P}_s \rho_{11}(\nu, E)|^2 d\nu \\ &\sim |A|^2 [\frac{h(\gamma, \widetilde{\omega}_1)}{s^4} + \frac{h_2(\gamma, \widetilde{\omega}_1)}{s^2} + e^{\gamma s} h_1(s, \gamma, \widetilde{\omega}_1)] \end{aligned} \tag{9.81}$$

[2]In the exponential decay law the survival probability is $\sim e^{-\gamma t}$, $t > 0$ and $t = -s$. Consequently, the decay probability is equal to $q_\rho(t) = 1 - e^{-\gamma t}$, then, we have $\frac{\partial}{\partial t} q_\rho(t)]_{t=0} = \gamma$. However, In Zeno effect the continuous measurement effects does not allow the particle to decay as $\frac{\partial}{\partial t} q_\rho(t)]_{t=0} = 0$ [94, 95].

where:

$$\begin{aligned} h(\gamma,\widetilde{\omega}_1) &= (\frac{1}{\pi(\gamma/2)^6})\big[\frac{32}{105}+\frac{53\pi}{128}-\frac{53\beta}{64}-\frac{25}{64}\sin\beta \\ &- \frac{41}{64}\sin 2\beta-\frac{23}{192}\sin 3\beta-\frac{5}{32}\sin 4\beta-\frac{13}{320}\sin 5\beta-\frac{7}{192}\sin 6\beta \\ &- \frac{3}{448}\sin 7\beta-\frac{21}{3584}\sin 8\beta+\frac{2}{7(\gamma/2)}\frac{1}{(1+\frac{\widetilde{\omega}_1^2}{(\gamma/2)^2})^{7/2}}\big], \end{aligned} \tag{9.82}$$

$$h_1(s,\gamma,\widetilde{\omega}_1)=\frac{2\pi}{\gamma^2}\left(-2\arctan\beta+\frac{1}{\gamma s}+\frac{\gamma\sin 2\widetilde{\omega}_1 s}{s(\widetilde{\omega}_1^2+\frac{\gamma^2}{4})}+\frac{(\widetilde{\omega}_1^2-\frac{\gamma^2}{4})\cos 2\widetilde{\omega}_1 s-\gamma\widetilde{\omega}_1\sin 2\widetilde{\omega}_1 s}{s(\widetilde{\omega}_1^2+\frac{\gamma^2}{4})^2}\right) \tag{9.83}$$

and

$$h_2(\gamma,\widetilde{\omega}_1)=\frac{32}{\gamma^3}\left(-\frac{1}{3\big(1+\frac{\widetilde{\omega}_1^2}{(\gamma/2)^2}\big)^{3/2}}+\frac{1}{3}-\frac{3\beta}{8}-\frac{1}{4}\sin 2\beta-\frac{1}{32}\sin 4\beta\right) \tag{9.84}$$

where $\beta=\arctan(\frac{-2\widetilde{\omega}_1}{\gamma})$.

Equation (9.81) shows an algebraically decreasing function and an exponentially decreasing oscillating functions.

9.7 Conclusion

We have studied the projection of the initial pure state $\rho(t)=|\psi_t\rangle\langle\psi_t|$, onto unstable state space of time operator. Since $\mathcal{P}_0\rho$ is not factorizable each of these states has a positive von Neumann entropy, where the von Neumann entropy of ρ is $\mathcal{S}_{vn}=-\mathrm{Tr}(\rho\log\rho)$. Moreover, the entropy of $\mathcal{P}_0\rho(t)$ increases to zero when $t\to\infty$.

Our result shows that the survival probability is decreasing like an exponential function for short time and both algebraically and exponentially for long time. We have also shown that the action of the projection operator in the Friedrichs model is to eleminate the Zeno effect. That is one of the major effects of using time operator on unstable states. This is not surprising since the effect of the projection operator $\mathcal{P}_0$ is to prepare the system in an unstable state. Preparation in experimental high energy physics is currently used (see [99, 100, 103]). Although, the Zeno effect has been observed in some cases, its universality is far from being verified.

It would be interesting to compute if from (9.75) and (9.77), the short time estimate of the survival probability turns out to be less than purely exponentially decreasing function of time which corresponds to quantum anti-Zeno effect [63, 104].

Recently, we have studied 2-level Friedrichs model with weak coupling interaction for kaonic system [105, 106]. In the next publication, we shall consider 2-level or n-level Friedrichs by using time super-operator in the Liouville space to study decoherence of kaonic particles.

9.8 Appendix A

In the usual formulation of the Friedrichs model, the border line between system and environment is ill defined because the Hilbert spaces associated to those degrees of freedom is not the tensorial product of their respective Hilbert spaces but is rather their direct sum. Nevertheless it is possible, as we shall see below, to imbed the direct sum of the Hilbert spaces associated to the discrete and continuous degrees of freedom into a larger space in which those subspaces (tensorially) factorize, and to formulate an equivalent Hamiltonian dynamics that contains as a special subset of solutions all the solutions of the original model.

This modified Friedrichs model can be explained heuristically as follows. Instead of representing the state of the system at time t by a direct sum of the Hilbert spaces associated to the discrete and continuous degrees of freedom, we imbed it into the tensorial products of a two-dimensional Hilbert space $\mathcal{H}^2$ (that corresponds to the discrete level plus their decay product) and of a Fock space; $\mathcal{H}^2 \bigotimes \mathcal{H}_{\text{photon}}$,

$$\psi_{\text{discret}} = \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} \text{ and } \psi_{\text{photon}} = \begin{pmatrix} f^0 \\ f^1(\mu') \\ f^2(\mu', \mu'') \\ \dots \end{pmatrix} \text{ and the state is given by:}$$

$$\Psi_{0,1,\mu^i} = \begin{pmatrix} f_0 \\ 0 \end{pmatrix} \bigotimes \begin{pmatrix} 0 \\ f^1(\mu') \\ f^2(\mu', \mu'') \\ \vdots \\ f^2(\mu', \mu'', \dots, \mu^{(n)}) \\ \dots \end{pmatrix} + \begin{pmatrix} 0 \\ f_1 \end{pmatrix} \bigotimes \begin{pmatrix} f^0 \\ 0 \\ \vdots \end{pmatrix} \tag{9.85}$$

where f_0 represents the amplitude of a new discrete state $|0\rangle$ that is assumed to contain the "decay products" resulting from the disintegration of the discrete kaonic state $|1\rangle$; besides, $f^n(\mu', \mu'', \dots, \mu^{(n)})$ $(n = 1, 2, \dots)$ represents the amplitude of the n environment particles.

Now that we defined our representation of the state of the system, we can define the free Hamiltonian:

$$H_0 = \begin{pmatrix} \omega_1 & 0 \\ 0 & \mu \end{pmatrix} \otimes Id.^{\mu} + Id.^{0,1} \otimes \mu a^{\dagger}.a \tag{9.86}$$

The first part of it represents the energies of the discrete mode, while the second one contains the energies of the excited modes. Here the operators $a^{\dagger}.a$ count the number of excitations in the mode μ.

The interaction Hamiltonian, $H_{\text{int}} = \lambda V$, is equal to

$$H_{\text{int}} = \begin{pmatrix} 0 & \lambda v(\mu) \\ 0 & 0 \end{pmatrix} \otimes a^{\dagger} + \begin{pmatrix} 0 & 0 \\ \lambda v^*(\mu) & 0 \end{pmatrix} \otimes a. \tag{9.87}$$

In analogy with quantum optics, this interaction represents the decay of the kaonic "excited" state (1) to the "ground" state (0), with excitation of a mode of energy (μ) while by unitarity the inverse process is also possible (diminution of the energy of a continuous mode by one quantum of energy μ (here $\hbar = 1$), and repopulation of

the discrete state $|1\rangle$). If the initial state is such that no continuous mode is excited $(f^i(\mu^{'}, \mu^{''}, \ldots, \mu^{(i)}, t = 0) = 0 \forall i > 0)$, then, the dynamics of the state $\Psi_{0,1,\mu}(t)$ is considerably simplified because there will never occur more than one excitation.

In that case $f_1(t)$ and $f^1(\mu, t))$ obey a closed system of three equations:

$$\omega_1 f_1(t) + \lambda \int d\mu v^*(\mu) f^1(\mu, t) = \mathrm{i}\frac{\partial f_1(t)}{\partial t}, \tag{9.88}$$

and

$$\lambda v(\mu) f_1(t) + \mu f^1(\mu, t) = \mathrm{i}\frac{\partial f^1(\mu, t)}{\partial t}. \tag{9.89}$$

where we used $\langle v(\mu), f^1(\mu)\rangle = \int d\mu v^*(\mu) f^1(\mu)$, and the components f_0 and f^0 remain unaffected on the evolution so we take them equal to 1, all the other modes are zero.

9.9 Appendix B

To obtain the $G_s(\nu, E)$, at first, we take the principal value integral in the equation (9.64), i.e.

$$\mathsf{P}\int_0^{+\infty} \frac{e^{\mathrm{i}sx}}{\nu_0^*(x-\nu)(\nu_0 + x)}\, dx, \tag{9.90}$$

using the contour of the Fig. 9.2, we have

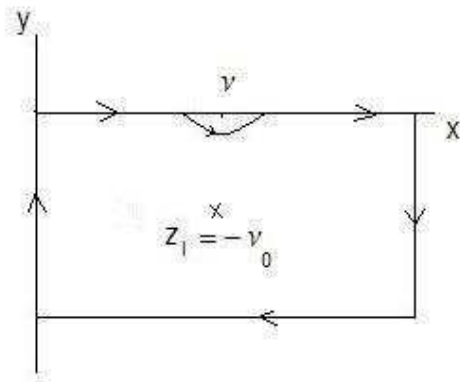

Figure 9.2: .

$$\oint \frac{e^{\mathrm{i}sz}}{\nu_0^*(z-\nu)(\nu_0+z)}\,dy = \lim_{\epsilon\to 0}\lim_{R\to\infty}\Bigg(\int_0^{\nu-\epsilon}+\int_{c_1}+\int_{\nu+\epsilon}^{R}+\int_0^{-R}+\int_R^0 + \int_{-R}^{0}\frac{e^{-sy}}{\nu_0^*(\mathrm{i}y-\nu)(\nu_0+\mathrm{i}y)}\,\mathrm{i}dy\Bigg) = 2\pi\mathrm{i}\sum a_{-1}. \tag{9.91}$$

We note that for $a<0$, i.e. $E<\widetilde{\omega}_1$ we have a simple pole as $z_I=-\nu_0$, then, its residues is $a_{-1}=\frac{-2\pi\mathrm{i}e^{-\mathrm{i}s\nu_0}}{\nu_0^*(\nu_0+\nu)}$, and for $a>0$, i.e. $E>\widetilde{\omega}_1$, we do not have any pole in the contours then, $a_{-1}=0$. Here the fourth and fifth integrals in the above equation are zeros, and the second integral gives:

$$\int_{c_1} = \lim_{\epsilon\to 0}\int_{\pi}^{2\pi}\frac{e^{\mathrm{i}s\epsilon e^{\mathrm{i}\theta}}}{\nu_0^*((\nu+\epsilon e^{\mathrm{i}\theta})-\nu)(\nu_0+(\nu+\epsilon e^{\mathrm{i}\theta}))}\mathrm{i}\epsilon e^{\mathrm{i}\theta}d\theta = \frac{\pi\mathrm{i}}{\nu_0^*(\nu_0+\nu)}. \tag{9.92}$$

Finally we have

$$\mathsf{P}\int_0^{+\infty}\frac{e^{\mathrm{i}sx}}{\nu_0^*(x-\nu)(\nu_0+x)}\,dx = \frac{-\pi\mathrm{i}}{\nu_0^*(\nu+\nu_0)} + \lim_{R\to\infty}\frac{\mathrm{i}}{\nu_0^*}\int_{-R}^{0}\frac{e^{-sy}}{(y+\mathrm{i}\nu)(y-\mathrm{i}\nu_0)}\,dy + \begin{cases}\frac{2\pi\mathrm{i}e^{-\mathrm{i}s\nu_0}}{\nu_0^*(\nu_0+\nu)} & E<\widetilde{\omega}_1\\ 0 & E>\widetilde{\omega}_1,\end{cases} \tag{9.93}$$

and the integral in the right-hand-side becomes:

$$\int_{-R}^{0}\frac{e^{-sy}}{(y+\mathrm{i}\nu)(y-\mathrm{i}\nu_0)}\,dy = \frac{\mathrm{i}}{\nu+\nu_0}\Bigg(\int_{-R}^{0}\frac{e^{-sy}}{y-\mathrm{i}\nu_0}dy - \int_{-R}^{0}\frac{e^{-sy}}{y+\mathrm{i}\nu}dy\Bigg). \tag{9.94}$$

To calculate the first integral in (9.64), i.e.

$$\int_{-\infty}^{0}\frac{e^{\mathrm{i}sx}}{\nu_0(x-\nu)(\nu_0^*-x)}\,dx. \tag{9.95}$$

we use the contour of the Fig. 9.3, the above integral can be written as

$$\oint\frac{e^{\mathrm{i}sz}}{\nu_0(z-\nu)(\nu_0^*-z)}\,dz = \lim_{R\to\infty}\int_{-R}^{0}\frac{e^{-sy}}{\nu_0(\mathrm{i}y-\nu)(\nu_0^*-\mathrm{i}y)}\,\mathrm{i}dy = 2\pi\mathrm{i}\sum a_{-1}\ , \tag{9.96}$$

where the other terms in above integration are zero. By using the contour in Fig. 9.3 we have a simple pole as $z_{II}=\nu_0^*$ for $a<0$, i.e. $E<\widetilde{\omega}_1$ and corresponding residues

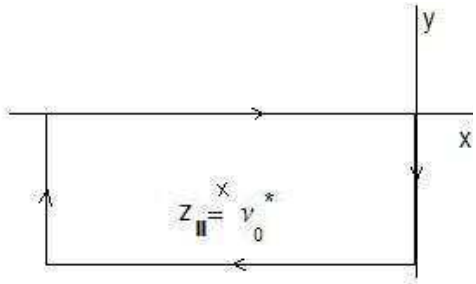

Figure 9.3: .

is $a_{-1} = \frac{2\pi i e^{is\nu_0^*}}{\nu_0(\nu_0^* - \nu)}$. It has no pole for $a > 0$, i.e. $E > \widetilde{\omega}_1$ and $a_{-1} = 0$. Thus, we have

$$\begin{aligned}\int_{-\infty}^{0} \frac{e^{isx}}{\nu_0(x-\nu)(\nu_0^* - x)}\, dx &= \frac{1}{\nu_0^* - \nu}\left(\int_{-R}^{0} \frac{e^{-sy}}{y + i\nu_0^*} dy - \int_{-R}^{0} \frac{e^{-sy}}{y + i\nu} dy\right) \\ &+ \begin{cases} \frac{2\pi i e^{is\nu_0^*}}{\nu_0(\nu_0^* - \nu)} & E < \widetilde{\omega}_1 \\ 0 & E > \widetilde{\omega}_1. \end{cases}\end{aligned} \tag{9.97}$$

Now, by using the equations (9.32), (9.60), (9.64), (9.93), (9.94) and (9.97) we can obtain equation (9.65).

9.10 Appendix C

To prove the equation (9.81). In the first step, we use the following approximation as $s \to -\infty$

$$\begin{aligned}\int_{-\infty}^{0} \frac{e^{-sz}}{y+z} dy &= e^{sx} \int_{-\infty}^{z} \frac{e^{-su}}{u} du \\ &= e^{sz}\left\{\left[\frac{e^{-su}}{-su}\right]_{-\infty}^{z} - \int_{-\infty}^{z} \frac{e^{-su}}{su^2}\, du\right\} \\ &= \frac{1}{(-zs)}\left[1 + \frac{1}{(-zs)} + \frac{2!}{(-zs)^2} + \cdots + \frac{n!}{(-zs)^n} + r_n(-zs)\right]\end{aligned} \tag{9.98}$$

where the last result was obtained by integral part by part repetitions, z can be a complex number, and

$$r_n(z) = (n+1)!ze^{-z}\int_{-\infty}^{z}\frac{e^t}{t^{n+2}}dt. \tag{9.99}$$

Let $z = x + \mathrm{i}y$ then along the segment $t = \sigma + \mathrm{i}y$ $(-\infty < \sigma \leq x,\ x \leq 0)$ we have ,

$$|e^{t-z}| = e^{\sigma - x}, \qquad |t| \geq |z| \tag{9.100}$$

and hence

$$|r_n(z)| \leq \frac{(n+1)!}{|z|^{n+1}}\int_{-\infty}^{x} e^{\sigma-x}d\sigma = \frac{(n+1)!}{|z|^{n+1}} = O(|z|^{-n-1}). \tag{9.101}$$

Therefore we have the asymptotic representation

$$\int_{-\infty}^{0}\frac{e^{-sz}}{y+z}dy = \frac{1}{(-sz)}[\sum_{k=0}^{n}\frac{k!}{(-sz)^k} + O(|sz|^{-n-1})]. \tag{9.102}$$

It follows from (9.102) that the convergent series

$$\frac{1}{(-sz)}\sum_{k=0}^{n}\frac{k!}{(-sz)^k} \tag{9.103}$$

is asymptotic series for $\int_{-\infty}^{0}\frac{e^{-sz}}{y+z}dy$, and we have the estimate

$$|r_n(-sz)| \leq \frac{(n+1)!}{|-sz|^{n+1}} \tag{9.104}$$

In this case the error committed in approximation of $\int_{-\infty}^{0}\frac{e^{-sz}}{y+z}dy$ by the finite number of terms does not exceed the first neglected term in absolute value [102].

Finally, as follows we show that $|r_n(z)| = r_n(|z|)$:

$$\begin{aligned} r_n(|z|) &= (n+1)!|z|e^{-|z|}\int_{-\infty}^{|z|}\frac{e^t}{t^{n+2}}dt \\ &\leq (n+1)!|z|\int_{-\infty}^{|z|}\frac{e^{t-|z|}}{|z|^{n+2}}dt \\ &\leq \frac{(n+1)!}{|z|^{n+1}} \end{aligned} \tag{9.105}$$

where for $r_n(|z|)$ we arrived at the same relation as we arrived at for $|r_n(z)|$ in (9.104), which means that not only we can replace $r_n(|z|)$ by $|r_n(z)|$ and vice versa but also we can show

$$r_n(z) = r_n(|z|e^{\mathrm{i}\theta}) = |r_n(z)|e^{\mathrm{i}\theta} \tag{9.106}$$

where $\theta = \arg(z)$. Thus, the four integrals in equation (9.65), can be written as:

$$\begin{aligned}
\mathfrak{I} \;\sim\; & \frac{-1}{\nu_0(\nu_0^* - \nu)}\Big[\Big(\frac{1}{(-\mathrm{i}\nu_0^* s)} + \frac{1}{(-\mathrm{i}\nu_0^* s)^2} + r_1(-\mathrm{i}\nu_0^* s)\Big) - \Big(\frac{1}{(-\mathrm{i}\nu s)} + \frac{1}{(-\mathrm{i}\nu s)^2} + r_1(-\mathrm{i}\nu s)\Big)\Big] \\
+ \; & \frac{1}{\nu_0^*(\nu_0 + \nu)}\Big[\Big(\frac{1}{(\mathrm{i}\nu_0 s)} + \frac{1}{(\mathrm{i}\nu_0 s)^2} + r_1(\mathrm{i}\nu_0 s)\Big) - \Big(\frac{1}{(-\mathrm{i}\nu s)} + \frac{1}{(-\mathrm{i}\nu s)^2} + r_1(-\mathrm{i}\nu s)\Big)\Big] \\
\sim \; & \frac{-2a}{|\nu_0|^4 \nu s^2} - \frac{1}{\nu_0(\nu_0^* - \nu)}\big(r_1(-\mathrm{i}\nu_0^* s) - r_1(-\mathrm{i}\nu s)\big) + \frac{1}{\nu_0^*(\nu_0 + \nu)}\big(r_1(\mathrm{i}\nu_0 s) - r_1(-\mathrm{i}\nu s)\big).
\end{aligned} \tag{9.107}$$

by using (9.106) we obtain

$$\begin{aligned}
\mathfrak{I} \sim \frac{-2a}{|\nu_0|^4 \nu s^2} \; & + \; \Big(-\frac{e^{-\mathrm{i}\delta}}{\nu_0(\nu_0^* - \nu)} + \frac{e^{\mathrm{i}\delta}}{\nu_0^*(\nu_0 + \nu)}\Big)|r_1(\mathrm{i}\nu_0 s)| \\
& - \; \Big(-\frac{1}{\nu_0(\nu_0^* - \nu)} + \frac{1}{\nu_0^*(\nu_0 + \nu)}\Big)e^{i\pi/2}|r_1(-\mathrm{i}\nu s)|
\end{aligned} \tag{9.108}$$

where $\delta = \arg(\nu_0) = \arctan(\frac{b}{a})$. Similarly, we can write $\mathfrak{I}^*$ as:

$$\begin{aligned}
\mathfrak{I}^* \sim \frac{-2a}{|\nu_0|^4 \nu s^2} \; & + \; \Big(-\frac{e^{\mathrm{i}\delta}}{\nu_0^*(\nu_0 - \nu)} + \frac{e^{-\mathrm{i}\delta}}{\nu_0(\nu_0^* + \nu)}\Big)|r_1(\mathrm{i}\nu_0 s)| \\
& - \; \Big(-\frac{1}{\nu_0^*(\nu_0 - \nu)} + \frac{1}{\nu_0(\nu_0^* + \nu)}\Big)e^{-i\pi/2}|r_1(-\mathrm{i}\nu s)|.
\end{aligned} \tag{9.109}$$

Now,

$$\mathfrak{I}^2 = \mathfrak{I}^*\mathfrak{I} \sim \mathfrak{I}_1 + \mathfrak{I}_2 + \mathfrak{I}_3 + \mathfrak{I}_4 \tag{9.110}$$

where

$$|\mathfrak{I}_1|^2 = \frac{-4a^2}{|\nu_0|^8\nu^2 s^4} + \Big(\frac{1}{|\nu_0|^2|\nu_0^*-\nu|^2} + \frac{1}{|\nu_0|^2|\nu_0+\nu|^2}\Big)\big(|r_1(\mathrm{i}\nu_0 s)|^2 + |r_1(-\mathrm{i}\nu s)|^2\big) \tag{9.111}$$

$$\begin{aligned}|\mathfrak{I}_2|^2 &= \frac{-2a}{|\nu_0|^4\nu s^2}\Big[\Big(-\frac{e^{-\mathrm{i}\delta}}{\nu_0(\nu_0^*-\nu)} + \frac{e^{\mathrm{i}\delta}}{\nu_0^*(\nu_0+\nu)} + \text{c.c.}\Big)|r_1(\mathrm{i}\nu_0 s)| \\ &\quad -\mathrm{i}\Big(-\frac{1}{\nu_0(\nu_0^*-\nu)} + \frac{1}{\nu_0^*(\nu_0+\nu)} - \text{c.c.}\Big)|r_1(-\mathrm{i}\nu s)|\Big]\end{aligned} \tag{9.112}$$

$$\begin{aligned}|\mathfrak{I}_3|^2 &= \Big(-\frac{e^{-2\mathrm{i}\delta}}{\nu_0^2(\nu_0^{*2}-\nu^2)} + \frac{e^{2\mathrm{i}\delta}}{\nu_0^{*2}(\nu_0^2-\nu^2)}\Big)|r_1(\mathrm{i}\nu_0 s)|^2 \\ &\quad -\Big(-\frac{1}{\nu_0^2(\nu_0^{*2}-\nu^2)} + \frac{1}{\nu_0^{*2}(\nu_0^2-\nu^2)}\Big)|r_1(-\mathrm{i}\nu s)|^2\end{aligned} \tag{9.113}$$

$$\begin{aligned}|\mathfrak{I}_4|^2 &= -\mathrm{i}\Big(\frac{e^{-\mathrm{i}\delta}}{|\nu_0|^2|\nu_0^*-\nu|^2} + \frac{e^{\mathrm{i}\delta}}{|\nu_0|^2|\nu_0+\nu|^2} \\ &\quad -\frac{e^{-\mathrm{i}\delta}}{\nu_0^2(\nu_0^{*2}-\nu^2)} - \frac{e^{\mathrm{i}\delta}}{\nu_0^{*2}(\nu_0^2-\nu^2)}\Big)|r_1(\mathrm{i}\nu s)||r_1(\mathrm{i}\nu_0 s)|\end{aligned} \tag{9.114}$$

where "c.c." is indicated to "complex conjugate". Now, we replace $|r_1(z)| \sim \frac{2}{|z_1|^2}$ from (9.104), in the above equations and then we calculate $\int_{-\infty}^{+\infty}|\mathfrak{I}_i|^2 d\nu,\ i = 1,\ldots,4$. After, taking some contour integrations we obtain:

$$\int_{-\infty}^{\infty}|\mathfrak{I}|^2 d\nu \sim \Big(\frac{4\pi}{|\nu_0|^6 s^4}\Big)\Big(\frac{2}{b} - \frac{5b}{|\nu_0|^2} + \frac{6b^3}{|\nu_0|^4} + \frac{3b^2}{|\nu_0|^2} - \frac{2}{|\nu_0|} - \frac{2ab}{|\nu_0|^3}\Big). \tag{9.115}$$

Now, we shall take the integral on $E(0 \le E < \infty)$ of the above equation. But at first, we remember the two following integrals:

$$\begin{aligned}\int_0^{\infty}\frac{dE}{|\nu_0|^n} &= \int_0^{\infty}\frac{dE}{(E-\widetilde{\omega}_1)^2+b^2)^{n/2}} \\ &= \int_{-\widetilde{\omega}_1}^{\infty}\frac{du}{(u^2+b^2)^{n/2}}, \quad (u = E-\widetilde{\omega}_1) \\ &= \frac{1}{b^{n-1}}\int_{\beta}^{\frac{\pi}{2}}\cos^{n-2}\theta d\theta, \quad (b\tan\theta = u).\end{aligned} \tag{9.116}$$

and

$$\begin{aligned}\int_0^{\infty}\frac{a}{|\nu_0|^n}\,dE &= \int_0^{\infty}\frac{(E-\widetilde{\omega}_1)}{(E-\widetilde{\omega}_1)^2+b^2)^{n/2}}\,dE \\ &= \frac{1}{2(\frac{n}{2}-1)(\widetilde{\omega}_1^2+b^2)^{n/2-1}}\,, \qquad (n \neq 1).\end{aligned} \tag{9.117}$$

where $\beta = \arctan(\frac{-\widetilde{\omega}_1}{b})$. Then, we arrive at $h(\gamma, \widetilde{\omega}_1)/s^4$ where $h(\gamma, \widetilde{\omega}_1)$ is defined in(9.82).

Now, we compute the square of the remainder (non-integral) part of the equation (9.65) called $\mathfrak{I}_R$.

$$|\mathfrak{I}_R|^2 = \begin{cases} |e^{-\mathrm{i}s\nu}[\frac{e^{\mathrm{i}s\nu_0^*}}{\nu_0(\nu_0^*-\nu)} - \frac{e^{-\mathrm{i}s\nu_0}}{\nu_0^*(\nu_0+\nu)}]|^2, & E < \widetilde{\omega}_1 \\ \\ 0, & E > \widetilde{\omega}_1. \end{cases} \tag{9.118}$$

Then integrating on ν yields:

$$\int_{-\infty}^{+\infty} |\mathfrak{I}_R|^2 d\nu = \begin{cases} \frac{\pi e^{\gamma s}}{|\nu_0|^2}[\frac{2}{\gamma} - \frac{\mathrm{i}e^{2\mathrm{i}(E-\widetilde{\omega}_1)s}}{\nu_0^*} + \frac{\mathrm{i}e^{-2\mathrm{i}(E-\widetilde{\omega}_1)s}}{\nu_0}], & E < \widetilde{\omega}_1 \\ 0, & E > \widetilde{\omega}_1. \end{cases} \tag{9.119}$$

Finally, by integrating on E from 0 to ∞ and by using the above relation we obtain

$$\int_0^{\widetilde{\omega}_1} dE \int_{-\infty}^{+\infty} |\mathfrak{I}_R|^2 d\nu \sim h_1(s, \gamma, \widetilde{\omega}_1) e^{\gamma s} \tag{9.120}$$

where $h_1(s, \gamma, \widetilde{\omega}_1)$ is defined in (9.83).

In the last step we must computed $\int_0^{+\infty} dE \int_{-\infty}^{+\infty} d\nu(\mathfrak{I}_R^* \mathfrak{I} + \text{c.c.})$. First, we calculate the integral on ν, it is obtained.

$$\int_{-\infty}^{+\infty} (\mathfrak{I}_R^* \mathfrak{I} + \text{c.c.}) d\nu = \frac{4\pi}{|\nu_0|^5 s^2}(-\frac{a}{b} + \frac{b}{|\nu_0|}). \tag{9.121}$$

Taking integral on E yields:

$$\int_0^{\widetilde{\omega}_1} dE \int_{-\infty}^{+\infty} (\mathfrak{I}_R^* \mathfrak{I} + \text{c.c.}) d\nu = \frac{h_2(\gamma, \widetilde{\omega}_1)}{s^2} \tag{9.122}$$

where $h_2(\gamma, \widetilde{\omega}_1)$ is defined in (9.84). We note that the integration on E in (9.122) is taken between 0 and $\widetilde{\omega}_1$ because for $E > \widetilde{\omega}_1$ we have $\mathfrak{I}_R = 0$.

By adding all the terms we have

$$\int_0^{\infty} dE \int_{-\infty}^{+\infty} |\mathcal{P}_s f(\nu, E)|^2 d\nu \sim \frac{h(\gamma, \widetilde{\omega}_1)}{s^4} + \frac{h_2(\gamma, \widetilde{\omega}_1)}{s^2} + e^{\gamma s} h_1(s, \gamma, \widetilde{\omega}_1), \tag{9.123}$$

and finally, we can obtain (9.81).

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