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– Appendices –

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Contents

Appendix A

Definitions, conventions and properties

Abstract: This chapter presents all mathematical objects that are used throughout the main dissertation and the present appendices. Extra care is enforced to define a consistent set of equations, in particular regarding phase and normalization conventions. Additionnally, building blocks that are required for a partial wave expansion of a given function are introduced. Many formulæ come from Refs. [1–3].

Contents

A.1 Common operators

$\bar{f}(r)$	Radial part of an arbitrary function $f(\vec{r})$
$[L]$	Degeneracy $[L] = 2L + 1$
$L^{\pm}$	Shortcut for $L \pm 1$
$\|1 : i, 2 : j\rangle$	Normalized non-antisymmetrized two-particle product state
$\|i\, j\rangle$	Normalized antisymmetrized two-particle product state $\|i\, j\rangle = \hat{a}_i^\dagger\, \hat{a}_j^\dagger\, \|0\rangle = \dfrac{\|1 : i, 2 : j\rangle - \|1 : j, 2 : i\rangle}{\sqrt{2}}$
$P_{\vec{r}/\sigma/\tau}$	Position/spin/isospin-flip operator $P_{\vec{r}}\, \|1 : \vec{r}\,\sigma\, q, 2 : \vec{r}\,'\,\sigma'\, q'\rangle = \|1 : \vec{r}\,'\,\sigma\, q, 2 : \vec{r}\,\sigma'\, q'\rangle$ $P_{\sigma}\, \|1 : \vec{r}\,\sigma\, q, 2 : \vec{r}\,'\,\sigma'\, q'\rangle = \|1 : \vec{r}\,\sigma'\, q, 2 : \vec{r}\,'\,\sigma\, q'\rangle$ $P_{\tau}\, \|1 : \vec{r}\,\sigma\, q, 2 : \vec{r}\,'\,\sigma'\, q'\rangle = \|1 : \vec{r}\,\sigma\, q', 2 : \vec{r}\,'\,\sigma'\, q\rangle$
P_{12}	Two-particle exchange operator $P_{12} = P_{\vec{r}}\, P_{\sigma}\, P_{\tau}$ $P_{12}\, \|1 : i, 2 : j\rangle = \|1 : j, 2 : i\rangle$
$\mathcal{A}_{12}$	Two-particle antisymmetrization operator $\mathcal{A}_{12} = \mathbb{I} - P_{12}$
$\mathcal{A}_{123}$	Three-particle antisymmetrization operator $\mathcal{A}_{123} = (\mathbb{I} + P_{23}P_{12} + P_{31}P_{12})(\mathbb{I} - P_{12})$
$\prod_{S/T/S_z/T_z}$	Projector on specific two-body spin/isospin state $\prod_{S} = \left[\dfrac{1 + (-1)^{1-S} P_{\sigma}}{2}\right]$ $\prod_{S_z} = \left[(1 - S_z^2) + \dfrac{1}{2}\, S_z\, S_z + (\dfrac{3}{2} S_z^2 - 1)\, S_z^2\right]$
$T^{[f]}$	Rank-k tensor
$T_{\mu}^{[f]}$	Component μ of a rank-k tensor
$[T_1 \otimes T_2]^{[k]\,\mu}$	Component μ of the rank-k tensorial product of two tensors T_1 and T_2

$\langle \ell_1\, m_1\, \ell_2\, m_2\, \vert \ell_1\, \ell_2\, \ell\, m\rangle$	Clebsh-Gordan coefficient
$\begin{pmatrix} \ell_1 & \ell_2 & \ell \\ m_1 & m_2 & m \end{pmatrix}$	Wigner $3j$ coefficient
$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{Bmatrix}$	Wigner $6j$ coefficient
$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix}$	Wigner $9j$ coefficient

To keep track of all angular momenta, the following short notations will be used in place of Dirac ones for a given operator O, where Υ denotes all other dependencies beyond the relative momenta $\vec{k}$ and $\vec{k}\,'$

$$\langle k\,(LS)JS_z\,TT_z|O(\Upsilon)|k'\,(L'S)JS_z\,TT_z\rangle \equiv \langle k\,|O^{JSS_zTT_z}_{LL'}(\Upsilon)|k'\,\rangle \equiv O^{JST}_{LL'}(k,k';\Upsilon)\,, \tag{A.1a}$$

$$\langle k\,(LS)J\,T|O(\Upsilon)|k'\,(L'S)J\,T\rangle \equiv \langle k\,|O^{JST}_{LL'}(\Upsilon)|k'\,\rangle \equiv O^{JST}_{LL'}(k,k';\Upsilon)\,, \tag{A.1b}$$

$$O^{LST}_{LL}(k,k';\Upsilon) \equiv O^{JST}_{L}(k,k';\Upsilon)\,. \qquad \text{(Uncoupled channels)} \tag{A.1c}$$

A.2 Mathematical functions

A.2.1 Clebsh-Gordan and Wigner coefficients

A.2.1.1 Transformation rules

In the following, we note $j = j_1 + j_2 + j_3$. One has then

$$\langle \ell_1\, m_1\, \ell_2\, m_2\, \vert \ell_1\, \ell_2\, \ell_3\, m_3\rangle = (-1)^{\ell_1-\ell_2-m_3}\,\sqrt{[\ell_3]}\,\langle \ell_1\, m_1\, \ell_2\, m_2\, \vert \ell_1\, \ell_2\, \ell_3\, -m_3\rangle\,, \tag{A.2a}$$

$$\langle \ell_1\, 0\, \ell_2\, 0\, \vert \ell_1\, \ell_2\, \ell\, 0\rangle = (-1)^{\ell_1+\ell_2}\,\sqrt{[\ell]}\begin{pmatrix} \ell_1 & \ell_2 & \ell \\ 0 & 0 & 0 \end{pmatrix}, \tag{A.2b}$$

$$\sum_{m_s\,m_j} \left\langle \ell'\, m_\ell\, s\, m_s \,\middle|\, \ell'\, s\, j\, m_j\right\rangle \langle \ell\, m_\ell\, s\, m_s\, \vert \ell\, s\, j\, m_j\rangle = \delta_{\ell\ell'}\,\frac{[j]}{[\ell]}\,, \tag{A.2c}$$

$$\begin{pmatrix} j' & 0 & j \\ -m'_j & 0 & m_j \end{pmatrix} = \delta_{jj'}\,\delta_{m_j m'_j}(-1)^{j-m}\,\frac{1}{\sqrt{[j]}}\,, \tag{A.2d}$$

$$\begin{pmatrix} j & j & 1 \\ m_j & -m_j & 0 \end{pmatrix} = (-1)^{j-m}\,\frac{m}{\sqrt{j\,(j+1)\,[j]}}\,, \tag{A.2e}$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = (-1)^{\frac{1}{2}J}\,\sqrt{\frac{(j_1+j_2-j_3)!(j_1-j_2+j_3)!(-j_1+j_2+j_3)!}{(j_1+j_2+j_3+1)!}} \times \frac{\left(\frac{1}{2}J\right)!}{\left(\frac{1}{2}J-j_1\right)!\left(\frac{1}{2}J-j_2\right)!\left(\frac{1}{2}J-j_3\right)!}\,, \tag{A.2f}$$

$$\begin{pmatrix} \ell & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} = (-1)^{\ell+\frac{1}{2}\ell'}\, \ell'! \sqrt{\frac{(2\ell-\ell')!}{(2\ell+\ell'+1)!}} \frac{\left(\ell+\frac{1}{2}\ell'\right)!}{\left(\frac{1}{2}\ell'\right)!\left(\frac{1}{2}\ell'\right)!\left(\ell-\frac{1}{2}\ell'\right)!} \qquad \text{for } \ell' \text{ even}\,, \tag{A.2g}$$

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ 0 & j_3 & j_2 \end{Bmatrix} = (-1)^J \frac{1}{\sqrt{[j_2][j_3]}}\,, \tag{A.2h}$$

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ 1 & j_3 & j_2 \end{Bmatrix} = (-1)^{J+1} \frac{2(j_2(j_2+1)+j_3(j_3+1)-j_1(j_1+1))}{\sqrt{2j_2(2j_2+1)(2j_2+2)2j_3(2j_3+1)(2j_3+2)}}\,, \tag{A.2i}$$

$$\begin{Bmatrix} f & f & 0 \\ d & c & e \\ b & a & e \end{Bmatrix} = \begin{Bmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{Bmatrix} = \frac{(-1)^{b+c+e+f}}{\sqrt{[e][f]}} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}. \tag{A.2j}$$

A.2.1.2 Specific values

$$\langle 2\,0\,1\,0\,|2\,1\,1\,0\rangle = \langle 1\,0\,2\,0\,|1\,2\,1\,0\rangle = -\sqrt{\frac{2}{5}}\,, \tag{A.3a}$$

$$\langle 3\,0\,1\,0\,|3\,1\,2\,0\rangle = -\sqrt{\frac{3}{7}} \qquad \langle 2\,0\,2\,0\,|2\,2\,2\,0\rangle = -\sqrt{\frac{2}{35}}\,, \tag{A.3b}$$

$$\begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} = -\frac{1}{\sqrt{3}} \qquad \begin{pmatrix} 2 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \sqrt{\frac{2}{15}} \qquad \begin{pmatrix} 3 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix} = -\sqrt{\frac{3}{35}}\,, \tag{A.3c}$$

$$\begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix} = \sqrt{\frac{2}{15}}\,, \tag{A.3d}$$

$$\begin{Bmatrix} 1 & 1 & 0 \\ 1 & 1 & 2 \end{Bmatrix} = \frac{1}{3} \qquad \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \end{Bmatrix} = \frac{1}{6} \qquad \begin{Bmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \end{Bmatrix} = \frac{1}{30}\,, \tag{A.3e}$$

$$\begin{Bmatrix} 2 & 1 & 0 \\ 1 & 0 & 2 \end{Bmatrix} = 0 \qquad \begin{Bmatrix} 2 & 1 & 1 \\ 1 & 0 & 2 \end{Bmatrix} = \frac{1}{\sqrt{15}} \qquad \begin{Bmatrix} 2 & 1 & 2 \\ 1 & 0 & 2 \end{Bmatrix} = 0\,, \tag{A.3f}$$

$$\begin{Bmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{Bmatrix} = -\begin{Bmatrix} 0 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{Bmatrix} = \frac{1}{3\sqrt{3}} \qquad \begin{Bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{Bmatrix} = -\begin{Bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{Bmatrix} = \frac{1}{9}\,, \tag{A.3g}$$

$$\begin{Bmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{Bmatrix} = \frac{1}{3\sqrt{3}} \qquad \begin{Bmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{Bmatrix} = -\frac{1}{6\sqrt{15}}\,,$$

$$\begin{Bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 2 & 2 & 1 \end{Bmatrix} = \frac{1}{6\sqrt{5}} \qquad \begin{Bmatrix} 3 & 3 & 0 \\ 1 & 1 & 1 \\ 2 & 2 & 1 \end{Bmatrix} = \frac{1}{3\sqrt{105}}\,, \tag{A.3h}$$

(A.3i)

$$\left\{\begin{array}{ccc} 0 & 0 & 0 \\ 1 & 1 & 2 \\ 1 & 1 & 2 \end{array}\right\} = \frac{1}{3\sqrt{5}} \qquad \left\{\begin{array}{ccc} 2 & 2 & 0 \\ 1 & 1 & 2 \\ 1 & 1 & 2 \end{array}\right\} = \frac{1}{150}\,, \tag{A.3j}$$

$$\left\{\begin{array}{ccc} 1 & 1 & 0 \\ 1 & 1 & 2 \\ 2 & 2 & 2 \end{array}\right\} = \frac{\sqrt{7}}{30\sqrt{5}} \qquad \left\{\begin{array}{ccc} 3 & 3 & 0 \\ 1 & 1 & 2 \\ 2 & 2 & 2 \end{array}\right\} = \frac{1}{35\sqrt{15}}\,, \tag{A.3k}$$

$$\left\{\begin{array}{ccc} 1 & 1 & 0 \\ 0 & 2 & 2 \\ 1 & 1 & 2 \end{array}\right\} = \frac{1}{15} \qquad \left\{\begin{array}{ccc} 2 & 2 & 0 \\ 0 & 2 & 2 \\ 2 & 2 & 2 \end{array}\right\} = \frac{1}{25}\,, \tag{A.3l}$$

$$\left\{\begin{array}{ccc} 1 & 1 & 0 \\ 1 & 1 & 2 \\ 2 & 0 & 2 \end{array}\right\} = \frac{1}{15} \qquad \left\{\begin{array}{ccc} 2 & 2 & 0 \\ 0 & 2 & 2 \\ 2 & 0 & 2 \end{array}\right\} = \frac{1}{25}\,, \tag{A.3m}$$

$$\left\{\begin{array}{ccc} 0 & 0 & 0 \\ 2 & 0 & 2 \\ 2 & 0 & 2 \end{array}\right\} = \frac{1}{5}\,, \tag{A.3n}$$

$$\left\{\begin{array}{ccc} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 0 \\ 1 & 1 & 1 \end{array}\right\} = \frac{1}{3\sqrt{6}} \qquad \left\{\begin{array}{ccc} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 1 \\ 1 & 1 & 2 \end{array}\right\} = \frac{1}{9} \qquad \left\{\begin{array}{ccc} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 0 \\ 1 & 1 & 1 \end{array}\right\} = \frac{1}{3\sqrt{6}}\,. \tag{A.3o}$$

A.2.2 Tensorial representations

Spherical components of a vector $\vec{r}$ can be defined as

$$r_0 = r_z\,, \qquad r_{\pm 1} = \mp \frac{x \pm i\,y}{\sqrt{2}}\,, \tag{A.4}$$

in such a way that we have

$$\vec{r} = r^{[1]} = r\sqrt{\frac{4\pi}{3}}\,Y^{[1]}(\hat{r})\,. \tag{A.5}$$

Two vectors $\vec{a}$ and $\vec{b}$ can be combined into a tensor of rank 0, 1 or 2, with

$$\vec{a}\cdot\vec{b} = -\sqrt{3}\,\left[a^{[1]}\otimes b^{[1]}\right]^{[0]\,0}\,, \tag{A.6a}$$

$$i\,\vec{a}\wedge\vec{b} = \sqrt{2}\,\left[a^{[1]}\otimes b^{[1]}\right]^{[1]}\,. \tag{A.6b}$$

More generally, the scalar product of two tensors of same rank is

$$T^{[k]}\cdot U^{[k]} = (-1)^k\,\sqrt{[k]}\,\left[T^{[k]}\otimes U^{[k]}\right]^{[0]}\,. \tag{A.7}$$

A spherical tensor of rank l can be constructed from components of two other tensors as

$$T^{[\ell]}_m = \sum_{m_1,m_2} R^{[\ell_1]}_{m_1}\,S^{[\ell_2]}_{m_2}\,\langle \ell_1\,m_1\,\ell_2\,m_2\,|\ell_1\,\ell_2\,\ell\,m\rangle\,. \tag{A.8}$$

A.2.3 Spherical harmonics

Standard spherical harmonics are defined as normalized eigenstates of angular momentum operators L^2 and L_z

$$Y_\ell^m(\theta,\varphi) = \frac{(-1)^{\ell+m}}{2^\ell\,\ell!}\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi\,(\ell+m)!}}\,\sin(\theta)^m\,\left[\frac{\partial}{\partial\,\cos(\theta)}\right]^{\ell+m}\sin(\theta)^{2\ell}\,e^{i\,m\,\varphi}\,. \tag{A.9}$$

Those functions have the following properties

$$Y_\ell^{-m}(\theta,\varphi) = (-1)^m\,Y_\ell^{m*}(\theta,\varphi)\,, \tag{A.10a}$$

$$\int_0^\pi \sin(\theta)\,\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\,Y_\ell^{m*}(\theta,\varphi)\,Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\,\delta_{mm'}\,. \tag{A.10b}$$

One has also

$$Y_\ell^m(\widehat{\vec{p}+\vec{p}\,'}) = \sum_{\ell_1+\ell_2=\ell}\frac{p^{\ell_1}\,p'^{\ell_2}}{|\vec{p}+\vec{p}\,'|^\ell}\sqrt{\frac{4\pi\,[\ell]!}{[\ell_1]![\ell_2]!}}\,\left[Y^{[\ell_1]}(\hat{p})\otimes Y^{[\ell_2]}(\hat{p}')\right]^{[\ell]\,m}\,. \tag{A.11}$$

The inverse relation for the expansion of the tensorial product of spherical harmonics reads

$$\left[Y^{[\ell_1]}(\hat{p})\otimes Y^{[\ell_2]}(\hat{p})\right]^{[\ell]\,m} = \sqrt{\frac{[\ell_1][\ell_2]}{4\pi\,[\ell]}}\,\langle\ell_1\,0\,\ell_2\,0\,|\ell_1\,\ell_2\,\ell\,0\rangle\;Y_\ell^m(\hat{p})\,. \tag{A.12}$$

A.2.4 Tensor spherical harmonics

The definition of spherical harmonics can be extended to more general objects arising when considering a $L+S$ coupling. Starting from the standard unit vectors $u_i, i=1/x,2/y,3/z$, one can define the irreducible representation of rank $(2S+1)$ of the rotation group through

$$C^{S\,M_S} = \sum_{\alpha_i} C^{S\,M_S}_{\alpha_1\ldots\alpha_S}\,u^{(1)}_{\alpha_1}\otimes\ldots\otimes u^{(S)}_{\alpha_S}\,, \qquad S=0,1\ldots\quad M_S=-S\ldots S\,. \tag{A.13}$$

For instance

$$C^{0\,0} = 1\,, \tag{A.14a}$$

$$C^{1\,1}_\alpha = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\-i\\0\end{pmatrix}\qquad C^{1\,0}_\alpha = \begin{pmatrix}0\\0\\1\end{pmatrix}\qquad C^{1\,-1}_\alpha = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\\0\end{pmatrix}\,, \tag{A.14b}$$

that is for $S=1$, cartesian components of C transform a vector from cartesian to spherical coordinates. One can then define tensor spherical harmonics [4] as

$$\mathcal{Y}^{M_J}_{(LS)J}(\Omega) = \sum_{M_L\,M_S}\langle L\,M_L\,S\,M_S\,|L\,S\,J\,M_J\rangle\;Y_L^{M_L}(\Omega)\,C^{S\,M_S}\,, \tag{A.15}$$

For $S=0$ one recovers

$$\mathcal{Y}^{M_J}_{(L0)J}(\Omega) = \delta_{LJ}\,\delta_{M_LM_J}\,Y_L^{M_L}(\Omega)\,, \tag{A.16}$$

using

$$C^{0\,0} = 1\,, \qquad \langle L\,M_L\,0\,0\,|L\,0\,J\,M_J\rangle = \delta_{LJ}\,\delta_{M_LM_J}\,. \tag{A.17}$$

Those tensor spherical harmonics are spinors, that is they are of dimension $2S+1$. Finally, orthogonality of tensor spherical harmonics reads for the same spin S

$$\int\mathrm{d}\Omega\,\mathcal{Y}^{M'_J\,*}_{(L'S)J'}(\Omega)\,\mathcal{Y}^{M_J}_{(LS)J}(\Omega) = \delta_{LL'}\,\delta_{JJ'}\,\delta_{M_JM'_J}\,. \tag{A.18}$$

A.2.5 Spherical Bessel functions

The radial Helmoltz equation

$$x^2 \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + 2x \frac{\mathrm{d}f}{\mathrm{d}x} + (x^2 - \nu(\nu+1))f = 0\,, \tag{A.19}$$

has two linearly independent solutions, i.e. spherical Bessel functions $j_\nu(x)$ and Neumann functions $n_\nu(x)$. In particular, spherical Bessel functions are defined as

$$j_\nu(x) \equiv \sqrt{\frac{\pi}{2x}} J_{\nu+1/2}(x) \equiv (-x)^\nu \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^\nu \frac{\sin(x)}{x}\,, \tag{A.20}$$

where J_ν are ordinary Bessel functions. They have the following properties, for $\nu \in \mathbb{Z}$:

$$j_{\nu-1}(z) + j_{\nu+1}(z) = (2\nu+1)\frac{j_\nu(z)}{z}\,, \tag{A.21a}$$

$$\nu\, j_{\nu-1}(z) - (\nu+1)\, j_{\nu+1}(z) = (2\nu+1)\frac{\mathrm{d}}{\mathrm{d}z} j_\nu(z)\,, \tag{A.21b}$$

$$\frac{\nu+1}{z}\, j_\nu(z) + \frac{\mathrm{d}}{\mathrm{d}z} j_\nu(z) = j_{\nu-1}(z)\,, \tag{A.21c}$$

$$\frac{\nu}{z}\, j_\nu(z) - \frac{\mathrm{d}}{\mathrm{d}z} j_\nu(z) = j_{\nu+1}(z)\,. \tag{A.21d}$$

First spherical Bessel functions, presented in FIG. A.1, and their derivatives read

$$j_0(x) = \frac{\sin(x)}{x}\,, \tag{A.22a}$$

$$j_1(x) = \frac{1}{x}\frac{\sin(x)}{x} - \frac{\cos(x)}{x}\,, \tag{A.22b}$$

$$j_2(x) = \left(\frac{3}{x^2} - 1\right)\frac{\sin(x)}{x} - \frac{3}{x}\frac{\cos(x)}{x}\,, \tag{A.22c}$$

$$j_3(x) = \left(\frac{15}{x^3} - \frac{6}{x}\right)\frac{\sin(x)}{x} - \left(\frac{15}{x^2} - 1\right)\frac{\cos(x)}{x}\,, \tag{A.22d}$$

$$j_4(x) = \left(\frac{105}{x^4} - \frac{45}{x^2} + 1\right)\frac{\sin(x)}{x} - \left(\frac{105}{x^3} - \frac{10}{x}\right)\frac{\cos(x)}{x}\,, \tag{A.22e}$$

$$j_5(x) = \dots$$

$$\frac{dj_0(x)}{dx} = -\frac{1}{x}\frac{\sin(x)}{x} + \frac{\cos(x)}{x}\,, \tag{A.23a}$$

$$\frac{dj_1(x)}{dx} = -\left(\frac{2}{x^2} - 1\right)\frac{\sin(x)}{x} + \frac{2}{x}\frac{\cos(x)}{x}\,, \tag{A.23b}$$

$$\frac{dj_2(x)}{dx} = -\left(\frac{9}{x^3} - \frac{4}{x}\right)\frac{\sin(x)}{x} + \left(\frac{9}{x^2} - 1\right)\frac{\cos(x)}{x}\,, \tag{A.23c}$$

$$\frac{dj_3(x)}{dx} = -\left(\frac{60}{x^4} - \frac{27}{x^2} + 1\right)\frac{\sin(x)}{x} + \left(\frac{60}{x^3} - \frac{7}{x}\right)\frac{\cos(x)}{x}\,, \tag{A.23d}$$

$$\frac{dj_4(x)}{dx} = -\left(\frac{525}{x^5} - \frac{240}{x^3} + \frac{11}{x}\right)\frac{\sin(x)}{x} + \left(\frac{525}{x^4} - \frac{65}{x^2} + 1\right)\frac{\cos(x)}{x}\,, \tag{A.23e}$$

$$\frac{dj_5(x)}{dx} = \dots$$

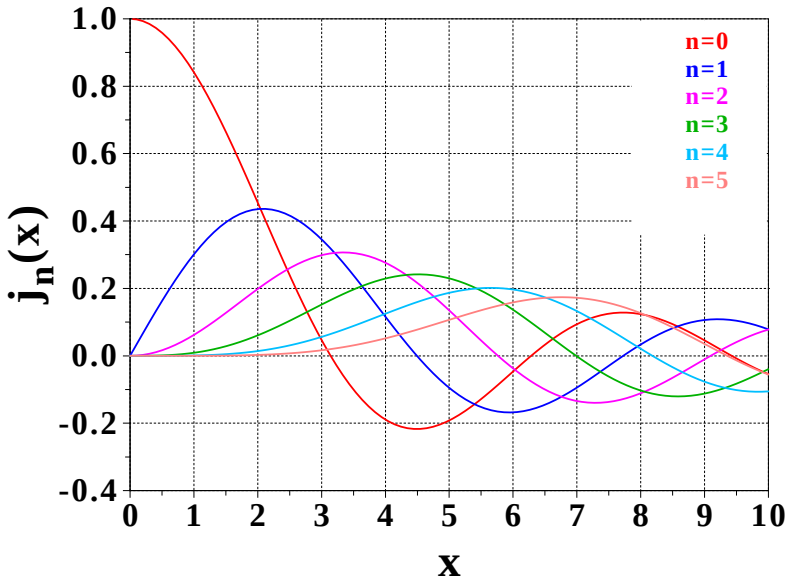


Figure A.1: First spherical Bessel functions.

A.2.6 Legendre polynomials

Legendre polynomials $P_\ell(x)$ are defined by the relationships

$$\frac{1}{\sqrt{1-2\,x\,h+h^2}} = \sum_\ell h^\ell\, P_\ell(x)\,, \tag{A.24a}$$

$$P_\ell(x) = \sum_{r=0}^{[\ell/2]} (-1)^r\, \frac{(2\ell-2r)!\, x^{\ell-2r}}{2^\ell\, r!\, (\ell-r)!\, (\ell-2r)!}\,, \tag{A.24b}$$

$$P_\ell(x) = \frac{1}{2^\ell\, \ell!}\, \frac{d^\ell}{d\, x^\ell} (x^2-1)^\ell\,. \tag{A.24c}$$

One can also define associated Legendre functions of the first kind $P_\ell^m(x)$ for $|m| \leq \ell$ through

$$P_\ell^m(x) = (1-x^2)^{m/2}\, \frac{d^m}{d\, x^m} P_\ell(x) = \frac{(1-x^2)^{m/2}}{2^\ell\, \ell!}\, \frac{d^{\ell+m}}{d\, x^{\ell+m}} (x^2-1)^\ell\,. \tag{A.25}$$

In particular

$$P_\ell(0) = 1 \tag{A.26a}$$

$$P_\ell(-x) = (-1)^\ell\, P_\ell(x)\,, \quad P_\ell^m(-x) = (-1)^{\ell+m}\, P_\ell^m(x)\,, \quad P_\ell^{-m}(x) = (-1)^m\, \frac{(\ell-m)!}{(\ell+m)!}\, P_\ell^m(x)\,. \tag{A.26b}$$

For any (θ, φ) one has also

$$P_\ell(\cos(\theta)) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^0(\theta,\varphi)\,, \tag{A.27a}$$

$$Y_\ell^0(\theta,\varphi) = (-1)^m \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi\,(\ell+m)!}}\, P_\ell^m(\cos(\theta))\, e^{i\,m\,\varphi}\,, \tag{A.27b}$$

thus Legendre polynomials are only defined in theory for arguments lower than 1 in absolute value. They have the following properties

$$\int_{-1}^{+1} P_\ell(x)\, P_{\ell'}(x)\, \mathrm{d}x = \frac{\delta_{\ell\ell'}}{\ell+\frac{1}{2}}\,, \qquad j_\ell(y) = \frac{(-i)^\ell}{2} \int_{-1}^{+1} e^{i\,x\,y}\, P_\ell(x)\, \mathrm{d}x\,. \tag{A.28}$$

First Legendre polynomials read

$$P_0(x) = 1\,, \tag{A.29a}$$
$$P_1(x) = x\,, \tag{A.29b}$$
$$P_2(x) = \frac{1}{2}(3x^2 - 1)\,, \tag{A.29c}$$
$$P_3(x) = \frac{1}{2}(5x^3 - 3x)\,, \tag{A.29d}$$
$$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)\,, \tag{A.29e}$$
$$P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)\,, \tag{A.29f}$$
$$P_6(x) = \frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)\,, \tag{A.29g}$$
$$P_7(x) = \dots$$

and are represented in Fig. A.2. They verify orthogonality relations

$$\int_{-1}^{1} P_\ell(x)\, P_{\ell'}(x)\, \mathrm{d}x = \frac{2\,\delta_{\ell\ell'}}{[\ell]}\,, \tag{A.30}$$

and

$$P_\lambda(\cos(\omega)) = \frac{4\pi}{[\lambda]} \sum_{m=-\lambda}^{\lambda} Y_\lambda^{m*}(\theta,\varphi)\, Y_\lambda^{m}(\theta',\varphi')\,. \tag{A.31}$$

They also verify

$$P_n(z)\, P_m(z) = \sum_{k=|m-n|}^{m+n} b(n,m,k)\, P_k(z)\,, \tag{A.32}$$

where

$$b(n,m,k) = \delta_{0\gamma}\, \frac{[k]\,(k+m-n-1)!!\,(k-m+n-1)!!\,(m+n-k-1)!!\,(k+m+n)!!}{(k+m-n)!!\,(k-m+n)!!\,(m+n-k)!!\,(k+m+n-1)!!}\,, \tag{A.33a}$$

$$\gamma = \frac{1}{2}(k+m+n)\; MOD\, 1\,. \tag{A.33b}$$

In particular for $n = 1$, one has:

	$b(1,m,k)$				
m \ k	0	1	2	3	4
0	0	1	0	0	0
1	$\frac{1}{3}$	0	$\frac{2}{3}$	0	0
2	0	$\frac{2}{5}$	0	$\frac{3}{5}$	0
3	0	0	$\frac{3}{7}$	0	$\frac{4}{7}$

$$x\,P_0(x) = P_1(x) \tag{A.34a}$$
$$x\,P_1(x) = \frac{2}{3}\,P_2(x) + \frac{1}{3}\,P_2(x) \tag{A.34b}$$
$$x\,P_2(x) = \frac{3}{5}\,P_3(x) + \frac{2}{5}\,P_1(x) \tag{A.34c}$$
$$x\,P_3(x) = \frac{4}{7}\,P_4(x) + \frac{3}{7}\,P_2(x)\,. \tag{A.34d}$$

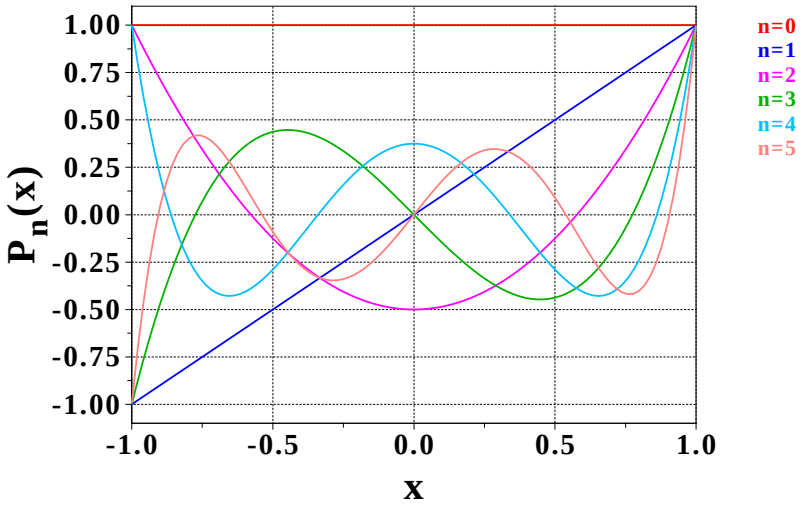


Figure A.2: First Legendre polynomials.

A.2.7 Jacobi polynomials

Jacobi Polynomials are defined as

$$\begin{aligned} P_n^{\alpha,\beta}(x) =& \frac{(-1)^n}{2^n\, n!} \frac{1}{(1-x)^\alpha\,(1-x)^\beta} \frac{d^n}{\mathrm{d}x^n} \left[(1-x)^{\alpha+n}\,(1-x)^{\beta+n}\right] \\ =& \frac{1}{2^n} \sum_{\nu=0}^{n} \begin{pmatrix} n+\alpha \\ \nu \end{pmatrix} \begin{pmatrix} n+\beta \\ n-\nu \end{pmatrix} (x-1)^{n-\nu}\,(x+1)^\nu\,, \end{aligned} \tag{A.35}$$

and normalized such that

$$P_n^{\alpha,\beta}(1) = \begin{pmatrix} n+\alpha \\ n \end{pmatrix}. \tag{A.36}$$

In particular, Legendre polynomials are defined as

$$P_n(x) = P_n^{0,0}(x)\,. \tag{A.37}$$

Jacobi polynomials $P_n^{\alpha,\beta}(x)$ are orthogonal for the scalar product

$$(f_n|f_m)^{\alpha,\beta)} = \int_{-1}^{1} (1-x)^\alpha\,(1-x)^\beta\, f_n(x)\, f_m(x)\,\mathrm{d}x\,, \tag{A.38}$$

thus, using the normalization condition from Eq. (A.36)

$$\int_{-1}^{1} (1-x)^\alpha\,(1-x)^\beta\, P_n^{\alpha,\beta}(x)\, P_m^{\alpha,\beta}(x)\,\mathrm{d}x = \frac{2^{1+\alpha+\beta}}{2n+\alpha+\beta+1} \frac{\Gamma(n+\alpha+1)\,\Gamma(n+\beta+1)}{\Gamma(n+1)\,\Gamma(n+\alpha+\beta+1)}\,\delta_{mn}\,. \tag{A.39}$$

A.3 Angular expansions

A.3.1 Legendre polynomials expansion

Any function $g(\vec{k},\vec{k}\,')$ can be expanded in terms of Legendre polynomials, e.g.

$$g(\vec{k},\vec{k}\,') = \sum_\lambda P_\lambda(\cos(\omega))\,\bar{g}_\lambda(k,k')\,, \tag{A.40}$$

where $\omega = (\vec{k}, \vec{k}\,')$. Therefore one has

$$\bar{g}_\lambda(k,k') = \frac{[\lambda]}{2}\int_{-1}^{1} P_\lambda(x)\, g(\vec{k},\vec{k}\,')\,\mathrm{d}x. \tag{A.41}$$

Using Eq. (A.31), Eq. (A.40) can be written as

$$\begin{aligned} g(\vec{k},\vec{k}\,') =& \sum_\lambda \frac{4\pi}{[\lambda]} \sum_{m=-\lambda}^{\lambda} Y_\lambda^{m*}(\theta,\phi)\, Y_\lambda^m(\theta',\phi')\, \bar{g}_\lambda(k,k') \\ =& \sum_\lambda 4\pi \sum_{m=-\lambda}^{\lambda} \frac{(-1)^m}{[\lambda]}\, Y_\lambda^{-m}(\hat{k})\, Y_\lambda^m(\hat{k}')\, \bar{g}_\lambda(k,k') \\ =& 4\pi\,(-1)^\lambda \sum_\lambda \langle \lambda\, m\, \lambda\, -m\, |\lambda\, \lambda\, 0\, 0\rangle\; Y_\lambda^{-m}(\hat{k})\, Y_\lambda^m(\hat{k}')\, \bar{g}_\lambda(k,k') \\ =& 4\pi\,(-1)^\lambda \sum_\lambda \left[Y^{[\lambda]}(\hat{k}) \otimes Y^{[\lambda]}(\hat{k}')\right]^{[0]}\; \bar{g}_\lambda(k,k')\,, \end{aligned} \tag{A.42}$$

where one used Eq. (A.63) with the specific case $\ell = m = 0$. Thus one has

$$g(\vec{k},\vec{k}\,') = \sum_\lambda \left[Y^{[\lambda]}(\hat{k}) \otimes Y^{[\lambda]}(\hat{k}')\right]^{[0]}\; \tilde{g}_\lambda(k,k'), \tag{A.43}$$

where

$$\tilde{g}_\lambda(k,k') = 2\pi\,(-1)^\lambda \sqrt{[\lambda]}\int_{-1}^{1} P_\lambda(x)\, g(\vec{k},\vec{k}\,')\,\mathrm{d}x = \frac{4\pi}{\sqrt{[\lambda]}}\,(-1)^\lambda\, \bar{g}_\lambda(k,k')\,. \tag{A.44}$$

A.3.2 Dirac 3D delta function decomposition

To evaluate the proper normalization factor for our matrix elements (see Sec. D.2), a partial wave expansion of the 3D Dirac delta function is needed. The latter is defined as

$$\nabla^2 \frac{1}{r} = -4\pi\,\delta(\vec{r})\,, \qquad \int \mathrm{d}\vec{r}\,\delta(\vec{r}-\vec{r}\,') = 1\,. \tag{A.45}$$

Let $j(\vec{k},\vec{k}\,') = \delta\vec{k} - \vec{k}\,'$. One can use the representation of the delta function in spherical coordinates

$$\delta(\vec{r}-\vec{r}\,') = \frac{1}{r^2\,\sin(\theta)}\,\delta(r-r')\,\delta(\theta-\theta')\,\delta(\varphi-\varphi')\,, \tag{A.46}$$

such that

$$\int \mathrm{d}\vec{r}\,\delta(\vec{r}-\vec{r}\,') = \int_0^{+\infty}\delta(r-r')\,\mathrm{d}r \int_0^{\pi}\delta(\theta-\theta')\,\mathrm{d}\theta \int_0^{2\pi}\delta(\varphi-\varphi')\,\mathrm{d}\varphi = 1\,. \tag{A.47}$$

To evaluate the coefficients $\bar{j}_\lambda(k,k')$ of the partial wave expansion using Eq. (A.41) or Eq. (A.44), the integration domain relates to the relative angle ω between $\vec{k}$ and $\vec{k}\,'$ such that

$$\cos(\omega) = \cos(\theta)\,\cos(\theta') + \sin(\theta)\,\sin\theta'\,\cos(\varphi-\varphi')\,. \tag{A.48}$$

Using the rotational invariance, one can put $\vec{k}\,'$ on the z axis such that $\theta' = \varphi' = 0$, and use the representation of the delta function

$$\delta(\vec{r}-\vec{r}\,') = \frac{1}{2\pi\,r^2\,\sin(\theta)}\,\delta(r-r')\,\delta(\theta)\,. \tag{A.49}$$

One has then

$$\begin{aligned}\bar{j}_\lambda(k,k') =& \frac{[\lambda]}{2}\,\frac{1}{2\pi}\,\frac{\delta(k-k')}{k^2}\int_0^\pi \mathrm{d}\theta\, P_\lambda(\cos(\theta))\,\delta(\theta)\\ =& \frac{[\lambda]}{4\pi}\,\frac{\delta(k-k')}{k^2}\,P_\lambda(\cos(0))\\ =& \frac{[\lambda]}{4\pi}\,\frac{\delta(k-k')}{k^2}\,.\end{aligned} \tag{A.50}$$

Thus one recovers the usual expansion

$$\delta(\vec{k}-\vec{k}\,') = \frac{\delta(k-k')}{k^2}\sum_\lambda \frac{[\lambda]}{4\pi}\,P_\lambda(\cos(\omega))\,. \tag{A.51}$$

Equivalently

$$\tilde{j}_\lambda(k,k') = (-1)^\lambda\,\sqrt{[\lambda]}\,\frac{\delta(k-k')}{k^2}\,. \tag{A.52}$$

A.3.3 Polynomial decomposition

We start for the direct term from

$$f(\vec{k},\vec{k}\,') = q^2 = \left(k^2 + k'^2 - 2\,kk'\,\cos(\theta)\right)\,. \tag{A.53}$$

This gives easily

$$\tilde{f}_0(k,k') = 2\pi\int_{-1}^1 \left(k^2+k'^2-2\,kk'\,x\right)\,\mathrm{d}x = 4\pi\left(k^2+k'^2\right)\,, \tag{A.54a}$$

$$\tilde{f}_1(k,k') = -\,2\pi\sqrt{3}\int_{-1}^1 \left(k^2+k'^2-2\,kk'\,x\right)\,x\,\mathrm{d}x = \frac{8\pi}{\sqrt{3}}kk'\,, \tag{A.54b}$$

$$\tilde{f}_{\lambda\geq 2}(k,k') = 0\,. \tag{A.54c}$$

The exchange term reads simply $f(\vec{k},-\vec{k}\,')$, that is the values of $\tilde{f}_i$ are the same.

A.3.4 Gaussian decomposition

We start for the direct term from

$$g^i(\vec{k},\vec{k}\,') = e^{-\frac{1}{4}\mu_i^2\,q^2} = e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}\,e^{\frac{1}{2}\mu_i^2\,kk'\,\cos(\theta)}\,. \tag{A.55}$$

For the leading orders one has then

$$\int_{-1}^1 e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,P_0(x)\,\mathrm{d}x = \int_{-1}^1 e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,\mathrm{d}x = 4\,\frac{\mathrm{sh}\left(\frac{1}{2}\mu_i^2\,kk'\right)}{\mu_i^2\,kk'} \equiv 2\frac{\mathrm{sh}(\Gamma_i)}{\Gamma_i} \tag{A.56a}$$

$$\begin{aligned}\int_{-1}^1 e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,P_1(x)\,\mathrm{d}x =& \int_{-1}^1 e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,x\,\mathrm{d}x\\ =& \frac{2}{\mu_i^2\,kk'}\left[e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,x\right]_{-1}^1 - \frac{2}{\mu_i^2\,kk'}\int_{-1}^1 e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,\mathrm{d}x\\ =& \frac{4}{\mu_i^2\,kk'}\mathrm{ch}\left(\frac{1}{2}\mu_i^2\,kk'\right) - \frac{2}{\mu_i^2\,kk'}\int_{-1}^1 e^{\frac{1}{2}\mu_i^2\,kk'\,x}\,\mathrm{d}x\\ =& \frac{4}{\mu_i^4\,k^2k'^2}\left(\mu_i^2\,kk'\,\mathrm{ch}\left(\frac{1}{2}\mu_i^2\,kk'\right) - 2\,\mathrm{sh}\left(\frac{1}{2}\mu_i^2\,kk'\right)\right)\\ \equiv& \frac{2}{\Gamma_i^2}\left(\Gamma_i\,\mathrm{ch}(\Gamma_i) - \mathrm{sh}(\Gamma_i)\right)\end{aligned} \tag{A.56b}$$

$$\int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, P_2(x)\,\mathrm{d}x = \int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, \frac{1}{2}(3x^2-1)\,\mathrm{d}x$$
$$= \frac{4}{\mu_i^6\, k^3 k'^3}\left(-6\mu_i^2\, kk'\,\mathrm{ch}\left(\frac{1}{2}\mu_i^2\, kk'\right) + sh\left(\frac{1}{2}\mu_i^2\, kk'\right)(12+\mu_i^4\, k^2 k'^2)\right)$$
$$\equiv \frac{2}{\Gamma_i^3}\left(-3\Gamma_i\,\mathrm{ch}(\Gamma_i) + (3+\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right) \tag{A.56c}$$

$$\int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, P_3(x)\,\mathrm{d}x = \int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, \frac{1}{2}(5x^3-3x)\,\mathrm{d}x$$
$$\equiv \frac{2}{\Gamma_i^4}\left(\Gamma_i\,(15+\Gamma_i^2)\mathrm{ch}(\Gamma_i) - 3\,(5+2\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right) \tag{A.56d}$$

$$\int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, P_4(x)\,\mathrm{d}x = \int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, \frac{1}{8}(35x^4-30x^2+3)\,\mathrm{d}x$$
$$\equiv \frac{2}{\Gamma_i^5}\left(-5\Gamma_i\,(21+2\Gamma_i^2)\mathrm{ch}(\Gamma_i) + (105+45\Gamma_i^2+\Gamma_i^4)\mathrm{sh}(\Gamma_i)\right) \tag{A.56e}$$

$$\int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, P_5(x)\,\mathrm{d}x = \int_{-1}^{1} e^{\frac{1}{2}\mu_i^2\, kk'\, x}\, \frac{1}{8}(63x^5-70x^3+15x)\,\mathrm{d}x$$
$$\equiv \frac{2}{\Gamma_i^6}\left(\Gamma_i\,(945+105\Gamma_i^2+\Gamma_i^4)\mathrm{ch}(\Gamma_i) - 15(63+28\Gamma_i^2+\Gamma_i^4)\mathrm{sh}(\Gamma_i)\right)\,, \tag{A.56f}$$

for $\Gamma_i = \dfrac{1}{2}\,\mu_i^2\, kk'$. Therefore

$$\tilde{g}_0^i(k,k') = 4\pi\frac{e^{-\frac{1}{4}\,\mu_i^2\,(k^2+k'^2)}}{\Gamma_i}\,\mathrm{sh}(\Gamma_i) \tag{A.57a}$$
$$\tilde{g}_1^i(k,k') = -\,4\pi\,\sqrt{3}\,\frac{e^{-\frac{1}{4}\,\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^2}\,(\Gamma_i\,\mathrm{ch}(\Gamma_i) - \mathrm{sh}(\Gamma_i)) \tag{A.57b}$$
$$\tilde{g}_2^i(k,k') = 4\pi\,\sqrt{5}\,\frac{e^{-\frac{1}{4}\,\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^3}\left(-3\Gamma_i\,\mathrm{ch}(\Gamma_i) + (3+\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right) \tag{A.57c}$$
$$\tilde{g}_3^i(k,k') = -\,4\pi\,\sqrt{7}\,\frac{e^{-\frac{1}{4}\,\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^4}\left(\Gamma_i\,(15+\Gamma_i^2)\,\mathrm{ch}(\Gamma_i) - 3\,(5+2\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right) \tag{A.57d}$$
$$\tilde{g}_4^i(k,k') = 4\pi\,\sqrt{9}\,\frac{e^{-\frac{1}{4}\,\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^5}\left(-5\Gamma_i\,(21+2\Gamma_i^2)\mathrm{ch}(\Gamma_i) + (105+45\Gamma_i^2+\Gamma_i^4)\mathrm{sh}(\Gamma_i)\right) \tag{A.57e}$$
$$\tilde{g}_5^i(k,k') = -\,4\pi\,\sqrt{11}\,\frac{e^{-\frac{1}{4}\,\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^6}\left(\Gamma_i\,(945+105\Gamma_i^2+\Gamma_i^4)\mathrm{ch}(\Gamma_i) - 15(63+28\Gamma_i^2+\Gamma_i^4)\mathrm{sh}(\Gamma_i)\right)\,. \tag{A.57f}$$

Exchange terms are identical with the variable change $\Gamma_i \to -\Gamma_i$. The first functions $\tilde{g}_n^i(k;k')$ are represented in FIG. A.3 for $k = k'$. One sees there expected convergence properties of the series as a function of n, since the overall magnitude of the functions g_n^i decrease with n.

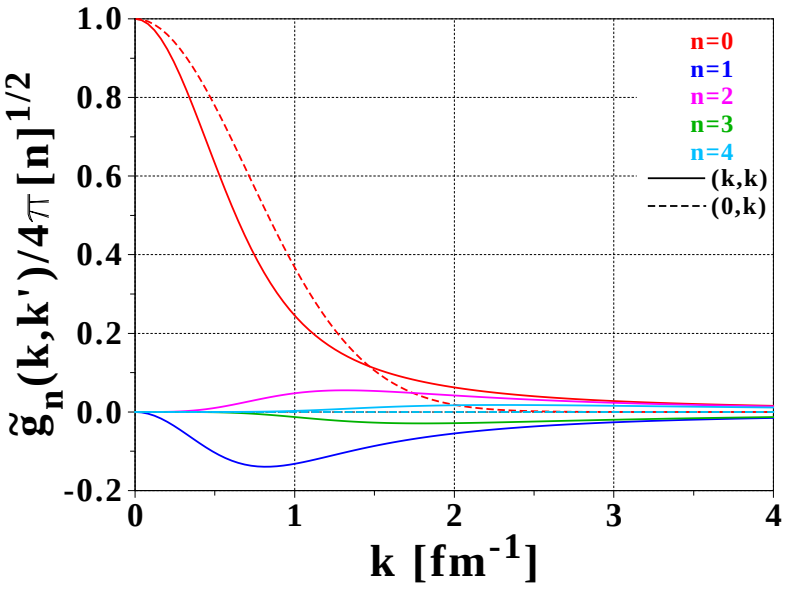


Figure A.3: Form factors $g_n^i(k,k)$ for $\mu = 1$ and various values of n.

A.3.5 One-pion-exchange form factor decomposition

In this case one will have to consider for the direct terms the form factors

$$p^f(\vec{k},\vec{k}\,') = \frac{q^2}{q^2+m_\pi^2}\,\frac{1}{q^f} = \frac{k^2+k'^2-2\,kk'\,\cos(\theta)}{k^2+k'^2-2\,kk'\,\cos(\theta)+m_\pi^2}\,\frac{1}{|\vec{k}-\vec{k}\,'|^f}\,, \tag{A.58}$$

for $f = 0, 1, 2$. The $f = 1$ block is irrelevant for the partial wave decomposition, while one gets in the $f = 0$ block

$$\begin{aligned}\tilde{p}_0^0(k,k') =& 2\pi\int_{-1}^{1}\frac{k^2+k'^2-2\,kk'\,x}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\mathrm{d}x\\ =& 2\pi\int_{-1}^{1}\left(1-\frac{m_\pi^2}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right)\mathrm{d}x\\ =& 4\pi\left[1+\frac{m_\pi^2}{4\,kk'}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right],\end{aligned} \tag{A.59a}$$

$$\begin{aligned}\tilde{p}_1^0(k,k') =& -2\pi\sqrt{3}\int_{-1}^{1}\frac{k^2+k'^2-2\,kk'\,x}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,x\,\mathrm{d}x\\ =& -2\pi\sqrt{3}\int_{-1}^{1}\left(x-\frac{m_\pi^2\,x}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right)\mathrm{d}x\\ =& -2\pi\sqrt{3}\int_{-1}^{1}\frac{m_\pi^2}{2\,kk'}\left(1+\frac{k^2+k'^2+m_\pi^2}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right)\mathrm{d}x\\ =& -4\pi\sqrt{3}\left[\frac{m_\pi^2}{2\,kk'}+\frac{m_\pi^2\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right],\end{aligned} \tag{A.59b}$$

$$
\begin{aligned}
\tilde{p}_2^0(k,k') =& 2\pi\sqrt{5}\int_{-1}^{1}\frac{k^2+k'^2-2\,kk'\,x}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\frac{1}{2}(3x^2-1)\,\mathrm{d}x \\
=& 2\pi\sqrt{5}\left[\int_{-1}^{1}\left(\frac{3}{2}\,x^2-\frac{3}{2}\,\frac{m_\pi^2\,x^2}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right)\mathrm{d}x-\frac{1}{2}\,\tilde{p}_0^0(k,k')\right] \\
=& 2\pi\sqrt{5}\left[\int_{-1}^{1}\left(\frac{3}{2}\,x^2-\frac{3}{2}\,\frac{m_\pi^2}{2\,kk'}\left[x+\frac{(k^2+k'^2+m_\pi^2)\,x}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right]\right)\mathrm{d}x-\frac{1}{2}\,\tilde{p}_0^0(k,k')\right] \\
=& 2\pi\sqrt{5}-\frac{\sqrt{5}}{2}\,\tilde{p}_0^0(k,k') \\
&+2\pi\sqrt{5}\int_{-1}^{1}\frac{3}{2}\,\frac{m_\pi^2\,(k^2+k'^2+m_\pi^2)}{4\,k^2k'^2}\left(1+\frac{(k^2+k'^2+m_\pi^2)}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right)\mathrm{d}x \\
=& 2\pi\sqrt{5}-\frac{\sqrt{5}}{2}\,\tilde{p}_0^0(k,k') \\
&+3\pi\sqrt{5}\,\frac{m_\pi^2\,(k^2+k'^2+m_\pi^2)}{4\,k^2k'^2}\left(2+\frac{(k^2+k'^2+m_\pi^2)}{2\,kk'}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right) \\
=& 4\pi\sqrt{5}\left[\frac{3m_\pi^2\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\right. \\
&\left.++\frac{m_\pi^2}{2\,kk'}\left(-\frac{1}{4}\frac{3m_\pi^2\,(k^2+k'^2+m_\pi^2)}{16\,k^2k'^2}\right)\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right]. \qquad \text{(A.59c)}
\end{aligned}
$$

Likewise for the $f=2$ block one gets

$$
\begin{aligned}
\tilde{p}_0^2(k,k') =& 2\pi\int_{-1}^{1}\frac{1}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\mathrm{d}x \\
=& -4\pi\left[\frac{1}{4\,kk'}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right], \qquad \text{(A.60a)}
\end{aligned}
$$

$$
\begin{aligned}
\tilde{p}_1^2(k,k') =& -2\pi\sqrt{3}\int_{-1}^{1}\frac{1}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,x\,\mathrm{d}x \\
=& \frac{2\pi\sqrt{3}}{2\,kk'}\int_{-1}^{1}\left(1+\frac{(k^2+k'^2+m_\pi^2)}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\right)\mathrm{d}x \\
=& 4\pi\sqrt{3}\left[\frac{1}{2\,kk'}+\frac{(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right], \qquad \text{(A.60b)}
\end{aligned}
$$

$$
\begin{aligned}
\tilde{p}_2^2(k,k') =& 2\pi\sqrt{5}\int_{-1}^{1}\frac{1}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\frac{1}{2}(3x^2-1)\,\mathrm{d}x \\
=& -\frac{\sqrt{5}}{2}\,\tilde{p}_0^2(k,k') - 2\pi\sqrt{5}\int_{-1}^{1}\frac{3}{4\,kk'}\left(x+\frac{(k^2+k'^2+m_\pi^2)\,x}{2\,kk'\,x-k^2-k'^2-m_\pi^2}\,\mathrm{d}x\right) \\
=& -\frac{\sqrt{5}}{2}\,\tilde{p}_0^2(k,k') \\
& -4\pi\sqrt{5}\,\frac{3\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\left(1+\frac{(k^2+k'^2+m_\pi^2)}{4\,kk'}\,\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right) \\
=& -4\pi\sqrt{5}\left[\frac{3\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\right. \\
& \left.+\frac{1}{4\,kk'}\left(-\frac{1}{2}+\frac{3\,(k^2+k'^2+m_\pi^2)^2}{8\,k^2k'^2}\right)\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right],
\end{aligned}
\tag{A.60c}
$$

$$
\begin{aligned}
\tilde{p}_3^2(k,k') =& -2\pi\sqrt{7}\int_{-1}^{1}\frac{1}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\frac{1}{2}(5x^3-3x)\,\mathrm{d}x \\
=& -\sqrt{7}\left[-\frac{3}{2}\,\frac{p_1^2(k,k')}{-\sqrt{3}}+\frac{10\pi}{2}\int_{-1}^{1}\frac{x^3}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\mathrm{d}x\right] \\
=& -\sqrt{7}\left[-\frac{3}{2}\,\frac{p_1^2(k,k')}{-\sqrt{3}}-\frac{10\pi}{4\,kk'}\int_{-1}^{1}x^2\,\mathrm{d}x\right. \\
& \left.-\frac{10\pi\,(k^2+k'^2+m_\pi^2)}{4\,kk'}\int_{-1}^{1}\frac{x^2}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\,\mathrm{d}x\right] \\
=& -\sqrt{7}\left[-\frac{3}{2}\,\frac{p_1^2(k,k')}{-\sqrt{3}}-\frac{10\pi}{6\,kk'}\right. \\
& \left.-\frac{10\pi\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\int_{-1}^{1}\left(x-(k^2+k'^2+m_\pi^2)\frac{x}{k^2+k'^2-2\,kk'\,x+m_\pi^2}\right)\mathrm{d}x\right] \\
=& -\sqrt{7}\left[-\frac{5\pi}{3\,kk'}+\left(\frac{5\,(k^2+k'^2+m_\pi^2)^2}{8\,k^2k'^2}-\frac{3}{2}\right)\,\frac{p_1^2(k,k')}{-\sqrt{3}}\right] \\
=& -4\pi\sqrt{7}\left[\frac{1}{kk'}\left(\frac{1}{3}-\frac{5\,(k^2+k'^2+m_\pi^2)^2}{16\,k^2k'^2}\right)\right. \\
& \left.+\frac{(k^2+k'^2+m_\pi^2)}{16\,k^2k'^2}\left(3-\frac{5\,(k^2+k'^2+m_\pi^2)^2}{4\,k^2\,k'^2}\right)\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right)\right].
\end{aligned}
\tag{A.60d}
$$

A.4 Reduced matrix elements

Reduced matrix elements are defined using standard convention, i.e. such that

$$
(\ell'||\hat{\mathbb{I}}||\ell) = \sqrt{[\ell]}\,\delta\ell\ell' \qquad\qquad ((\ell's')j'||\hat{\mathbb{I}}||(\ell s)j) = \sqrt{[j]}\,\delta_{\ell\ell'}\,\delta_{ss'}\,. \tag{A.61}
$$

A.4.1 General relations

For two tensors $T^{[k_1]}$ and $T^{[k_2]}$ of ranks k_1 and k_2 respectively, acting on the same system, reduced matrix elements of the tensorial product $X^{[k]}$ of rank k of $T^{[k_1]}$ and $T^{[k_2]}$ read

$$(\gamma'\, J'||X^{[k]}||\gamma\, J) = \sqrt{[k]}\,(-1)^{k+J+J'} \sum_{\gamma'',J''} \left\{ \begin{array}{ccc} k_1 & k_2 & k \\ J & J' & J'' \end{array} \right\} (\gamma'\, J'||T^{[k_1]}||\gamma''\, J'')\,(\gamma''\, J''||T^{[k_2]}||\gamma\, J)\,, \tag{A.62}$$

where γ stands for other degrees of freedom. If $T^{[k_1]}$ and $U^{[k_2]}$ act on different coupled systems, one has instead

$$\begin{aligned}(\gamma'\,(J_1'J_2')J'||X^{[k]}||\gamma\,(J_1J_2)J) = \sqrt{[J][J'][k]} \left\{ \begin{array}{ccc} J_1' & J_1 & k_1 \\ J_2' & J_2 & k_2 \\ J' & J & k \end{array} \right\} \\ \times \sum_{\gamma''} (\gamma'\, J_1'||T^{[k_1]}||\gamma''\, J_1)\,(\gamma''\, J_2'||U^{[k_2]}||\gamma\, J_2)\,. \end{aligned} \tag{A.63}$$

Matrix elements of the scalar product of two commuting operators of same rank $T^{[k]}$ and $U^{[k]}$ read then

$$\begin{aligned}(\gamma'\,(J_1'J_2')J'||(T^{[k]}\cdot U^{[k]})||\gamma\,(J_1J_2)J) = \sqrt{[J]}\,(-1)^{J_1+J_2'+J} \left\{ \begin{array}{ccc} J_1' & J_2' & J \\ J_2 & J_1 & k \end{array} \right\} \delta_{JJ'} \\ \times \sum_{\gamma''} (\gamma'\, J_1'||T^{[k]}||\gamma''\, J_1)\,(\gamma''\, J_2'||U^{[k]}||\gamma\, J_2)\,. \end{aligned} \tag{A.64}$$

In particular, if $T^{[k]}$ and $U^{[k]}$ are scalars, one finds

$$\begin{aligned}(\gamma'\,(J_1'J_2')J'|(T^{[0]}\cdot U^{[0]})|\gamma\,(J_1J_2)J) = \sqrt{\frac{[J]}{[J_1][J_2]}}\,\delta_{JJ'}\,\delta_{J_1J_1'}\,\delta_{J_2J_2'} \\ \times \sum_{\gamma''} (\gamma'\, J_1'||T^{[0]}||\gamma''\, J_1)\,(\gamma''\, J_2'||U^{[0]}||\gamma\, J_2)\,. \end{aligned} \tag{A.65}$$

Finally, for a tensor $T^{[k]}$ acting only on one part of a coupled scheme, one gets

$$(\gamma'\,(J_1'J_2)J'||T^{[k]}||\gamma\,(J_1J_2)J) = (-1)^{J_1'+J_2+J+k}\sqrt{[J][J']} \left\{ \begin{array}{ccc} J_1' & J' & J_2 \\ J & J_1 & k \end{array} \right\} (\gamma'\, J_1'||T^{[k]}||\gamma''\, J_1)\,. \tag{A.66}$$

A.4.2 Exchange terms

Reduced matrix elements are computed in the following only for the direct terms, e.g.

$$(k'\, J'||O(\vec{k}\,',\vec{k})||k\, J) \equiv (k'\, J'||O(\vec{q})||k\, j)\,. \tag{A.67}$$

Exchange terms are equal to the direct ones, as they read

$$\begin{aligned}(k'\, J'||O(\vec{q}\,')||k\, J) =& (k'\, J'||O(\vec{k}\,',-\vec{k})||k\, J) \\ =& \sum_{\lambda} \tilde{O}_\lambda(k',-(-k))\,(k'\, J'||\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(-(-\hat{k}))\right]^{[0]}||k\, J) \\ =& (k'\, J'||O(\vec{q})||k\, J). \end{aligned} \tag{A.68}$$

The treatment of exchange terms will therefore only require an additional factor two in the partial wave decomposition.

A.4.3 Reduced matrix elements of selected operators

A.4.3.1 $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ operator

One has

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \frac{\vec{S}^{\,2} - \vec{\sigma}_1^2 - \vec{\sigma}_2^2}{2} \,. \tag{A.69}$$

Thus

$$\begin{aligned}
(S'||\vec{\sigma}_1 \cdot \vec{\sigma}_2||S) =& \frac{\langle S'\, M'_S|\vec{\sigma}_1 \cdot \vec{\sigma}_2|S\, M_S\rangle}{(-1)^{S-M'_S}\begin{pmatrix} S' & 0 & S \\ -M'_S & 0 & M_S \end{pmatrix}} \\
=& \frac{\sqrt{[S]}}{2}\,\delta_{SS'}\,\delta_{M_S M'_S}\,\langle S'\, M'_S|\vec{S}^{\,2} - \vec{\sigma}_1^2 - \vec{\sigma}_2^2|S\, M_S\rangle \\
=& \frac{\sqrt{[S]}}{2}\,\delta_{SS'}\,\delta_{M_S M'_S}\,(4S(S+1) - 6) \\
=& \sqrt{[S]}\,\delta_{SS'}\,(2S(S+1) - 3) \,.
\end{aligned} \tag{A.70}$$

A.4.3.2 $P_{\sigma/\tau}$ operator

By definition

$$P_\sigma = \frac{1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2}{2} \,. \tag{A.71}$$

One gets easily from Eqs. (A.70,A.61)

$$\begin{aligned}
(S'||P_\sigma||S) =& \frac{1}{2}\left[\sqrt{[S]}\,\delta_{SS'} + \sqrt{[S]}\,\delta_{SS'}\,(2S(S+1) - 3)\right] \\
=& \sqrt{[S]}\,\delta_{SS'}\,(S(S+1) - 1) \\
=& \sqrt{[S]}\,\delta_{SS'}\,(-1)^{S+1}.
\end{aligned} \tag{A.72}$$

Another way to obtain the latter result stems from

$$\begin{aligned}
(S'||P_\sigma||S) =& \frac{\langle S'\, M'_S|P_\sigma|S\, M_S\rangle}{(-1)^{S-M'_S}\begin{pmatrix} S' & 0 & S \\ -M'_S & 0 & M_S \end{pmatrix}} \\
=& \sqrt{[S]}\,\delta_{SS'}\,\left\langle (\tfrac{1}{2}\,\tfrac{1}{2})S'\, M'_S\right|\, P_\sigma\, \left|(\tfrac{1}{2}\,\tfrac{1}{2})S\, M_S\right\rangle \\
=& \sqrt{[S]}\,\delta_{SS'}\sum_{S_1,S_2}\left\langle (\tfrac{1}{2}\,\tfrac{1}{2})S'\, M'_S\right|\left\langle \tfrac{1}{2}\,S_1\,\tfrac{1}{2}\,S_2\right|\left.\tfrac{1}{2}\,\tfrac{1}{2}\,S\, M_S\right\rangle P_\sigma\left|\tfrac{1}{2}\,S_1\,\tfrac{1}{2}\,S_2\right\rangle \\
=& \sqrt{[S]}\,\delta_{SS'}\sum_{S_1,S_2}\left\langle (\tfrac{1}{2}\,\tfrac{1}{2})S'\, M'_S\right|\left\langle \tfrac{1}{2}\,S_1\,\tfrac{1}{2}\,S_2\right|\left.\tfrac{1}{2}\,\tfrac{1}{2}\,S\, M_S\right\rangle \left|\tfrac{1}{2}\,S_2\,\tfrac{1}{2}\,S_1\right\rangle \\
=& \sqrt{[S]}\,\delta_{SS'}\sum_{S_1,S_2}\left\langle (\tfrac{1}{2}\,\tfrac{1}{2})S'\, M'_S\right|\left\langle \tfrac{1}{2}\,S_2\,\tfrac{1}{2}\,S_1\right|\left.\tfrac{1}{2}\,\tfrac{1}{2}\,S\, M_S\right\rangle \left|\tfrac{1}{2}\,S_1\,\tfrac{1}{2}\,S_2\right\rangle \\
=& \sqrt{[S]}\,\delta_{SS'}\,(-1)^{1+S}\sum_{S_1,S_2}\left\langle (\tfrac{1}{2}\,\tfrac{1}{2})S'\, M'_S\right|\left\langle \tfrac{1}{2}\,S_1\,\tfrac{1}{2}\,S_2\right|\left.\tfrac{1}{2}\,\tfrac{1}{2}\,S\, M_S\right\rangle \left|\tfrac{1}{2}\,S_1\,\tfrac{1}{2}\,S_2\right\rangle \\
=& \sqrt{[S]}\,\delta_{SS'}\,(-1)^{1+S}\,\langle\, S'\, M'_S|S\, M_S\rangle \\
=& \sqrt{[S]}\,\delta_{SS'}\,(-1)^{1+S} \,.
\end{aligned} \tag{A.73}$$

A.4.3.3 $\prod_{S/T}$ operator

By definition

$$\prod_S = \frac{1+(-1)^{1-S}\,P_\sigma}{2}\,. \tag{A.74}$$

One gets easily from Eqs. (A.72,A.61)

$$\begin{aligned}(S'||\prod_{S_0}||S) =& \frac{1}{2}\left[\sqrt{[S]}\,\delta_{SS'} + (-1)^{1-S_0}\,\sqrt{[S]}\,\delta_{SS'}\,(-1)^{S+1}\right]\\ =& \frac{1}{2}\,\sqrt{[S]}\,\delta_{SS'}\,(1+(-1)^{S+S_0})\\ =& \sqrt{[S]}\,\delta_{SS'}\,\delta_{SS_0}\,.\end{aligned} \tag{A.75}$$

A.4.3.4 Total angular momentum L

We have immediately, using results from Sec. A.2.1.1

$$(L||L||L') = \frac{\langle L\,M_L|L_0|L'\,M'_L\rangle}{(-1)^{L-M_L}\begin{pmatrix} L & 1 & L'\\ -M_L & 0 & M'_L\end{pmatrix}} = \delta_{LL'}\,\sqrt{L\,(L+1)\,(2L+1)}\,. \tag{A.76}$$

A.4.3.5 $(\vec{\sigma}_1+\vec{\sigma}_2)$ operator

The easiest way is to use the result from the previous section

$$(S||\vec{\sigma}_1+\vec{\sigma}_2||S') = 2\,(S||\vec{S}\,||S') = \delta_{SS'}\,2\,\sqrt{S\,(S+1)\,(2S+1)} = \delta_{SS'}\,\delta_{S1}\,2\,\sqrt{6}\,, \tag{A.77}$$

since $S=0,1$. Another method can be used as a check, involving Eq. (A.63), that reads

$$\begin{aligned}(S||\vec{\sigma}_1+\vec{\sigma}_2||S') =& ((\tfrac{1}{2}\,\tfrac{1}{2})S||\vec{\sigma}_1+\vec{\sigma}_2||(\tfrac{1}{2}\,\tfrac{1}{2})S')\\ =& ((\tfrac{1}{2}\,\tfrac{1}{2})S||\sigma_1||(\tfrac{1}{2}\,\tfrac{1}{2})S') + ((\tfrac{1}{2}\,\tfrac{1}{2})S||P_\sigma^\dagger\,P_\sigma\,\sigma_2\,P_\sigma\,P_\sigma^\dagger||(\tfrac{1}{2}\,\tfrac{1}{2})S')\\ =& ((\tfrac{1}{2}\,\tfrac{1}{2})S||\sigma_1||(\tfrac{1}{2}\,\tfrac{1}{2})S') + ((\tfrac{1}{2}\,\tfrac{1}{2})S||P_\sigma^\dagger\,\sigma_1\,P_\sigma^\dagger||(\tfrac{1}{2}\,\tfrac{1}{2})S')\\ =& ((\tfrac{1}{2}\,\tfrac{1}{2})S||\sigma_1||(\tfrac{1}{2}\,\tfrac{1}{2})S') + (-1)^{S+S'}\,((\tfrac{1}{2}\,\tfrac{1}{2})S||\sigma_1||(\tfrac{1}{2}\,\tfrac{1}{2})S')\\ =& (1+(-1)^{S+S'})\,((\tfrac{1}{2}\,\tfrac{1}{2})S||\sigma_1||(\tfrac{1}{2}\,\tfrac{1}{2})S')\,,\end{aligned} \tag{A.78}$$

where

$$\begin{aligned}((\tfrac{1}{2}\,\tfrac{1}{2})S||\sigma_1||(\tfrac{1}{2}\,\tfrac{1}{2})S') =& (\tfrac{1}{2}||\sigma_1||\tfrac{1}{2})\,(\tfrac{1}{2}||\hat{\mathbb{I}}||\tfrac{1}{2})\,\sqrt{[S][S'][1]}\begin{Bmatrix} 1/2 & 1/2 & 1\\ 1/2 & 1/2 & 0\\ S & S' & 1\end{Bmatrix}\\ =& \frac{\langle \frac{1}{2}\,\frac{1}{2}|\sigma_{1,0}|\frac{1}{2}\,\frac{1}{2}\rangle}{(-1)^0\begin{pmatrix} 1/2 & 1 & 1/2\\ -1/2 & 0 & 1/2\end{pmatrix}}\,\sqrt{2}\,\sqrt{[S][S'][1]}\begin{Bmatrix} 1/2 & 1/2 & 1\\ 1/2 & 1/2 & 0\\ S & S' & 1\end{Bmatrix}\\ =& \sqrt{12}\,\sqrt{[S][S'][1]}\,\frac{\delta_{S1}\,\delta_{S'1}}{3\sqrt{6}}\,.\end{aligned} \tag{A.79}$$

Thus

$$(S||\vec{\sigma}_1+\vec{\sigma}_2||S') = (1+(-1)^{S+S'})\,\delta_{S1}\,\delta_{S'1}\,\sqrt{6} = \delta_{SS'}\,\delta_{S1}\,2\,\sqrt{6}\,. \tag{A.80}$$

Using Eq. (A.66) directly would have led to the same result for $((\frac{1}{2}\,\frac{1}{2})S||\sigma_1||(\frac{1}{2}\,\frac{1}{2})S')$.

A.4.3.6 $\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]}\right]^{[f]}$ operator

This is only a small generalization of the previous results, and one has using Eq. (A.63)

$$\begin{aligned}(S||\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]}\right]^{[f]}||S') =& \sqrt{[f][S][S']} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 1 \\ S & S' & f \end{Bmatrix} (\tfrac{1}{2}||\sigma_1^{[1]}||\tfrac{1}{2})^2 \\ =& 6\sqrt{[f][S][S']} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 1 \\ S & S' & f \end{Bmatrix}. \end{aligned} \tag{A.81}$$

For $f = 0$, one recovers easily the results from the previous sections. Indeed

$$\begin{aligned}(S||\vec{\sigma}_1 \cdot \vec{\sigma}_2||S') =& -\sqrt{3}\,(S||\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]}\right]^{[0]}||S') \\ =& -6\sqrt{3}\sqrt{[0][S][S']} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 1 \\ S & S' & 0 \end{Bmatrix} \\ =& -6\sqrt{3}\,\delta_{SS'}\,[S]\frac{(-1)^{2+S}}{\sqrt{[1][S]}} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & S \end{Bmatrix} \\ =& -6\,\delta_{SS'}\sqrt{[S]}\,(-1)^{2+S}\,(-1)^{2+S}\,\frac{3-2S(S+1)}{6} \\ =& \delta_{SS'}\sqrt{[S]}\,(2S(S+1)-3)\,. \end{aligned} \tag{A.82}$$

A.4.3.7 Spherical harmonics

Any finite rotation can be characterized by three Euler angles (α, β, γ), and the associated operator is noted

$$D(\alpha,\beta,\gamma) = e^{\frac{i\gamma}{\hbar}J_z}\,e^{\frac{i\beta}{\hbar}J_y}\,e^{\frac{i\alpha}{\hbar}J_z}\,. \tag{A.83}$$

Its matrix elements in the representation $|j\,m_j\rangle$ are

$$\mathcal{D}^{(j)}_{m,m'}(\alpha,\beta,\gamma) \equiv \langle j\,m'_j|D(\alpha,\beta,\gamma)|j\,m_j\rangle\,. \tag{A.84}$$

In the representations we are using J_z is diagonal, thus

$$\mathcal{D}^{(j)}_{m,m'}(\alpha,\beta,\gamma) = e^{i\,m'\,\gamma}\,\mathcal{D}^{(j)}_{m,m'}(0,\beta,0)\,e^{i\,m\,\alpha} \equiv e^{i\,m'\,\gamma}\,d^{(j)}_{m,m'}(\beta)\,e^{i\,m\,\alpha}\,. \tag{A.85}$$

Matrix elements $d^{(j)}_{m,m'}(\beta)$ can be evaluated using Jacobi Polynomials (Sec. A.2.7), and read

$$d^{(j)}_{m,m'}(\beta) = \sqrt{\frac{(j+m')!\,(j-m')!}{(j+m)!\,(j-m)!}}\,\cos^{m'+m}\left(\frac{\beta}{2}\right)\,\sin^{m'-m}\left(\frac{\beta}{2}\right)\,P^{m'-m,m'+m}_{j-m'}(\cos(\beta))\,. \tag{A.86}$$

Therefore, using Eqs. (A.85,A.39,A.86), one has for $t \equiv \cos(\beta)$

$$\begin{aligned}
&\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \mathcal{D}^{(j_1)\,*}_{m_1',m_1}(\alpha,\beta,\gamma)\,\mathcal{D}^{(j_2)}_{m_2',m_2}(\alpha,\beta,\gamma)\,\mathrm{d}\alpha\,\sin(\beta)\,\mathrm{d}\beta\,\mathrm{d}\gamma \\
&\qquad = \frac{\delta_{m_1'm_2'}\,\delta_{m_1m_2}}{2}\sqrt{\frac{(j_1+m_1')!\,(j_1-m_1')!\,(j_2+m_2')!\,(j_2-m_2')!}{(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!}} \\
&\qquad\quad \times \int_{-1}^{1}\left(\frac{1+t}{2}\right)^{m_1'+m_1}\left(\frac{1-t}{2}\right)^{m_1'-m_1} P^{m_1'-m_1,m_1'+m_1}_{j_1-m_1'}(t)\,P^{m_1'-m_1,m_1'+m_1}_{j_2-m_1'}(t)\,\mathrm{d}t \\
&\qquad = \frac{\delta_{m_1'm_2'}\,\delta_{m_1m_2}\,\delta_{j_1j_2}}{[j_1]}\,.
\end{aligned} \tag{A.87}$$

Transformation rules for the finite rotations read on the other hand

$$\mathcal{D}^{(j_1)}_{m_1',m_1}(\alpha,\beta,\gamma)\,\mathcal{D}^{(j_2)}_{m_2',m_2}(\alpha,\beta,\gamma) = \sum_{j,m',m}[j]\begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & m' \end{pmatrix}\mathcal{D}^{(j)\,*}_{m',m}(\alpha,\beta,\gamma)\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix}. \tag{A.88}$$

This leads to

$$\begin{aligned}
&\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \mathcal{D}^{(j_1)}_{m_1',m_1}(\alpha,\beta,\gamma)\,\mathcal{D}^{(j_2)}_{m_2',m_2}(\alpha,\beta,\gamma)\,\mathcal{D}^{(j_3)}_{m_3',m_3}(\alpha,\beta,\gamma)\,\mathrm{d}\alpha\,\sin(\beta)\,\mathrm{d}\beta\,\mathrm{d}\gamma \\
&\qquad = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3' \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.
\end{aligned} \tag{A.89}$$

Finally, one has

$$\mathcal{D}^{(\ell)}_{0,m}(\alpha,\beta,\gamma) = \sqrt{\frac{4\pi}{[\ell]}}\,Y^m_\ell(\beta,\gamma)\,, \tag{A.90}$$

and Eq. (A.89) becomes

$$\begin{aligned}
&\int_0^{2\pi}\int_0^{\pi} Y^{m_1}_{\ell_1}(\theta,\varphi)\,Y^{m_1}_{\ell_1}(\theta,\varphi)\,Y^{m_1}_{\ell_1}(\theta,\varphi)\,\sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\varphi \\
&\qquad = \sqrt{\frac{[\ell_1][\ell_2][\ell_3]}{4\pi}}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.
\end{aligned} \tag{A.91}$$

This amounts to

$$(k'\,L'||Y^{[k]}(\hat{k})||k\,L) = \frac{\langle k\,L'M_L'|Y^\mu_k(\hat{k})|k\,L\,M_L\rangle}{(-1)^{L'-M_L'}\begin{pmatrix} L' & k & L \\ -M_L' & \mu & M_L \end{pmatrix}} = (-1)^{L'}\sqrt{\frac{[L'][k][L]}{4\pi}}\begin{pmatrix} L' & k & L \\ 0 & 0 & 0 \end{pmatrix}. \tag{A.92}$$

A.4.4 Tensorial product of spherical harmonics

Using Eqs. (A.62,A.92), we get

$$\begin{aligned}(k'\,L'||\left[Y^{[a]}(\hat{k}')\otimes Y^{[b]}(\hat{k})\right]^{[f]}||k\,L) =&(-1)^{f+L+L'}\sqrt{[f]}\begin{Bmatrix} a & b & f\\ L' & L & 0\end{Bmatrix}\\ &\times(k'\,L'||Y^{[a]}(\hat{k}')||k'\,0)\,(k\,0||Y^{[b]}(\hat{k})||k\,L)\\ =&(-1)^{f+L+L'}\sqrt{[f]}\begin{Bmatrix} a & b & f\\ L & L' & 0\end{Bmatrix}(-1)^{L'}\\ &\times\sqrt{\frac{[0][a][L']}{4\pi}}\begin{pmatrix} L' & a & 0\\ 0 & 0 & 0\end{pmatrix}\sqrt{\frac{[L][b][0]}{4\pi}}\begin{pmatrix} 0 & b & L\\ 0 & 0 & 0\end{pmatrix}\\ =&(-1)^{f+L}\sqrt{[f]}\frac{(-1)^{L+L'+f}}{\sqrt{[L][L']}}\frac{[L][L']}{4\pi}\delta_{aL'}\,\delta_{bL}\frac{(-1)^{L+L'}}{\sqrt{[L][L']}}\\ =&(-1)^{L}\frac{\sqrt{[f]}}{4\pi}\,\delta_{aL'}\,\delta_{bL}\,.\end{aligned}\tag{A.93}$$

A.4.5 Quadratic terms

Using Eq. (A.92) and results from Sec. A.3.3, one has

$$\begin{aligned}(k'\,L'||q^2||k\,L) =&\sum_\lambda \tilde{f}_\lambda(k',k)\,(k'\,L'||\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\right]^{[0]}||k\,L)\\ =&\sum_\lambda\frac{\tilde{f}_\lambda(k',k)}{4\pi}\,\delta_{\lambda L}\,\delta_{\lambda L'}\,(-1)^{L'}\\ =&\frac{\delta_{LL'}}{4\pi}\left[4\pi\left(k^2+k'^2\right)\,\delta_{L0}-\frac{8\pi}{\sqrt{3}}kk'\,\delta_{L1}\right]\\ =&\delta_{LL'}\left[\left(k^2+k'^2\right)\,\delta_{L0}-\frac{2}{\sqrt{3}}kk'\,\delta_{L1}\right]\,.\end{aligned}\tag{A.94}$$

A.4.6 Gaussian terms

Applying the same method from the previous section, one gets for the direct terms

$$\begin{aligned}(k'\,L'||e^{-\frac{1}{4}\mu_i^2\,q^2}||k\,L) =&\sum_\lambda \tilde{g}^i_\lambda(k',k)\,(k'\,L'||\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\right]^{[0]}||k\,L)\\ =&\sum_\lambda\frac{\tilde{g}^i_\lambda(k',k)}{4\pi}\,\delta_{\lambda L}\,\delta_{\lambda L'}\,(-1)^{L'}\\ =&\frac{\delta_{LL'}}{4\pi}(-1)^{L'}\,\tilde{g}^i_L(k',k)\,.\end{aligned}\tag{A.95}$$

Appendix B

Hartree-Fock-Bogoliubov formalism in the traditional and Russian representations

Abstract: The present chapter provides an extended set of general equations about HFB formalism. The focus is put on the link between the so-called *traditional* and *Russian* representations in the case where time-reversal symmetry is not assumed. All equations of interest are especially given in both configuration and coordinate spaces and are further specified for time-reversal symmetric systems, spherical systems and infinite nuclear matter.

Contents

B.1 One-body states

B.1.1 Representation

Spin and isospin indices will be noted $\sigma = \pm 1/2$ and $q = \pm 1/2$, respectively, with the notation $\bar{\sigma} = -\sigma$, and

$$2\sigma = -2\bar{\sigma} = (-1)^{s-\sigma}\,, \tag{B.1}$$

with $s = 1/2$. Single-nucleon spinors $\{\varphi_\mu\}$ have good isospin projections and are represented by

$$\langle \vec{r}\,|\,\mu\rangle \equiv \varphi_\mu(\vec{r}\,q) = \begin{pmatrix} \langle \vec{r}\;\sigma = +1/2\,q\,|\,\mu\rangle \\ \langle \vec{r}\;\sigma = -1/2\,q\,|\,\mu\rangle \end{pmatrix} = \begin{pmatrix} \varphi_\mu(\vec{r}+1/2\,q) \\ \varphi_\mu(\vec{r}-1/2\,q) \end{pmatrix}. \tag{B.2}$$

Orthonormality and closure relationships in a given isospin subspace read for the set of spinors $\{\varphi_\mu\}$ as

$$\int \mathrm{d}\vec{r}\,\varphi_\mu^\dagger(\vec{r}\,q)\,\varphi_\nu(\vec{r}\,q) = \sum_\sigma \int \mathrm{d}\vec{r}\,\varphi_\mu^*(\vec{r}\,\sigma\,q)\,\varphi_\nu(\vec{r}\,\sigma\,q) = \delta_{\mu\nu}\,, \tag{B.3a}$$

$$\sum_\mu \varphi_\mu(\vec{r}\,\sigma\,q)\,\varphi_\mu^*(\vec{r}\,'\,\sigma'\,q) = \delta(\vec{r}-\vec{r}\,')\,\delta_{\sigma\sigma'}\,. \tag{B.3b}$$

In Dirac notations, closure relationships read as

$$\sum_\mu |\mu\rangle\,\langle\mu| = 1\,, \qquad \sum_q \sum_\sigma \int \mathrm{d}\vec{r}\,|\vec{r}\,\sigma\,q\rangle\,\langle\vec{r}\,\sigma\,q| = 1\,, \tag{B.4}$$

whereas those within a given isospin subspace are obtained by limiting the above sums to states corresponding to a given isospin projection.

B.1.2 Symmetries

Symmetries and associated quantum numbers μ used to designate single-particle states depend on the situation and cannot be given once and for all. Pairing requires at least the existence of one good quantum number (beyond isospin) to split the basis into two halves that are coupled by the Bogoliubov transformation. Because it is general enough to cover most of the situations of interest, we use the z-signature ζ_z as the transformation that provides this quantum number [5]. To be complete, one should characterize transformation properties of basis states under a complete symmetry group.

Signature transformations correspond to three rotations by an angle π around the reference axes, that is

$$\hat{R}_j = e^{i\pi\hat{J}_j} = e^{i\pi\hat{L}_j} e^{i\pi\hat{S}_j} = i\,e^{i\pi\hat{L}_j}\,\hat{\sigma}_j \qquad \text{for } j = x,\,y,\,z, \tag{B.5}$$

where $\hat{\sigma}_j$ are the Pauli spin-matrices. The third signature depends on the other two, since

$$\hat{R}_i\hat{R}_j = \epsilon_{ijk}\hat{R}_k - \delta_{ij}\,, \tag{B.6}$$

where ϵ_{ijk} is the Levi-Civita symbol and δ_{ij} the Kronecker symbol.

It is essential to also introduce the time-reversal operator $\hat{\mathcal{T}} = e^{i\,\pi\,\hat{S}_y}\,\hat{K}$, where $\hat{K}$ is an operator which associates to a wave function its complex conjugate and $\hat{S}_y$ is the spin-projection operator of the N-body system. For single-nucleon spinors the time-reversal operator reduces to $i\,\hat{\sigma}_y\,\hat{K}$. We will come back extensively to the properties of $\hat{\mathcal{T}}$ below. Squares of these basic operators for a N-body state are given by

$$\hat{\mathcal{T}}^2 = (-1)^N, \quad \hat{R}_i^2 = -1\,. \tag{B.7}$$

Single-particle eigenstates of $\hat{R}_z$ have eigenvalues $i\zeta_\mu = \pm i$ ($\zeta_\mu = \pm 1$). The z-signature relates, in the restrictive case of an axially symmetric system, to the projection of orbital momentum m_ℓ and spin σ on the z-axis according to

ζ_μ	m_ℓ	σ
+ 1	even	+1/2
+ 1	odd	-1/2
- 1	even	-1/2
- 1	odd	+1/2

As already said, the basis will be split into two halves according to the z-signature quantum number and pairing is assumed to take place between states of opposite signature. Consequently, the Bogoliubov transformation only pairs states of opposite signature, noted $(\mu, \hat{\nu})$. However, this notation does not specify which of the two states has a positive signature.

B.2 Two-body states

Normalized and antisymmetrized two-body states will be noted $|i\,j\rangle$, and non-antisymmetrized states $|1:i\,,\,2:j\rangle$. It will sometimes be useful to introduce non-normalized and antisymmetrized two-body states $\|\,i\,j\gg$ as

$$|i\,j\rangle = \frac{|1:i\,,\,2:j\rangle - |1:j\,,\,2:i\rangle}{\sqrt{2}}\,, \qquad \|\,i\,j\gg = |1:i\,,\,2:j\rangle - |1:j\,,\,2:i\rangle = \sqrt{2}\,|i\,j\rangle\,. \tag{B.8}$$

Starting from these states, several types of two-body wave functions can be obtained, depending on the scalar product considered. Typically, one can have

$$\langle 1:\vec{r},\,2:\vec{r}\,'|1:\mu,\,2:\mu'\rangle = \varphi_\mu(\vec{r}\,q)\,\varphi_{\mu'}(\vec{r}\,'\,q)\,, \tag{B.9a}$$

$$\langle 1:\vec{r}\sigma,\,2:\vec{r}\,'\sigma'|1:\mu,\,2:\mu'\rangle = \varphi_\mu(\vec{r}\,\sigma\,q)\,\varphi_{\mu'}(\vec{r}\,'\sigma'\,q)\,, \tag{B.9b}$$

$$\langle \vec{r}\,\vec{r}\,'|\mu\,\mu'\rangle = \varphi_\mu(\vec{r}\,q)\,\varphi_{\mu'}(\vec{r}\,'\,q) - \varphi_{\mu'}(\vec{r}\,q)\,\varphi_\mu(\vec{r}\,'\,q)\,, \tag{B.9c}$$

$$\langle \vec{r}\sigma\,\vec{r}\,'\sigma'|\mu\,\mu'\rangle = \varphi_\mu(\vec{r}\,\sigma\,q)\,\varphi_{\mu'}(\vec{r}\,'\sigma'\,q) - \varphi_{\mu'}(\vec{r}\,\sigma\,q)\,\varphi_\mu(\vec{r}\,'\sigma'\,q)\,, \tag{B.9d}$$

$$\langle 1:\vec{r},\,2:\vec{r}\,'|\mu\,\mu'\rangle = \frac{1}{\sqrt{2}}\left[\varphi_\mu(\vec{r}\,q)\,\varphi_{\mu'}(\vec{r}\,'\,q) - \varphi_{\mu'}(\vec{r}\,q)\,\varphi_\mu(\vec{r}\,'\,q)\right]\,, \tag{B.9e}$$

$$\langle 1:\vec{r}\sigma,\,2:\vec{r}\,'\sigma'|\mu\,\mu'\rangle = \frac{1}{\sqrt{2}}\left[\varphi_\mu(\vec{r}\,\sigma\,q)\,\varphi_{\mu'}(\vec{r}\,'\sigma'\,q) - \varphi_{\mu'}(\vec{r}\,\sigma\,q)\,\varphi_\mu(\vec{r}\,'\sigma'\,q)\right]\,. \tag{B.9f}$$

Then, care must be considered when defining closure relationships in the two-body space, depending on the antisymmetry and normalization of the two-body states considered. The two choices of main interest are

$$\sum_{qq'}\sum_{\sigma\sigma'}\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,|1:\vec{r}\sigma q,\,2:\vec{r}\,'\sigma'q'\rangle\,\langle 1:\vec{r}\sigma q,\,2:\vec{r}\,'\sigma'q'| = 1\,, \tag{B.10a}$$

$$\sum_{qq'}\sum_{\sigma\sigma'}\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,|\vec{r}\,\sigma\,q\,\vec{r}\,'\,\sigma'\,q'\rangle\,\langle \vec{r}\,\sigma\,q\,\vec{r}\,'\,\sigma'\,q'| = 2\,. \tag{B.10b}$$

Those results are obtained through

$$\begin{aligned}
&\langle 1:\mu,\,2:\nu|\left[\sum_{qq'}\sum_{\sigma\sigma'}\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,|1:\vec{r}\sigma q,\,2:\vec{r}\,'\sigma'q'\rangle\,\langle 1:\vec{r}\sigma q,\,2:\vec{r}\,'\sigma'q'|\right]\,|1:\mu',\,2:\nu'\rangle \\
&= \left(\sum_{\sigma\,q}\int \mathrm{d}\vec{r}\,\varphi^*_\mu(\vec{r}\,\sigma\,q)\,\varphi_{\mu'}(\vec{r}\,\sigma\,q)\right)\,\left(\sum_{\sigma'\,q'}\int \mathrm{d}\vec{r}\,'\,\varphi^*_\nu(\vec{r}\,'\,\sigma'\,q')\,\varphi_{\nu'}(\vec{r}\,'\,\sigma'\,q')\right) \\
&= \delta_{\mu\mu'}\,\delta_{\nu\nu'} \\
&= \langle 1:\mu,\,2:\nu|1:\mu',\,2:\nu'\rangle\,,
\end{aligned} \tag{B.11}$$

and

$$\begin{aligned}
&\langle \mu\,\nu| \left[\sum_{qq'} \sum_{\sigma\sigma'} \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \,|\vec{r}\,\sigma\,q,\,\vec{r}\,'\,\sigma'\,q'\rangle\,\langle \vec{r}\,\sigma\,q,\,\vec{r}\,'\,\sigma'\,q'| \right] \,|\mu'\,\nu'\rangle \\
&= \sum_{qq'} \sum_{\sigma\sigma'} \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \left(\varphi^*_\mu(\vec{r}\,\sigma\,q)\,\varphi^*_\nu(\vec{r}\,'\,\sigma'\,q') - \varphi^*_\nu(\vec{r}\,\sigma\,q)\,\varphi^*_\mu(\vec{r}\,'\,\sigma'\,q') \right) \\
&\qquad\qquad \times \left(\varphi_{\mu'}(\vec{r}\,\sigma\,q)\,\varphi_{\nu'}(\vec{r}\,'\,\sigma'\,q) - \varphi_{\nu'}(\vec{r}\,\sigma\,q)\,\varphi_{\mu'}(\vec{r}\,'\,\sigma'\,q) \right) \\
&= 2 \left[\left(\sum_{q\sigma} \int \mathrm{d}\vec{r}\,\varphi^*_\mu(\vec{r}\,\sigma\,q)\,\varphi_{\mu'}(\vec{r}\,\sigma\,q) \right) \left(\sum_{q'\sigma'} \int \mathrm{d}\vec{r}\,'\,\varphi^*_\nu(\vec{r}\,'\,\sigma'\,q')\,\varphi_{\nu'}(\vec{r}\,'\,\sigma'\,q') \right) \right. \\
&\qquad \left. - \left(\sum_{q\sigma} \int \mathrm{d}\vec{r}\,\varphi^*_\mu(\vec{r}\,\sigma\,q)\,\varphi_{\nu'}(\vec{r}\,\sigma\,q) \right) \left(\sum_{q'\sigma'} \int \mathrm{d}\vec{r}\,'\,\varphi^*_\nu(\vec{r}\,'\,\sigma'\,q')\,\varphi_{\mu'}(\vec{r}\,'\,\sigma'\,q') \right) \right] \\
&= 2 \left[\delta_{\mu\mu'}\,\delta_{\nu\nu'} - \delta_{\mu\nu'}\,\delta_{\nu\mu'} \right] \\
&= 2\,\langle \mu\,\nu|\mu'\,\nu'\rangle\,,
\end{aligned} \tag{B.12}$$

where Kronecker symbols also relates to the isospin of the states. Equivalently, in configuration space one has

$$\sum_{\mu\nu} |1:\mu,\,2:\nu\rangle\,\langle 1:\mu,\,2:\nu| = 1\,, \qquad\qquad \sum_{\mu\nu} |\mu\,\nu\rangle\,\langle \mu\,\nu| = 2\,. \tag{B.13}$$

B.3 Time-reversal operator

B.3.1 Definition

In the N-body Hilbert space, one has

$$\hat{\mathcal{T}} \equiv e^{i\,\pi\,\hat{S}_y}\,\hat{K}\,, \qquad\qquad \hat{\mathcal{T}}^2 = (-1)^N\,, \tag{B.14}$$

The operator $\hat{\mathcal{T}}$ is antiunitary (unitary and antilinear), with the following properties:

$$\hat{\mathcal{T}}^\dagger = \hat{\mathcal{T}}^{-1}\,, \tag{B.15a}$$

$$\lambda\,\hat{\mathcal{T}} = \hat{\mathcal{T}}\,\lambda^*\,, \qquad \forall\,\lambda \in \mathbb{C}\,, \tag{B.15b}$$

$$\langle u|\big(\hat{\mathcal{T}}|v\rangle\big) = \Big[\langle u|\big(\hat{\mathcal{T}}|v\rangle\big)\Big]^*\,, \tag{B.15c}$$

$$\langle u|\big(\hat{\mathcal{T}}^\dagger|v\rangle = \langle v|\big(\hat{\mathcal{T}}|u\rangle\,. \tag{B.15d}$$

In particular, the basis vector, bra or ket, on which such operators are applied needs to be specified. Representation and transformation rules differ between the Hilbert and Fock (second quantization) spaces.

Indeed, it is important to know the number of fermions on which $\hat{\mathcal{T}}$ is applied. For even-even systems $\hat{\mathcal{T}}^2 = 1$, and one can find time-invariant states such that $\hat{\mathcal{T}}\,|\Psi\rangle = |\Psi\rangle$. For single-nucleon spinors $\hat{\mathcal{T}}^2 = -1$, and no state is invariant under the action of $\hat{\mathcal{T}}$. Its action on a given basis state $|\mu\rangle$ defines the state $|\bar{\mu}\rangle$ according to

$$\hat{\mathcal{T}}\,|\mu\rangle = |\bar{\mu}\rangle\,, \qquad\qquad \hat{\mathcal{T}}\,|\bar{\mu}\rangle = -|\mu\rangle\,. \tag{B.16}$$

In particular $|\bar{\mu}\rangle$ and $|\mu\rangle$ are orthogonal to each other. Indeed, one has $\hat{\mathcal{T}}^\dagger = \hat{\mathcal{T}}^{-1} = -\hat{\mathcal{T}}$, thus

$$\langle\mu|\bar{\mu}\rangle = \langle\mu|\big(\hat{\mathcal{T}}|\mu\rangle = -\langle\mu|\big(\hat{\mathcal{T}}^\dagger|\mu\rangle = -\langle\mu|\big(\hat{\mathcal{T}}|\mu\rangle = -\langle\mu|\bar{\mu}\rangle = 0\,. \tag{B.17}$$

In the $N = 1$ case, the complex conjugate operator $\hat{K}$ does not act on the Hibert basis states, but ensures that $\hat{\mathcal{T}}$ is antilinear through

$$\hat{K}\,|\mu\rangle = |\mu\rangle\,, \qquad\qquad \hat{K}\,\left[\alpha\,|\mu\rangle\right] = \alpha^*\,|\mu\rangle\,. \tag{B.18}$$

B.3.2 Action on single-particle wave functions

The transformation of a single-particle wave function under the application of $\hat{\mathcal{T}}$ is given by

$$(\hat{\mathcal{T}}\,\varphi)_\mu(\vec{r}\,\sigma\,q) = 2\sigma\,\varphi^*_\mu(\vec{r}\,\bar{\sigma}\,q)\,, \tag{B.19}$$

thus $\hat{\mathcal{T}}$ does not change the parity of the state. It can be easily checked that $(\hat{\mathcal{T}}^2\varphi)_\mu = -\varphi_\mu$.

B.3.3 Transformation of creation and annihilation operators

One can introduce the time-reversal operator in Fock space $\hat{\tilde{\mathcal{T}}}$ through its transformation rules for standard creation and annihilation operators defined on the tensorial product of space, spin and isospin as well as on the particle vacuum $|0\rangle$ as

$$\hat{\tilde{\mathcal{T}}}^\dagger\,\hat{a}^\dagger_{\vec{r}\sigma q}\,\hat{\tilde{\mathcal{T}}} = 2\sigma\,\hat{a}^\dagger_{\vec{r}\bar{\sigma}q}\,, \qquad\qquad \hat{\tilde{\mathcal{T}}}\,\hat{a}^\dagger_{\vec{r}\sigma q}\,\hat{\tilde{\mathcal{T}}}^\dagger = 2\bar{\sigma}\,\hat{a}^\dagger_{\vec{r}\bar{\sigma}q}\,, \tag{B.20a}$$

$$\hat{\tilde{\mathcal{T}}}^\dagger\,\hat{a}_{\vec{r}\sigma q}\,\hat{\tilde{\mathcal{T}}} = 2\sigma\,\hat{a}_{\vec{r}\bar{\sigma}q}\,, \qquad\qquad \hat{\tilde{\mathcal{T}}}\,\hat{a}_{\vec{r}\sigma q}\,\hat{\tilde{\mathcal{T}}}^\dagger = 2\bar{\sigma}\,\hat{a}_{\vec{r}\bar{\sigma}q}\,, \tag{B.20b}$$

$$\hat{\tilde{\mathcal{T}}}\,|0\rangle = |0\rangle\,. \tag{B.20c}$$

In any arbitrary basis, one can define

$$\overline{\hat{a}^\dagger_k} \equiv \hat{\mathcal{T}}\,\hat{a}^\dagger_k\,\hat{\mathcal{T}}^\dagger\,, \tag{B.21}$$

and obtain an explicit representation of $\hat{\tilde{\mathcal{T}}}$ under the form

$$\hat{\tilde{\mathcal{T}}} = \exp\left[\frac{\pi}{2}\sum_k\left(\overline{\hat{a}^\dagger_k}\,\hat{a}_k - \hat{a}^\dagger_k\,\overline{\hat{a}_k}\right)\right]\,. \tag{B.22}$$

One says that the basis is *closed* under time-reversal symmetry when, starting from the basis state $|k\rangle$, one can find another basis state $|\tilde{k}\rangle$ such that

$$\overline{\hat{a}^\dagger_k} \equiv \eta_k\,\hat{a}^\dagger_{\tilde{k}}\,. \tag{B.23}$$

This is for instance the case of the eigenbasis of the position, spin and isospin operators $\{\hat{a}^\dagger_{\vec{r}\sigma q}\}$. In this case $\{\widetilde{\vec{r}\sigma q}\} \equiv \{\vec{r}\,\bar{\sigma}q\}$ and $\eta_{\vec{r}\sigma q} \equiv 2\bar{\sigma}$.

B.3.4 Action on one-body Dirac bras and kets

The representation of the same operator in Hilbert space $\hat{\mathcal{T}}$ is obtained through its action on a basis ket $|\vec{r}\,\sigma\,q\rangle$ and bra $\langle\vec{r}\,\sigma\,q|$ as

$$\hat{\mathcal{T}}|\vec{r}\,\sigma\,q\rangle = 2\bar{\sigma}|\vec{r}\,\bar{\sigma}\,q\rangle \qquad\qquad \langle\vec{r}\,\sigma\,q|\hat{\mathcal{T}} = 2\sigma\,\langle\vec{r}\,\bar{\sigma}\,q|\,, \tag{B.24}$$

which is consistent with Eqs. (B.20a,B.20c). This allows one to recover Eq. (B.19) through

$$(\hat{\mathcal{T}}\,\varphi)_\mu(\vec{r}\,\sigma\,q) = \langle\vec{r}\,\sigma\,q|\big(\hat{\mathcal{T}}|\mu\rangle = \langle\vec{r}\,\sigma\,q|\hat{\mathcal{T}}\big)|\mu\rangle^* = 2\sigma\,\langle\vec{r}\,\bar{\sigma}\,q|\mu\rangle^* = 2\sigma\,\varphi^*_\mu(\vec{r}\,\bar{\sigma}\,q)\,. \tag{B.25}$$

Note that the different signs appearing above come from a specific choice of phase in the definition of $\hat{\mathcal{T}} = e^{\pm i\,\pi\hat{\sigma}_y}\,\hat{K}^{(1)}$. In the following no distinction between $\hat{\mathcal{T}}$ and $\hat{\tilde{\mathcal{T}}}$ will be made.

[1] In the present case $\hat{\mathcal{T}} = e^{+i\,\pi\hat{\sigma}_y}\,\hat{K}$.

B.3.5 Matrix representation

One has to be very careful when representing $\hat{\mathcal{T}}$ through a matrix acting in the one-body Hilbert space. We define

$$\mathcal{T}_{\mu\nu} \equiv \langle\mu|\big(\hat{\mathcal{T}}|\nu\rangle = \int \mathrm{d}\vec{r} \sum_{\sigma} \varphi^*_\mu(\vec{r}\,\sigma\,q)\,(\hat{\mathcal{T}}\,\varphi)_\nu(\vec{r}\,\sigma\,q) = \int \mathrm{d}\vec{r} \sum_{\sigma} 2\sigma\,\varphi^*_\mu(\vec{r}\,\sigma q)\,\varphi^*_\nu(\vec{r}\,\bar{\sigma}\,q)\,. \quad \text{(B.26)}$$

Some care must be taken when defining the matrix representation of related operators. Although one naturally has $\mathcal{T}^*_{\mu\nu} = \langle\mu|\big(\hat{\mathcal{T}}^*|\nu\rangle$, $\mathcal{T}^{-1}_{\mu\nu} = \langle\mu|\big(\hat{\mathcal{T}}^{-1}|\nu\rangle$ and $\mathcal{T}^\dagger_{\mu\nu} = \langle\mu|\big(\hat{\mathcal{T}}^\dagger|\nu\rangle$, the matrix representation of $\hat{\mathcal{T}}^2$ is less trivially obtained as

$$\langle\mu|\big(\hat{\mathcal{T}}^2|\nu\rangle = \langle\mu|\hat{\mathcal{T}}\big)\big(\hat{\mathcal{T}}|\nu\rangle^* = \sum_{\kappa}\langle\mu|\big(\hat{\mathcal{T}}|\kappa\rangle\langle\kappa|\big(\hat{\mathcal{T}}|\nu\rangle^* \equiv (\mathcal{T}\mathcal{T}^*)_{\mu\nu} \neq \mathcal{T}^2_{\mu\nu}\,. \quad \text{(B.27)}$$

Then, one can check in matrix representation the properties of $\hat{\mathcal{T}}$ when acting on the single-particle Hilbert space, i.e.

$$\begin{aligned}
\mathcal{T}_{\nu\mu} &= \int \mathrm{d}\vec{r} \sum_{\sigma} 2\sigma\varphi^*_\nu(\vec{r}\,\sigma q)\,\varphi^*_\mu(\vec{r}\,\bar{\sigma}\,q) \\
&= \int \mathrm{d}\vec{r} \sum_{\sigma} 2\bar{\sigma}\varphi^*_\nu(\vec{r}\,\bar{\sigma} q)\,\varphi^*_\mu(\vec{r}\,\sigma\,q) \\
&= -\,\mathcal{T}_{\mu\nu}\,. && \text{hence } \mathcal{T}^T = -\mathcal{T}\,, \quad \text{(B.28a)}
\end{aligned}$$

$$\begin{aligned}
(\mathcal{T}\mathcal{T}^*)_{\mu\nu} &= \sum_{\kappa} \mathcal{T}_{\mu\kappa}\,\mathcal{T}^*_{\kappa\nu} \\
&= \sum_{\mu} \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} 2\sigma\,\varphi^*_\mu(\vec{r}\,\sigma\,q)\,\varphi^*_\kappa(\vec{r}\,\bar{\sigma}\,q)\,2\sigma'\,\varphi_\kappa(\vec{r}\,'\,\sigma'\,q)\,\varphi_\nu(\vec{r}\,'\,\bar{\sigma}'\,q) \\
&= \int \mathrm{d}\vec{r} \sum_{\sigma} 2\sigma\,\varphi^*_\mu(\vec{r}\,\sigma\,q)\,2\bar{\sigma}\,\varphi_\nu(\vec{r}\,\sigma\,q) \\
&= -\,\delta_{\mu\nu} && \text{hence } \mathcal{T}^2 = -1\,, \quad \text{(B.28b)}
\end{aligned}$$

$$\begin{aligned}
(\mathcal{T}^\dagger\,\mathcal{T})_{\mu\nu} &= \sum_{\kappa} \mathcal{T}^*_{\kappa\mu}\,\mathcal{T}_{\kappa\nu} \\
&= \sum_{\mu} \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} 2\sigma\,\varphi_\kappa(\vec{r}\,\sigma\,q)\,\varphi_\mu(\vec{r}\,\bar{\sigma}\,q)\,2\sigma'\,\varphi^*_\kappa(\vec{r}\,'\,\sigma'\,q)\,\varphi^*_\nu(\vec{r}\,'\,\bar{\sigma}'\,q) \\
&= \int \mathrm{d}\vec{r} \sum_{\sigma} 2\sigma\,\varphi_\mu(\vec{r}\,\bar{\sigma}\,q)\,2\sigma\,\varphi^*_\nu(\vec{r}\,\bar{\sigma}\,q) \\
&= \delta_{\mu\nu} && \text{hence } \mathcal{T}^{-1} = \mathcal{T}^\dagger\,. \quad \text{(B.28c)}
\end{aligned}$$

Since a state and its time-reversed partners have opposite signatures, non-zero matrix elements of $\mathcal{T}$ necessarily couple two different halves of the basis. $\mathcal{T}$ denotes the transformation matrix within each signature block from the basis φ to the basis formed out of their time-reversed

partners. It takes the form

$$\mathcal{T} = \begin{array}{c|cc|cc} & (\hat{\mathcal{T}}\,\varphi)_\mu & & (\hat{\mathcal{T}}\,\varphi)_{\hat{\nu}} & \\ & & & & \\ & 0 & & \mathcal{T}_{\mu\hat{\nu}} & \varphi_\mu \\ & & & & \\ \hline & & & & \\ & \mathcal{T}_{\hat{\nu}\mu} & & 0 & \varphi_{\hat{\nu}} \\ & & & & \end{array} \tag{B.29}$$

which, if the ordering of the starting basis of size M is such that the first $M/2$ states have a positive signature, shows that the ordering in the transformed basis has changed in such a way that states of negative signature now come first. This is again because $(\hat{\mathcal{T}}\,\varphi)_\mu$ has the opposite signature to φ_μ. Finally, a representation of the time-reversed states of a given spinor is achieved through

$$(\hat{\mathcal{T}}\,\varphi)_{\hat{\nu}}(\vec{r}\,\sigma\,q) = \langle \vec{r}\,\sigma\,q|\big(\hat{\mathcal{T}}|\hat{\nu}\rangle = \sum_\mu \langle \vec{r}\,\sigma\,q|\mu\rangle\,\langle\mu|\big(\hat{\mathcal{T}}|\hat{\nu}\rangle = \sum_\mu \varphi_\mu(\vec{r}\,\sigma\,q)\,\mathcal{T}_{\mu\hat{\nu}}\,, \tag{B.30}$$

whereas the inverse equation reads

$$\varphi_\mu(\vec{r}\,\sigma\,q) = \sum_{\hat{\nu}} (\hat{\mathcal{T}}\,\varphi)_{\hat{\nu}}(\vec{r}\,\sigma\,q)\,\mathcal{T}^\dagger_{\hat{\nu}\mu}\,. \tag{B.31}$$

B.4 Energy density functional formalism

In the energy Density functional (EDF) formalism, the ground-state energy is postulated under the form of a functional $\mathcal{E}[\rho,\kappa,\kappa^*]$ of the one-body density ρ^q and the pairing tensor κ^q, defined as

$$\rho^q_{\nu\mu} \equiv \langle\Phi|\hat{a}^{q\,\dagger}_\mu\,\hat{a}_\nu|\Phi\rangle\,, \qquad\qquad \kappa^q_{\nu\mu} \equiv \langle\Phi|\hat{a}_\mu\,\hat{a}_\nu|\Phi\rangle\,, \tag{B.32}$$

where $|\Phi\rangle$ is an auxiliary quasiparticle product state for the Hartree-Fock-Bogoliubov (HFB) realization of Single-Reference EDF (SR-EDF). Without going into any details concerning the actual form of the nuclear EDF, it is important to know that $\mathcal{E}[\rho,\kappa,\kappa^*]$ splits into the uncorrelated[2] kinetic energy and the remaining correlation energy[3].

B.4.1 Normal density matrix, pair density matrix and pairing tensor

The normal one-body density matrix is defined in coordinate representation through

$$\rho(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q') \equiv \langle\Phi|\hat{a}^\dagger_{\vec{r}\,'\sigma'q'}\,\hat{a}_{\vec{r}\sigma q}|\Phi\rangle = \sum_{\mu\nu}\varphi^*_\mu(\vec{r}\,'\,\sigma'\,q')\,\varphi_\nu(\vec{r}\,\sigma\,q)\,\rho^q_{\nu\mu}\,\delta_{qq'}\,, \tag{B.33}$$

where $\{\varphi_\mu\}$ denotes an arbitrary single-particle basis.

[2] In the HFB implementation of the EDF formalism, the kinetic energy is partly correlated through smooth occupation numbers associated with the explicit treatment of pair scattering.

[3] Such correlation energy also accounts for the correlated part of the kinetic energy which is not treated explicitly through the first contribution to $\mathcal{E}[\rho,\kappa,\kappa^*]$.

- In the so-called *traditional representation* of the HFB formalism, the pairing tensor is introduced through

$$\kappa(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q'\,)\equiv\langle\Phi|\hat{a}_{\vec{r}\,'\sigma'q'}\,\hat{a}_{\vec{r}\sigma q}|\Phi\rangle=\sum_{\mu\hat{\nu}}\varphi_{\hat{\nu}}(\vec{r}\,'\,\sigma'\,q'\,)\,\varphi_{\mu}(\vec{r}\,\sigma\,q)\,\kappa^{q}_{\mu\hat{\nu}}\,\delta_{qq'}\,, \tag{B.34}$$

  and is such that $\kappa^{q}_{\mu\nu}=\kappa^{q}_{\mu\nu}\,\delta_{-\zeta_\nu\zeta_\mu}$, as the Bogoliubov transformation only couples states of opposite signatures.

- In the so-called *Russian representation* of the HFB formalism, it is rather the pair density which is used, and it is defined as

$$\tilde{\rho}(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q'\,)\equiv 2\bar{\sigma}'\,\kappa(\vec{r}\,\sigma\,q,\vec{r}\,'\,\bar{\sigma}'\,q')=2\bar{\sigma}'\sum_{\mu\hat{\nu}}\varphi_{\hat{\nu}}(\vec{r}\,'\,\bar{\sigma}'\,q'\,)\,\varphi_{\mu}(\vec{r}\,\sigma\,q)\,\kappa^{q}_{\mu\hat{\nu}}\,\delta_{qq'}\,. \tag{B.35}$$

Since nucleons are chosen to have a good isospin projection, all densities and fields are isospin-block diagonal. This suggests to introduce the notations[4]

$$X^{q}(\vec{r}\,\sigma,\vec{r}\,'\,\sigma')\equiv X(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q')\,\delta_{qq'}\,,\qquad\qquad X=\rho,\tilde{\rho},\kappa,h,\tilde{h},\Delta\ldots \tag{B.36}$$

The scalar part of the normal and pair density matrices, the latter being of particular interest when pairing is restricted to the spin-singlet/isospin-triplet channel, can be introduced for a given isospin q through

$$\rho^{q}(\vec{r},\vec{r}\,')\equiv\sum_{\sigma}\rho^{q}(\vec{r}\,\sigma,\vec{r}\,'\,\sigma)\,,\qquad\qquad\tilde{\rho}^{q}(\vec{r},\vec{r}\,')\equiv\sum_{\sigma}\tilde{\rho}^{q}(\vec{r}\,\sigma,\vec{r}\,'\,\sigma)\,, \tag{B.37}$$

which leads naturally to the definition of the local scalar normal and pair densities

$$\rho^{q}(\vec{r}\,)\equiv\rho^{q}(\vec{r},\vec{r}\,)\,,\qquad\qquad\tilde{\rho}^{q}(\vec{r}\,)\equiv\tilde{\rho}^{q}(\vec{r},\vec{r}\,)\,, \tag{B.38}$$

which cannot be introduced for the pairing tensor κ as it is skew symmetric ($\kappa^{\mathrm{T}}=-\kappa$).

From Eqs. (B.31,B.35), one finds that

$$\begin{aligned}\tilde{\rho}(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q'\,)=&2\bar{\sigma}'\sum_{\mu\hat{\nu}}\sum_{\mu'}\mathcal{T}^{*}_{\hat{\nu}\mu'}\,(\hat{\mathcal{T}}\,\varphi)_{\mu'}(\vec{r}\,'\,\bar{\sigma}'\,q'\,)\,\varphi_{\mu}(\vec{r}\,\sigma\,q)\,\kappa^{q}_{\mu\hat{\nu}}\,\delta_{qq'}\\=&\sum_{\mu\hat{\nu}}\sum_{\mu'}\mathcal{T}^{*}_{\hat{\nu}\mu'}\,\varphi^{*}_{\mu'}(\vec{r}\,'\,\sigma'\,q'\,)\,\varphi_{\mu}(\vec{r}\,\sigma\,q)\,\kappa^{q}_{\mu\hat{\nu}}\,\delta_{qq'}\\\equiv&\sum_{\mu\mu'}\varphi^{*}_{\mu'}(\vec{r}\,'\,\sigma'\,q'\,)\,\varphi_{\mu}(\vec{r}\,\sigma\,q)\,\tilde{\rho}^{q}_{\mu\mu'}\,\delta_{qq'}\,,\end{aligned} \tag{B.39}$$

which defines the matrix elements of $\tilde{\rho}^{q}_{\mu\mu'}$ in any arbitrary single-particle basis in terms of those of κ and of the time-reversal operator $\hat{\mathcal{T}}$, i.e.

$$\tilde{\rho}^{q}_{\mu\mu'}=\sum_{\hat{\nu}}\kappa^{q}_{\mu\hat{\nu}}\,\mathcal{T}^{*}_{\hat{\nu}\mu'}\,,\qquad\qquad\kappa^{q}_{\mu\hat{\nu}}=\sum_{\mu'}\tilde{\rho}^{q}_{\mu\mu'}\,\mathcal{T}^{T}_{\mu'\hat{\nu}}\,, \tag{B.40}$$

or, equivalently, $\tilde{\rho}^{q}=\kappa^{q}\,\mathcal{T}^{*}$ and $\kappa^{q}=\tilde{\rho}^{q}\,\mathcal{T}^{T}$. In a similar way, one can show that:

$$\tilde{\rho}^{q\,\dagger}_{\mu\mu'}=\sum_{\hat{\nu}}\mathcal{T}_{\hat{\nu}\mu}\,\kappa^{q\,*}_{\mu'\hat{\nu}}\,,\qquad\qquad\kappa^{q\,*}_{\mu'\hat{\nu}}=\sum_{\mu}\mathcal{T}^{*}_{\hat{\nu}\mu}\,\tilde{\rho}^{q\,\dagger}_{\mu\mu'}\,, \tag{B.41}$$

[4] In configuration space, one will also use matrix elements of the kind X^{q}_{ij} where the superscript is a reminder that the field and densities are diagonal in isospin. In all rigor however, matrix elements should be noted X_{ij}, the isospin superscript appearing for matrix elements of the kind $X_{\vec{r}\sigma q\,\vec{r}\,'\sigma' q}\equiv X^{q}_{\vec{r}\sigma\,\vec{r}\,'\sigma'}$.

or, equivalently, $\tilde{\rho}^{q\,\dagger} = \mathcal{T}^T\,\kappa^{q\,\dagger}$ and $\kappa^{q\,\dagger} = \mathcal{T}^*\,\tilde{\rho}^{q\,\dagger}$. Eq. (B.40) is the matrix representation of the definition of the pair density matrix in an arbitrary matrix through

$$\tilde{\rho}^q_{\mu\nu} \equiv \langle\Phi|\,\overline{\hat{a}^q_\nu}\,\hat{a}^q_\mu\,|\Phi\rangle\,, \tag{B.42}$$

which can be used to prove that, for time-reversal invariant systems $\hat{\mathcal{T}}\,|\Phi\rangle = |\Phi\rangle$, the pairing tensor becomes hermitian. Indeed

$$\begin{aligned}\tilde{\rho}^q_{\mu\nu} =&\langle\Phi|\,\hat{\mathcal{T}}^\dagger\big)\,\big(\hat{\mathcal{T}}\,\hat{a}^q_\nu\,\hat{\mathcal{T}}^\dagger\,\hat{a}^q_\mu\,|\Phi\rangle\\ =&-\langle\Phi|\,\hat{a}^q_\nu\,\big(\hat{\mathcal{T}}^\dagger\,\hat{\mathcal{T}}^2\,\hat{a}^q_\mu\,\hat{\mathcal{T}}^\dagger\,\hat{\mathcal{T}}\,|\Phi\rangle^*\\ =&\langle\Phi|\,\overline{\hat{a}^q_\mu}\,\hat{a}^q_\nu\,|\Phi\rangle^*\\ =&\tilde{\rho}^{q\,*}_{\nu\mu}\,,\end{aligned} \tag{B.43}$$

where $\langle\Phi|\,\hat{\mathcal{T}}^\dagger\big) = \langle\Phi|$, $\hat{\mathcal{T}}^\dagger\,\hat{\mathcal{T}} = 1$ and $\hat{\mathcal{T}}^2 = -1$ have been used. This result provides one advantage to using the Russian representation in the case of time-reversal invariant systems.

B.4.2 Generalized density matrices

Since the many-body auxiliary HFB state is an independent quasiparticle state, the normal density matrix ρ does not contain enough information to characterize the state. The generalized one-body density matrix which does so is defined in the traditional representation as

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} = \begin{pmatrix} \langle\Phi|\hat{a}^\dagger\hat{a}|\Phi\rangle & \langle\Phi|\hat{a}\hat{a}|\Phi\rangle \\ \langle\Phi|\hat{a}^\dagger\hat{a}^\dagger|\Phi\rangle & \langle\Phi|\hat{a}\hat{a}^\dagger|\Phi\rangle \end{pmatrix}, \tag{B.44}$$

and is idempotent $\mathcal{R}^2 = \mathcal{R}$, as it should be for an independent quasiparticle state. This leads to various relations between ρ and κ, e.g.

$$\rho\cdot\rho - \kappa\cdot\kappa^* = \rho\,, \qquad \rho\cdot\kappa - \kappa\cdot\rho^* = 0\,, \tag{B.45a}$$

$$\kappa^*\cdot\rho - \rho^*\cdot\kappa^* = 0\,, \qquad \rho^*\cdot\rho^* - \kappa^*\cdot\kappa = \rho^*\,. \tag{B.45b}$$

The pairing tensor being skew symmetric, its trace vanishes, that is

$$\mathrm{Tr}\{\kappa^q\} = \mathrm{Tr}\{\kappa^{q\,*}\} = \sum_\mu \kappa^q_{\mu\mu} = \int \mathrm{d}\vec{r}\sum_\sigma \kappa(\vec{r}\,\sigma\,q,\vec{r}\,\sigma\,q) = \int \mathrm{d}\vec{r}\sum_\sigma \kappa^*(\vec{r}\,\sigma\,q,\vec{r}\,\sigma\,q) = 0\,. \tag{B.46}$$

A generalized density matrix can also be introduced in the Russian representation through

$$\tilde{\mathcal{R}} = \begin{pmatrix} \rho & \tilde{\rho} \\ \tilde{\rho}^\dagger & 1-\rho^* \end{pmatrix}, \tag{B.47}$$

which contains the same information as $\mathcal{R}$, and shares the property $\tilde{\mathcal{R}}^2 = \tilde{\mathcal{R}}$, leading to

$$\rho\cdot\rho + \tilde{\rho}\cdot\tilde{\rho}^\dagger = \rho\,, \qquad \rho\cdot\tilde{\rho} - \tilde{\rho}\cdot\rho^* = 0\,, \tag{B.48a}$$

$$\tilde{\rho}^\dagger\cdot\rho - \rho^*\cdot\tilde{\rho}^\dagger = 0\,, \qquad \rho^*\cdot\rho^* + \tilde{\rho}^\dagger\cdot\tilde{\rho} = \rho^*\,. \tag{B.48b}$$

B.5 Hartree-Fock-Bogoliubov equations

B.5.1 Traditional representation

The equations of motion for the single-particle states and the occupation amplitudes are determined self-consistently from the variation of the total constrained energy. The second constraint makes the many-body state to remain an independent quasiparticle state whereas the first one fixes the average particle number to the actual number of particles. This is the minimum set of constraints. The minimization reads

$$\delta\Big(\mathcal{E}[\rho,\kappa,\kappa^*] - \frac{1}{2}\sum_q \lambda^q(\mathrm{Tr}\{\rho^q\} + \mathrm{Tr}\{\rho^{q\,*}\}) - \sum_q \mathrm{Tr}\{\Lambda^q(\mathcal{R}^{q\,2} - \mathcal{R}^q)\}\Big) = 0\,, \tag{B.49}$$

with the additional conditions

$$\mathrm{Tr}\{\rho^q\} = \mathrm{Tr}\{\rho^{q\,*}\} = \langle\hat{N}_q\rangle = \langle\hat{N}_q^\dagger\rangle = N_q\,, \tag{B.50a}$$

$$\mathcal{R}^{q\,2} - \mathcal{R}^q = 0\,, \tag{B.50b}$$

which have to be met by adjusting the Lagrange parameters λ^q and Λ^q accordingly. The variation is expressed through a variation of the matrix elements of the generalized density matrix $\mathcal{R}^q$. We have to remember, however, that $\mathcal{R}^q$ contains redundant information since only half of its matrix elements are independent, i.e.

$$\rho^{q\,*}_{ij} = \rho^q_{ji}\,, \qquad \kappa^q_{ij} = -\kappa^q_{ji}\,, \qquad \kappa^{q\,*}_{ij} = -\kappa^{q\,*}_{ji}\,. \tag{B.51}$$

One chooses the irreducible set of independent variables $\rho^q_{ij}, \rho^{q\,*}_{ij}, \kappa^q_{ij}, \kappa^{q\,*}_{ij}$ for $j < i$ as well as ρ^q_{ii} for all i. The variation of $\mathcal{R}^q$ can be written as

$$\delta\mathcal{R}^q_{kl} = \begin{pmatrix} \delta\rho^q_{kl} & \delta\kappa^q_{kl} \\ -\delta\kappa^{q\,*}_{kl} & -\delta\rho^{q\,*}_{kl} \end{pmatrix}. \tag{B.52}$$

Then, the variation of the energy gives

$$\begin{aligned}\delta\mathcal{E} =& \sum_{j<iq}\left(\frac{\delta\mathcal{E}}{\delta\rho^q_{ij}}\,\delta\rho^q_{ij} + \frac{\delta\mathcal{E}}{\delta\rho^{q\,*}_{ij}}\,\delta\rho^{q\,*}_{ij} + \frac{\delta\mathcal{E}}{\delta\kappa^q_{ij}}\,\delta\kappa^q_{ij} + \frac{\delta\mathcal{E}}{\delta\kappa^{q\,*}_{ij}}\,\delta\kappa^{q\,*}_{ij}\right) + \sum_{iq}\frac{\delta\mathcal{E}}{\delta\rho^q_{ii}}\,\delta\rho^q_{ii} \\ \equiv& \frac{1}{2}\sum_{ijq}\left(h^q_{ji}\delta\rho^q_{ij} + h^{q\,*}_{ji}\delta\rho^{q\,*}_{ij} - \Delta^{q\,*}_{ji}\delta\kappa^q_{ij} - \Delta^q_{ji}\delta\kappa^{q\,*}_{ij}\right) \\ =& \frac{1}{2}\,\mathrm{Tr}\left\{h\delta\rho + h^*\delta\rho^* - \Delta^*\delta\kappa - \Delta\delta\kappa\right\}\,,\end{aligned} \tag{B.53}$$

where we have introduced, for $j \le i$,

$$h^q_{ji} \equiv \frac{\delta\mathcal{E}}{\delta\rho^q_{ij}} = h^{q\,*}_{ij}\,, \qquad \Delta^q_{ij} \equiv \frac{\delta\mathcal{E}}{\delta\kappa^{q\,*}_{ij}} = -\Delta^q_{ji}\,, \tag{B.54}$$

$$h^{q\,*}_{ji} \equiv \frac{\delta\mathcal{E}}{\delta\rho^{q\,*}_{ij}} = h^q_{ij}\,, \qquad \Delta^{q\,*}_{ij} \equiv \frac{\delta\mathcal{E}}{\delta\kappa^q_{ij}} = -\Delta^{q\,*}_{ji}\,. \tag{B.55}$$

The concept of trace can also be used for the combined spaces of particle indices and submatrices of HFB theory. Introducing the generalized HFB matrix $\mathcal{H}^q$ in analogy to $\mathcal{R}^q$ as

$$\mathcal{H}^q = \begin{pmatrix} h^q & \Delta^q \\ -\Delta^{q\,*} & -h^{q\,*} \end{pmatrix}, \tag{B.56}$$

the variation of the energy can be rewritten as

$$\begin{aligned}\delta\mathcal{E} = \sum_{ijq} \mathcal{H}^q_{ij}\delta\mathcal{R}^q_{ji} = \mathrm{Tr}\{\mathcal{H}\delta\mathcal{R}\} =& \frac{1}{2}\mathrm{Tr}\left\{\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} \delta\rho & \delta\kappa \\ -\delta\kappa^* & -\delta\rho^* \end{pmatrix}\right\} \\ =& \frac{1}{2}\mathrm{Tr}\left\{h\delta\rho - \Delta\delta\kappa^* - \Delta^*\delta\kappa + h^*\delta\rho^*\right\}. \end{aligned} \tag{B.57}$$

The trace has to be taken in the space of single-particle states and, if applicable, in the space of 2×2 matrices. If the index q is absent (present), the trace in isospin space is (not) considered. The variation of the constraint on particle number gives

$$\delta\mathrm{Tr}\{\rho^q\} = \sum_{ij}\delta\rho^q_{ij}\frac{\delta}{\delta\rho^q_{ij}}\sum_k \rho^q_{kk} = \sum_{ij}\delta_{ij}\,\delta\rho^q_{ij}\,, \tag{B.58a}$$

$$\delta\mathrm{Tr}\{\rho^{q\,*}\} = \sum_{ij}\delta\rho^{q*}_{ij}\frac{\delta}{\delta\rho^{q*}_{ij}}\sum_k \rho^{q*}_{kk} = \sum_{ij}\delta_{ij}\,\delta\rho^{q*}_{ij}\,. \tag{B.58b}$$

The variations of the constraint and of the energy functional can be combined into

$$\delta\big(\mathcal{E} - \frac{1}{2}\sum_q \lambda^q(\mathrm{Tr}\{\rho^q\} + \mathrm{Tr}\{\rho^{q\,*}\})\big) = \mathrm{Tr}\{\mathcal{H}'\delta\mathcal{R}\}\,, \tag{B.59}$$

where

$$\mathcal{H}^{q\,\prime} = \begin{pmatrix} h^q - \lambda^q & \Delta^q \\ -\Delta^{q\,*} & -(h^{q\,*} - \lambda^q) \end{pmatrix} \equiv \begin{pmatrix} h^{q\prime} & \Delta^q \\ -\Delta^{q\,*} & -h^{q\prime *} \end{pmatrix}. \tag{B.60}$$

On the other hand, the variation of $\mathrm{Tr}\{\Lambda^q(\mathcal{R}^{q\,2} - \mathcal{R}^q)\}$ leads to

$$\begin{aligned}\delta\mathrm{Tr}\{\Lambda^q(\mathcal{R}^{q\,2} - \mathcal{R}^q)\} =& \sum_{mn}\frac{\delta}{\delta\mathcal{R}^q_{mn}}\sum_{ij}\Lambda^q_{ij}\left(\sum_k \mathcal{R}^q_{jk}\mathcal{R}^q_{ki} - \mathcal{R}^q_{ji}\right)\delta\mathcal{R}^q_{mn} \\ =& \sum_{ij}\Lambda^q_{ij}\left[\sum_k(\delta_{jm}\delta_{kn}\mathcal{R}^q_{ki} + \mathcal{R}^q_{jk}\delta_{km}\delta_{in}) - \delta_{jm}\delta_{in}\right]\delta\mathcal{R}^q_{mn} \\ =& \left(\sum_i \Lambda^q_{im}\mathcal{R}^q_{ni} + \sum_j \Lambda^q_{nj}\mathcal{R}^q_{jm} - \Lambda^q_{nm}\right)\delta\mathcal{R}^q_{mn} \\ =& (\mathcal{R}^q\Lambda^q + \Lambda^q\mathcal{R}^q - \Lambda^q)_{nm}\,\delta\mathcal{R}^q_{mn} \\ =& \mathrm{Tr}\{(\mathcal{R}^q\Lambda^q + \Lambda^q\mathcal{R}^q - \Lambda^q)\,\delta\mathcal{R}^q\}\,, \end{aligned} \tag{B.61}$$

in such a way that the variational equation finally reads

$$\mathrm{Tr}\{\left(\mathcal{H}^{q\,\prime} - \mathcal{R}^q\Lambda^q - \Lambda^q\mathcal{R}^q + \Lambda^q\right)\delta\mathcal{R}^q\} = 0\,. \tag{B.62}$$

The latter equation has to hold for an arbitrary variation $\delta\mathcal{R}^q$. This means that the rest of the expression has to be zero, i.e.

$$\mathcal{H}^{q\,\prime} - \mathcal{R}^q\Lambda^q - \Lambda^q\mathcal{R}^q + \Lambda^q = 0\,. \tag{B.63}$$

In the next step we eliminate the matrix of Lagrange parameters Λ^q. Subtraction of $\mathcal{R}^q \times$ Eq. (B.63)) from Eq. (B.63) $\times\,\mathcal{R}^q$ yields to

$$\begin{aligned} 0 =& \mathcal{H}^{q\,\prime}\mathcal{R}^q - \mathcal{R}^q\Lambda^q\mathcal{R}^q - \Lambda^q\mathcal{R}^{q\,2} + \Lambda^q\mathcal{R}^q - \mathcal{R}^q\mathcal{H}^{q\,\prime} + \mathcal{R}^{q\,2}\Lambda^q + \mathcal{R}^q\Lambda^q\mathcal{R}^q - \mathcal{R}^q\Lambda^q \\ =& [\mathcal{H}^{q\,\prime}, \mathcal{R}^q] - \Lambda^q(\mathcal{R}^{q\,2} - \mathcal{R}^q) + (\mathcal{R}^{q\,2} - \mathcal{R}^q)\Lambda^q \\ =& [\mathcal{H}^{q\,\prime}, \mathcal{R}^q]\,. \end{aligned} \tag{B.64}$$

This means that the solution of the minimization problem is a basis which diagonalizes simultaneously $\mathcal{H}^{q\prime}$ and $\mathcal{R}^q$. Finally, one obtains the HFB eigenvalues problem in the traditional representation under the form

$$\begin{pmatrix} h^q - \lambda^q & \Delta^q \\ -\Delta^{q\,*} & -h^{q\,*} + \lambda^q \end{pmatrix} \begin{pmatrix} \mathcal{U}^{q[\kappa]} \\ \mathcal{V}^{q[\kappa]} \end{pmatrix}_\mu = E^q_\mu \begin{pmatrix} \mathcal{U}^{q[\kappa]} \\ \mathcal{V}^{q[\kappa]} \end{pmatrix}_\mu , \tag{B.65}$$

where $(\mathcal{U}^{q[\kappa]}_\mu, \mathcal{V}^{q[\kappa]}_\mu)$ are the upper and lower components of the quasiparticle eigenstate expanded in the single-particle basis of interest one starts with, whereas E^q_μ denotes the corresponding quasiparticle energy. Having those quasiparticle eigenstates at hand, the normal density matrix and pairing tensor can be calculated as

$$\rho = \mathcal{V}^{q[\kappa]\,*}\,\mathcal{V}^{q[\kappa]\,\mathrm{T}}\,, \qquad \kappa = \mathcal{V}^{q[\kappa]\,*}\,\mathcal{U}^{q[\kappa]\,\mathrm{T}} = -\mathcal{U}^{q[\kappa]}\,\mathcal{V}^{q[\kappa]\,\dagger}\,. \tag{B.66}$$

B.5.2 Russian representation

We introduce the $(2N \times 2N)$ unitary matrix G as

$$G = \begin{pmatrix} 0 & 1 \\ \mathcal{T}^* & 0 \end{pmatrix}, \tag{B.67}$$

and perform the associated basis transformation on Eq. (B.65), that is

$$G^\dagger \begin{pmatrix} h^q - \lambda^q & \Delta^q \\ -\Delta^{q\,*} & -h^{q\,*} + \lambda^q \end{pmatrix} G\,G^\dagger \begin{bmatrix} \mathcal{U}^{q[\kappa]} \\ \mathcal{V}^{q[\kappa]} \end{bmatrix}_\mu = E^q_\mu\,G^\dagger \begin{bmatrix} \mathcal{U}^{q[\kappa]} \\ \mathcal{V}^{q[\kappa]} \end{bmatrix}_\mu , \tag{B.68}$$

to obtain

$$\begin{pmatrix} -\mathcal{T}^T h^{q\,*} \mathcal{T}^* + \lambda^q & \tilde{h}^{q\,\dagger} \\ \tilde{h}^q & h^q - \lambda^q \end{pmatrix} \begin{bmatrix} \mathcal{V}^{q[\tilde{\rho}]} \\ \mathcal{U}^{q[\tilde{\rho}]} \end{bmatrix}_\mu = E^q_\mu \begin{bmatrix} \mathcal{V}^{q[\tilde{\rho}]} \\ \mathcal{U}^{q[\tilde{\rho}]} \end{bmatrix}_\mu , \tag{B.69}$$

or equivalently

$$\begin{pmatrix} h^q - \lambda^q & \tilde{h}^q \\ \tilde{h}^{q\,\dagger} & -(\mathcal{T}^{-1} h^q \mathcal{T})^* + \lambda^q \end{pmatrix} \begin{bmatrix} \mathcal{U}^{q[\tilde{\rho}]} \\ \mathcal{V}^{q[\tilde{\rho}]} \end{bmatrix}_\mu = E^q_\mu \begin{bmatrix} \mathcal{U}^{q[\tilde{\rho}]} \\ \mathcal{V}^{q[\tilde{\rho}]} \end{bmatrix}_\mu , \tag{B.70}$$

with the quasiparticle states in the Russian representation defined as

$$\begin{bmatrix} \mathcal{U}^{q[\tilde{\rho}]} \\ \mathcal{V}^{q[\tilde{\rho}]} \end{bmatrix}_\mu \equiv \begin{bmatrix} \mathcal{U}^{q[\kappa]} \\ \mathcal{T}^T\,\mathcal{V}^{q[\kappa]} \end{bmatrix}_\mu . \tag{B.71}$$

and the pair field $\tilde{h}$ as

$$\tilde{h}^q \equiv \Delta^q\,\mathcal{T}^*\,, \tag{B.72a}$$

$$\tilde{h}^q \equiv -\,\mathcal{T}^T\,\Delta^{q\,*}\,. \tag{B.72b}$$

Coming back to the definition of the pairing field in the traditional representation, that is

$$\Delta^q_{i\hat{j}} = \frac{\partial \mathcal{E}}{\partial \kappa^{q\,*}_{i\hat{j}}} = \sum_{kl} \frac{\partial \mathcal{E}}{\partial \tilde{\rho}^{q\,\dagger}_{kl}} \frac{\partial \tilde{\rho}^{q\,\dagger}_{kl}}{\partial \kappa^{q\,*}_{i\hat{j}}} = \sum_k \frac{\partial \mathcal{E}}{\partial \tilde{\rho}^{q\,\dagger}_{ki}}\,\mathcal{T}_{\hat{j}k} \equiv \sum_k \tilde{h}^q_{ik}\,\mathcal{T}^T_{k\hat{j}}\,, \tag{B.73a}$$

$$\Delta^{q\,*}_{i\hat{j}} = \frac{\partial \mathcal{E}}{\partial \kappa^q_{i\hat{j}}} = \sum_{kl} \frac{\partial \mathcal{E}}{\partial \tilde{\rho}^q_{kl}} \frac{\partial \tilde{\rho}^q_{kl}}{\partial \kappa^q_{i\hat{j}}} = \sum_l \frac{\partial \mathcal{E}}{\partial \tilde{\rho}^q_{il}}\,\mathcal{T}^*_{\hat{j}l} \equiv \sum_l \mathcal{T}^*_{\hat{j}l}\,\tilde{h}^{q\,\dagger}_{li}\,, \tag{B.73b}$$

and posing

$$\tilde{h}^q_{ij} \equiv \frac{\partial \mathcal{E}}{\partial \tilde{\rho}^{q\,\dagger}_{ji}}\,, \qquad \tilde{h}^{q\,\dagger}_{ij} \equiv \frac{\partial \mathcal{E}}{\partial \tilde{\rho}^{q}_{ji}}\,, \tag{B.74}$$

one can show that

$$\Delta^q = \tilde{h}^q\,\mathcal{T}^T\,, \tag{B.75a}$$
$$\Delta^{q\,*} = \tilde{h}^{q\,*}\,\mathcal{T}^\dagger = -(\tilde{h}^q\,\mathcal{T}^T)^\dagger\,, \tag{B.75b}$$

which indeed is consistent with Eqs. (B.72a,B.72b).

Using Eq. (B.71), the one-body and pair density matrices read as

$$\rho^q = \mathcal{V}^{q[\kappa]\,*}\,\mathcal{V}^{q[\kappa]\,\mathrm{T}} = \mathcal{T}\,\mathcal{V}^{q[\tilde{\rho}]\,*}\,\mathcal{V}^{q[\tilde{\rho}]\,\mathrm{T}}\,\mathcal{T}^\dagger\,, \tag{B.76a}$$
$$\tilde{\rho}^q = \kappa^q\,\mathcal{T}^* = -\mathcal{U}^{q[\kappa]}\,\mathcal{V}^{q[\kappa]\,\dagger}\,\mathcal{T}^* = -\mathcal{U}^{q[\tilde{\rho}]}\,\mathcal{V}^{q[\tilde{\rho}]\,\dagger}\,, \tag{B.76b}$$

which shows in particular that the one-body density expressed in terms of the quasiparticle components does not read generally the same in the traditional and Russian representations. Of course, the representations using κ and $\tilde{\rho}$ are fully equivalent, but one or the other may present advantages under certain circumstances. The pair density matrix is particularly suited to quasi-local pairing functionals, in particular when the corresponding effective vertex is limited to the spin-singlet/isospin-triplet channel. When the system is invariant under time-reversal, the pair density $\tilde{\rho}$ becomes hermitian which leads to simplifications. Note however that Eq. (B.70) demonstrates that quasiparticle wave functions in the Russian representation are not solutions of the HFB equations when time-reversal invariance is not assumed [6].

According to Eq. (B.71), the Russian representation amounts to representing the lower component of the quasiparticle wave functions in the basis constructed with the time-reversed states of the ones used to express the upper component. Because of the properties of the $M \times M$ unitary matrix G, the first $M/2$ components of $\mathcal{V}^{q[\tilde{\rho}]}$ have now an opposite signature to the first $M/2$ components of $\mathcal{U}^{q[\tilde{\rho}]}$.

B.5.3 Coordinate ⊗ spin ⊗ isospin space

B.5.3.1 Standard notations

Two typical notations used to represent quasiparticle states in the κ representation (equivalently in the $\tilde{\rho}$ representation) are

$$\begin{bmatrix} \mathcal{U}^{q[\kappa]}_{\mu}(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{q[\kappa]}_{\mu}(\vec{r}\,\sigma\,q) \end{bmatrix} \equiv \begin{bmatrix} \mathcal{U}^{q[\kappa]}_{\vec{r}\sigma q,\mu} \\ \mathcal{V}^{q[\kappa]}_{\vec{r}\sigma q,\mu} \end{bmatrix}\,. \tag{B.77}$$

The first notation is specifically used when expanding the quasiparticle states in coordinate, spin and isospin spaces. Indeed, one then talks about the upper and lower components of the quasiparticle *wave functions*. The second notation is a classic matrix notation which is more general and used for any arbitrary single-particle basis. Using the latter notation, it becomes obvious that the first index always refers to the particle basis used to expand the quasiparticle states whereas the second corresponds to the quasiparticle basis.

The upper and lower components of the quasiparticle wave function are obtained explicitly from the quasiparticle creation and annihilation operators defined in Eq. (B.110) (or Eq. (B.116))

according to

$$\begin{bmatrix} \mathcal{U}_\mu^{q[\kappa]}(\vec{r}\,\sigma\,q) \\ \mathcal{V}_\mu^{q[\kappa]}(\vec{r}\,\sigma\,q) \end{bmatrix} \equiv \begin{bmatrix} \langle \vec{r}\,\sigma\,q\,|\hat{\beta}_\mu^{q\,\dagger}|0\rangle \\ \langle \vec{r}\,\sigma\,q\,|\hat{\beta}_\mu^{q}|0\rangle^* \end{bmatrix} . \tag{B.78}$$

B.5.3.2 Dirac notations

The introduction of Dirac notations in the HFB formalism raises questions because of the use of particle and quasiparticle operators/states. First, and in order to differentiate between those two types of bases, the notation $\underline{\mu}$ will be used when needed to characterize quasiparticle states. Such a notation will allow one to write kets of the form $|i\,\underline{\mu}\rangle$ where the two states belong to different spaces (particle or quasiparticle). Because the two states belong to different spaces, the symmetry of the state $|i\,\underline{\mu}\rangle$ under the exchange of the indices does not need to be specified.

With such a notation, one can now resolve unambiguously scalar products of the type

$$|i\,\underline{\mu}\rangle = \sum_k |k\rangle\,\langle k|i\,\underline{\mu}\rangle = \sum_k \langle k|i\rangle\,|k\,\underline{\mu}\rangle = \sum_k \delta_{ki}\,|k\,\underline{\mu}\rangle\,. \tag{B.79}$$

Although the notations as matrix elements (or wave functions) are similar for quasiparticle states used in the traditional and Russian representations, their Dirac notations differ in a very significant manner. While the Dirac notation of the upper and lower components of the quasiparticle states are those of usual one-body operators in the Russian representation, the lower component in the traditional representation behaves as a pair destruction that connects different Hilbert spaces for two particles. This leads to

$$\begin{bmatrix} \mathcal{U}_{i,\mu}^{q[\tilde{\rho}]} \\ \mathcal{V}_{i,\mu}^{q[\tilde{\rho}]} \end{bmatrix} \equiv \begin{bmatrix} \langle i|\mathcal{U}^{q[\tilde{\rho}]}|\underline{\mu}\rangle \\ \langle i|\mathcal{V}^{q[\tilde{\rho}]}|\underline{\mu}\rangle \end{bmatrix} \qquad \begin{bmatrix} \mathcal{U}_{i,\mu}^{q[\kappa]} \\ \mathcal{V}_{i,\mu}^{q[\kappa]} \end{bmatrix} \equiv \begin{bmatrix} \langle i|\mathcal{U}^{q[\kappa]}|\underline{\mu}\rangle \\ \langle \mathcal{V}^{q[\kappa]}|i\,\underline{\mu}\rangle \end{bmatrix} , \tag{B.80}$$

where i can denote a state in configuration or coordinate space. Dirac notations in a given single-particle basis for the fields h^q, $\tilde{h}^q$ and Δ^q, as well as of the densities ρ^q, $\tilde{\rho}^q$ and κ^q are also to be defined properly. For instance, matrix elements of the pairing field Δ^q in coordinate space are usually defined through

$$\Delta_{ij}^q \equiv \sum_{\sigma_1\sigma_2} \int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q)\,\Delta^q(\vec{r}_1\,\sigma_1,\vec{r}_2\,\sigma_2)\,. \tag{B.81}$$

The corresponding Dirac notation is

$$\begin{aligned} \Delta_{ij}^q \equiv \langle i\,j|\Delta^q\rangle =& \frac{1}{2}\int \mathrm{d}\vec{r}_1\mathrm{d}\vec{r}_2 \sum_{\sigma_1\,\sigma_2} \langle i\,j|\vec{r}_1\,\sigma_1\,q\,\vec{r}_2\,\sigma_2\,q\rangle\,\langle \vec{r}_1\,\sigma_1\,q\,\vec{r}_2\,\sigma_2\,q|\Delta^q\rangle \\ \equiv& \frac{1}{2}\int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2 \sum_{\sigma_1\,\sigma_2} \langle i\,j|\vec{r}_1\,\sigma_1\,\vec{r}_2\,\sigma_2\rangle\,\Delta^q(\vec{r}_1\,\sigma_1,\vec{r}_2\,\sigma_2)\,. \end{aligned} \tag{B.82}$$

and carries the skew symmetry of the pairing field through the antisymmetry of $\langle i\,j|$. To recover exactly Eq. (B.81), the skew symmetry of the pairing field in coordinate space is used to write

$$\begin{aligned}\Delta^q_{ij} \equiv \langle i\,j|\Delta^q\rangle =& \frac{1}{2}\int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2 \sum_{\sigma_1\,\sigma_2} \langle i\,j|\vec{r}_1\,\sigma_1\,\vec{r}_2\,\sigma_2\rangle\,\Delta^q(\vec{r}_1\,\sigma_1,\vec{r}_2\,\sigma_2)\\ =& \frac{1}{2}\int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2 \sum_{\sigma_1\,\sigma_2} \Big[\varphi^*_i(\vec{r}_1\,\sigma_1\,q)\,\varphi^*_j(\vec{r}_2\,\sigma_2\,q)\\ &\qquad - \varphi^*_j(\vec{r}_1\,\sigma_1\,q)\,\varphi^*_i(\vec{r}_2\,\sigma_2\,q)\Big]\langle\vec{r}_1\,\sigma_1\,q\,\vec{r}_2\,\sigma_2\,q|\Delta^q\rangle\\ =& \int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2 \sum_{\sigma_1\,\sigma_2} \varphi^*_i(\vec{r}_1\,\sigma_1\,q)\,\varphi^*_j(\vec{r}_2\,\sigma_2\,q)\,\Delta^q(\vec{r}_1\,\sigma_1,\vec{r}_2\,\sigma_2)\,. \end{aligned} \tag{B.83}$$

Once again, one should write $\Delta^q_{ij} \equiv \langle i\,j|\Delta\rangle$ in all rigor since the isospin superscript should not be further specified as it is part of the quantum numbers i/j. The latter will be kept nevertheless to remember that the fields and densities are diagonal in isospin space. Note finally that the most proper notation should be $\Delta^q_{ij} \equiv \langle i\,j|\Delta^q|0\rangle$.

In a similar fashion, we introduce the notations

$$h^q_{ij} \equiv \langle i|h^q|j\rangle \qquad\qquad h^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') \equiv \langle\vec{r}\,\sigma\,q|h^q|\vec{r}\,'\,\sigma'\,q\rangle\,, \tag{B.84a}$$

$$\tilde{h}^q_{ij} \equiv \langle i|\tilde{h}^q|j\rangle \qquad\qquad \tilde{h}^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') \equiv \langle\vec{r}\,\sigma\,q|\tilde{h}^q|\vec{r}\,'\,\sigma'\,q\rangle\,, \tag{B.84b}$$

$$\Delta^q_{ij} \equiv \langle i\,j|\Delta^q\rangle \qquad \Delta^{q\,*}_{ij} \equiv \langle ij|\Delta^q\rangle^* = \langle\Delta^q|i\,j\rangle \qquad \Delta^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') \equiv \langle\vec{r}\,\sigma\,q\,\vec{r}\,'\,\sigma'\,q|\Delta^q\rangle\,, \tag{B.84c}$$

$$\rho^q_{ij} \equiv \langle i|\rho^q|j\rangle \qquad\qquad \rho^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') \equiv \langle\vec{r}\,\sigma\,q|\rho^q|\vec{r}\,'\,\sigma'\,q\rangle\,, \tag{B.84d}$$

$$\tilde{\rho}^q_{ij} \equiv \langle i|\tilde{\rho}^q|j\rangle \qquad\qquad \tilde{\rho}^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') \equiv \langle\vec{r}\,\sigma\,q|\tilde{\rho}^q|\vec{r}\,'\,\sigma'\,q\rangle\,, \tag{B.84e}$$

$$\kappa^q_{ij} \equiv \langle i\,j|\kappa^q\rangle \qquad \kappa^{q\,*}_{ij} \equiv \langle ij|\kappa^q\rangle^* = \langle\kappa^q|i\,j\rangle \qquad \kappa^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') \equiv \langle\vec{r}\,\sigma\,q\,\vec{r}\,'\,\sigma'\,q|\kappa^q\rangle\,. \tag{B.84f}$$

For instance, Eqs. (B.84c,B.84f) allows to write the gap equation obtained from a bilinear EDF (see Sec. B.11) as

$$\Delta^q_{ij} = \frac{1}{2}\sum_{kl} \bar{v}^{\kappa\kappa}_{ijkl}\,\kappa^q_{kl} \qquad \Leftrightarrow \qquad \langle i\,j|\Delta^q\rangle = \frac{1}{2}\sum_{kl}\langle i\,j|v^{\kappa\kappa}|k\,l\rangle\,\langle k\,l|\kappa^q\rangle = \langle i\,j|v^{\kappa\kappa}\,\kappa^q\rangle\,. \tag{B.85}$$

In the previous example, the operator product can be naturally worked out through the use of a completeness relationship in the two-body Hilbert space because κ^q is multiplied with a two-body operator. In other cases, such as the product of one-body-like operators with two-body-like ones or the product of an operator carrying a quasiparticle label with one carrying two single-particle ones, one must be very careful when inserting or removing completeness relationships in Dirac notations (matrix-product notations is always safe). This is due to the specificity of Dirac notation for quantities like Δ^q, κ^q or $\mathcal{V}^{q[\kappa]}$. Products like $\rho^q = \mathcal{V}^{q[\kappa]*}\mathcal{V}^{q[\kappa]\mathrm{T}}$ have to be worked out in matrix notations in order to make both indices of each quantity explicit before Dirac notations can be used. Then, additional closure relationships can be used. For instance[5]

CANNOT DO	CAN DO
$\rho^q_{\vec{r}\sigma,\vec{r}\,'\sigma'} = \langle\vec{r}\,\sigma\,q|\mathcal{V}^{q[\kappa]*}\,\mathcal{V}^{q[\kappa]\mathrm{T}}|\vec{r}\,'\,\sigma'\,q\rangle$	$\rho^q_{\vec{r}\sigma,\vec{r}\,'\sigma'} = \Big[\mathcal{V}^{q[\kappa]*}\,\mathcal{V}^{q[\kappa]\mathrm{T}}\Big]_{\vec{r}\sigma q,\vec{r}\,'\sigma' q}$
$= \sum_\mu \langle\vec{r}\,\sigma\,q|\mathcal{V}^{q[\kappa]*}|\mu\rangle\,\langle\mu|\mathcal{V}^{q[\kappa]\mathrm{T}}|\vec{r}\,'\,\sigma'\,q\rangle$	$= \sum_\mu \mathcal{V}^{q[\kappa]*}_{\vec{r}\sigma q,\mu}\,\mathcal{V}^{q[\kappa]\ \mathrm{T}}_{\mu,\vec{r}\,'\sigma' q}$

[5] Note that because of its definition in Eq. (B.78), the Dirac notation of $\mathcal{V}^{q[\kappa]*}_{\vec{r}\sigma q,\mu}$ resembles that of a complex conjugate.

$$= \sum_{\mu} \langle \mathcal{V}^{q[\kappa]} | \vec{r}\,' \sigma'\, q\, \underline{\mu} \rangle \langle \vec{r}\, \sigma\, q\, \underline{\mu} | \mathcal{V}^{q[\kappa]} \rangle$$

Finally, one can provide a Dirac notation for the matrix elements of the time-reversal operator as

$$\mathcal{T}_{ij} \equiv \langle i | (\hat{\mathcal{T}} | j \rangle \equiv \langle i\, j | \hat{\mathcal{T}} \rangle \,, \tag{B.86}$$

with the same care required when writing matrix elements and products. Said in a crude way, the Dirac notation of $\hat{\mathcal{T}}$ is related to the fact that "it changes a bra into a ket". It is crucial to remember that $\hat{\mathcal{T}}$ always acts on the second index in Eq. (B.86). Using the Dirac notation given above, it is easy to recover that $\mathcal{T}^T = -\mathcal{T}$, as stated in Eq. (B.28a), since

$$\mathcal{T}^T_{ij} = \mathcal{T}_{ji} \equiv \langle j\, i | \hat{\mathcal{T}} \rangle = -\langle i\, j | \hat{\mathcal{T}} \rangle = -\mathcal{T}_{ij} \,. \tag{B.87}$$

B.5.3.3 Traditional representation

Starting from Eq. (B.65), we represent the HFB equations in the traditional representation in an arbitrary single-particle basis. Although we could directly expand them in the basis of present interest, the derivation below underlines the necessary care when going from one basis to another through the insertion of completeness relationships (at the positions indicated by •) in Dirac notations. Focusing on the upper component $\mathcal{U}^{q[\kappa]}_{\mu}$, this leads to[6] for all i

$$\begin{aligned}
0 =& - E^q_\mu \mathcal{U}^{q[\kappa]}_{i\mu} + \sum_j (h^q_{ij} - \lambda^q \delta_{ij}) \mathcal{U}^{q[\kappa]}_{j\mu} + \Delta^q_{ij} \mathcal{V}^{q[\kappa]}_{j\mu} \\
=& - E^q_\mu \langle i | \bullet \mathcal{U}^{[q\,\kappa]} | \underline{\mu} \rangle + \sum_j (\langle i | \bullet\, h^q \bullet | j \rangle - \lambda^q \langle i | \bullet\bullet | j \rangle) \langle j | \bullet \mathcal{U}^{[q\,\kappa]} | \underline{\mu} \rangle + \langle i\, j | \bullet\bullet\, \Delta^q \rangle \langle \mathcal{V}^{[q\,\kappa]} \bullet | j\, \underline{\mu} \rangle \\
=& \sum_{\sigma\sigma'\sigma''} \int \mathrm{d}\vec{r}\, \mathrm{d}\vec{r}\,' \mathrm{d}\vec{r}\,'' \Bigg[-E^q_\mu \varphi^*_i(\vec{r}\, \sigma\, q) \mathcal{U}^{[q\,\kappa]}_\mu(\vec{r}\, \sigma\, q) \\
& \qquad + \sum_j \Bigg[\varphi^*_i(\vec{r}\, \sigma\, q) \Big(h^q(\vec{r}\, \sigma, \vec{r}\,' \sigma') - \lambda^q \delta_{\sigma\sigma'} \delta(\vec{r} - \vec{r}\,') \Big) \\
& \qquad\qquad \times \varphi_j(\vec{r}\,' \sigma'\, q) \varphi^*_j(\vec{r}\,'' \sigma''\, q) \mathcal{U}^{[q\,\kappa]}_\mu(\vec{r}\,'' \sigma''\, q) \\
& \qquad + \varphi^*_i(\vec{r}\, \sigma\, q) \varphi^*_j(\vec{r}\,' \sigma'\, q) \Delta^q(\vec{r}\, \sigma, \vec{r}\,' \sigma') \varphi_j(\vec{r}\,'' \sigma''\, q) \mathcal{V}^{[q\,\kappa]}_\mu(\vec{r}\,'' \sigma''\, q) \Bigg] \Bigg] \\
=& \sum_\sigma \int \mathrm{d}\vec{r} \varphi^*_i(\vec{r}\, \sigma\, q) \Bigg[E^q_\mu \mathcal{U}^{[q\,\kappa]}_\mu(\vec{r}\, \sigma\, q) \\
& \qquad - \sum_{\sigma'} \int \mathrm{d}\vec{r}\,' \Big[\Big(h^q(\vec{r}\, \sigma, \vec{r}\,' \sigma') - \lambda^q \delta_{\sigma\sigma'} \delta(\vec{r} - \vec{r}\,') \Big) \mathcal{U}^{[q\,\kappa]}_\mu(\vec{r}\,' \sigma'\, q) \\
& \qquad\qquad - \Delta^q(\vec{r}\, \sigma, \vec{r}\,' \sigma') \mathcal{V}^{[q\,\kappa]}_\mu(\vec{r}\,' \sigma'\, q) \Big] \Bigg] \,.
\end{aligned} \tag{B.88}$$

The latter is true for all i thus, as the set $\{\varphi_i\}$ forms a complete basis, one has

$$\sum_{\sigma'} \int \mathrm{d}\vec{r}\,' \Big[h'^q(\vec{r}\, \sigma, \vec{r}\,' \sigma') \mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,' \sigma'\, q) - \Delta^q(\vec{r}\, \sigma, \vec{r}\,' \sigma') \mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,' \sigma'\, q) \Big] = E^q_\mu \mathcal{U}^{q[\kappa]}_\mu(\vec{r}\, \sigma\, q) \,, \tag{B.89}$$

[6] At the level of $\langle i\, j | \bullet\bullet\, \Delta^q \rangle$ a closure relationship on the antisymmetrized two-body state $|\vec{r}\, \sigma\, q\, \vec{r}\,' \sigma'\, q\rangle$ is used. However, using the skew symmetry of Δ^q, one can "reduce" $[\varphi^*_i(\vec{r}\, \sigma\, q) \varphi^*_j(\vec{r}\,' \sigma'\, q) - \varphi^*_j(\vec{r}\, \sigma\, q) \varphi^*_i(\vec{r}\,' \sigma'\, q)]/2$ into $\varphi^*_i(\vec{r}\, \sigma\, q) \varphi^*_j(\vec{r}\,' \sigma'\, q)$.

where $h'^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') = h^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') - \lambda^q\,\delta_{\sigma\sigma'}\,\delta(\vec{r}-\vec{r}\,')$. The same method applied for the lower quasiparticle component $\mathcal{V}^{q[\kappa]}$ leads to the HFB equations in coordinate space, i.e.

$$\int \mathrm{d}\vec{r}\,' \sum_{\sigma'} \begin{pmatrix} h'^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') & \Delta^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') \\ -\Delta^{q*}(\vec{r}\,\sigma,\vec{r}\,'\sigma') & -h'^{q\,*}(\vec{r}\,\sigma,\vec{r}\,'\sigma') \end{pmatrix} \begin{bmatrix} \mathcal{U}_\mu^{q\,[\kappa]}(\vec{r}\,'\sigma'\,q) \\ \mathcal{V}_\mu^{q\,[\kappa]}(\vec{r}\,'\sigma'\,q) \end{bmatrix} = E_\mu^q \begin{bmatrix} \mathcal{U}_\mu^{q\,[\kappa]}(\vec{r}\,\sigma\,q) \\ \mathcal{V}_\mu^{q\,[\kappa]}(\vec{r}\,\sigma\,q) \end{bmatrix}, \tag{B.90}$$

B.5.3.4 Russian representation

One can use the same method as in the traditional representation to obtain the HFB equations in the $\tilde{\rho}$ representation in coordinate space. To do so, one needs first to work out

$$\begin{aligned} (\mathcal{T}^T\,h^*\,\mathcal{T}^*)_{\vec{r}\sigma q\,,\,\vec{r}\,'\sigma' q} &= \int \mathrm{d}\vec{r}_{12} \sum_{\sigma_{12}} \mathcal{T}_{\vec{r}_1\sigma_1 q\,,\,\vec{r}\sigma q}\,h^{q\,*}_{\vec{r}_1\sigma_1 q\,,\,\vec{r}_2\sigma_2 q}\,\mathcal{T}^*_{\vec{r}_2\sigma_2 q\,,\,\vec{r}\,'\sigma' q} \\ &= \int \mathrm{d}\vec{r}_{12} \sum_{\sigma_{12}} \langle\vec{r}_1\sigma_1 q|\big(\hat{\mathcal{T}}\,|\vec{r}\sigma q\rangle\,h^*(\vec{r}_1\sigma_1 q\,,\,\vec{r}_2\sigma_2 q)\,\langle\vec{r}_2\sigma_2 q|\big(\hat{\mathcal{T}}|\vec{r}\,'\sigma' q\rangle^* \\ &= \int \mathrm{d}\vec{r}_{12} \sum_{\sigma_{12}} 2\bar{\sigma}\,\langle\vec{r}_1\sigma_1 q|\vec{r}\bar{\sigma}q\rangle\,h^*(\vec{r}_1\sigma_1 q\,,\,\vec{r}_2\sigma_2 q)\,2\bar{\sigma}'\,\langle\vec{r}_2\sigma_2 q|\vec{r}\,'\bar{\sigma}'q\rangle^* \\ &= 2\bar{\sigma}\,2\bar{\sigma}'\,h^{q\,*}(\vec{r}\,\bar{\sigma},\vec{r}\,'\,\bar{\sigma}')\,. \end{aligned} \tag{B.91}$$

Representing Eq. (B.70) for the lower component of the quasiparticle, one finds easily

$$\begin{aligned} &\int \mathrm{d}\vec{r}\,' \sum_{\sigma'} \tilde{h}^{q\dagger}(\vec{r}\,\sigma,\vec{r}\,'\sigma')\,\mathcal{U}_\mu^{q[\tilde{\rho}]}(\vec{r}\,'\sigma'\,q) \\ &\qquad - \big[2\bar{\sigma}\,2\bar{\sigma}'h^{q*}(\vec{r}\,\bar{\sigma},\vec{r}\,'\,\bar{\sigma}') - \lambda^q\,\delta_{\sigma\sigma'}\,\delta(\vec{r}-\vec{r}\,')\big]\,\mathcal{V}_\mu^{q[\tilde{\rho}]}(\vec{r}\,'\sigma'\,q) = E_\mu^q\,\mathcal{V}_\mu^{q[\tilde{\rho}]}(\vec{r}\,\sigma\,q)\,, \end{aligned} \tag{B.92}$$

which finally leads to

$$\begin{aligned} E_\mu^q &\begin{bmatrix} \mathcal{U}_\mu^{q[\tilde{\rho}]}(\vec{r}\,\sigma\,q) \\ \mathcal{V}_\mu^{q[\tilde{\rho}]}(\vec{r}\,\sigma\,q) \end{bmatrix} = \\ &\int \mathrm{d}\vec{r}\,' \sum_{\sigma'} \begin{pmatrix} h^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') - \lambda^q\,\delta_{\sigma\sigma'}\,\delta(\vec{r}-\vec{r}\,') & \tilde{h}^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') \\ \tilde{h}^{q*}(\vec{r}\,'\sigma',\vec{r}\,\sigma) & -2\bar{\sigma}\,2\bar{\sigma}'\,h^{q*}(\vec{r}\,\bar{\sigma},\vec{r}\,'\,\bar{\sigma}') + \lambda^q\,\delta_{\sigma\sigma'}\,\delta(\vec{r}-\vec{r}\,') \end{pmatrix} \begin{bmatrix} \mathcal{U}_\mu^{q[\tilde{\rho}]}(\vec{r}\,'\sigma'\,q) \\ \mathcal{V}_\mu^{q[\tilde{\rho}]}(\vec{r}\,'\sigma'\,q) \end{bmatrix}. \end{aligned} \tag{B.93}$$

B.5.3.5 Further connections between traditional and Russian representations

Starting from Eq. (B.75a), one can use the same type of derivation as in Eq. (B.91) to show that

$$\Delta^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') = 2\sigma'\,\tilde{h}^q(\vec{r}\,\sigma,\vec{r}\,'\bar{\sigma}')\,. \tag{B.94}$$

In the exact same manner, one obtains from Eq. (B.71)

$$\begin{bmatrix} \mathcal{U}_\mu^{q[\tilde{\rho}]}(\vec{r}\,\sigma\,q) \\ \mathcal{V}_\mu^{q[\tilde{\rho}]}(\vec{r}\,\sigma\,q) \end{bmatrix} = \begin{bmatrix} \mathcal{U}_\mu^{q[\kappa]}(\vec{r}\,\sigma\,q) \\ 2\bar{\sigma}\,\mathcal{V}_\mu^{q[\kappa]}(\vec{r}\,\bar{\sigma}\,q) \end{bmatrix}. \tag{B.95}$$

B.6 Time-reversal invariant systems

B.6.1 Basic properties

In case the system is time-reversal invariant (i.e., $\hat{\mathcal{T}}|\Phi\rangle = |\Phi\rangle$), all single-particle basis of interest[7] are closed under the action of $\hat{\mathcal{T}}$. Thus, one can always find a state $\varphi_{\tilde{\mu}}(\vec{r}\sigma q)$ in the basis fulfilling

$$\varphi_{\bar{\mu}}(\vec{r}\,\sigma\,q) = (\hat{\mathcal{T}}\,\varphi)_\mu(\vec{r}\,\sigma\,q) \equiv \eta_\mu\,\varphi_{\tilde{\mu}}(\vec{r}\,\sigma\,q)\,, \tag{B.96}$$

where $\eta_{\tilde{\mu}} = -\eta_\mu$ and $|\eta_\mu| = 1$ (this quantum number can be taken real), with the additional result that $\varphi_{\tilde{\mu}}$ has an opposite signature to φ_μ. In such a basis, the time-reversal operator becomes

$$\mathcal{T}_{\mu\hat{\nu}} = \eta_{\hat{\nu}}\,\delta_{\tilde{\mu}\hat{\nu}}\,. \tag{B.97}$$

This can be seen with the example of an eigenbasis $\{|\mu\rangle\}$ of a time-reversal invariant one-body field $\hat{h}^q$

$$\hat{\mathcal{T}}\,\hat{h}^q\,\hat{\mathcal{T}}^\dagger = \hat{h}^q\,. \tag{B.98}$$

If $|\mu\rangle$ is eigenstate of $\hat{h}^q$ with the eigenvalue ϵ_μ, one finds

$$\hat{\mathcal{T}}\,\hat{h}^q\,|\mu\rangle = \hat{h}^q\,\hat{\mathcal{T}}\,|\mu\rangle = \hat{h}^q\,|\bar{\mu}\rangle\,, \tag{B.99a}$$

$$= \hat{\mathcal{T}}\,\epsilon_\mu\,|\mu\rangle = \epsilon_\mu\,|\bar{\mu}\rangle\,, \tag{B.99b}$$

and thus $\eta_\mu\,|\bar{\mu}\rangle \equiv |\tilde{\mu}\rangle$ is also an eigenstate of $\hat{h}^q$ with the same eigenvalue ϵ_μ. Eigenstates of $\hat{h}$ are then two-fold degenerated for time-reversal invariant systems.

B.6.2 Quasiparticle states

Starting from Eq. (B.97), the relationships between the lower quasiparticle components $\mathcal{V}^{q[\tilde{\rho}]}$ and $\mathcal{V}^{q[\kappa]}$ become

$$\mathcal{U}^{q[\tilde{\rho}]}_{i\mu} = \mathcal{U}^{q[\kappa]}_{i\mu}\,, \tag{B.100a}$$

$$\mathcal{V}^{q[\tilde{\rho}]}_{i\mu} = \sum_j \mathcal{T}^T_{ij}\,\mathcal{V}^{q[\kappa]}_{j\mu} = \sum_j \eta_i\,\delta_{j\tilde{\imath}}\,\mathcal{V}^{q[\kappa]}_{j\mu} = \eta_i\,\mathcal{V}^{q[\kappa]}_{\tilde{\imath}\mu}\,, \tag{B.100b}$$

which matches with Eq. (B.95) as the coordinate $\otimes$ spin $\otimes$ isospin basis is indeed closed under time-reversal symmetry.

B.6.3 Densities

As already shown in Eq. (B.43), the pair density matrix is hermitian for time-reversal invariant systems ($\tilde{\rho}^{q\dagger} = \tilde{\rho}^q$). As a result, Eq. (B.76b) becomes

$$\tilde{\rho}^q = -\mathcal{U}^{q[\tilde{\rho}]}\,\mathcal{V}^{q[\tilde{\rho}]^\dagger} = -\mathcal{V}^{q[\tilde{\rho}]}\,\mathcal{U}^{q[\tilde{\rho}]^\dagger}\,, \tag{B.101}$$

which is precisely the definition of $\tilde{\rho}^q$ where only time-reversal invariant systems have been considered [6]. Equivalently, using that $\mathcal{T}\,\rho^q\,\mathcal{T}^\dagger = \rho^q$, one obtains

$$\rho^q = \mathcal{T}^\dagger\,(\mathcal{T}\,\mathcal{V}^{q[\tilde{\rho}]^*}\,\mathcal{V}^{q[\tilde{\rho}]^{\mathrm{T}}}\,\mathcal{T}^\dagger)\,\mathcal{T} = \mathcal{V}^{q[\tilde{\rho}]^*}\,\mathcal{V}^{q[\tilde{\rho}]^{\mathrm{T}}}\,. \tag{B.102}$$

[7] The basis which diagonalizes h^q, the canonical basis, ...

B.6.4 Fields

One finds from Eq. (B.75a) that the pairing gap

$$\Delta^q_{i\tilde{j}} = \eta_j \, \tilde{h}^q_{ij} = \eta_j \, \tilde{h}^{q\,*}_{\tilde{j}i} \,, \tag{B.103}$$

is hermitian for time-reversal invariant systems. Furthermore, one can use that $h^q = \mathcal{T}\, h^q \, \mathcal{T}^\dagger$ to obtain

$$\begin{aligned} h^q(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') =& \langle \vec{r}\,\sigma | h^q | \vec{r}\,'\,\sigma' \rangle \\ =& \langle \vec{r}\,\sigma | \big(\hat{\mathcal{T}}^\dagger \, h^q \, \hat{\mathcal{T}} | \vec{r}\,'\,\sigma' \rangle \\ =& \langle \vec{r}\,\sigma | \hat{\mathcal{T}}^\dagger \big) \, h^q \, \big(\hat{\mathcal{T}} | \vec{r}\,'\,\sigma' \rangle^* \\ =& 2\bar{\sigma}\, 2\bar{\sigma}' \, \langle \vec{r}\,\bar{\sigma} | h^q | \vec{r}\,'\,\bar{\sigma}' \rangle^* \\ =& 2\bar{\sigma}\, 2\bar{\sigma}' \, h^{q*}(\vec{r}\,\bar{\sigma}, \vec{r}\,'\,\bar{\sigma}') \,. \end{aligned} \tag{B.104}$$

Finally, the pair field $\tilde{h}^q$ has the same symmetries of $\tilde{\rho}^q$, i.e.

$$\tilde{h}^{q*}(\vec{r}\,'\,\sigma', \vec{r}\,\sigma) = \tilde{h}^q(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') \,. \tag{B.105}$$

B.6.5 HFB equations

The HFB eigenvalues problem in the $\tilde{\rho}$ representation can be simplified using Eqs. (B.104,B.105). Traditional HFB equations [6] can now be recovered from Eq. (B.70) using the time-reversal invariance of the system

$$\int \mathrm{d}\vec{r}\,' \sum_{\sigma'} \begin{pmatrix} h'^q(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') & \tilde{h}^q(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') \\ \tilde{h}^q(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') & -h'^q(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') \end{pmatrix} \begin{bmatrix} \mathcal{U}^{q\,[\tilde{\rho}]}_\mu(\vec{r}\,'\,\sigma'\,q) \\ \mathcal{V}^{q\,[\tilde{\rho}]}_\mu(\vec{r}\,'\,\sigma'\,q) \end{bmatrix} = E^q_\mu \begin{bmatrix} \mathcal{U}^{q\,[\tilde{\rho}]}_\mu(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{q\,[\tilde{\rho}]}_\mu(\vec{r}\,\sigma\,q) \end{bmatrix} . \tag{B.106}$$

Such form of the HFB equations could also be obtained in configuration space through

$$\big[\mathcal{T}^T \, h^{q*} \, \mathcal{T}^* \big]_{ij} = \sum_{kl} \mathcal{T}_{ki} \, h^{q*}_{kl} \, \mathcal{T}^*_{lj} = \eta_i \, \eta_j \, h^{q*}_{\tilde{i}\tilde{j}} \,, \tag{B.107}$$

and

$$\begin{aligned} \eta_i \, \eta_j \, h^{q*}_{\tilde{i}\tilde{j}} =& \eta_i \, \eta_j \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} \varphi^*_{\tilde{i}}(\vec{r}\,\sigma\,q) \, h^{q*}(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') \, \varphi_{\tilde{j}}(\vec{r}\,'\,\sigma'\,q) \\ =& \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} 2\sigma \, \varphi_i(\vec{r}\,\bar{\sigma}\,q) \, h^{q*}(\vec{r}\,\sigma, \vec{r}\,'\,\sigma') \, 2\sigma' \, \varphi^*_j(\vec{r}\,'\,\bar{\sigma}'\,q) \\ =& \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} 2\sigma \, \varphi_i(\vec{r}\,\bar{\sigma}\,q) \, h^{q}(\vec{r}\,'\,\sigma', \vec{r}\,\sigma) \, 2\sigma' \, \varphi^*_j(\vec{r}\,'\,\bar{\sigma}'\,q) \\ =& \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} 2\bar{\sigma} \, \varphi_i(\vec{r}\,\sigma\,q) \, h^{q}(\vec{r}\,'\,\bar{\sigma}', \vec{r}\,\bar{\sigma}) \, 2\bar{\sigma}' \, \varphi^*_j(\vec{r}\,'\,\sigma'\,q) \\ =& \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,' \sum_{\sigma\sigma'} \varphi_i(\vec{r}\,\sigma\,q) \, h^{q*}(\vec{r}\,'\,\sigma', \vec{r}\,\sigma) \, \varphi^*_j(\vec{r}\,'\,\sigma'\,q) \\ =& h^{q\,*}_{ji} = h^q_{ij} \,. \end{aligned} \tag{B.108}$$

Independently of any single-particle representation, one thus finds that the HFB equations, in the Russian representation, take for time-reversal invariant systems the form

$$\begin{pmatrix} h^q - \lambda^q & \tilde{h}^q \\ \tilde{h}^q & -h^q + \lambda^q \end{pmatrix} \begin{bmatrix} \mathcal{U}^{q[\tilde{\rho}]} \\ \mathcal{V}^{q[\tilde{\rho}]} \end{bmatrix}_\mu = E^q_\mu \begin{bmatrix} \mathcal{U}^{q[\tilde{\rho}]} \\ \mathcal{V}^{q[\tilde{\rho}]} \end{bmatrix}_\mu . \tag{B.109}$$

Except for the fact that h^q is real because it is time-reversal invariant, the HFB equations in the traditional representation do not significantly simplify for time-reversal invariant systems.

B.7 Canonical basis

B.7.1 Bloch-Messiah-Zumino decomposition in the traditional representation

In the traditional representation, the Bogoliubov transformation leading to the quasiparticle states solution of the HFB problem takes the form

$$\begin{pmatrix} \hat{\beta}^q \\ \hat{\beta}^{q\dagger} \end{pmatrix} = W^{q[\kappa]\dagger} \begin{pmatrix} \hat{a}^q \\ \hat{a}^{q\dagger} \end{pmatrix} = \begin{pmatrix} \mathcal{U}^{q[\kappa]\dagger} & \mathcal{V}^{q[\kappa]\dagger} \\ \mathcal{V}^{q[\kappa]\mathrm{T}} & \mathcal{U}^{q[\kappa]\mathrm{T}} \end{pmatrix} \begin{pmatrix} \hat{a}^q \\ \hat{a}^{q\dagger} \end{pmatrix} , \tag{B.110}$$

where $\hat{\beta}^q$ and $\hat{\beta}^{q\dagger}$ on the one hand and $\hat{a}^q$ and $\hat{a}^{q\dagger}$ on the other obey fermionic anticommutation rules. The Bloch-Messiah-Zumino theorem [7–9] states that $W^{q[\kappa]}$ may be decomposed into a set of three consecutive transformations

$$W^{q[\kappa]\dagger} = \begin{pmatrix} C^{q\,\dagger} & 0 \\ 0 & C^{q\,\mathrm{T}} \end{pmatrix} \begin{pmatrix} \bar{\mathcal{U}}^{q[\kappa]\dagger} & \bar{\mathcal{V}}^{q[\kappa]\dagger} \\ \bar{\mathcal{V}}^{q[\kappa]\mathrm{T}} & \bar{\mathcal{U}}^{q[\kappa]\mathrm{T}} \end{pmatrix} \begin{pmatrix} D^{q\,\dagger} & 0 \\ 0 & D^{q\,\mathrm{T}} \end{pmatrix} , \tag{B.111}$$

where D^q and C^q are unitary, while $\bar{\mathcal{U}}^{q[\kappa]}$ is diagonal and $\bar{\mathcal{V}}^{q[\kappa]}$ is canonical (see below). This decomposition of the matrix establishes the following bases of interest:

1. An arbitrary basis of single-particle states $(\hat{a}^q, \hat{a}^{q\dagger})$. This can be for instance the basis in which the one-body field h^q is diagonal.

2. D^q is a unitary transformation among the single-particle states, which leads to the canonical basis $(\hat{c}^q, \hat{c}^{q\dagger})$

$$\begin{pmatrix} \hat{c}^q \\ \hat{c}^{q\dagger} \end{pmatrix} = \begin{pmatrix} D^{q\,\dagger} & 0 \\ 0 & D^{q\,\mathrm{T}} \end{pmatrix} \begin{pmatrix} \hat{a}^q \\ \hat{a}^{q\dagger} \end{pmatrix} , \tag{B.112}$$

   in which the one-body density matrix is diagonal while the pairing tensor is canonical. In the absence of pairing the HF and canonical bases are identical, as in this case the mean-field Hamiltonian solves the HF equation $[h^q, \rho^q] = 0$. Thus, a set of single-particle states can be chosen that diagonalises h^q and ρ^q at the same time. The two bases are also identical for what is usually called the HF+BCS approximation to HFB.

3. $\bar{\mathcal{U}}^{q[\kappa]}$ and $\bar{\mathcal{V}}^{q[\kappa]}$ define the special Bogoliubov transformation

$$\begin{pmatrix} \hat{\alpha}^q \\ \hat{\alpha}^{q\dagger} \end{pmatrix} = \begin{pmatrix} \bar{\mathcal{U}}^{q[\kappa]\dagger} & \bar{\mathcal{V}}^{q[\kappa]\dagger} \\ \bar{\mathcal{V}}^{q[\kappa]\mathrm{T}} & \bar{\mathcal{U}}^{q[\kappa]\mathrm{T}} \end{pmatrix} \begin{pmatrix} \hat{c}^q \\ \hat{c}^{q\dagger} \end{pmatrix} , \tag{B.113}$$

   where only pairs of single-particle states are mixed, leading to a set of quasiparticle states which diagonalizes the generalized density matrix $\mathcal{R}^q$ with eigenvalues of 1 (0) for occupied (unoccupied) quasiparticle states. In general, this basis will not yet diagonalize the HFB Hamiltonian $\mathcal{H}^q$.

4. A further unitary transformation C^q among the quasiparticle states leads then to a set of quasiparticle states which solve the HFB equation $[\mathcal{R}^q, \mathcal{H}^{q\,\prime}] = 0$, and therefore diagonalise $\mathcal{R}$ and the HFB Hamiltonian $\mathcal{H}^{q\,\prime}$:

$$\begin{pmatrix} \hat{\beta}^q \\ \hat{\beta}^{q\dagger} \end{pmatrix} = \begin{pmatrix} C^{q\,\dagger} & 0 \\ 0 & C^{q\,\mathrm{T}} \end{pmatrix} \begin{pmatrix} \hat{\alpha}^q \\ \hat{\alpha}^{q\dagger} \end{pmatrix} . \tag{B.114}$$

One has then

$$\mathcal{U}^{q[\kappa]} = D^q \bar{\mathcal{U}}^{q[\kappa]} C^q , \qquad \mathcal{V}^{q[\kappa]} = D^{q*} \bar{\mathcal{V}}^{q[\kappa]} C^q , \tag{B.115}$$

and quasiparticle operators are defined as

$$\hat{\beta}^{q\,\dagger}_\mu = \sum_j \mathcal{U}^{q[\kappa]}_{j\mu}\, \hat{a}^{q\dagger}_j + \mathcal{V}^{q[\kappa]}_{j\mu}\, \hat{a}^q_j = \sum_j \sum_{kl} D^q_{jk}\, \bar{\mathcal{U}}^{q[\kappa]}_{kl}\, C^q_{l\mu}\, \hat{a}^{q\dagger}_j + D^{q\,*}_{jk}\, \bar{\mathcal{V}}^{q[\kappa]}_{kl}\, C^q_{l\mu}\, \hat{a}^q_j . \tag{B.116}$$

B.7.2 General case

The canonical basis $\{\phi_\mu(\vec{r}q)\}$ diagonalizes the one-body density matrix according to the transformation

$$\rho^{q\,\mathrm{can}}_{\nu\mu} = \left(D^q \rho^q D^{q\,\dagger} \right)_{\nu\mu} = \rho^{q\,\mathrm{can}}_{\mu\mu}\, \delta_{\nu\mu} , \tag{B.117}$$

while the pairing tensor is put in its canonical form $\kappa^{q\,\mathrm{can}}_{\mu\hat{\nu}} = \kappa^{q\,can}_{\mu\hat{\mu}}\, \delta_{\nu\mu}$, where $\hat{\mu}$ designates the pair conjugate state of μ[8]. In the HFB formalism, states are not paired a priori as in the BCS approximation, except for the fact that only states with opposite signatures are coupled through the Bogoliubov transformation.

If the canonical basis is ordered in such a way that conjugate states $(\mu, \hat{\mu})$ come next to each other, the special matrices $(\bar{\mathcal{U}}^{q[\kappa]}, \bar{\mathcal{V}}^{q[\kappa]})$ are 2×2 block diagonal, where the blocks have the following structure:

$$\bar{\mathcal{U}}^{q[\kappa]} \equiv \begin{pmatrix} u^q_\mu & 0 \\ 0 & u^q_{\hat{\mu}} \end{pmatrix} = \begin{pmatrix} u^q_\mu & 0 \\ 0 & u^q_\mu \end{pmatrix} , \tag{B.118a}$$

$$\bar{\mathcal{V}}^{q[\kappa]} \equiv \begin{pmatrix} 0 & v^q_\mu \\ v^q_{\hat{\mu}} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \zeta_\mu\, v^q_\mu \\ \zeta_{\hat{\mu}}\, v^q_\mu & 0 \end{pmatrix} , \tag{B.118b}$$

$u^q_\mu > 0$ and v^q_μ being real BCS-like coefficients. Thus, one has $\bar{\mathcal{U}}^{q[\kappa]}_{\mu\nu} = \bar{\mathcal{U}}^{q[\kappa]}_{\mu\mu}\, \delta_{\mu\nu}$ and $\bar{\mathcal{V}}^{q[\kappa]}_{\mu\nu} = \bar{\mathcal{V}}^{q[\kappa]}_{\mu\hat{\mu}}\, \delta_{\hat{\mu}\nu}$, such that

$$\bar{\mathcal{U}}^{q[\kappa]}_{\mu\mu} = +\bar{\mathcal{U}}^{q[\kappa]}_{\hat{\mu}\hat{\mu}} = \quad u^q_\mu , \qquad \bar{\mathcal{V}}^{q[\kappa]}_{\mu\hat{\mu}} = -\bar{\mathcal{V}}^{q[\kappa]}_{\hat{\mu}\mu} = \zeta_\mu\, v^q_\mu . \tag{B.119}$$

As a result, the normal density matrix and pairing tensor are such that

$$\rho^q_{\mu\mu} = +\rho^q_{\hat{\mu}\hat{\mu}} = v^{q\,2}_\mu , \qquad \kappa^q_{\mu\hat{\mu}} = -\kappa^q_{\hat{\mu}\mu} = \zeta_\mu\, u^q_\mu\, v^q_\mu . \tag{B.120}$$

In the canonical basis, $\bar{\mathcal{V}}^{q[\bar{\rho}]}$ and thus $\tilde{\rho}^q$ do not take canonical forms in general, i.e. if time-reversal invariance of the system is not assumed. For instance, one has

$$\tilde{\rho}^q_{\mu\mu'} = \kappa^q_{\mu\hat{\mu}}\, \hat{\mathcal{T}}^*_{\hat{\mu}\mu'} , \qquad \kappa^q_{\mu\hat{\mu}} = \sum_{\mu'} \tilde{\rho}^q_{\mu\mu'}\, \mathcal{T}^{\mathrm{T}}_{\mu'\hat{\mu}} . \tag{B.121}$$

[8] We omit the subscript can in the following when it is not necessary.

Also, one can write

$$\rho^q(\vec{r},\vec{r}\,') = \sum_{\mu} \phi^\dagger_\mu(\vec{r}\,' q)\,\phi_\mu(\vec{r}\,q)\,\rho^q_{\mu\mu}\,, \tag{B.122a}$$

$$\rho^q(\vec{r}) = \sum_{\mu} \phi^\dagger_\mu(\vec{r}\,q)\,\phi_\mu(\vec{r}\,q)\,\rho^q_{\mu\mu}\,, \tag{B.122b}$$

$$\tilde{\rho}^q(\vec{r},\vec{r}\,') = \sum_{\mu'\mu} \phi^\dagger_{\mu'}(\vec{r}\,' q)\,\phi_\mu(\vec{r}\,q)\,\tilde{\rho}^q_{\mu\mu'}\,, \tag{B.122c}$$

$$\tilde{\rho}^q(\vec{r}) = \sum_{\mu'\mu} \phi^\dagger_{\mu'}(\vec{r}\,q)\,\phi_\mu(\vec{r}\,q)\,\tilde{\rho}^q_{\mu\mu'} = -\sum_{\mu} \psi_{\mu\hat{\mu}}(\vec{r}\,q)\,\kappa^q_{\mu\hat{\mu}}\,, \tag{B.122d}$$

where the local spin-singlet part of the two-body wave function has been introduced through

$$\psi_{\mu\nu}(\vec{r}\,q) \equiv \sum_{\sigma} 2\sigma\,\phi_\mu(\vec{r}\,\sigma\,q)\,\phi_\nu(\vec{r}\,\bar{\sigma}\,q)\,. \tag{B.123}$$

B.7.3 BCS-like occupation numbers

In the HFB theory, explicit expressions of $(u^{q\,2}_\mu, v^{q\,2}_\mu)$ can be obtained by using the fact that the minimization principle amounts to canceling the part of the Hamiltonian $\hat{H}$ corresponding to two-quasiparticle excitations, i.e.

$$\mathcal{H}^{q\,20} = \bar{\mathcal{U}}^{q[\kappa]\,\dagger}\,(h^q - \lambda^q)\,\bar{\mathcal{V}}^{q[\kappa]\,*} - \bar{\mathcal{V}}^{q[\kappa]\,\dagger}\left(h^{q\,\mathrm{T}} - \lambda^q\right)\bar{\mathcal{U}}^{q[\kappa]\,*} + \bar{\mathcal{U}}^{q[\kappa]\,\dagger}\,\Delta^q\,\bar{\mathcal{U}}^{q[\kappa]\,*} - \bar{\mathcal{V}}^{q[\kappa]\,\dagger}\,\Delta^{q\,*}\,\bar{\mathcal{V}}^{q[\kappa]\,*} = 0\,. \tag{B.124}$$

For a given matrix element, this identity reads as

$$\zeta_\mu\,u^q_\mu\,v^q_\mu\left(h^q_{\mu\mu} + h^q_{\hat{\mu}\hat{\mu}} - 2\lambda^q\right) + \Delta^q_{\mu\hat{\mu}}\left(u^{q\,2}_\mu - v^{q\,2}_\mu\right) = 0\,. \tag{B.125}$$

Such a set of equations leads to the well-known BCS-like expressions

$$\left[\begin{array}{c} u^{q\,2}_\mu \\ v^{q\,2}_\mu \end{array}\right] = \frac{1}{2}\left(1 \pm \frac{\left(h^q_{\mu\mu} + h^q_{\hat{\mu}\hat{\mu}}\right)/2 - \lambda^q}{\sqrt{\left[\left(h^q_{\mu\mu} + h^q_{\hat{\mu}\hat{\mu}}\right)/2 - \lambda^q\right]^2 + \Delta^{q\,2}_{\mu\hat{\mu}}}}\right)\,, \tag{B.126}$$

which leaves the sign of v^q_μ undecided.

B.7.4 Time-reversal invariant systems

For time-reversal invariant systems, the canonical basis is closed under the action of $\hat{\mathcal{T}}$, thus

$$\phi_{\hat{\mu}}(\vec{r}\,\sigma\,q) \equiv \phi_{\tilde{\mu}}(\vec{r}\,\sigma\,q) = \eta_\mu\,\phi_{\bar{\mu}}(\vec{r}\,\sigma\,q) = \eta_\mu\,2\sigma\,\phi^*_\mu(\vec{r}\,\bar{\sigma}\,q)\,, \tag{B.127}$$

As a result, $\mathcal{T}_{\mu\hat{\nu}} = \eta_{\hat{\nu}}\,\delta_{\tilde{\mu}\hat{\nu}}$ and

$$\tilde{\rho}^q_{\mu\mu'} = \eta_\mu\,\kappa^q_{\mu\tilde{\mu}}\,\delta_{\mu\mu'} = \eta_\mu\,\zeta_\mu\,u^q_\mu\,v^q_\mu\,\delta_{\mu\mu'}\,. \tag{B.128}$$

This shows that, while κ^q is canonical, $\tilde{\rho}^q$ becomes diagonal in the canonical basis and thus

$$\tilde{\rho}^q(\vec{r},\vec{r}\,') = \sum_{\mu} \phi^\dagger_\mu(\vec{r}\,' q)\,\phi_\mu(\vec{r}\,q)\,\eta_\mu\,\zeta_\mu\,u^q_\mu\,v^q_\mu\,. \tag{B.129}$$

At the same time, one finds that the lower component of the Russian quasiparticle states becomes diagonal and the 2×2 $(\mu, \tilde{\mu})$ blocks of the special transformation take the form

$$\left(\bar{\mathcal{U}}^{q[\bar{\rho}]}\right)_{\mu\tilde{\mu}} = \quad u^q_\mu \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \left(\bar{\mathcal{V}}^{q[\bar{\rho}]}\right)_{\mu\tilde{\mu}} = \eta_\mu \, \zeta_\mu \, v^q_\mu \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{B.130}$$

Indeed

$$\begin{aligned} \bar{\mathcal{V}}^{q[\bar{\rho}]}_{\mu\nu} = (\mathcal{T}^T \, \bar{\mathcal{V}}^{q[\kappa]})_{\mu\nu} &= \sum_k \mathcal{T}_{\mu k} \, \bar{\mathcal{V}}^{[q\,\kappa]}_{k\nu} \\ &= \sum_k \eta_k \, \delta_{\mu\tilde{k}} \, \delta_{k\tilde{\nu}} \, \zeta_k v^q_\nu \\ &= \eta_{\tilde{\mu}} \, \zeta_{\tilde{\mu}} \, v^q_\mu \, \delta_{\mu\nu} = \eta_\mu \, \zeta_\mu \, v^q_\mu \, \delta_{\mu\nu} \, . \end{aligned} \tag{B.131}$$

The subtlety here is that, for a given pair $(\mu, \tilde{\mu})$, the quantum number ζ_μ originally used to separate the basis into two halves coupled by the Bogoliubov transformation is not necessarily the same as the (real) phase η_μ, i.e. $\eta_\mu \, \zeta_\mu = \pm 1$ depending on the quantum number μ. For time-reversal systems, it might thus be useful to reorder each pair of canonical states $(\mu, \tilde{\mu})$ according to η_μ and not ζ_μ as done in general. This is equivalent to saying that one can redefine the BCS-like coefficient v^q_μ whose sign, as opposed to u^q_μ, cannot been specified anyway. This redefinition corresponds to the replacement $\eta_\mu \, \zeta_\mu \, v^q_\mu \to v^q_\mu$ in the previous formulæ. In such a case, one will have

$$\bar{\mathcal{U}}^{q[\kappa]} \equiv \quad u^q_\mu \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \bar{\mathcal{V}}^{q[\kappa]} \equiv \eta_\mu \, v^q_\mu \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{B.132}$$

and

$$\bar{\mathcal{U}}^{q[\bar{\rho}]} \equiv u^q_\mu \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \bar{\mathcal{V}}^{q[\bar{\rho}]} \equiv v^q_\mu \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{B.133}$$

However, if the system is not time-reversal invariant, the definition of v^q_μ has to be made according to ζ_μ.

B.8 Quasiparticle basis

B.8.1 Quasiparticle states

Quasiparticle operators in the traditional representation are related to the canonical ones using the Bloch-Messiah decomposition through

$$\hat{\beta}^{q\,\dagger}_\mu = \sum_k \bar{\mathcal{U}}^{q[\kappa]}_{kk} \, C^q_{k\mu} \, \hat{c}^{q\,\dagger}_k + \sum_k \bar{\mathcal{V}}^{q[\kappa]}_{k\hat{k}} \, C^q_{\hat{k}\mu} \, \hat{c}^q_k = \sum_k u^q_k \, C^q_{k\mu} \, \hat{c}^{q\,\dagger}_k + \sum_k \zeta_k \, v^q_k \, C^q_{\hat{k}\mu} \, \hat{c}^q_k \, , \tag{B.134a}$$

$$\hat{\beta}^q_\mu = \sum_k \bar{\mathcal{U}}^{q[\kappa]*}_{kk} \, C^{q\,*}_{k\mu} \, \hat{c}^q_k + \sum_k \bar{\mathcal{V}}^{q[\kappa]*}_{k\hat{k}} \, C^{q\,*}_{\hat{k}\mu} \, \hat{c}^{q\,\dagger}_k = \sum_k u^q_k \, C^{q\,*}_{k\mu} \, \hat{c}^q_k + \sum_k \zeta_k \, v^q_k \, C^{q\,*}_{\hat{k}\mu} \, \hat{c}^{q\,\dagger}_k \, , \tag{B.134b}$$

which can be further simplified by using the fact that the transformation C^q only couples states with the same signature. Using Eq. (B.78) one has

$$\begin{bmatrix} \mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q) \end{bmatrix} = \sum_k \begin{bmatrix} \phi_k(\vec{r}\,\sigma\,q) \, u^q_k \, C^q_{k\mu} \\ \eta_k \, \phi^*_k(\vec{r}\,\sigma\,q) \, v^q_k \, C^q_{\hat{k}\mu} \end{bmatrix}, \tag{B.135}$$

B.8.2 Normal and pair density matrices, pairing tensor

We now give the expressions of the densities expressed in the traditional and Russian quasiparticle bases and recover, using Eq. (B.135), the corresponding formulæ in the canonical basis. Using Eq. (B.66), it is obvious that

$$\begin{aligned}\rho^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') &= \sum_\mu \mathcal{V}^{q[\kappa]\,*}_{\vec{r}\sigma q,\mu}\,\mathcal{V}^{q[\kappa]\;\mathrm{T}}_{\mu,\vec{r}\,'\sigma' q} = \sum_\mu \mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q)^*\,\mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,'\,\sigma'\,q) \\ &= \sum_\mu 2\sigma\,\mathcal{V}^{q[\tilde{\rho}]*}_\mu(\vec{r}\,\bar{\sigma}\,q)\,2\sigma'\,\mathcal{V}^{q[\tilde{\rho}]}_\mu(\vec{r}\,'\,\bar{\sigma}'\,q)\,, \end{aligned} \tag{B.136}$$

which leads, using $\sum_\mu C^{q\;*}_{k\mu}\,C^q_{k'\mu} = \delta_{kk'}$ and $\zeta_k^2 = 1$, to

$$\begin{aligned}\rho^q(\vec{r}\,\sigma,\vec{r}\,'\,\sigma') &= \sum_\mu \sum_{kk'} \zeta_k\,\zeta_{k'}\,\phi_k(\vec{r}\,\sigma\,q)\,v^q_k\,C^{q\;*}_{\bar{k}\mu}\,\phi^*_{k'}(\vec{r}\,'\,\sigma'\,q)\,v^q_{k'}\,C^q_{\bar{k}'\mu} \\ &= \sum_k \phi_k(\vec{r}\,\sigma\,q)\,\phi^*_k(\vec{r}\,'\,\sigma'\,q)\,{v^q_k}^2\,, \end{aligned} \tag{B.137}$$

which is compliant with Eq. (B.122a).

In the same fashion, Eq. (B.66) leads to two formulations for the pairing tensor and pair densities in terms of the quasiparticle basis, i.e.

$$\kappa(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q) = \sum_\mu \mathcal{V}^{q[\kappa]\,*}_{\vec{r}\sigma q,\mu}\mathcal{U}^{q[\kappa]\;\mathrm{T}}_{\mu,\vec{r}\,'\sigma' q} = -\sum_\mu \mathcal{U}^{q[\kappa]}_{\vec{r}\sigma q,\mu}\,\mathcal{V}^{q[\kappa]\;\dagger}_{\mu,\vec{r}\,'\sigma' q}, \tag{B.138a}$$

$$= \sum_\mu \mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q)^*\,\mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,'\,\sigma'\,q) = -\sum_\mu \mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q)\,\mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,'\,\sigma'\,q)^*\,, \tag{B.138b}$$

$$\tilde{\rho}(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q) = \sum_\mu 2\bar{\sigma}'\,\mathcal{V}^{q[\kappa]*}_\mu(\vec{r}\,\sigma\,q)\,\mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,'\,\bar{\sigma}'\,q) = -\sum_\mu 2\bar{\sigma}'\,\mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q)\,\mathcal{V}^{q[\kappa]*}_\mu(\vec{r}\,'\,\bar{\sigma}'\,q)\,, \tag{B.138c}$$

$$= \sum_\mu 2\sigma\,\mathcal{V}^{q[\tilde{\rho}]*}_\mu(\vec{r}\,\bar{\sigma}\,q)\,2\bar{\sigma}'\,\mathcal{U}^{q[\tilde{\rho}]}_\mu(\vec{r}\,'\,\bar{\sigma}'\,q) = -\sum_\mu \mathcal{U}^{q[\tilde{\rho}]}_\mu(\vec{r}\,\sigma\,q)\,\mathcal{V}^{q[\tilde{\rho}]*}_\mu(\vec{r}\,'\,\sigma'\,q)\,. \tag{B.138d}$$

Finally, one recovers

$$\begin{aligned}\tilde{\rho}(\vec{r}\,\sigma\,q,\vec{r}\,'\,\sigma'\,q) &= \sum_\mu 2\bar{\sigma}'\,\mathcal{V}^{q[\kappa]*}_\mu(\vec{r}\,\sigma\,q)\,\mathcal{U}^{q[\kappa]}_\mu(\vec{r}\,'\,\bar{\sigma}'\,q) \\ &= \sum_\mu \sum_{kk'} 2\bar{\sigma}'\,\zeta_k\,\phi_k(\vec{r}\,\sigma\,q)\,v^q_k\,C^*_{\hat{k}\mu}\,\phi_{k'}(\vec{r}\,'\,\bar{\sigma}'\,q)\,u^q_{k'}\,C_{k'\mu} \\ &= 2\bar{\sigma}'\sum_k \phi_k(\vec{r}\,\sigma\,q)\,\phi_\nu(\vec{r}\,'\,\bar{\sigma}'\,q)\,\kappa_{k\hat{k}}\,, \end{aligned} \tag{B.139}$$

which is compliant with Eq. (B.35) if the latter were to be written in the canonical basis.

B.8.3 Local normal and pair scalar densities

Using Eq. (B.136), the local scalar normal density is obtained as

$$\rho^q(\vec{r}\,) = \sum_\mu \sum_\sigma \left|\mathcal{V}^{q[\kappa]}_\mu(\vec{r}\,\sigma\,q)\right|^2 = \sum_\mu \sum_\sigma \left|\mathcal{V}^{q[\tilde{\rho}]}_\mu(\vec{r}\,\sigma\,q)\right|^2\,, \tag{B.140}$$

whereas Eq. (B.138d) leads to a local scalar pair density of the form

$$\tilde{\rho}^{q}(\vec{r}) = -\sum_{\mu}\sum_{\sigma} 2\bar{\sigma}\,\mathcal{U}_{\mu}^{q[\kappa]}(\vec{r}\,\sigma\,q)\,\mathcal{V}_{\mu}^{q[\kappa]*}(\vec{r}\,\bar{\sigma}\,q) = -\sum_{\mu}\sum_{\sigma}\mathcal{U}_{\mu}^{q[\tilde{\rho}]}(\vec{r}\,\sigma\,q)\,\mathcal{V}_{\mu}^{q[\tilde{\rho}]*}(\vec{r}\,\sigma\,q)\,. \tag{B.141}$$

B.9 Spherical systems

B.9.1 Basic properties

Different phase conventions exist to define single-particle states in such a context. We chose to write the spinors as

$$\langle\,\vec{r}\,|\,\mu\rangle = \varphi_{\mu}(\vec{r}\,q) = \frac{u_{n\ell j}(r\,q)}{r}\sum_{m_\ell\sigma} Y_{\ell}^{m_\ell}(\hat{r})\,\langle\ell\,m_\ell\,\tfrac{1}{2}\,\sigma|j\,m\rangle\,|\sigma\rangle \equiv \frac{u_{n\ell j}(rq)}{r}\,\Omega_{\ell jm}(\hat{r})\,, \tag{B.142}$$

where $\mu \equiv n\ell jmq$. $\Omega_{j\ell m}(\hat{r})$ are spherical spinors that couple the angular part of the wave function to spinors associated with spin 1/2. They have the properties

$$\hat{\vec{J}}^{\,2}\,\Omega_{j\ell m}(\hat{r}) = \hbar^2\,j(j+1)\,\Omega_{j\ell m}(\hat{r})\,, \tag{B.143a}$$

$$\hat{\vec{L}}^{\,2}\,\Omega_{j\ell m}(\hat{r}) = \hbar^2\,\ell(\ell+1)\,\Omega_{j\ell m}(\hat{r})\,, \tag{B.143b}$$

$$\hat{\vec{S}}^{\,2}\,\Omega_{j\ell m}(\hat{r}) = \hbar^2\,s(s+1)\,\Omega_{j\ell m}(\hat{r}) = \frac{3}{4}\,\hbar^2\,\Omega_{j\ell m}(\hat{r})\,, \tag{B.143c}$$

$$\hat{J}_z\,\Omega_{j\ell m}(\hat{r}) = \hbar\,m\,\Omega_{j\ell m}(\hat{r})\,. \tag{B.143d}$$

Spherical spinors are orthonormal, i.e.

$$\int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)\,\Omega_{j\ell m}^{\dagger}(\theta,\varphi)\,\Omega_{j'\ell'm'}(\theta,\varphi) = \delta_{jj'}\,\delta_{\ell\ell'}\,\delta_{mm'}\,. \tag{B.144}$$

and also have the properties

$$\sum_{m=-j}^{j}\Omega_{j\ell m}^{\dagger}(\hat{r})\,\Omega_{j\ell m}(\hat{r}) = \frac{2j+1}{4\pi}\,, \qquad \sum_{m=-j}^{j}\Omega_{j\ell m}^{\dagger}(\hat{r})\,\hat{\vec{\sigma}}\,\Omega_{j\ell m}(\hat{r}) = 0\,. \tag{B.145}$$

The quantum numbers of a spinor are given by its total angular momentum j, the projection of the angular momentum m along the z axis and the value of the orbital angular momentum ℓ. For a given j, only $\ell = j \pm \frac{1}{2}$ are possible values. The total spin quantum number S is a good quantum number but corresponds to the same $S = \frac{1}{2}$ for all nucleons. The spin projection is *not* a good quantum number since single-particle states mix $\sigma = \pm\frac{1}{2}$. For states defined by Eq. (B.142), parity and z-signature are given by $\pi_\mu = (-1)^{\ell}$ and $\zeta_\mu = -i^{2m+1} = (-1)^{m-\frac{1}{2}}$, respectively.

B.9.2 Time-reversal symmetry

The time-reversed state of $\varphi_{n\ell jm}$ is obtained by applying the operator $\hat{\mathcal{T}}$, i.e.

$$\begin{aligned}(\hat{\mathcal{T}}\,\varphi)_{n\ell jm}(\vec{r}\,q) =& \frac{u_{nlj}(r\,q)}{r}\sum_{\sigma}\langle\ell\,(m-\sigma)\,\tfrac{1}{2}\,\sigma|j\,m\rangle\,Y_{\ell}^{m-\sigma\,*}(\hat{r})\,(-2\sigma)\,|\bar{\sigma}\rangle \\ =& \frac{u_{nlj}(r\,q)}{r}\sum_{\sigma}(-1)^{\ell+\frac{1}{2}-j}\,(-1)^{\sigma-\frac{1}{2}}\,(-1)^{-m-\sigma} \\ & \qquad\times\langle\ell\,(-m-\sigma)\,\tfrac{1}{2}\,\sigma|j\,(-m)\rangle\,Y_{\ell}^{-m-\sigma}(\hat{r})\,|\sigma\rangle \\ =& (-1)^{\ell-j-m}\,\varphi_{n\ell j-m}(\vec{r}\,q)\,,\end{aligned} \tag{B.146}$$

where the relationships

$$Y_\ell^{m_\ell *}(\hat{r}) = (-1)^{m_\ell}\, Y_\ell^{-m_\ell}(\hat{r})\,, \tag{B.147a}$$

$$2\sigma = (-1)^{\sigma-\frac{1}{2}}\,, \tag{B.147b}$$

$$\langle \ell\, m_\ell\, \tfrac{1}{2}\, \bar{\sigma} | j\, m\rangle = (-1)^{\ell+\frac{1}{2}-j}\, \langle \ell\, (-m_\ell)\, \tfrac{1}{2}\, \sigma | j\, (-m)\rangle\,, \tag{B.147c}$$

have been used. Thus, the basis is closed with respect to the action of $\hat{\mathcal{T}}$. We obtain in the present case that $\tilde{\mu} \equiv n\ell j(-m)q$ and $\eta_\mu \equiv (-1)^{\ell-j-m} = (-1)^{\ell-j-\frac{1}{2}}\,\zeta_\mu$. This relates to the fact that, in a time-independent calculation, a system that sustains a self-consistent spherical symmetry is necessarily time-reversal invariant.

The quantum number ζ_μ is the one used to differentiate between the two halves of the basis ($\zeta_\mu > 0$ and $\zeta_\mu < 0$). The real number η_μ is the phase connecting a state with a time-reversed one of opposite signature when the system is time-reversal invariant. Here are typical values of η_μ and ζ_μ for a selection of spherical shells

$p_{3/2}$	j=3/2	l=1		$d_{3/2}$	j=3/2	l=2
m	ζ_μ	η_μ	—	m	ζ_μ	η_μ
+ 3/2	-	-		+ 3/2	-	+
+ 1/2	+	+		+ 1/2	+	-
- 1/2	-	-		- 1/2	-	+
- 3/2	+	+		- 3/2	+	-

which shows that η_μ has opposite signs for states belonging to two different halves of the basis but that it is not necessarily equal to ζ_μ.

B.9.3 Canonical basis

The canonical states $\phi_{n\ell jm}$ verify all the properties discussed above. Note that the principal quantum number n does not necessarily denote the number of nodes in the canonical wave function. This property is due to the fact the D^q transformation amounts to mixing states originating from major shells characterized by different number of nodes in order to make the canonical states localized in space.

Because of spherical symmetry, BCS-like occupation numbers are independent on the magnetic quantum number m. As already discussed, the time-reversal invariance of the system allows us to order each conjugated pair $(\mu, \tilde{\mu})$ according to the number η_μ rather than ζ_μ. In the end, the 2×2 blocks read as

$$\bar{\mathcal{U}}^{q[\kappa]} \equiv \begin{pmatrix} \bar{\mathcal{U}}^{n\ell jq[\kappa]}_{mm} & 0 \\ 0 & \bar{\mathcal{U}}^{n\ell jq[\kappa]}_{(-m)(-m)} \end{pmatrix} = u^q_{n\ell j} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{B.148a}$$

$$\bar{\mathcal{V}}^{q[\kappa]} \equiv \begin{pmatrix} 0 & \bar{\mathcal{V}}^{n\ell jq[\kappa]}_{m(-m)} \\ \bar{\mathcal{V}}^{n\ell jq[\kappa]}_{(-m)m} & 0 \end{pmatrix} = (-1)^{\ell-j-m}\, v^q_{n\ell j} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{B.148b}$$

and in the same way,

$$\bar{\mathcal{U}}^{q[\tilde{\rho}]} = u^q_{n\ell j} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{B.149a}$$

$$\bar{\mathcal{V}}^{q[\tilde{\rho}]} = v^q_{n\ell j} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{B.149b}$$

while the *non-zero* matrix elements of the density matrices are

$$\rho^{n\ell jq}_{mm} = +\rho^{n\ell jq}_{(-m)(-m)} = v^{q\,2}_{n\ell j}, \tag{B.150a}$$

$$\kappa^{n\ell jq}_{m(-m)} = -\kappa^{n\ell jq}_{(-m)m} = (-1)^{\ell-j-m}\, u^q_{n\ell j}\, v^q_{n\ell j}, \tag{B.150b}$$

$$\tilde{\rho}^{n\ell jq}_{mm} = +\tilde{\rho}^{n\ell jq}_{(-m)(-m)} = u^q_{n\ell j}\, v^q_{n\ell j}. \tag{B.150c}$$

Using the previous expressions, the scalar local densities are obtained from Eqs. (B.122b,B.122d) as

$$\rho_q(\vec{r}) = \sum_{n\ell j} \frac{2j+1}{4\pi} \frac{u^2_{n\ell j}(rq)}{r^2}\, v^{q\,2}_{n\ell j}, \tag{B.151a}$$

$$\tilde{\rho}_q(\vec{r}) = \sum_{n\ell j} \frac{2j+1}{4\pi} \frac{u^2_{n\ell j}(rq)}{r^2}\, u^q_{n\ell j}\, v^q_{n\ell j}, \tag{B.151b}$$

and are manifestly spherically symmetric.

B.9.4 Quasiparticle basis

Due to spherical symmetry, the traditional and Russian quasiparticle wave functions are also characterized by the quantum numbers (ℓjm). The connection between the canonical and traditional quasiparticle wave functions is provided by Eq. (B.135) with the third part C^q of the Bogoliubov transformation which can only mix states with different principal quantum numbers but same (ℓjm), i.e. $C^q_{n\ell jm,n'\ell'j'm'} \equiv C^{\ell jq}_{nn'}\delta_{jj'}\,\delta_{\ell\ell'}\,\delta_{mm'}$. Starting from canonical states from Eq. (B.142) and using Eq. (B.135), one finds traditional quasiparticle wave functions of the form

$$\begin{bmatrix} \mathcal{U}^{n\ell jq[\kappa]}_m(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{n\ell jq[\kappa]}_m(\vec{r}\,\sigma\,q) \end{bmatrix} \equiv \sum_{n'} C^{\ell jq}_{n'n} \frac{u_{n'\ell j}(rq)}{r} \sum_{m_\ell} Y^{m_\ell}_\ell(\hat{r}) \begin{bmatrix} u^q_{n'\ell j}\, \langle \ell\, m_\ell\, \frac{1}{2}\, \sigma | j\, m\rangle \\ 2\bar{\sigma}\, v^q_{n'\ell j}\, \langle \ell\, m_\ell\, \frac{1}{2}\, \bar{\sigma} | j\, m\rangle \end{bmatrix}, \tag{B.152}$$

whereas Eq. (B.95) allows one to recover the quasiparticle wave functions in the Russian representation as

$$\begin{bmatrix} \mathcal{U}^{n\ell jq[\tilde{\rho}]}_m(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{n\ell jq[\tilde{\rho}]}_m(\vec{r}\,\sigma\,q) \end{bmatrix} \equiv \sum_{n'} C^{\ell jq}_{n'n} \frac{u_{n'\ell j}(rq)}{r} \sum_{m_\ell} Y^{m_\ell}_\ell(\hat{r}) \begin{bmatrix} u^q_{n'\ell j}\, \langle \ell\, m_\ell\, \frac{1}{2}\, \sigma | j\, m\rangle \\ -v^q_{n'\ell j}\, \langle \ell\, m_\ell\, \frac{1}{2}\, \sigma | j\, m\rangle \end{bmatrix}. \tag{B.153}$$

The latter relationships prove that the upper and lower components of the quasiparticle wave functions are indeed eigenstates of $(\hat{\vec{L}}^2, \hat{\vec{J}}^2, \hat{J}_z)$ with eigenvalues (ljm) and can be written as

$$\mathcal{U}_m^{n\ell jq[\kappa]}(\vec{r}\,q) \equiv \frac{\mathcal{U}^q_{n\ell j}(r\,q)}{r} \sum_{m_\ell\sigma} Y_l^{m_l}(\hat{r})\,\langle \ell\, m_\ell\, \tfrac{1}{2}\,\sigma | j\, m\rangle\,|\sigma\rangle\,, \tag{B.154a}$$

$$\mathcal{V}_m^{n\ell jq[\kappa]}(\vec{r}\,q) \equiv \frac{\mathcal{V}^q_{n\ell j}(r\,q)}{r} \sum_{m_\ell\sigma} Y_l^{m_l}(\hat{r})\,2\sigma\,\langle \ell\, m_\ell\, \tfrac{1}{2}\,\bar{\sigma} | j\, m\rangle\,|\sigma\rangle\,, \tag{B.154b}$$

$$\mathcal{U}_m^{n\ell jq[\tilde{\rho}]}(\vec{r}\,q) \equiv \frac{\mathcal{U}^q_{n\ell j}(r\,q)}{r} \sum_{m_\ell\sigma} Y_l^{m_l}(\hat{r})\,\langle \ell\, m_\ell\, \tfrac{1}{2}\,\sigma | j\, m\rangle\,|\sigma\rangle\,, \tag{B.154c}$$

$$\mathcal{V}_m^{n\ell jq[\tilde{\rho}]}(\vec{r}\,q) \equiv \frac{\mathcal{V}^q_{n\ell j}(r\,q)}{r} \sum_{m_\ell\sigma} Y_l^{m_l}(\hat{r})\,\langle \ell\, m_\ell\, \tfrac{1}{2}\,\sigma | j\, m\rangle\,|\sigma\rangle\,, \tag{B.154d}$$

where the radial parts $(\mathcal{U}^q_{n\ell j}(r\,q), \mathcal{V}^q_{n\ell j}(r\,q))$ are independent of the representation (traditional or Russian) and are connected to canonical states through

$$\begin{bmatrix} \mathcal{U}^q_{n\ell j}(r\,q) \\ \mathcal{V}^q_{n\ell j}(r\,q) \end{bmatrix} \equiv \sum_{n'} \begin{bmatrix} +u^q_{n'\ell j} \\ -v^q_{n'\ell j} \end{bmatrix} u_{n'\ell j}(rq)\, C^{\ell jq}_{n'n}\,. \tag{B.155}$$

It it interesting to note, although this should not come as a surprise, that the only difference between traditional and Russian quasiparticles in spherical symmetry relates to the angular⊗spin part of the lower component. Basically, to produce a given magnetic quantum number m, the spin-up (-down) component of $\mathcal{V}^{q[\tilde{\rho}]}$ couples to the orbital angular momentum as if it were a spin-down (-up) component.

B.9.5 Local densities

Starting from Eqs. (B.140,B.141) and using the expressions of quasiparticle wave functions from above, or starting from Eqs. (B.151a,B.151b) and using the (inverse of the) transformation from Eq. (B.155), one finds

$$\rho^q(\vec{r}\,) = \sum_{n\ell j} \frac{2j+1}{4\pi} \frac{\mathcal{V}^{q\,2}_{n\ell j}(rq)}{r^2}\,, \tag{B.156a}$$

$$\tilde{\rho}^q(\vec{r}\,) = -\sum_{n\ell j} \frac{2j+1}{4\pi} \frac{\mathcal{U}^q_{n\ell j}(rq)\,\mathcal{V}^q_{n\ell j}(rq)}{r^2}\,. \tag{B.156b}$$

More elaborate quasi-local and fully non-local densities can be easily expressed too, e.g. first in the canonical basis and transformed if necessary into the quasiparticle basis using Eq. (B.155).

B.9.6 HFB equations

In spherical symmetry, HFB equations can be solved independently within each (lj) block. For a non-local EDF, e.g. Gogny EDF, they do not simplify significantly in coordinate space, although one may take advantage of symmetries of non-local densities at play to perform a partial wave expansion of the fields. For a quasi-local EDF, e.g. Skyrme EDF, HFB equations in coordinate space become purely radial.

B.10 Infinite nuclear matter

B.10.1 Basic properties

Due to the translational invariance of infinite nuclear matter, the spatial part of the single-particle wave functions of interest is known a priori and take the form of a plane wave. In addition, nucleons are considered to have a good spin projection. The latter property leads to great simplification but can also leads to confusion if one does not use very explicit notations. Thus, let us use explicit notations in the first two parts of the section. A given state is going to be characterized by the set of quantum numbers $\mu \equiv \vec{k}_\mu \sigma_\mu q_\mu$, where the index μ underlines that those denote the quantum numbers of the state and not the components of the spin-isospin spinor. In this way, basis kets are given by $|\mu\rangle \equiv |\vec{k}_\mu \sigma_\mu q_\mu\rangle$, whereas their components are obtained as

$$\langle \vec{r}\,\sigma\, q|\vec{k}_\mu \sigma_\mu q_\mu\rangle \equiv \varphi_{\vec{k}_\mu \sigma_\mu q_\mu}(\vec{r}\,\sigma\, q) = e^{i\,\vec{k}_\mu\cdot\vec{r}}\,\delta_{\sigma\sigma_\mu}\,\delta_{qq_\mu}\,. \tag{B.157}$$

B.10.2 Time-reversal symmetry

Starting from $|\mu\rangle = |\vec{k}_\mu \sigma_\mu q_\mu\rangle$, we calculate the component of its time-reversed partner according to

$$(\hat{\mathcal{T}}\,\varphi)_\mu(\vec{r}\,\sigma\, q) = \langle \vec{r}\,\sigma\, q|\big(\hat{\mathcal{T}}\,|\mu\rangle = 2\sigma\,\langle \vec{r}\,\bar{\sigma}\, q|\vec{k}_\mu \sigma_\mu q_\mu\rangle^* = 2\bar{\sigma}_\mu\, e^{-i\,\vec{k}_\mu\cdot\vec{r}}\,\delta_{\sigma\bar{\sigma}_\mu}\,\delta_{qq_\mu} = 2\bar{\sigma}_\mu\,\varphi_{(-\vec{k}_\mu)(-\sigma_\mu)q_\mu}(\vec{r}\,\sigma\, q)\,, \tag{B.158}$$

which demonstrates that the basis is closed with respect to the action of $\hat{\mathcal{T}}$. The corresponding conjugated state in the basis is $\tilde{\mu} \equiv (-\vec{k}_\mu)(-\sigma_\mu)q_\mu$ and $\eta_{\vec{k}_\mu\sigma_\mu q_\mu} = 2\bar{\sigma}_\mu$. This relates to the fact that, in a time-independent calculation, a system that sustains a self-consistent translational symmetry is necessarily time-reversal invariant. When it is not misleading, we drop the index μ in the following and sometimes confuse quantum numbers of a state with the ones of its spin-isospin components.

One can see easily that $|\vec{k}\sigma q\rangle$ are not eigenstates of the z-signature operator. Such a quantum number is however unnecessary in the present case as the pairing is restricted from the outset to time-reversed states[9]. Thus, only the phase $\eta_{\vec{k}\,\sigma\,q}$ is of importance.

B.10.3 Canonical basis

Canonical states $\phi_{\vec{k}\sigma q}$ verify all properties discussed above. In the present case, the pairing treatment reduces to a BCS approximation since the Bogoliubov transformation is known a priori. Because of translational symmetry, BCS occupation numbers are independent of the direction of $\vec{k}$. Because of time-reversal invariance, they also are independent of σ. In the end, the 2×2 blocks of the special Bogoliubov transformations read in the canonical basis as

$$\bar{\mathcal{U}}^{q[\kappa]} \equiv \begin{pmatrix} \bar{\mathcal{U}}^{q[\kappa]}_{\vec{k}\sigma,\vec{k}\sigma} & 0 \\ 0 & \bar{\mathcal{U}}^{q[\kappa]}_{-\vec{k}-\sigma,-\vec{k}-\sigma} \end{pmatrix} = \quad u^q_k \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{B.159a}$$

$$\bar{\mathcal{V}}^{q[\kappa]} \equiv \begin{pmatrix} 0 & \bar{\mathcal{V}}^{q[\kappa]}_{\vec{k}\sigma,-\vec{k}-\sigma} \\ \bar{\mathcal{V}}^{q[\kappa]}_{-\vec{k}-\sigma,\vec{k}\sigma} & 0 \end{pmatrix} = 2\bar{\sigma}\, v^q_k \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{B.159b}$$

[9] The fact that the pairing only couples $\varphi_{\vec{k}}$ and $\varphi_{-\vec{k}}$ is dictated by translational symmetry and the fact that we are considering static uniform matter. However, nothing fundamental, except for the pairing interaction that we have in mind, prevents nucleons to pair in the spin-triplet state.

and

$$\bar{\mathcal{U}}^{q[\bar{\rho}]} = u_k^q \begin{pmatrix} 1 & 0 \\ & \\ 0 & 1 \end{pmatrix}, \qquad \bar{\mathcal{V}}^{q[\bar{\rho}]} = v_k^q \begin{pmatrix} 1 & 0 \\ & \\ 0 & 1 \end{pmatrix}, \tag{B.160}$$

while *non-zero* matrix elements of the density matrices are

$$\rho^q_{\vec{k}\sigma,\vec{k}\sigma} = +\rho^q_{-\vec{k}-\sigma,-\vec{k}-\sigma} = v_k^{q\,2}\,, \tag{B.161a}$$

$$\kappa^q_{\vec{k}\sigma,-\vec{k}-\sigma} = -\kappa^q_{-\vec{k}-\sigma,\vec{k}\sigma} = 2\bar{\sigma}\,u_k^q\,v_k^q\,, \tag{B.161b}$$

$$\tilde{\rho}^q_{\vec{k}\sigma,\vec{k}\sigma} = +\tilde{\rho}^q_{-\vec{k}-\sigma,-\vec{k}-\sigma} = u_k^q\,v_k^q\,. \tag{B.161c}$$

Using the previous expressions, the non-local scalar densities are obtained from Eqs. (B.122a,B.122c) as[10]

$$\rho_q(\vec{r},\vec{r}\,') = 2\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,e^{i\,\vec{k}\cdot(\vec{r}-\vec{r}\,')}\,v_k^{q\,2}\,, \tag{B.162a}$$

$$\tilde{\rho}_q(\vec{r},\vec{r}\,') = 2\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,e^{i\,\vec{k}\cdot(\vec{r}-\vec{r}\,')}\,u_k^q\,v_k^q\,, \tag{B.162b}$$

and naturally lead to constant local densities of the form

$$\rho_q(\vec{r}\,) = 2\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,v_k^{q\,2}\,, \tag{B.163a}$$

$$\tilde{\rho}_q(\vec{r}\,) = 2\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,u_k^q\,v_k^q\,. \tag{B.163b}$$

Note that the integration over the angle can be trivially done in the four equations above thanks to the independence of u_k^q and v_k^q on the direction of $\vec{k}$.

B.10.4 Quasiparticle basis

Since we are presently dealing with a BCS approximation, it is easy to find the results "directly" without relying on the general HFB formalism. However, our goal is precisely to recover "intuitive" results from the most general formalism.

Due to symmetries, traditional and Russian quasiparticle wave functions are also characterized by the quantum numbers $\vec{k}\sigma q$ in nuclear matter. The connection between the canonical and traditional quasiparticle wave functions is provided by Eq. (B.135) where the third part C^q of the Bogoliubov transformation is trivial as one deals with a BCS approximation, i.e. $C^q_{\vec{k}\sigma q,\vec{k}\,'\sigma q} \equiv \delta(\vec{k}-\vec{k}\,')\,\delta_{\sigma\sigma'}\,\delta_{qq'}$. One thus finds traditional quasiparticle wave functions of the form

$$\begin{bmatrix} \mathcal{U}^{q[\kappa]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{q[\kappa]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,\sigma\,q) \end{bmatrix} \equiv e^{i\,\vec{k}_\mu\cdot\vec{r}} \begin{bmatrix} u^q_{k_\mu}\,\delta_{\sigma\sigma_\mu} \\ 2\bar{\sigma}\,v^q_{k_\mu}\,\delta_{\sigma\bar{\sigma}_\mu} \end{bmatrix} \delta_{qq_\mu}\,, \tag{B.164}$$

whereas Eq. (B.95) allows to recover quasiparticle wave functions in the Russian representation as

$$\begin{bmatrix} \mathcal{U}^{q[\bar{\rho}]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,\sigma\,q) \\ \mathcal{V}^{q[\bar{\rho}]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,\sigma\,q) \end{bmatrix} \equiv e^{i\,\vec{k}_\mu\cdot\vec{r}} \begin{bmatrix} u^q_{k_\mu} \\ -v^q_{k_\mu} \end{bmatrix} \delta_{\sigma\sigma_\mu}\,\delta_{qq_\mu}\,. \tag{B.165}$$

[10] It is interesting to note a subtlety relative to the use of Eqs. (B.122a,B.122d) in the present case. One the one hand, the sum over σ that appears from the scalar product of the spinors $\phi^\dagger_\mu(\vec{r}\,'\,q)$ and $\phi_\mu(\vec{r}\,q)$ provides only one term in spin space since only one component is zero. On the other hand, the sum over μ contains a sum over σ_μ which provides the factor of 2 in Eqs. (B.162a,B.163b)

The latter relationships prove that upper and lower components of quasiparticle wave functions are indeed eigenstates of $\hat{\vec{k}}$ with eigenvalues $\vec{k}_\mu$ and can be written as

$$\mathcal{U}^{q[\kappa]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,q) \equiv \mathcal{U}^{q}_{\vec{k}_\mu}(\vec{r}\,q)\,\delta_{\sigma\sigma_\mu}\,\delta_{qq_\mu}\,, \tag{B.166a}$$

$$\mathcal{V}^{q[\kappa]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,q) \equiv \mathcal{V}^{q}_{\vec{k}_\mu}(\vec{r}\,q)\,2\sigma\,\delta_{\sigma\bar{\sigma}_\mu}\,\delta_{qq_\mu}\,, \tag{B.166b}$$

$$\mathcal{U}^{q[\tilde{\rho}]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,q) \equiv \mathcal{U}^{q}_{\vec{k}_\mu}(\vec{r}\,q)\,\delta_{\sigma\sigma_\mu}\,\delta_{qq_\mu}\,, \tag{B.166c}$$

$$\mathcal{V}^{q[\tilde{\rho}]}_{\vec{k}_\mu\sigma_\mu q_\mu}(\vec{r}\,q) \equiv \mathcal{V}^{q}_{\vec{k}_\mu}(\vec{r}\,q)\,\delta_{\sigma\sigma_\mu}\,\delta_{qq_\mu}\,, \tag{B.166d}$$

where the spatial parts $(\mathcal{U}^{q}_{\vec{k}_\mu}(\vec{r}\,q), \mathcal{V}^{q}_{\vec{k}_\mu}(\vec{r}\,q))$ are independent of the representation (traditional or Russian) and are connected to canonical states through

$$\begin{bmatrix} \mathcal{U}^{q}_{\vec{k}_\mu}(\vec{r}\,q) \\ \mathcal{V}^{q}_{\vec{k}_\mu}(\vec{r}\,q) \end{bmatrix} \equiv e^{i\,\vec{k}_\mu\cdot\vec{r}} \begin{bmatrix} +u^{q}_{k_\mu} \\ -v^{q}_{k_\mu} \end{bmatrix}. \tag{B.167}$$

In the present case, the only difference between traditional and Russian quasiparticles in INM relates to the spin part of the lower component. In particular, upper and lower components of traditional quasiparticles are eigenstates of $\hat{\sigma}_z$ with *opposite* eigenvalues.

B.10.5 Densities

Although the spatial part of all wave functions of interest is known explicitly in the present case, one can re-express non-local densities given by Eqs. (B.162a,B.162b) in terms of the spatial parts of the quasiparticle wave functions, that is

$$\rho_q(\vec{r},\vec{r}\,') = \;\; 2\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,\mathcal{V}^{q}_{\vec{k}}(\vec{r}\,q)\,\mathcal{V}^{q*}_{\vec{k}}(\vec{r}\,'\,q)\,, \tag{B.168a}$$

$$\tilde{\rho}_q(\vec{r},\vec{r}\,') = -\,2\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,\mathcal{U}^{q}_{\vec{k}}(\vec{r}\,q)\,\mathcal{V}^{q*}_{\vec{k}}(\vec{r}\,'\,q)\,, \tag{B.168b}$$

B.10.6 Gap equation

We are now interested in obtaining the (neutron-neutron or proton-proton) gap equation in INM from a pairing vertex vertex $v^{\kappa\kappa}$ which is restricted to the spin-singlet/isospin-triplet channel (see Sec. B.11). More specifically, one starts from the general gap equation given in coordinate space by Eq. (B.187) as

$$\Delta^q(\vec{r}_1\,\sigma_1,\vec{r}_2\,\sigma_2) = 2\sigma_2\,\delta_{\bar{\sigma}_1\sigma_2}\,\frac{1}{2}\int \mathrm{d}\vec{r}_3\,\mathrm{d}\vec{r}_4\,v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4)\,\tilde{\rho}^q(\vec{r}_3,\vec{r}_4)\,. \tag{B.169}$$

and add the fact that the interaction is Galilean invariant, i.e.

$$v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2,\vec{r}_3,\,\vec{r}_4) \equiv v^{\kappa\kappa}_r(\vec{r},\vec{r}\,')\,\delta(\vec{R}-\vec{r}\,')\,, \tag{B.170}$$

where

$$\vec{r} \equiv \vec{r}_1 - \vec{r}_2\,, \qquad \vec{R} \equiv \frac{\vec{r}_1+\vec{r}_2}{2}\,, \tag{B.171a}$$

$$\vec{r}\,' \equiv \vec{r}_3 - \vec{r}_4\,, \qquad \vec{R}\,' \equiv \frac{\vec{r}_3+\vec{r}_4}{2}\,. \tag{B.171b}$$

One starts without assessing a priori the states coupled by the pairing tensor[11]. Thus, one starts with two canonical states $\mu \equiv \vec{k}_\mu\,\sigma_\mu q_\mu$ and $\mu' \equiv \vec{k}_{\mu'}\,\sigma_{\mu'} q_{\mu'}$ such that $q_\mu = q_{\mu'} = q$. Using Eqs. (B.83,B.162b), one obtains

$$\begin{aligned}\Delta^q_{\mu\mu'} &= \int \mathrm{d}\vec{r}_3\,\mathrm{d}\vec{r}_4 \sum_{\sigma_1\sigma_2} \phi^*_\mu(\vec{r}_1\sigma_1 q)\,\phi^*_{\mu'}(\vec{r}_2\sigma_2 q)\,2\sigma_2\,\delta_{\sigma_2\bar{\sigma}_1}\,\frac{1}{2}\int \mathrm{d}\vec{r}'\,v^{\kappa\kappa}_r(\vec{r},\vec{r}')\,\tilde{\rho}^q(\vec{r}') \\ &= \int \mathrm{d}\vec{R}\,\mathrm{d}\vec{r}\,e^{-i\,\vec{R}\cdot(\vec{k}_\mu+\vec{k}_{\mu'})/2}\,e^{-i\,\vec{r}\cdot(\vec{k}_\mu-\vec{k}_{\mu'})/2}\,2\bar{\sigma}_\mu\,\delta_{\sigma_{\mu'}\bar{\sigma}_\mu}\,\frac{1}{2}\int \mathrm{d}\vec{r}'\,v^{\kappa\kappa}_r(\vec{r},\vec{r}')\,\tilde{\rho}^q(\vec{r}') \\ &= 2\bar{\sigma}_\mu\,\delta_{\sigma_{\mu'}\bar{\sigma}_\mu}\,\delta_{-\vec{k}_{\mu'}\vec{k}_\mu}\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,u^q_k\,v^q_k\int \mathrm{d}\vec{r}'\,e^{-i\,\vec{k}_\mu\cdot\vec{r}}\,v^{\kappa\kappa}_r(\vec{r},\vec{r}')\,e^{i\,\vec{k}\cdot\vec{r}'}\,, \end{aligned} \tag{B.172}$$

which actually proves that the gap field only has non-zero matrix elements between μ and $\mu' = \tilde{\mu}$ which are characterized by a total momentum zero $\vec{k}_\mu + \vec{k}_{\tilde{\mu}} = \vec{0}$. As a result, the gap field only depends on one momentum and is thus isotropic. In order to remove the irrelevant spin dependence of the pairing gap, one usually isolate the (positive) spatial part Δ^q_k of the pairing matrix elements through $\Delta^q_{\vec{k}\sigma\vec{k}'\sigma'} \equiv 2\sigma\,\Delta^q_k\,\delta_{(-\vec{k}')\vec{k}}\,\delta_{\sigma'\bar{\sigma}}$ with[12]

$$\Delta^q_k = -\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,v^{\kappa\kappa}_r(\vec{k},\vec{k}')\,u^q_k\,v^q_k\,, \tag{B.173}$$

where the center-of-mass part of two-body matrix elements of the effective pairing vertex has been introduced in moment space through

$$v^{\kappa\kappa}_r(\vec{k},\vec{k}') \equiv \int \mathrm{d}\vec{r}'\,e^{-i\,\vec{k}_\mu\cdot\vec{r}}\,v^{\kappa\kappa}_r(\vec{r},\vec{r}')\,e^{i\,\vec{k}\cdot\vec{r}'}\,. \tag{B.174}$$

A last point needs to be addressed in order to reach the final expression of the gap equation. As discussed in Sec. B.7.3, explicit BCS-like expressions of $(u^{q\,2}_\mu, v^{q\,2}_\mu)$ leaves the sign of v^q_μ undecided. Presently, we fix it by requiring that the gap Δ^q_k defined above is positive for an attractive interaction. This leads to the final expression of the BCS gap equation in INM

$$\Delta^q_k = -\int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,v^{\kappa\kappa}_r(\vec{k},\vec{k}')\,\frac{\Delta^q_{k'}}{\sqrt{(\epsilon^q_{k'}-\lambda^q)^2+\Delta^{q\,2}_{k'}}}\,, \tag{B.175}$$

where $\epsilon^q_{k'}$ is the (spin-independent) eigenvalue of h^q. Note that if the pairing vertex is reduced to the s-wave as it is often done due to the properties of the bare nucleon-nucleon interaction, the integration over the angles can be trivially done.

B.11 Application to the bilinear EDF

For the sake of illustration, one can consider a simple bilinear functional of the form

$$\mathcal{E}[\rho,\kappa,\kappa^*] = \sum_{ij}\sum_q t^q_{ij}\,\rho^q_{ji} + \frac{1}{2}\sum_{ijkl}\sum_{qq'}\bar{v}^{\rho\rho}_{ikjl}\,\rho^q_{ji}\,\rho^{q'}_{lk} + \frac{1}{4}\sum_{ijkl}\sum_q \bar{v}^{\kappa\kappa}_{ikjl}\,\kappa^{q\,*}_{ik}\,\kappa^q_{jl}\,, \tag{B.176}$$

where t^q_{ij} denote the matrix element of the one-body kinetic operator whereas $\bar{v}^{\rho\rho}_{ikjl}$ and $\bar{v}^{\kappa\kappa}_{ikjl}$ represent (potentially) (right-)antisymmetrized and non-normalized matrix elements. With

[11] In full HFB, the matrix Δ^q is indeed full in the canonical basis even though the pairing tensor is canonical.
[12] The pairing gap relates to the negative pair field through $\Delta^q_k = -\tilde{h}^q_k$.

a simple bilinear EDF, $\bar{v}^{\rho\rho}_{ikjl}$ and $\bar{v}^{\kappa\kappa}_{ikjl}$ represent potentially (right-)antisymmetrized and non-normalized matrix elements[13] of two-body effective vertices in particle-hole and particle-particle channels, defined as

$$\bar{v}^{\rho\rho/\kappa\kappa}_{ikjl} = \langle 1:i,\, 2:j|v^{\rho\rho/\kappa\kappa}(1 - P_\sigma\, P_\sigma\, P_{\vec{r}})|1:k,\, 2:l\rangle = \langle 1:i,\, 2:j|v^{\rho\rho/\kappa\kappa} \parallel j\, l \gg \,. \tag{B.177}$$

Using symmetries of non-antisymmetrized matrix elements of the effective vertices under the exchange of two indistinguishable fermions, one can write for isospin q

$$\begin{aligned}
\langle i\, j|v^{\rho\rho/\kappa\kappa}|k\, l\rangle &= \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \langle i\, j|1:\vec{r}_1\sigma_1 q,\, 2:\vec{r}_2\sigma_2 q\rangle \\
&\qquad \times \langle 1:\vec{r}_1\sigma_1 q,\, 2:\vec{r}_2\sigma_2 q|v^{\rho\rho/\kappa\kappa}|1:\vec{r}_3\sigma_3 q,\, 2:\vec{r}_4\sigma_4 q\rangle\, \langle 1:\vec{r}_3\sigma_3 q,\, 2:\vec{r}_4\sigma_4 q|k\, l\rangle \\
&= \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_k(\vec{r}_3\,\sigma_3\,q)\, \varphi_l(\vec{r}_4\,\sigma_4\,q) \\
&\quad - \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_l(\vec{r}_3\,\sigma_3\,q)\, \varphi_k(\vec{r}_4\,\sigma_4\,q) \\
&= \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_k(\vec{r}_3\,\sigma_3\,q)\, \varphi_l(\vec{r}_4\,\sigma_4\,q) \\
&\quad - \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_4\sigma_4 q, \vec{r}_3\sigma_3 q)\, \varphi_l(\vec{r}_4\,\sigma_4\,q)\, \varphi_k(\vec{r}_3\,\sigma_3\,q) \\
&= \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_k(\vec{r}_3\,\sigma_3\,q)\, \varphi_l(\vec{r}_4\,\sigma_4\,q) \\
&\quad - \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_2\sigma_2 q, \vec{r}_1\sigma_1 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_l(\vec{r}_3\,\sigma_3\,q)\, \varphi_k(\vec{r}_4\,\sigma_4\,q) \\
&= \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_k(\vec{r}_3\,\sigma_3\,q)\, \varphi_l(\vec{r}_4\,\sigma_4\,q) \\
&\quad - \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\,\varphi_j^*(\vec{r}_1\,\sigma_1\,q) - \varphi_j^*(\vec{r}_2\,\sigma_2\,q)\,\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_l(\vec{r}_3\,\sigma_3\,q)\, \varphi_k(\vec{r}_4\,\sigma_4\,q) \\
&= 2 \times \frac{1}{2} \int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}} \left[\varphi_i^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_j^*(\vec{r}_2\,\sigma_2\,q) - \varphi_j^*(\vec{r}_1\,\sigma_1\,q)\,\varphi_i^*(\vec{r}_2\,\sigma_2\,q)\right] \\
&\qquad \times v^{\rho\rho/\kappa\kappa}(\vec{r}_1\sigma_1 q, \vec{r}_2\sigma_2 q; \vec{r}_3\sigma_3 q, \vec{r}_4\sigma_4 q)\, \varphi_k(\vec{r}_3\,\sigma_3\,q)\, \varphi_l(\vec{r}_4\,\sigma_4\,q) \\
&= \sqrt{2}\, \langle i\, j|v^{\rho\rho/\kappa\kappa}|1:k,\, 2:l\rangle \\
&= \sqrt{2}\, \langle 1:i,\, 2:j|v^{\rho\rho/\kappa\kappa}|k\, l\rangle \,.
\end{aligned} \tag{B.178}$$

[13] the exchange operator $(1 - P_\sigma\, P_\sigma\, P_{\vec{r}})$ is not normalized.

The latter result leads to

$$|i\,j\rangle = \frac{1 - P_\sigma\,P_\sigma\,P_{\vec{r}}}{\sqrt{2}}\,|1:i,\,2:j\rangle\,, \qquad \bar{v}^{\rho\rho/\kappa\kappa}_{ijkl} = \langle 1:i,\,2:j|v^{\rho\rho/\kappa\kappa} \parallel k\,l \gg = \langle i\,j|v^{\rho\rho/\kappa\kappa}|k\,l\rangle\,. \tag{B.179}$$

The particle-particle effective nucleon-nucleon vertex $v^{\kappa\kappa}$ is usually restricted to the spin-singlet/isospin-triplet channel (possibly further restricted to the s-wave, i.e. to the $^1\mathrm{S}_0$ partial wave). In this case

$$v^{\kappa\kappa} \equiv v^{\kappa\kappa}_r \prod_{S=0} \prod_{T=1} = v^{\kappa\kappa}_r \left[\frac{1-P_\sigma}{2}\right] \left[\frac{1+P_\tau}{2}\right]\,, \tag{B.180}$$

where $v^{\kappa\kappa}_r$ denotes the spatial part of the vertex.

Antisymmetrized and non-normalized matrix elements of such an interaction in coordinate, spin and isospin space read for particles with identical isospins as

$$\begin{aligned}
\bar{v}^{\kappa\kappa}_{1234} =& \langle 1:\vec{r}_1\sigma_1 q,\,2:\vec{r}_2\sigma_2 q|v^{\kappa\kappa} \parallel \vec{r}_3\sigma_3 q,\,\vec{r}_4\sigma_4 q \gg \\
=& \langle 1:\vec{r}_1\sigma_1 q,\,2:\vec{r}_2\sigma_2 q|v^{\kappa\kappa}\,(1 - P_{\vec{r}}\,P_\sigma\,P_\tau)\,|1:\vec{r}_3\sigma_3 q,\,2:\vec{r}_4\sigma_4 q\rangle \\
=& \langle 1:\vec{r}_1,\,2:\vec{r}_2|v^{\kappa\kappa}_r|1:\vec{r}_3,\,2:\vec{r}_4\rangle\,\langle 1:\sigma_1,\,2:\sigma_2|1 - P_\sigma|1:\sigma_3,\,2:\sigma_4\rangle \\
\equiv& v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4)\left(\delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4} - \delta_{\sigma_1\sigma_4}\,\delta_{\sigma_3\sigma_2}\right) \\
=& v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4)\,2\sigma_2\,2\sigma_4\,\delta_{\sigma_1\bar{\sigma}_2}\,\delta_{\sigma_3\bar{\sigma}_4}\,,
\end{aligned} \tag{B.181}$$

since fermion selection rules imply that $P_\tau = P_{\vec{r}} = 1$, and

$$\prod_{S=0}(1 - P_\sigma) = \frac{1-P_\sigma}{2}\,(1-P_\sigma) = \frac{2 - 2\,P_\sigma}{2} = 1 - P_\sigma\,. \tag{B.182}$$

In this case, one finds[14]

$$h^q_{ij} = t^q_{ij} + \frac{1}{2}\sum_{klq'}\left(\bar{v}^{\rho\rho}_{ikjl} + \bar{v}^{\rho\rho}_{kilj}\right)\,\rho^{q'}_{lk}\,, \tag{B.183a}$$

$$\Delta^q_{ij} = \frac{1}{2}\sum_{kl}\bar{v}^{\kappa\kappa}_{ijkl}\,\kappa^q_{kl}\,, \tag{B.183b}$$

where the anti-symmetry of $\bar{v}^{\rho\rho}$ has not been used explicitly. Equivalently in coordinate space

$$\begin{aligned}
h^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') =& \frac{\delta\mathcal{E}}{\delta\rho^q(\vec{r}\,'\sigma'\,q,\vec{r}\,\sigma\,q)} \\
=& t^q(\vec{r},\vec{r}\,')\,\delta_{\sigma\sigma'} + \int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\sum_{\sigma_1\sigma_2}\bar{v}^{\rho\rho}(\vec{r}\sigma q,\vec{r}_1\sigma_1 q;\vec{r}\,'\sigma' q,\vec{r}_2\sigma_2 q)\,\rho(\vec{r}_2\,\sigma_2\,q,\vec{r}_1\,\sigma_1\,q)\,,
\end{aligned} \tag{B.184}$$

[14] In order to derive the fields, one needs to split the sums in Eq. (B.176) in terms of contractions with $j \leq i$ only.

For the gap field, we start from its matrix elements in an arbitrary basis and use the restriction $v^{\kappa\kappa}$ of the pairing vertex to the spin-singlet/isospin-triplet channel

$$\begin{aligned}
\Delta^q_{ij} =& \frac{1}{2}\sum_{kl}\langle 1:i,\, 2:j|\bullet v^{\kappa\kappa}\bullet \parallel k,\, l \gg \kappa^q_{kl} \\
=& \frac{1}{2}\int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_{1234}}\sum_{kl} \langle 1:i,\, 2:j\,|1:\vec{r}_1\sigma_1,\, 2:\vec{r}_2\sigma_2\,\rangle \\
& \times \langle 1:\vec{r}_1\sigma_1 q,\, 2:\vec{r}_2\sigma_2 q|v^{\kappa\kappa} \parallel \vec{r}_3\sigma_3 q,\, \vec{r}_4\sigma_4 q \gg \langle 1:\vec{r}_3\,\sigma_3,\, 2:\vec{r}_4\,\sigma_4\,|1:k,\, 2:l\,\rangle\,\kappa^q_{kl} \\
=& \frac{1}{2}\int \mathrm{d}\vec{r}_{1234} \sum_{\sigma_1\sigma_3}\sum_{kl} \varphi^*_i(\vec{r}_1\,\sigma_1\,q)\,\varphi^*_j(\vec{r}_2\,\bar{\sigma}_1\,q) \\
& \times v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4)\,2\sigma_1\,2\sigma_3\,\varphi_k(\vec{r}_3\,\sigma_3\,q)\,\varphi_l(\vec{r}_4\,\bar{\sigma}_3\,q)\,\kappa^q_{kl} \\
=& \frac{1}{2}\int \mathrm{d}\vec{r}_{1234} \left[\sum_{\sigma_1} 2\sigma_1\,\varphi^*_i(\vec{r}_1\,\sigma_1\,q)\,\varphi^*_j(\vec{r}_2\,\bar{\sigma}_1\,q)\right] v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4) \\
& \times \left[\sum_{\sigma_3} 2\sigma_3 \sum_{kl}\varphi_k(\vec{r}_3\,\sigma_3\,q)\,\varphi_l(\vec{r}_4\,\bar{\sigma}_3\,q)\,\kappa^q_{kl}\right] \\
=& -\frac{1}{2}\int \mathrm{d}\vec{r}_{1234}\,\Psi^{q\,*}_{ij}(\vec{r}_1,\vec{r}_2)\; v^{\kappa\kappa}_r(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4)\,\tilde{\rho}^q(\vec{r}_3,\vec{r}_4)\,, \qquad \text{(B.185)}
\end{aligned}$$

where the singlet part of the two-body wave function has been used

$$\Psi^q_{ij}(\vec{r}_1,\vec{r}_2) \equiv \sum_{\sigma} 2\sigma\,\varphi_i(\vec{r}_1\,\sigma\,q)\,\varphi_j(\vec{r}_2\,\bar{\sigma}\,q)\,. \qquad \text{(B.186)}$$

The previous result combined with Eq. (B.81) allows to identify the matrix elements of the gap field in coordinate space as

$$\Delta^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') \equiv \frac{\delta\mathcal{E}}{\delta\kappa^{q\,*}(\vec{r}\,\sigma\,q,\vec{r}\,'\sigma'\,q)} = 2\sigma'\,\delta_{\sigma\bar{\sigma}'}\,\frac{1}{2}\int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,v^{\kappa\kappa}_r(\vec{r},\vec{r}\,';\vec{r}_1,\vec{r}_2)\,\tilde{\rho}^q(\vec{r}_1,\vec{r}_2)\,. \qquad \text{(B.187)}$$

On the other hand, the pair field reads in coordinate space as

$$\begin{aligned}
\tilde{h}^q(\vec{r}\,\sigma,\vec{r}\,'\sigma') =& \frac{\delta\mathcal{E}}{\delta\tilde{\rho}(\vec{r}\,'\,\sigma'\,q,\vec{r}\,\sigma\,q)} \\
=& \int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2 \sum_{\sigma_1\sigma_2} 2\sigma_1\sigma_2\,\bar{v}^{\kappa\kappa}(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}'q;\vec{r}_1\sigma_1 q,\vec{r}_2\bar{\sigma}_2 q)\,\tilde{\rho}(\vec{r}_1\,\sigma_1\,q,\vec{r}_2\,\sigma_2\,q) \\
=& \frac{1}{2}\int \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\delta_{\sigma\sigma'}\,v^{\kappa\kappa}_r(\vec{r},\vec{r}\,';\vec{r}_1,\vec{r}_2)\,\tilde{\rho}^q(\vec{r}_1,\vec{r}_2)\,. \qquad \text{(B.188)}
\end{aligned}$$

Appendix C

Many-body wave function and one-body density

Abstract: The present chapter contains detailed notes concerning properties of the many-body wave function and its possible decomposition in terms of single-particle states, in the case of self-bound systems and quantum systems bound by a central potential. Internal overlap functions are properly introduced in both cases, as they lead to the definition of the internal one-body density. The latter is the object of interest for self-bound EDF systems.

Contents

C.1 Spectroscopic amplitudes without center-of-mass correlations

At first center-of-mass degrees of freedom are neglected, leading to a fixed-center framework.

C.1.1 Basis sets for the N-body problem

If spin and isospin degrees of freedom are suppressed[1], and the Coulomb potential is neglected, the exact non-relativistic Hamiltonian for a N-body system reads

$$\hat{\mathcal{H}}^N(\vec{r}_1 \dots \vec{r}_N) = \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^{\,2}}{2m} + \sum_{\substack{i,j=1 \\ i<j}}^{N} \hat{v}_s(r_{ij})\,, \tag{C.1}$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j\,|$ and v_s is the bare nucleon-nucleon interaction. Without treating the center-of-mass motion, one can consider the equivalent Hamiltonian for the $(N-1)$-body system, i.e.

$$\hat{\mathcal{H}}^{N-1}(\vec{r}_1 \dots \vec{r}_N) = \sum_{i=1}^{N-1} \frac{\hat{\vec{p}}_i^{\,2}}{2m} + \sum_{\substack{i,j=1 \\ i<j}}^{N-1} \hat{v}_s(r_{ij})\,, \tag{C.2}$$

Fully antisymmetrized eigenstates of $\hat{\mathcal{H}}^{N-1}$ are noted $\Psi_i^{N-1}(\vec{r}_1 \dots \vec{r}_{N-1})$ and are associated to the energy E_i^{N-1}, E_0^{N-1} being the ground-state energy. Including bound and continuum states, $\{\Psi_i^{N-1}\}$ forms a complete set in the space $\mathcal{E}_{\mathcal{A}}^{N-1}$ of antisymmetric $(N-1)$-body wave functions. Orthonormalization of this set reads

$$\int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_{N-1}\, \Psi_i^{N-1*}(\vec{r}_1 \dots \vec{r}_{N-1})\, \Psi_j^{N-1}(\vec{r}_1 \dots \vec{r}_{N-1}) = \delta_{ij}\,, \tag{C.3}$$

and its completeness in the space of antisymmetric $(N-1)$-body wave functions, for any $\psi^{N-1} \in \mathcal{E}_{\mathcal{A}}^{N-1}$, is expressed as

$$\sum\!\!\!\!\!\!\int_i \int \mathrm{d}\vec{r}'_1 \dots \mathrm{d}\vec{r}'_{N-1}\, \Psi_i^{N-1}(\vec{r}_1 \dots \vec{r}_{N-1})\, \Psi_i^{N-1*}(\vec{r}'_1 \dots \vec{r}'_{N-1}) \times \psi^{N-1}(\vec{r}'_1 \dots \vec{r}'_{N-1}) = \psi^{N-1}(\vec{r}_1 \dots \vec{r}_{N-1})\,, \tag{C.4}$$

[1] All spin and isospin dependences of the N-body wave function will be dropped here, and $\mathcal{H}^N(\vec{r}_1 \dots \vec{r}_N) \equiv \mathcal{H}^N(\vec{r}_1\sigma_1 q_1 \dots \vec{r}_N\sigma_N q_N)$.

where $\sum\!\!\!\!\!\!\int_i$ stands for a discrete sum over bound states and an integral over continuum states. The set $\{\Psi_i^{N-1}\}$ can be used as a basis for the space $\mathcal{E}_{\mathcal{A}}^N$ of N-body antisymmetrized wave functions by defining[2] [10]

$$ {}_{\mathcal{A}}\Psi_{i,\vec{r}}^N(\vec{r}_1 \dots \vec{r}_N) = \mathcal{A}_{1..N}\, \Psi_{i,\vec{r}}^N(\vec{r}_1 \dots \vec{r}_N)\,, \tag{C.5} $$

where

$$ \Psi_{i,\vec{r}}^N(\vec{r}_1 \dots \vec{r}_N) = \Psi_i^{N-1}(\vec{r}_1 \dots \vec{r}_{N-1})\, \delta(\vec{r} - \vec{r}_N)\,, \tag{C.6} $$

and $\mathcal{A}_{1..N}$ antisymmetrizes between the N coordinates $\vec{r}_i$ appearing in Eq. (C.5), i.e.

$$ \mathcal{A}_{1..N}\, \Psi_{i,\vec{r}}^N(\vec{r}_1 \dots \vec{r}_N) = \frac{\sqrt{N}}{N!} \int \mathrm{d}\vec{r}'_1 \dots \mathrm{d}\vec{r}'_N \quad \det_{i,j=1..N} \left[\delta(\vec{r}_i - \vec{r}'_j)\, \Psi_{i,\vec{r}}^N(\vec{r}'_1 \dots \vec{r}'_N)\right]\,. \tag{C.7} $$

This "intercluster" antisymmetrization operator is normalized so as to satisfy

$$ \mathcal{A}_{1..N}^2 = \sqrt{N}\mathcal{A}_{1..N}\,. \tag{C.8} $$

C.1.1.1 Properties of the set $\{\Psi_{i,\vec{r}}^N\}$

Wave functions $\{\Psi_{i,\vec{r}}^N\}$ span a space $\mathcal{E}^N$ which is a direct sum of the space $\mathcal{E}_{\mathcal{A}}^N$ containing totally antisymmetric N-body states, and $\mathcal{E}_{\mathcal{M}}^N$ containing mixed-symmetric N-body states. The latter are antisymmetric in their first $N-1$ coordinates and symmetric with any exchange involving the N^{th} coordinate[3]. Any wave function ψ^N in $\mathcal{E}^N$ can be written as the sum of an antisymmetric and a mixed-symmetric component, i.e.

$$ \psi^N(\vec{r}_1 \dots \vec{r}_N) \equiv \psi_{\mathcal{A}}^N(\vec{r}_1 \dots \vec{r}_N) + \psi_{\mathcal{M}}^N(\vec{r}_1 \dots \vec{r}_N) \tag{C.9a} $$

$$ \equiv \frac{\mathcal{A}_{1..N}}{\sqrt{N}}\psi^N(\vec{r}_1 \dots \vec{r}_N) + \left(1 - \frac{\mathcal{A}_{1..N}}{\sqrt{N}}\right)\psi^N(\vec{r}_1 \dots \vec{r}_N)\,. \tag{C.9b} $$

Since $\left(1 - \frac{\mathcal{A}_{1..N}}{\sqrt{N}}\right)\left(\frac{\mathcal{A}_{1..N}}{\sqrt{N}}\right) = 0$, the two subspaces $\mathcal{E}_{\mathcal{M}}^N$ and $\mathcal{E}_{\mathcal{A}}^N$ are orthogonal to each other, i.e.

$$ \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N\, \Psi_{\mathcal{A}}^{N*}(\vec{r}_1 \dots \vec{r}_N)\, \Psi_{\mathcal{M}}^N(\vec{r}_1 \dots \vec{r}_N) = 0\,. \tag{C.10} $$

Furthermore, a symmetric operator $\hat{\mathcal{O}}_{\mathcal{S}}$ cannot connect those subspaces, that is

$$ \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N\, \Psi_{\mathcal{A}}^{N*}(\vec{r}_1 \dots \vec{r}_N)\, \hat{\mathcal{O}}_{\mathcal{S}}\, \Psi_{\mathcal{M}}^N(\vec{r}_1 \dots \vec{r}_N) = 0\,. \tag{C.11} $$

This is in particular the case for the Hamiltonian of the N-body system $\hat{\mathcal{O}}_{\mathcal{S}} = \hat{\mathcal{H}}^N$. This may have important consequences, as it will be shown later on.

The set $\{\Psi_{i,\vec{r}}^N\}$ is orthonormal with respect to both i and $\vec{r}$, using Eq. (C.3)

$$ \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N\, \Psi_{i,\vec{r}}^{N\,*}(\vec{r}_1 \dots \vec{r}_N)\, \Psi_{j,\vec{r}'}^N(\vec{r}_1 \dots \vec{r}_N) = \delta_{ij}\delta(\vec{r} - \vec{r}')\,, \tag{C.12} $$

and completeness reads for any state $\psi^N \in \mathcal{E}^N$ as

$$ \int \mathrm{d}\vec{r}'_1 \dots \mathrm{d}\vec{r}'_N \left(\sum\!\!\!\!\!\!\int_i \int \mathrm{d}\vec{r}\; \Psi_{i,\vec{r}}^N(\vec{r}_1 \dots \vec{r}_N)\, \Psi_{i,\vec{r}}^{N\,*}(\vec{r}'_1 \dots \vec{r}'_N)\right)\psi^N(\vec{r}'_1 \dots \vec{r}'_N) = \psi^N(\vec{r}_1 \dots \vec{r}_N)\,. \tag{C.13} $$

[2] This is equivalent to $|{}_{\mathcal{A}}\Psi_{i,\vec{r}}^N\rangle = \hat{a}_{\vec{r}}^\dagger|\Psi_i^{N-1}\rangle$, where $\hat{a}_{\vec{r}}^\dagger$ creates a nucleon at position $\vec{r}$.

[3] For $N = 2$, $\mathcal{E}_{\mathcal{M}}^N$ is empty.

C.1.1.2 Properties of the set $\{{}_{\mathcal{A}}\Psi^N_{i,\vec{r}}\}$

The set $\{{}_{\mathcal{A}}\Psi^N_{i,\vec{r}}\}$ spans the space of antisymmetrized N-body wave functions $\mathcal{E}^N_{\mathcal{A}}$. However, these states are no longer orthonormal, since

$$\int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N \, {}_{\mathcal{A}}\Psi^{N\,*}_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N) \, {}_{\mathcal{A}}\Psi^N_{j,\vec{r}'}(\vec{r}_1 \dots \vec{r}_N) \equiv \mathcal{N}(i\vec{r}, j\vec{r}') \,, \tag{C.14}$$

where $\mathcal{N}(i\vec{r}, j\vec{r}')$ is the kernel of the norm operator $\hat{\mathcal{N}}$[4]. Basis states ${}_{\mathcal{A}}\Psi^N_{i,\vec{r}}$ are not linearly independent, and related through the norm operator

$${}_{\mathcal{A}}\Psi^N_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N) = \frac{1}{N} \sum\!\!\!\!\!\!\int_j \mathrm{d}\vec{r}' \, \mathcal{N}(i\vec{r}, j\vec{r}') \, {}_{\mathcal{A}}\Psi^N_{j,\vec{r}'}(\vec{r}_1 \dots \vec{r}_N) \,. \tag{C.17}$$

The basis $\{{}_{\mathcal{A}}\Psi^N_{i,\vec{r}}\}$ is thus overcomplete and spans $\mathcal{E}^N_{\mathcal{A}}$ exactly N times[5], which explains the $\frac{1}{N}$ factor in Eq. (C.17). Completeness conditions for the set $\{{}_{\mathcal{A}}\Psi^N_{i,\vec{r}}\}$ become

- for $\psi^N \in \mathcal{E}^N_{\mathcal{A}}$

$$\int \mathrm{d}\vec{r}'_1 \dots \mathrm{d}\vec{r}'_N \left(\frac{1}{N} \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r} \, {}_{\mathcal{A}}\Psi^N_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N) \, {}_{\mathcal{A}}\Psi^{N\,*}_{i,\vec{r}}(\vec{r}'_1 \dots \vec{r}'_N) \right) \psi^N(\vec{r}'_1 \dots \vec{r}'_N) = \psi^N(\vec{r}_1 \dots \vec{r}_N) \,, \tag{C.18}$$

- for $\psi^N \in \mathcal{E}^N_{\mathcal{M}}$

$$\int \mathrm{d}\vec{r}'_1 \dots \mathrm{d}\vec{r}'_N \left(\frac{1}{N} \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r} \, {}_{\mathcal{A}}\Psi^N_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N) \, {}_{\mathcal{A}}\Psi^{N\,*}_{i,\vec{r}}(\vec{r}'_1 \dots \vec{r}'_N) \right) \psi^N(\vec{r}'_1 \dots \vec{r}'_N) = 0 \,. \tag{C.19}$$

This shows that the operator

$$\hat{\mathcal{P}}_{\mathcal{A}} = \frac{1}{N} \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r} \, |{}_{\mathcal{A}}\Psi^N_{i,\vec{r}}\rangle\langle {}_{\mathcal{A}}\Psi^N_{i,\vec{r}}| \,, \tag{C.20}$$

is a projection operator which projects any function in $\mathcal{E}^N$ onto its fully antisymmetrized component[6].

C.1.2 Decomposition of the N-body wave function

Using the basis sets previously defined, any antisymmetric wave function ψ^N_ν can be expanded in several ways. First, using the basis set $\{\Psi^N_{i,\vec{r}}\}$

$$\psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) = \frac{1}{\sqrt{N}} \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r} \, \Psi^N_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N) \, \varphi^N_{\nu i}(\vec{r}) \,. \tag{C.21}$$

[4] This is the equivalent of a generating function for a series

$$G(a_n, x) = \sum_{n=0}^{+\infty} a_n \, x^n \,, \tag{C.15}$$

or the integrand $k(x, x')$ that defines an integral transform through

$$(Tf)(x) = \int_{\mathsf{X}} \mathrm{d}x' \, k(x, x') \, f(x') \,. \tag{C.16}$$

The latter applies in the case when T is an operator.

[5] This is easily seen when the initial basis $\{\Psi^N_{i,\vec{r}}\}$ is composed of Slater determinants.

[6] $\hat{\mathcal{P}}^2_{\mathcal{A}} = \hat{\mathcal{P}}_{\mathcal{A}}$ is proven using Eq. (C.17).

Applying the antisymmetrization operator $\mathcal{A}_{1..N}$ to each side of Eq. (C.21) allows to decompose ψ^N_ν in terms of the basis set $\{{}_{\mathcal{A}}\Psi^N_{i,\vec{r}}\}$, that is

$$\psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) = \frac{1}{N} \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r}\, {}_{\mathcal{A}}\Psi^N_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N)\, \varphi^N_{\nu i}(\vec{r})\,, \tag{C.22}$$

where the following identity is used:

$$\frac{\mathcal{A}_{1..N}}{\sqrt{N}} \psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) = \psi^N_\nu(\vec{r}_1 \dots \vec{r}_N)\,, \tag{C.23}$$

as ψ^N is fully antisymmetric. Finally, the bare definition of $\Psi^N_{i,\vec{r}}$ (Eq. (C.6)) put into the same equation (Eq. (C.21)) provides with a decomposition in term of the basis set $\{\Psi^{N-1}_i\}$ that reads

$$\psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) = \frac{1}{\sqrt{N}} \sum\!\!\!\!\!\!\int_i \Psi^{N-1}_i(\vec{r}_1 \dots \vec{r}_{N-1})\, \varphi^N_{\nu i}(\vec{r}_N)\,. \tag{C.24}$$

In those three equations, the expansion coefficients $\varphi^N_{\nu i}$, also called **overlap functions**, are identical and expressed in different ways, i.e.

$$\varphi^N_{\nu i}(\vec{r}) = \sqrt{N} \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N\, \Psi^{N\,*}_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N)\, \psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) \qquad = \sqrt{N} \langle \Psi^N_{i,\vec{r}} | \psi^N_\nu \rangle\,, \tag{C.25a}$$

$$= \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N\, {}_{\mathcal{A}}\Psi^{N\,*}_{i,\vec{r}}(\vec{r}_1 \dots \vec{r}_N)\, \psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) \qquad = \langle {}_{\mathcal{A}}\Psi^N_{i,\vec{r}} | \psi^N_\nu \rangle\,, \tag{C.25b}$$

$$= \sqrt{N} \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_{N-1} \Psi^{N-1\,*}_i(\vec{r}_1 \dots \vec{r}_{N-1}) \psi^N_\nu(\vec{r}_1 \dots \vec{r}_{N-1}, \vec{r}) \qquad = \langle \Psi^{N-1}_i | \hat{a}_{\vec{r}} | \psi^N_\nu \rangle\,, \tag{C.25c}$$

from Eq. (C.21), Eq. (C.23), and Eq. (C.24), respectively. The expansion is explicitly antisymmetric in Eq. (C.22), while in Eqs. (C.21,C.24) the antisymmetry is carried by the expansion coefficients. In those cases only the whole sum $\sum\!\!\!\!\!\!\int_i$ is antisymmetric, whereas each individual term is not.

C.1.3 Spectroscopic quantities

C.1.3.1 Spectroscopic factors

When ψ^N_ν is a bound eigenstate Ψ^N_ν of the N-body Hamiltonian, the expansion coefficients $\varphi^N_{\nu i}(\vec{r})$ are called spectroscopic amplitudes, and their norms

$$S_{\nu i} = \int \mathrm{d}\vec{r} |\varphi^N_{\nu i}(\vec{r})|^2\,, \tag{C.26}$$

are called **spectroscopic factors**. Squaring Eq. (C.21), integrating over the coordinates and using Eq. (C.13) gives the spectroscopic factor sum rule [11]

$$\sum_i \int \mathrm{d}\vec{r} |\varphi^N_{\nu i}(\vec{r})|^2 = N\,. \tag{C.27}$$

As a property, spectroscopic amplitudes completely determine the wave function Ψ^N_ν. Their spatial dependence is related to properties of single-particle states of the N-body system, and their norm provides a measure of the structural similarity between the n^{th} excited $(N-1)$-body state and a cluster of $N-1$ particles taken from the N-body initial state.

C.1.3.2 Upper bound for spectroscopic factors

One defines normalized spectroscopic amplitudes as

$$\overline{\varphi}^N_{\nu i}(\vec{r}) = \frac{1}{\sqrt{S_{\nu i}}}\varphi^N_{\nu i}(\vec{r})\,, \tag{C.28}$$

where

$$\sqrt{S_{\nu i}} = \int \mathrm{d}\vec{r}\,\overline{\varphi}^{N*}_{\nu i}(\vec{r})\varphi^N_{\nu i}(\vec{r}) = \langle \mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]|\Psi^N_\nu\rangle\,. \tag{C.29}$$

One can then introduce the projector

$$\hat{P}_{\nu i} = \frac{|\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]\rangle\langle\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]|}{\langle\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]|\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]\rangle} \equiv \frac{|\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]\rangle\langle\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]|}{N_{\nu i}}\,. \tag{C.30}$$

Any antisymmetric state $|\Psi^N_\nu\rangle$ can then be decomposed using $\hat{P}_{\nu i}$ into components parallel and orthogonal to $|\mathcal{A}_{1..N}\,[\overline{\varphi}^N_{\nu i}\,\Psi^{N-1}_i]\rangle$, and reads

$$|\Psi^N_\nu\rangle = \hat{P}_{\nu i}|\Psi^N_\nu\rangle + (1-\hat{P}_{\nu i})|\Psi^N_\nu\rangle \equiv |\Psi^N_{\nu i,\|}\rangle + |\Psi^N_{\nu i,\perp}\rangle\,. \tag{C.31}$$

Thus one has for the spectroscopic factor

$$S_{\nu i} = N_{\nu i}\langle\Psi^N_{\nu i,\|}|\Psi^N_{\nu i,\|}\rangle = N_{\nu i}\left(\langle\Psi^N_\nu|\Psi^N_\nu\rangle - \langle\Psi^N_{\nu i,\perp}|\Psi^N_{\nu i,\perp}\rangle\right)\,. \tag{C.32}$$

The factor $N_{\nu i}$ is expressed as

$$N_{\nu i} = 1 - \sum\!\!\!\!\!\!\int_j \left(\int \mathrm{d}\vec{r}\,\varphi^{N-1*}_{ji}(\vec{r})\,\overline{\varphi}^N_{\nu i}(\vec{r})\right)^2\,. \tag{C.33}$$

Thus $N_{\nu i} \leq 1$ carries the effect of antisymmetrization. It is equal to one only if $\varphi^N_{\nu i}(\vec{r})$ is orthogonal to all $\varphi^{N-1}_{ji}(\vec{r})$. It is also the upper bound for the spectroscopic factor $S_{\nu i}$, as both $\langle\Psi^N_{\nu i,\|}|\Psi^N_{\nu i,\|}\rangle$ and $\langle\Psi^N_{\nu i,\perp}|\Psi^N_{\nu i,\perp}\rangle$ in Eq. (C.32) are positive definite and $|\Psi^N_\nu\rangle$ is normalized. When the $(N-1)$-body system is completely described by the wave function $|\Psi^{N-1}_i\rangle$[7], i.e. when there are no distortions due to the potential of the N^{th} nucleon, $\langle\Psi^N_{\nu i,\perp}|\Psi^N_{\nu i,\perp}\rangle$ vanishes. Thus $\langle\Psi^N_{\nu i,\|}|\Psi^N_{\nu i,\|}\rangle$ provides with a measure of the dynamic distortions induced by the presence of the extra particle.

C.1.3.3 Reaction rates

The spectroscopic amplitudes can be used to calculate reaction rates. Let us consider a simplified case of neutron capture, where both the N-body final bound state $|\Psi^N_i\rangle$ and the wave function in the incident channel $|\vec{\Psi}^N_j\rangle$ ($(N-1)$-body system + incoming nucleon) are expanded for an arbitrary n in terms of overlap functions under the form

$$\varphi^N_{in}(\vec{r}) = \sqrt{N}\langle\Psi^N_{n,\vec{r}}|\Psi^N_i\rangle\,, \qquad \vec{\varphi}^N_{jn}(\vec{r}) = \sqrt{N}\langle\Psi^N_{n,\vec{r}}|\vec{\Psi}^N_j\rangle\,. \tag{C.34}$$

In particular in the entrance channel, the expansion coefficient $\vec{\varphi}^N_{0n}$ is a continuum wave function (the entrance channel is unbound). Matrix elements of the one-body transition operator $\hat{\mathcal{O}}(\vec{r})$

[7] That is, using $\langle\Psi^N_{\nu i,\|}|\Psi^N_{\nu i,\|}\rangle = 1$, this means that the N-body system is exactly the antisymmetrized superposition of the $(N-1)$-body state and the overlap function.

read then

$$\begin{aligned}\mathcal{M}_{ij} =&\langle\Psi_i^N|\hat{\mathcal{O}}(\vec{r})|\vec{\Psi}_j^N\rangle\\ =&\sum\!\!\!\!\!\!\int_n \mathrm{d}\vec{r}\,\varphi_{in}^{N\,*}(\vec{r})\,\hat{\mathcal{O}}(\vec{r})\,\vec{\varphi}_{jn}^{N}(\vec{r})\\ =&\sum\!\!\!\!\!\!\int_n \sqrt{S_{in}}\int \mathrm{d}\vec{r}\,\overline{\varphi}_{in}^{N\,*}(\vec{r})\,\hat{\mathcal{O}}(\vec{r}_N)\,\vec{\varphi}_{jn}^{N}(\vec{r})\,.\end{aligned} \tag{C.35}$$

Capture reactions being peripherical, the process takes mostly place at large distance from the center of the target nucleus, which remains in its ground state. Thus only the first term in the expansion of the entrance channel $|\vec{\Psi}_j^N\rangle$ significantly contributes to the total matrix element. The total cross-section is then proportional to $|\mathcal{M}_{i0}|$, thus linearly dependent on the spectroscopic factor associated with the ground state of the $(N-1)$-body system S_{i0}.

C.1.4 Properties of the norm kernel $\mathcal{N}(i\vec{r}, j\vec{r}')$

Following the initial definition of the kernel $\mathcal{N}(i\vec{r}, j\vec{r}')$ of the norm operator $\hat{\mathcal{N}}$ (Eq. (C.14)), one has

$$\mathcal{N}(i\vec{r}, j\vec{r}') = \int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\;{}_{\mathcal{A}}\Psi_{i,\vec{r}}^{N\,*}(\vec{r}_1\ldots\vec{r}_N)\;{}_{\mathcal{A}}\Psi_{j,\vec{r}'}^{N}(\vec{r}_1\ldots\vec{r}_N) \tag{C.36a}$$

$$=\sqrt{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\;\Psi_{i,\vec{r}}^{N\,*}(\vec{r}_1\ldots\vec{r}_N)\;{}_{\mathcal{A}}\Psi_{j,\vec{r}'}^{N}(\vec{r}_1\ldots\vec{r}_N) \tag{C.36b}$$

$$=N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\;\Psi_{i,\vec{r}}^{N\,*}(\vec{r}_1\ldots\vec{r}_N)\,\frac{\mathcal{A}_{1..N}}{\sqrt{N}}\,\Psi_{j,\vec{r}'}^{N}(\vec{r}_1\ldots\vec{r}_N) \tag{C.36c}$$

$$=\langle\Psi_i^{N-1}|\hat{a}_{\vec{r}}\,\hat{a}_{\vec{r}'}^{\dagger}|\Psi_j^{N-1}\rangle\,, \tag{C.36d}$$

which shows that $\mathcal{N}(i\vec{r}, j\vec{r}')$ is

- The kernel of the norm operator for the basis set $\{{}_{\mathcal{A}}\Psi_{i,\vec{r}}^{N}\}$ (Eq. (C.36a)).
- proportional to the overlap of an element from $\{{}_{\mathcal{A}}\Psi_{i,\vec{r}}^{N}\}$ and an element from $\{\Psi_{i,\vec{r}}^{N}\}$ (Eq. (C.36b)).
- such as $\dfrac{\mathcal{N}(i\vec{r}, j\vec{r}')}{N}$ is the matrix element of the projector $\dfrac{\mathcal{A}_{1..N}}{\sqrt{N}}$ in the basis $\{\Psi_{i,\vec{r}}^{N}\}$ (Eq. (C.36c)).

In particular, for any antisymmetric wave function ψ_ν^N the decomposition from Eq. (C.21) becomes

$$\psi_\nu^N(\vec{r}_1\ldots\vec{r}_N) = \frac{1}{\sqrt{N}}\sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r}\,\Psi_{i,\vec{r}}^{N}(\vec{r}_1\ldots\vec{r}_N)\,\varphi_{\nu i}^{N}(\vec{r})\,. \tag{C.37}$$

Multiplying the latter by ${}_{\mathcal{A}}\Psi_{j,\vec{r}'}^{N}(\vec{r}_1\ldots\vec{r}_N)$ and integrating over the coordinates $\vec{r}_1\ldots\vec{r}_N$, one gets

$$\varphi_{\nu i}^{N}(\vec{r}) = \frac{1}{N}\sum\!\!\!\!\!\!\int_j \mathrm{d}\vec{r}'\,\mathcal{N}(i\vec{r}, j\vec{r}')\,\varphi_{\nu j}^{N}(\vec{r}')\,. \tag{C.38}$$

Likewise, if ψ_ν^N is mixed-symmetric, one has

$$0 = \frac{1}{N}\sum\!\!\!\!\!\!\int_j \mathrm{d}\vec{r}'\,\mathcal{N}(i\vec{r}, j\vec{r}')\,\varphi_{\nu j}^{N}(\vec{r}')\,. \tag{C.39}$$

Thus $\frac{\mathcal{A}_{1..N}}{\sqrt{N}}$ acts like a projection operator when acting on a set of expansion coefficients. In particular, its restriction to the subspace of totally antisymmetric N-body wave functions is the identity.

This kernel can also be written in terms of particle or hole states. Inserting a complete set of N-body states $|\Psi_p^N\rangle$[8], with associated overlaps $\varphi_{pi}^N(\vec{r})$ with $|{}_{\mathcal{A}}\Psi_{i,\vec{r}'}^N\rangle$, in Eq. (C.36d), one finds

$$\mathcal{N}(i\vec{r}, j\vec{r}') = \sum\!\!\!\!\!\!\int_{p(N)} \varphi_{pi}^N(\vec{r})\, \varphi_{pj}^{N*}(\vec{r}')\,, \tag{C.40}$$

where $p(N)$ denotes that the sum runs over states of the N-body system. This expression is only valid in the case of fixed-center systems, where the second quantization formalism can be used. In the case of self-bound systems another definition for the kernel is used (see below). On the other hand, using the definition of ${}_{\mathcal{A}}\Psi_{i,\vec{r}}^N$ (Eq. (C.6)), the kernel can be expressed in terms of the $(N-1)$-body overlap functions as

$$\begin{aligned}
\mathcal{N}(i\vec{r}, j\vec{r}') =& N \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N\, \Psi_{i,\vec{r}}^{N*}(\vec{r}_1 \ldots \vec{r}_N)\, \frac{\mathcal{A}_{1..N}}{\sqrt{N}}\, \Psi_{j,\vec{r}'}^N(\vec{r}_1 \ldots \vec{r}_N) \\
=& N \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N\, \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{N-1})\, \delta(\vec{r} - \vec{r}_N)\, \frac{\mathcal{A}_{1..N}}{\sqrt{N}}\, \Psi_j^{N-1}(\vec{r}_1 \ldots \vec{r}_{N-1})\, \delta(\vec{r}' - \vec{r}_N) \\
=& \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N\, \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{N-1})\, \delta(\vec{r} - \vec{r}_N)\, \delta(\vec{r}' - \vec{r}_N)\, \Psi_j^{N-1}(\vec{r}_1 \ldots \vec{r}_{N-1}) \\
& - \sum_{n=1}^{N-1} (-1)^n \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N\, \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{N-1})\, \delta(\vec{r} - \vec{r}_N) \\
& \qquad \times \delta(\vec{r}_n - \vec{r}')\, \Psi_j^{N-1}(\vec{r}_1 \ldots \vec{r}_{n-1}, \vec{r}_{n+1} \ldots \vec{r}_N) \\
=& \delta(\vec{r} - \vec{r}')\, \delta_{ij} - \sum_{n=1}^{N-1} (-1)^n \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{n-1}\, \mathrm{d}\vec{r}_{n+1} \ldots \mathrm{d}\vec{r}_{N-1} \\
& \qquad \times \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{n-1}, \vec{r}', \vec{r}_{n+1} \ldots \vec{r}_{N-1}) \Psi_j^{N-1}(\vec{r}_1 \ldots \vec{r}_{n-1}, \vec{r}_{n+1} \ldots \vec{r}) \\
=& \delta(\vec{r} - \vec{r}')\, \delta_{ij} - (N-1) \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-2} \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{N-2}, \vec{r}') \Psi_j^{N-1}(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}) \\
=& \delta(\vec{r} - \vec{r}')\, \delta_{ij} - (N-1) \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-2} \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{N-2}, \vec{r}') \Psi_j^{N-1}(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}) \\
=& \delta(\vec{r} - \vec{r}')\, \delta_{ij} - \sum\!\!\!\!\!\!\int_{h(N-2)} \varphi_{ih}^{N-1*}(\vec{r}')\, \varphi_{jh}^{N-1}(\vec{r})\,,
\end{aligned} \tag{C.41}$$

where one used an expansion of the antisymmetrization operator according to its last determinant column, starting from the bottom ($\vec{r}_N$,$\vec{r}'_N$), i.e.

$$\begin{aligned}
\frac{\mathcal{A}_{1..N}}{\sqrt{N}}\, \Psi_{j,\vec{r}'}^N(\vec{r}_1 \ldots \vec{r}_N) =& \frac{1}{N!} \int \mathrm{d}\vec{r}'_1 \ldots \mathrm{d}\vec{r}'_N \quad \det_{k,l=1..N} \left[\delta(\vec{r}_k - \vec{r}'_l) \Psi_j^N(\vec{r}'_1 \ldots \vec{r}'_N)\right] \\
=& \frac{1}{N!} \int \mathrm{d}\vec{r}'_1 \ldots \mathrm{d}\vec{r}'_N \quad \det_{k,l=1..N} \left[\delta(\vec{r}_k - \vec{r}'_l) \Psi_j^{N-1}(\vec{r}'_1 \ldots \vec{r}'_{N-1})\, \delta(\vec{r}' - \vec{r}'_N)\right]
\end{aligned}$$

[8] They are taken here as eigenstates of $\hat{\mathcal{H}}^N$ but this is not mandatory.

$$
\begin{aligned}
=&\frac{\delta(\vec{r}\,'-\vec{r}_N)}{N!}\int \mathrm{d}\vec{r}\,'_1\ldots\mathrm{d}\vec{r}\,'_{N-1}\quad \det_{k,l=1..N-1}\left[\delta(\vec{r}_k-\vec{r}\,'_l)\Psi_j^{N-1}(\vec{r}\,'_1\ldots\vec{r}\,'_{N-1})\right]\\
&-\frac{1}{N!}\sum_{n=1}^{N-1}(-1)^n\int \mathrm{d}\vec{r}\,'_1\ldots\mathrm{d}\vec{r}\,'_N\,\delta(\vec{r}_n-\vec{r}\,'_N)\\
&\qquad\qquad\times\quad \det_{\substack{k,l=1..N\\ k\neq n,l\neq N}}\left[\delta(\vec{r}_k-\vec{r}\,'_l)\Psi_j^{N-1}(\vec{r}\,'_1\ldots\vec{r}\,'_{N-1})\right]\,\delta(\vec{r}\,'-\vec{r}\,'_N)\\
=&\frac{\delta(\vec{r}\,'-\vec{r}_N)}{N}\Psi_j^{N-1}(\vec{r}_1\ldots\vec{r}_{N-1})\\
&-\frac{1}{N}\sum_{n=1}^{N-1}(-1)^n\,\delta(\vec{r}_n-\vec{r}\,')\,\Psi_j^{N-1}(\vec{r}_1\ldots\vec{r}_{n-1},\vec{r}_{n+1}\ldots\vec{r}_N)\,, \qquad \text{(C.42)}
\end{aligned}
$$

using the fact that Ψ_j^{N-1} is totally antisymmetric. Combining Eqs. (C.41,C.40) gives the completeness relationship for the spectroscopic amplitudes

$$
\delta(\vec{r}-\vec{r}\,')\,\delta_{ij}=\sum\!\!\!\!\!\!\int_{h(N-2)}\varphi_{ih}^{N-1\,*}(\vec{r}\,')\,\varphi_{jh}^{N-1}(\vec{r})+\sum\!\!\!\!\!\!\int_{p(N)}\varphi_{pj}^{N\,*}(\vec{r}\,')\,\varphi_{pi}^{N}(\vec{r})\,. \qquad \text{(C.43)}
$$

The sum over h runs over states of the $(N-2)$-body system (e.g. the "hole" states of the $(N-1)$-body system), and the one over p runs over states of the N-body system (e.g. the "particle" states of the $(N-1)$-body system). It shows that spectroscopic amplitudes for particle states of the $(N-1)$-body system are not complete by themselves as they lack the contribution of Pauli blocking, i.e. contributions from holes states.

C.1.5 Coupled equations for the overlap functions

The N-body Hamiltonian can be further decomposed into

$$
\begin{aligned}
\hat{\mathcal{H}}^N(\vec{r}_1\ldots\vec{r}_N)=&\sum_{i=1}^{N}\frac{\hat{\vec{p}}_i^{\,2}}{2m}+\sum_{\substack{i,j=1\\ i<j}}^{N}\hat{v}_s(r_{ij})\\
=&\hat{\mathcal{H}}^{N-1}(\vec{r}_1\ldots\vec{r}_{N-1})-\frac{\hbar^2\,\hat{\partial}_N^2}{2m}+\sum_{i=1}^{N-1}\hat{v}_s(r_{iN})\,. \qquad \text{(C.44)}
\end{aligned}
$$

One defines $|\Psi_\nu^N\rangle$ and $|\Psi_i^{N-1}\rangle$ as eigenvectors of $\hat{\mathcal{H}}^N$ and $\hat{\mathcal{H}}^{N-1}$ respectively[9]. The associated eigenvalues problem leads to

$$
\langle\Psi_i^{N-1}|\hat{\mathcal{H}}^N|\Psi_\nu^N\rangle=E_\nu^N\langle\Psi_i^{N-1}|\Psi_\nu^N\rangle=E_i^{N-1}\langle\Psi_i^{N-1}|\Psi_\nu^N\rangle+\langle\Psi_i^{N-1}|-\frac{\hbar^2\hat{\partial}_N^2}{2m}+\sum_{k=1}^{N-1}\hat{v}_s(r_{kN})|\Psi_\nu^N\rangle\,. \qquad \text{(C.45)}
$$

Inserting the expansion from Eq. (C.24) for $|\Psi_\nu^N\rangle$ gives a set of Schrödinger-like coupled equations for the overlaps $\varphi_{\nu i}^N(\vec{r})$, that reads

$$
(E_\nu^N-E_i^{N-1})\varphi_{\nu i}^N(\vec{r})=-\frac{\hbar^2\,\hat{\partial}^2}{2m}\varphi_{\nu i}^N(\vec{r})+\sum\!\!\!\!\!\!\int_j\langle\Psi_i^{N-1}|\sum_{k=1}^{N-1}\hat{v}_s(|\vec{r}_k-\vec{r}\,|)|\Psi_j^{N-1}\rangle\,\varphi_{\nu j}^N(\vec{r})\,. \qquad \text{(C.46)}
$$

In this form, the "potential" reads

$$
v_{ij}(\vec{r})=\langle\Psi_i^{N-1}|\sum_{k=1}^{N-1}\hat{v}_s(|\vec{r}_k-\vec{r}\,|)|\Psi_j^{N-1}\rangle\,, \qquad \text{(C.47)}
$$

[9] The following is valid for the ground state $|\Psi_0^N\rangle$ of the N-body system and its exited states.

and involves an infinite sum of terms, thus it cannot be solved directly.

C.1.6 Approximate decoupling of the problem

Solutions of Eq. (C.46) include the completely antisymmetrized states, but also mixed-symmetric states, i.e. unphysical states. If the coupled equations are solved exactly this is not a problem as the two subspaces do not mix (Eq. (C.11)). When approximations are performed this can become a serious issue.

The N-body state $|\Psi_\nu^N\rangle$ can be approximated by a Slater determinant constructed from the spectroscopic amplitudes $\{\varphi_{\nu j}^N(\vec{r})\}_{j=1..N}$. In this case N Hartree-Fock (HF) orbitals can be identified as approximations to spectroscopic amplitudes and single-particle energies approximate single-nucleon separation energies. The local (Hartree) part comes from the diagonal v_{jj} terms in Eq. (C.46) and the non-local/exchange (Fock) potential comes from off-diagonal matrix elements, thus from channel couplings. From these starting points, a one-body potential model may be obtained, treating the nucleus as a system of N non-interacting nucleons. Indeed,

- Starting from the Hartree approximation, which consists in neglecting of-diagonal terms, this amounts to imposing that the one-body potential is the same for each single particle orbital, i.e. $v_{jj}(\vec{r}) = v(\vec{r})$.
- Starting from the Hartree-Fock approximation, one can use the replacement $v_{ij}(\vec{r}) = \delta_{ij} v(\vec{r})$.

This gives in both case the usual one-body equation for the spectroscopic amplitudes

$$(E_\nu^N - E_i^{N-1})\varphi_{\nu i}^N(\vec{r}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{}\varphi_{\nu i}^N(\vec{r}) + v(\vec{r})\,\varphi_{\nu i}^N(\vec{r})\,. \tag{C.48}$$

The use of Slater determinant ensures proper antisymmetrization of the equations. In particular, when calculating the expectation value of a one-body operator $\hat{\mathcal{O}}(\vec{r})$, the $(N-2)$ remaining states can be integrated out and only active orbitals remain. Thus the associated matrix element $\int \mathrm{d}\vec{r}\varphi_{\nu i}^{N*}(\vec{r})\hat{\mathcal{O}}(\vec{r})\varphi_{\nu j}^N(\vec{r})$ looks like a pure one-body expression. Finally, the potential model gives exactly N spectroscopic factors equal to one, all the other ones being zero, that is without pairing nor many-body correlations. Adding correlations beyond the HF picture allows for instance single-particle orbitals of the N- and $(N-1)$-body systems to be different. In this case the expansion of $|\Psi_\nu^N\rangle$ will contain contributions from more than N terms. As a consequence, it is usually admitted that spectroscopic factors are all less than 1. This is however a consequence of the antisymmetrization of the wave functions and distortion effects, as it will be shown later.

C.1.7 Asymptotic behavior of the expansion coefficients

One has to separate here between several cases.

- If one of the states $|\Psi_i^{N-1}\rangle$ or $|\Psi_j^{N-1}\rangle$ in Eq. (C.46) corresponds to a bound state of the $(N-1)$-body system, matrix elements $v_{ij}(\vec{r})$ have a short range, as a result of the convolution of the short-range two-body potential and a bound state wave function.
- When both $|\Psi_i^{N-1}\rangle$ or $|\Psi_j^{N-1}\rangle$ describe continuum states, matrix elements $v_{ij}(\vec{r})$ take a long range tail, but infinitesimal in amplitude (continuum normalization).

In the first case, overlap functions become asymptotically solutions of the free Schrödinger equation

$$\left[\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l_\nu(l_\nu+1)}{\hbar^2 r^2}\right) - \kappa_{\nu i}^2\right]\varphi_{\nu i}^{N\infty}(\vec{r}) = 0\,, \tag{C.49}$$

with

$$\kappa_{\nu i} = \sqrt{-\frac{2m^*(E^N_\nu - E^{N-1}_i)}{\hbar^2}}\,, \tag{C.50}$$

Solutions of Eq. (C.49) take in the asymptotic region $r > R$ the form

$$\varphi^{N\,\infty}_{\nu i}(\vec{r}) = B_\nu h_{l_\nu}(i\,\kappa_{\nu i} r) Y^{m_\nu}_{l_\nu}(\hat{r})\,, \tag{C.51}$$

where the spherical Hankel functions are defined as

$$h_l(i\,\kappa r) \equiv j_l(i\,\kappa r) + i\,n_l(i\,\kappa r) = i^l \frac{e^{-\kappa r}}{(\kappa r)} \sum_{k=0}^{l} \frac{1}{(2\kappa r)^k} \frac{(l+k)!}{k!(l-k)!}\,. \tag{C.52}$$

This shows the overlap functions $\varphi^N_{\nu i}(\vec{r})$ fall off exponentially at large distance where they decouple from each other, i.e.

$$\varphi^N_{\nu i}(\vec{r}) \underset{r\to+\infty}{\longrightarrow} \sim \frac{e^{-\kappa_{\nu i}\, r}}{r}\, Y^{m_l}_l(\hat{r})\,. \tag{C.53}$$

The exponential decay is the smallest for $i = 0$. Thus processes with reaction probabilities peaked in the asymptotic region only only on the asymptotic normalization coefficient (ANC) given by

$$\mathcal{ANC}_\nu = \lim_{r\to+\infty} \left[\varphi^N_{\nu 0}(\vec{r}) \times r\, e^{\kappa_{\nu i}\, r}\right]\,. \tag{C.54}$$

The ANC is a property of the spectroscopic amplitude which implicitly includes the spectroscopic factor. Its expression comes from the Fourier transform of the coupled equation Eq. (C.46), that is

$$\tilde{\varphi}^N_{\nu i}(\vec{k}\,) = \frac{1}{E^N_\nu - E^{N-1}_i - \frac{k^2}{2m}} \sum\!\!\!\!\!\!\int_j \mathrm{d}\vec{r}\, e^{i\,\vec{k}\cdot\vec{r}} \langle \Psi^{N-1}_i | \sum_{k=1}^{N-1} \hat{v}_s(|\vec{r}_k - \vec{r}\,|) | \Psi^{N-1}_j \rangle\, \varphi^N_{\nu j}(\vec{r})\,, \tag{C.55}$$

where a pole in the Fourier transform appears. It has been shown that the ANC can be obtained by an integration over the nuclear interior with a sum over spectroscopic amplitudes by taking the residue of this pole for $i = 0$ [12], i.e.

$$\mathcal{ANC}_\nu = \lim_{k\to -i\,\kappa_{\nu 0}} \left[4m\pi^2 \sum\!\!\!\!\!\!\int_j \mathrm{d}\vec{r}\, e^{i\,\vec{k}\cdot\vec{r}} \langle \Psi^{N-1}_0 | \sum_{k=1}^{N-1} \hat{v}_s(|\vec{r}_k - \vec{r}\,|) | \Psi^{N-1}_j \rangle\, \varphi^N_{\nu j}(\vec{r}) \right]\,, \tag{C.56}$$

for $\kappa_{\nu 0} = \sqrt{2m(E^N_\nu - E^{N-1}_0)}$.

C.2 Center-of-mass correlations

In the previous section, the Hartree-Fock approximation or the definition of a one-body potential confines the center-of-mass at a given position. The picture radically changes with the explicit treatment of the center-of-mass motion. We start from the exact non-relativistic Hamiltonian of a N-body system. $\hat{\mathcal{H}}^N$ is invariant under translation, and can be decomposed into a center-of-mass (c.o.m.) $\hat{\mathcal{H}}^N_{\text{c.o.m.}}$ and an internal part $\hat{\mathcal{H}}^N_{\text{int}}$

$$\begin{cases} \hat{\mathcal{H}}^N_{\text{c.o.m.}}(\vec{r}_1 \ldots \vec{r}_N) = & -\dfrac{\hbar^2}{2mN} \left(\displaystyle\sum_{i=1}^{N} \hat{\partial}_i \right)^2 \\ \\ \hat{\mathcal{H}}^N_{\text{int}}(\vec{r}_1 \ldots \vec{r}_N) = & \displaystyle\sum_{\substack{i,j=1 \\ i<j}}^{N} \left[-\dfrac{\hbar^2}{2mN} \left(\hat{\partial}_i - \hat{\partial}_j \right)^2 + \hat{v}_s(r_{ij}) \right]\,, \end{cases} \tag{C.57}$$

C.2.1 Internal N-body wave function

Eigenstates of $\hat{\mathcal{H}}^N$ are noted $\Psi^N_{i,\vec{K}}(\vec{r}_1 \dots \vec{r}_N)$ to account for the center-of-mass momentum $\vec{K}$. Because of the explicit decomposition of the Hamiltonian from Eq. (C.57), $\Psi^N_{i,\vec{K}}(\vec{r}_1 \dots \vec{r}_N)$ can be factorized into center-of-mass (plane wave) and internal contributions, i.e.

$$\Psi^N_{i,\vec{K}}(\vec{r}_1 \dots \vec{r}_N) = e^{i\,\vec{K}\cdot\vec{R}_N}\,\Phi^N_i(\vec{r}_1 \dots \vec{r}_N)\,, \tag{C.58}$$

where $\vec{R}_N$ is the center-of-mass coordinate

$$\vec{R}_N = \frac{1}{N}\sum_{i=1}^{N}\vec{r}_i\,. \tag{C.59}$$

The internal wave function Φ^N_i may also be noted $\Phi^N_i(\vec{r}_1 \dots \vec{r}_N) \equiv \ddot{\Phi}^N_i(\vec{\xi}_1 \dots \vec{\xi}_{N-1})$, using the $N-1$ independent internal variables expressed in terms of the Jacobi coordinates [10; 13]

$$\vec{\xi}_i = \vec{r}_{i+1} - \frac{1}{i}\sum_{j=1}^{i}\vec{r}_j = -\vec{\rho}_i\,, \tag{C.60}$$

which all are invariant under translation. For any $\vec{a}$ one has

$$\Phi^N_i(\vec{r}_1 + \vec{a} \dots \vec{r}_N + \vec{a}\,) = \Phi^N_i(\vec{r}_1 \dots \vec{r}_N)\,, \tag{C.61}$$

which leads to

$$\Psi^N_{i,\vec{K}}(\vec{r}_1 + \vec{a} \dots \vec{r}_N + \vec{a}\,) = e^{i\,\vec{K}\cdot\vec{a}}\,\Psi^N_{i,\vec{K}}(\vec{r}_1 \dots \vec{r}_N)\,. \tag{C.62}$$

C.2.1.1 Orthonormalization properties

Orthonormalization of the set $\{\Psi^N_{i,\vec{K}}\}$ reads

$$\begin{aligned}(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\delta_{ij} &= \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_N\,\Psi^{N\,*}_{i,\vec{K}}(\vec{r}_1 \dots \vec{r}_N)\,\Psi^N_{j,\vec{K}\,'}(\vec{r}_1 \dots \vec{r}_N)\\ &= \int \mathrm{d}\vec{\xi}_1 \dots \mathrm{d}\vec{\xi}_{N-1}\,d\vec{R}_N\,e^{i\,\vec{R}_N\cdot(\vec{K}-\vec{K}\,')}\ddot{\Phi}^{N*}_i(\vec{\xi}_1 \dots \vec{\xi}_{N-1})\,\ddot{\Phi}^N_j(\vec{\xi}_1 \dots \vec{\xi}_{N-1})\\ &= (2\pi)^3\delta(\vec{K}-\vec{K}\,')\int \mathrm{d}\vec{\xi}_1 \dots \mathrm{d}\vec{\xi}_{N-1}\,\ddot{\Phi}^{N*}_i(\vec{\xi}_1 \dots \vec{\xi}_{N-1})\,\ddot{\Phi}^N_j(\vec{\xi}_1 \dots \vec{\xi}_{N-1})\,.\end{aligned} \tag{C.63}$$

Note that the variable change $(\vec{r}_1 \dots \vec{r}_N) \to (\vec{\xi}_1 \dots \vec{\xi}_{N-1}, \vec{R}_N)$ is bijective. Indeed,

- the system $(\vec{\xi}_i)_{i=1,N-1}$ is linearly independent, as only $\vec{\xi}_{i\geq n-1}$ contain $\vec{r}_n$, so the linear problem $\sum_{i=1}^{N-1} a_i\vec{\xi}_i = \vec{0}$ can be solved iteratively from $i = N-1$ to $i = 1$, leading for all i to $a_i = 0$.
- one has $\vec{R}_N \cdot \vec{\xi}_i = 0$ for all i in $[1 \dots N-1]$, thus $(\vec{\xi}_1 \dots \vec{\xi}_{N-1}, \vec{R}_N)$ is a linearly independent system of cardinal $N = \mathrm{card}(\vec{r}_1 \dots \vec{r}_N)$.

The orthonormalization of the set $\{\Phi^N_i\}$ can therefore be carried out in as

$$\int \mathrm{d}\vec{\xi}_1 \dots \mathrm{d}\vec{\xi}_{N-1}\,\ddot{\Phi}^{N*}_i(\vec{\xi}_1 \dots \vec{\xi}_{N-1})\,\ddot{\Phi}^N_j(\vec{\xi}_1 \dots \vec{\xi}_{N-1}) = \delta_{ij}\,. \tag{C.64}$$

or using an explicit removal of the center-of-mass degree of freedom in the integrand, that is

$$\int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N \, \Phi_i^{N*}(\vec{r}_1 \ldots \vec{r}_N) \, \delta(\vec{R}_N) \, \Phi_j^N(\vec{r}_1 \ldots \vec{r}_N) = \delta_{ij} \, . \tag{C.65}$$

In an equivalent way, by enclosing the system in a large box of volume $\mathcal{V}$, we get

$$\lim_{\mathcal{V}\to+\infty} \frac{1}{\mathcal{V}} \int_{\mathcal{V}} \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N \, \Phi_i^{N*}(\vec{r}_1 \ldots \vec{r}_N) \Phi_j^N(\vec{r}_1 \ldots \vec{r}_N) = \delta_{ij} \, . \tag{C.66}$$

C.2.1.2 Completeness relationships

Completeness property of the set $\{\Psi^N_{i,\vec{K}}\}$ reads

$$\begin{aligned} \int d\vec{K} \sum\!\!\!\!\!\!\int_i \Psi^N_{i,\vec{K}}{}^*(\vec{r}_1 \ldots \vec{r}_N) \, \Psi^N_{i,\vec{K}}(\vec{r}\,'_1 \ldots \vec{r}\,'_N) &= \sum\!\!\!\!\!\!\int_i \Phi_i^{N*}(\vec{r}_1 \ldots \vec{r}_N) \, \Phi_i^N(\vec{r}\,'_1 \ldots \vec{r}\,'_N) \, (2\pi)^3 \, \delta(\vec{K} - \vec{K}\,') \\ &= \int \mathrm{d}\vec{r} \frac{1}{A!} \det_{i,j=1\ldots N} \left[\delta(\vec{r}_i - \vec{r}\,'_j + \vec{r}\,)\right] \, (2\pi)^3 \, \delta(\vec{K} - \vec{K}\,') \, . \end{aligned} \tag{C.67}$$

The extra integral over $\vec{r}$ in Eq. (C.67) expresses the equivalence of translated configurations. Indeed, in the case of fixed-center systems, we would have had

$$\sum\!\!\!\!\!\!\int_i \Psi_i^{N*}(\vec{r}_1 \ldots \vec{r}_N) \, \Psi_i^N(\vec{r}\,'_1 \ldots \vec{r}\,'_N) = \frac{1}{A!} \det_{i,j=1\ldots N} \left[\delta(\vec{r}_i - \vec{r}\,'_j)\right] \, , \tag{C.68}$$

where the determinant accounts for the antisymmetrization of the wave functions. However, using Eq. (C.68) one would from Eq. (C.61) for any arbitrary $\vec{a}$

$$\sum\!\!\!\!\!\!\int_i \Phi_i^{N*}(\vec{r}_1 \ldots \vec{r}_N) \, \Phi_i^N(\vec{r}\,'_1 \ldots \vec{r}\,'_N) = \sum\!\!\!\!\!\!\int_i \Phi_i^{N*}(\vec{r}_1 \ldots \vec{r}_N) \, \Phi_i^N(\vec{r}\,'_1 + \vec{a} \ldots \vec{r}\,'_N + \vec{a}\,) \, , \tag{C.69}$$

thus

$$\frac{1}{A!} \det_{i,j=1\ldots N} \left[\delta(\vec{r}_i - \vec{r}\,'_j)\right] = \frac{1}{A!} \det_{i,j=1\ldots N} \left[\delta\left(\vec{r}_i - \vec{r}\,'_j - \vec{a}\,\right)\right] \, , \tag{C.70}$$

which is inexact. Explicit use of Eq. (C.67) will be done later. Similarly we have for reference in momentum space

$$\sum\!\!\!\!\!\!\int_i \tilde{\Phi}_i^{N*}(\vec{q}_1 \ldots \vec{q}_N) \, \tilde{\Phi}_i^N(\vec{q}\,'_1 \ldots \vec{q}\,'_N) = \frac{1}{(2\pi)^3} \int \mathrm{d}\vec{Q} \frac{1}{A!} \det_{i,j=1\ldots N} \left[\delta\left(\vec{q}_i - \vec{q}\,'_j + \frac{1}{A}\vec{Q}\right)\right] \, , \tag{C.71}$$

where

$$\tilde{\Phi}_i^N(\vec{q}_1 \ldots \vec{q}_N) = \frac{1}{(2\pi)^{3N/2}} \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N \, \Phi_i^N(\vec{r}_1 \ldots \vec{r}_N) \exp\left[-i \sum_{i=1}^N \vec{q}_i \cdot \vec{r}_i\right] \, \delta(\vec{R}_N) \, . \tag{C.72}$$

C.2.2 Decomposition of the N-body wave function

C.2.2.1 Standard and internal spectroscopic amplitudes

In the case of systems localized around a fixed center like the electrons of an atom, one defined a single-particle overlap function between N and $(N-1)$-body particle systems Ψ^N and Ψ^{N-1} as

$\breve{\varphi}^N_{\nu i} = \sqrt{N}\langle\Psi^N_{i,\vec{r}}|\Psi^N_\nu\rangle$ (Eq. (C.25c))[10]. In the case of nuclei there is no fixed external force center. Nucleons are localized around their center of mass, and standard overlap functions read [10]

$$\begin{aligned}\breve{\varphi}^N_{\nu i}(\vec{r},\vec{K}_N,\vec{K}_{N-1}) =&\sqrt{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\,\delta(\vec{r}-\vec{r}_N)\,\Psi^{N-1\ *}_{i,\vec{K}_{N-1}}(\vec{r}_1\ldots\vec{r}_{N-1})\,\Psi^N_{\nu,\vec{K}_N}(\vec{r}_1\ldots\vec{r}_N)\\ =&\sqrt{N}\,e^{i\,\vec{r}.(\vec{K}_N-\vec{K}_{N-1})}\int \mathrm{d}\vec{\xi}_1\ldots\mathrm{d}\vec{\xi}_{N-1}\,e^{-i\,\vec{\xi}_{N-1}.\left(\frac{N-1}{N}\vec{K}_N-\vec{K}_{N-1}\right)}\\ &\times\ddot{\Phi}^{N-1*}_i(\vec{\xi}_1\ldots\vec{\xi}_{N-2})\,\ddot{\Phi}^N_\nu(\vec{\xi}_1\ldots\vec{\xi}_{N-1})\\ \equiv& e^{i\,\vec{r}.(\vec{K}_N-\vec{K}_{N-1})}\,\varphi^N_{\nu i}\left(\frac{N-1}{N}\vec{K}_N-\vec{K}_{N-1}\right). \end{aligned}\tag{C.73}$$

Thus the spatial dependence of spectroscopic amplitudes is given by a plane wave, as a consequence of the translational invariance. Indeed, $\frac{N-1}{N}\vec{K}_N-\vec{K}_{N-1}$ is Galilean invariant. On the other hand, the spectroscopic factor reads $\left|\tilde{\varphi}^N_{\nu i}\left(\frac{N-1}{N}\vec{K}_N-\vec{K}_{N-1}\right)\right|^2$ and is the Fourier transform of the **internal spectroscopic amplitude**, which can be defined by removing from Eq. (C.73) the center-of-mass contribution, that is

$$\begin{aligned}\varphi^N_{\nu i}(\vec{r}) =&\frac{1}{(2\pi)^{3/2}}\int \mathrm{d}\vec{K}_{N-1}\,e^{i\,\vec{r}.\vec{K}_{N-1}}\,\tilde{\varphi}_{\nu i}(\vec{K}_{N-1})\\ =&\frac{1}{(2\pi)^{3/2}}\int \mathrm{d}\vec{K}_{N-1}\,\breve{\varphi}^N_{\nu,i}(\vec{r},\vec{0},\vec{K}_{N-1})\\ =&\frac{1}{(2\pi)^{3/2}}\sqrt{N}\int \mathrm{d}\vec{K}_{N-1}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\,\delta(\vec{r}-\vec{r}_N)\,e^{-i\,\vec{R}_{N-1}.\vec{K}_{N-1}}\\ &\times\Phi^{N-1*}_i(\vec{r}_1\ldots\vec{r}_{N-1})\,\Phi^N_\nu(\vec{r}_1\ldots\vec{r}_N)\\ =&\sqrt{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\,\delta(\vec{r}-\vec{r}_N)\,\delta(\vec{R}_{N-1})\,\Phi^{N-1*}_i(\vec{r}_1\ldots\vec{r}_{N-1})\,\Phi^N_\nu(\vec{r}_1\ldots\vec{r}_N). \end{aligned}\tag{C.74}$$

Thus internal overlaps can be defined as [14]

$$\varphi^N_{\nu i}(\vec{r}) =\sqrt{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\Phi^{N-1*}_i(\vec{r}_1\ldots\vec{r}_{N-1})\delta(\vec{R}_{N-1})\Phi^N_\nu(\vec{r}_1\ldots\vec{r}_{N-1},\vec{r})\tag{C.75a}$$

$$=\sqrt{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\Phi^{N-1*}_i(\vec{r}_1\ldots\vec{r}_{N-1})\delta(\vec{R}_{N-1}+\vec{r})\Phi^N_\nu(\vec{r}_1\ldots\vec{r}_{N-1},\vec{0}).\tag{C.75b}$$

In particular, this shows an internal wave function of the N-body system can be expanded on a complete set of internal eigenstates of the $(N-1)$-body system using Eq. (C.67), i.e

$$\Phi^N_\nu(\vec{r}_1\ldots\vec{r}_N)=\frac{1}{\sqrt{A}}\sum\!\!\!\!\!\!\int_i \Phi^{N-1}_i(\vec{r}_1\ldots\vec{r}_{N-1})\varphi^N_{\nu i}(\vec{r}_N-\vec{R}_{N-1}).\tag{C.76}$$

One can also define overlap functions by replacing the center-of-mass projection $\delta(\vec{R}_{N-1})$ in Eq. (C.75a) by the total c.o.m. projection for the N-body system $\delta(\vec{R}_N)$, leading to another expression $\dot{\varphi}^N_{ij}(\vec{r})$. Then, $\dot{\varphi}^N_{ij}(\vec{r})$ and $\varphi^N_{ij}(\vec{r})$ are related by a trivial scale transformation that reads [15]

$$\dot{\varphi}^N_{ij}(\vec{r})=\left[\frac{N}{N-1}\right]^3\varphi^N_{ij}\left(\frac{N}{N-1}\vec{r}\right).\tag{C.77}$$

[10] From this point on for more convenience, standard overlap functions will be noted $\breve{\varphi}$, whereas the internal overlaps will be φ. One may note in this case that the standard overlap functions depend on the center-of-mass momenta of the two convoluted states.

C.2.2.2 Relation with knockout reactions

The definition from Eq. (C.75a) is the most accurate for one-neutron knockout studies, but will also be convenient for the internal one-body density matrix. Indeed, when looking at the overlap function in momentum space by Fourier transforming

$$\begin{aligned}\tilde{\varphi}^N_{\nu i}(\vec{q}) =& \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}\vec{r}\, e^{-i\,\vec{q}\cdot\vec{r}}\, \varphi^N_{\nu i}(\vec{r}) \\ =& \sqrt{N} \int \mathrm{d}\vec{q}_1 \ldots \mathrm{d}\vec{q}_{N-1} \Phi_i^{N-1\,*}(\vec{q}_1 \ldots \vec{q}_{N-1}) (2\pi)^3 \delta \left(\sum_{i=1}^{A} \vec{q}_i \right) \Phi^N_\nu(\vec{q}_1 \ldots \vec{q}_N)\,, \end{aligned} \tag{C.78}$$

we find that if the N-body system is in its ground state, then $\varphi^N_{0i}(\vec{q}) \equiv \varphi^N_i(\vec{q})$ is the amplitude for extracting a particle with momentum $\vec{q}$ from the internal ground state of the "target" Φ^N_0 ending up in the internal eigenstate Φ^{N-1}_i of the residual system. This is closely related to the description of one-particle knockout reactions, and in compliance with previous definitions of the overlap functions [11; 16; 17]. In Ref. [11], the cross-section for knockout reactions is proportional, in the plane wave impulse approximation (PWIA)[11], to the spectral function, and it reads

$$P(\vec{k}, E) = \sum_i |A_i(\vec{k})|^2 \delta(E - E^{N-1}_i + E^N_0)\,, \tag{C.79}$$

where $\vec{k}$ and E are respectively the momentum and energy transferred to the nucleus, and the amplitude $A_i(\vec{k})$ is the Fourier transform of the overlap integral of the initial and final state nuclear wave functions

$$A_i(\vec{k}) = \int \mathrm{d}\vec{r}_N\, e^{i\,\vec{k}\cdot\vec{r}_N} \ll \Psi^{N-1}_i | \Psi^N_0 \gg \tag{C.80}$$

where the notation $\ll .|. \gg$ means integration on the fewer number of coordinates, i.e.

$$\ll \Psi^{N-1}_i | \Psi^N_0 \gg = \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1} \Psi^{N-1\,*}_i(\vec{r}_1 \ldots \vec{r}_{N-1}) \Psi^N_0(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}_N)\,. \tag{C.81}$$

To account for translational invariance, internal quantities E^{N-1}_i have then been introduced, noting that the residual nucleus recoils with momentum $\vec{k}$

$$E^{N-1}_{i,\vec{k}} = E^{N-1}_i + \frac{k^2}{2m(A-1)}\,, \tag{C.82}$$

one finds

$$P(\vec{k}, E) = \sum_i |A'_i(\vec{k})|^2 \delta \left(E + \epsilon_i - \frac{k^2}{2m(A-1)} \right)\,, \tag{C.83}$$

where the amplitude is now

$$A'_i(\vec{k}) = \int \mathrm{d}\vec{r}'_N\, e^{i\,\vec{k}\cdot\vec{r}'_N} \ll \Phi^{N-1}_i | \Phi^N_0 \gg\,. \tag{C.84}$$

The following quantities have been defined here:

$$\vec{r}'_i = \vec{r}_i - \vec{R}_{N-1}\,, \qquad \epsilon_i = E^N_0 - E^{N-1}_i\,. \tag{C.85}$$

[11] That is, neglecting final state interactions for the ejected particle, that is the outgoing nucleon is a plane wave. The coincidence cross-section is then the product of the nucleon-nucleon cross-section and the spectral function.

The overlap between internal wave functions is related to the overlap between the wave functions in the laboratory frame through

$$\langle \Psi^{N-1}_{i,\vec{K}} | \Psi^N_0 \rangle = \frac{1}{\mathcal{V}} \int \mathrm{d}\vec{R}_{N-1}\, e^{-i\,\vec{K}\cdot\vec{R}_{N-1}} \ll \Phi^{N-1}_i | \Phi^N_0 \gg$$
$$= \int \mathrm{d}\vec{R}_{N-1}\, e^{-i\,\vec{K}\cdot\vec{R}_{N-1}} \ll \Phi^{N-1}_i | \Phi^N_0 \gg \delta(\vec{R}_N)\,. \quad \text{(C.86)}$$

Eq. (C.76) expresses the distribution of the hole strength among various eigenstates of the final nucleus, and the spectral function becomes

$$P(\vec{k},E) = \sum_{ij} \varphi^{N*}_{0i}(\vec{k})\varphi^N_{0j}(\vec{k}) \sum_k S^k_{ij}\, \delta\left(E + \epsilon_i - \frac{k^2}{2m(A-1)}\right), \quad \text{(C.87)}$$

where

$$S^k_{ij} = \ll \Phi^{N-1}_i | \Phi^{N-1}_k \gg \ll \Phi^{N-1}_k | \Phi^{N-1}_j \gg, \quad \text{(C.88)}$$

single-particle occupation probabilities

$$S_{ij} = \sum_k S^k_{ij} = \langle \Phi^{N-1}_i | \Phi^{N-1}_j \rangle, \quad \text{(C.89)}$$

as well as the single-particle removal energies

$$\epsilon'_i = \frac{1}{S_{ii}} \sum_k S^k_{ii}\epsilon_k = \langle \Phi^N_0 | \hat{H}^N | \Phi^N_0 \rangle - \frac{1}{S_{ii}} \langle \Phi^{N-1}_i | \hat{H}^{N-1} | \Phi^{N-1}_i \rangle, \quad \text{(C.90)}$$

have been defined.

C.2.3 Internal spectroscopic factors

Second quantization formalism cannot be used any more when taking into account center-of-mass correlations. In particular, the definition of the spectroscopic factors from Eq. (C.26)

$$\breve{S}_{\nu i} = \int \mathrm{d}\vec{r} \left| \langle \Psi^{N-1}_i | \hat{a}_{\vec{r}} | \Psi^N_\nu \rangle \right|^2, \quad \text{(C.91)}$$

is now invalid. However, the normalization of the internal overlaps $\varphi^N_{\nu i}$

$$S_{\nu i} = \int \mathrm{d}\vec{r} |\varphi^N_{\nu i}(\vec{r})|^2, \quad \text{(C.92)}$$

can be defined as the internal spectroscopic factors. Using Eq. (C.67), it appears then that one still has

$$\sum_{i=0}^{+\infty} S_{\nu i} = N\,. \quad \text{(C.93)}$$

Actually, those are the true spectroscopic factors of the system appearing in dynamic equations. Indeed, when taking into account center-of-mass correlations, Eq. (C.35) reads as a plane wave transition operator[12]

$$\mathcal{M}_{ij} = \langle \Psi^N_i | \sum_{n=1}^N e^{-i\,\vec{k}\cdot\vec{r}_n} | \vec{\Psi}^N_j \rangle$$
$$= \frac{N}{(2\pi)^3} \int \mathrm{d}\vec{K}_{N-1} \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r}\, \frac{\breve{\varphi}^{N*}_{ni}(\vec{r},\vec{K}_i,\vec{K}_{N-1})}{\sqrt{N}}\, e^{-i\,\vec{k}\cdot\vec{r}}\, \frac{\breve{\varphi}^N_{nj}(\vec{r},\vec{K}_j,\vec{K}_{N-1})}{\sqrt{N}}$$
$$= \delta(\vec{k}+\vec{K}_i-\vec{K}_j) \sum\!\!\!\!\!\!\int_i \mathrm{d}\vec{r}\, \varphi^{N*}_{ni}(\vec{r})\, e^{-i\,\frac{N-1}{N}\vec{k}\cdot\vec{r}}\, \bar{\varphi}^N_{nj}(\vec{r})\,. \quad \text{(C.94)}$$

[12] This is the appropriate transition operator for radiative capture processes.

The delta factor ensures momentum conservation in the process, and the $\frac{N-1}{N}$ factor represents the laboratory to center-of-mass frame transformation. It appears that internal spectroscopic amplitudes are indeed the relevant objects for nuclear dynamics.

It must be kept in mind that individual (internal) spectroscopic factors can be greater than one for fermion systems, because of the center-of-mass motion [11; 16; 17]. For instance in the case of $N = 2$ [15; 18], any internal wave function reads $\Phi^{(2)}(\vec{r}_1, \vec{r}_2) = f(\vec{r}_1 - \vec{r}_2)$ with $\int r^2 \, \mathrm{d}r \, |f(\vec{r})|^2 = 1$. The only internal one-body state is $\Phi^{(1)}(\vec{r}_1) = 1$, and its overlap φ_1 with $\Phi^{(2)}$ reads $\varphi_1(\vec{r}) = \sqrt{2} f(-\vec{r})$. The associated spectroscopic factor is then 2. Discussions concerning the upper bound for spectroscopic factors are not pursued here and can be found in Refs. [15; 19]. In particular, it has been found for N fermions in an harmonic oscillator model that the upper bound for occupation numbers (eigenvalues of the internal one-body density matrix discussed later) is $n_{max} = \left[\frac{N}{N-1}\right]^{N-1}$.

C.2.4 Coupled equations for the internal spectroscopic amplitudes

To obtain the equations satisfied by the internal spectroscopic amplitudes, $\hat{\mathcal{H}}^N_{\mathrm{int}}(\vec{r}_1 \dots \vec{r}_N)$ can be further decomposed into [15]

$$\hat{\mathcal{H}}^N_{\mathrm{int}}(\vec{r}_1 \dots \vec{r}_N) = \hat{\mathcal{H}}^{N-1}_{\mathrm{int}}(\vec{r}_1 \dots \vec{r}_{N-1}) - \hbar^2 \frac{N-1}{2mN} \left(\hat{\partial}_N - \frac{1}{N-1} \sum_{i=1}^{N-1} \hat{\partial}_i \right)^2 + \sum_{i=1}^{N-1} \hat{v}_s(|\vec{r}_N - \vec{r}_i|) \,. \tag{C.95}$$

This expression can be substituted in the identity

$$0 = \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_{N-1} \, \delta(\vec{R}_{N-1}) \, \Psi_i^{N-1\,*}(\vec{r}_1 \dots \vec{r}_{N-1}) \left[\hat{\mathcal{H}}^N_{\mathrm{int}}(\vec{r}_1 \dots \vec{r}_N) - E^N_\nu \right] \Psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) \,. \tag{C.96}$$

This leads after some manipulations to the coupled equations

$$\begin{aligned} &-\frac{\hbar^2}{2m^*} \partial^2 \varphi^N_{\nu i}(\vec{r}) - (E^N_\nu - E^{N-1}_i) \varphi^N_{\nu i}(\vec{r}) = \\ &-(N-1)\sqrt{N} \int \mathrm{d}\vec{r}_1 \dots \mathrm{d}\vec{r}_{N-1} \, \delta(\vec{R}_{N-1}) \, \Psi_i^{N-1\,*}(\vec{r}_1 \dots \vec{r}_{N-1}) \, v_s(|\vec{r} - \vec{r}_{N-1}|) \, \Psi^N_\nu(\vec{r}_1 \dots \vec{r}_{N-1}, \vec{r}), \end{aligned} \tag{C.97}$$

where $m^* = \frac{N-1}{N} m$ is the reduced mass, $E^N_\nu = E^N_{\nu,\vec{K}} - \frac{K^{N\,2}}{2mN}$ the internal eigenenergy, and using that

$$\sum_{i=1}^{N} \vec{\nabla}_i \Psi^N_\nu(\vec{r}_1 \dots \vec{r}_N) = 0 \,. \tag{C.98}$$

In particular, coupled equations from Eq. (C.97) show that internal spectroscopic amplitudes follow asymptotically the free Schrödinger equation, thus have exponential decays. One may note that standard spectroscopic amplitudes $\breve{\varphi}$ still fulfill the initial coupled equations system but they are now plane waves.

C.2.5 Koltun sum rules

The Koltun sum rules gives a final consistency check concerning the decomposition of the N-body wave function. It is assumed that the Hamiltonian contains only two-body forces[13]. The total

[13] An experimental violation of this sum rule could prove the existence of 3NF, although other effects may explain it [20].

energy of the nucleus is then [11; 21]

$$E_0^N = \frac{1}{2}\int \mathrm{d}\vec{k} \int \mathrm{d}E \left(-E + \frac{k^2}{2m}\right) P(\vec{k}, E)\,. \tag{C.99}$$

The energy E is the energy transfer in the laboratory frame, and not the internal energy transfer $E_{\rm int} = E - \frac{1}{N-1}\frac{k^2}{2m}$. In terms of $E_{\rm int}$ the sum rule reads

$$E_0^N = \frac{1}{2}\int \mathrm{d}\vec{k} \int \mathrm{d}E_{\rm int} \left(-E_{\rm int} + \frac{N-2}{N-1}\frac{k^2}{2m}\right) P(\vec{k}, E_{\rm int})\,. \tag{C.100}$$

In the single-particle basis this can be expressed as

$$E_0^N = \frac{1}{2}\sum\!\!\!\!\!\!\int_i S_{ii}\epsilon'_i + \frac{1}{2}\frac{N-2}{N-1}T^N\,, \tag{C.101}$$

where T^N is the kinetic energy. The correction factor $\frac{N-2}{N-1}$ accounts for the recoil factor, and cancels the extra kinetic energy in the expression of ϵ'_i arising from the reduced mass effect $\frac{N}{N-1}$[14].

In the present case, the Koltun sum rule is checked for the internal energy E_0^N, where the internal kinetic energy reads [15]

$$\begin{aligned} T^N &= \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N\, \delta(\vec{R}_N)\, \Psi_0^{N*}(\vec{r}_1 \ldots \vec{r}_N) \left[-\frac{\hbar^2}{2mN}\sum_{\substack{i,j=1\\ i<j}}^{N} (\partial_i - \partial_j)^2\right] \Psi_0^N(\vec{r}_1 \ldots \vec{r}_N) \\ &= -\frac{\hbar^2}{2m}\int \mathrm{d}\vec{r}_N\, [\partial^2_{\vec{r}'_N}\, \rho^{[1]}(\vec{r}_N, \vec{r}'_N)]_{\vec{r}'_N = \vec{r}_N} \\ &= -\frac{\hbar^2}{2m}\int \mathrm{d}\vec{q}_N\, q_N^2\, \eta(\vec{q}_N)\,, \end{aligned} \tag{C.102}$$

using the definition of the internal density matrix (Sec. C.3.2) and the associated momentum distribution (Eq. (C.150)). From the coupled equations for the overlap (Eq. (C.97)), multiplied by $\varphi_{0i}^{N*}(\vec{r})$, integrated over $\vec{r}$, and after summation on the states i of the $(N-1)$-body system, one obtains

$$\begin{aligned} \frac{N}{N-1}T^N + (N-1)\sqrt{N}\int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1}\, d\vec{r}\, \delta(\vec{R}_{N-1}) \sum\!\!\!\!\!\!\int_i \Psi_i^{N-1*}(\vec{r}_1 \ldots \vec{r}_{N-1})\, \varphi_{0i}^{N*}(\vec{r}\,) \\ \times v_s(|\vec{r} - N\vec{-}1|)\, \Psi_0^N(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}\,) = -\langle E_r\rangle_N\,, \end{aligned} \tag{C.103}$$

where one defines the mean removal energy as

$$\langle E_r\rangle_N = \sum\!\!\!\!\!\!\int_i (E_i^{N-1} - E_0^N) S_{0i}\,. \tag{C.104}$$

Using the completeness relationship for the set $\{\Psi_i^{N-1}\}$, the second term in Eq. (C.103) can be converted to twice the potential energy v^N in the system, reading

$$\begin{aligned} v^N &= E_0^N - T^N \\ &= \frac{N(N-1)}{2}\int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_N\, \delta(\vec{R}_N)\, v_s(|\vec{r}_N - N\vec{-}1|)\, |\Psi_0^N(\vec{r}_1 \ldots \vec{r}_N)|^2\,. \end{aligned} \tag{C.105}$$

As a result the Koltun sum rule is retrieved, and it reads

$$E_0^N = \frac{1}{2}\left(\frac{N-2}{N-1}T^N - \langle E_r\rangle_N\right)\,. \tag{C.106}$$

[14] This correction can be justified when looking at the deuteron, where $E_0^2 = \epsilon'_0$.

C.2.6 Self-consistent translationally invariant theories

The decomposition from Eq. (C.76) is the most adequate when dealing with self-consistent theories for translationally invariant systems, without substraction of the center-of-mass contribution. In the Hartree-Fock case, it was found [22] that generalized equations could be found without the use of Slater determinants for a set of N amplitudes $\{\phi_j\}$. Those equations are translationally invariant, but do not come from a variational principle. In the limit of large N, those may be then identified to the standard HF orbitals.

Figure C.1: Diagrammatic definition of the amplitudes $\langle\Psi^{N-1}_{j,\vec{P}'}|\,\hat{a}_{\vec{p}}\,|\Psi^N_{i,\vec{P}}\rangle$ (left-hand side) and $\langle\Psi^{N-2}_{j,\vec{P}'}|\,\hat{a}_{\vec{p}}\,|\Psi^{N-1}_{i,\vec{P}}\rangle$ (right-hand side). nucleon lines (double lines) are on mass shells.

As suggested by Fig. C.1, one starts by defining the set of amplitudes $\{\phi^i_j\}$ and $\{\breve{\phi}^i_j\}$ as

$$\delta(\vec{P}\,'+\vec{p}+\vec{P}\,)\phi^i_j\left(\frac{(N-1)\vec{p}-(\vec{P}-\vec{p}\,)}{N}\right)=\langle\Psi^{N-1}_{j,\vec{P}'}|\,\hat{a}_{\vec{p}}\,|\Psi^N_{i,\vec{P}}\rangle \tag{C.107a}$$

$$\delta(\vec{P}\,'+\vec{p}+\vec{P}\,)\breve{\phi}^i_j\left(\frac{(N-2)\vec{p}-(\vec{P}-\vec{p}\,)}{N-1}\right)=\langle\Psi^{N-2}_{j,\vec{P}'}|\,\hat{a}_{\vec{p}}\,|\Psi^{N-1}_{i,\vec{P}}\rangle\,. \tag{C.107b}$$

Now when considering the ground state $|\Psi^N_0\rangle\equiv|\Psi^N_{0,\vec{0}}\rangle$, one can assume that only N amplitudes $\phi_j(\vec{p}\,)$ are needed, which are defined as

$$\delta(\vec{P}\,'+\vec{p}\,)\phi_j\left(\frac{(N-1)\vec{p}-(\vec{P}-\vec{p}\,)}{N}\right)=\langle\Psi^{N-1}_{j,\vec{P}'}|\hat{a}_{\vec{p}}|\Psi^N_0\rangle\,. \tag{C.108}$$

They describe the relative motion of a nucleon of momentum $\vec{q}$ and a $(N-1)$-body system. To prove that this decomposition in terms of the relative motion with respect to the $(N-1)$-body system is the most accurate, the equations satisfied by the amplitudes ϕ_i can be derived. One starts from an Hamiltonian using only two body interactions, of the form

$$\hat{\mathcal{H}}^N=\int \mathrm{d}\vec{p}\,\hat{a}^\dagger_{\vec{p}}\,\frac{p^2}{2m}\,\hat{a}_{\vec{p}}+\frac{1}{2}\int \mathrm{d}\vec{p}_1\,\mathrm{d}\vec{p}_2\,\mathrm{d}\vec{p}_3\,d\tilde{\mathrm{p}}_4\,\hat{\mathrm{a}}^\dagger_{\tilde{\mathrm{p}}_1}\,\hat{\mathrm{a}}^\dagger_{\tilde{\mathrm{p}}_2}\,\langle\tilde{\mathrm{p}}_1\;\tilde{\mathrm{p}}_2|\mathrm{v_s}|\tilde{\mathrm{p}}_3\;\tilde{\mathrm{p}}_4\rangle\,\hat{\mathrm{a}}_{\tilde{\mathrm{p}}_3}\,\hat{\mathrm{a}}_{\tilde{\mathrm{p}}_4}\,. \tag{C.109}$$

This leads to

$$\begin{aligned}\langle\Psi^{N-1}_{j,\vec{P}'}|[\hat{H},\hat{a}_{\vec{p}}]|\Psi^N_0\rangle&=\left(\bar{E}^{N-1}_j+\frac{P'^2}{2m(N-1)}-E^N_0\right)\langle\Psi^{N-1}_{j,\vec{P}'}|\hat{a}_{\vec{p}}|\Psi^N_0\rangle\\&=\langle\Psi^{N-1}_{j,\vec{P}'}|[\hat{T},\hat{a}_{\vec{p}}]|\Psi^N_0\rangle+\langle\Psi^{N-1}_{j,\vec{P}'}|[\hat{v_s},\hat{a}_{\vec{p}}]|\Psi^N_0\rangle\,.\end{aligned} \tag{C.110}$$

After some manipulations and assumptions, in particular that the interaction is local and only depends on the momentum transfer [22], one finds HF-like equations for the functions ϕ_j, i.e.

$$\left(\epsilon'_j + \frac{\hbar^2\partial^2}{2m^*}\right)\phi_j(\vec{r}) = \left(\frac{N-2}{N-1}\right)^3 \left[\int \mathrm{d}\vec{r}\,' \sum_{k=1}^{N} \phi_k^*\left(\frac{N-2}{N-1}\vec{r}\,'\right) v(|\vec{r}-\vec{r}\,'|)\,\phi_k\left(\frac{N-2}{N-1}\vec{r}\,'\right)\right]\phi_j(\vec{r}) \tag{C.111a}$$

$$- \left(\frac{N-2}{N-1}\right)^3 \left[\int \mathrm{d}\vec{r}\,' \sum_{k=1}^{N} \phi_k^*\left(\frac{N-2}{N-1}\vec{r}\,'\right) v(|\vec{r}-\vec{r}\,'|)\,\phi_k\left(\vec{r}+\frac{1}{N-1}\vec{r}\,'\right)\right] \times \phi_j\left(\vec{r}\,' - \frac{1}{N-1}(\vec{r}-\vec{r}\,')\right) . \tag{C.111b}$$

Standard HF equations can be retrieved in the limit of large N. To simplify the exchange term (Eq. (C.111b)), one may consider the case of a potential with a short range in comparison to the size of the system, ie $\vec{r} \approx \vec{r}\,'$, which leads to

$$\left(\epsilon'_j + \frac{\hbar^2\partial^2}{2m^*}\right)\phi_j(\vec{r}) = \left(\frac{N-2}{N-1}\right)^3 \left[\int \mathrm{d}\vec{r}\,' \sum_{k=1}^{N} \phi_k^*\left(\frac{N-2}{N-1}\vec{r}\,'\right) v(|\vec{r}-\vec{r}\,'|)\,\phi_k\left(\frac{N-2}{N-1}\vec{r}\,'\right)\right]\phi_j(\vec{r}) \tag{C.112a}$$

$$- \left(\frac{N-2}{N-1}\right)^3 \left[\int \mathrm{d}\vec{r}\,' \sum_{k=1}^{N} \phi_k^*\left(\frac{N-2}{N-1}\vec{r}\,'\right) v(|\vec{r}-\vec{r}\,'|)\,\phi_k(\vec{r})\,\phi_j(\vec{r}\,')\right] , \tag{C.112b}$$

which are indeed HF-like equations.

C.2.7 Internal Slater determinants

An interesting way to understand the expansion of Eq. (C.76) comes from the use of internal Slater determinants (ISDs) to describe the uncorrelated motion of the N particles in N orbits around their center-of-mass[15] [18], that is

$$\Phi^N_{SD}(\vec{r}_1 \ldots \vec{r}_N) = \frac{1}{\sqrt{N!}} \det_{i,j=1\ldots N}\left[\phi_j(\vec{r}_i - \vec{R}_N)\right] , \tag{C.113}$$

and

$$\Phi^{N-1}_{i,SD}(\vec{r}_1 \ldots \vec{r}_{N-1}) = \frac{1}{\sqrt{(N-1)!}} \det_{\substack{i,j=1\ldots N \\ i\neq N, j\neq i}}\left[\phi_j(\vec{r}_i - \vec{R}_{N-1})\right] . \tag{C.114}$$

ISDs can then be used to evaluate single-particle overlap functions and spectroscopic factors using Eq. (C.75a). Likewise, the expansion from Eq. (C.76) can be interpreted as an expansion with respect to the first column of the determinant, followed by a translation of $\vec{R}_N - \vec{R}_{N-1}$

[15] This corresponds to remove the spurious c.o.m. motion in the usual fixed-frame Slater determinants.

(ISDs are translational invariants), i.e.

$$\Phi^N_{SD}(\vec{r}_1 \dots \vec{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\vec{r}_1 - \vec{R}_N) & \phi_1(\vec{r}_2 - \vec{R}_N) & \dots & \phi_1(\vec{r}_N - \vec{R}_N) \\ \phi_2(\vec{r}_1 - \vec{R}_N) & \phi_2(\vec{r}_2 - \vec{R}_N) & \dots & \phi_2(\vec{r}_N - \vec{R}_N) \\ \dots & \dots & & \dots \\ \phi_N(\vec{r}_1 - \vec{R}_N) & \phi_N(\vec{r}_2 - \vec{R}_N) & \dots & \phi_N(\vec{r}_N - \vec{R}_N) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_{i=1}^{N} (-1)^{i+1} \phi_i(\vec{r}_1 - \vec{R}_N) \begin{vmatrix} \phi_1(\vec{r}_2 - \vec{R}_N) & \dots & \phi_1(\vec{r}_N - \vec{R}_N) \\ \dots & & \dots \\ \phi_{i-1}(\vec{r}_2 - \vec{R}_N) & \dots & \phi_{i-1}(\vec{r}_N - \vec{R}_N) \\ \phi_{i+1}(\vec{r}_2 - \vec{R}_N) & \dots & \phi_{i+1}(\vec{r}_N - \vec{R}_N) \\ \dots & & \dots \\ \phi_N(\vec{r}_2 - \vec{R}_N) & \dots & \phi_N(\vec{r}_N - \vec{R}_N) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_{i=1}^{N} (-1)^{i+1} \phi_i(\vec{r}_1 - \vec{R}_{N-1}) \begin{vmatrix} \phi_1(\vec{r}_2 - \vec{R}_{N-1}) & \dots & \phi_1(\vec{r}_N - \vec{R}_{N-1}) \\ \dots & & \dots \\ \phi_{i-1}(\vec{r}_2 - \vec{R}_{N-1}) & \dots & \phi_{i-1}(\vec{r}_N - \vec{R}_{N-1}) \\ \phi_{i+1}(\vec{r}_2 - \vec{R}_{N-1}) & \dots & \phi_{i+1}(\vec{r}_N - \vec{R}_{N-1}) \\ \dots & & \dots \\ \phi_N(\vec{r}_2 - \vec{R}_{N-1}) & \dots & \phi_N(\vec{r}_N - \vec{R}_{N-1}) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i+1} \phi_i(\vec{r}_1 - \vec{R}_{N-1}) \, \Phi^{N-1}_{i,SD}(\vec{r}_2 \dots \vec{r}_{N-1}) \, . \tag{C.115}$$

The phase $(-1)^{i+1}$ is then to be recast in either $(N-1)$-body ISDs or the overlap functions. For more details regarding the antisymmetrization, we refer to Ref. [10].

C.3 One-body density

The ground state of the N-body system will be noted hereafter as $\Psi^N_{0,\vec{0}}(\vec{r}_1 \dots \vec{r}_N) \equiv \Psi^N_0(\vec{r}_1 \dots \vec{r}_N)$.

C.3.1 Laboratory frame

C.3.1.1 Definition

In the laboratory frame, second quantization formalism can be used, and the density matrix reads

$$\rho(\vec{r}, \vec{r}\,') = \langle \Psi^N_0 | \hat{a}^\dagger_{\vec{r}\,'} \, \hat{a}_{\vec{r}} | \Psi^N_0 \rangle \, . \tag{C.116}$$

In the general case, the non-local one-body density operator $\hat{\rho}(\vec{r}, \vec{r}\,')$ takes the form

$$\hat{\rho}(\vec{r}, \vec{r}\,') = \frac{1}{N!} \det_{i,j=1\dots N} \left[\delta(\vec{r} - \hat{\vec{r}}_i) \delta(\vec{r}\,' - \hat{\vec{r}}\,'_j) \frac{1}{(N-2)!} \det_{k \neq i, l \neq j} \left[\delta(\hat{\vec{r}}_k - \hat{\vec{r}}\,'_l) \right] \right] . \tag{C.117}$$

However because N-body wave functions are antisymmetrized one can use a reduced form which reads

$$\hat{\rho}(\vec{r}, \vec{r}\,') = \sum_{i=1}^{N} \delta(\vec{r} - \hat{\vec{r}}_i) \delta(\vec{r}\,' - \hat{\vec{r}}\,'_i) \prod_{j \neq i} \delta(\hat{\vec{r}}_j - \hat{\vec{r}}\,'_j) \, , \tag{C.118}$$

so that for any Slater determinant[16]

$$|\Phi\rangle = \frac{1}{\sqrt{N!}} \begin{bmatrix} \phi_1(\vec{r}_1) & \phi_2(\vec{r}_1) & \dots & \phi_N(\vec{r}_1) \\ \phi_1(\vec{r}_2) & \phi_2(\vec{r}_2) & \dots & \phi_N(\vec{r}_2) \\ & \dots\dots\dots\dots & & \\ \phi_1(\vec{r}_N) & \phi_2(\vec{r}_N) & \dots & \phi_N(\vec{r}_N) \end{bmatrix}, \tag{C.119}$$

the expectation value of $\hat{\rho}(\vec{r},\vec{r}\,')$ is

$$\langle\Phi|\hat{\rho}(\vec{r},\vec{r}\,')|\Phi\rangle = \frac{1}{N!}\sum_{j=1}^{N}\sum_{\hat{\mathcal{P}}_{\|j}}\Big(\langle 1\,2..N|\hat{\mathcal{P}}^{\dagger}_{\|j}\hat{\rho}(\vec{r},\vec{r}\,')\hat{\mathcal{P}}_{\|j}|1\,2..N\rangle + \sum_{k\neq j}\sum_{\hat{\mathcal{P}}_{\|k}\neq\hat{\mathcal{P}}_{\|j}} \epsilon_{\hat{\mathcal{P}}_{\|k}}\epsilon_{\hat{\mathcal{P}}_{\|j}}\langle 1\,2..N|\hat{\mathcal{P}}^{\dagger}_{\|k}\hat{\rho}(\vec{r},\vec{r}\,')\hat{\mathcal{P}}_{\|j}|1\,2..N\rangle\Big), \tag{C.120}$$

where $|i_1\,i_2..i_N\rangle \equiv |\phi_1(\vec{r}_{i_1})\,\phi_2(\vec{r}_{i_2})..\phi_N(\vec{r}_{i_N})\rangle$, and $\hat{\mathcal{P}}_{\|k}$ is a permutation matrix in the uplet $\{1,2,..,N\}\backslash\{k\}$ of signature $\epsilon_{\hat{\mathcal{P}}_{\|k}}$. If there is at least one permutation between the bra $\langle 1\,2\,..k_1..k_2..N|\rightarrow\langle 1\,2..k_2..k_1..N|$ and the ket $|1\,2..k_1..k_2..N\rangle$[17], one obtains

$$\begin{aligned}\langle 1\,2..k_2..k_1..N|\hat{\rho}(\vec{r},\vec{r}\,')|1\,2..N\rangle =& \sum_{i=1}^{N}\int \mathrm{d}\vec{r}\,'_{1..N}\int \mathrm{d}\vec{r}_{1..N}\phi_1^*(\vec{r}\,'_1)..\phi_{k_1}^*(\vec{r}\,'_{k_2})..\phi_{k_2}^*(\vec{r}\,'_{k_1})..\phi_N^*(\vec{r}\,'_N)\\ &\times\delta(\vec{r}-\vec{r}_i)\delta(\vec{r}\,'-\vec{r}\,'_i)\prod_{j\neq i}\delta(\vec{r}_j-\vec{r}\,'_j)\phi_1(\vec{r}_1)..\phi_N(\vec{r}_N)\\ =& \sum_{\substack{i=1\\ i\neq k_1,k_2}}^{N}\prod_{\substack{j=1\\ j\neq k_1,k_2,i}}^{N}\langle\phi_j|\phi_j\rangle\langle\phi_{k_1}|\phi_{k_2}\rangle\langle\phi_{k_2}|\phi_{k_1}\rangle\phi_i^*(\vec{r}\,')\phi_i(\vec{r})\\ &+\prod_{\substack{j=1\\ j\neq k_2,i}}^{N}\langle\phi_j|\phi_j\rangle\langle\phi_i|\phi_{k_2}\rangle\phi_{k_2}^*(\vec{r}\,')\phi_i(\vec{r})\\ &+\prod_{\substack{j=1\\ j\neq k_1,i}}^{N}\langle\phi_j|\phi_j\rangle\langle\phi_i|\phi_{k_1}\rangle\phi_{k_1}^*(\vec{r}\,')\phi_i(\vec{r})\\ =&0\,.\end{aligned} \tag{C.121}$$

Thus

$$\forall k\neq j\,,\qquad \sum_{\hat{\mathcal{P}}_{\|k}\neq\hat{\mathcal{P}}_{\|j}}\langle 1\,2..N|\hat{\mathcal{P}}^{\dagger}_{\|k}\hat{\rho}(\vec{r},\vec{r}\,')\hat{\mathcal{P}}_{\|j}|1\,2..N\rangle = 0\,, \tag{C.122}$$

[16] Obviously the Slater determinant is not a good solution, as it is not translationally invariant. However, it gives us a good insight of the way the one-body density operator acts.

[17] For symmetry reasons, we can keep the ket $|\,2..i..j..N\rangle$ unchanged.

and

$$\begin{aligned}\langle\Phi|\hat{\rho}(\vec{r},\vec{r}\,')|\Phi\rangle =& \frac{1}{N!}\sum_{j=1}^{N}\sum_{\hat{\mathcal{P}}_{\|j}}\langle 1\,2..N|\hat{\mathcal{P}}_{\|j}^{\dagger}\hat{\rho}(\vec{r},\vec{r}\,')\hat{\mathcal{P}}_{\|j}|1\,2..N\rangle \\ =& \frac{1}{N!}\sum_{i=1}^{N}\sum_{j=1}^{N}\mathrm{card}(\{\hat{\mathcal{P}}_{\|j}\})\langle 1\,2..N|\delta(\vec{r}-\hat{\vec{r}}_i)\delta(\vec{r}\,'-\hat{\vec{r}}\,'_i)\prod_{k\neq i}\delta(\hat{\vec{r}}_k-\hat{\vec{r}}\,'_k)|1\,2..N\rangle \\ =& \frac{1}{N!}\sum_{i=1}^{N}\sum_{j=1}^{N}(N-1)!\int \mathrm{d}\vec{r}\,'_1\ldots\int \mathrm{d}\vec{r}\,'_N\int \mathrm{d}\vec{r}_1\ldots\int \mathrm{d}\vec{r}_N\phi_1^*(\vec{r}\,'_1)\ldots\phi_N^*(\vec{r}\,'_N) \\ & \times\delta(\vec{r}-\vec{r}_i)\delta(\vec{r}\,'-\vec{r}\,'_i)\prod_{k\neq i}\delta(\vec{r}_k-\vec{r}\,'_k)\phi_1(\vec{r}_1)\ldots\phi_N(\vec{r}_N) \\ =& \sum_{i=1}^{N}\phi_i^*(\vec{r}\,')\phi_i(\vec{r})\,. \end{aligned} \tag{C.123}$$

In the second quantization formalism, any one-body operator is implicitly considered as local in all other variables, thus the product running over Dirac functions $\delta(\hat{\vec{r}}_j-\hat{\vec{r}}\,'_j)$ in Eq. (C.118) is automatically resolved in integrals like $\langle 1\,2..k_2..k_1..N|\hat{\rho}(\vec{r},\vec{r}\,')|1\,2..N\rangle$, but integrals running on those variables are supposed to be trivial. We will use then the following compact notations, which make explicit use of the antisymmetrisation.

- For the one-body density matrix

$$\hat{\rho}(\vec{r},\vec{r}\,') \equiv N\,\delta(\vec{r}-\hat{\vec{r}}_N)\,\delta(\vec{r}\,'-\hat{\vec{r}}_N)\,, \tag{C.124}$$

  such that

$$\rho(\vec{r},\vec{r}\,') \equiv \langle\Psi_0^N|\hat{\rho}(\vec{r},\vec{r}\,')|\Psi_0^N\rangle \equiv N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,\Psi_0^{N*}(\vec{r}_1\ldots\vec{r}_{N-1}\,,\vec{r})\,\Psi_0^N(\vec{r}_1\ldots\vec{r}_{N-1}\,,\vec{r}\,')\,. \tag{C.125}$$

- For its local part

$$\hat{\rho}(\vec{r}) \equiv \hat{\rho}(\vec{r},\vec{r}) \equiv N\,\delta(\vec{r}-\hat{\vec{r}}_i)\,, \tag{C.126}$$

  such that

$$\rho(\vec{r}) = \langle\Psi_0^N|\hat{\rho}(\vec{r})|\Psi_0^N\rangle \equiv N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,|\Psi_0^N(\vec{r}_1\ldots\vec{r}_{N-1}\,,\vec{r})|^2\,. \tag{C.127}$$

These expressions assume that N-body wave functions are normalized to 1, thus the local density integrates to N.

C.3.1.2 Laboratory density for self-bound systems

Using Eq. (C.127) and Eq. (C.58), one finds for the one-body density in the laboratory frame

$$\rho(\vec{r}) = N\int \mathrm{d}\vec{\xi}_1\,'\ldots\mathrm{d}\vec{\xi}\,'_{N-1}\,|\Phi_0^N(\vec{\xi}\,'_1\ldots\vec{\xi}\,'_{N-1})|^2\,, \tag{C.128}$$

where the Jacobi coordinates are defined here as

$$\begin{cases}\vec{\xi}\,'_i = \vec{r}_{i+1} - \dfrac{1}{i}\displaystyle\sum_{j=1}^{i}\vec{r}_j & \text{for } i < N-1\,, \\ \vec{\xi}\,'_{N-1} = \vec{r} - \dfrac{1}{N-1}\displaystyle\sum_{j=1}^{N-1}\vec{r}_j\,. \end{cases} \tag{C.129}$$

Using a trivial variable change we find that the one-body density is invariant under any translation $\vec{r} \to \vec{r} + \vec{a}$, thus $\rho(\vec{r})$ is a constant. Indeed, using Eq. (C.116), the density matrix in the laboratory frame is the sum of the spectroscopic amplitudes $\breve{\varphi}^N_{0i}$ in the same frame, i.e.

$$\rho(\vec{r}, \vec{r}') = \langle \Psi^N_0 | \, \hat{a}^\dagger_{\vec{r}'} \, \hat{a}_{\vec{r}} \, | \Psi^N_0 \rangle = \sum\!\!\!\!\!\!\int_i \breve{\varphi}^{N*}_{0i}(\vec{r}') \, \breve{\varphi}^N_{0i}(\vec{r}) \, . \tag{C.130}$$

Thus one has for the one-body density, using Eq. (C.73)

$$\rho(\vec{r}) = \rho(\vec{r}, \vec{r}') = \sum\!\!\!\!\!\!\int_i |\varphi^N_{0i}(-\vec{K}_i)|^2 = \sum\!\!\!\!\!\!\int_i \breve{S}_{0i} = N \, , \tag{C.131}$$

using the sum rule for the spectroscopic factors $\breve{S}_{0i}$. As a verification, the number of nucleons is then

$$\frac{1}{\mathcal{V}} \int \mathrm{d}\vec{r} \, \rho(\vec{r}) = N \frac{\mathcal{V}}{\mathcal{V}} = N \, . \tag{C.132}$$

This is a consequence of the fact that standard spectroscopic amplitudes are now plane waves. They still verify asymptotically the free Schrödinger equation, but with positive energy, which explains how the density in the laboratory frame can be uniform.

C.3.2 Internal density

From this point on, it is crucial to find an expression for the internal one-body density operator. However, there are several ways to define it. We compare here two possible definitions:

- The first possible solution reads

$$\begin{aligned} \rho^{[1]}(\vec{r}, \vec{r}') =& \langle \Psi^N_0 | \hat{\rho}^{[1]}(\vec{r}, \vec{r}') | \Psi^N_0 \rangle \\ =& N \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1} \, \delta(\vec{R}_{N-1}) \, \Psi^{N*}_0(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}') \, \Psi^N_0(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}) \, . \end{aligned} \tag{C.133}$$

  The variable change $(\vec{r}_1 \ldots \vec{r}_N) \to (\vec{\xi}_1 \ldots \vec{\xi}_{N-1}, \vec{r}_N)$ has been used. Its diagonal part $\rho^{[1]}(\vec{r})$ represents the probability to find a particle at position $\vec{r}$ with respect to the center-of-mass **of the remaining** $(N-1)$ **particles**.

- On the other hand one may also define the internal density such that its diagonal part is the probability to find a particle with respect to the **total c.o.m. of the** N**-body system**

$$\begin{aligned} \rho^{[2]}(\vec{r}, \vec{r}') =& \langle \Psi^N_0 | \hat{\rho}^{[2]}(\vec{r}, \vec{r}') | \Psi^N_0 \rangle \\ =& N \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1} \, \delta(\overline{\vec{R}}_N) \, \Psi^{N*}_0(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}') \, \Psi^N_0(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}) \, . \end{aligned} \tag{C.134}$$

  In this case the c.o.m. position is defined as

$$\overline{\vec{R}}_N = \frac{1}{N} \sum_{i=1}^{N-1} \vec{r}_i + \frac{1}{2N} (\vec{r} + \vec{r}') \, . \tag{C.135}$$

C.3.2.1 Operatorial form of $\hat{\rho}^{[1]}$

Let us start in the fictious case where the operator for the local part of the density matrix $\rho^{[1]}(\vec{r}) \equiv \rho^{[1]}(\vec{r},\vec{r}\,)$ only acts on the internal wave functions $\Phi^N/\ddot{\Phi}^N$. One has then [13]

$$\hat{\rho}^{[1]}(\vec{r}) = N\,\delta(\vec{r}-\vec{\xi}_{N-1}) = N\,\delta(\vec{r}-\vec{r}_N+\vec{R}_{N-1})\,. \tag{C.136}$$

Using Eq. (C.136) applied only to the internal wave functions, one finds

$$\begin{aligned}
\rho^{[1]}(\vec{r}) =& N\int \mathrm{d}\vec{\xi}_1\ldots\mathrm{d}\vec{\xi}_{N-1}\,\ddot{\Phi}_0^{N*}(\vec{\xi}_1\ldots\vec{\xi}_{N-1})\,\delta(\vec{r}-\vec{\xi}_{N-1})\,\ddot{\Phi}_0^{N}(\vec{\xi}_1\ldots\vec{\xi}_{N-1})\\
=& N\int \mathrm{d}\vec{\xi}_1\ldots\mathrm{d}\vec{\xi}_{N-2}\,|\ddot{\Phi}_0^N(\vec{\xi}_1\ldots\vec{\xi}_{N-2},\vec{r}\,)|^2\\
=& N\int \mathrm{d}\vec{\xi}_1\ldots\mathrm{d}\vec{\xi}_{N-2}\,d\vec{R}_{N-1}\,\delta(\vec{R}_{N-1})\,|\ddot{\Phi}_0^N(\vec{\xi}_1\ldots\vec{\xi}_{N-2},\vec{r}\,)|^2\\
=& N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,\delta(\vec{R}_{N-1})\,|\Phi_0^N(\vec{r}_1\ldots\vec{r}_{N-1},\vec{r}+\vec{R}_{N-1})|^2 \qquad \text{(C.137a)}\\
=& N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,\delta(\vec{R}_{N-1})\,|\Phi_0^N(\vec{r}_1-\vec{R}_{N-1}\ldots\vec{r}_{N-1}-\vec{R}_{N-1},\vec{r}\,)|^2\\
=& N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,\delta(\vec{R}_{N-1})\,|\Phi_0^N(\vec{r}_1\ldots\vec{r}_{N-1},\vec{r}\,)|^2\,, \qquad \text{(C.137b)}
\end{aligned}$$

where Eq. (C.137a) is the exact expression one would have directly obtained using Eq. (C.136). To find the definition of the internal density operator in the full Hilbert space, Eq. (C.136) can be generalized into

$$\hat{\rho}^{[1]}(\vec{r}) = \delta(\hat{\vec{R}}_N)\sum_{i=1}^{N}\delta(\vec{r}-\vec{r}_i+\vec{R}_{N-1}^{(i)})\,, \tag{C.138}$$

where

$$\vec{R}_{N-1}^{(i)} = \frac{1}{N-1}\sum_{\substack{j=1\\ j\neq i}}^{N}\vec{r}_j\,. \tag{C.139}$$

More generally, one has for an arbitrary translation of the center-of-mass of the system

$$\hat{\rho}^{[1]}(\vec{r}) = \delta(\hat{\vec{R}}_N+\vec{a}\,)\sum_{i=1}^{N}\delta(\vec{r}-\vec{r}_i+\vec{R}_{N-1}^{(i)})\,, \tag{C.140}$$

This leads to

$$\begin{aligned}
\rho^{[1]}(\vec{r}) =& \sum_{i=1}^{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\,|\Phi_0^N(\vec{r}_1\ldots\vec{r}_N)|^2\,\delta(\hat{\vec{R}_N})\,\delta(\vec{r}-\vec{r}_i+\vec{R}_{N-1}^{(i)})\\
=& N^3\sum_{i=1}^{N}\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{i-1}\,d\vec{r}_{i+1}\ldots d\vec{r}_N\\
&\qquad\times|\Phi_0^N(\vec{r}_1\ldots\vec{r}_{i-1},-(N-1)\vec{R}_{N-1}^{(i)},\vec{r}_{i+1}\ldots\vec{r}_N)|^2\,\delta(\vec{r}+N\vec{R}_{N-1}^{(i)}) \qquad \text{(C.141a)}\\
=& N^4\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,|\Phi_0^N(\vec{r}_1\ldots\vec{r}_{N-1},-(N-1)\vec{R}_{N-1})|^2\,\delta(\vec{r}+N\vec{R}_{N-1})\\
=& N^4\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\,|\Phi_0^N(\vec{r}_1\ldots\vec{r}_N)|^2\,\delta(\vec{r}+N\vec{R}_{N-1})\,\delta(\vec{r}_N+(N-1)\vec{R}_{N-1}) \qquad \text{(C.141b)}\\
=& N^4\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_N\,|\ddot{\Phi}_0^N(\vec{\xi}_1\ldots\vec{\xi}_{N-1})|^2\,\delta(\vec{r}+N\vec{R}_{N-1})\,\delta(\vec{r}_N+(N-1)\vec{R}_{N-1})
\end{aligned}$$

$$
\begin{aligned}
&= N^4 \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1} \, |\ddot{\Phi}_0^N(\vec{\xi}_1 \ldots - N\vec{R}_{N-1})|^2 \, \delta(\vec{r} + N\vec{R}_{N-1}) \\
&= N^4 \int \mathrm{d}\vec{\xi}_1 \ldots \mathrm{d}\vec{\xi}_{N-2} d\vec{R}_{N-1} \, |\ddot{\Phi}_0^N(\vec{\xi}_1 \ldots \vec{\xi}_{N-1}, -N\vec{R}_{N-1})|^2 \, \delta(\vec{r} + N\vec{R}_{N-1}) \\
&= N^4 \int \mathrm{d}\vec{\xi}_1 \ldots \mathrm{d}\vec{\xi}_{N-2} d\vec{R}_{N-1} \, |\ddot{\Phi}_0^N(\vec{\xi}_1 \ldots - N\vec{R}_{N-1})|^2 \, \delta(\vec{r} + N\vec{R}_{N-1}) \\
&= N \int \mathrm{d}\vec{\xi}_1 \ldots \mathrm{d}\vec{\xi}_{N-2} \, |\ddot{\Phi}_0^N(\vec{\xi}_1 \ldots \vec{\xi}_{N-1}, \vec{r})|^2 \,, \qquad \text{(C.141c)}
\end{aligned}
$$

since

$$
\vec{R}_N = \vec{0} \Rightarrow \frac{1}{N}\vec{r}_i = -\frac{1}{N}\sum_{\substack{j=1 \\ \neq i}}^{N} \vec{r}_j \Rightarrow \frac{1}{N}\vec{r}_i = \frac{N-1}{N}\vec{R}_{N-1}^{(i)} \Rightarrow \delta(\vec{r} - \vec{r}_i + \vec{R}_{N-1}^{(i)}) = \delta(\vec{r} + N\vec{R}_{N-1}^{(i)}) \,, \qquad \text{(C.142)}
$$

which corresponds to Eq. (C.137b). In particular, Eq. (C.141b) shows that the one-body density operator also reads

$$
\begin{aligned}
\hat{\rho}^{[1]}(\vec{r}) &= N^4 \, \delta(\vec{r} + N\vec{R}_{N-1}) \, \delta(\vec{r}_N + (N-1)\vec{R}_{N-1}) \\
&= N^3 \sum_{i=1}^{N} \delta(\vec{r} + N\vec{R}_{N-1}^{(i)}) \, \delta(\vec{r}_i + (N-1)\vec{R}_{N-1}^{(i)}) \,. \qquad \text{(C.143)}
\end{aligned}
$$

Using the previous arguments, the one-body internal density matrix can therefore be expressed as

$$
\begin{aligned}
\hat{\rho}^{[1]}(\vec{r}, \vec{r}\,') &= N \, \delta(\vec{r} - \hat{\vec{\xi}}_{N-1}) \, \delta(\vec{r}\,' - \hat{\vec{\xi}}_{N-1}{}') \\
&= \delta(\vec{R}_N) \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i + \vec{R}_{N-1}^{(i)}) \times \delta(\vec{R}_N') \sum_{j=1}^{N} \delta(\vec{r}\,' - \vec{r}_j' + \vec{R}_{N-1}^{(i)'}) \\
&= N^3 \sum_{i=1}^{N} \delta(\vec{r} + N\vec{R}_{N-1}^{(i)}) \delta(\vec{r}_i + (N-1)\vec{R}_{N-1}^{(i)}) \\
&\quad \times \sum_{j=1}^{N} \delta(\vec{r}\,' + N\vec{R}_{N-1}^{(j)'}) \delta(\vec{r}_j' + (N-1)\vec{R}_{N-1}^{(j)'}) \,, \qquad \text{(C.144)}
\end{aligned}
$$

which leads to [13; 15]

$$
\begin{aligned}
\rho^{[1]}(\vec{r}, \vec{r}\,') &= \langle \Psi_0^N | \hat{\rho}^{[1]}(\vec{r}, \vec{r}\,') | \Psi_0^N \rangle \\
&= N \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1} \, \Psi_0^{N*}(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}\,') \, \delta(\vec{R}_{N-1}) \Psi_0^N(\vec{r}_1 \ldots \vec{r}_{N-1}, \vec{r}) \qquad \text{(C.145a)} \\
&= N \int \mathrm{d}\vec{\xi}_1 \ldots \mathrm{d}\vec{\xi}_{N-2} \, \Psi_0^{N*}(\vec{\xi}_1 \ldots \vec{\xi}_{N-2}, \vec{r}\,') \, \Psi_0^N(\vec{\xi}_1 \ldots \vec{\xi}_{N-2}, \vec{r}) \,. \qquad \text{(C.145b)}
\end{aligned}
$$

A similar expression for Eq. (C.145a) reads

$$
\overline{\rho}^{[1]}(\vec{y}, \vec{y}\,') = N \int \mathrm{d}\vec{r}_1 \ldots \mathrm{d}\vec{r}_{N-1} \, \Psi_0^{N*}\left(\vec{r}_1 \ldots \vec{r}_{N-1}, \frac{\vec{y}\,'}{2}\right) \delta(\vec{y} + \vec{R}_{N-1}) \Psi_0^N\left(\vec{r}_1 \ldots \vec{r}_{N-1}, \frac{\vec{y}\,'}{2}\right) ,
$$

using the relative and center-of-mass coordinates $\vec{y} = \frac{\vec{r}+\vec{r}\,'}{2}$ and $\vec{y}\,' = \vec{r}\,' - \vec{r}$.

C.3.2.2 Properties of $\hat{\rho}^{[1]}$

$\hat{\rho}^{[1]}(\vec{r},\vec{r}')$ is a N-body operator, thus includes more correlations than tye laboratory density $\hat{\rho}^{\text{lab}}(\vec{r},\vec{r}')$. This may be the reason the densities in the internal and laboratory frame have different transformation rules under a translation of the system. Indeed, $\hat{\rho}^{\text{lab}}(\vec{r},\vec{r}')$ transforms as a scalar, $\hat{\rho}^{[1]}(\vec{r},\vec{r}')$ is invariant. Using Eq. (C.67), the ground state one-body internal density becomes a function of the overlaps, i.e.

$$\rho^{[1]}(\vec{r},\vec{r}') = \sum_{i=0}^{+\infty} \varphi_{0i}^{*}(\vec{r}')\varphi_{0i}(\vec{r})\,. \tag{C.146}$$

Eq. (C.146) shows immediately that $\hat{\rho}^{[1]}$ has positive eigenvalues and its trace is normalized to the total particle number. On the other hand the trace of $\hat{\rho}^{[1]}$ is immediately

$$Tr(\hat{\rho}^{[1]}) = \int \mathrm{d}\vec{r}\,\rho^{[1]}(\vec{r},\vec{r}) = \sum_{i} S_{0i} = N\,, \tag{C.147}$$

using the spectroscopic factors sum rule. According to the coupled equation for the internal overlap function (Eq. (C.97)), one finds that the asymptotics of the internal one-body density reads[18]

$$\rho^{[1]}(r,r') \underset{r'\to+\infty}{\longrightarrow} \varphi_{00}^{N}(r)\,\mathcal{C}_0\,\frac{e^{-\kappa_0 r'}}{r'}\,, \tag{C.148}$$

where $\kappa_0 = \frac{1}{\hbar}\sqrt{2m(E_0^{N-1} - E_0^{N})}$. Thus

$$\rho^{[1]}(r) = \rho^{[1]}(r,r) \underset{r\to+\infty}{\longrightarrow} |\mathcal{C}_0|^2\,\frac{e^{-2\kappa_0 r}}{r^2}\,. \tag{C.149}$$

The associated momentum distribution becomes, using Eq. (C.72)

$$\begin{aligned}\eta(\vec{q}) =& \frac{1}{(2\pi)^3}\int \mathrm{d}\vec{y}\,\mathrm{d}\vec{y}'\,e^{-i\,\vec{q}\cdot\vec{y}'}\overline{\rho}^{[1]}(\vec{y},\vec{y}') \\ =& N\int \mathrm{d}\vec{q}_1\ldots\mathrm{d}\vec{q}_{N-1}|\Psi_0^N(\vec{q}_1\ldots\vec{q}_{N-1},\vec{q})|^2\,\delta\left(\vec{q}+\sum_{i=1}^{N-1}\vec{q}_i\right)\,.\end{aligned} \tag{C.150}$$

Finally, Eq. (C.137b) shows that the internal density in invariant under an arbitrary translation $\hat{T}_{\vec{a}}$ of the system of vector $\vec{a}$, that is

$$\rho^{[1]}_{\vec{a}}(\vec{r}) = \langle\Psi_0^N|\hat{T}_{\vec{a}}\,\hat{\rho}^{[1]}\,\hat{T}_{\vec{a}}^{\dagger}|\Psi_0^N\rangle = \rho^{[1]}(\vec{r})\,. \tag{C.151}$$

Generalization of this property to other kinds of internal density (i.e. with respect to rotation, particle number...) is still an open question, although it seems somewhat natural.

C.3.2.3 Properties of $\hat{\rho}^{[2]}$

The local part of $\hat{\rho}^{[2]}$ reads

$$\rho^{[2]}(\vec{r}) = N\int \mathrm{d}\vec{r}_1\ldots\mathrm{d}\vec{r}_{N-1}\,\delta(\overline{\vec{R}}_N^{[1]})\,|\Psi_0^N(\vec{r}_1\ldots\vec{r}_{N-1},\vec{r})|^2\,, \tag{C.152}$$

where the c.o.m. position is defined as

$$\overline{\vec{R}}_N^{[1]} = \frac{1}{N}\sum_{i=1}^{N-1}\vec{r}_i + \frac{1}{N}\vec{r}\,. \tag{C.153}$$

[18] Note that overlaps are assimilated to their radial parts here.

It appears that $\rho^{[2]}(\vec{r})$ is the expectation value of

$$\hat{\rho}^{[2]}(\vec{r}) = N\,\delta(\vec{R}_N)\,\delta(\vec{r}-\vec{r}_N) = \delta(\vec{R}_N)\sum_{i=1}^{N}\delta(\vec{r}-\vec{r}_i) = N\,\delta\left(\vec{r}-\frac{N-1}{N}\vec{\xi}_{N-1}\right). \tag{C.154}$$

Equivalently, for the one-body density matrix one has

$$\hat{\rho}^{[2]}(\vec{r},\vec{r}\,') = N\,\delta\left(\vec{r}-\frac{N-1}{N}\vec{\xi}_{N-1}\right)\,\delta\left(\vec{r}\,'-\frac{N-1}{N}\vec{\xi}\,'_{N-1}\right). \tag{C.155}$$

The one-body matrices $\rho^{[1]}$ and $\rho^{[2]}$ are related through

$$\rho^{[2]}(\vec{r},\vec{r}\,') = \left(\frac{N}{N-1}\right)^3\rho^{[1]}\left(\vec{r}+\frac{\vec{r}+\vec{r}\,'}{2(N-1)},\vec{r}\,'+\frac{\vec{r}+\vec{r}\,'}{2(N-1)}\right), \tag{C.156a}$$

$$\rho^{[2]}(\vec{r}) = \left(\frac{N}{N-1}\right)^3\rho^{[1]}\left(\frac{N}{N-1}\vec{r}\right). \tag{C.156b}$$

In particular, contrary to $\rho^{[1]}$, $\rho^{[2]}(\vec{r},\vec{r}\,')$ does not have any simple decomposition in terms of single-particle overlaps. However, its local part $\rho^{[2]}(\vec{r})$ does in terms of the overlaps $\dot{\varphi}^N_{\nu i}$ previously defined, and Eq. (C.156b) can be derived from Eq. (C.77).

However, eigenvalues of $\hat{\rho}^{[2]}$ are not necessarily positive. Indeed, let us consider the $N=2$ d-dimension case [23], where an internal two-body wave function reads $\Psi^2(x_1,x_2) = f(x_1-x_2)$, with $\int \mathrm{d}x\,|f(x)|^2 = 1$. Because of permutation symmetry, Φ^2 has good parity, i.e. $f(-x) = \eta\,f(x)$, $\eta=+1$ for bosons, $\eta=-1$ for fermions. In this case one has

$$\rho^{[2]}(x,x') = 2^{d+1}\,f\left(\frac{3}{2}x+\frac{1}{2}x'\right)\,f\left(\frac{1}{2}x+\frac{3}{2}x'\right). \tag{C.157}$$

$\rho^{[2]}(x,x')$ is invariant under a parity transformation, thus $\rho^{[2]}(-x,-x') = \rho^{[2]}(x,x')$, and its eigenfunctions also have good parities. However, both parities $\pm\eta$ are present. Indeed, $\rho^{[2]}(x,x')$ can be projected on its even and odd parity eigenspaces such that

$$\begin{aligned}\rho^{[2]}_{\pm}(x,x') =& \frac{1}{2}\left[\rho^{[2]}(x,x')\pm\rho^{[2]}(x,-x')\right]\\ =& 2^d\left[f\left(\frac{3}{2}x+\frac{1}{2}x'\right)\,f\left(\frac{1}{2}x+\frac{3}{2}x'\right)\pm f\left(\frac{3}{2}x-\frac{1}{2}x'\right)\,f\left(\frac{1}{2}x-\frac{3}{2}x'\right)\right].\end{aligned} \tag{C.158}$$

The trace of those components reads

$$Tr[\rho^{[2]}_{\pm}] = \int \mathrm{d}x\rho^{[2]}_{\pm}(x,x) = 2^d\int \mathrm{d}x\,\left[|f(2x)|^2\pm\eta|f(x)|^2\right] = 1\pm\eta\,2^d. \tag{C.159}$$

This shows that eigenfunctions with the wrong parity $-\eta$ have a negative summed eigenvalue strength, i.e.

$$\int \mathrm{d}x\rho^{[2]}_{-\eta}(x,x) = 1-2^d<0, \tag{C.160}$$

proving that negative eigenvalues are present. For $d=1$ explicit examples can be constructed. Indeed, harmonic oscillator wave functions read

$$f_0(a,x) = \frac{1}{a^{1/2}\pi^{1/4}}e^{-\frac{x^2}{2a^2}} \tag{C.161a}$$

$$f_0(a,x) = \frac{\sqrt{2}}{a^{1/2}\pi^{1/4}}e^{-\frac{x^2}{2a^2}}\frac{x}{a} \tag{C.161b}$$

$$f_0(a,x) = \frac{\sqrt{2}}{a^{1/2}\pi^{1/4}}e^{-\frac{x^2}{2a^2}}\left[\left(\frac{x}{a}\right)^2-\frac{1}{2}\right], \tag{C.161c}$$

and associated density matrices can be numerically diagonalized into

$$\rho_i^{[2]}(x,x') = 4\, f_i\left(\frac{3}{2}x+\frac{1}{2}x'\right)\, f_i\left(\frac{1}{2}x+\frac{3}{2}x'\right)\,. \tag{C.162}$$

One finds then for $i=0$ a lowest eigenvalue of -0.8888888888 and for $i=1$ a lowest one of -1.481481. Both are in the wrong parity eigenspace, odd for $i=0$ and even for $i=1$. It is found actually after some trial and error that the corresponding eigenfunctions are

- $f_1(a/\sqrt{2},x)$ in the $i=0$ subspace, corresponding to an eigenvalue of $-8/9$.
- $f_2(a/\sqrt{2},x)$ in the $i=1$ subspace, corresponding to an eigenvalue of $-40/27$.

For this reason, $\rho^{[2]}(\vec{r},\vec{r}\,')$ appears to be a bad definition for the internal one-body density[19]. $\rho^{[1]}(\vec{r},\vec{r}\,')$ was found to be the tool of choice for knockout reactions, but $\rho^{[2]}(\vec{r},\vec{r}\,')$ is the one involved when looking at electron scattering [13; 22]. Indeed, in the case of a three-momentum transfer $\vec{q}$ to the N-body system, as depicted in FIG. C.2, the proton matter form factor is written as

$$F_M(\vec{q}^{\,2}) = \frac{1}{Z}\sum_{j=1}^{N}\int \mathrm{d}\vec{k}\,'\,\phi_j^*\left(\frac{(N-1)(\vec{k}-\vec{k}\,')-\vec{k}\,'}{N-1}\right)\phi_j\left(\frac{(N-1)(\vec{k}-\vec{k}\,'+\vec{q})-\vec{k}\,'}{N-1}\right)\,, \tag{C.163}$$

where the proton internal form factor is neglected. This gives for the charge density, after a Fourier transform

$$\rho_C(\vec{r}) = \frac{1}{Z}\left(\frac{N}{N-1}\right)^3\sum_{j=1}^{N}\phi_j^*\left(\frac{N}{N-1}\vec{r}\right)\phi_j\left(\frac{N}{N-1}\vec{r}\right)\,. \tag{C.164}$$

Indeed, the charge density is defined with the origin of the coordinate system to be the center-of-mass of the N-body system. The factor $\frac{N}{N-1}$ relates to this coordinate system the coordinates variables of the ϕ_j overlaps, defined with the center-of-mass of the $(N-1)$-body frame in the origin.

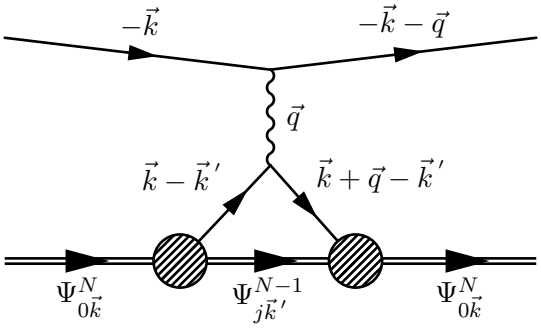


Figure C.2: Electron scattering in the center-of-mass frame for a momentum transfer $\vec{q}$.

[19] It may be worth checking if one may use it anyway if the problem is correctly written to eliminate the wrong parity subspace.

C.4 Energy density functional framework

It appears that a connection with the energy density functional framework is possible by considering that EDF auxiliary states aim at mapping the internal density $\rho^{[1]}(\vec{r})$. In this case the EDF one-body density is computed using the usual formula in the "laboratory frame". The next step is to approximate further the internal overlap by either HF or HFB wave functions. In particular spectroscopic factors are then equal to quasiparticle occupations. However, several points have been raised and should be kept in mind:

- for self-bound systems, spectroscopic factors might be greater than one in some cases. One has to be careful here, as the spectroscopic factors in the EDF method are by essence lower than one.
- When computing the charge density, correction factors from Eq. (C.164) have to be taken into account for the coordinate change.
- The definition of ISDs with respect to either $\vec{R}_N$ and $\vec{R}_{N-1}$ has to be studied. In particular, it should be interesting to apply $\hat{\rho}^{[1]}(\vec{r},\vec{r}')$ and $\hat{\rho}^{[2]}(\vec{r},\vec{r}')$ to those ISDs and find associated instrinsic densities, and whether they take a "canonical" form or not.
- One the other hand, it should be interesting, starting from a Slater determinant to evaluate numerically the density in its three definitions, and compare it to exact formulæ [24].

Following the analysis from Ref. [19], one can introduce the natural orbitals ϕ_α defined as the complete orthonormal set of single-particle wave functions which diagonalizes $\hat{\rho}^{[1]}$, i.e.

$$\hat{\rho}^{[1]}(\vec{r},\vec{r}') = \sum_\alpha n_\alpha\, \phi_\alpha^*(\vec{r}')\phi_\alpha(\vec{r})\,, \tag{C.165}$$

where corresponding eigenvalues n_α are called the natural occupation numbers. For fixed-center systems, those are lower or equal to one, but may be larger in the present case of self-bound systems. Indeed, in the $N=2$ case from Sec. C.2.3, one gets $\rho^{[1]}(x,x') = 2\,f(x)\,f^*(x')$, which has a $n_\alpha = 2$ eigenvalue.

One the one hand occupation numbers of the overlap functions $\varphi^N_{\nu i}$ can be defined as [25]

$$N_{\nu i} = \frac{1}{S_{\nu i}} \int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}'\varphi^{N*}_{\nu i}(\vec{r}')\,\rho^{[1]}(\vec{r},\vec{r}')\,\varphi^N_{\nu i}(\vec{r}) = \frac{1}{S_{\nu i}} \sum_\alpha n_\alpha\, |\langle\varphi^N_{\nu i}|\phi_\alpha\rangle|^2\,. \tag{C.166}$$

Thus one has

$$S^2_{\nu i} = |\langle\varphi^N_{\nu i}|\varphi^N_{\nu i}\rangle|^2 \leq \cancel{\sum_j} |\langle\varphi^N_{\nu i}|\varphi^N_{\nu j}\rangle|^2 = \sum_\alpha n_\alpha\, |\langle\varphi^N_{\nu i}|\phi_\alpha\rangle|^2\,, \tag{C.167}$$

and one always has

$$S_{\nu i} \leq N_{\nu i} \leq n_{max}\,, \tag{C.168}$$

where d_{max} is the largest occupation number.

On the other hand natural orbitals are defined as the solutions of the eigenvalues equation

$$\int \mathrm{d}r'\, r'^2\, \rho^{[1]}(r,r')\,\phi_\alpha(r') = n_\alpha\,\phi_\alpha(r)\,. \tag{C.169}$$

Taking the limit $r \to +\infty$ for occupied natural orbitals[20], one finds

$$\phi_\alpha(r) \underset{r\to+\infty}{\longrightarrow} \mathcal{C}_0\, \frac{e^{-\kappa_0\, r}}{r}\, \frac{\langle\varphi^N_{00}|\phi_\alpha\rangle}{d_\alpha}\,, \tag{C.170}$$

[20] For $d_\alpha = 0$, one has $\cancel{\sum}_j |\langle\phi_\alpha|\varphi^N_{\nu j}\rangle|^2$, thus a zero overlap between ϕ_α and all the overlap functions.

Thus all natural orbitals have the same decay as the lowest bound eigenstate, as long as the overlap $\langle\varphi^N_{00}|\phi_\alpha\rangle$ does not vanish, which is true only for non-interacting systems where natural and overlap bases coincide. Expanding the overlaps in the natural basis

$$\varphi^N_{\nu i}(r) = \sum_\alpha \langle\varphi^N_{\nu i}|\phi_\alpha\rangle\, \phi_\alpha(r)\,, \tag{C.171}$$

and taking the limit of large r gives the sum rule

$$\sum_\alpha \frac{\langle\varphi^N_{00}|\phi_\alpha\rangle\langle\phi_\alpha|\varphi^N_{0i}\rangle}{d_\alpha} = \delta_{0\nu}\,. \tag{C.172}$$

C.5 Possible extensions

Internal degrees of freedom can be easily defined in the case of translational invariance, since the center-of-mass motion is directly separated at the wave function level. Similar definitions would be of very interest for other symmetries, such as rotational or particle number ones, however they would involve more complex derivations. Nevertheless, this would allow to interpret accurately the mapping between the EDF one-body density and the true internal one of the many-body system for these additional symmetries. This might also help devising a proper Hohenberg-Kohn-like theorem including the internal density with respect to all underlying symmetries of the problem, as it is under study for the translational symmetry [24].

Appendix D

Properties of nuclear forces

Abstract: This chapter presents detailed calculations concerning the properties of nuclear forces, such as scattering phase shifts, nuclear matter equation of state or gap equation.

Contents

D.1 Tensor interaction

D.1.1 One-pion exchange interaction and Yukawa potential

D.1.1.1 Scalar mesons

In non-relativistic field theory, the coupling between nucleons of mass m and scalar mesons is described by the Lagrangian density

$$\delta\mathcal{L}(\vec{x}\,) = g\,\Psi^{\dagger}(\vec{x}\,)\,\phi(\vec{x}\,)\,\Psi(\vec{x}\,) = -\delta\mathcal{H}(\vec{x}\,)\,, \tag{D.1}$$

where $\Psi(\vec{x}\,)$ is the nucleon wave function and $\phi(\vec{x}\,)$ the scalar meson field. The latter can be expanded in a Fourier series as

$$\phi(\vec{x}\,) \equiv \sum_{q=0}^{+\infty} \sqrt{\frac{2\pi}{\omega_q}} k_q \, e^{i\,\vec{q}\cdot\vec{x}}\,, \tag{D.2}$$

where

$$\omega_q = \sqrt{q^2+\mu^2}\,, \tag{D.3}$$

μ being the meson mass, such that the meson density is $\rho = 2\omega_q|\phi|^2$. The hamiltonian of the meson field can be cast into a superposition of harmonic oscillators of energies ω_q and coordinates k_q. Taking a number of quanta n_q in those oscillators equal to 0 (no meson) or 1 (one meson), the resulting nucleon-nucleon interaction is obtained in second-order perturbation theory from the time-ordered diagrams presented in Fig. D.1.

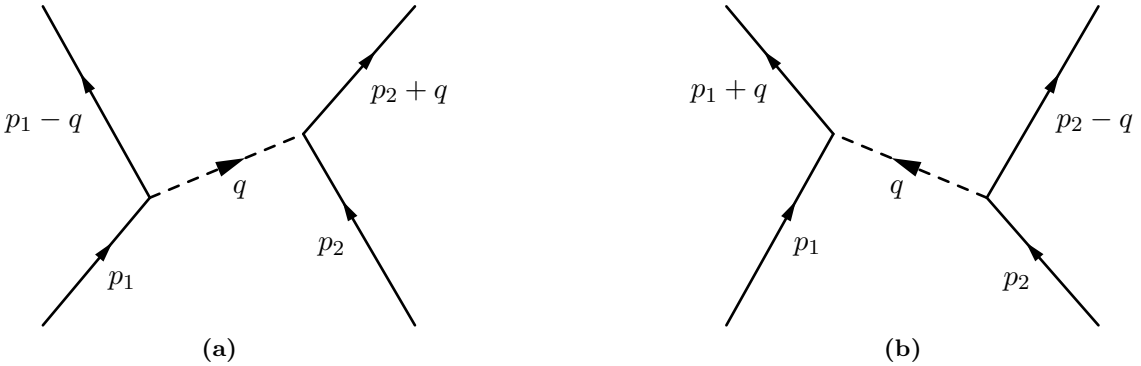


Figure D.1: Time-ordered diagrams for the one-meson scalar exchange. Time flows from bottom to top.

In both cases the initial energy reads

$$E_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m}\,, \tag{D.4}$$

whereas the intermediate state energy is

$$E_i^{(a)} = \omega_q + \frac{(p_1-q)^2}{2m} + \frac{p_2^2}{2m} \qquad \text{for the diagram of Fig. D.1a,} \tag{D.5a}$$

$$E_i^{(b)} = \omega_q + \frac{(p_2+q)^2}{2m} + \frac{p_1^2}{2m} \qquad \text{for the diagram of Fig. D.1b.} \tag{D.5b}$$

The entire expression for the process reads in second-order perturbation theory

$$\left(\frac{\langle f|\delta\mathcal{H}|i\rangle\langle i|\delta\mathcal{H}|0\rangle}{E_0 - E_i^{(a)}}\right)^{(a)} = g^2 \left(\frac{2\pi}{\omega_q}\right) \frac{1}{\frac{p_1^2}{2m} - \omega_q - \frac{(p_1-q)^2}{2m}} \qquad \text{for Fig. D.1a,} \tag{D.6a}$$

$$\left(\frac{\langle f|\delta\mathcal{H}|i\rangle\langle i|\delta\mathcal{H}|0\rangle}{E_0 - E_i^{(b)}}\right)^{(b)} = g^2 \left(\frac{2\pi}{\omega_q}\right) \frac{1}{\frac{p_2^2}{2m} - \omega_q - \frac{(p_2+q)^2}{2m}} \qquad \text{for Fig. D.1b,} \tag{D.6b}$$

where $|0\rangle$ is the initial state, $|i\rangle$ the intermediate state and $|f\rangle$ the final one. It is assumed that all momenta involved are of the same order of magnitude. The meson resonance occurs for $q \sim \mu$,

thus $\frac{p_i^2}{2m}$ and $\frac{(p_i \pm q)^2}{2m}$ terms are of order $\frac{\mu}{m}$, and for light mesons $\mu \ll m$ they are all small in comparison with ω_q. The total matrix element for the nucleon-nucleon interaction becomes then

$$\frac{\langle f|\delta\mathcal{H}|i\rangle\langle i|\delta\mathcal{H}|0\rangle}{E_0 - E_i} = -g^2\frac{4\pi}{\omega_q^2} = -g^2\frac{4\pi}{q^2+\mu^2} \equiv v(\vec{q}\,)\,. \tag{D.7}$$

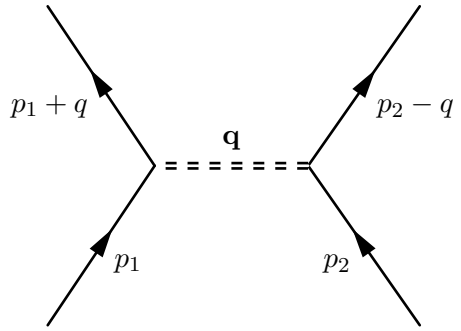


Figure D.2: Feynman diagram for the one-scalar meson exchange.

Another method consists in evaluating directly the scattering amplitude of the Feynman diagram from Fig. D.2. Using the usual Feynman rules, the matrix element for nucleon scattering reads

$$\mathcal{M} = 2 \times \Psi^*\, g\, \Psi \frac{-2i\,\pi}{\mathbf{q}^2 - \mu^2 + i\,\epsilon}\, \Psi^*\, g\, \Psi\,, \tag{D.8}$$

where implicit integrations on the nucleon fields are left out, and $\mathbf{q} \equiv (q^0, \vec{q}\,)$ is the momentum transfer. The static potential is obtained by setting $q^0 = 0$ and looking at the three-momentum transfer only, i.e.

$$\mathcal{M} = \Psi^*\,\Psi\,\left[\frac{4i\,\pi\,g^2}{q^2+\mu^2}\right]\,\Psi^*\,\Psi = \langle f| - i\,v(\vec{q}\,)|0\rangle\,. \tag{D.9}$$

Thus one finds for the interaction potential $v(\vec{q}\,)$ the same expression than in Eq. (D.7). Its Fourier transform gives the interaction in coordinate space under the form of the well-known Yukawa potential

$$v(\vec{r}\,) = \int \frac{\mathrm{d}\vec{q}}{(2\pi)^3} v(\vec{q}\,) = -g^2\frac{e^{-\mu r}}{r}\,. \tag{D.10}$$

D.1.1.2 Pseudoscalar mesons

In the low energy limit, the long-range part of the vacuum nucleon-nucleon interaction is dominated, in the meson exchange model, by the exchange of the lightest strongly interacting particle, which is known to be the pion. For low energy processes, one can neglect virtual nucleon pair and π productions, given that the characteristic momentum transfer is of the order of $\frac{q^2}{m}$. The non-relativistic Lagrangian for the axial nucleon-pion $N\pi$ coupling reads

$$\delta\mathcal{L}(\vec{x}\,) = -g_A\,\Psi^\dagger(\vec{x}\,)\left[\vec{\sigma}\cdot\vec{\Pi}\right]\Psi(\vec{x}\,)\,, \tag{D.11}$$

where $g_A = 1.25$ is the axial coupling constant, and $\vec{\Pi}$ is the pseudo-scalar pion propagator

$$\vec{\Pi} = \frac{1}{\sqrt{2}f_\pi}\left[\tau^x\vec{\nabla}\pi^x + \tau^y\vec{\nabla}\pi^y + \tau^z\vec{\nabla}\pi^z\right]\,, \tag{D.12}$$

$f_\pi = 132$ MeV being the pion decay constant. π^{xyz} are components of the pion field, i.e.

$$\pi^\pm = \frac{\pi^x \pm i\,\pi^y}{\sqrt{2}}\,, \qquad \pi^0 = \pi^z\,. \tag{D.13}$$

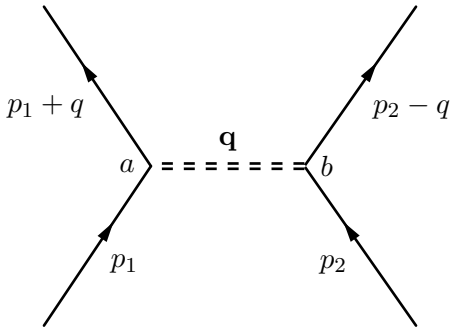


Figure D.3: Feynman diagram for one-pion exchange (pseudo-scalar meson).

The nucleon-nucleon scattering matrix element becomes using an implicit summation rule

$$\mathcal{M} = 2 \times \Psi^* \, \frac{-g_A}{\sqrt{2} f_\pi} \sigma^i \tau^a q^i \, \Psi \frac{-2i\,\pi \delta_{ab}}{\mathbf{q}^2 - \mu^2 + i\,\epsilon} \, \Psi^* \, \frac{g_A}{\sqrt{2} f_\pi} \sigma^j \tau^b q^j \, \Psi \,, \tag{D.14}$$

with the convention that $\partial\phi = -i\,q\phi$ for an incoming scalar field. Thus for the static potential, one finds

$$\begin{aligned} \mathcal{M} =& i\,\Psi^*\,\sigma^i\tau^a\,\Psi 4\pi \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 \frac{q^i q^j}{q^2+\mu^2}\,\Psi^*\,\sigma^j\tau^a\,\Psi, \\ =& -i\,\langle f| \left[-4\pi \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 (\vec{\tau}_1\cdot\vec{\tau}_2\,)\,\frac{(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)}{q^2+\mu^2}\right]|0\rangle \\ =& \langle f| - i\,v_\pi(\vec{q})|0\rangle \,. \end{aligned} \tag{D.15a}$$

The one-pion interaction reads then in momentum space

$$v_\pi(\vec{q}) = -4\pi \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 (\vec{\tau}_1\cdot\vec{\tau}_2\,)\,\frac{(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)}{q^2+\mu^2}\,. \tag{D.16}$$

This potential can be separated in a central part and a pure tensor one according to

$$\begin{aligned} v_\pi(\vec{q}) = -4\pi \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 (\vec{\tau}_1\cdot\vec{\tau}_2\,) \Bigg[& \frac{(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,) - \frac{1}{3}\,(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\,q^2}{q^2+\mu^2} \\ & + \frac{1}{3}\,(\vec{\sigma}_1\cdot\vec{\sigma}_2\,) - \frac{1}{3}\mu^2 \frac{(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)}{q^2+\mu^2}\Bigg]\,. \end{aligned} \tag{D.17}$$

One the other hand, one gets in coordinate space

$$\begin{aligned} v_\pi(\vec{r}\,) =& \int \frac{\mathrm{d}\vec{q}}{(2\pi)^3} e^{i\,\vec{q}\cdot\vec{r}}\, v_\pi(\vec{q}\,) \\ =& -4\pi \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 (\vec{\tau}_1\cdot\vec{\tau}_2\,) \int \frac{\mathrm{d}\vec{q}}{(2\pi)^3} e^{i\,\vec{q}\cdot\vec{r}} \frac{(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\vec{q}\,)}{q^2+\mu^2} \\ =& +4\pi \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 (\vec{\tau}_1\cdot\vec{\tau}_2\,) \left(\vec{\sigma}_1\cdot\vec{\nabla}\right)\left(\vec{\sigma}_2\cdot\vec{\nabla}\right) \int \frac{\mathrm{d}\vec{q}}{(2\pi)^3} e^{i\,\vec{q}\cdot\vec{r}} \frac{1}{q^2+\mu^2} \\ =& \left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 (\vec{\tau}_1\cdot\vec{\tau}_2\,) \left(\vec{\sigma}_1\cdot\vec{\nabla}\right)\left(\vec{\sigma}_2\cdot\vec{\nabla}\right) \frac{e^{-\mu r}}{r}\,. \end{aligned} \tag{D.18a}$$

To recover the tensor operator S_{12}, gradients have to be evaluated, starting in the cartesian basis where $\vec{r} = \sum x^i \vec{e}_i$. We obtain

$$\partial^i \partial^j \left(\frac{e^{-\mu r}}{r}\right) = e^{-\mu r}\, \partial^i \partial^j \left(\frac{1}{r}\right) + \partial^i e^{-\mu r} \times \partial^j \left(\frac{1}{r}\right) + \partial^j e^{-\mu r} \times \partial^i \left(\frac{1}{r}\right) + \frac{1}{r}\, \partial^i \partial^j e^{-\mu r}\,. \quad \text{(D.19)}$$

The action of partial derivatives in Eq. (D.18a) can then be computed using

$$\partial^i r = \partial^i \sqrt{x^{i\,2} + x^{j\,2} + x^{k\,2}} = \frac{2x^i}{2\sqrt{x^{i\,2} + x^{j\,2} + x^{k\,2}}} = \overline{r}^{\,i}\,, \quad \text{(D.20a)}$$

$$\partial^i e^{-\mu r} = \partial^i e^{-\mu\sqrt{x^{i\,2}+x^{j\,2}+x^{k\,2}}} = -\mu \frac{2x^i}{2\sqrt{x^{i\,2} + x^{j\,2} + x^{k\,2}}} e^{\mu r} = -\mu \overline{r}^{\,i} e^{-\mu r}\,, \quad \text{(D.20b)}$$

$$\partial^i e^{-\mu r^2} = \partial^i e^{-\mu\left(x^{i\,2}+x^{j\,2}+x^{k\,2}\right)} = -2\mu\, r\, \overline{r}^{\,i}\, e^{-\mu r^2}\,, \quad \text{(D.20c)}$$

$$\partial^i \left(\frac{1}{r}\right) = -\frac{\overline{r}^{\,i}}{r^2}\,, \quad \text{(D.20d)}$$

$$\partial^i \left(\frac{1}{r^2}\right) = -2\frac{\overline{r}^{\,i}}{r^3}\,, \quad \text{(D.20e)}$$

$$\partial^i \overline{r}^{\,j} = \partial^i \left(\frac{x^j}{\sqrt{x^{i\,2} + x^{j\,2} + x^{k\,2}}}\right) = \frac{\delta_{ij}}{r} - x^j\, \partial^i \left(\frac{1}{r}\right) = \frac{\delta_{ij}}{r} - \frac{\overline{r}^{\,i}\,\overline{r}^{\,j}}{r}\,, \quad \text{(D.20f)}$$

where the normalized vector $\vec{\overline{r}} = \frac{\vec{r}}{r}$, and its components $\overline{r}^{\,i} = \frac{x^i}{r}$ have been defined. This leads to

$$\partial^i e^{-\mu r} \times \partial^j \left(\frac{1}{r}\right) = \mu \frac{\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^2}\, e^{-\mu r} = \partial^j e^{-\mu r} \times \partial^i \left(\frac{1}{r}\right)\,, \quad \text{(D.21a)}$$

$$\frac{1}{r}\, \partial^i \partial^j e^{-\mu r} = \frac{1}{r} \partial^i \left(-\mu\, \overline{r}^{\,j}\, e^{-\mu r}\right) \mu \left[\frac{\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^2} - \frac{\delta_{ij}}{r^2} + \mu \frac{\overline{r}^{\,i}\,\overline{r}^{\,j}}{r}\right] e^{-\mu r}\,, \quad \text{(D.21b)}$$

$$\begin{aligned} e^{-\mu r}\, \partial^i \partial^j \left(\frac{1}{r}\right) &= \left[(1-\delta_{ij})\, \partial^i \partial^j \left(\frac{1}{r}\right) + \delta_{ij}\, \partial^i \partial^j \left(\frac{1}{r}\right)\right] e^{-\mu r} \\ &= \left[(1-\delta_{ij})\, \partial^i \left(-\overline{r}^{\,j} \frac{1}{r^2}\right) + \frac{1}{3}\delta_{ij}\, \Delta \left(\frac{1}{r}\right)\right] e^{-\mu r} \\ &= \left[(1-\delta_{ij}) \left(-\frac{1}{r^2}\, \partial^i \overline{r}^{\,j} - \overline{r}^{\,j}\, \partial^i \left(\frac{1}{r^2}\right)\right) - \frac{4\pi}{3}\delta_{ij}\delta(\vec{r})\right] e^{-\mu r} \\ &= \left[(1-\delta_{ij}) \left(\frac{3\,\overline{r}^{\,i}\,\overline{r}^{\,j} - \delta_{ij}}{r^3}\right) - \frac{4\pi}{3}\delta_{ij}\delta(\vec{r})\right] e^{-\mu r} \\ &= \left[(1-\delta_{ij}) \left(\frac{3\,\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^3}\right) - \frac{4\pi}{3}\delta_{ij}\delta(\vec{r})\right] e^{-\mu r}\,, \end{aligned} \quad \text{(D.21c)}$$

where an explicit separation of the cases $i = j$ and $i \neq j$ is done, and the Poisson law

$$\Delta \left(\frac{1}{r}\right) = -4\pi\, \delta(\vec{r})\,, \quad \text{(D.22)}$$

is used for $i = j$. Likewise, the spherical symmetry of $\frac{1}{r}$ allows to write

$$\delta_{ij}\, \partial^i \partial^j \left(\frac{1}{r}\right) = \delta_{ij}\, \partial^{i\,2} \left(\frac{1}{r}\right) = \frac{1}{3}\delta_{ij}\, \Delta \left(\frac{1}{r}\right)\,. \quad \text{(D.23)}$$

Therefore, one gets for the action of spin dot gradient operators on the Yukawa potential

$$\begin{aligned}
\left(\vec{\sigma}_1\cdot\vec{\nabla}\right)\left(\vec{\sigma}_2\cdot\vec{\nabla}\right)\frac{e^{-\mu r}}{r} &= \sum_{i,j=1}^{3}\sigma_1^i\,\sigma_2^j\,\partial^i\,\partial^j\,\left(\frac{e^{-\mu r}}{r}\right)\\
&= \sum_{i,j=1}^{3}\sigma_1^i\,\sigma_2^j\left[(1-\delta_{ij})\left(\frac{3\,\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^3}\right)-\frac{4\pi}{3}\delta_{ij}\delta(\vec{r}\,)\right.\\
&\qquad\left.+\,\mu\left(\frac{3\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^2}-\frac{\delta_{ij}}{r^2}+\mu\frac{\overline{r}^{\,i}\,\overline{r}^{\,j}}{r}\right)\right]e^{-\mu r}\\
&= \sum_{i,j=1}^{3}\sigma_1^i\,\sigma_2^j\left[\left(\frac{3\,\overline{r}^{\,i}\,\overline{r}^{\,j}-\delta_{ij}}{r^3}\right)+\mu\left(\frac{3\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^2}-\frac{\delta_{ij}}{r^2}+\mu\frac{\overline{r}^{\,i}\,\overline{r}^{\,j}}{r}\right)\right]e^{-\mu r}\\
&\qquad-\sum_{i,j=1}^{3}\sigma_1^i\,\sigma_2^j\,\frac{4\pi}{3}\delta_{ij}\delta(\vec{r}\,)\,e^{-\mu r}\\
&=\mu^3\sum_{i,j=1}^{3}\sigma_1^i\,\sigma_2^j\left[\left(3\,\overline{r}^{\,i}\,\overline{r}^{\,j}-\delta_{ij}\right)\left(1+\frac{1}{3\mu r}+\frac{1}{(\mu r)^2}+\frac{1}{(\mu r)^3}\right)\right.\\
&\qquad\left.+\,\frac{1}{3\mu r}\delta_{ij}\right]e^{-\mu r}-\frac{4\pi}{3}(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\delta(\vec{r}\,)\\
&=\mu^3\left[\left(3\frac{(\vec{\sigma}_1\cdot\vec{r}\,)(\vec{\sigma}_2\cdot\vec{r}\,)}{r^2}-(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\right)\left(1+\frac{1}{3\mu r}+\frac{1}{(\mu r)^2}+\frac{1}{(\mu r)^3}\right)\right.\\
&\qquad\left.+\,\frac{1}{3\mu r}(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\right]e^{-\mu r}-\frac{4\pi}{3}(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\delta(\vec{r}\,)\,,
\end{aligned}\tag{D.24}$$

using

$$\sum_{i,j=1}^{3}\delta_{ij}\frac{3\,\overline{r}^{\,i}\,\overline{r}^{\,j}}{r^3}=\frac{3\,\sum_{i=1}^{3}\overline{r}^{\,i}\,\overline{r}^{\,i}}{r^3}=\frac{3}{r^3}=\sum_{i,j=1}^{3}\frac{\delta_{ij}}{r^3}\,.\tag{D.25}$$

The one-pion interaction reads thus in coordinate space

$$\begin{aligned}
v_\pi(\vec{r}\,)=\mu^3\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2(\vec{\tau}_1\cdot\vec{\tau}_2\,)\left[\mathsf{S}_{12}\left(1+\frac{1}{3\mu r}+\frac{1}{(\mu r)^2}+\frac{1}{(\mu r)^3}\right)e^{-\mu r}\right.\\
\left.+\,\frac{1}{3}(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\left[\frac{e^{-\mu r}}{\mu r}-\frac{4\pi}{3\mu^3}\delta(\vec{r}\,)\right]\right],
\end{aligned}\tag{D.26}$$

with the usual definition for the tensor operator

$$\mathsf{S}_{12}=\frac{3}{r^2}\,(\vec{\sigma}_1\cdot\vec{r}\,)\;(\vec{\sigma}_2\cdot\vec{r}\,)-\vec{\sigma}_1\cdot\vec{\sigma}_2\,.\tag{D.27}$$

The last term in Eq. (D.26) is usually recast into the central part of the effective vertex, and the "tensor interaction" corresponds only to the pure tensor contribution from one-pion exchange.

D.1.2 Properties of the tensor operator

The operator $(3\overline{r}^{\,i}\overline{r}^{\,j}-\delta_{ij})$ is traceless (given that $\sum_i \overline{r}^{\,i}\overline{r}^{\,i}=1$) and symmetric, thus transforms as a $\ell=2$ object under rotations, since

$$\overline{r}^{\,1}=\sin(\theta)\,\cos(\varphi)\,,\qquad \overline{r}^{\,2}=\sin(\theta)\,\sin(\varphi)\,,\qquad \overline{r}^{\,3}=\cos(\theta)\,.\tag{D.28}$$

therefore

$$3\overline{r}^{\,1}\overline{r}^{\,1} - \delta_{11} = 3\,\sin^2(\theta)\,\cos^2(\varphi) - 1 \quad = +3\sqrt{\frac{2\pi}{15}}\left[-\sqrt{\frac{2}{3}}Y_2^0(\theta,\varphi) + Y_2^2(\theta,\varphi) + Y_2^{-2}(\theta,\varphi)\right], \tag{D.29a}$$

$$3\overline{r}^{\,2}\overline{r}^{\,2} - \delta_{22} = 3\,\sin^2(\theta)\,\sin^2(\varphi) - 1 \quad = -3\sqrt{\frac{2\pi}{15}}\left[\sqrt{\frac{2}{3}}Y_2^0(\theta,\varphi) + Y_2^2(\theta,\varphi) + Y_2^{-2}(\theta,\varphi)\right], \tag{D.29b}$$

$$3\overline{r}^{\,3}\overline{r}^{\,3} - \delta_{33} = 3\,\cos^2(\theta) - 1 \quad = +4\frac{\sqrt{\pi}}{5}Y_2^0(\theta,\varphi), \tag{D.29c}$$

$$3\overline{r}^{\,1}\overline{r}^{\,2} - \delta_{12} = 3\,\sin^2(\theta)\,\cos(\varphi)\,\sin(\varphi) \quad = -3i\,\frac{\sqrt{2\pi}}{15}\left[Y_2^2(\theta,\varphi) - Y_2^{-2}(\theta,\varphi)\right], \tag{D.29d}$$

$$3\overline{r}^{\,1}\overline{r}^{\,3} - \delta_{13} = 3\,\sin(\theta)\,\cos(\theta)\,\cos(\varphi) \quad = +3\frac{\sqrt{2\pi}}{15}\left[Y_2^{-1}(\theta,\varphi) - Y_2^1(\theta,\varphi)\right], \tag{D.29e}$$

$$3\overline{r}^{\,2}\overline{r}^{\,3} - \delta_{23} = 3\,\sin(\theta)\,\cos(\theta)\,\sin(\varphi) \quad = +3i\,\frac{\sqrt{2\pi}}{15}\left[Y_2^{-1}(\theta,\varphi) + Y_2^1(\theta,\varphi)\right]. \tag{D.29f}$$

We recall here the expressions of some spherical harmonics in spherical coordinates

$$Y_2^{-2}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\,e^{-2i\,\varphi}\,\sin(\theta)\,\cos\theta\,, \tag{D.30a}$$

$$Y_2^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\,e^{-i\,\varphi}\,\sin(\theta)\,\cos\theta\,, \tag{D.30b}$$

$$Y_2^{0}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta - 1\right), \tag{D.30c}$$

$$Y_2^{1}(\theta,\varphi) = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,e^{i\,\varphi}\,\sin(\theta)\,\cos\theta\,, \tag{D.30d}$$

$$Y_2^{2}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\,e^{2i\,\varphi}\,\sin(\theta)\,\cos\theta\,. \tag{D.30e}$$

Thus S_{12} can be written entirely in terms of $Y_2^n(\theta,\varphi)$ components, thus only contributes when the angular momentum difference between the initial and final state is $\Delta L = 0, \pm 2$, except for $L = L' = 0$ matrix elements which are forbidden. For instance such a tensor will couple s and d waves, and have non-zero matrix elements within p waves.

D.2 Partial wave expansion

The standard expansion of a plane wave in terms of spherical harmonics reads [26]

$$e^{i\,\vec{k}\cdot\vec{r}} \equiv \langle\vec{r}|\vec{k}\,\rangle = 4\pi\sum_{\ell\,m_\ell} i^\ell\,Y_\ell^{m_\ell *}(\hat{k})\,Y_\ell^{m_\ell}(\hat{r})\,j_\ell(k\,r) = \sum_\ell i^\ell\,[\ell\,]\,P_\ell(\hat{k}\cdot\hat{r})\,j_\ell(k\,r)\,, \tag{D.31}$$

using spherical Bessel functions of the first kind j_ℓ, Legendre polynomials P_ℓ, and with $[\ell] \equiv 2\ell+1$. Thus a given state $|\,\vec{k}\,\rangle$ is expanded into

$$|\,\vec{k}\,\rangle \equiv 4\pi\sum_{\ell\,m_\ell} i^\ell\,|\,k\,\ell\,m_\ell\,\rangle\,Y_\ell^{m_\ell *}(\hat{k})\,. \tag{D.32}$$

For two-nucleon scattering, the relative orbital angular momentum L couples to the total spin S of the nucleon pair to give a total two-body angular momentum J, which complexifies the

problem. Still, a partial wave expansion of the nuclear potential $v(\vec{k},\vec{k}\,)$ can be given. Indeed, by analogy with Eq. (D.31), one can expand the spinor $|\vec{k}\,SS_z\,TT_z\rangle$ describing the two-body relative motion[1] into

$$|\vec{k}\,SS_z\,TT_z\rangle \equiv 4\pi \sum_{L}\sum_{JJ_z} i^L\, \mathcal{Y}^{J_z}_{(LS)J}{}^{*}(\hat{k})\,\sqrt{\frac{\pi}{2}}\,|k\,(LS)JJ_zS_z\,TT_z\rangle\,, \tag{D.33}$$

in terms of spin 0 or 1 tensor spherical harmonics $\mathcal{Y}^{J_z}_{(LS)J}(\hat{k})$ (Sec. A.2.4), and with

$$\langle\vec{r}\,|k\,(LS)JJ_zS_z\,TT_z\rangle \equiv \sqrt{\frac{2}{\pi}}\,\mathcal{Y}^{J_z}_{(LS)J}(\hat{r})\,j_L(k\,r)\,|TT_z\rangle\,|S_z\rangle\,. \tag{D.34}$$

One has then

$$\langle\,\vec{r}\,|\vec{k}\,SS_z\,TT_z\rangle = 4\pi \sum_{LJJ_z} i^L\,\mathcal{Y}^{J_z}_{(LS)J}{}^{*}(\hat{k})\,\mathcal{Y}^{J_z}_{(LS)J}(\hat{r})\,j_L(kr)\,|TT_z\rangle\,|S_z\rangle\,, \tag{D.35}$$

such that Eq. (D.31) can be easily recovered for both $S=0$ and $S=1$ spinors. Indeed

- $S=0$ spinors can be identified with scalars, i.e.

$$e^{i\,\vec{k}\cdot\vec{r}} = 4\pi \sum_{LJJ_z} i^L\,\delta_{LJ} Y_L^{J_z}{}^{*}(\hat{k})\,Y_L^{J_z}(\hat{r})\,j_L(kr) = 4\pi \sum_{LL_z} i^L\,Y_L^{L_z}{}^{*}(\hat{k})\,Y_L^{L_z}(\hat{r})\,j_L(kr)\,, \tag{D.36}$$

- for $S=1$ one can take any component of the dimension-3 spinor to evaluate $e^{i\,\vec{k}\cdot\vec{r}}$, that is

$$\begin{aligned} e^{i\,\vec{k}\cdot\vec{r}} =& u_\alpha\cdot 4\pi \sum_{LJJ_z} i^L \sum_{L_zS_z}\sum_{L'_zS'_z} Y_L^{L_z}{}^{*}(\hat{k})\langle L\,L_z\,1\,S_z\,|L\,1\,J\,J_z\rangle^{*}\,\big\langle L\,L'_z\,1\,S'_z\,\big|L\,1\,J\,J_z\big\rangle \\ &\times Y_L^{L'_z}(\hat{r})\,j_L(kr)\,C_1^{S_z}{}^{*}\,C_1^{S'_z} \\ =& u_\alpha\cdot 4\pi \sum_{L} i^L \sum_{L_zS_z} Y_L^{L_z}{}^{*}(\hat{k})Y_L^{L_z}(\hat{r})\,j_L(kr)\,C_1^{S_z}{}^{*}\,C_1^{S_z} \\ =& 4\pi \sum_{LL_z} i^L\,Y_L^{L_z}{}^{*}(\hat{k})Y_L^{L_z}(\hat{r})\,j_L(kr)\,. \end{aligned} \tag{D.37}$$

One cannot couple states with different spins S/S' since the bra and kets would correspond to different $L+S$ coupling schemes. Using a representation where nucleons have a good isospin, and from the fundamental symmetries of the nuclear interaction[2] the dependence of partial waves on T is trivial and no recoupling is needed. The partial wave expansion of potential matrix elements $v(\vec{k},\vec{k}\,')$ reads in a coupled scheme as

$$\begin{aligned} \langle\vec{k}\,SS_z\,TT_z|v|\vec{k}\,'\,SS_z\,TT_z\rangle = \frac{\pi}{2}\,(4\pi)^2 \sum_{LL'}\sum_{JJ'}\sum_{J_zJ'_z} i^{L'-L}\,\mathcal{Y}^{J'_z}_{(L'S)J'}{}^{*}(\hat{k}')\,\mathcal{Y}^{J_z}_{(LS)J}(\hat{k}) \\ \times\langle k\,(LS)JJ_zS_z\,TT_z|v|k'\,(L'S)J'J'_zS_z\,TT_z\rangle\,. \end{aligned} \tag{D.38}$$

The latter expression can be further simplified for realistic nuclear interactions using that (i) v is invariant under the rotation of two particles, i.e. it does not depend on J_z/J'_z, (ii) the total angular momentum J is conserved, (iii) the spin/isospin and their projections are conserved, and (iv) in the absence of tensor force or for $S=0$ states, the orbital momentum L is also conserved.

[1] We choose here to use the spin/isospin projections S_z/T_z rather that projections of spin/isospin angular momenta M_S/M_T. This constitutes a fully equivalent convention.

[2] That is, it only couples between states of same spin S and isospin T.

If a tensor interaction is present it only couples states such that $|L-L'|=0,2$ and $L,L'>0$. One has then

$$\langle \vec{k}\, SS_z\, TT_z|v|\vec{k}\,'\, SS_z\, TT_z\rangle = \frac{\pi}{2}\,(4\pi)^2 \sum_{LL'}\sum_{JJ_z} i^{L'-L}\, \mathcal{Y}^{J_z}_{(L'S)J}{}^{*}(\hat{k}')\, \mathcal{Y}^{J_z}_{(LS)J}(\hat{k})\, v^{JSS_zTT_z}_{LL'}(k,k')\,, \tag{D.39}$$

where the short notation from Eq. (A.1a) is used. In most case one will not consider CIB/CSB forces, or the isospin projection will be specified, that is the superscripts S_z/T_z can be dropped. One is left with partial wave matrix elements of the kind $v^{JST}_{LL'}(k,k')$, with conventions from Eqs. (A.1b,A.1c), that are called matrix elements of the interaction in a given partial wave.

Regarding the partial wave expansion of a nuclear potential v, the following remarks will hold.

- The capital angular momentum notation $L, J\ldots$ will denote relative angular momenta for two-body states.
- All terms involved are scalar under the rotation of the two particles, thus one has using Wigner-Eckart's theorem

$$\begin{aligned}\langle k'\ (L'S')J'J'_zS'_z|v|k\ (LS)JJ_zS_z\rangle&\\ =(-1)^{J-J'_z}&\begin{pmatrix} J' & 0 & J\\ -J'_z & 0 & J_z\end{pmatrix}(k'\ (L'S')J'S'_z||v||k\ (LS)JS_z)\\ =\frac{\delta_{JJ'}\,\delta_{J_zJ'_z}}{\sqrt{[J]}}&\,(k'\ (L'S')JS'_z||v||k\ (LS)JS_z)\,.\end{aligned} \tag{D.40}$$

  Equivalently, in the total scheme $|(LS)JJ_zS_z\,TT_z\rangle$, the interaction is separable into its isospin part v^T and the angular momentum part v^J, and

$$\begin{aligned}&\langle k'\ (L'S')J'J'_zS'_z\,T'T'_z|v|k\ (LS)JJ_zS_z\,TT_z\rangle\\ &\quad=\frac{\delta_{JJ'}\,\delta_{J_zJ'_z}\,\delta_{S_zS'_z}}{\sqrt{[J]}}\,(k'\ (L'S')JS'_z||v^J||k\ (LS)JS_z)\,\frac{\delta_{TT'}\,\delta_{T_zT'_z}}{\sqrt{[T]}}\,(TT_z||v^T||TT_z)\,.\end{aligned} \tag{D.41}$$

  Standard or reduced matrix elements of the interaction can thus be evaluated, whichever is the easiest. Unless specified, J_z-, S_z- and T_z-dependencies will be dropped thereafter.

  Note that in all rigor reduced matrix elements should be written as $(L'||f(\vec{k},\vec{k}\,')||L)$, however we denote them by $(k'\ L'||f(\vec{k},\vec{k}\,')||k\ L)$ to keep in mind that they represent projected quantities which only depend on k and k'.

- Spin and isospin operators are defined such as (Pauli matrices)

$$\hat{\sigma}_z\,|S\,S_z\rangle = S_z\,|S\,S_z\rangle\,,\qquad \hat{\sigma}^2\,|S\,S_z\rangle = 4\,S(S+1)|S\,S_z\rangle\,. \tag{D.42}$$

The states $|k\,(LS)JJ_zS_z\,TT_z\rangle$ in the $V_{\mathrm{low}\,k}$ code are normalized according to the convention

$$\begin{aligned}
&\langle k'\,(L'S')J'J'_zS'_z\,T'T'_z|k\,(LS)JJ_zS_z\,TT_z\rangle \\
&\quad=\delta_{SS'}\,\delta_{TT'}\,\delta_{T_zT'_z}\int \mathrm{d}\vec{r}\,\langle k'\,(L'S)J'J'_zS'_z\,T'T'_z|\vec{r}\,\rangle\,\langle\vec{r}\,|k\,(LS)JJ_zS_z\,TT_z\rangle \\
&\quad=\delta_{SS'}\,\delta_{TT'}\,\delta_{T_zT'_z}\,\frac{2}{\pi}\int \mathrm{d}\vec{r}\,\mathcal{Y}^{J'_z}_{(L'S)J'}{}^{*}(\hat{r})\,j_{L'}(k'\,r)\;\mathcal{Y}^{J_z}_{(LS)J}(\hat{r})\,j_L(k\,r) \\
&\quad=\delta_{SS'}\,\delta_{TT'}\,\delta_{T_zT'_z}\,\frac{2}{\pi}\,\delta_{LL'}\,\delta_{JJ'}\,\delta_{J_zJ'_z}\int_0^{+\infty} r^2\,\mathrm{d}r\,j_L(k'\,r)\,j_L(k\,r) \\
&\quad=\delta_{SS'}\,\delta_{TT'}\,\delta_{T_zT'_z}\,\delta_{LL'}\,\delta_{JJ'}\,\delta_{J_zJ'_z}\,\frac{\delta(k-k')}{kk'}\,. \qquad \text{(D.43)}
\end{aligned}$$

In the following decoupling, we have used states $|k\,(LS)JJ_zS_z\,TT_z\rangle$ with a different normalization. Indeed, according to our conventions the partial wave expansion of the Dirac delta 3D function (Eq. (A.52)) reads

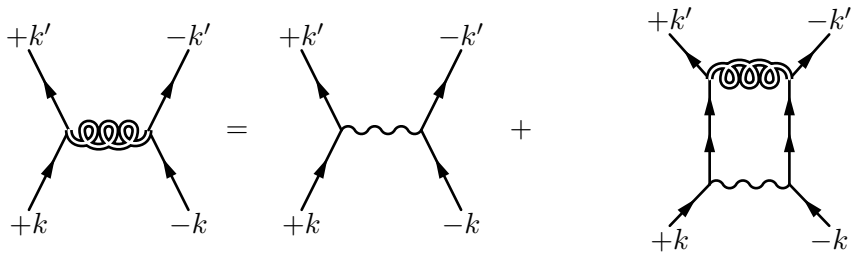
$$\begin{aligned}
&\langle k'\,(L'S')J'J'_zS'_z\,T'T'_z|k\,(LS)JJ_zS_z\,TT_z\rangle \\
&\quad=\langle k'\,(L'S')J'J'_zS'_z\,T'T'_z|\mathbb{I}|k\,(LS)JJ_zS_z\,TT_z\rangle \qquad \text{(D.44)}\\
&\quad=\delta_{JJ'}\,\delta_{J_zJ'_z}\,\delta_{SS'}\,\delta_{S_zS'_z}\,\delta_{TT'}\,\delta_{T_zT'_z}\,\frac{(k'\,L'||\delta(\vec{k}-\vec{k}\,')||k\,L)}{\sqrt{[L]}} \qquad \text{(D.45)}\\
&\quad=\delta_{JJ'}\,\delta_{J_zJ'_z}\,\delta_{SS'}\,\delta_{S_zS'_z}\,\delta_{TT'}\,\delta_{T_zT'_z} \qquad \text{(D.46)}\\
&\qquad\times\frac{1}{\sqrt{[L]}}\sum_{\lambda}(-1)^{\lambda}\,\frac{\delta(k-k')}{k^2}\,\sqrt{[\lambda]}(k\,L'||\left[Y^{[\lambda]}(\hat{k})\otimes Y^{[\lambda]}(\hat{k}')\right]^{[0]}||k\,L) \\
&\quad=\delta_{JJ'}\,\delta_{J_zJ'_z}\,\delta_{SS'}\,\delta_{S_zS'_z}\,\delta_{TT'}\,\delta_{T_zT'_z}\,\delta_{LL'}\,\frac{\delta(k-k')}{k^2}\,\frac{1}{4\pi}\,. \qquad \text{(D.47)}
\end{aligned}$$

Hence in our conventions we must carry an extra $1/4\pi$ factor to have consistent results with the $V_{\mathrm{low}\,k}$ code.

Values of L, S, J and T for the first few partial waves that are to be evaluated are found in Tab. {D.1}.

D.3 Scattering phase shifts

Scattering phase shifts will be defined through matrix elements of the scattering T-matrix. The latter is best expressed in momentum space, and reads



$$\langle\vec{k}\,|T(E)|\vec{k}\,'\rangle \quad=\quad \frac{m}{\hbar^2}\langle\vec{k}\,|v|\vec{k}\,'\rangle \quad +\mathcal{P}\int\frac{\mathrm{d}\vec{k}\,''}{(2\pi)^3}\frac{\langle\vec{k}\,|v|\vec{k}\,''\rangle\,\langle\vec{k}\,''\,|T(E)|\vec{k}\,'\rangle}{E-E(k'')}\,, \qquad \text{(D.48)}$$

	L	S	J	T
$^1S_0$	0	0	0	1
$^3S_1$	0	1	1	0
$^1P_1$	1	0	1	0
$^3P_0$	1	1	0	1
$^3P_1$	1	1	1	1
$^3P_2$	1	1	2	1
$^1D_2$	2	0	2	1
$^3D_1$	2	1	1	0
$^3D_2$	2	1	2	0
$^3D_3$	2	1	3	0

Table D.1: First partial waves that are to be evaluated.

where $\mathcal{P}$ denotes a principal value integration.

The nucleon-nucleon scattering phase shifts are defined through the scattering matrix. In the case of a rapidly decreasing (more than $1/r$) potential $v(r)$, the scattering solution $\Psi_{\vec{k}}$ at a given energy $E = \hbar^2\, k^2/2m$, m being the reduced mass, is a solution of the Schrödinger equation

$$(H_0 + v)\, \Psi_{\vec{k}} = E\, \Psi_{\vec{k}}\,. \tag{D.49}$$

One can write $\Psi_{\vec{k}}$ as $\phi_{\vec{k}} + \chi_{\vec{k}}$, where $\phi_{\vec{k}}$ is a solution of the free Schrödinger equation with energy E

$$H_0\, \phi_{\vec{k}} = E\, \phi_{\vec{k}}\,, \tag{D.50}$$

and the normalization $\langle\phi_{\vec{k}}|\phi_{\vec{k}}\rangle = \langle\Psi_{\vec{k}}|\Psi_{\vec{k}}\rangle = \langle\phi_{\vec{k}}|\Psi_{\vec{k}}\rangle$. By definition of the T-matrix one has then for uncoupled channels

$$T_L^{JST}(k,k';E)\, \phi_{L,\vec{k}}^{JST} = \delta(k-k')\delta\left(E - \frac{\hbar^2\, k^2}{2\mu}\right)\, v_L^{JST}\, \Psi_{L,\vec{k}}^{JST}\,, \tag{D.51}$$

where a wave function is expanded into

$$\phi_{\vec{k}}(\vec{r}) = \sum_L (2L+1)\, i^L\, \phi_{L,\vec{k}}(r)\, P_L(\cos\theta)\,. \tag{D.52}$$

One has in particular

$$H_0\, \phi_{\vec{k}}(\vec{r}) = E\, \phi_{\vec{k}}(\vec{r}) \qquad \Rightarrow \qquad \left[\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{L\,(L+1)}{r^2}\right]\, \phi_{L,\vec{k}}(r) = 0\,. \tag{D.53}$$

For a plane wave one has $\phi_{L,\vec{k}}^{JST}(r) = j_L(kr)$, and in the absence of any scattering potential the scattering solution corresponds asymptotically to a superposition of ingoing and outgoing spherical waves, i.e.

$$\phi_{L,\vec{k}}^{JST}(r) \underset{r\to+\infty}{\longrightarrow} \frac{1}{kr}\sin\left(kr - L\frac{\pi}{2}\right) = \frac{1}{2i\, kr}\left[e^{+i(kr-L\pi/2)} - e^{-i(kr-L\pi/2)}\right]\,. \tag{D.54}$$

The scattering matrix is defined through the expression of the asymptotic behavior of $\Psi_{\vec{k}}$ as an equivalent linear superposition.

D.3.1 Uncoupled channels

The restriction S_L^{JST} of the scattering matrix to an uncoupled channel is a scalar, and the scattered wave can be written as

$$\Psi_{L,\vec{k}}^{JST}(r) \underset{r\to+\infty}{\longrightarrow} A\,\frac{-1}{2i\,kr}\left[e^{-i(kr-L\pi/2)} - S_L^{JST}(E)\,e^{+i(kr-L\pi/2)}\right]. \tag{D.55}$$

The flux conservation ensures that $|S_L^{JST}|^2 = 1$, thus

$$S_L^{JST}(E) \equiv e^{2i\,\delta_L^{JST}(E)}, \tag{D.56}$$

where $\delta_L^{JST}(E)$ is the scattering phase shift at a given energy E. One has then, disregarding an arbitrary phase

$$\Psi_{L,\vec{k}}^{JST}(r) \underset{r\to+\infty}{\longrightarrow} \mathcal{A}\,\frac{1}{kr}\sin\left(kr - L\frac{\pi}{2} + \delta_L^{JST}(E)\right). \tag{D.57}$$

The normalization constant $\mathcal{A}$ is fixed by the condition $\langle\Psi_{L,\vec{k}}^{JST}|\phi_{L,\vec{k}}\rangle = \langle\phi_{L,\vec{k}}|\phi_{L,\vec{k}}\rangle$, and is easily obtained from boundary conditions on the radial scattering function [27], i.e.

$$\begin{aligned}\Psi_{L,\vec{k}}^{JST}(r) &\underset{r\to+\infty}{\longrightarrow} j_L(kr) + \tan(\delta_L^{JST}(E))\,n_l(kr)\\ &\underset{r\to+\infty}{\longrightarrow} \frac{1}{kr}\sin\left(kr - L\frac{\pi}{2}\right) + \tan(\delta_L^{JST}(E))\frac{1}{kr}\cos\left(kr - L\frac{\pi}{2}\right)\\ &\underset{r\to+\infty}{\longrightarrow} \frac{1}{\cos(\delta_L^{JST}(E))}\frac{1}{kr}\sin\left(kr - L\frac{\pi}{2} + \delta_L^{JST}(E)\right).\end{aligned} \tag{D.58a}$$

One gets then

$$\phi_{L,\vec{k}}(r) \underset{r\to+\infty}{\longrightarrow} \frac{1}{kr}\sin\left(kr - L\frac{\pi}{2}\right), \tag{D.59a}$$

$$\Psi_{L,\vec{k}}^{JST}(r) \underset{r\to+\infty}{\longrightarrow} \frac{1}{\cos(\delta_L^{JST}(E))}\frac{1}{kr}\sin\left(kr - L\frac{\pi}{2} + \delta_L^{JST}(E)\right). \tag{D.59b}$$

In the framework of Ref. [26], the connection between the scattering phase shifts and the T-matrix for uncoupled channels is obtained through the following procedure.

1. From Eqs. (D.49,D.50), we have

$$\left\{\begin{array}{cc} \left[\times\phi_{\vec{k}}^*\right] & (H_0+v)\,\Psi_{\vec{k}} = E\,\Psi_{\vec{k}} \\ & \updownarrow - \\ & \phi_{\vec{k}}^*\,H_0^\dagger = E\,\phi_{\vec{k}}^* \qquad \left[\times\Psi_{\vec{k}}\right] \end{array}\right. \Rightarrow \phi_{\vec{k}}^*\,H_0\,\Psi_{\vec{k}} - \phi_{\vec{k}}^*\,H_0^\dagger\,\Psi_{\vec{k}} = -\phi_{\vec{k}}^*\,v\,\Psi_{\vec{k}}. \tag{D.60}$$

2. From Eq. (D.53) and a projection on the angular momentum into, one gets then

$$\phi_{L,\vec{k}}^*(r)\,\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,\Psi_{L,\vec{k}}^{JST}(r) - \Psi_{L,\vec{k}}^{JST}(r)\,\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,\phi_{L,\vec{k}}^*(r) = -\frac{m}{\hbar^2}\,\phi_{L,\vec{k}}^*(r)\,v_L^{JST}(r)\,\Psi_{L,\vec{k}}^{JST}(r). \tag{D.61}$$

3. Integrating over r leads to

$$\begin{aligned}\int_{r=0}^{R}\mathrm{d}r\,r^2\left[\phi_{L,\vec{k}}^*(r)\,\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,\Psi_{L,\vec{k}}^{JST}(r) - \Psi_{L,\vec{k}}^{JST}(r)\,\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,\phi_{L,\vec{k}}^*(r)\right]\\ = -\frac{m}{\hbar^2}\int_{r=0}^{R} r^2\,\mathrm{d}r\,\phi_{L,\vec{k}}^*(r)\,v_L^{JST}(r)\,\Psi_{L,\vec{k}}^{JST}(r).\end{aligned} \tag{D.62}$$

4. Using an integration by parts, we obtain

$$-\int_{r=0}^{R} \mathrm{d}r\, \frac{\mathrm{d}}{\mathrm{d}r}\left[r\,\phi^*_{L,\vec{k}}(r)\,\frac{\mathrm{d}}{\mathrm{d}r}\big(r\,\Psi^{JST}_{L,\vec{k}}(r)\big) - r\,\Psi^{JST}_{L,\vec{k}}(r)\,\frac{\mathrm{d}}{\mathrm{d}r}\left(r\,\phi^*_{L,\vec{k}}(r)\right)\right] = -\frac{m}{\hbar^2}\int_{r=0}^{R} r^2\,\mathrm{d}r\,\phi^*_{L,\vec{k}}(r)\,v_L(r)\,\Psi_{L,\vec{k}}(r)\,. \quad \text{(D.63)}$$

5. One gets then

$$-\left[r\,\phi^*_{L,\vec{k}}(r)\,\frac{\mathrm{d}}{\mathrm{d}r}\big(r\,\Psi^{JST}_{L,\vec{k}}(r)\big) - r\,\Psi^{JST}_{L,\vec{k}}(r)\,\frac{\mathrm{d}}{\mathrm{d}r}\left(r\,\phi^*_{L,\vec{k}}(r)\right)\right]_{r=R} = -\frac{m}{\hbar^2}\int_{r=0}^{R} r^2\,\mathrm{d}r\,\phi^*_{L,\vec{k}}(r)\,v^{JST}_L(r)\,\Psi^{JST}_{L,\vec{k}}(r)\,. \quad \text{(D.64)}$$

For very large distances $r > R$, the asymptotic solutions from Eqs. (D.59a,D.59b) can be used, whereas the fully on-shell T-matrix, expressed in fm units, is recovered in the right-hand side. One gets then

$$-\int_0^R \mathrm{d}r\, r^2\,\phi^*_{\vec{k}}(r)\,T^{JST}_L(E,r)\,\phi_{\vec{k}}(r) = \frac{1}{k}\left[-\sin\left(kR+L\frac{\pi}{2}\right)\,\frac{1}{\cos(\delta^{JST}_L(E))}\cos\left(kR+L\frac{\pi}{2}+\delta^{JST}_L(E)\right) + \cos\left(kR+L\frac{\pi}{2}\right)\,\frac{1}{\cos(\delta^{JST}_L(E))}\sin\left(kR+L\frac{\pi}{2}+\delta^{JST}_L(E)\right)\right] \quad \text{(D.65a)}$$

$$\frac{\tan(\delta^{JST}_L(E))}{k} = -\,\langle k|T^{JST}_L(E)|k\rangle\,, \quad \text{(D.65b)}$$

with the fully on-shell condition $E = \hbar^2\,k^2/m$. Thus one recovers for uncoupled channels the usual expression

$$T^{JST}_L\left(k,k;\frac{\hbar^2\,k^2}{m}\right) = -\frac{\tan\left(\delta^{JST}_L(k)\right)}{k}\,. \quad \text{(D.66)}$$

D.3.2 Uncoupled channels: alternate method

Now let us present another method to recover Eq. (D.66) which will be useful for coupled channels. Different methods exists to regularize the Lippmann-Schwinger equation stemming from

$$\lim_{\epsilon\to 0}\frac{1}{k^2-q^2\pm i\epsilon} = \mathcal{P}\frac{1}{k^2-q^2} \mp i\pi\,\delta(k^2-q^2)\,. \quad \text{(D.67)}$$

This allows to define alternate T-matrices, i.e. such that

$$T^{\pm} = v + v\frac{1}{E-H_0\pm i\epsilon}T^{\pm}\,. \quad \text{(D.68)}$$

Within the formalism of Ref. [28]

- the representation T, called reactance matrix, reaction matrix or Heitler's matrix, is related to an hermitian representation of the scattering matrix in a stationary state formalism through

$$S = \frac{1-\frac{1}{2}i\,T}{1+\frac{1}{2}i\,T}\,, \quad \text{(D.69)}$$

- the representations $T^{\pm}$ provide a time-independent formulation of the scattering problem in which the small positive/negative imaginary part selects an incoming or outgoing waves formalism[3]. One has then

$$T^{\pm} = S \mp 1. \tag{D.70}$$

From Eqs. (D.69,D.70), one gets

$$T^{+} + \frac{1}{2} i\, T\, T^{+} = -i\, T\,. \tag{D.71}$$

Non-vanishing matrix elements for the latter expression can be obtained on the energy shell using

$$T^{+}_{ab} \equiv -2\pi\, i\, \delta(E_a - E_b)\, T^{+}_{ab}\,, \qquad T_{ab} \equiv 2\pi\, \delta(E_a - E_b)\, T_{ab}\,. \tag{D.72}$$

This leads, on the energy shell, to

$$T^{+}\left(k, k, \frac{\hbar^2\, k^2}{m}\right) = T\left(k, k, \frac{\hbar^2\, k^2}{m}\right) - i\,\pi\, T^{+}\left(k, k, \frac{\hbar^2\, k^2}{m}\right) T\left(k, k, \frac{\hbar^2\, k^2}{m}\right)\,. \tag{D.73}$$

Now one has to advocate a different normalization to remain in agreement with Ref. [26]. Indeed, different conventions are possible for uncoupled channels scattering, e.g.

Ref. [26]	Ref. [28]	
$T_L^{JST} = -\frac{1}{\pi}\,\tan(\delta_L^{JST})$	$T_L^{JST} = -\frac{1}{k}\,\tan(\delta_L^{JST})$	(D.74)
$T^{+}{}_L^{JST} = -\frac{1}{\pi}\, e^{i\,\delta_L^{JST}}\,\sin(\delta_L^{JST})$	$T^{+}{}_L^{JST} = -\frac{1}{k}\, e^{i\,\delta_L^{JST}}\,\sin(\delta_L^{JST})$	(D.75)

which suggests that a normalization factor of $\frac{k}{\pi}$ must be carried out at the level of Eq. (D.73)[4] to recover the usual expression [29]

$$T^{+}\left(k, k, \frac{\hbar^2\, k^2}{m}\right) = T\left(k, k, \frac{\hbar^2\, k^2}{m}\right) - i\, k T^{+}\left(k, k, \frac{\hbar^2\, k^2}{m}\right) T\left(k, k, \frac{\hbar^2\, k^2}{m}\right)\,. \tag{D.76}$$

The same renormalization leads, using Eq. (D.70), to

$$S_L^{JST} = 1 - 2i\, k\, T^{+}{}_L^{JST}\,, \tag{D.77}$$

which allows to recover Eq. (D.75). One gets then easily

$$T^{+}{}_L^{JST} = \frac{T_L^{JST}}{1 + i\, k\, T_L^{JST}}\,, \qquad S_L^{JST} = 1 - 2i\, k\, \frac{T_L^{JST}}{1 + i\, k\, T_L^{JST}}\,, \qquad T_L^{JST} = -\frac{1}{ik}\,\frac{S_L^{JST} - 1}{S_L^{JST} + 1}\,, \tag{D.78}$$

that is (Eq. (D.56))

$$T_L^{JST} = -\frac{1}{k}\,\tan(\delta_L^{JST})\,. \tag{D.79}$$

[3] In all rigor, the T-matrix as defined by Lippmann and Schwinger is T^{+} while the T-matrix defined at the level of Eq. (D.48) is usually called the reactance K-matrix.

[4] This k/π factor comes from the use of non-normalized Bessel function.

D.3.3 Coupled channels

For channels coupled by the tensor force (hence $S = 1$), each channel ${}^3(J^\pm)_J$ is not an eigenstate of the scattering matrix. The wave function for a state with total angular momentum J reads

$$\phi^{JST}_{\vec{k}}(\vec{r}) \equiv \tilde{\phi}^{JST}_{J^-}(r)\, \mathcal{Y}^{J_z}_{(J^-\,1)J}(\Omega) + \tilde{\phi}^{JST}_{J^+}(r)\, \mathcal{Y}^{J_z}_{(J^+\,1)J}(\Omega)\,. \tag{D.80}$$

The latter is written as a spinor

$$\phi^{JST}_{\vec{k}}(\vec{r}) \equiv \left\{ \begin{array}{c} \tilde{\phi}^{JST}_{J^-,\vec{k}}(\vec{r}) \\ \tilde{\phi}^{JST}_{J^+,\vec{k}}(\vec{r}) \end{array} \right\}. \tag{D.81}$$

Likewise

$$\Psi^{JST}_{\vec{k}}(\vec{r}) \equiv \left\{ \begin{array}{c} \tilde{\Psi}^{JST}_{J^-,\vec{k}}(\vec{r}) \\ \tilde{\Psi}^{JST}_{J^+,\vec{k}}(\vec{r}) \end{array} \right\}. \tag{D.82}$$

For large values of r each radial function can be written as a linear superposition of an incoming and an outgoing spherical wave, i.e.

$$\tilde{\phi}_{J^\pm}(r) \underset{r\to+\infty}{\longrightarrow} \frac{1}{2i\,kr}\left[e^{-i(kr-J^\pm\pi/2)} - e^{+i(kr-J^\pm\pi/2)}\right], \tag{D.83a}$$

$$\tilde{\Psi}^{J1T}_{J^-}(r) \underset{r\to+\infty}{\longrightarrow} \frac{1}{2i\,kr}\left[A_1\, e^{-i(kr-J^-\pi/2)} - B_1\, e^{+i(kr-J^-\pi/2)}\right], \tag{D.83b}$$

$$\tilde{\Psi}^{J1T}_{J^+}(r) \underset{r\to+\infty}{\longrightarrow} \frac{1}{2i\,kr}\left[A_2\, e^{-i(kr-J^+\pi/2)} - B_2\, e^{+i(kr-J^+\pi/2)}\right]. \tag{D.83c}$$

The 2×2 restriction of the S-matrix between states $L, L' = J^\pm$ is then introduced as $B \equiv S^{J1T}\, A$. Two parametrizations of the scattering matrix, leading to different definitions for the phase shifts, are commonly used[(5)].

1. The eigenphase shifts convention [30] where

$$S^{J1T} \equiv {U^{J1T}}^{-1}\, \exp(2i\,\Delta^{J1T})\, U^{J1T}\,, \tag{D.84a}$$

$$U^{J1T} = \begin{pmatrix} \cos(\epsilon_J) & \sin(\epsilon_J) \\ -\sin(\epsilon_J) & \cos(\epsilon_J) \end{pmatrix}, \tag{D.84b}$$

$$\Delta^{J1T} = \begin{pmatrix} \delta_{J\alpha} & 0 \\ 0 & \delta_{J\beta} \end{pmatrix} \equiv \begin{pmatrix} \delta_\alpha & 0 \\ 0 & \delta_\beta \end{pmatrix}, \tag{D.84c}$$

$$S^{J1T} = \begin{pmatrix} \cos^2(\epsilon_J)\, e^{2i\,\delta_\alpha} + \sin^2(\epsilon_J)\, e^{2i\,\delta_\beta} & \cos(\epsilon_J)\,\sin(\epsilon_J)\left[e^{2i\,\delta_\alpha} - e^{2i\,\delta_\beta}\right] \\ \cos(\epsilon_J)\,\sin(\epsilon_J)\left[e^{2i\,\delta_\alpha} - e^{2i\,\delta_\beta}\right] & \cos^2(\epsilon_J)\, e^{2i\,\delta_\beta} + \sin^2(\epsilon_J)\, e^{2i\,\delta_\alpha} \end{pmatrix}. \tag{D.84d}$$

   The latter corresponds, in first approximation, to writing the two eigenstates $\tilde{\Psi}_\alpha$ and $\tilde{\Psi}_\beta$ of the T-matrix as a superposition of the uncoupled solutions in the $J^\pm$ states, with a

[5] To not overload the notations the E-dependence of the phase shifts will be dropped in the following and reintroduced in the final results.

mixture parameter ϵ_J. These eigenstates are defined such that ratios between incoming and outgoing waves in $J^\pm$ channels are equal, i.e. $B_2/B_1 = A_2/A_1$ hence

$$A_2^\alpha/A_1^\alpha = \tan(\epsilon_J)\,, \qquad A_2^\beta/A_1^\beta = -\frac{1}{\tan(\epsilon_J)}\,. \tag{D.85}$$

Using Eqs. (D.84a-D.84d), the equations that connect the amplitudes of incoming A_i and outgoing B_i waves take the usual form for uncoupled channels for the eigenstates α and β, that is[6]

$$B_i^\alpha = e^{2i\,\delta_\alpha}\,A_i^\alpha\,, \qquad B_i^\beta = e^{2i\,\delta_\beta}\,A_i^\beta\,. \tag{D.86}$$

The convention

$$\lim_{E\to 0}\epsilon_J = 0\,, \tag{D.87}$$

ensures that near zero energy (no scattering) the α wave is mainly constituted by $\tilde{\Psi}^{J1T}_{J^-,\vec{k}}$.

To relate these eigenphase shifts to the matrix elements of the T-matrix T^{J1T}, the easiest way consists in using the alternate approach from Sec. D.3.2. The easiest starting point is[7]

$$T^{J1T}_{L_1L_2} = \big[-\frac{1}{i\,k}\,(S-\mathbb{I})\times(S+\mathbb{I})^{-1}\big]^{J1T}_{L_1L_2}\,, \tag{D.88}$$

where, in the 2×2 subspace $L = J^\pm$

$$(S_J+\mathbb{I})^{-1} = \frac{1}{\Gamma}\begin{pmatrix} (1+e^{2i\delta_\beta})\cos(2\epsilon_J) & -(e^{2i\delta_\alpha}-e^{2i\delta_\beta})\cos(\epsilon_J)\sin(\epsilon_J) \\ \quad +(1+e^{2i\delta_\alpha})\sin(2\epsilon_J) & \\ -(e^{2i\delta_\alpha}-e^{2i\delta_\beta})\cos(\epsilon_J)\sin(\epsilon_J) & (1+e^{2i\delta_\alpha})\cos(2\epsilon_J) \\ & \quad +(1+e^{2i\delta_\beta})\sin(2\epsilon_J) \end{pmatrix}, \tag{D.89a}$$

$$T_J = -\frac{1}{ik\Gamma}\begin{pmatrix} (e^{2i\delta_\alpha}-e^{2i\delta_\beta})\cos(2\epsilon_J) & (e^{2i\delta_\alpha}-e^{2i\delta_\beta})\sin(2\epsilon_J) \\ \quad +e^{2i(\delta_\alpha+\delta_\beta)}-1 & \\ (e^{2i\delta_\alpha}-e^{2i\delta_\beta})\sin(2\epsilon_J) & (e^{2i\delta_\beta}-e^{2i\delta_\alpha})\cos(2\epsilon_J) \\ & \quad +e^{2i(\delta_\alpha+\delta_\beta)}-1 \end{pmatrix}, \tag{D.89b}$$

$$\Gamma = (1+e^{2i\,\delta_\alpha})(1+e^{2i\,\delta_\beta})\,. \tag{D.89c}$$

One gets then after some manipulations

$$\frac{T^{J1T}_{J^+J^-}+T^{J1T}_{J^-J^+}}{T^{J1T}_{J^-J^-}-T^{J1T}_{J^+J^+}} = \tan(2\,\epsilon_J)\,, \tag{D.90a}$$

$$T^{J1T}_{J^-J^-}+T^{J1T}_{J^+J^+}+\frac{T^{J1T}_{J^-J^-}-T^{J1T}_{J^+J^+}}{\cos(2\,\epsilon_J)} = -\frac{2}{i\,k}\,\frac{e^{2i\,\delta_\alpha}-1}{e^{2i\,\delta_\alpha}+1} = \frac{2}{k}\,\tan(\delta_\alpha)\,, \tag{D.90b}$$

$$T^{J1T}_{J^-J^-}+T^{J1T}_{J^+J^+}-\frac{T^{J1T}_{J^-J^-}-T^{J1T}_{J^+J^+}}{\cos(2\,\epsilon_J)} = \frac{2}{k}\,\tan(\delta_\beta)\,. \tag{D.90c}$$

[6] Equations for β relate to those for α by the phase change $\epsilon_J \to \epsilon_J + \frac{\pi}{2}$.

[7] Given that S and T are matrices one has to take matrix inverses instead of simple quotients.

This leads to the usual expression [26]

$$\tan\left[2\,\epsilon_J\left(E\right)\right] = \frac{T^{J1T}_{J^-J^+}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) + T^{J1T}_{J^+J^-}\left(k,k;\frac{\hbar^2\,k^2}{m}\right)}{T^{J1T}_{J^-J^-}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) - T^{J1T}_{J^+J^+}\left(k,k;\frac{\hbar^2\,k^2}{m}\right)}\,, \tag{D.91a}$$

$$\tan\left[\delta^{J1T}_{J^-}\left(E\right)\right] = -\frac{k}{2}\left[T^{J1T}_{J^-J^-}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) + T^{J1T}_{J^+J^+}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) + \frac{T^{J1T}_{J^-J^-}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) - T^{J1T}_{J^+J^+}\left(k,k;\frac{\hbar^2\,k^2}{m}\right)}{\cos(2\,\epsilon_J)}\right], \tag{D.91b}$$

$$\tan\left[\delta^{J1T}_{J^+}\left(E\right)\right] = -\frac{k}{2}\left[T^{J1T}_{J^-J^-}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) + T^{J1T}_{J^+J^+}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) - \frac{T^{J1T}_{J^-J^-}\left(k,k;\frac{\hbar^2\,k^2}{m}\right) - T^{J1T}_{J^+J^+}\left(k,k;\frac{\hbar^2\,k^2}{m}\right)}{\cos(2\,\epsilon_J)}\right], \tag{D.91c}$$

where one does the usual (wrong) approximation, coming from the zero coupling limit $\epsilon_j \to 0$ where the identification $\alpha \equiv J^-$ and $\beta \equiv J^+$ is exact, i.e.

$$\delta_\alpha \equiv \delta^{J1T}_{J^-}\left(E\right)\,, \qquad \delta_\beta \equiv \delta^{J1T}_{J^+}\left(E\right)\,. \tag{D.92}$$

2. The bar-phaseshifts [31], where the scattering matrix is now defined as

$$S^{J1T} \equiv \exp(i\,\bar{\delta})\,\exp(2i\,\bar{\epsilon})\,\exp(i\,\bar{\delta})\,, \tag{D.93a}$$

$$S^{J1T} = \begin{pmatrix} \exp(i\,\bar{\delta}^{J1T}_{J^-}) & 0 \\ 0 & \exp(i\,\bar{\delta}^{J1T}_{J^+}) \end{pmatrix} \begin{pmatrix} \cos(2\,\bar{\epsilon}_J) & i\,\sin(2\,\bar{\epsilon}_J) \\ i\,\sin(2\,\bar{\epsilon}_J) & \cos(2\,\bar{\epsilon}_J) \end{pmatrix} \times \begin{pmatrix} \exp(i\,\bar{\delta}^{J1T}_{J^-}) & 0 \\ 0 & \exp(i\,\bar{\delta}^{J1T}_{J^+}) \end{pmatrix}. \tag{D.93b}$$

In this case $\bar{\epsilon}_J$ provides the proportions into which an incoming beam of a given channel divides between the two outgoing channels. Bar- and eigen-phaseshifts are related through

$$\delta^{J1T}_{J^+} + \delta^{J1T}_{J^-} = \bar{\delta}^{J1T}_{J^+} + \bar{\delta}^{J1T}_{J^-}\,, \tag{D.94a}$$

$$\sin(\bar{\delta}^{J1T}_{J^-} - \bar{\delta}^{J1T}_{J^+}) = \frac{\tan 2\,\bar{\epsilon}_J}{\tan(2\,\epsilon_J)}\,, \tag{D.94b}$$

$$\sin(\delta^{J1T}_{J^-} - \delta^{J1T}_{J^+}) = \frac{\sin 2\,\bar{\epsilon}_J}{\sin(2\,\epsilon_J)}\,. \tag{D.94c}$$

Both of these conventions are equivalent for uncoupled channels. In the present work one will use the bar-phaseshift convention, as it is done for the reference PWA93, and will remove the overbar on the notations δ and ϵ. Scattering phase shifts can be given either as a function of the relative momentum k or the energy in the laboratory frame $E_{\rm lab}$, which reads

$$E_{\rm lab} = 4\,\frac{\hbar^2\,k^2}{m}\,. \tag{D.95}$$

D.3.3.1 Coulomb corrections for proton-proton phase shifts

In the case of proton-proton scattering, the long-range Coulomb interaction modifies the previous picture. Indeed, the scattering matrix has to be formulated in terms of asymptotic electromagnetic states, since plane waves are not good asymptotic solutions any more. Different formulations of the phase shifts in the presence of the electromagnetic interaction are then possible corresponding to the type of functions that are used to match asymptotically the interacting and non-interacting scattering solutions. They correspond to the notation δ_X^Y, denoting the phase shift solution with potential X with respect to the asymptotic solution of the potential Y. For instance for neutron-neutron scattering if the nuclear strong interaction is noted N, the scattering phase shifts defined at the level of Eq. (D.56) and Eqs. (D.84a-D.84d) correspond to δ_N^0, since the plane waves used for the matching are solutions of the free Schrödinger equation. In the presence of long-range electromagnetic interactions, the total potential is usually decomposed into

$$v = v_N + v_{EM}\,, \tag{D.96}$$

where the electromagnetic interaction v_{EM} contains

- the improved Coulomb potential $v_{C1} + v_{C2}$ including relativistic $1/m^2$ corrections and contributions of the 2γ-exchange diagrams [32]

$$v_{C1}(r) = \frac{\alpha'}{r}\,, \tag{D.97a}$$

$$v_{C2}(r) = -\frac{1}{2\,m_p^2}\left[(\Delta + k^2)\,\frac{\alpha}{r} + \frac{\alpha}{r}\,(\Delta + k^2)\right]\,, \tag{D.97b}$$

  where the energy-dependent coupling constant α' is given from the fine structure constant α by

$$\alpha' = \alpha\,\frac{m_p^2 + 2\,k^2}{m_p\,\sqrt{m_p^2 + 2\,k^2}}\,, \tag{D.98}$$

- the magnetic moment interaction v_{MM}, which reads for the proton-proton interaction [33]

$$v_{MM}(r) = -\frac{\alpha}{4\,m_p^2\,r^3}\left[\mu_p^2\,\mathsf{S}_{12} + (6 + 8\,\kappa_p)\,\mathbf{L}\cdot\mathbf{S}\right]\,, \tag{D.99}$$

  where μ_p is the proton magnetic moment and $\kappa_p = \mu_p - 1$ the anomalous magnetic moment,

- the vaccuum polarization v_{VP} [34; 35]

$$v_{VP}(r) = \frac{2\,\alpha\,\alpha'}{3\pi\,r}\int_1^{+\infty} \mathrm{d}x\, e^{-2m_e\,r\,x}\left(1 + \frac{1}{2x^2}\right)\frac{\sqrt{x^2-1}}{x^2}\,. \tag{D.100}$$

The proton-proton scattering phase shifts are then usually defined as nuclear-electromagnetic phase shifts δ_{N+EM}^{EM}, that is with respect to electromagnetic wave functions.

The easiest way to compute them is to use an an intermediate step the phase shift δ_{N+C1}^{C1} of the Coulomb+nuclear interaction with respect to Coulomb wave functions (see for instance Ref. [36]). For uncoupled channels, the asymptotic wave function can be written as

$$\Psi_{L,k}^{JST}(r) \underset{r\to+\infty}{\longrightarrow} F_L^c(r) + \tan(\delta_L^{JST})\,G_L^c(r)\,, \tag{D.101}$$

where F_L^c and G_L^c are regular and irregular Coulomb wave functions [37; 38]. Likewise, for a short-range vanishing potential one has

$$\tilde{\Psi}_{L,k}^{JST}(r) \underset{r\to+\infty}{\longrightarrow} F_L^0(r) + \tan(\tilde{\delta}_L^{JST})\,G_L^0(r)\,, \tag{D.102}$$

where F_L^0 and G_L^0 are so-called solutions of the Coulomb problem with zero charge, and usually expressed in terms of Bessel and Neumann functions (Eq. (D.58a)). Now the two solutions can be matched at an arbitrary distance R where $\tilde{\delta}_L^{JST}$ has been calculated with a Fourier-transformed Coulomb potential integrated up to the radius R [39]. Indeed, the two wave functions $\Psi_{L,k}^{JST}$ and $\tilde{\Psi}_{L,k}^{JST}$ describe the same system on the sphere with radius $R+\varepsilon$. By matching logarithmic derivatives, the phase shift δ_L^{JST}, corresponding to δ_{N+C}^{C}, can then be obtained from $\tilde{\delta}_L^{JST}$ in a Wronskian form by

$$\tan(\delta_L^{JST}) = \frac{\tan(\tilde{\delta}_L^{JST})\,[F_L, G_L^0] + [F_L, F_L^0]}{[F_L^0, G_L] + \tan(\tilde{\delta}_L^{JST})\,[G_L^0, G_L]}\,, \tag{D.103}$$

where

$$[X_L, Y_L] \equiv \left(Y_L \frac{d\,X_L}{d\,r} - X_L \frac{d\,Y_L}{d\,r} \right)_{r=R}\,. \tag{D.104}$$

For instance, for vacuum NN forces such as AV18 that are expressed in momentum space through a Fourier transform, phase shifts δ_L^{JST} are easily obtained by setting the value of R and computing accordingly the values of $\tilde{\delta}_L^{JST}$. The radius R is determined such that the short-range nuclear interaction vanishes beyond this value. At the same time, the truncated Fourier transform of the Coulomb potential will have rapid oscillations for too large values of R. For these reasons, a value $R \approx 10$ fm is usually used [40]. For coupled channels, e.g. $^3\mathrm{P}_2$-$^3\mathrm{F}_2$, the same prescription can be applied in the 2×2 subspace of the scattering matrix [36].

Since electromagnetic corrections beyond the Coulomb potential are small, the phase shifts δ_{N+EM}^{EM} can then be expanded into [33; 36]

$$\begin{aligned}\delta_{N+EM}^{EM} = \delta_{N+C1}^{C1} + \delta_{C1+C2}^{C1} + \delta_{C1+C2+MM}^{C1+C2} \\ + \delta_{C1+C2+MM+VP}^{C1+C2+MM} - \delta_{N+C1+C2+MM+VP}^{C1+N} \equiv \delta_{N+C1}^{C1}\rho + \phi + \tau - \tilde{\Delta}\,,\end{aligned} \tag{D.105}$$

where ρ is the improved Coulomb phase shift [41], ϕ the magnetic moment phase shift [33], τ the vaccuum polarization phase shift [42] and $\tilde{\Delta}$ the improved Coulomb-Foldy correction [41], and are usually computed using a distorted-wave Born approximation. Now all $L \geq 1$ partial waves are only weakly affected by eletromagnetic corrections, and one has in first approximation

$$\delta_{N+EM}^{EM} \approx \delta_{N+C1}^{C1}\,. \tag{D.106}$$

On the other hand, the phase shifts ρ, ϕ, τ and $\tilde{\Delta}$ have to be explicitly computed for $L = 0$ partial waves, that is the $^1\mathrm{S}_0$ channel (there is no proton-proton interaction in the coupled $^3\mathrm{S}_1$-$^3\mathrm{D}_1$ channel corresponding to $T = 0$). However (i) the first three are independent of the nuclear strong interaction v_N, and (ii) the improved Coulomb-Foldy correction $\tilde{\Delta}_0$ is found to be independent of v_N at a reasonable precision [41]. For these reasons, tabulated values at low energy can be used [41] instead of exact computations with a suitable precision for the scope of this thesis.

Finally, the contribution of the magnetic moment interaction v_{MM} is supposed to be small for np and nn interactions, that is one will use in these channels the standard phase shifts δ_N^0.

D.3.3.2 Scattering parameters

In addition to the scattering phase shifts, other quantities can be derived. In the case of a short-range two-body potential, it can be shown that the phase shifts behave like

$$\delta_L^{JST} \underset{k\to 0}{\sim} k^{2L+1}\,, \tag{D.107}$$

which implies that s-wave scattering dominates at low-energy limit[8]. At low energy, one can expand the s-wave effective range function $F_0(k)$ in powers of k^2 into [43]

$$F_0(k) \approx -\frac{1}{a_S} + \frac{1}{2}\, r_S\, k^2 + v_2\, k^4 + v_3\, k^6 + v_4\, k^8 + \dots \tag{D.108}$$

where the s-wave scattering length a_S, effective range r_S and shape parameters $v_{2/3/4}$ have been introduced. For s waves the effective range function is written as

$$F_0(k) = A_0\, k \cot\left[\delta_0^{JST}\right] + B_0\,. \tag{D.109}$$

For uncharged particles, the effective range function corresponds to $A_0 = 1$ and $B_0 = 0$, that is [44]

$$F_0(k) = k \cot\left[\left(\delta_N^0\right)_0^{JST}\right]\,. \tag{D.110}$$

In the case of proton-proton scattering, the effective range function has to be modified to take into account electromagnetic corrections. Two solutions are possible, i.e.

- the effective range function using the Coulomb potential for the long-range part of the interaction [45; 46], which reads

$$F_0(k) = C_0(\eta')\, k \cot\left[\left(\delta_{N+C1}^{C1}\right)_0^{JST}\right] + 2\, k\, \eta'\, h(\eta')\,, \tag{D.111}$$

  where η' is the relativistic Coulomb parameter [47]

$$\eta' = \frac{\alpha\, m_p}{2k} \frac{1 + 2\frac{k^2}{m_p^2}}{\sqrt{1 + \frac{k^2}{m_p^2}}}\,, \tag{D.112}$$

  and

$$C_0^2(\eta') = \frac{2\pi\,\eta'}{e^{2\pi\,\eta'} - 1}\,, \qquad h(\eta') = \mathrm{Re}[\Psi(1 + i\,\eta')] - \ln(\eta')\,, \tag{D.113}$$

  Ψ being the digamma function [3],

- the effective range function with respect to the full electromagnetic potential, which reads [48; 49]

$$F_0(k) = C_0(\eta')\, k\, \frac{(1+\chi_0)\cot\left[\left(\delta_{N+EM}^{EM}\right)_0^{JST}\right] - \tan\tau_0}{(1+A_1)(1-\chi_0)} + (1-A_2)\, 2\, k\, \eta'\, h(\eta') + k^2\, d\,[C_0^4(\eta') - 1] + 2\,\eta'\, k\, \ell_0\,. \tag{D.114}$$

D.4 Nuclear matter equation of state

The total energy per particle of spin-unpolarized infinite matter calculated via MBPT can be decomposed into an uncorrelated kinetic energy term and a correlation part as

$$\frac{E}{A}(k_F^n, k_F^p) = \frac{E^K}{A}(k_F^n, k_F^p) + \frac{E^V}{A}(k_F^n, k_F^p). \tag{D.115}$$

The kinetic part can be evaluated exactly, while the calculation of the correlation energy at lowest (HF) order using a two-body interaction expanded in partial waves is given below in

[8] As long as the nucleons are not identical, in which case p-wave scattering dominates, but this is not the case here.

Sec. D.4.3. Similar formulæ may be applied for calculations at second order in MBPT or resumming particle-particle ladders to all orders once (i) the vacuum interaction has been replaced by an effective one, and (ii) the additional dependencies of the latter, for instance on the total momentum $\vec{K}$ or the G-matrix starting energy ω, have been specified and properly treated. Such a derivation uses a partial wave expansion of the vertex, and thus consists in a converging series.

The system is put in a box of arbitrary volume $\mathcal{V}$, in which case the transformation from discrete sums to continuous integrals reads

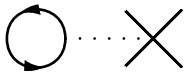
$$\sum_{\vec{k}} \longrightarrow \frac{\mathcal{V}}{(2\pi)^3} \int \mathrm{d}\vec{k}\,. \tag{D.116}$$

Obviously dependencies on the volume should disappear in the final expression with the introduction of the total particle number $A = \rho\,\mathcal{V}$.

In the following, one assumes that the effect of superfluidity can be neglected for the EOS[9] and pairing properties are treated separately by solving the gap equation without any feedback on occupations numbers nor the binding energy.

D.4.1 Kinetic energy

The uncorrelated kinetic energy is immediately

$E^K(k_F^n, k_F^p) \equiv$ 

$$= \sum_{\sigma\, q} \frac{\mathcal{V}}{(2\pi)^3} \int_{k<k_F^q} \mathrm{d}\vec{k}\, \frac{\hbar^2\, k^2}{2\, m} = \sum_q \frac{3}{5} \frac{\hbar^2\, (k_F^q)^2}{2\, m}\, \rho^q\, \mathcal{V}\,. \tag{D.117}$$

The kinetic energy per nucleon is thus

$$\frac{E^K}{A}(k_F^n, k_F^p) = \sum_q \frac{3}{5} \frac{\hbar^2\, (k_F^q)^2}{2\, m}\, \frac{\rho^q}{\rho_0}\,. \tag{D.118}$$

Symetric matter

For symmetric matter, one has $\beta = 0$, that is

$$\frac{E^K}{A}(k_F) = \frac{3}{10} \frac{\hbar^2\, k_F^2}{m}\,. \tag{D.119}$$

Neutron matter

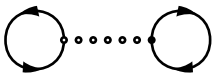
For neutron matter, one has $\beta = 1$, that is

$$\frac{E^K}{A}(k_F^n) = \frac{3}{5} \frac{\hbar^2\, k_F^{n\,2}}{2m} = 2^{2/3}\, \frac{3}{5} \frac{\hbar^2\, k_F^2}{2m}\,. \tag{D.120}$$

[9] This is incorrect for low-density neutron matter where one approaches a BCS-BEC phase transition.

D.4.2 Correlation energy at the Hartree-Fock level: generalities

The correlation energy of spin-unpolarized INM reads at the Hartree-Fock level as a double trace over the closed loops of the two-body potential v, i.e.

$E^V(k_F^n, k_F^p) \equiv$ 

$$= \frac{1}{2} \sum_{ijkl} \langle\, i\, j \,|\, v\,(1 - P_{12}) \,|\, k\, l \,\rangle\, \rho_{ki}\, \rho_{lj} \tag{D.121a}$$

$$= \frac{1}{2} \sum_{q_1\, q_2} \int_{|\vec{k}_1|<k_F^{q_2}} \int_{|\vec{k}_2|<k_F^{q_2}} \frac{\mathcal{V}\,\mathrm{d}\vec{k}_1}{(2\pi)^3} \frac{\mathcal{V}\,\mathrm{d}\vec{k}_2}{(2\pi)^3} \sum_{S\,S_z} \sum_{T\,T_z} \langle \tfrac{1}{2}\tfrac{1}{2}\, q_1 q_2 | T\, T_z \rangle^2\, \rho^{q_1}_{\vec{k}_1\vec{k}_1}\, \rho^{q_2}_{\vec{k}_2\vec{k}_2}$$
$$\times \langle\, \vec{k}_1\, \vec{k}_2\, S\, S_z\, T\, T_z \,|\, v\,(1 - P_{\vec{k}}\, P_\sigma\, P_\tau) \,|\, \vec{k}_1\, \vec{k}_2\, S\, S_z\, T\, T_z \,\rangle\,. \tag{D.121b}$$

The summations over $\vec{k}_i$ run over occupied states $k_i < k_F^{q_i}$, and thus implicitly depend on the associated isospin q_i, which explains why the sum over q_1 and q_2 cannot be resolved yet, contrary to the one over σ_1 and σ_2. One has however

$$\sum_{T_z} \langle \tfrac{1}{2}\tfrac{1}{2}\, qq | T\, T_z \rangle^2 = T\,, \qquad \sum_{T_z} \langle \tfrac{1}{2}\tfrac{1}{2}\, (-q)q | T\, T_z \rangle^2 = \frac{1}{2}\,. \tag{D.122}$$

D.4.3 Correlation energy at the Hartree-Fock level: partial wave expansion

The following derivation allows to evaluate the correlation energy of nuclear matter at the Hartree-Fock level for a generic vertex v. It will be only valid when the Fermi sea is unique (PNM) or identical for protons and neutrons (INM). In this case one will note $E(k_F^n, k_F^q) \equiv E(k_F)$. One has

$$E^V(k_F^n, k_F^p) = \frac{1}{2} \sum_{\vec{k}_1\,\vec{k}_2} \sum_{S\,S_z} \sum_{T\,T_z} \rho_{\vec{k}_1\,\vec{k}_1}\, \rho_{\vec{k}_2\,\vec{k}_2}\, \langle\, \vec{k}_1\, \vec{k}_2\, S\, S_z\, T\, T_z \,|\, v\,(1 - P_{\vec{k}}\, P_\sigma\, P_\tau) \,|\, \vec{k}_1\, \vec{k}_2\, S\, S_z\, T\, T_z \,\rangle \tag{D.123a}$$

$$= \frac{(2\pi)^3}{2\,\mathcal{V}} \sum_{\vec{k}\,\vec{K}} \sum_{S\,S_z} \sum_{T\,T_z} \theta\left(k_F - \left|\vec{K}/2 + \vec{k}\right|\right)\, \theta\left(k_F - \left|\vec{K}/2 - \vec{k}\right|\right)$$
$$\times \langle\, \vec{k}\, S\, S_z\, T\, T_z \,|\, v\,(1 - P_{\vec{k}}\, P_\sigma\, P_\tau) \,|\, \vec{k}\, S\, S_z\, T\, T_z \,\rangle\,, \tag{D.123b}$$

using from the momentum space transformation

$$\langle\, \vec{k}_1\, \vec{k}_2 \,|\, v \,|\, \vec{k}_1\, \vec{k}_2 \,\rangle = \frac{1}{\mathcal{V}} \langle\, \vec{k} \,|\, v \,|\, \vec{k} \,\rangle\,, \tag{D.124}$$

and with

$$\rho_{\vec{K}\,\vec{K}} = \Theta(k_F - K)\,, \tag{D.125}$$

that is

- for symmetric matter $k_F = k_F^n = k_F^p$ and $\rho_{\vec{K}} = \Theta(k_F - K)$,
- for neutron matter $k_F^3 = \frac{1}{2} k_F^n$ and $\rho_{\vec{K}} = \Theta(k_F^n - K)$.

From a partial wave expansion one gets then

$$E^V(k_F^n,k_F^p) = \frac{(4\pi)^2\,\mathcal{V}}{2}\int\frac{\mathrm{d}\vec{k}}{(2\pi)^3}\int\frac{\mathrm{d}\vec{K}}{(2\pi)^3}\,\theta\left(k_F-\left|\vec{K}/2+\vec{k}\right|\right)\,\theta\left(k_F-\left|\vec{K}/2-\vec{k}\right|\right) \times\sum_{\substack{S\,S_z\\T\,T_z\\L\,L_z\\L'\,L'_z\\J\,J_z}} Y_L^{L_z}(\hat{k})\,Y_{L'}^{L'_z\,*}(\hat{k})\,C^{L'\,S\,J}_{L'_z\,S_z\,J_z}\,C^{L\,S\,J}_{L_z\,S_z\,J_z}\,\left(1-(-1)^{L+S+T}\right)\,v_{LL'}^{JSS_zTT_z}(k,k)\,. \tag{D.126}$$

using Eq. (A.10a), a $L+S$ summation, and

$$P_{\vec{k}}\,P_\sigma\,P_\tau\,|\,\vec{k}\,S\,S_z\,T\,T_z\,\rangle = (-1)^{S+T}\,|\,-\vec{k}\,S\,S_z\,T\,T_z\,\rangle\,. \tag{D.127}$$

The product of Clebsh-Gordan coefficients implies that $L_z = L'_z$, and since the interaction does not depend on the angular momentum projection J_z, one gets

$$E^V(k_F^n,k_F^p) = \frac{(4\pi)^2\,\mathcal{V}}{2}\int\frac{\mathrm{d}\vec{k}}{(2\pi)^3}\int\frac{\mathrm{d}\vec{K}}{(2\pi)^3}\,\theta\left(k_F-\left|\vec{K}/2+\vec{k}\right|\right)\,\theta\left(k_F-\left|\vec{K}/2-\vec{k}\right|\right) \times\sum_{\substack{L\,L_z\,J\\S\,T\,T_z}}\left(1-(-1)^{L+S+T}\right)\,\frac{[J]}{[L]}\,Y_L^{L_z}(\hat{k})\,Y_L^{L_z\,*}(\hat{k})\,v_L^{JSTT_z}(k,k)\,. \tag{D.128}$$

The computation of the integral

$$\mathcal{I}(k,\bar{k}_F) \equiv \int\frac{\mathrm{d}\vec{K}}{(2\pi)^3}\rho_{\frac{\vec{K}}{2}+\vec{k}}\,\rho_{\frac{\vec{K}}{2}-\vec{k}}\,, \tag{D.129}$$

uses the properties of the polynomials

$$P_\theta^\pm(K,k_F) = \frac{K^2}{4}\pm k\,K\,\cos(\theta)+k^2-{k_F}^2\,, \tag{D.130}$$

such that

$$\theta\left(k_F-\left|\vec{K}/2\pm\vec{k}\right|\right)=1\Leftrightarrow P^\pm(K)\le 0\,. \tag{D.131}$$

The determinant of $P_\theta^\pm$ reads in both cases

$$\Delta = k^2\,\cos^2(\theta)-k^2+{k_F}^2 = {k_F}^2-k^2\,\sin^2(\theta)\,, \tag{D.132}$$

from which two cases have to be considered.

1. $\Delta<0$ in which case $P_\theta^\pm(K)$ is of the sign of $k^2-{k_F}^2$. That is $P_\theta^\pm(K)\le 0$ requires $k<k_F$, while $\Delta<0$ requires at the same time $\sin(\theta)>k_F/k$. Both conditions are exclusive, thus the case $\Delta<0$ is not possible.
2. $\Delta\ge 0$ in which case $\sin(\theta)\le k_F/k$. We note θ_0 the critical angle verifying $\sin(\theta_0)=k_F/k$. In this case $P_\theta^\pm$ has two roots

$$K_1^\pm = \mp 2k\,\cos(\theta)-2\sqrt{{k_F}^2-k^2\,\sin^2(\theta)}\,,\qquad K_2^\pm = \mp 2k\,\cos(\theta)+2\sqrt{{k_F}^2-k^2\,\sin^2(\theta)}\,, \tag{D.133}$$

and for $\bar{K}^\pm = (K_1^\pm+K_2^\pm)/2$

$$P_\theta^\pm(\bar{K}^\pm) = k^2\,\sin^2(\theta)-{k_F}^2\le 0\,. \tag{D.134}$$

One has then

	$K_1^\pm$		$K_2^\pm$	
$P_\theta^\pm$	+ 0	-	0	+

In $\mathcal{I}(k,k_F)$ both P_θ^- and P_θ^+ have to be negative at the same time, and one will have to consider two cases:

1. for $\theta \leq \pi/2$ one has $\cos(\theta) \geq 0$ thus $\bar{K}^+ \leq \bar{K}^-$. The condition $P_\theta^\pm(K) \leq 0$ can only be fulfilled if $K_1^- \leq K_2^+$, that is

$$K_1^- < K_2^+ \,, \qquad k < k_F \,, \tag{D.135a}$$

$$k\,\cos(\theta) - \sqrt{\Delta} < -\,k\,\cos(\theta) + \sqrt{\Delta}\,, \qquad k\,\cos(\theta) < \sqrt{{k_F}^2 - k^2\,\sin^2(\theta)}\,. \tag{D.135b}$$

   That means that there is actually no critical angle θ_0 in this case and the upper limit of the integral over θ can be set to $\pi/2$. On the other hand one has $K_1^- \leq 0$, that is for an integral running on K in $\mathcal{I}(k,k_F)$ one has to take the interval $[0, K_2^+]$,

2. equivalently for $\theta > \pi/2$ one finds that the integral on K in $\mathcal{I}(k,k_F)$ runs on $[0, K_2^-]$.

One gets then

$$\begin{aligned}
\mathcal{I}(k,k_F) =& \Theta(k_F-k)\,\frac{1}{(2\pi)^2}\int \sin(\theta)\,\mathrm{d}\theta \int_{K\in\mathcal{D}} K^2\,\mathrm{d}K \\
=& \Theta(k_F-k)\,\frac{1}{(2\pi)^2}\int_0^{\pi/2} \sin(\theta)\,\mathrm{d}\theta \int_0^{K_2^+} K^2\,\mathrm{d}K \\
&+ \Theta(k_F-k)\,\frac{1}{(2\pi)^2}\int_{\pi/2}^{\pi} \sin(\theta)\,\mathrm{d}\theta \int_0^{K_2^-} K^2\,\mathrm{d}K \\
=& \frac{1}{(2\pi)^3}\,\Theta(k_F-k)\,\frac{2\pi}{3}\int_0^{\pi/2}\sin(\theta)\,\mathrm{d}\theta\,{K_2^+}^3 + \frac{1}{(2\pi)^3}\,\Theta(k_F-k)\,\frac{2\pi}{3}\int_{\pi/2}^{\pi}\sin(\theta)\,\mathrm{d}\theta\,{K_2^-}^3 \\
=& \frac{1}{(2\pi)^3}\,\Theta(k_F-k)\,\frac{32\pi}{3}\left[k^3 - 3\,k\,{k_F} + 2\,{k_F}^3\right] \,.
\end{aligned} \tag{D.136}$$

Symmetric matter

One has for symmetric matter

$$\rho = \frac{1}{(2\pi)^3}\sum_\sigma\sum_q \frac{4\pi}{3}k_F^3 = \frac{1}{(2\pi)^3}\,\frac{16\pi}{3}k_F^3\,, \tag{D.137}$$

that is

$$\mathcal{I}(k,k_F) = \Theta(k_F-k)\,2\,\rho\left(1 - \frac{3}{2}\frac{k}{k_F} + \frac{1}{2}\left[\frac{k}{k_F}\right]^3\right) \,. \tag{D.138}$$

One finds for symmetric matter $E^V(k_F,k_F) \equiv E^V(k_F)$, where

$$E^V(k_F) = (4\pi)^2\,\rho\,\mathcal{V}\int_0^{k_F}\frac{k^2\,\mathrm{d}k}{(2\pi)^3}\sum_{\substack{L\,S\,J\\T\,T_z}}\left(1-(-1)^{L+S+T}\right)[J]\,v_L^{JSTT_z}(k,k)\left(1 - \frac{3}{2}\frac{k}{k_F} + \frac{1}{2}\left[\frac{k}{k_F}\right]^3\right) , \tag{D.139}$$

where one recalls that $[J] \equiv J+1$. Thus, assuming charge-independence of the potential and summing over T_z[10]

$$\frac{E^V}{A}(k_F) = \frac{4}{\pi}\int_0^{k_F} k^2\,\mathrm{d}k \sum_{L\,S\,J\,T}{}' [J][T]\, v_L^{JST}(k,k)\left(1-\frac{3}{2}\frac{k}{k_F}+\frac{1}{2}\left[\frac{k}{k_F}\right]^3\right), \tag{D.140}$$

where $\sum'$ denotes that the sum runs only on odd values of $L+S+T$.

Neutron matter

For neutron matter one has equivalently

$$\rho = \frac{1}{(2\pi)^3}\sum_\sigma \frac{4\pi}{3}k_F^3 = \frac{1}{(2\pi)^3}\frac{8\pi}{3}k_F^3 = \frac{1}{(2\pi)^3}\frac{4\pi}{3}{k_F^n}^3, \tag{D.141}$$

that is using Eq. (D.136)

$$\int \frac{\mathrm{d}\vec{K}}{(2\pi)^3}\rho_{\frac{\vec{K}}{2}+\vec{k}}\,\rho_{\frac{\vec{K}}{2}-\vec{k}} = \mathcal{I}(k,k_F^n) = \Theta(k_F^n-k)\,8\,\rho\left(1-\frac{3}{2}\frac{k}{k_F^n}+\frac{1}{2}\left[\frac{k}{k_F^n}\right]^3\right). \tag{D.142}$$

Thus

$$\frac{E^V}{A}(k_F^n,0) \equiv \frac{E^V}{A}(k_F^n) = \frac{48}{\pi}\int_0^{k_F^n} k^2\,\mathrm{d}k \sum_{L\,S\,J}{}' [J]\, v_L^{JS1}(k,k)\left(1-\frac{3}{2}\frac{k}{k_F^n}+\frac{1}{2}\left[\frac{k}{k_F^n}\right]^3\right). \tag{D.143}$$

D.4.4 Correlation energy at the Hartree-Fock evel: gaussian vertices

With gaussian vertices, the computation of INM/PNM equations of state can be done exactly, without a (truncated) partial wave summation. One will consider a gaussian vertex of the kind

$$v(\vec{r}) = \sum_{ST}\sum_i C_i^{ST}[\rho_0]\, e^{-\frac{r^2}{\mu_i^2}} \prod_S\prod_T \equiv \sum_{ST}\sum_i v_i^{ST}(\vec{r}) \prod_S\prod_T, \tag{D.144}$$

containing if necessary density-dependent terms, depending on ρ_0 in INM. The correlation energy reads from Eq. (D.121b)

$$\begin{aligned} E^V(k_F^n,k_F^p) =& \frac{1}{2}\sum_{q_1\,q_2}\sum_{\vec{k}_1\,\vec{k}_2}\sum_{S\,S_z}\sum_{T\,T_z}\langle \tfrac{1}{2}\tfrac{1}{2}\,q_1q_2|T\,T_z\rangle^2\,\rho_{\vec{k}_1\,\vec{k}_1}\,\rho_{\vec{k}_2\,\vec{k}_2} \\ &\times \langle\,\vec{k}_1\,\vec{k}_2\,S\,S_z\,T\,T_z\,|\,v\,(1-P_{\vec{k}}\,P_\sigma\,P_\tau)\,|\,\vec{k}_1\,\vec{k}_2\,S\,S_z\,T\,T_z\,\rangle \qquad \text{(D.145a)} \\ =& \frac{1}{2}\sum_{q_1\,q_2}\sum_{\vec{k}_1\,\vec{k}_2}\sum_{S\,T}[S]\sum_{T_z}\langle \tfrac{1}{2}\tfrac{1}{2}\,q_1q_2|T\,T_z\rangle^2\,\rho_{\vec{k}_1\,\vec{k}_1}\,\rho_{\vec{k}_2\,\vec{k}_2} \\ &\times \sum_i\left[\langle\,\vec{k}_1\,\vec{k}_2\,|\,v_i^{ST}\,|\,\vec{k}_1\,\vec{k}_2\,\rangle - (-1)^{S+T}\langle\,\vec{k}_1\,\vec{k}_2\,|\,v_i^{ST}\,|\,\vec{k}_2\,\vec{k}_1\,\rangle\right], \qquad \text{(D.145b)} \end{aligned}$$

[10] This implies that one assumes that the vacuum interaction is charge-independent. In practical calculations, one takes usually $T_z = 0$ for CIB forces.

Now using the results from Sec. E.1, one finds directly

$$\langle \vec{k}_1\,\vec{k}_2\,|\,v_i^{ST}\,|\,\vec{k}_1\,\vec{k}_2\,\rangle = \frac{(\mu_i\sqrt{\pi})^3\,C_i^{ST}[\rho_0]}{\mathcal{V}}\,, \tag{D.146a}$$

$$\langle \vec{k}_1\,\vec{k}_2\,|\,v_i^{ST}\,|\,\vec{k}_2\,\vec{k}_1\,\rangle = \frac{(\mu_i\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_i^2\,|\vec{k}_1-\vec{k}_2|^2}\,C_i^{ST}[\rho_0]}{\mathcal{V}}\,. \tag{D.146b}$$

Thus

$$\sum_{\vec{k}_1\,\vec{k}_2}\langle \vec{k}_1\,\vec{k}_2\,|\,v_i^{ST}\,|\,\vec{k}_1\,\vec{k}_2\,\rangle\,\rho_{\vec{k}_1}\,\rho_{\vec{k}_2} = \mathcal{V}\,\frac{(\mu_i\sqrt{\pi})^3\,C_i^{ST}[\rho_0]}{(2\pi)^6}\,\frac{4\pi\,(k_F^{q_1})^3}{3}\,\frac{4\pi\,(k_F^{q_2})^3}{3}\,, \tag{D.147a}$$

$$\sum_{\vec{k}_1\,\vec{k}_2}\langle \vec{k}_1\,\vec{k}_2\,|\,v_i^{ST}\,|\,\vec{k}_2\,\vec{k}_1\,\rangle\,\rho_{\vec{k}_1}\,\rho_{\vec{k}_2} = \mathcal{V}\,\frac{(\mu_i\sqrt{\pi})^3\,C_i^{ST}[\rho_0]}{(2\pi)^6}J(X_i^{q_1},X_i^{q_2})\,, \tag{D.147b}$$

where

$$X_i^{q_1} = \mu_i\,k_F^{q_i}\,, \tag{D.148a}$$

$$X_i = \mu_i\,k_F\,, \tag{D.148b}$$

$$J(X_i^{q_1},X_i^{q_2}) = \frac{\pi^2}{6}\left(\frac{2}{\mu_i}\right)^6 F(X_i^{q_1},X_i^{q_2}) \tag{D.148c}$$

$$\begin{aligned} F(X,Y) =& e^{-\left(\frac{X+Y}{2}\right)^2}(X^2+Y^2-XY-2) - e^{-\left(\frac{X-Y}{2}\right)^2}(X^2+Y^2+XY-2) \\ &+ \frac{\sqrt{\pi}}{2}\,\mathrm{erf}\left(\frac{X+Y}{2}\right)(X^3+Y^3) + \frac{\sqrt{\pi}}{2}\,\mathrm{erf}\left(\frac{X-Y}{2}\right)(X^3-Y^3)\,, \end{aligned} \tag{D.148d}$$

$$\mathrm{erf}(X) = \frac{2}{\sqrt{\pi}}\int_0^X e^{-u^2}\,\mathrm{d}u\,. \tag{D.148e}$$

The box volume can be noted as

$$\mathcal{V} = \frac{A}{\rho} = A\,\frac{3\pi^2\,\mu_i^3}{2\,X_i^3}\,. \tag{D.149}$$

The correlation energy reads then

$$\begin{aligned} E^V(k_F^n,k_F^p) =& A\sum_{S\,T}[S]\,C_i^{ST}[\rho_0]\sum_{T_z}\sum_{q_1\,q_2}\sum_i \langle \tfrac{1}{2}\,\tfrac{1}{2}\,q_1 q_2|T\,T_z\rangle^2 \\ &\times\left[\frac{1}{48\sqrt{\pi}}\left(\frac{X_i^{q_1}\,X_i^{q_2}}{X_i}\right)^3 - (-1)^{S+T}\frac{1}{8\sqrt{\pi}}\frac{F(X_i^{q_1},X_i^{q_2})}{X_i^3}\right] \end{aligned} \tag{D.150a}$$

$$\begin{aligned} =& \frac{A}{8\sqrt{\pi}}\sum_{S\,T}[S]\sum_i\frac{C_i^{ST}[\rho_0]}{X_i^3}\left[\frac{1}{6}\left(T\,X_i^{n6}+T\,X_i^{p6}+(X_i^n\,X_i^p)^3\right)\right. \\ &\left. -(-1)^{S+T}\left(T\,F(X_i^n,X_i^n)+T\,F(X_i^p,X_i^p)+\frac{F(X_i^n,X_i^p)+F(X_i^p,X_i^n)}{2}\right)\right]. \end{aligned} \tag{D.150b}$$

Symmetric matter

One has for symmetric matter

$$X_i^n = X_i^p = X_i\,, F(X_i,X_i) = \qquad e^{-X_i^2}(X_i^2-2) - 3\,X_i^2 + 2 + \sqrt{\pi}\,\mathrm{erf}(X_i)\,X_i^3\,. \tag{D.151a}$$

The potential energy is then

$$\frac{E^V}{A}(k_F) = \sum_{S\,T}\frac{1}{8\sqrt{\pi}}\,[S]\,[T]\sum_i C_i^{ST}[\rho_0]\left[\frac{X_i^3}{6} - (-1)^{S+T}\frac{F(X_i,X_i)}{X_i^3}\right]. \tag{D.152}$$

The decomposition in (S,T) channels is thus explicit.

Neutron matter

Likewise for neutron matter

$$X_i^{n3} = 2\,X_i^3 \qquad X_i^p = 0\,, \tag{D.153a}$$
$$F(X_i,0) = F(0,X_i) = F(0,0) = 0\,. \tag{D.153b}$$

The potential energy is then

$$\frac{E^V}{A}(k_F^n) = \sum_S \frac{1}{4\sqrt{\pi}}\,[S] \sum_i C_i^{S1}[\rho_0] \left[\frac{X_i^{n3}}{6} + (-1)^S \frac{F(X_i^n, X_i^n)}{X_i^{n3}}\right]. \tag{D.154}$$

D.4.5 Equivalence between the two methods

To check the consistency between the two approaches, we will consider the case of symmetric matter. One gets from Eq. (D.140) with an explicit decomposition into direct and exchange terms

$$\begin{aligned}
\frac{E^V}{A}(k_F) =& \frac{2}{\pi}\int_0^{k_F} k^2\,\mathrm{d}k \sum_{L\,S\,J\,T} [J][T] \\
&\times \left[{v_{dir}}_L^{JST}(k,k) - (-1)^{L+S+T}\,{v_{ex}}_L^{JST}(k,k)\right] \left(1 - \frac{3}{2}\frac{k}{k_F} + \frac{1}{2}\left[\frac{k}{k_F}\right]^3\right) \\
=& \frac{1}{\pi}\,\frac{1}{4\pi}\int_0^{k_F} k^2\,\mathrm{d}k \sum_{L\,S\,J\,T} [J][T] \int_0^{\pi} P_L(\cos(\theta))\,\sin(\theta)\,\mathrm{d}\theta \\
&\times \left[v_{dir}^{ST}(\vec{k},\vec{k}) - (-1)^{L+S+T} v_{exc}^{ST}(\vec{k},\vec{k})\right] \left(1 - \frac{3}{2}\frac{k}{k_F} + \frac{1}{2}\left[\frac{k}{k_F}\right]^3\right) \\
=& \frac{1}{\pi}\,\frac{1}{4\pi}\int_0^{k_F} k^2\,\mathrm{d}k \sum_{L\,S\,J\,T} \sum_i C_i^{ST}[\rho_0]\,(\mu_i\sqrt{\pi})^3 [J][T] \\
&\times \int_0^{\pi} P_L(\cos(\theta))\,\sin(\theta)\,\mathrm{d}\theta \left[1 - (-1)^{L+S+T}\,e^{-\mu_i^2 k^2}\right] \left(1 - \frac{3}{2}\frac{k}{k_F} + \frac{1}{2}\left[\frac{k}{k_F}\right]^3\right) \\
=& \frac{2}{\pi}\,\frac{1}{4\pi} \sum_{L\,S\,J\,T} \sum_i C_i^{ST}[\rho_0]\,(\mu_i\sqrt{\pi})^3 [J][T]\,\delta_{L0} \\
&\times \int_0^{k_F} k^2\,\mathrm{d}k \left[1 - (-1)^{S+T}\,e^{-\mu_i^2 k^2}\right] \left(1 - \frac{3}{2}\frac{k}{k_F} + \frac{1}{2}\left[\frac{k}{k_F}\right]^3\right) \\
=& \frac{2}{\pi}\,\frac{1}{4\pi} \sum_{S\,T} \sum_i C_i^{ST}[\rho_0]\,(\mu_i\sqrt{\pi})^3 [S][T] \\
&\times \left[\frac{k_F^3}{24} - (-1)^{S+T}\left(\frac{2 - 3\,{k_F}^2\,\mu_i^2 + e^{-{k_F}^2\,\mu_i^2}({k_F}^2\,\mu_i^2 - 2) + \sqrt{\pi}\,\mathrm{erf}(k_F\,\mu_i)\,{k_F}^3\,\mu_i^3}{4\,{k_F}^3\,\mu_i^6}\right)\right] \\
=& \sum_{S\,T} [S][T]\,\frac{1}{8\sqrt{\pi}} \sum_i C_i^{ST}[\rho_0] \left[\frac{X_i^3}{6} - (-1)^{S+T}\frac{F(X_i,X_i)}{X_i^3}\right],
\end{aligned} \tag{D.155}$$

that is the expression found in Eq. (D.152).

Appendix E

Properties of $v_{\mathrm{BDRS}}^{[\mathrm{X}]}$

Abstract: this chapter presents the formal derivations of the properties of v_{BDRS} in its different realizations, in particular concerning momentum-space and partial-wave expressions that are carried out in a pedestrian way.

Contents

Let us recall that the Gogny effective force D1S is defined as a finite-range local effective vertex that reads [50–53]

$$v(\vec{r}_i) = \delta(\vec{r}_1 - \vec{r}_3\,)\delta(\vec{r}_2 - \vec{r}_4\,)\, v_{\rm D1X}(\vec{r}, \vec{R}, \overleftarrow{k}', \overrightarrow{k}\,), \tag{E.1}$$

where

$$v_{\rm D1X}(\vec{r}, \vec{R}\,) = \sum_{i=1}^{2} [W_i + B_i\, P_\sigma - H_i\, P_\tau - M_i\, P_\sigma\, P_\tau]\, e^{-\frac{r^2}{\mu_i^2}} \tag{E.2a}$$

$$+ t_0(1 + x_0 P_\sigma)\rho^\alpha(\vec{R}\,)\delta(\vec{r}\,) \tag{E.2b}$$

$$+ i\, W_{LS}\, (\vec{\sigma}_1 + \vec{\sigma}_2)\, \overleftarrow{k}' \wedge \delta(\vec{r}\,)\, \overrightarrow{k}\,. \tag{E.2c}$$

that is, the Gogny vertex consists of a finite-range central force plus zero-range spin-orbit and density-dependent terms. Recently, improved parametrizations have been recently proposed that contain finite-range density-dependent terms, leading to the D2 parametrization [54]. It reads

$$v_{\rm D2}(\vec{r}, \vec{R}\,) = \sum_{i=1}^{2} [W_i + B_i\, P_\sigma - H_i\, P_\tau - M_i\, P_\sigma\, P_\tau]\, e^{-\frac{r^2}{\mu_i^2}} \tag{E.3a}$$

$$+ [W_3 + B_3\, P_\sigma - H_3\, P_\tau - M_3\, P_\sigma\, P_\tau]\, e^{-\frac{r^2}{\mu_3^2}} \left(\frac{\rho^\alpha(\vec{r}_1\,) + \rho^\alpha(\vec{r}_2\,)}{2}\right) \tag{E.3b}$$

$$+ i\, W_{LS}\, (\vec{\sigma}_1 + \vec{\sigma}_2)\, \overleftarrow{k}' \wedge \delta(\vec{r}\,)\, \overrightarrow{k}\,. \tag{E.3c}$$

On the other hand, the finite-range non-empirical vertex $v^{[X]}_{BDRS}$ reads in all its realizations

$$v^{[X]}_{\rm BDRS}(\vec{r}, \vec{R}, \Lambda) = \sum_{i=1}^{N} \left[\sum_{ST} C_i^{ST}[\rho_0(\vec{R}\,), \rho_1(\vec{R}\,), \vec{s}_0(\vec{R}\,), \vec{s}_1(\vec{R}\,), \Lambda]\, e^{-\frac{r^2}{\mu_i^2}} \prod_S \prod_T\right] \tag{E.4a}$$

$$+ \sum_T C_{so}^{1T}[\rho_0(\vec{R}\,), \rho_1(\vec{R}\,), \vec{s}_0(\vec{R}\,), \vec{s}_1(\vec{R}\,), \Lambda]$$

$$\times e^{-\frac{r^2}{\mu_{so}^2}}\, (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{r} \wedge \overrightarrow{k} \prod_{S=1} \prod_T \tag{E.4b}$$

$$+ \sum_T C_t^{1T}[\rho_0(\vec{R}\,), \rho_1(\vec{R}\,), \vec{s}_0(\vec{R}\,), \vec{s}_1(\vec{R}\,), \Lambda]\, e^{-\frac{r^2}{\mu_t^2}}\, r^2\, \mathsf{S}_{12} \prod_{S=1} \prod_T\,. \tag{E.4c}$$

In the following we neglect CIB/CSB effects, that is $v^{[X]}_{BDRS}$ is independent of S_z and T_z. If it were the case, neither the expressions in momentum space or the partial wave expansion would change since the nuclear interaction is always diagonal in such projections.

E.1 Matrix elements in momentum space

E.1.1 Conventions and preliminary remarks

In momentum space the plane wave basis is the natural basis of interest. The single-particle basis is composed of plane waves with good spin and isospin projection, i.e.

$$\langle \vec{r}\,|\vec{k}\,\sigma\, q\rangle = \varphi_{\vec{k}}(\vec{r}\sigma q) = e^{i\vec{k}\cdot\vec{r}}\, \chi^\sigma\, \chi^q\,, \tag{E.5}$$

whose scalar product is given by

$$\langle \vec{k}\,\sigma\,q|\vec{k}\,'\,\sigma'\,q'\rangle \;=\; (2\pi)^3\,\delta(\vec{k}-\vec{k}\,')\,\delta_{\sigma\sigma'}\,\delta_{qq'}\,. \tag{E.6}$$

Because of the convention used to define plane waves, integrals in momentum space are characterized by $\int \mathrm{d}\vec{k}\,/\,(2\pi)^3$, such that [1]

$$\langle \vec{r}|\vec{r}\,'\rangle = \int \frac{\mathrm{d}\vec{k}}{(2\pi)^3}\,e^{i\,\vec{k}\cdot(\vec{r}-\vec{r}\,')} = \delta(\vec{r}-\vec{r}\,')\,. \tag{E.8}$$

One has then

$$v(\vec{k}_{1234}) = \int \mathrm{d}\vec{r}_{1234}\,e^{-i[+\vec{k}_1\cdot\vec{r}_1+\vec{k}_2\cdot\vec{r}_2-\vec{k}_3\cdot\vec{r}_3-\vec{k}_4\cdot\vec{r}_4]}\,v(\vec{r}_{1234})\,, \tag{E.9a}$$

$$v(\vec{k}_{1234}) = \frac{1}{(2\pi)^{12}}\int \mathrm{d}\vec{k}_{1234}\,e^{-i[-\vec{k}_1\cdot\vec{r}_1-\vec{k}_2\cdot\vec{r}_2+\vec{k}_3\cdot\vec{r}_3+\vec{k}_4\cdot\vec{r}_4]}\,v(\vec{k}_{1234})\,. \tag{E.9b}$$

E.1.2 Gogny interaction

E.1.2.1 Central terms

Disregarding the initial prefactor (WBHM terms) that only depends on spin and isospin degrees of freedom and decouple from the radial part, the vertex reduces to a pure gaussian $e^{-\frac{r^2}{\mu_i}}$, which leads for the direct term to

$$\begin{aligned}\langle \vec{k}_k\;\vec{k}_l|V_{\mathrm{D1X}}|\vec{k}_i\;\vec{k}_j\rangle^{SS_zTT_z}_{i,dir} &= \int \mathrm{d}\vec{r}_1\,d\vec{r}_2\,e^{i\,[\vec{r}_1\cdot(\vec{k}_i-\vec{k}_k\,)+\vec{r}_2\cdot(\vec{k}_j-\vec{k}_l\,)]}\,e^{-\frac{r^2}{\mu_i}}\\ &= \int \mathrm{d}\vec{R}\,e^{i\,\vec{R}\cdot(\vec{K}-\vec{K}\,')}\int \mathrm{d}\vec{r}\,e^{i\,\vec{r}\cdot\vec{q}}\,e^{-\frac{r^2}{\mu_i}}\\ &= (\mu_i\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_i^2q^2}\,(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\,.\end{aligned} \tag{E.10}$$

For the exchange term, one finds equivalently

$$\langle \vec{k}_k\;\vec{k}_l|V_{\mathrm{D1X}}|\vec{k}_i\;\vec{k}_j\rangle^{SS_zTT_z}_{i,ex} = (\mu_i\sqrt{\pi})^3 e^{-\frac{1}{4}\mu_i^2q'^2}\,(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\,.$$

E.1.2.2 Spin-orbit term

The spin-orbit part reads for the direct term

$$\begin{aligned}\langle \vec{k}_k\;\vec{k}_l|V_{\mathrm{D1X}}|\vec{k}_i\;\vec{k}_j\rangle^{1S_zTT_z}_{so,dir} &= i\,W_{LS}\int \mathrm{d}\vec{r}_1\,d\vec{r}_2\,e^{-i\,(\vec{r}_1\cdot\vec{k}_k+\vec{r}_2\cdot\vec{k}_l)}\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\overleftarrow{k'}\wedge\delta(\vec{r})\,\overrightarrow{k}\,e^{i\,(\vec{r}_1\cdot\vec{k}_i+\vec{r}_2\cdot\vec{k}_j)}\\ &= i\,W_{LS}\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\left[\int \mathrm{d}\vec{r}_1\,d\vec{r}_2\;\vec{r}\;e^{i\,[\vec{r}_1\cdot(\vec{k}_i-\vec{k}_k\,)+\vec{r}_2\cdot(\vec{k}_j-\vec{k}_l\,)]}\delta(\vec{r}\,)\right]\vec{k}\\ &= i\,W_{LS}\,(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\;(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\left[\int \mathrm{d}\vec{r}\,e^{i\,\vec{r}\cdot\vec{q}}\,\delta(\vec{r}\,)\right]\vec{k}\\ &= i\,W_{LS}\,(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\;(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\vec{k}\,.\end{aligned} \tag{E.11}$$

[1] That is, we are using non-unitary Fourier transforms:

$$\tilde{f}(k) = \int_{-\infty}^{+\infty} f(r)\,e^{-i\,k\,r}\,\mathrm{d}r\,, \qquad f(r) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\tilde{f}(k)\,e^{+i\,k\,r}\,\mathrm{d}k\,. \tag{E.7}$$

E.1.2.3 Density-dependent terms: D1X

In the case of D1X, the density-dependent term is zero range, thus

$$\begin{aligned}\langle \vec{k}_k\ \vec{k}_l|V_{\mathrm{D1X}}|\vec{k}_i\ \vec{k}_j\rangle^{SS_zTT_z}_{\rho,dir} &= \int \mathrm{d}\vec{r}_1\, d\vec{r}_2\, e^{i\,[\vec{r}_1\cdot(\vec{k}_i-\vec{k}_k\,)+\vec{r}_2\cdot(\vec{k}_j-\vec{k}_l\,)]}\,\rho^\alpha(\vec{R}\,)\,\delta(\vec{r}\,)\\ &= \int \mathrm{d}\vec{R}\, e^{i\,\vec{R}\cdot(\vec{K}-\vec{K}\,')}\rho^\alpha(\vec{R}\,)\int \mathrm{d}\vec{r}\, e^{i\,\vec{r}\cdot\vec{q}}\,\delta(\vec{r}\,)\\ &= \tilde{\rho}^\alpha(\vec{K}-\vec{K}\,')\,. \end{aligned} \tag{E.12}$$

In unpolarized symmetric infinite nuclear matter, $\rho^\alpha(\vec{R}\,)=\rho_0$, thus one gets

$$\langle \vec{k}_k\ \vec{k}_l|V_{\mathrm{D1X}}|\vec{k}_i\ \vec{k}_j\rangle^{SS_zTT_z}_{\rho,dir} = \rho_0^\alpha\,(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\,.$$

E.1.2.4 Density-dependent terms: D2

In the case of the D2 interaction, the expression of the density-dependent term does not allow to decouple the dependencies on $(\vec{r}_1,\vec{r}_2)$ through the variable change $(\vec{r},\vec{R}\,)$. However, this can be achieved in infinite nuclear matter, where

$$\frac{\rho(\vec{r}\,)^\alpha+\rho(\vec{r}\,)^\alpha}{2}=\rho_0^\alpha\,. \tag{E.13}$$

By analogy with central terms, one gets then

$$\langle \vec{k}_k\ \vec{k}_l|V_{\mathrm{D2}}|\vec{k}_i\ \vec{k}_j\rangle^{SS_zTT_z}_{\rho,dir} = \rho_0^\alpha\,(\mu_3\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_3^2q^2}\,(2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\,. \tag{E.14}$$

E.1.3 Microscopic vertex

In the following all realizations $v^{[\mathrm{X}]}_{\mathrm{BDRS}}$ are treated simultaneously. At the [bare(2)] level, density dependencies of the coupling constants vanish. In this section a compact notation for the coupling constants $C_x^{ST}[\rho_0(\vec{R}\,),\rho_1(\vec{R}\,),\vec{S}_0(\vec{R}\,),\vec{S}_1(\vec{R}\,),\Lambda]\equiv C_x^{ST}(\vec{R},\Lambda)$ will be used.

E.1.3.1 Central terms

The vertex is here a pure gaussian term $C_i^{ST}(\vec{R},\Lambda)e^{-\frac{r^2}{\mu_i}}$, which leads to

$$\begin{aligned}\langle \vec{k}_k\ \vec{k}_l|v^{[\mathrm{X}]}_{\mathrm{BDRS}}|\vec{k}_i\ \vec{k}_j\rangle^{ST}_{i,dir} &= \int \mathrm{d}\vec{r}_1\, d\vec{r}_2\, e^{i\,[\vec{r}_1\cdot(\vec{k}_i-\vec{k}_k\,)+\vec{r}_2\cdot(\vec{k}_j-\vec{k}_l\,)]}\,C_i^{ST}(\vec{R},\Lambda)\,e^{-\frac{r^2}{\mu_i}}\\ &= \int \mathrm{d}\vec{R}\, e^{i\,\vec{R}\cdot(\vec{K}-\vec{K}\,')}\,C_i^{ST}(\vec{R},\Lambda)\int \mathrm{d}\vec{r}\, e^{i\,\vec{r}\cdot\vec{q}}\,e^{-\frac{r^2}{\mu_i}}\\ &= (\mu_i\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_i^2q^2}\,\tilde{C}_i^{ST}(\vec{K}\,'-\vec{K},\Lambda)\,, \end{aligned} \tag{E.15a}$$

where $\tilde{C}_i^{ST}(\vec{K}\,'-\vec{K},\Lambda)$ is the Fourier transform of the coupling constant that reads

$$\tilde{C}_i^{ST}(\vec{K}\,'-\vec{K},\Lambda)=\int \mathrm{d}\vec{R}\; e^{-i\,\vec{R}\cdot(\vec{K}\,'-\vec{K}\,)}\,C_i^{ST}(\vec{R},\Lambda)\,. \tag{E.16}$$

In the case of infinite nuclear matter, the coupling constant is independent of the center-of-mass position, hence

$$\langle \vec{k}_k\ \vec{k}_l|v^{[\mathrm{X}]}_{\mathrm{BDRS}}|\vec{k}_i\ \vec{k}_j\rangle^{ST}_{i,dir} = C_i^{ST}[\rho_0,\rho_1,\vec{S}_0,\vec{S}_1,\Lambda](2\pi)^3(\mu_i\sqrt{\pi})^3e^{-\frac{1}{4}\mu_i^2q^2}\delta(\vec{K}-\vec{K}\,')\,. \tag{E.17}$$

For the exchange term, one finds

$$\langle \vec{k}_k\ \vec{k}_l|v^{[\mathrm{X}]}_{\mathrm{BDRS}}|\vec{k}_i\ \vec{k}_j\rangle^{ST}_{i,ex} = (\mu_i\sqrt{\pi})^3e^{-\frac{1}{4}\mu_i^2q'^2}C_i^{ST}[\rho_0,\rho_1,\vec{S}_0,\vec{S}_1,\Lambda](2\pi)^3\,\delta(\vec{K}-\vec{K}\,')\,. \tag{E.18}$$

E.1.3.2 Spin-orbit terms

The matrix elements in momentum space read for the direct term

$$\begin{aligned}
\langle \vec{k}_k\ \vec{k}_l|v^{[\mathrm{X}]}_{\mathrm{BDRS}}|\vec{k}_i\ \vec{k}_j\rangle^{1T}_{so,dir} &= \int \mathrm{d}\vec{r}_1\, d\vec{r}_2\, e^{-i\,(\vec{r}_1\cdot\vec{k}_k+\vec{r}_2\cdot\vec{k}_l)} C^{1T}_{so}(\vec{R},\Lambda) \\
&\qquad \times e^{-\frac{r^2}{\mu_{so}}}\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{r}\wedge\overrightarrow{k}\; e^{i\,(\vec{r}_1\cdot\vec{k}_i+\vec{r}_2\cdot\vec{k}_j)} \\
&= (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\left[\int \mathrm{d}\vec{r}_1\, d\vec{r}_2\ \vec{r}\, e^{i\,[\vec{r}_1\cdot(\vec{k}_i-\vec{k}_k)+\vec{r}_2\cdot(\vec{k}_j-\vec{k}_l)]}\right. \\
&\qquad \left. \times\, C^{1T}_{so}(\vec{R},\Lambda)\, e^{-\frac{r^2}{\mu_{so}}}\right]\wedge\frac{\vec{k}_i-\vec{k}_j}{2} \\
&= i\,\tilde{C}^{1T}_{so}(\vec{K}\,'-\vec{K},\Lambda)\ (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\left[\int \mathrm{d}\vec{r}\, e^{-\frac{r^2}{\mu_{so}}}\, e^{i\,\vec{r}\cdot\vec{q}}\,(-i\,\vec{r})\right]\wedge\vec{k} \\
&= -\,i\,\tilde{C}^{1T}_{so}(\vec{K}\,'-\vec{K},\Lambda)\ (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\nabla_{\vec{q}}\left[\int \mathrm{d}\vec{r}\, e^{-\frac{r^2}{\mu_{so}}}\, e^{i\,\vec{r}\cdot\vec{q}}\right]\wedge\vec{k} \\
&= -\,i\,(\mu_{so}\sqrt{\pi})^3\,\tilde{C}^{1T}_{so}(\vec{K}\,'-\vec{K},\Lambda)\ (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\nabla_{\vec{q}}\, e^{-\frac{1}{4}\mu^2_{so}q^2}\wedge\vec{k} \\
&= i\,\frac{\mu^2_{so}\,(\mu_{so}\sqrt{\pi})^3}{2}\, e^{-\frac{1}{4}\mu^2_{so}q^2}\,\tilde{C}^{1T}_{so}(\vec{K}\,'-\vec{K},\Lambda)\ (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{q}\wedge\vec{k} \\
&= i\,\frac{\mu^2_{so}\,(\mu_{so}\sqrt{\pi})^3}{2}\, e^{-\frac{1}{4}\mu^2_{so}q^2}\,\tilde{C}^{1T}_{so}(\vec{K}\,'-\vec{K},\Lambda)\ (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\vec{k}\,, \qquad \text{(E.19)}
\end{aligned}$$

where we used

$$\int \mathrm{d}\vec{r}\, e^{-\frac{r^2}{\mu_{so}}}\, e^{i\,\vec{r}\cdot\vec{q}}\,(i\,\vec{r}) = \nabla_{\vec{q}}\int \mathrm{d}\vec{r}\, e^{-\frac{r^2}{\mu_{so}}}\, e^{i\,\vec{r}\cdot\vec{q}}\,. \qquad \text{(E.20)}$$

Likewise, one gets for the exchange part

$$\langle \vec{k}_k\ \vec{k}_l|v^{[\mathrm{X}]}_{\mathrm{BDRS}}|\vec{k}_i\ \vec{k}_j\rangle^{1T}_{so,ex} = i\,\frac{\mu^2_{so}\,(\mu_{so}\sqrt{\pi})^3}{2}\, e^{-\frac{1}{4}\mu^2_{so}q'^2}\,\tilde{C}^{1T}_{so}(\vec{K}\,'-\vec{K},\Lambda)\ (\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\vec{k}\,. \qquad \text{(E.21)}$$

E.1.4 Tensor terms

E.1.4.1 Simple gaussian case

Let us look at the matrix elements in momentum space of a tensor term having a simple gaussian form factor, that is

$$v^t(\vec{r},\vec{R},\Lambda) \equiv C^{1T}_t(\vec{R},\Lambda)\, e^{-\frac{r^2}{\mu_t}}\,\mathsf{S}_{12}\,. \qquad \text{(E.22)}$$

In this case, following the same steps as in Sec. E.1.2.2 for the direct term leads to

$$\begin{aligned}
\langle \vec{k}_k\ \vec{k}_l|v^t|\vec{k}_i\ \vec{k}_j\rangle^{1T}_{dir} &= \int \mathrm{d}\vec{r}_1\, d\vec{r}_2\, e^{-i\,(\vec{r}_1\cdot\vec{k}_k+\vec{r}_2\cdot\vec{k}_l)} C^{1T}_t(\vec{R},\Lambda)\, e^{-\frac{r^2}{\mu_t}}\,\mathsf{S}_{12}\; e^{i\,(\vec{r}_1\cdot\vec{k}_i+\vec{r}_2\cdot\vec{k}_j)} \\
&= -\int \mathrm{d}\vec{R}\, C^{1T}_t(\vec{R},\Lambda)\, e^{i\,\vec{R}\cdot(\vec{K}-\vec{K}\,')}\left[3\,(\vec{\sigma}_1\cdot\nabla_{\vec{q}})\ (\vec{\sigma}_2\cdot\nabla_{\vec{q}}) + \vec{\sigma}_1\cdot\vec{\sigma}_2\right] \\
&\qquad \times \int \mathrm{d}\vec{r}\, e^{-\frac{r^2}{\mu_t}}\, e^{i\,\vec{r}\cdot\vec{q}}\, r^{-2}\,, \qquad \text{(E.23)}
\end{aligned}$$

and

$$\begin{aligned}\int \mathrm{d}\vec{r}\, e^{-\frac{r^2}{\mu_t}}\, e^{-i\,\vec{r}\cdot\vec{q}}\, r^{-2} =& 2\pi \int_{r=0}^{+\infty} \mathrm{d}r e^{-\frac{r^2}{\mu_t}} \int_{\theta=0}^{\pi} \mathrm{d}\theta\, \sin(\theta)\, e^{-i\,rq\,\cos(\theta)} \\ =& 4\pi \int_{r=0}^{+\infty} \mathrm{d}r e^{-\frac{r^2}{\mu_t}} \frac{\sin(rq)}{rq} \\ =& \frac{2\pi^2}{q}\left(\frac{2}{\pi}\int_0^{+\infty} \mathrm{d}r\, e^{-\frac{r^2}{\mu_t}} \frac{\sin(rq)}{r}\right) \\ =& \frac{2\pi^2}{q}\left(\frac{2}{\pi}\int_0^{+\infty} \mathrm{d}r'\, e^{-r'^2} \frac{\sin\left(2r\frac{q\mu_t}{2}\right)}{r}\right) \\ =& \frac{2\pi^2}{q}\mathrm{erf}\left(\frac{q\mu_t}{2}\right), \end{aligned} \tag{E.24}$$

where for $x \in \mathbb{R}$

$$\mathrm{erf}(x) = \frac{2}{\sqrt{x}}\int_0^z e^{-t^2}\mathrm{d}t = \frac{2}{\pi}\int_0^{+\infty} \frac{e^{-t^2}\,\sin(2xt)}{t}\mathrm{d}t\,. \tag{E.25}$$

Thus

$$\langle \vec{k}_k\ \vec{k}_l|v^t|\vec{k}_i\ \vec{k}_j\rangle_{dir}^{1T} = -2\pi^2\,\tilde{C}_t^{1T}(\vec{K}\,' - \vec{K}, \Lambda)\left[3\left(\vec{\sigma}_1\cdot\nabla_{\vec{q}}\right)\left(\vec{\sigma}_2\cdot\nabla_{\vec{q}}\right) + \vec{\sigma}_1\cdot\vec{\sigma}_2\right]\frac{\mathrm{erf}\left(\frac{q\mu_t}{2}\right)}{q}\,, \tag{E.26}$$

and for the exchange term

$$\langle \vec{k}_k\ \vec{k}_l|v^t|\vec{k}_i\ \vec{k}_j\rangle_{ex}^{1T} = -2\pi^2\,\tilde{C}_t^{1T}(\vec{K}\,' - \vec{K}, \Lambda)\left[3\left(\vec{\sigma}_1\cdot\nabla_{\vec{q}'}\right)\left(\vec{\sigma}_2\cdot\nabla_{\vec{q}'}\right) + \vec{\sigma}_1\cdot\vec{\sigma}_2\right]\frac{\mathrm{erf}\left(\frac{q'\mu_t}{2}\right)}{q'}\,. \tag{E.27}$$

The following relations may be useful for handling properly the erf function

$$\mathrm{erf}(+\infty) = 1 \tag{E.28a}$$

$$\mathrm{erf}(0) = 0 \tag{E.28b}$$

$$\int \mathrm{erf}(b+az)\,\mathrm{d}z = \frac{b\,\mathrm{erf}(b+az)}{a} + z\,\mathrm{erf}(b+az) + \frac{e^{-a^2z^2-2abz}}{a\sqrt{\pi}} \tag{E.28c}$$

$$\int z^{\alpha-1}\,\mathrm{erf}(az)\,\mathrm{d}z = \frac{z^\alpha}{a}\left(\frac{1}{(az)^\alpha\sqrt{\pi}}\Gamma\left(\frac{\alpha+1}{2}, a^2z^2\right) + \mathrm{erf}(az)\right), \tag{E.28d}$$

$$\Gamma(a,z) = \int_z^{+\infty} t^{a-1}\,e^{-t}\,\mathrm{d}t\,. \tag{E.28e}$$

In all cases, one sees that a subsequent partial wave decomposition of such a term would lead at best to a very complicated expression, and at worst to a non-analytical expression. This justifies the use of a modified gaussian expression for the tensor part of $v_{\rm BDRS}^{\rm [X]}$ that is easily expressed in coordinate and momentum spaces.

E.1.4.2 Convenient tensor term for $v_{\rm BDRS}$

We construct another expression for the tensor interaction, where we approximate the one-pion exchange iteraction *in momentum space* using a gaussian expression, i.e.

$$V_\pi(\vec{q}) \approx V_t(\vec{q}) = -\left(\vec{\tau}_1\cdot\vec{\tau}_2\right)\left(\vec{\sigma}_1\cdot\vec{q}\right)\left(\vec{\sigma}_2\cdot\vec{q}\right)\left(\mu_t\sqrt{\pi}\right)^3 e^{-\frac{1}{4}\mu_t^2q^2}\,, \tag{E.29}$$

which is equivalent, in coordinate space, to

$$V_t(\vec{r}) = \left(\vec{\tau}_1\cdot\vec{\tau}_2\right)\left(\vec{\sigma}_1\cdot\vec{\nabla}\right)\left(\vec{\sigma}_2\cdot\vec{\nabla}\right)e^{-\frac{r^2}{\mu_t^2}}\,. \tag{E.30}$$

The gradient operators are applied using Eqs. (D.20a-D.20f), which leads to

$$\begin{aligned}\partial^i\,\partial^j\,e^{-\frac{r^2}{\mu_t^2}} &= -\,2\mu_t\,\partial^j\left(x^i\,e^{-\frac{r^2}{\mu_t^2}}\right)\\ &= -\,\frac{2}{\mu_t^2}\left(\partial^j\,x^i\times e^{-\frac{r^2}{\mu_t^2}}+x^i\,\partial^j\,e^{-\frac{r^2}{\mu_t^2}}\right)\\ &= \left[\frac{4}{\mu_t^4}\,r^2\,\overline{r}^{\,i}\,\overline{r}^{\,j}-\frac{2}{\mu_t^2}\,\delta_{ij}\right]\,e^{-\frac{r^2}{\mu_t^2}}\\ &= \left[\frac{4}{3\mu_t^4}\,\left(3\,\overline{r}^{\,i}\,\overline{r}^{\,j}-\delta_{ij}\right)-\frac{2}{\mu_t^2}\delta_{ij}\left(\frac{1}{r^2}-\frac{2}{3\mu_t^2}\right)\right]\,r^2\,e^{-\frac{r^2}{\mu_t^2}}\,.\end{aligned}\tag{E.31}$$

Thus one has in coordinate space

$$V_t(\vec{r})=\frac{4}{3\mu_t^4}\,(\vec{\tau}_1\cdot\vec{\tau}_2\,)\,\mathsf{S}_{12}\,r^2\,e^{-\frac{r^2}{\mu_t^2}}-\frac{2}{\mu_t^2}\,(\vec{\tau}_1\cdot\vec{\tau}_2\,)\,(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\left(\frac{1}{r^2}-\frac{2}{3\mu_t^2}\right)\,r^2\,e^{-\frac{r^2}{\mu_t^2}}\,,\tag{E.32}$$

which can be recast into central and pure tensor contributions. Such a decomposition can be equivalently performed at the level of Eq. (E.29), i.e.

$$\begin{aligned}V_t(\vec{q})=-\,(\vec{\tau}_1\cdot\vec{\tau}_2\,)\left[(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)-\frac{1}{3}\,(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\,q^2\right]\,(\mu_t\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_t^2q^2}\\ +\,\frac{1}{3}\,(\vec{\sigma}_1\cdot\vec{\sigma}_2\,)\,q^2\,(\mu_t\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_t^2q^2}\,.\end{aligned}\tag{E.33}$$

The validity of this modified gaussian approximation has to be asserted a posteriori, by considering deuteron or INM properties of v_{BDRS}.

E.2 Partial wave expansion

In the following, the $(2\pi)^3$ factor that appears in momentum space vertices will be only reinjected in the final result. We did not a priori assume J-invariance of the nucleon-nucleon interaction but the former is recovered in the end.

E.2.1 D1X/D2 interaction

E.2.1.1 Brink-Booker terms

The interaction is already separable in angular momentum, spin and isospin parts, and reads for one Brink-Booker term

$$\begin{aligned}v_{\mathrm{D1X}}^{BB,i}(\vec{k}\,',\vec{k}\,)=&(\mu_i\,\sqrt{\pi})^3\,\left[W_i+B_i\,P_\sigma-H_i\,P_\tau-M_i\,P_\sigma\,P_\tau\right]\,e^{-\frac{1}{4}\mu_i^2\,q^2}\\ \equiv&(\mu_i\,\sqrt{\pi})^3\,\left[W_i+B_i\,P_\sigma-H_i\,P_\tau-M_i\,P_\sigma\,P_\tau\right]\,g^i(\vec{k}\,',\vec{k}\,)\,.\end{aligned}\tag{E.34}$$

Therefore, using Eqs. (D.41,A.65,A.70) one gets

$$\begin{aligned}\langle k'\;(L'S')J'\,T'|v_{\mathrm{D1X}}^{BB,i}|k\;(LS)J\,T\rangle =&\delta_{JJ'}\,\delta_{SS'}\,\delta_{TT'}\,(\mu_i\,\sqrt{\pi})^3\,\frac{(k'\,L'||e^{-\frac{1}{4}\mu_i^2\,q^2}||k\,L)}{\sqrt{[L]}}\\ &\times\left[W_i+(-1)^{S+1}\,B_i-(-1)^{T+1}\,H_i-(-1)^{S+T}\,M_i\right]\,,\end{aligned}\tag{E.35}$$

Using Eq. (A.95) leads then to

$$\langle k'\ (L'S')J'\,T'|v_{\rm D1X}^{BB,i}|k\ (LS)J\,T\rangle = (-1)^L\,\frac{\delta_{JJ'}\,\delta_{SS'}\,\delta_{TT'}\,\delta_{LL'}}{4\pi\,\sqrt{[L]}}\,(\mu_i\,\sqrt{\pi})^3\,\tilde{g}_L^i(k',k) \times\Big[W_i+(-1)^{S+1}\,B_i-(-1)^{T+1}\,H_i-(-1)^{S+T}\,M_i\Big]\,. \quad \text{(E.36)}$$

E.2.1.2 Density-dependent terms

Density-dependent terms for D1X and D2 in symmetric INM are trivial from this point on. This amounts to substituting in the previous expression for the central terms

$$(\mu_i\,\sqrt{\pi})^3\,\frac{\tilde{g}_L^i(k',k)}{4\pi}\to\delta_{L0}\,,\qquad W_i\to t_0\,,\qquad B_i\to t_0\,x_0\,,\qquad H_i=M_i\to 0\,. \quad \text{(E.37a)}$$

One finds then

$$\langle k'\ (L'S')J'\,T'|v_{\rm D1X}^{\rho}|k\ (LS)J\,T\rangle = \delta_{JJ'}\,\delta_{SS'}\,\delta_{TT'}\,\delta_{LL'}\,\delta_{L0}\,t_0\,\rho_0^\alpha\,\Big[1+(-1)^{S+1}\,x_0\Big]\,. \quad \text{(E.38)}$$

This term only contributes in the $L=0$ channel. On the other hand

$$\langle k'\ (L'S')J'\,T'|v_{\rm D2}^{\rho}|k\ (LS)J\,T\rangle = (-1)^L\,\frac{\delta_{JJ'}\,\delta_{SS'}\,\delta_{TT'}\,\delta_{LL'}}{4\pi\,\sqrt{[L]}}\,(\mu_i\,\sqrt{\pi})^3\,\rho_0^\alpha\,\tilde{g}_L^3(k',k) \times\Big[W_3+(-1)^{S+1}\,B_3-(-1)^{T+1}\,H_3-(-1)^{S+T}\,M_3\Big]\,. \quad \text{(E.39)}$$

E.2.1.3 Spin-orbit terms

There are both a very long and a very short way to perform the partial wave expansion. One has for both D1X and D2

$$V_{\rm D1X/D2}^{so}(\vec{k}\,',\vec{k}\,)=i\,W_{LS}\,(\vec{\sigma}_1+\vec{\sigma}_2)\ \vec{k}\,'\wedge\vec{k}\,. \quad \text{(E.40)}$$

Using Eqs. (A.5,A.6b), one has

$$i\vec{k}\,'\wedge\vec{k}=\frac{1}{2}\,i\vec{q}\wedge\vec{q}\,'=\frac{\sqrt{2}}{2}\,qq'\,\frac{4\pi}{3}\,\Big[Y^{[1]}(\hat{q})\otimes Y^{[1]}(\hat{q}')\Big]^{[1]}\,. \quad \text{(E.41)}$$

That is, Eq. (A.11) leads to

$$i\vec{k}\,'\wedge\vec{k}=\sqrt{2}\frac{4\pi}{3}\sum_{\substack{\lambda_1+\lambda_2=1\\ \mu_1+\mu_2=1}}(-1)^{\lambda_2}\,k'^{\lambda_1+\mu_1}\,k^{\lambda_2+\mu_2}\,\frac{12\pi}{\sqrt{[\lambda_1]![\lambda_2]![\mu_1]![\mu_2]!}} \times\Big[\Big[Y^{[\lambda_1]}(\hat{k}')\otimes Y^{[\lambda_2]}(\hat{k})\Big]^{[1]}\otimes\Big[Y^{[\mu_1]}(\hat{k}')\otimes Y^{[\mu_2]}(\hat{k})\Big]^{[1]}\Big]^{[1]}\,. \quad \text{(E.42)}$$

The two tensors can then be recoupled by analogy to LSJ coupling, then expanded using Eq. (A.12) such that

$$\begin{aligned}
i\vec{k}' \wedge \vec{k} =& \frac{4\pi}{3}\sqrt{2} \sum_{\substack{\lambda_1+\lambda_2=1\\ \mu_1+\mu_2=1}} (-1)^{\lambda_2}\, k'^{\lambda_1+\mu_1}\, k^{\lambda_2+\mu_2} \frac{12\pi}{\sqrt{[\lambda_1]![\lambda_2]![\mu_1]![\mu_2]!}} \sum_{f,g} \sqrt{[1][1][f][g]} \\
& \times \begin{Bmatrix} \lambda_1 & \lambda_2 & 1 \\ \mu_1 & \mu_2 & 1 \\ f & g & 1 \end{Bmatrix} \left[\left[Y^{[\lambda_1]}(\hat{k}') \otimes Y^{[\mu_1]}(\hat{k}') \right]^{[f]} \otimes \left[Y^{[\lambda_2]}(\hat{k}) \otimes Y^{[\mu_2]}(\hat{k}) \right]^{[g]} \right]^{[1]} \\
=& \frac{4\pi}{3}\sqrt{2} \sum_{\substack{\lambda_1+\lambda_2=1\\ \mu_1+\mu_2=1}} (-1)^{\lambda_2}\, k'^{\lambda_1+\mu_1}\, k^{\lambda_2+\mu_2} \frac{12\pi}{\sqrt{[\lambda_1]![\lambda_2]![\mu_1]![\mu_2]!}} \\
& \times \sum_{f,g} \sqrt{[1][1][f][g]} \begin{Bmatrix} \lambda_1 & \lambda_2 & 1 \\ \mu_1 & \mu_2 & 1 \\ f & g & 1 \end{Bmatrix} \langle \lambda_1\, 0\, \mu_1\, 0 \,|\lambda_1\, \mu_1\, f\, 0\rangle \, \langle \lambda_2\, 0\, \mu_2\, 0 \,|\lambda_2\, \mu_2\, g\, 0\rangle \\
& \times \frac{\sqrt{[\lambda_1][\lambda_2][\mu_1][\mu_2]}}{4\pi\sqrt{[f][g]}} \left[Y^{[f]}(\hat{k}') \otimes Y^{[g]}(\hat{k}) \right]^{[1]} .
\end{aligned} \tag{E.43}$$

Hence

$$\begin{aligned}
&(k'\, L' || i\vec{k}' \wedge \vec{k} || k\, L) \\
&\quad = \sqrt{2} \sum_{\substack{\lambda_1+\lambda_2=1\\ \mu_1+\mu_2=1}} (-1)^{\lambda_2}\, k'^{\lambda_1+\mu_1}\, k^{\lambda_2+\mu_2} \\
&\qquad \times \frac{1}{\sqrt{[\lambda_1]![\lambda_2]![\mu_1]![\mu_2]!}} \sqrt{[1][1][L][L']} \begin{Bmatrix} \lambda_1 & \lambda_2 & 1 \\ \mu_1 & \mu_2 & 1 \\ L' & L & 1 \end{Bmatrix} \\
&\qquad \times \left\langle \lambda_1\, 0\, \mu_1\, 0 \,\middle|\lambda_1\, \mu_1\, L'\, 0\right\rangle \, \langle \lambda_2\, 0\, \mu_2\, 0 \,|\lambda_2\, \mu_2\, L\, 0\rangle \, \frac{\sqrt{[\lambda_1][\lambda_2][\mu_1][\mu_2]}}{\sqrt{[L'][L]}} (-1)^L \sqrt{[1]} \\
&\quad = 3\sqrt{6} \sum_{\substack{\lambda_1+\lambda_2=1\\ \mu_1+\mu_2=1}} (-1)^{\lambda_2+L}\, k'^{\lambda_1+\mu_1}\, k^{\lambda_2+\mu_2} \frac{\sqrt{[\lambda_1][\lambda_2][\mu_1][\mu_2]}}{\sqrt{[\lambda_1]![\lambda_2]![\mu_1]![\mu_2]!}} \begin{Bmatrix} \lambda_1 & \lambda_2 & 1 \\ \mu_1 & \mu_2 & 1 \\ L' & L & 1 \end{Bmatrix} \\
&\qquad \times \left\langle \lambda_1\, 0\, \mu_1\, 0 \,\middle|\lambda_1\, \mu_1\, L'\, 0\right\rangle \, \langle \lambda_2\, 0\, \mu_2\, 0 \,|\lambda_2\, \mu_2\, L\, 0\rangle \, .
\end{aligned} \tag{E.44, E.45}$$

An alternative method is to apply directly Eq. (A.6b), i.e.

$$i\vec{k}' \wedge \vec{k} = \sqrt{2}\, kk' \frac{4\pi}{3} \left[Y^{[1]}(\hat{k}) \otimes Y^{[1]}(\hat{k}') \right]^{[1]} . \tag{E.46}$$

Therefore, using Eq. (A.93)

$$\begin{aligned}
(k'\, L' || i\vec{k}' \wedge \vec{k} || k\, L) =& \sqrt{2}\, kk' \frac{4\pi}{3} (k'\, L' || \left[Y^{[1]}(\hat{k}) \otimes Y^{[1]}(\hat{k}') \right]^{[1]} || k\, L) \\
=& -\delta_{L1}\, \delta_{L'1}\, \sqrt{2}\, kk' \frac{4\pi}{3} \frac{\sqrt{[1]}}{4\pi} \\
=& -\delta_{L1}\, \delta_{L'1} \frac{\sqrt{2}}{\sqrt{3}}\, kk' .
\end{aligned} \tag{E.47}$$

Thus the zero-range spin orbit only acts in the $L = 1$ partial waves, as it was expected (the angular dependence of $\vec{k}\,' \wedge \vec{k}$ is in $\sin(\hat{k}\,' \cdot \hat{k})$ which is a Legendre polynomial of first order. The two methods are obviously equivalent, given that

- the terms in Eq. (E.45) corresponding to $\lambda_1 = \mu_1 = 1$ and $\lambda_2 = \mu_2 = 1$ imply that one of the Clebsh-Gordan coefficient is zero (if $\lambda_1 = \mu_1 = 1$ then $L = 0$, thus we must have $L' = 1$ to have a non-zero $9j$, in which case $\langle 1\,0\,1\,0\,|1\,1\,1\,0\rangle = 0$),
- regardless of the values of λ_1, λ_2, μ_1, μ_2, one has two of the summed terms in Eq. (E.45) are equal to 0, and two equal to 1, thus

$$\frac{\sqrt{[\lambda_1][\lambda_2][\mu_1][\mu_2]}}{\sqrt{[\lambda_1]![\lambda_2]![\mu_1]![\mu_2]!}} = \frac{1}{2}\,. \tag{E.48}$$

- for $\lambda_1 = \mu_2 = 1$ and $\lambda_2 = \mu_1 = 0$, the $9j$ coefficient in Eq. (E.45) indicates that $L = L' = 1$. The product of the Clebsh-Gordan coefficients is (maximum coupling)

$$\langle 1\,0\,0\,0\,|1\,0\,1\,0\rangle\ \langle 0\,0\,1\,0\,|0\,1\,1\,0\rangle = 1\,. \tag{E.49}$$

  Using Eq. (A.3g), one has then

$$\begin{aligned}(k'\,L'||i\vec{k}\,' \wedge \vec{k}||k\,L) =& (-1)\,\delta_{L1}\,\delta_{L'1}\,\frac{3\sqrt{6}}{2}\,kk'\left[\begin{Bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{Bmatrix} - \begin{Bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{Bmatrix}\right] \\ =& -\,\delta_{L1}\,\delta_{L'1}\,\frac{\sqrt{2}}{\sqrt{3}}\,kk'\,.\end{aligned} \tag{E.50}$$

Thus one has, using the previous comments as well as Eqs. (A.64,A.80)

$$\begin{aligned}&\langle k'\ (L'S')J'\,T'|v^{so}_{\mathrm{D1X/D2}}|k\ (LS)J\,T\rangle \\ &=\frac{1}{\sqrt{[J]}}\,W_{LS}\,\langle k'\ (L'S')J'\,T'||\,(\vec{\sigma}_1+\vec{\sigma}_2)\,.\left(i\vec{k}\,' \wedge \vec{k}\right)||k\ (LS)J\,T\rangle \\ &=(-1)^{L+S'+J}\,\delta_{JJ'}\,\delta_{TT'}\,W_{LS}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix}(k'\,L'||i\vec{k}\,' \wedge \vec{k}||k\,L)\,(S||\vec{\sigma}_1+\vec{\sigma}_2||S') \\ &=(-1)^{S'+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{L1}\,\delta_{L'1}\,\delta_{S1}\,\delta_{S'1}\,W_{LS}\,2\,\sqrt{6}\,\frac{\sqrt{2}}{\sqrt{3}}\,kk'\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\ &=(-1)^{1+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{L1}\,\delta_{L'1}\,kk'\,\delta_{S1}\,\delta_{S'1}\,4\,W_{LS}\begin{Bmatrix} 1 & 1 & J \\ 1 & 1 & 1 \end{Bmatrix} \\ &=(-1)^{J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{L1}\,\delta_{L'1}\,kk'\,\delta_{S1}\,\delta_{S'1}\,4\,W_{LS}\,(-1)^{J+3}\frac{4-J(J+1)}{12} \\ &=W_{LS}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{L1}\,\delta_{L'1}\,\delta_{S1}\,\frac{4-J(J+1)}{3}\,kk'\,.\end{aligned} \tag{E.51}$$

E.2.1.4 Summary

For the final result one should not forget about exchange terms, which are equal to the direct ones in the expansion (see Sec. A.4.5), so there is an extra 2 factor that should be be carried

on. The latter is not written here to keep consistency with the conventions in the code that computes low-momentum interactions. One finds

$$V_{\mathrm{D1X}}({}^1S_0,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_0^i(k',k)}{4\pi}\,[W_i - B_i - H_i + M_i] + 2\,t_0\,\rho_0^\alpha\,(1-x_0)\,, \tag{E.52a}$$

$$V_{\mathrm{D1X}}({}^3S_1,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_0^i(k',k)}{4\pi}\,[W_i + B_i + H_i + M_i] + 2\,t_0\,\rho_0^\alpha\,(1+x_0)\,, \tag{E.52b}$$

$$V_{\mathrm{D1X}}({}^1P_1,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i - B_i + H_i - M_i]\,, \tag{E.52c}$$

$$V_{\mathrm{D1X}}({}^3P_0,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i + B_i - H_i - M_i] + \frac{8}{3}\,W_{LS}\,kk'\,, \tag{E.52d}$$

$$V_{\mathrm{D1X}}({}^3P_1,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i + B_i - H_i - M_i] + \frac{4}{3}\,W_{LS}\,kk'\,, \tag{E.52e}$$

$$V_{\mathrm{D1X}}({}^3P_2,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i + B_i - H_i - M_i] - \frac{4}{3}\,W_{LS}\,kk'\,, \tag{E.52f}$$

$$V_{\mathrm{D1X}}({}^1D_2,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}}\,[W_i - B_i - H_i + M_i]\,, \tag{E.52g}$$

$$\begin{aligned} V_{\mathrm{D1X}}({}^3D_1,k,k') &= V_{\mathrm{D1X}}({}^3D_2,k,k') = V_{\mathrm{D1X}}({}^3D_3,k,k') \\ &= \frac{1}{2\pi^2}\sum_{i=1}^{2}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}}\,[W_i + B_i + H_i - M_i]\,, \end{aligned} \tag{E.52h}$$

where (see Sec. A.3.1)

$$\frac{\tilde{g}_0^i(k',k)}{4\pi} = \frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i}\,\mathrm{sh}(\Gamma_i)\,, \tag{E.53a}$$

$$\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}} = -\frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^2}\,(\Gamma_i\,\mathrm{ch}(\Gamma_i) - \mathrm{sh}(\Gamma_i))\,, \tag{E.53b}$$

$$\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}} = \frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^3}\,\left(-3\Gamma_i\,\mathrm{ch}(\Gamma_i) + (3+\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right)\,, \tag{E.53c}$$

$$\Gamma_i = \frac{1}{2}\,\mu_i^2\,kk'\,. \tag{E.53d}$$

Equivalently for D2

$$V_{\mathrm{D2}}({}^1S_0,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_0^i(k',k)}{4\pi}\,[W_i - B_i - H_i + M_i]\,, \tag{E.54a}$$

$$V_{\mathrm{D2}}({}^3S_1,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_0^i(k',k)}{4\pi}\,[W_i + B_i + H_i + M_i]\,, \tag{E.54b}$$

$$V_{\rm D2}({}^1P_1,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i-B_i+H_i-M_i]\,, \tag{E.54c}$$

$$V_{\rm D2}({}^3P_0,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i+B_i-H_i-M_i]+\frac{8}{3}\,W_{LS}\,kk'\,, \tag{E.54d}$$

$$V_{\rm D2}({}^3P_1,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i+B_i-H_i-M_i]+\frac{4}{3}\,W_{LS}\,kk'\,, \tag{E.54e}$$

$$V_{\rm D2}({}^3P_2,k,k') = -\frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,[W_i+B_i-H_i-M_i]-\frac{4}{3}\,W_{LS}\,kk'\,, \tag{E.54f}$$

$$V_{\rm D2}({}^1D_2,k,k') = \sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}}\,[W_i-B_i-H_i+M_i]\,, \tag{E.54g}$$

$$\begin{aligned} V_{\rm D2}({}^3D_1,k,k') =& V_{\rm D2}({}^3D_2,k,k') = V_{\rm D2}({}^3D_3,k,k') \\ =& \frac{1}{2\pi^2}\sum_{i=1}^{3}(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}}\,[W_i+B_i+H_i-M_i]\,, \end{aligned} \tag{E.54h}$$

with the convention that $\tilde{g}_\lambda^3(k',k)$ includes the extra ρ_0^α factor for simplicity.

E.2.2 $v_{\rm BDRS}^{\rm [X]}$ vertex

The partial wave expansion is performed in unpolarized symmetric nuclear matter, where in-medium dependencies of the coupling constants of $v_{\rm BDRS}^{\rm [X]}$ only relate, when necessary, to ρ_0, i.e. they carry no angular dependency.

E.2.2.1 Central terms

The central terms of $v_{\rm BDRS}$ interaction are already separated in spin/isospin channels, i.e.

$$v_{\rm BDRS}^{ST,i}(\vec{k}\,',\vec{k}\,') = C_i^{ST}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,e^{-\frac{1}{4}\mu_i^2q^2}\prod_S\prod_T. \tag{E.55}$$

Using Eq. (A.75) and the results from Sec. E.2.1.1, one gets easily

$$\begin{aligned} &\langle k'\ (L'S')J'\,T'|v_{\rm BDRS}^{S_0T_0,i}|k\ (LS)J\,T\rangle \\ &\qquad = (-1)^L\,\frac{\delta_{JJ'}\,\delta_{SS'}\,\delta_{SS_0}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{LL'}}{4\pi\sqrt{[L]}}\,C_i^{S_0T_0}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\tilde{g}_L^i(k',k)\,. \end{aligned} \tag{E.56}$$

E.2.2.2 Finite-range spin-orbit

We have here

$$\begin{aligned} v_{\rm BDRS}^{1T,so}(\vec{k}\,',\vec{k}\,') =& i\,C_{so}^{1T}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}e^{-\frac{1}{4}\mu_{so}^2q^2}\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\vec{k}\prod_{S=1}\prod_T \\ \equiv& i\,C_{so}^{1T}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}g^{so}(\vec{k}\,',\vec{k}\,)\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\,'\wedge\vec{k}\prod_{S=1}\prod_T. \end{aligned} \tag{E.57}$$

Using the same approach than in Sec. E.2.1.3 for a zero-range spin-orbit, one gets from Eq. (A.43)

$$
\begin{aligned}
i\,e^{-\frac{1}{4}\mu_{so}^2 q^2}\,\vec{k}\,'\wedge\vec{k} =& \sqrt{2}\,kk'\,\frac{4\pi}{3}\,\Big[Y^{[1]}(\hat{k}')\otimes Y^{[1]}(\hat{k})\Big]^{[1]}\;e^{-\frac{1}{4}\mu_{so}^2 q^2}\\
=& \sqrt{2}\,kk'\,\frac{4\pi}{3}\,\Big[Y^{[1]}(\hat{k}')\otimes Y^{[1]}(\hat{k})\Big]^{[1]}\;\sum_\lambda \tilde{g}^{so}_\lambda(k',k)\,\Big[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\Big]^{[0]}\\
=& \sqrt{2}\,kk'\,\frac{4\pi}{3}\,\sum_\lambda \tilde{g}^{so}_\lambda(k',k)\,\Big[\Big[Y^{[1]}(\hat{k}')\otimes Y^{[1]}(\hat{k})\Big]^{[1]}\otimes\Big[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\Big]^{[0]}\Big]^{[1]}\\
=& \sqrt{2}\,kk'\,\frac{4\pi}{3}\,\sum_\lambda \tilde{g}^{so}_\lambda(k',k)\sum_{ab}\begin{Bmatrix}\lambda&\lambda&0\\1&1&1\\a&b&1\end{Bmatrix}\sqrt{[0][1][a][b]}\\
&\qquad\times\Big[\Big[Y^{[1]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k}')\Big]^{[a]}\otimes\Big[Y^{[1]}(\hat{k})\otimes Y^{[\lambda]}(\hat{k})\Big]^{[b]}\Big]^{[1]}\\
=& \sqrt{2}\,kk'\,\frac{4\pi}{3}\,\sum_\lambda \tilde{g}^{so}_\lambda(k',k)\sum_{ab}\begin{Bmatrix}\lambda&\lambda&0\\1&1&1\\a&b&1\end{Bmatrix}\sqrt{[0][1][a][b]}\,\frac{\sqrt{[\lambda][\lambda][1][1]}}{4\pi\sqrt{[a][b]}}\\
&\qquad\times\langle\lambda\,0\,1\,0\,|\lambda\,1\,a\,0\rangle\,\langle\lambda\,0\,1\,0\,|\lambda\,1\,b\,0\rangle\,\Big[Y^{[a]}(\hat{k}')\otimes Y^{[b]}(\hat{k})\Big]^{[1]}\\
=& \sqrt{6}\,kk'\,\sum_\lambda \tilde{g}^{so}_\lambda(k',k)\sum_{ab}\begin{Bmatrix}\lambda&\lambda&0\\1&1&1\\a&b&1\end{Bmatrix}[\lambda]\\
&\qquad\times\langle\lambda\,0\,1\,0\,|\lambda\,1\,a\,0\rangle\,\langle\lambda\,0\,1\,0\,|\lambda\,1\,b\,0\rangle\,\Big[Y^{[a]}(\hat{k}')\otimes Y^{[b]}(\hat{k})\Big]^{[1]}\,.
\end{aligned}
\tag{E.58}
$$

Hence, using Eq. (A.93)

$$
\begin{aligned}
&(k'\,L'||i\,e^{-\frac{1}{4}\mu_{so}^2 q^2}\,\vec{k}\,'\wedge\vec{k}||k\,L)\\
&=(-1)^{L'}\,3\sqrt{2}\,kk'\,\sum_\lambda[\lambda]\,\frac{\tilde{g}^{so}_\lambda(k',k)}{4\pi}\begin{Bmatrix}\lambda&\lambda&0\\1&1&1\\L'&L&1\end{Bmatrix}\langle\lambda\,0\,1\,0\,|\lambda\,1\,L'\,0\rangle\,\langle\lambda\,0\,1\,0\,|\lambda\,1\,L\,0\rangle\,.
\end{aligned}
\tag{E.59}
$$

Some remarks hold at this point

- one cannot have $L=L'=0$ otherwise the $9j$ coefficient would be zero,
- the product of the Clebsh-Gordan coefficients is non-zero if and only if $\lambda+1+L$ and $\lambda+1+L'$ are both even. Thta is, L and L' must be of same parity. On the other hand, the $9j$ coefficient requires $L'=L,L\pm1$, thus $L=L'$, such that the finite-range spin-orbit (i) does not couple between partial waves of different angular momenta, and (ii) acts on all $L>1$ partial waves,
- in the limit $\mu_{so}\to 0$, that is

$$
g^{so}_\lambda(\vec{k}\,',\vec{k}\,)=1\,,\qquad\qquad \tilde{g}^{so}_\lambda(k',k)=4\pi\,\delta_{\lambda 0}\,,
\tag{E.60}
$$

  using Eq. (A.3h) allows to recover the results from Sec. E.2.1.3.

Using the previous remarks one can write

$$
\begin{aligned}
&(k'\,L'||i\,e^{-\frac{1}{4}\mu_{so}^2 q^2}\,\vec{k}'\wedge\vec{k}||k\,L)\\
&\quad=(-1)^L\,\delta_{LL'}\,3\sqrt{2}\,kk'\sum_\lambda[\lambda]\,\frac{\tilde{g}_\lambda^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}\lambda&\lambda&0\\1&1&1\\L&L&1\end{array}\right\}\langle\lambda\,0\,1\,0\,|\lambda\,1\,L\,0\rangle^2\\
&\quad=(-1)^L\,\delta_{LL'}\,3\sqrt{2}\,kk'\,[L]\sum_\lambda[\lambda]\,\frac{\tilde{g}_\lambda^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}\lambda&\lambda&0\\1&1&1\\L&L&1\end{array}\right\}\left(\begin{array}{ccc}\lambda&1&L\\0&0&0\end{array}\right)^2. \qquad \text{(E.61)}
\end{aligned}
$$

Thus

$$
\begin{aligned}
&\langle k'\;(L'S')J'\,T'|v_{\rm BDRS}^{1T_0,so}|k\;(LS)J\,T\rangle\\
&\quad=\frac{1}{\sqrt{[J]}}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\\
&\qquad\qquad\times\langle\vec{k}'\;(L'S')J'||\left(\prod_{S_0=1}\vec{\sigma}_1+\vec{\sigma}_2\right)\cdot\left(ie^{-\frac{1}{4}\mu_{so}^2q^2}\,\vec{k}'\wedge\vec{k}\right)||k\;(LS)J\rangle\\
&\quad=(-1)^{L+S'+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\\
&\qquad\qquad\times\left\{\begin{array}{ccc}L'&S'&J\\S&L&1\end{array}\right\}(k'\,L'||ie^{-\frac{1}{4}\mu_{so}^2q^2}\,\vec{k}'\wedge\vec{k}||k\,L)\,(S||\prod_{S_0=1}\vec{\sigma}_1+\vec{\sigma}_2||S')\\
&\quad=(-1)^{L+1+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\delta_{LL'}\,2\sqrt{6}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\left\{\begin{array}{ccc}L&1&J\\1&L&1\end{array}\right\}\\
&\qquad\qquad\times(-1)^L\,3\sqrt{2}\,kk'\,[L]\sum_\lambda[\lambda]\,\frac{\tilde{g}_\lambda^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}\lambda&\lambda&0\\1&1&1\\L&L&1\end{array}\right\}\left(\begin{array}{ccc}\lambda&1&L\\0&0&0\end{array}\right)^2\\
&\quad=(-1)^{1+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\delta_{LL'}\,12\,\sqrt{3}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\left\{\begin{array}{ccc}L&1&J\\1&L&1\end{array}\right\}\\
&\qquad\qquad\times kk'\,[L]\sum_\lambda[\lambda]\,\frac{\tilde{g}_\lambda^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}\lambda&\lambda&0\\1&1&1\\L&L&1\end{array}\right\}\left(\begin{array}{ccc}\lambda&1&L\\0&0&0\end{array}\right)^2. \qquad \text{(E.62)}
\end{aligned}
$$

In particular the $L=1$ partial wave will involve $\lambda=0,2$ components, whereas in the $L=3$ waves one will have $\lambda=1,3$. The finite-range spin-orbit only acts by construction in the $S=1$ channel, but if the explicit projector $\prod_{S_0=1}$ were to be removed, the conclusion would be the same since $(\vec{\sigma}_1+\vec{\sigma}_2)$ already acts in the $S=1$ channel only. Thus the $S=1$ projection operator is redundant, but is kept for simplicity.

We provide here the matrix elements for the first partial waves.

1. For $L=L'=1$, one gets

   $\langle k'\;(1S')J'\,T'|v_{\rm BDRS}^{1T_0,so}|k\;(1S)J\,T\rangle$

$$
\begin{aligned}
=&(-1)^{1+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,36\sqrt{3}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,\left\{\begin{array}{ccc}1&1&J\\1&1&1\end{array}\right\}\\
&\times kk'\sum_{\lambda}[\lambda]\,\frac{\tilde{g}_{\lambda}^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}\lambda&\lambda&0\\1&1&1\\1&1&1\end{array}\right\}\left(\begin{array}{ccc}\lambda&1&1\\0&0&0\end{array}\right)^2\\
=&\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,3\sqrt{3}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,(4-J(J+1))\,kk'\\
&\times\left[\frac{\tilde{g}_0^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}0&0&0\\1&1&1\\1&1&1\end{array}\right\}\left(\begin{array}{ccc}0&1&1\\0&0&0\end{array}\right)^2\right.\\
&\left.+\,5\,\frac{\tilde{g}_2^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}2&2&0\\1&1&1\\1&1&1\end{array}\right\}\left(\begin{array}{ccc}2&1&1\\0&0&0\end{array}\right)^2\right]\\
=&\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,(4-J(J+1))\,kk'\\
&\times\left[\frac{1}{3}\,\frac{\tilde{g}_0^{so}(k',k)}{4\pi}-\frac{1}{3\sqrt{5}}\,\frac{\tilde{g}_2^{so}(k',k)}{4\pi}\right].
\end{aligned}
\tag{E.63}
$$

2. For $L=L'=2$ one gets

$$
\begin{aligned}
&\langle k'\ (2S')J'\,T'|v_{\rm BDRS}^{1T_0,so}|k\ (2S)J\,T\rangle\\
=&(-1)^{1+J}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,60\sqrt{3}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,\left\{\begin{array}{ccc}2&1&J\\1&2&1\end{array}\right\}\\
&\times kk'\sum_{\lambda}[\lambda]\,\frac{\tilde{g}_{\lambda}^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}\lambda&\lambda&0\\1&1&1\\2&2&1\end{array}\right\}\left(\begin{array}{ccc}\lambda&1&2\\0&0&0\end{array}\right)^2\\
=&\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\sqrt{15}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,(-8+J(J+1))\,kk'\\
&\times\left[3\frac{\tilde{g}_1^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}1&1&0\\1&1&1\\2&2&1\end{array}\right\}\left(\begin{array}{ccc}1&1&2\\0&0&0\end{array}\right)^2\right.\\
&\left.+\,7\,\frac{\tilde{g}_3^{so}(k',k)}{4\pi}\left\{\begin{array}{ccc}3&3&0\\1&1&1\\2&2&1\end{array}\right\}\left(\begin{array}{ccc}3&1&2\\0&0&0\end{array}\right)^2\right]\\
=&\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,(-8+J(J+1))\,kk'\\
&\times\left[\frac{1}{5\sqrt{3}}\,\frac{\tilde{g}_1^{so}(k',k)}{4\pi}-\frac{1}{5\sqrt{7}}\,\frac{\tilde{g}_3^{so}(k',k)}{4\pi}\right].
\end{aligned}
\tag{E.64}
$$

3. For $L=L'=3$

$$\langle k'\ (3S')J'\,T'|v_{\rm BDRS}^{1T_0,so}|k\ (3S)J\,T\rangle$$

$$=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,(14-J(J+1))\,kk' \times\left[\frac{1}{7\sqrt{5}}\,\frac{\tilde{g}_2^{so}(k',k)}{4\pi}-\frac{1}{7\sqrt{9}}\,\frac{\tilde{g}_4^{so}(k',k)}{4\pi}\right]. \tag{E.65}$$

4. For $L=L'=4$

$$\langle k'\;(4S')J'\,T'|v_{\rm BDRS}^{1T_0,so}|k\;(4S)J\,T\rangle =\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2}\,(-22+J(J+1))\,kk' \times\left[\frac{1}{9\sqrt{7}}\,\frac{\tilde{g}_3^{so}(k',k)}{4\pi}-\frac{1}{9\sqrt{11}}\,\frac{\tilde{g}_5^{so}(k',k)}{4\pi}\right]. \tag{E.66}$$

5. One can actually extrapolate from the previous results a generic formula for any angular momentum $L=L'$ under the form

$$\langle k'\;(LS')J'\,T'|v_{\rm BDRS}^{1T_0,so}|k\;(LS)J\,T\rangle =\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,C_{so}^{1T_0}[\rho_0,\Lambda]\frac{\mu_{so}^2(\mu_{so}\sqrt{\pi})^3}{2} \times(-1)^{1-L}\,(2+L(L+1)-J(J+1))\,kk' \times\left[\frac{1}{[L]\sqrt{[L-1]}}\,\frac{\tilde{g}_{L-1}^{so}(k',k)}{4\pi}-\frac{1}{[L]\sqrt{[L+1]}}\,\frac{\tilde{g}_{L+1}^{so}(k',k)}{4\pi}\right]. \tag{E.67}$$

E.2.2.3 Finite-range tensor

We consider here a generic tensor interaction with an arbitrary form factor $f(q)$, such that the formulæ obtained can be applied for the one-pion exchange and $v_{\rm BDRS}^{\rm [X]}$. We consider then[2]

$$v_{\rm ff}^{1T,t}(\vec{k}\,',\vec{k}\,)=g(q)\,\left[3\,(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)-(\vec{\sigma}_1\cdot\vec{\sigma}_2)\,q^2\right]\prod_{S=1}\prod_{T}. \tag{E.68}$$

By construction, and according to Sec. D.1, this tensor should only couple between states of angular momentum $L'=L\pm2$ because the $(\vec{\sigma}_1\cdot\vec{\sigma}_2)\,q^2$ counter term allows to write $v_{\rm ff}^{1T,t}(\vec{k}\,',\vec{k}\,)$ as a combination of Y_2^m spherical harmonics. One has then using Eqs. (A.5,A.6a)

$$\begin{aligned} g(q)\,&\left[3\,(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)-(\vec{\sigma}_1\cdot\vec{\sigma}_2)\,q^2\right]\\ &=g(q)\,\left[9\,\left[\sigma_1^{[1]}\otimes q^{[1]}\right]^{[0]}\,\left[\sigma_2^{[1]}\otimes q^{[1]}\right]^{[0]}-(\vec{\sigma}_1\cdot\vec{\sigma}_2)\,q^2\right]\\ &=q^2\,g(q)\,\left[12\pi\,\left[\sigma_1^{[1]}\otimes Y^{[1]}(\hat{q})\right]^{[0]}\,\left[\sigma_2^{[1]}\otimes Y^{[1]}(\hat{q})\right]^{[0]}-(\vec{\sigma}_1\cdot\vec{\sigma}_2)\right]\\ &=q^2\,g(q)\left(12\pi\sum_f\sqrt{[0][0][f][f]}\begin{Bmatrix}1&1&f\\1&1&f\\0&0&0\end{Bmatrix}\right.\\ &\qquad\left.\times\left[\sigma_1^{[1]}\otimes\sigma_2^{[1]}\right]^{[f]}\,\left[Y^{[1]}(\hat{q})\otimes Y^{[1]}(\hat{q})\right]^{[f]}-(\vec{\sigma}_1\cdot\vec{\sigma}_2)\right)\end{aligned}$$

[2] In the case of a one-pion exchange, the isospin projection operator $\prod_T$ has to be replaced by $\tau_1\cdot\tau_2$.

$$
\begin{aligned}
=&12\pi\, q^2\, g(q) \sum_f [f] \left\{ \begin{array}{ccc} 1 & 1 & f \\ 1 & 1 & f \\ 0 & 0 & 0 \end{array} \right\} \frac{\sqrt{[1][1]}}{\sqrt{4\pi\,[f]}} \, \langle 1\,0\,1\,0\,|1\,1\,f\,0\rangle \\
&\times \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[f]} \otimes Y^{[f]}(\hat{q}) \right]^{[0]} - q^2\, g(q)\ (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \\
=&12\pi\, q^2\, g(q) \sum_f [f] \frac{(-1)^f}{\sqrt{[f]}} \left\{ \begin{array}{ccc} 1 & 1 & f \\ 1 & 1 & 0 \end{array} \right\} \sqrt{[f]} \left(\begin{array}{ccc} 1 & 1 & f \\ 0 & 0 & 0 \end{array} \right) \frac{3}{\sqrt{4\pi\,[f]}} \\
&\times \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[f]} \otimes Y^{[f]}(\hat{q}) \right]^{[0]} - q^2\, g(q)\ (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \\
=&12\pi\, q^2\, g(q) \sum_f [f]\, (-1)^f \frac{(-1)^f}{\sqrt{[1][1]}} \left(\begin{array}{ccc} 1 & 1 & f \\ 0 & 0 & 0 \end{array} \right) \frac{3}{\sqrt{4\pi\,[f]}} \\
&\times \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[f]} \otimes Y^{[f]}(\hat{q}) \right]^{[0]} - q^2\, g(q)\ (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \\
=&12\pi\, q^2\, g(q) \sum_f \sqrt{[f]} \left(\begin{array}{ccc} 1 & 1 & f \\ 0 & 0 & 0 \end{array} \right) \frac{1}{\sqrt{4\pi}} \\
&\times \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[f]} \otimes Y^{[f]}(\hat{q}) \right]^{[0]} - q^2\, g(q)\ (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\ . \qquad \text{(E.69)}
\end{aligned}
$$

The $3j$ coefficient requires $f = 0, 1, 2$. However

- the $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ factor exactly cancels out the $f = 0$ component, since

$$
12\pi \left(\begin{array}{ccc} 1 & 1 & 0 \\ 0 & 0 & 0 \end{array} \right) \frac{1}{\sqrt{4\pi}} \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[0]} \otimes Y^{[0]}(\hat{q}) \right]^{[0]} = -\frac{3}{\sqrt{3}} \left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[0]} = \vec{\sigma}_1 \cdot \vec{\sigma}_2\,, \qquad \text{(E.70)}
$$

- for $f = 1$ the $3j$ coefficient is zero.

Thus we only have $f = 2$[(3)]. One has then

$$
\begin{aligned}
&\langle k'\,(L'S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(LS)J\,T\rangle \\
&\quad =\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,12\pi\,\sqrt{5} \left(\begin{array}{ccc} 1 & 1 & 2 \\ 0 & 0 & 0 \end{array} \right) \frac{1}{\sqrt{[j]}} \frac{1}{\sqrt{4\pi}} \\
&\qquad \times (k'\,(L'S')J'||q^2\, g(q) \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[2]} \otimes Y^{[2]}(\hat{q}) \right]^{[0]} ||k\,(LS)J) \\
&\quad =\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\frac{\sqrt{6}\,\sqrt{4\pi}}{\sqrt{[J]}} \\
&\qquad \times (k'\,(L'S')J'||q^2\, g(q) \left[\left[\sigma_1^{[1]} \otimes \sigma_2^{[1]} \right]^{[2]} \otimes Y^{[2]}(\hat{q}) \right]^{[0]} ||k\,(LS)J)\,. \qquad \text{(E.71)}
\end{aligned}
$$

[3] This was expected by construction of the operator S_{12} which is proportional to Y_2.

We need thus to evaluate

$$
\begin{aligned}
&(k'\,(L'S')J'||q^2\,g(q)\left[\left[\sigma_1^{[1]}\otimes\sigma_2^{[1]}\right]^{[2]}\otimes Y^{[2]}(\hat{q})\right]^{[0]}||k\,(LS)J)\\
&\quad=\sqrt{[J][J'][0]}\begin{Bmatrix} L' & L & 2\\ S' & S & 2\\ J' & J & 0\end{Bmatrix}(k'\,L'||q^2\,g(q)\,Y^{[2]}(\hat{q})||k\,L)\,(S'||\left[\sigma_1^{[1]}\otimes\sigma_2^{[1]}\right]^{[2]}||S)\\
&\quad=\delta_{JJ'}\frac{\sqrt{[J]}}{\sqrt{[2]}}\begin{Bmatrix} L' & S' & J\\ S & L & 2\end{Bmatrix}(k'\,L'||q^2\,g(q)\,Y^{[2]}(\hat{q})||k\,L)\,(S'||\left[\sigma_1^{[1]}\otimes\sigma_2^{[1]}\right]^{[2]}||S)\,,
\end{aligned}
\tag{E.72}
$$

where from Eq. (A.81)

$$
(S||\left[\sigma_1^{[1]}\otimes\sigma_2^{[1]}\right]^{[2]}||S')=6\sqrt{[2][S][S']}\begin{Bmatrix} 1/2 & 1/2 & 1\\ 1/2 & 1/2 & 1\\ S & S' & 2\end{Bmatrix}. \tag{E.73}
$$

Thus the $9j$ coefficient is only non-zero when $S=S'=1$. As expected, the finite-range tensor only acts in the spin-triplet partial waves and the $S_0=1$ projector in this term is also redundant. We have then

$$
(S||\left[\sigma_1^{[1]}\otimes\sigma_2^{[1]}\right]^{[2]}||S')=6\,\delta_{SS'}\,\delta_{S1}\sqrt{[2][1][1]}\begin{Bmatrix} 1/2 & 1/2 & 1\\ 1/2 & 1/2 & 1\\ 1 & 1 & 2\end{Bmatrix}=\delta_{SS'}\,\delta_{S1}\,2\sqrt{5}\,. \tag{E.74}
$$

On the other hand, we can use the same decoupling-recoupling method from Sec. E.2.2.2 to obtain

$$
\begin{aligned}
&(k'\,L'||q^2\,g(q)\,Y^{[2]}(\hat{q})||k\,L)\\
&\quad=\sum_{\mu_1+\mu_2=2}\sqrt{\frac{4\pi\,[2]!}{[\mu_1]![\mu_2]!}}(-1)^{\mu_2}\,k'^{\mu_1}\,k^{\mu_2}\,(k'\,L'||g(q)\,\left[Y^{[\mu_1]}(\hat{k}')\otimes Y^{[\mu_2]}(\hat{k})\right]^{[2]}||k\,L)\\
&\quad=\sum_{\mu_1+\mu_2=2}\sqrt{\frac{4\pi\,[2]!}{[\mu_1]![\mu_2]!}}(-1)^{\mu_2}\,k'^{\mu_1}\,k^{\mu_2}\\
&\qquad\qquad\times\sum_{\lambda}\tilde{g}_\lambda(q)(k'\,L'||\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\right]^{[0]}\left[Y^{[\mu_1]}(\hat{k}')\otimes Y^{[\mu_2]}(\hat{k})\right]^{[2]}||k\,L)\\
&\quad=\sum_{\mu_1+\mu_2=2}\sqrt{\frac{4\pi\,[2]!}{[\mu_1]![\mu_2]!}}(-1)^{\mu_2}\,k'^{\mu_1}\,k^{\mu_2}\\
&\qquad\qquad\times\sum_{\lambda}\tilde{g}_\lambda(q)(k'\,L'||\left[\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\right]^{[0]}\otimes\left[Y^{[\mu_1]}(\hat{k}')\otimes Y^{[\mu_2]}(\hat{k})\right]^{[2]}\right]^{[2]}||k\,L)\\
&\quad=\sum_{\mu_1+\mu_2=2}\sqrt{\frac{4\pi\,[2]!}{[\mu_1]![\mu_2]!}}(-1)^{\mu_2}\,k'^{\mu_1}\,k^{\mu_2}\sum_{\lambda}\tilde{g}_\lambda(q)\sum_{a,b}\begin{Bmatrix}\lambda & \lambda & 0\\ \mu_1 & \mu_2 & 2\\ a & b & 2\end{Bmatrix}\sqrt{[a][b][0][2]}\\
&\qquad\qquad\times(k'\,L'||\left[\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\mu_1]}(\hat{k}')\right]^{[a]}\otimes\left[Y^{[\lambda]}(\hat{k})\otimes Y^{[\mu_2]}(\hat{k})\right]^{[b]}\right]^{[2]}||k\,L)
\end{aligned}
\tag{E.75}
$$

$$= \sum_{\mu_1+\mu_2=2} \sqrt{\frac{4\pi\,[2]!}{[\mu_1]![\mu_2]!}} (-1)^{\mu_2}\, k'^{\mu_1}\, k^{\mu_2} \sum_{\lambda} \tilde{g}_\lambda(q) \sum_{a,b} \left\{ \begin{array}{ccc} \lambda & \lambda & 0 \\ \mu_1 & \mu_2 & 2 \\ a & b & 2 \end{array} \right\} \sqrt{[a][b][0][2]} \tag{E.76}$$

$$\times \frac{\sqrt{[\lambda][\mu_1][\lambda][\mu_2]}}{4\pi\,\sqrt{[a][b]}} (k'\,L' || \left[Y^{[a]}(\hat{k}') \otimes Y^{[b]}(\hat{k}) \right]^{[2]} || k\,L)$$

$$\times \langle \lambda\,0\,\mu_1\,0\,|\lambda\,\mu_1\,a\,0\rangle\, \langle \lambda\,0\,\mu_2\,0\,|\lambda\,\mu_2\,b\,0\rangle$$

$$= [2]\, \frac{(-1)^{L'}}{(4\pi)^{3/2}} \sum_{\mu_1+\mu_2=2} \sqrt{\frac{[2]![\mu_1][\mu_2]}{[\mu_1]![\mu_2]!}} (-1)^{\mu_2}\, k'^{\mu_1}\, k^{\mu_2} \sum_{\lambda} [\lambda]\, \tilde{g}_\lambda(q) \left\{ \begin{array}{ccc} \lambda & \lambda & 0 \\ \mu_1 & \mu_2 & 2 \\ L' & L & 2 \end{array} \right\}$$

$$\times \left\langle \lambda\,0\,\mu_1\,0\,\middle|\lambda\,\mu_1\,L'\,0\right\rangle\, \langle \lambda\,0\,\mu_2\,0\,|\lambda\,\mu_2\,L\,0\rangle\,. \tag{E.77}$$

Some comments can be made here and allow to recover generic features associated with tensor coupling:

- as expected, the tensor couples between partial waves such as $|L - L'| \leq 2$, otherwise the $6j$ coefficient would be zero,
- one cannot have $L = L' = 0$, thus the tensor does not act on $L = L' = 0$ partial waves,
- if $\mu_1 = 0$ then $\mu_2 = 2$ and $\lambda = L'$. To have $\left(\begin{array}{ccc} L' & 2 & L \\ 0 & 0 & 0 \end{array} \right)$ to be non-zero, L and L' have to be of same parity. Same goes if $\mu_1 = \mu_2 = 1$ to have a non-zero product of $3j$ symbols. As expected, the tensor term only couples a partial wave of angular momentum L to partial waves $L' = L, L \pm 2$, except for $L = L' = 0$.

Finally, one obtains

$$\langle k'\,(L'S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(LS)J\,T\rangle$$

$$= \delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\,(-1)^{L'} \left\{ \begin{array}{ccc} L' & S' & J \\ S & L & 2 \end{array} \right\}$$

$$\times \sum_{\mu_1+\mu_2=2} \sqrt{\frac{[2]![\mu_1][\mu_2]}{[\mu_1]![\mu_2]!}} (-1)^{\mu_2}\, k'^{\mu_1}\, k^{\mu_2} \sum_{\lambda} [\lambda]\, \tilde{g}_\lambda(q) \left\{ \begin{array}{ccc} \lambda & \lambda & 0 \\ \mu_1 & \mu_2 & 2 \\ L' & L & 2 \end{array} \right\}$$

$$\times \left\langle \lambda\,0\,\mu_1\,0\,\middle|\lambda\,\mu_1\,L'\,0\right\rangle\, \langle \lambda\,0\,\mu_2\,0\,|\lambda\,\mu_2\,L\,0\rangle\,. \tag{E.78}$$

Like in the finite-range spin-orbit case, we provide here the explicit contributions we are interested in.

1. For $L = L' = 1$, three terms are to be considered, i.e.

- $\mu_1 = \mu_2 = 1$, in which case $\lambda = 0, 2$, and

$$\begin{aligned}
&\langle k'\,(1S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(1S)J\,T\rangle \\
&\quad=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\,\left\{\begin{array}{ccc}1&1&J\\1&1&2\end{array}\right\}\,\sqrt{\frac{[2]![1][1]}{[1]![1]!}}\,kk' \\
&\qquad\times\Bigg[[0]\,\tilde{g}_0(q)\,\left\{\begin{array}{ccc}0&0&0\\1&1&2\\1&1&2\end{array}\right\}\,\langle 0\,0\,1\,0\,|0\,1\,1\,0\rangle\,\langle 0\,0\,1\,0\,|0\,1\,1\,0\rangle \\
&\qquad\quad+[2]\,\tilde{g}_2(q)\,\left\{\begin{array}{ccc}2&2&0\\1&1&2\\1&1&2\end{array}\right\}\,\langle 2\,0\,1\,0\,|2\,1\,1\,0\rangle\,\langle 2\,0\,1\,0\,|2\,1\,1\,0\rangle\Bigg] \\
&\quad=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\left\{\begin{array}{ccc}1&1&J\\1&1&2\end{array}\right\}\,kk'\left[\frac{5}{\pi}\,\tilde{g}_0(q)+\frac{1}{\pi\sqrt{5}}\,\tilde{g}_2(q)\right],
\end{aligned}\tag{E.79}$$

- $\mu_1 = 0, \mu_2 = 2$, in which case $\lambda = 1$, and

$$\begin{aligned}
&\langle k'\,(1S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(1S)J\,T\rangle \\
&\quad=-\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\,\left\{\begin{array}{ccc}1&1&j\\1&1&2\end{array}\right\}\,\sqrt{\frac{[2]![0][2]}{[0]![2]!}}\,k^2 \\
&\qquad\times[1]\,\tilde{g}_1(q)\,\left\{\begin{array}{ccc}1&1&0\\0&2&2\\1&1&2\end{array}\right\}\,\langle 1\,0\,0\,0\,|1\,0\,1\,0\rangle\,\langle 1\,0\,2\,0\,|1\,2\,1\,0\rangle \\
&\quad=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\left\{\begin{array}{ccc}1&1&J\\1&1&2\end{array}\right\}\,k^2\,\frac{\sqrt{3}}{\pi}\,\tilde{g}_1(q)\,,
\end{aligned}\tag{E.80}$$

- $\mu_1 = 2, \mu_2 = 0$, in which case $\lambda = 1$, and immediately

$$\langle k'\,(1S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(1S)J\,T\rangle=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\left\{\begin{array}{ccc}1&1&J\\1&1&2\end{array}\right\}\,k'^2\,\frac{\sqrt{3}}{\pi}\,\tilde{g}_1(q)\,.\tag{E.81}$$

2. For $L = L' = 2$, one has also three terms to evaluate, i.e.

- $\mu_1 = \mu_2 = 1$, in which case $\lambda = 1, 3$, and

$$\begin{aligned}
&\langle k'\,(2S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(2S)J\,T\rangle \\
&\quad=-\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\,\left\{\begin{array}{ccc}2&1&J\\1&2&2\end{array}\right\}\,\sqrt{\frac{[2]![1][1]}{[1]![1]!}}\,kk' \\
&\qquad\times\Bigg[[1]\,\tilde{g}_1(q)\,\left\{\begin{array}{ccc}1&1&0\\1&1&2\\2&2&2\end{array}\right\}\,\langle 1\,0\,1\,0\,|1\,1\,2\,0\rangle\,\langle 1\,0\,1\,0\,|1\,1\,2\,0\rangle \\
&\qquad\quad+[3]\,\tilde{g}_3(q)\,\left\{\begin{array}{ccc}3&3&0\\1&1&2\\2&2&2\end{array}\right\}\,\langle 3\,0\,1\,0\,|3\,1\,2\,0\rangle\,\langle 3\,0\,1\,0\,|3\,1\,2\,0\rangle\Bigg]
\end{aligned}$$

$$=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\begin{Bmatrix}2&1&J\\1&2&2\end{Bmatrix}kk'\Big[-\frac{\sqrt{15}}{\pi}\,\tilde{g}_1(q)+\frac{3\sqrt{5}}{\pi\sqrt{7}}\,\tilde{g}_3(q)\Big]\,, \tag{E.82}$$

- $\mu_1=0,\mu_2=2$, in which case $\lambda=2$, and

$$\begin{aligned}&\langle k'\,(2S')J'\,T'|v_{\rm ff}^{1T,t}|k\,(2S)J\,T\rangle\\&\quad=\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\begin{Bmatrix}2&1&J\\1&2&2\end{Bmatrix}\sqrt{\frac{[2]![0][2]}{[0]![2]!}}\,k^2\\&\qquad\times[2]\,\tilde{g}_2(q)\begin{Bmatrix}2&2&0\\0&2&2\\2&2&2\end{Bmatrix}\langle 2\,0\,0\,0\,|2\,0\,2\,0\rangle\,\langle 2\,0\,2\,0\,|2\,2\,2\,0\rangle\\&\quad=-\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\begin{Bmatrix}2&1&J\\1&2&2\end{Bmatrix}k^2\,\frac{\sqrt{15}}{\pi\sqrt{7}}\,\tilde{g}_2(q)\,,\end{aligned} \tag{E.83}$$

- $\mu_1=2,\mu_2=0$, in which case $\lambda=1$, and immediately

$$\langle k'\,(2S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(2S)J\,T\rangle=-\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\begin{Bmatrix}1&1&J\\1&1&2\end{Bmatrix}k'^2\,\frac{\sqrt{15}}{\pi\sqrt{7}}\,\tilde{g}_2(q)\,. \tag{E.84}$$

3. For the coupled channels $L'=0,L=2$, one has $\lambda=\mu_2$, the $6j$ coefficient $\begin{Bmatrix}2&1&J\\1&0&2\end{Bmatrix}$ is non-zero if and only if $J=1$ because of the triangle rule. This means the only diagonal coupling to be considered will be ^{3}S$_1$-^{3}D$_1$. We have then

- In the case $\mu_1=\mu_2=1$, $\lambda=1$ and

$$\begin{aligned}&\langle k'\,(0S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(2S)J\,T\rangle\\&\quad=-\,\delta_{JJ'}\,\delta_{J1}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\begin{Bmatrix}2&1&1\\1&0&2\end{Bmatrix}\sqrt{\frac{[2]![1][1]}{[1]![1]!}}\,kk'\\&\qquad\times[1]\,\tilde{g}_1(q)\begin{Bmatrix}1&1&0\\1&1&2\\2&0&2\end{Bmatrix}\langle 1\,0\,1\,0\,|1\,1\,2\,0\rangle\,\langle 1\,0\,1\,0\,|1\,1\,0\,0\rangle\\&\quad=\delta_{JJ'}\,\delta_{J1}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,kk'\,\frac{\sqrt{2}}{\pi\sqrt{3}}\,\tilde{g}_1(q)\,,\end{aligned} \tag{E.85}$$

- In the case $\mu_1=2,\mu_2=0$, $\lambda=2$ and

$$\begin{aligned}&\langle k'\,(2S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(0S)J\,T\rangle\\&\quad=\delta_{JJ'}\,\delta_{J1}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\begin{Bmatrix}2&1&1\\1&0&2\end{Bmatrix}\sqrt{\frac{[2]![0][2]}{[0]![2]!}}\,k'^2\\&\qquad\times[2]\,\tilde{g}_2(q)\begin{Bmatrix}2&2&0\\2&0&2\\0&2&2\end{Bmatrix}\langle 2\,0\,0\,0\,|2\,0\,2\,0\rangle\,\langle 2\,0\,2\,0\,|2\,2\,0\,0\rangle\\&\quad=\delta_{JJ'}\,\delta_{J1}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,k'^2\,\frac{1}{\pi\sqrt{10}}\,\tilde{g}_2(q)\,,\end{aligned} \tag{E.86}$$

- In the case $\mu_1 = 0, \mu_2 = 2$, one has $\lambda = 0$ and

$$\begin{aligned}
&\langle k'\,(0S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(2S)J\,T) \\
&\quad=\delta_{JJ'}\,\delta_{J1}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\frac{10\sqrt{6}}{4\pi}\,\left\{\begin{array}{ccc} 2 & 1 & 1 \\ 1 & 0 & 2 \end{array}\right\}\,\sqrt{\frac{[2]![0][2]}{[0]![2]!}}\,k^2 \\
&\qquad\times[0]\,\tilde{g}_0(q)\,\left\{\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 2 & 2 \\ 0 & 2 & 2 \end{array}\right\}\,\langle 0\,0\,2\,0\,|0\,2\,2\,0\rangle\,\langle 0\,0\,0\,0\,|0\,0\,0\,0\rangle \\
&\quad=\delta_{JJ'}\,\delta_{J1}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,k^2\,\frac{1}{\pi\sqrt{2}}\,\tilde{g}_0(q)\,.
\end{aligned} \tag{E.87}$$

4. Finally for the coupled channels $L = 0, L' = 2$, one simply has to invert the roles of k and k' in the $L = 2, L' = 0$ case.

There seems to be a general relation for these reduced matrix elements. Indeed, one can write

- for $L = L'$

$$\begin{aligned}
&\langle k'\,(L'S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(L'S)J\,T\rangle \\
&\quad=(-1)^{L'+1}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\mathcal{F}_1(L',J) \\
&\qquad\times\left[[L'+1]\,kk'\,\frac{\tilde{g}_{L'-1}(q)}{4\pi\,\sqrt{[L'-1]}}+[L']\,(k^2+k'^2)\,\frac{\tilde{g}_{L'}(q)}{4\pi\,\sqrt{[L']}}\right. \\
&\qquad\qquad\left.+[L'-1]\,kk'\,\frac{\tilde{g}_{L'+1}(q)}{4\pi\,\sqrt{[L'+1]}}\right],
\end{aligned} \tag{E.88}$$

where

$$\mathcal{F}_1(L',J)=\left\{\begin{array}{ccc} L' & 1 & J \\ 1 & L' & 2 \end{array}\right\}\,\frac{2\sqrt{30}\,\sqrt{L'\,(L'+1)}}{\sqrt{[L'-1]\,[L']\,[L'+1]}}\,, \tag{E.89}$$

- for $L = L' + 2$, one necessarily has $J = L' + 1$, and

$$\begin{aligned}
&\langle k'\,(L'S')J'\,T'|v_{\rm ff}^{1T_0,t}|k\,(L'+2\,S)J\,T\rangle \\
&\quad=(-1)^{L'}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{TT_0}\,\delta_{SS'}\,\delta_{S1}\,\mathcal{F}_2(L') \\
&\qquad\times\left[\frac{k^2}{2}\,\frac{\tilde{g}_{L'}(q)}{4\pi\,\sqrt{[L']}}+kk'\,\frac{\tilde{g}_{L'+1}(q)}{4\pi\,\sqrt{[L'+1]}}+\frac{k'^2}{2}\,\frac{\tilde{g}_{L'+2}(q)}{4\pi\,\sqrt{[L'+2]}}\right],
\end{aligned} \tag{E.90}$$

where

$$\mathcal{F}_2(L')=\frac{12\,\sqrt{(L'+1)(L'+2)}}{[L'+2]}\,. \tag{E.91}$$

E.2.2.4 One-pion exchange

For reference, we provide a partial wave decomposition of the one-pion exchange, whose associated vertex reads in momentum space

$$\begin{aligned}
v_\pi(\vec{q}\,) &= -\,4\pi\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\,(\vec{\tau}_1\cdot\vec{\tau}_2\,)\,\frac{(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)}{q^2+\mu^2} \\
&= -\,4\pi\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\,(\vec{\tau}_1\cdot\vec{\tau}_2\,)\,\frac{1}{q^2+\mu^2}\,\left[(\vec{\sigma}_1\cdot\vec{q}\,)\,(\vec{\sigma}_2\cdot\vec{q}\,)-\frac{1}{3}\,q^2\,\,(\vec{\sigma}_1\cdot\vec{\sigma}_2)+\frac{1}{3}\,q^2\,\,(\vec{\sigma}_1\cdot\vec{\sigma}_2)\right].
\end{aligned} \tag{E.92}$$

To achieve this, we need to decompose in partial waves the counter term

$$v_\pi^{ct}(\vec{k}\,',\vec{k}\,) = g(q)\,q^2\ (\vec{\sigma}_1\cdot\vec{\sigma}_2)\ (\vec{\tau}_1\cdot\vec{\tau}_2)\ , \tag{E.93}$$

which is trivial. Indeed, let $G(q)=q^2\,g(q)$, one has then

$$\begin{aligned}
&\langle k'\,(L'S')J'\,T'|v_\pi^{ct}|k\,(LS)J\,T\rangle \\
&\quad=\delta_{JJ'}\,\delta_{TT'}\,\delta_{SS'}\sum_\lambda \tilde{G}_\lambda(q)\,\frac{1}{\sqrt{[L]}}\,(k'\,L'||\left[Y^{[\lambda]}(\hat{k}')\otimes Y^{[\lambda]}(\hat{k})\right]^{[0]}\,||k\,L) \\
&\qquad\qquad\times(2S(S+1)-3)\,(2T(T+1)-3) \\
&\quad=(-1)^{L+S+T}\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{SS'}\,\delta_{LL'}\,\frac{\tilde{G}_l(q)}{4\pi}\,\frac{1}{\sqrt{[L]}}\,(2S(S+1)-3)\,(2T(T+1)-3) \\
&\quad=-\,\delta_{JJ'}\,\delta_{TT'}\,\delta_{SS'}\,\delta_{LL'}\,\frac{\tilde{G}_l(q)}{4\pi}\,\frac{1}{\sqrt{[L]}}\,(2S(S+1)-3)\,(2T(T+1)-3)\,.
\end{aligned} \tag{E.94}$$

For the one-pion exchange v_π, one introduces (see Sec. A.3.5)

$$p^f(\vec{k}\,',\vec{k}\,)\equiv\frac{q^2}{q^2+m_\pi^2}\,\frac{1}{q^f}\,, \tag{E.95}$$

in which case

$$g(q)=-\,\frac{4\pi}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{1}{q^2+\mu^2}\equiv-\frac{4\pi}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 p^2(\vec{k}\,',\vec{k}\,)\,, \tag{E.96a}$$

$$G(q)=-\,\frac{4\pi}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{q^2}{q^2+\mu^2}\equiv-\frac{4\pi}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 p^0(\vec{k}\,',\vec{k}\,)\,. \tag{E.96b}$$

Thus after some manipulations, without the extra 2 factor for the exchange terms

$$\begin{aligned}
v_\pi({}^1S_0,k,k') =&v_\pi({}^3S_1,k,k') \\
=&-\,(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_0^0(k',k)}{4\pi}\,,
\end{aligned} \tag{E.97a}$$

$$v_\pi({}^1P_1,k,k') =3\,(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_1^0(k',k)}{4\pi\sqrt{3}}\,, \tag{E.97b}$$

$$\begin{aligned}
v_\pi({}^3P_0,k,k') =&\frac{(4\pi)^2}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_1^0(k',k)}{4\pi\sqrt{3}} \\
&-\frac{(4\pi)^2}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{4}{3}\left[5\,kk'\,\frac{\tilde{p}_0^2(k',k)}{4\pi}+3(k^2+k'^2)\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+kk'\,\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}\right]\,,
\end{aligned} \tag{E.97c}$$

$$\begin{aligned}
v_\pi({}^3P_1,k,k') =&\frac{(4\pi)^2}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_1^0(k',k)}{4\pi\sqrt{3}} \\
&-\frac{(4\pi)^2}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{4}{6}\left[5\,kk'\,\frac{\tilde{p}_0^2(k',k)}{4\pi}+3(k^2+k'^2)\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+kk'\,\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}\right]\,,
\end{aligned} \tag{E.97d}$$

$$\begin{aligned}
v_\pi({}^3P_2,k,k') =&\frac{(4\pi)^2}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_1^0(k',k)}{4\pi\sqrt{3}} \\
&-\frac{(4\pi)^2}{3}\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{4}{30}\left[5\,kk'\,\frac{\tilde{p}_0^2(k',k)}{4\pi}+3(k^2+k'^2)\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+kk'\,\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}\right]\,,
\end{aligned} \tag{E.97e}$$

$$v_\pi({}^1D_2,k,k') = -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_2^0(k',k)}{4\pi\sqrt{5}}\,, \tag{E.97f}$$

$$\begin{aligned} v_\pi({}^3D_1,k,k') =& -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_2^0(k',k)}{4\pi\sqrt{5}} \\ & -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{4}{10}\left[7\,kk'\,\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+5(k^2+k'^2)\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}+3\,kk'\,\frac{\tilde{p}_3^2(k',k)}{4\pi\sqrt{7}}\right], \end{aligned} \tag{E.97g}$$

$$\begin{aligned} v_\pi({}^3D_2,k,k') =& -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_2^0(k',k)}{4\pi\sqrt{5}} \\ & -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{4}{10}\left[7\,kk'\,\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+5(k^2+k'^2)\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}+3\,kk'\,\frac{\tilde{p}_3^2(k',k)}{4\pi\sqrt{7}}\right], \end{aligned} \tag{E.97h}$$

$$\begin{aligned} v_\pi({}^3D_3,k,k') =& -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{\tilde{p}_2^0(k',k)}{4\pi\sqrt{5}} \\ & -(4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2\frac{4}{35}\left[7\,kk'\,\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+5(k^2+k'^2)\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}+3\,kk'\,\frac{\tilde{p}_3^2(k',k)}{4\pi\sqrt{7}}\right], \end{aligned} \tag{E.97i}$$

$$v_\pi(\epsilon_1,k,k') = (4\pi)^2\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2 4\pi\sqrt{2}\left[\frac{1}{2}\,k^2\,\frac{\tilde{p}_0^2(k',k)}{4\pi}+kk'\,\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}}+\frac{1}{2}\,k'^2\,\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}}\right], \tag{E.97j}$$

where

$$\frac{\tilde{p}_0^0(k',k)}{4\pi} = 1+\frac{m_\pi^2}{4\,kk'}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right), \tag{E.98a}$$

$$\frac{\tilde{p}_1^0(k',k)}{4\pi\sqrt{3}} = -\frac{m_\pi^2}{2\,kk'}-\frac{m_\pi^2\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right), \tag{E.98b}$$

$$\frac{\tilde{p}_2^0(k',k)}{4\pi\sqrt{5}} = \frac{3m_\pi^2\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}+\frac{m_\pi^2}{2\,kk'}\left(-\frac{1}{4}+\frac{3m_\pi^2\,(k^2+k'^2+m_\pi^2)}{16\,k^2k'^2}\right)\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right), \tag{E.98c}$$

$$\frac{\tilde{p}_0^2(k',k)}{4\pi} = -\frac{1}{4\,kk'}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right), \tag{E.98d}$$

$$\frac{\tilde{p}_1^2(k',k)}{4\pi\sqrt{3}} = \frac{1}{2\,kk'}+\frac{(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right), \tag{E.98e}$$

$$\frac{\tilde{p}_2^2(k',k)}{4\pi\sqrt{5}} = -\frac{3\,(k^2+k'^2+m_\pi^2)}{8\,k^2k'^2}-\frac{1}{4\,kk'}\left(-\frac{1}{2}+\frac{3\,(k^2+k'^2+m_\pi^2)^2}{8\,k^2k'^2}\right)\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right), \tag{E.98f}$$

$$\begin{aligned} \frac{\tilde{p}_3^2(k',k)}{4\pi\sqrt{7}} =& -\frac{1}{kk'}\left(\frac{1}{3}-\frac{5\,(k^2+k'^2+m_\pi^2)^2}{16\,k^2k'^2}\right) \\ & -\frac{(k^2+k'^2+m_\pi^2)}{16\,k^2k'^2}\left(3-\frac{5\,(k^2+k'^2+m_\pi^2)^2}{4\,k^2\,k'^2}\right)\ln\left(\frac{m_\pi^2+(k-k')^2}{m_\pi^2+(k+k')^2}\right). \end{aligned} \tag{E.98g}$$

E.2.2.5 Summary

Using the previous work, matrix elements in the $L \leq 2$ partial waves for $v^{[\mathrm{X}]}_{\mathrm{BDRS}}$ read

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^1S_0,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{01}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_0^i(k',k)}{4\pi}\,, \tag{E.99a}$$

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3S_1,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{10}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_0^i(k',k)}{4\pi}\,, \tag{E.99b}$$

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^1P_1,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{00}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}}\,, \tag{E.99c}$$

$$\begin{aligned} v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3P_0,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{11}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}} \\ &+ 4\,\frac{1}{2\pi^2}\,C_{so}^{11}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,kk'\left[\frac{1}{3}\,\frac{\tilde{g}_0^{so}(k',k)}{4\pi} - \frac{1}{3}\,\frac{\tilde{g}_2^{so}(k',k)}{4\pi\sqrt{5}}\right] \\ &- \frac{1}{2\pi^2}\,C_t^{11}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\ &\qquad\times\frac{4}{3}\left[5\,\frac{\tilde{g}_0^t(k',k)}{4\pi}\,kk' + 3\,(k^2+k'^2)\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + \frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}}\,kk'\right], \end{aligned} \tag{E.99d}$$

$$\begin{aligned} v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3P_1,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{11}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}} \\ &+ 2\,\frac{1}{2\pi^2}\,C_{so}^{11}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,kk'\left[\frac{1}{3}\,\frac{\tilde{g}_0^{so}(k',k)}{4\pi} - \frac{1}{3}\,\frac{\tilde{g}_2^{so}(k',k)}{4\pi\sqrt{5}}\right] \\ &- \frac{1}{2\pi^2}\,C_t^{11}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\ &\qquad\times\frac{2}{3}\left[5\,\frac{\tilde{g}_0^t(k',k)}{4\pi}\,kk' + 3\,(k^2+k'^2)\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + \frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}}\,kk'\right], \end{aligned} \tag{E.99e}$$

$$\begin{aligned} v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3P_2,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{11}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_1^i(k',k)}{4\pi\sqrt{3}} \\ &- 2\,\frac{1}{2\pi^2}\,C_{so}^{11}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,kk'\left[\frac{1}{3}\,\frac{\tilde{g}_0^{so}(k',k)}{4\pi} - \frac{1}{3}\,\frac{\tilde{g}_2^{so}(k',k)}{4\pi\sqrt{5}}\right] \\ &- \frac{1}{2\pi^2}\,C_t^{11}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\ &\qquad\times\frac{2}{15}\left[5\,\frac{\tilde{g}_0^t(k',k)}{4\pi}\,kk' + 3\,(k^2+k'^2)\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + \frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}}\,kk'\right], \end{aligned} \tag{E.99f}$$

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^1D_2,k,k') = \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{01}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}}\,, \tag{E.99g}$$

$$
\begin{aligned}
v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3D_1,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{10}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}} \\
&- 6\,\frac{1}{2\pi^2}\,C_{so}^{10}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,\frac{kk'}{5}\,\left[\frac{\tilde{g}_1^{so}(k',k)}{4\pi\sqrt{3}} - \frac{\tilde{g}_3^{so}(k',k)}{4\pi\sqrt{7}}\right] \qquad \text{(E.99h)} \\
&+ \frac{1}{2\pi^2}\,C_t^{10}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\
&\qquad \times \frac{2}{5}\left[7\,kk'\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + 5(k^2+k'^2)\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}} + 3\,kk'\,\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}}\right], \\
v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3D_2,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{10}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}} \\
&- 2\,\frac{1}{2\pi^2}\,C_{so}^{10}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,\frac{kk'}{5}\,\left[\frac{\tilde{g}_1^{so}(k',k)}{4\pi\sqrt{3}} - \frac{\tilde{g}_3^{so}(k',k)}{4\pi\sqrt{7}}\right] \qquad \text{(E.99i)} \\
&+ \frac{1}{2\pi^2}\,C_t^{10}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\
&\qquad \times \frac{2}{5}\left[7\,kk'\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + 5(k^2+k'^2)\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}} + 3\,kk'\,\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}}\right], \\
v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3D_3,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{10}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_2^i(k',k)}{4\pi\sqrt{5}} \\
&+ 4\,\frac{1}{2\pi^2}\,C_{so}^{10}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,\frac{kk'}{5}\,\left[\frac{\tilde{g}_1^{so}(k',k)}{4\pi\sqrt{3}} - \frac{\tilde{g}_3^{so}(k',k)}{4\pi\sqrt{7}}\right] \qquad \text{(E.99j)} \\
&+ \frac{1}{2\pi^2}\,C_t^{10}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\
&\qquad \times \frac{4}{35}\left[7\,kk'\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + 5(k^2+k'^2)\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}} + 3\,kk'\,\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}}\right],
\end{aligned}
$$

$$
\begin{aligned}
v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3F_2,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{11}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_3^i(k',k)}{4\pi\sqrt{5}} \\
&+ \frac{1}{2\pi^2}\,C_{so}^{11}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,kk'\,\frac{8}{7}\,\left[\frac{\tilde{g}_2^{so}(k',k)}{4\pi\sqrt{5}} - \frac{\tilde{g}_4^{so}(k',k)}{4\pi\sqrt{9}}\right] \qquad \text{(E.99k)} \\
&- \frac{1}{2\pi^2}\,C_t^{11}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\
&\qquad \times \frac{8}{35}\left[9\,kk'\,\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}} + 7(k^2+k'^2)\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}} + 5\,kk'\,\frac{\tilde{g}_4^t(k',k)}{4\pi\sqrt{9}}\right],
\end{aligned}
$$

$$
\begin{aligned}
v^{[\mathrm{X}]}_{\mathrm{BDRS}}({}^3G_3,k,k') =& \frac{1}{2\pi^2}\sum_{i=1}^{N} C_i^{10}[\rho_0,\Lambda]\,(\mu_i\sqrt{\pi})^3\,\frac{\tilde{g}_4^i(k',k)}{4\pi\sqrt{5}} \\
&- \frac{1}{2\pi^2}\,C_{so}^{10}[\rho_0,\Lambda]\,\frac{\mu_{so}^2\,(\mu_{so}\sqrt{\pi})^3}{2}\,kk'\,\frac{10}{9}\,\left[\frac{\tilde{g}_3^{so}(k',k)}{4\pi\sqrt{7}} - \frac{\tilde{g}_5^{so}(k',k)}{4\pi\sqrt{11}}\right] \qquad \text{(E.99l)} \\
&+ \frac{1}{2\pi^2}\,C_t^{10}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \\
&\qquad \times \frac{10}{63}\left[11\,kk'\,\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}} + 9(k^2+k'^2)\frac{\tilde{g}_4^t(k',k)}{4\pi\sqrt{9}} + 7\,kk'\,\frac{\tilde{g}_5^t(k',k)}{4\pi\sqrt{11}}\right],
\end{aligned}
$$

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}(\epsilon_1,k,k') = -\frac{1}{2\pi^2}\,C_t^{10}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \times\ 4\sqrt{2}\left[\frac{1}{2}\,k^2\,\frac{\tilde{g}_0^t(k',k)}{4\pi} + kk'\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + \frac{1}{2}\,k'^2\,\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}}\right], \tag{E.99m}$$

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}(\epsilon_2,k,k') = +\frac{1}{2\pi^2}\,C_t^{11}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \times \frac{12\sqrt{6}}{5}\left[\frac{1}{2}\,k^2\,\frac{\tilde{g}_1^t(k',k)}{4\pi\sqrt{3}} + kk'\,\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}} + \frac{1}{2}\,k'^2\,\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}}\right], \tag{E.99n}$$

$$v^{[\mathrm{X}]}_{\mathrm{BDRS}}(\epsilon_3,k,k') = -\frac{1}{2\pi^2}\,C_t^{10}[\rho_0,\Lambda]\,\frac{\mu_t^4\,(\mu_t\sqrt{\pi})^3}{4} \times \frac{24\sqrt{3}}{7}\left[\frac{1}{2}\,k^2\,\frac{\tilde{g}_2^t(k',k)}{4\pi\sqrt{5}} + kk'\,\frac{\tilde{g}_3^t(k',k)}{4\pi\sqrt{7}} + \frac{1}{2}\,k'^2\,\frac{\tilde{g}_4^t(k',k)}{4\pi\sqrt{9}}\right], \tag{E.99o}$$

where

$$\frac{\tilde{g}_0^i(k,k')}{4\pi} = \frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i}\,\mathrm{sh}(\Gamma_i)\,, \tag{E.100a}$$

$$\frac{\tilde{g}_1^i(k,k')}{4\pi\sqrt{3}} = -\frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^2}\left[\Gamma_i\,\mathrm{ch}(\Gamma_i) - \mathrm{sh}(\Gamma_i)\right], \tag{E.100b}$$

$$\frac{\tilde{g}_2^i(k,k')}{4\pi\sqrt{5}} = \frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^3}\left[-3\Gamma_i\,\mathrm{ch}(\Gamma_i) + (3+\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right], \tag{E.100c}$$

$$\frac{\tilde{g}_3^i(k,k')}{4\pi\sqrt{7}} = -\frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^4}\left[\Gamma_i\,(15+\Gamma_i^2)\,\mathrm{ch}(\Gamma_i) - 3\,(5+2\Gamma_i^2)\mathrm{sh}(\Gamma_i)\right], \tag{E.100d}$$

$$\frac{\tilde{g}_4^i(k,k')}{4\pi\sqrt{9}} = \frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^5}\left[-5\Gamma_i\,(21+2\Gamma_i^2)\mathrm{ch}(\Gamma_i) + (105+45\Gamma_i^2+\Gamma_i^4)\mathrm{sh}(\Gamma_i)\right], \tag{E.100e}$$

$$\frac{\tilde{g}_5^i(k,k')}{4\pi\sqrt{11}} = -\frac{e^{-\frac{1}{4}\mu_i^2\,(k^2+k'^2)}}{\Gamma_i^6}\left[\Gamma_i\,(945+105\Gamma_i^2+\Gamma_i^4)\mathrm{ch}(\Gamma_i) - 15(63+28\Gamma_i^2+\Gamma_i^4)\mathrm{sh}(\Gamma_i)\right], \tag{E.100f}$$

$$\Gamma_i = \frac{1}{2}\,\mu_i^2\,kk'\,. \tag{E.100g}$$

Appendix F

Utilities for fitpack

Abstract: This chapter presents different objects that are used in FITPACK, i.e. as standard benchmark cost functions or the algorithm for generating random curves and surfaces.

Contents

F.1 Benchmarking cost functions

To evaluate the performances of the simplex and FITPACK algorithms, several cost functions f_i have been considered [55], corresponding to different situations in terms of (i) the existence of secondary minima (multimodal functions), (ii) the smoothness of the cost surface around the global minimum, and (iii) the dimensionality. For some of them we represent the surface in the two-dimension case for illustration purpose. n corresponds to the dimension of the problem, and the absolute optimum will be noted x^*. We also suggest values for the initial search space that are large enough to catch the complexity of the problem.

F.1.1 Unimodal functions

Unimodal functions are rather easy to optimize, although the problem becomes complex when the dimension increases.

- The so-called sphere function f_1 is defined as a simple sum of squares, i.e.

$$f_1(x) \equiv \sum_{i=1}^{n} x_i^2 \,, \tag{F.1a}$$

$$x_i \in [-100, +100] \,, \qquad x_i^* = 0 \,, \qquad f_1(x^*) = 0 \,. \tag{F.1b}$$

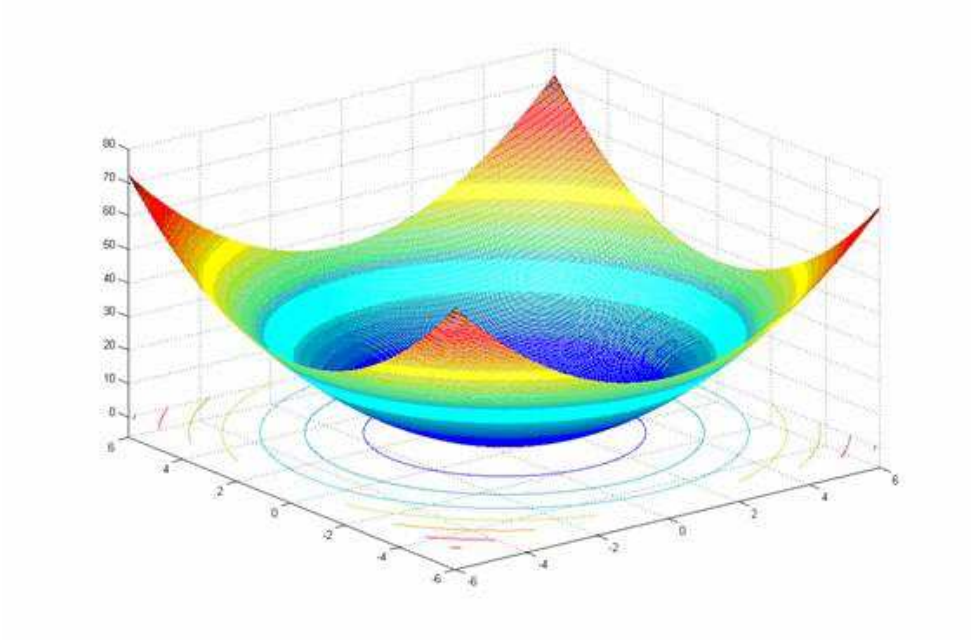


Figure F.1: The sphere function f_1 for $n = 2$.

- The function f_2 is defined as

$$f_2(x) \equiv \sum_{i=1}^{n} |x_i| + \prod_{i=1}^{n} |x_i| \,, \tag{F.2a}$$

$$x_i \in [-10, +10] \,, \qquad x_i^* = 0 \,, \qquad f_2(x^*) = 0 \,. \tag{F.2b}$$

- The function f_3 is defined as a Schwefels's double sum function [56]. Its gradient is not oriented along the principal axis due to the epistasis among their variables, such that any algorithms that use the gradient converges very slowly.

$$f_3(x) \equiv \sum_{i=1}^{n} \left[\sum_{j=1}^{i} x_j \right]^2 \,, \tag{F.3a}$$

$$x_i \in [-65, +65] \,, \qquad x_i^* = 0 \,, \qquad f_3(x^*) = 0 \,. \tag{F.3b}$$

- The function f_4 is defined as

$$f_4(x) \equiv \max_i |x_i| \,, \tag{F.4a}$$

$$x_i \in [-100, +100] \,, \qquad x_i^* = 0 \,, \qquad f_4(x^*) = 0 \,. \tag{F.4b}$$

- The function f_5 corresponds to Rosenbrock's function [57], which is unimodal for $n > 3$, and multimodal for $n \leq 3$. The global minimum is inside a long, narrow, parabolic-shaped flat valley, which is why f_5 is often called Rosenbrock's valley function. Due to the non-linearity of the valley, many algorithms converge slowly because they change the direction of the search repeatedly. To find the valley is trivial, however to converge to the global minimum is difficult. One has then

$$f_5(x) \equiv \sum_{i=1}^{n-1} \left[100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2 \right] \,, \tag{F.5a}$$

$$x_i \in [-30, +30] \,, \qquad x_i^* = 1 \,, \qquad f_5(x^*) = 0 \,. \tag{F.5b}$$

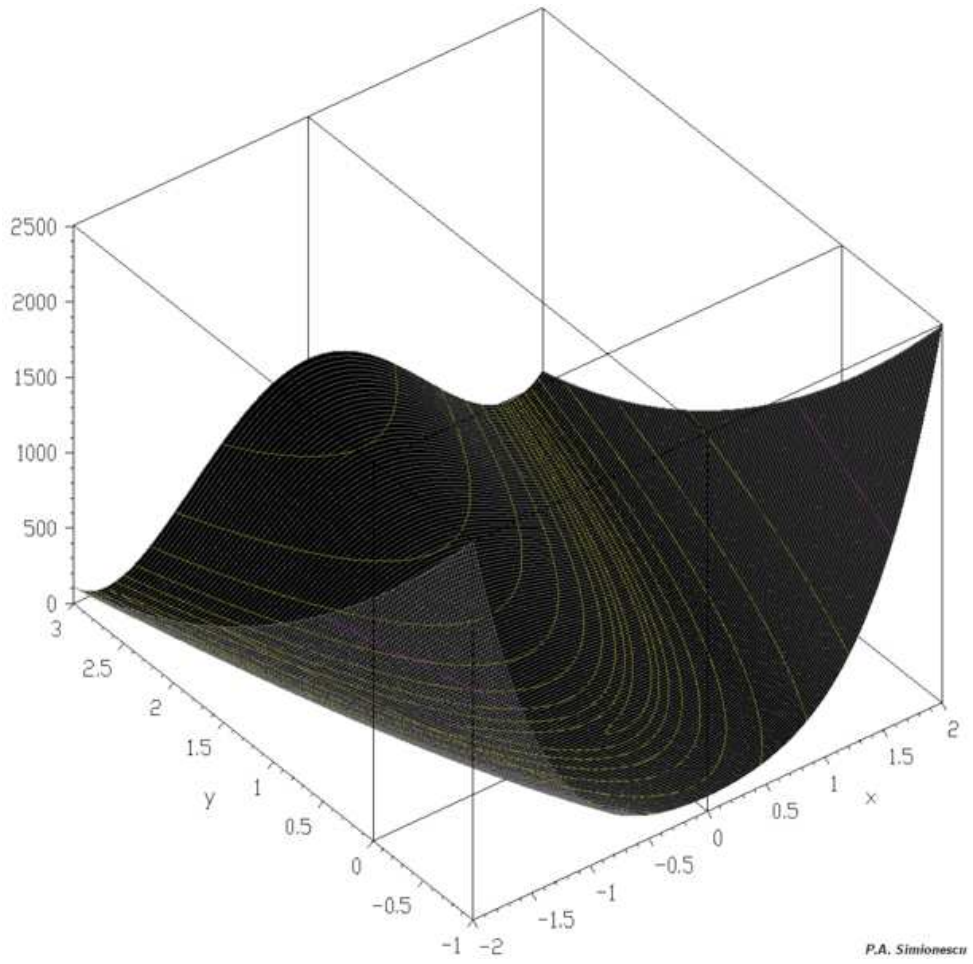


Figure F.2: The Rosenbrock's function f_5 for $n = 2$.

- The function f_6 corresponds to a discontinuous step function, defined as

$$f_6(x) \equiv \sum_{i=1}^{n} (\lfloor x_i + 0.5 \rfloor) \,, \tag{F.6a}$$

$$x_i \in [-100, +100] \,, \qquad x_i^* \in [0, 0.5) \,, \qquad f_6(x^*) = 0 \,. \tag{F.6b}$$

F.1.2 Multimodal functions with many local optima

This class of functions corresponds to the most complex optimization problems, since they contain many metastable traps that must be avoided.

- The function f_7 corresponds to Salomon's function, i.e.

$$f_7(x) \equiv -\cos\left(2\pi\sqrt{\sum_{i=1}^{n} x_i^2}\right) + \frac{1}{10}\sqrt{\sum_{i=1}^{n} x_i^2} + 1 \,, \tag{F.7a}$$

$$x_i \in [-100, +100] \,, \qquad x_i^* = 0 \,, \qquad f_7(x^*) = 0 \,. \tag{F.7b}$$

- The function f_8 corresponds to the normalized Schwefel's function [56], where the global minimum is geometrically distant, over the parameter space, from the next best local

minima. Therefore, search algorithms are potentially prone to convergence in the wrong direction. It reads

$$f_8(x) \equiv \frac{1}{n}\sum_{i=1}^{n} -x_i \sin(\sqrt{|x_i|}) + 418.982887272(...)\,, \tag{F.8a}$$

$$x_i \in [-500, +500]\,, \qquad x_i^* = 420.968746(...)\,, \qquad f_8(x^*) = 0\,. \tag{F.8b}$$

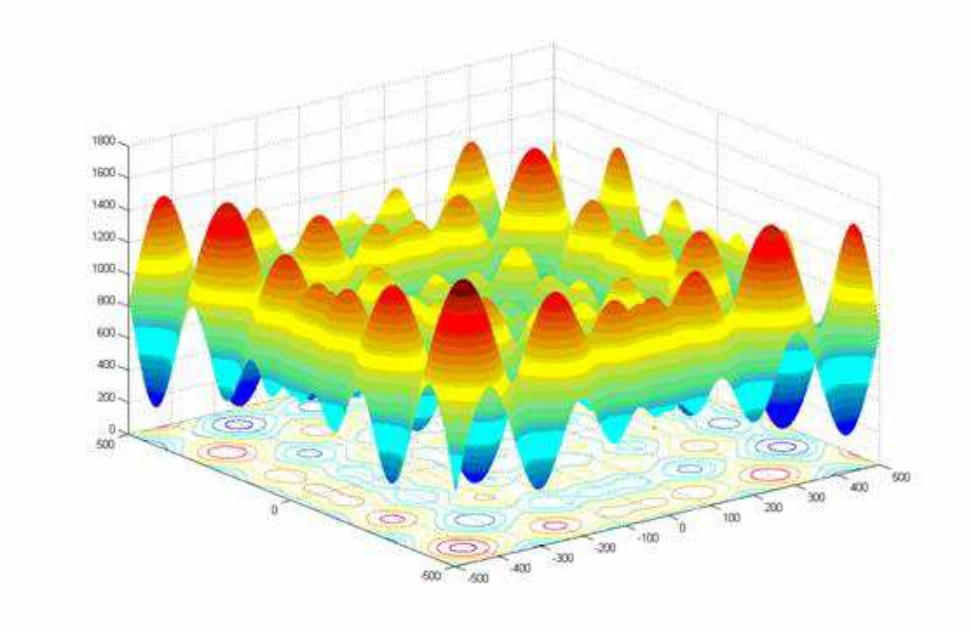


Figure F.3: The Schwefel's function f_8 for $n = 2$.

- The function f_9 is defined as the highly multimodal Rastrigin's function [58], i.e.

$$f_9(x) \equiv \sum_{i=1}^{n} \left[x_i^2 - 10\,\cos(2\pi\, x_i) + 10\right]\,, \tag{F.9a}$$

$$x_i \in [-5.12, +5.12]\,, \qquad x_i^* = 0\,, \qquad f_9(x^*) = 0\,. \tag{F.9b}$$

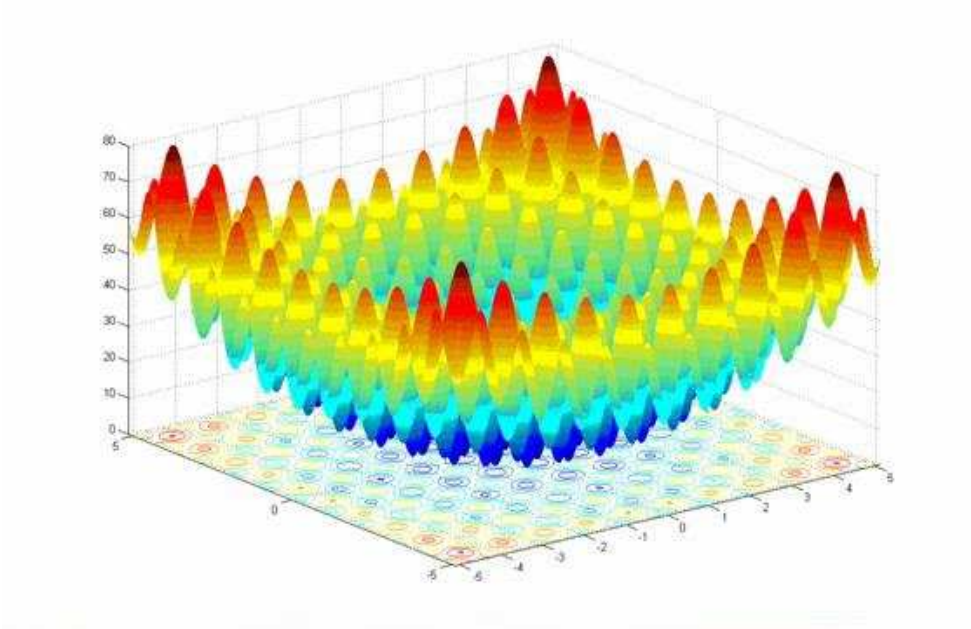


Figure F.4: The Rastringin's function f_9 for $n = 2$.

- The function f_{10} corresponds to Whitley's function defined as

$$f_{10}(x) \equiv \sum_{i=1}^{n} \sum_{j=1}^{n} \left[\frac{(100(x_i^3 - x_j)^2 + (1 - x_j))^2}{4000} - \cos\left(100(x_i^3 - x_j)^2 + (1 - x_j)^2\right) + 1 \right], \tag{F.10a}$$

$$x_i \in [-500, +500], \qquad x_i^* = 1, \qquad f_{10}(x^*) = 0. \tag{F.10b}$$

- The function f_{11} is the Griewank's function that reads

$$f_{11}(x) \equiv \frac{1}{4000} \sum_{i=1}^{n} x_i^2 - \prod_{i=1}^{n} \cos\left(\frac{x_i}{\sqrt{i}}\right) + 1, \tag{F.11a}$$

$$x_i \in [-500, +500], \qquad x_i^* = 0, \qquad f_{11}(x^*) = 0. \tag{F.11b}$$

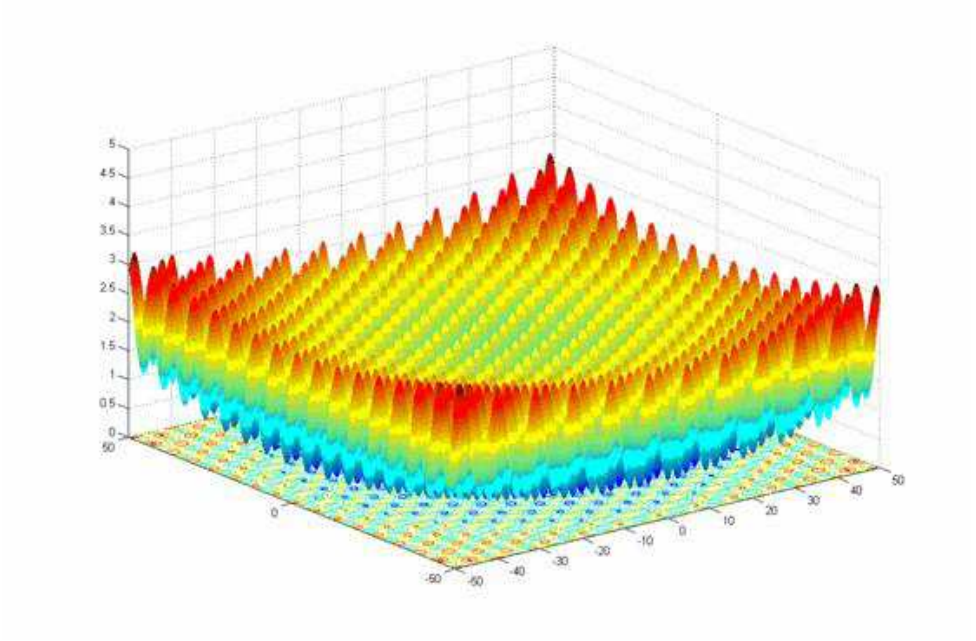


Figure F.5: The Griewank's function f_{11} for $n = 2$.

- the generalized penalized functions f_{12} and f_{13} are defined as

$$f_{12}(x) \equiv \frac{\pi}{30}\left[10\sin^2(\pi\, y_1) + \sum_{i=1}^{n-1}(y_i-1)^2(1+10\sin^2(\pi\, y_{i+1})) + (y_n-1)^2\right], \tag{F.12a}$$

$$x_i \in [-50,+50]\,, \qquad x_i^* = -1\,, \qquad f_{12}(x^*) = 0\,, \tag{F.12b}$$

$$u(x,a,k,m) = \begin{cases} k(x-a)^m\,, & x > a\,, \\ 0\,, & -a \le x \le a\,, \\ k(-x-a)^m\,, & -a > x\,, \end{cases} \qquad y_i = 1 + \frac{x_i+1}{4}\,, \tag{F.12c}$$

and

$$f_{13}(x) \equiv \frac{1}{10}\Big[10\sin^2(3\pi\, x_1) + \sum_{i=1}^{n-1}(x_i-1)^2(1+\sin^2(3\pi\, x_{i+1})) + (x_n-1)^2(1+\sin^2(2\pi\, x_n))\Big], \tag{F.13a}$$

$$x_i \in [-500,+500]\,, \qquad x_i^* = 1\,, \qquad f_{13}(x^*) = 0\,. \tag{F.13b}$$

- The function f_{14} corresponds to Ackley's function [59] that reads

$$f_{14}(x) \equiv -20\exp\left[-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n}x_i^2}\right] - \exp\left[\frac{1}{n}\sum_{i=1}^{n}\cos(2\pi\, x_i)\right] + 20 + e\,, \tag{F.14a}$$

$$x_i \in [-32,+32]\,, \qquad x_i^* = 0\,, \qquad f_{14}(x^*) = 0\,. \tag{F.14b}$$

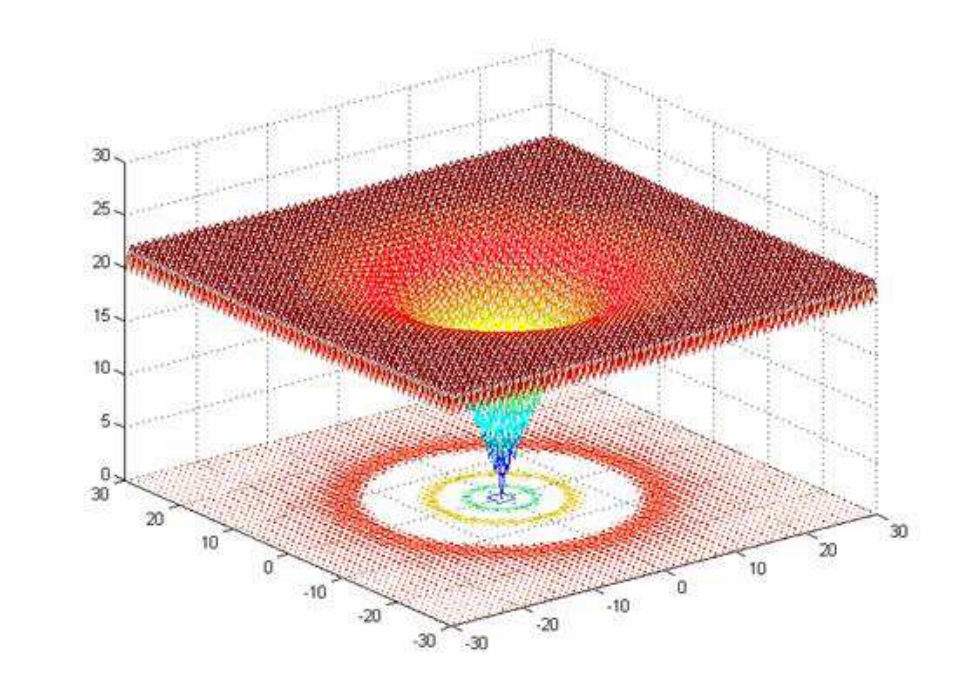


Figure F.6: The Ackley's function f_{14} for $n = 2$.

- The function f_{15} is Easom's function defined in two dimension, i.e.

$$f_{15}(x) \equiv -\cos(x_1)\,\cos(x_2)\,\exp[-(x_1-\pi)^2-(x_2-\pi)^2]\,, \tag{F.15a}$$

$$x_i \in [-100,+100]\,, \qquad x_i^* = \pi\,, \qquad f_{15}(x^*) = -1\,. \tag{F.15b}$$

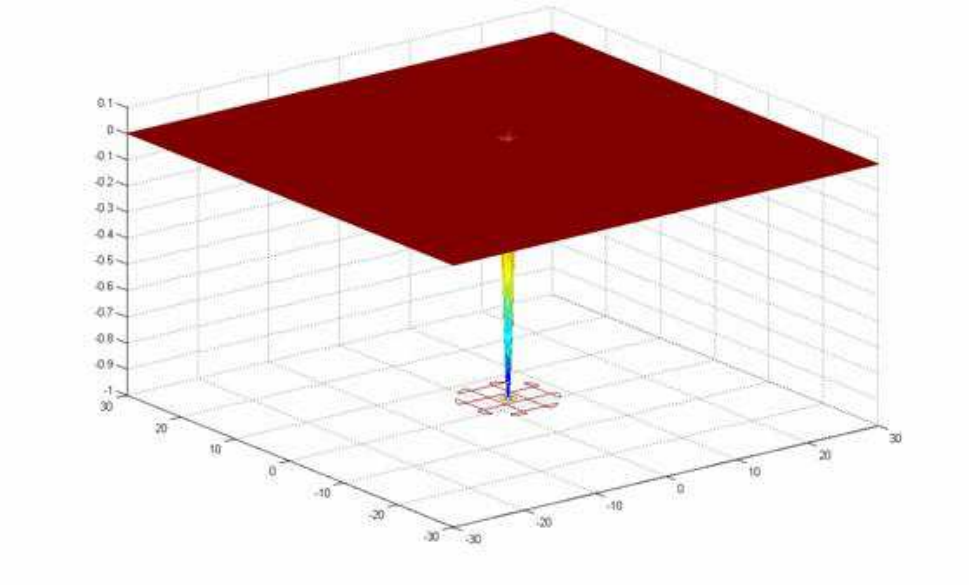


Figure F.7: The Easom's function f_{15}.

F.1.3 Multimodal functions with few local optima

- The function f_{16} is defined as Hump's "camel back" function, which posseses two global optima in two dimension, i.e.

$$f_{16}(x) \equiv \left(4 - 2.1x_2^2 + \frac{x_1^4}{3}\right) x_1^2 + x_1\, x_2 + (4x_2^2 - 4)x_2^2\,, \tag{F.16a}$$

$$x_i \in [-5, +5]\,, \tag{F.16b}$$

$$x^* = [0.089842(...), -0.712656(...)], [-0.089842(...), 0.712656(...)]\,, \tag{F.16c}$$

$$f_{15}(x^*) = -\,1.031628453(...)\,. \tag{F.16d}$$

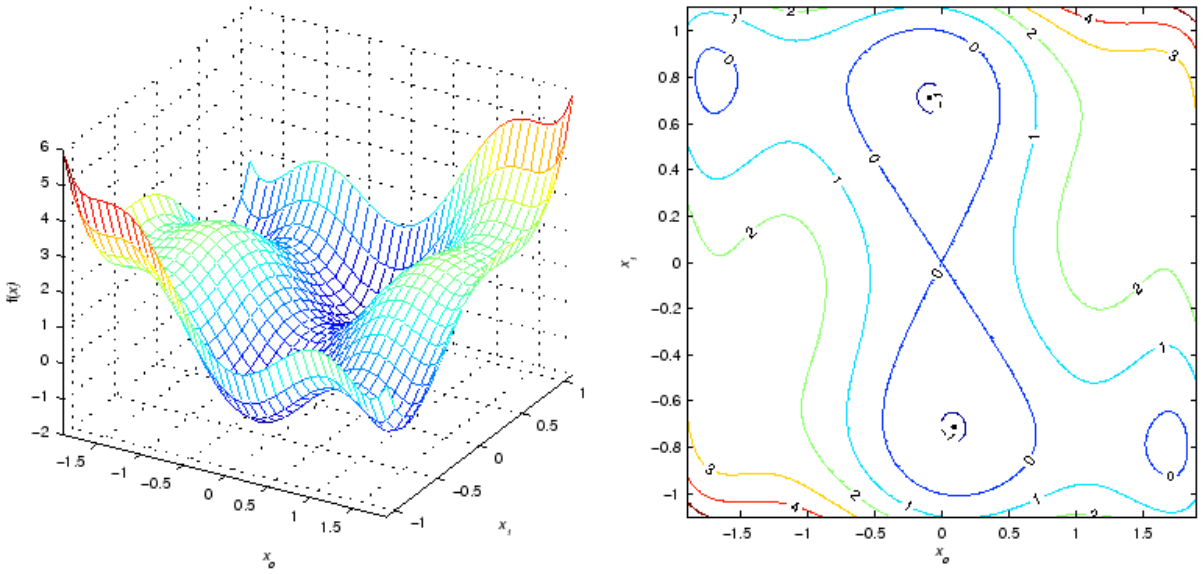


Figure F.8: The Hump's function f_{16}.

- The function f_{17} is Branin's function, which posseses three global optima in two dimension, i.e.

$$f_{17}(x) \equiv \left(x_2 - \frac{5.1}{4\pi^2}x_1^2 + \frac{5}{\pi}x_1 - 6\right)^2 + 10\left(1 - \frac{1}{8\pi}\right)\cos(x_1) + 10\,, \tag{F.17a}$$

$$x_1 \in [-5, +10]\,, \qquad x_2 \in [0, +15]\,, \tag{F.17b}$$

$$x^* = [-\pi, 12.275(...)], [\pi, 2.275(...)], [9.4278(...), 2.475(...)]\,, \tag{F.17c}$$

$$f_{17}(x^*) = 0.397887346(...)\,. \tag{F.17d}$$

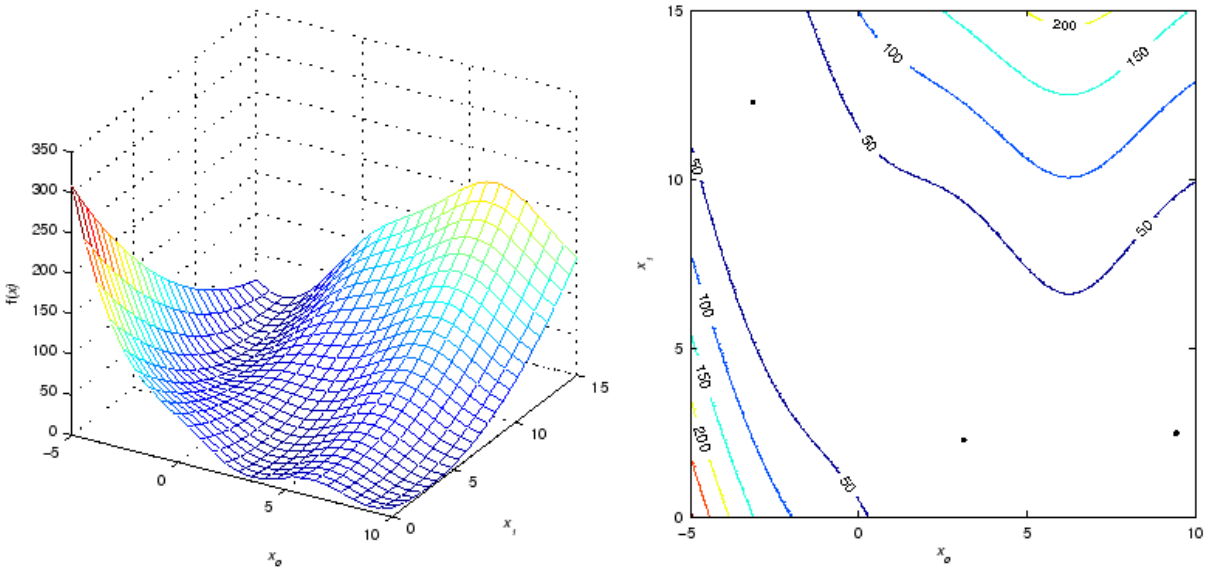


Figure F.9: The Branin's function f_{17}.

- The functions f_{18}, f_{19} and f_{20} corresponds to Shekel's foxhole functions in four dimension [60], for $m = 5$, 7 and 10, respectively, where

$$f_{17/18/19}(x) \equiv -\sum_{i=1}^{m} \frac{1}{\sum_{j=1}^{4}(x_j - a_{ij})^2 + c_i}\,, \tag{F.18a}$$

$$x_i \in [-10, +10]\,, \qquad x^* = [4, 4, 4, 4]\,, \tag{F.18b}$$

$$f_{17}(x^*) = -\,10.1422(...)\,, \qquad f_{18}(x^*) = -10.3909(...)\,, \qquad f_{19}(x^*) = -10.5300(...)\,. \tag{F.18c}$$

where the various coefficients are defined in Tab. {F.1}.

i	1	2	3	4	5	6	7	8	9	10
a_{i1}	4	1	8	6	3	2	5	8	6	7
a_{i2}	4	1	8	6	7	9	5	1	2	3.6
a_{i3}	4	1	8	6	3	2	3	8	6	7
a_{i4}	4	1	8	6	7	9	3	1	2	3.6
c_i	0.1	0.2	0.2	0.4	0.4	0.6	0.3	0.7	0.5	0.5

Table F.1: Parameters of the Shekel's modified foxhole functions.

- The function f_{21} is another class of two-dimension Shekel's function that reads

$$f_{21}(x) \equiv \left[\frac{1}{500} + \sum_{j=1}^{25}\left(j + (x_1 - a_{1j})^6 + (x_2 - a_{2j})^6\right)^{-1}\right]^{-1}\,, \tag{F.19a}$$

$$x_i \in [-65, +65]\,, \qquad x_i^* = -32\,, \qquad f_{21}(x^*) \approx 1\,, \tag{F.19b}$$

where the various coefficients are defined in Tab. {F.2}

i	1	2	3	4	5	6	7	8	9	10
a_{1i}	−32	−16	0	16	32	−32	−16	0	16	32
a_{2i}	−32	−32	−32	−32	−32	−16	−16	−16	−16	−16
i	11	12	13	14	15	16	17	18	19	20
a_{1i}	−32	−16	0	16	32	−32	−16	0	16	32
a_{2i}	0	0	0	0	0	16	16	16	16	16
i	21	22	23	24	25					
a_{1i}	−32	−16	0	16	32					
a_{2i}	32	32	32	32	32					

Table F.2: Parameters of the Shekel's alternative foxhole function.

- The function f_{22} is defined as Kowalik's function in four dimension [61] and reads

$$f_{22}(x) \equiv \sum_{i=1}^{11} \left[a_i - \frac{x_1(b_i^2 + b_i\, x_2)}{b_i^2 + b_i\, x_3 + x_4} \right]^2 , \tag{F.20a}$$

$$x_i \in [-5, +5] , \qquad x^* = [0.1928(...), 0.1908(...), 0.1231(...), 0.1358(...)] , \tag{F.20b}$$

$$f_{22}(x^*) = 0.0003075(...) , \tag{F.20c}$$

where the various coefficients are defined in Tab. {F.3}

i	a_i	$1/b_i$
1	0.1957	0.25
2	0.1947	0.5
3	0.1735	1
4	0.1600	2
5	0.0844	4
6	0.0627	6
7	0.0456	8
8	0.0342	10
9	0.0323	12
10	0.0235	14
11	0.0246	16

Table F.3: Parameters of the Kowalik's function.

F.2 Random surface generator

As explained in the main document, the computation of theoretical error bars using the bootstrap algorithm requires the construction of smooth random surfaces $\mathcal{R}$ in the interval $[-1, +1]$ that allows to compute variations of $V_{\mathrm{low}\,k}$ within a given tolerance around an initial input, i.e. such that

$$\forall\, i, j = 1 \ldots N , \qquad \langle \mathcal{R}(k_i, k_j) \rangle = 0 , \qquad \mathrm{Var}\left[\mathcal{R}(k_i, k_j)\right] = 0 . \tag{F.21}$$

We have devised a simple method to construct such functions in the case of a **regular** mesh $X_i = X_0 + (i-1)\Delta_X$.

F.2.1 One-dimension case

The idea consists in computing at each bin a uniform random value α in $[0,1)$, then convoluting it with the values obtained for all neighbors using an effective range function. Thus we define

$$\forall\, i = 1 \dots N\,, \qquad \alpha(X_i) = U(0,1)\,, \tag{F.22a}$$

$$\beta(X_i) \equiv \sum_{j=1}^{N} \alpha(X_j)\, f_{K\sigma}(X_i, X_j)\,, \tag{F.22b}$$

$$f_{K\sigma}(X_i, X_j) \equiv \exp\left[-\left(\frac{X_i - X_j}{\sigma}\right)^2\right] \Theta(|X_i - X_j| - K)\,, \tag{F.22c}$$

$$\gamma(X_i) \equiv 2\left(\frac{\beta(X_i)}{\beta_{\max}(X_i)}\right) - 1\,, \qquad \beta_{\max}(X_i) \equiv \sum_{j=1}^{N} f_{K\sigma}(X_i, X_j)\,, \tag{F.22d}$$

where $f_{K\sigma}$ is taken as a gaussian smoothing function. The former definition allows the random drawings at two separate bins to interact with each other. The γ curve verifies then for each i

$$\begin{aligned}\langle\gamma(X_i)\rangle =& 2\left(\frac{\langle\beta(X_i)\rangle}{\beta_{\max}(X_i)}\right) - 1 = \frac{2}{\beta_{\max}(X_i)}\left(\sum_{j=1}^{N}\langle\alpha(X_j)\rangle\, f_{K\sigma}(X_i, X_j)\right) - 1 \\ =& \frac{2}{\beta_{\max}(X_i)}\frac{\beta_{\max}(X_i)}{2} - 1 = 0\,.\end{aligned} \tag{F.23}$$

Finally, one renormalizes γ into a distribution of variance $1/4$, such that in average the random variable

$$\forall\, i = 1 \dots N\,, \qquad \mathcal{R}(X_i) \equiv \frac{\gamma(X_i)}{4\sqrt{\mathrm{Var}\,[\gamma(X_i)]}}\,, \tag{F.24}$$

remains most of the time in the interval $[-1,+1]$, using the property that a random variable almost never deviates over twice its standard deviation, by analogy with the normal distribution. Finally, we evaluate

$$\begin{aligned}\mathrm{Var}\,[\gamma(X_i)] &= \left(\frac{2}{\beta_{\max}(X_i)}\right)^2 \mathrm{Var}\,[\beta(X_i)] \\ &= \left(\frac{2}{\beta_{\max}(X_i)}\right)^2 \left(\sum_{j=1}^{N} \mathrm{Var}\,[\alpha(X_j)]\; f_{K\sigma}^2(X_i, X_j)\right) \\ &= \frac{1}{3\,\beta_{\max}^2(X_i)} \sum_{j=1}^{N} f_{K\sigma}^2(X_i, X_j)\,,\end{aligned} \tag{F.25}$$

using the fact that the random variables $\alpha(X_i)$ and $\alpha(X_j)$ are decorrelated for $i \neq j$, and

$$\mathrm{Var}\,[U(0,1)] = \frac{1}{12}\,. \tag{F.26}$$

Results are presented in Fig. F.10 for $\sigma = 0.1$, $K = 0.5$ and a mesh of 50 points equally spaced in $[0, 2.6]$[1]. We consider different cases, i.e.

[1] Obviously we have in mind the application of this method for realistic calculations where the mesh is defined in momentum space. These values for σ and K correspond to a good compromise for practical applications with no brutal variations of $\mathcal{R}$.

1. one random drawing of α in $[0, 1)$,
2. distribution of α according to a step function,
3. distribution of α where all values except one are zero,
4. large number of random drawings.

While the first three situations probe different regimes of the algorithm, the last one allows to compute the distribution of $\mathcal{R}(X_i)$ for each i.

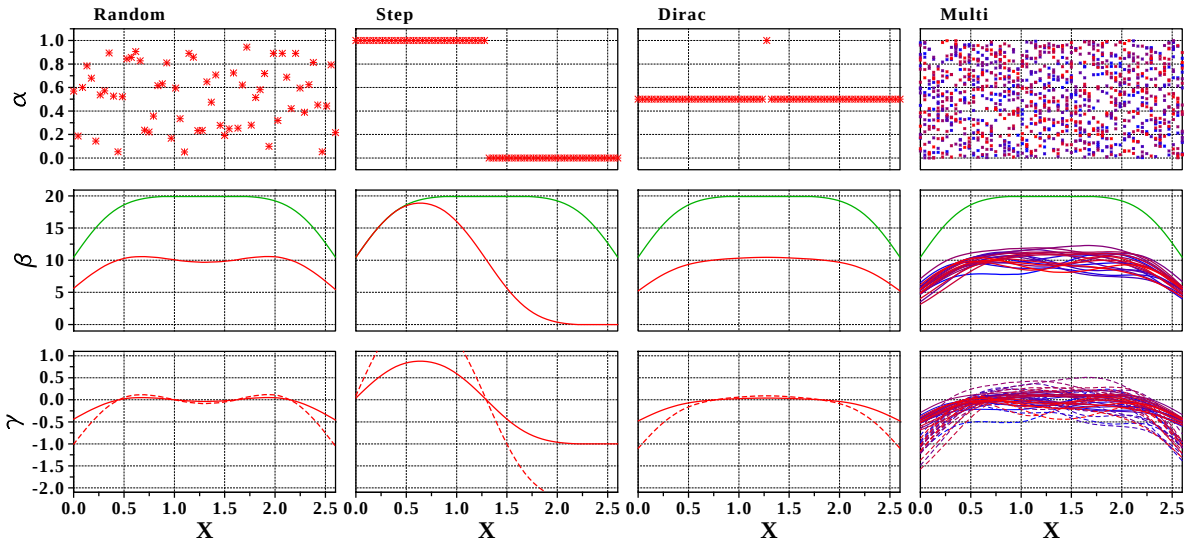


Figure F.10: Generation of random curves in one dimension for different cases presented in the text. The green curve presents the value of $\beta_{\max}(X_i)$, while in the lower panels solid and dashed lines correspond to γ and $\mathcal{R}$, respectively.

We find that using simple algorithm leads to a biaised definition of $\mathcal{R}$, as shown in Fig. F.11 on the distribution of $\mathcal{R}(X_i)$ at different points. Indeed (i) the distribution of $\mathcal{R}(X_{N/2})$ is of mean zero and variance one, but (ii) for $i = 1$ or $i = N$, it is of variance one but is not centered. This unwanted property corresponds to the fact that β is statistically more likely to reach β_{max} at the boundaries of the problem, where only one half of the mesh is fully weighted by the effective range function $f_{K\sigma}$. A signature of such a problem is the non-constant value of $\beta_{\max}$ over the mesh.

The solution consists in considering extra points below X_1 and over X_N, i.e. a mesh $\{X'\}$ which verifies

$$\forall i = 1 \dots N\,,\ X'_i = X_i\,, \qquad \forall j\,,\ X'_{j+1} - X'_j = \Delta_X\,, \tag{F.27}$$

such that $\beta_{\max}(X_i) \equiv \beta_{\max}$, as well as $\mathrm{Var}\,[\gamma(X_i)] \equiv \mathrm{Var}\,[\gamma]$, are independent of X_i[2]. One has then

$$\forall\, i = 1 \dots N\,, \qquad \alpha(X_i) = U(0,1)\,, \tag{F.28a}$$

$$\beta(X_i) \equiv \sum_{j=-\infty}^{+\infty} \alpha(X'_j)\, f_{K\sigma}(X_i, X'_j)\,, \tag{F.28b}$$

$$\gamma(X_i) \equiv 2\left(\frac{\beta(X_i)}{\beta_{\max}}\right) - 1\,, \tag{F.28c}$$

[2]This justifies the use of the Θ function in the expression of $f_{K\sigma}$, which defines K as the maximum range of the smoothing.

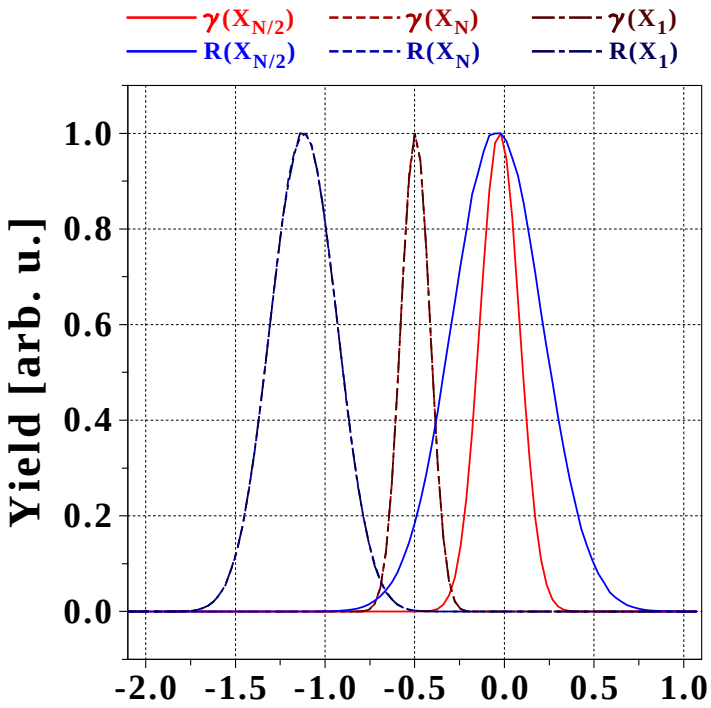


Figure F.11: Distributions of $\gamma(X_i)$ and $\mathcal{R}(X_i)$ at different positions.

$$\mathcal{R}(X_i) \equiv \frac{\gamma(X_i)}{4\sqrt{\mathrm{Var}\,[\gamma]}}\,, \tag{F.28d}$$

$$\forall j_0\,, \qquad \beta_{\max} \equiv \sum_{j=-\infty}^{+\infty} f_{K\sigma}(X'_{j_0}, X'_j)\,, \tag{F.28e}$$

$$\mathrm{Var}\,[\gamma] = \frac{1}{3\,\beta_{\max}^2} \sum_{j=-\infty}^{+\infty} f_{K\sigma}^2(X'_{j_0}, X'_j)\,, \tag{F.28f}$$

Results for this so-called *unbiased* case are presented in FIGS. (F.12,F.13). One sees immediately that (i) $\beta_{\max}$ is indeed independent of X in the area of interest (between the blue lines), (ii) the distribution of $\mathcal{R}$ is also independent of X and corresponds at each point to a random variable of mean zero and variance one, i.e. $\mathcal{R}$ is indeed a "random curve" in $[-1, +1]$ (in average).

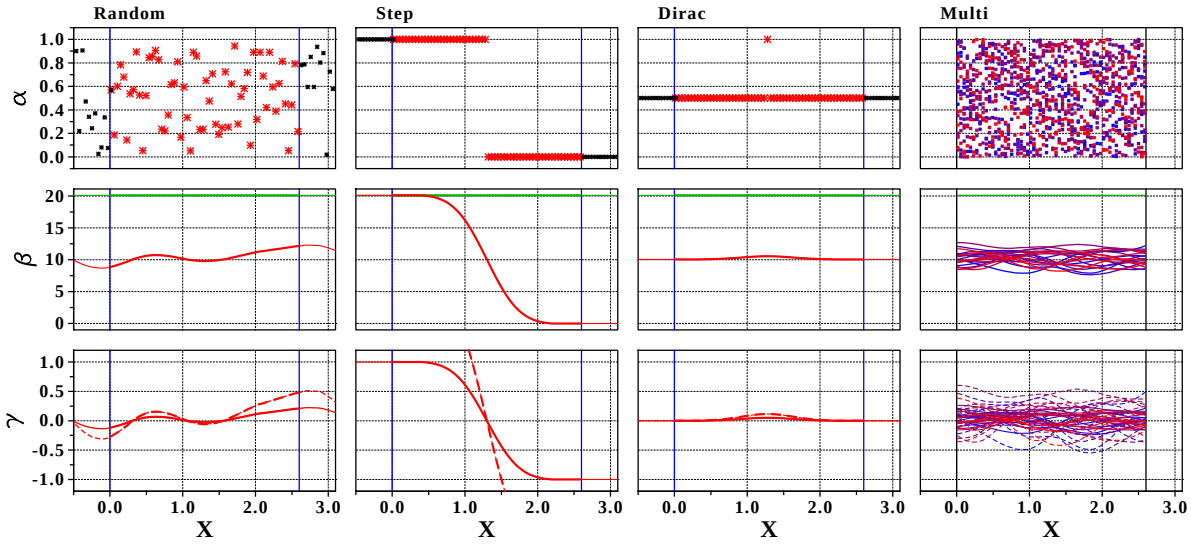


Figure F.12: Same as in FIG. F.10 in the unbiased case. Only values between the blue lines are actually considered in the end, other bins are only in intermediate steps of the generator.

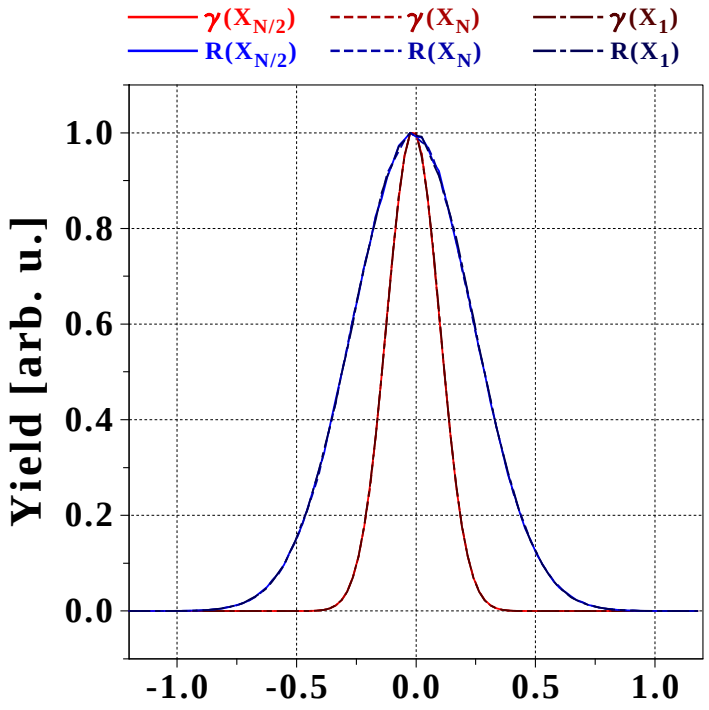


Figure F.13: Same as in FIG. F.11 in the unbiased case.

F.2.2 Two-dimension case

The generalization of the previous algorithm for the two-dimension case, after all biases are removed, reads then easily

$$\forall\, i,j = 1 \dots N\,, \qquad \alpha(X_i, X_j) = U(0,1)\,, \tag{F.29a}$$

$$\beta(X_i, X_j) \equiv \sum_{k=-\infty}^{+\infty} \sum_{\ell=-\infty}^{+\infty} \alpha(X'_k, X'_\ell)\, f_{K\sigma}(X_i, X'_k)\, f_{K\sigma}(X_j, X'_\ell)\,, \tag{F.29b}$$

$$\gamma(X_i, X_j) \equiv 2\left(\frac{\beta(X_i, X_j)}{\beta_{\max}}\right) - 1\,, \tag{F.29c}$$

$$\mathcal{R}(X_i, X_j) \equiv \frac{\gamma(X_i, X_j)}{4\sqrt{\mathrm{Var}\,[\gamma]}}\,, \tag{F.29d}$$

$$\forall k_0, \ell_0\,, \qquad \beta_{\max} \equiv \sum_{k=-\infty}^{+\infty} \sum_{\ell=-\infty}^{+\infty} f_{K\sigma}(X'_{k_0}, X'_k)\, f_{K\sigma}(X'_{\ell_0}, X'_\ell)$$

$$= \left(\sum_{k=-\infty}^{+\infty} f_{K\sigma}(X'_{k_0}, X'_k)\right)^2\,, \tag{F.29e}$$

$$\mathrm{Var}\,[\gamma] = \frac{1}{3\,\beta_{\max}^2} \left(\sum_{k=-\infty}^{+\infty} f_{K\sigma}^2(X'_{k_0}, X'_k)\right)^2\,. \tag{F.29f}$$

Results are presented in Figs. (F.14,F.15) for equivalent cases as in the previous section[3]. For large number of samplings one sees that the distribution of $\mathcal{R}(X_i, X_j)$ is also independent of X_i and X_j and corresponds at each point to a random variable of mean zero and variance one, i.e. $\mathcal{R}$ is indeed a "random surface" in $[-1, +1]$ (in average).

[3] The "Dirac" case corresponds to all values are zero except in a small region.

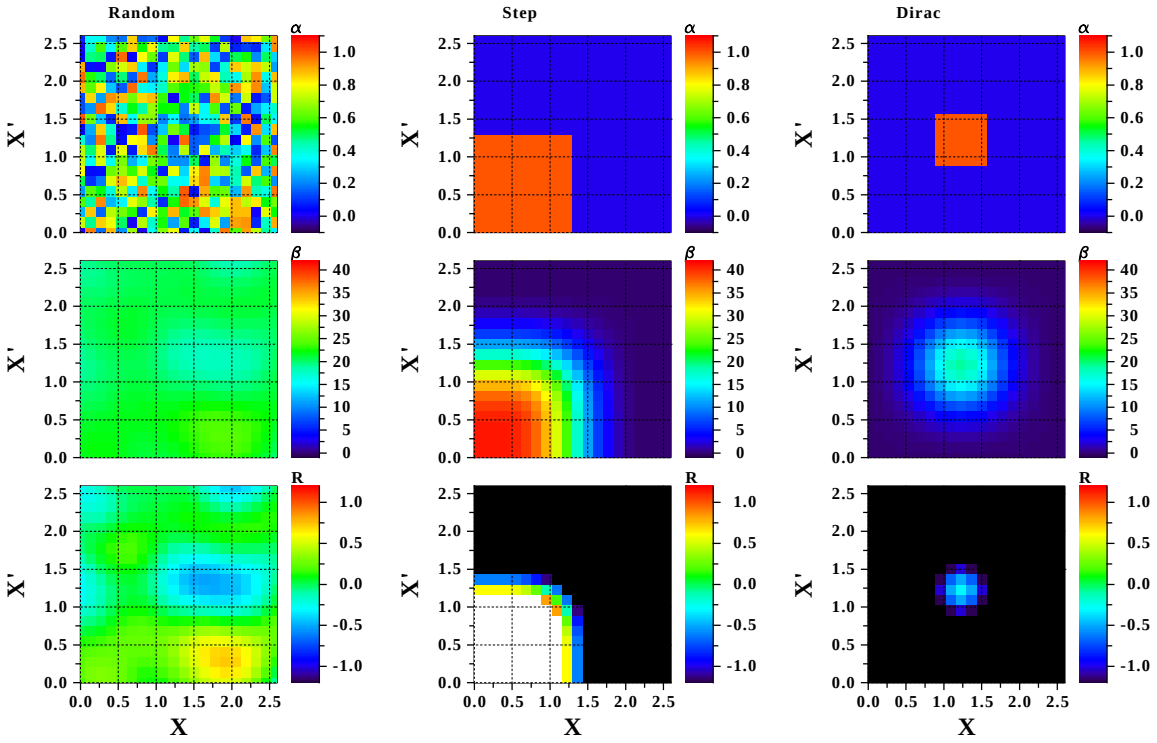


Figure F.14: Generation of unbiased random curves in two dimensions for different cases presented in the text. from top to bottom are displayed surface plots of α, β and $\mathcal{R}$.

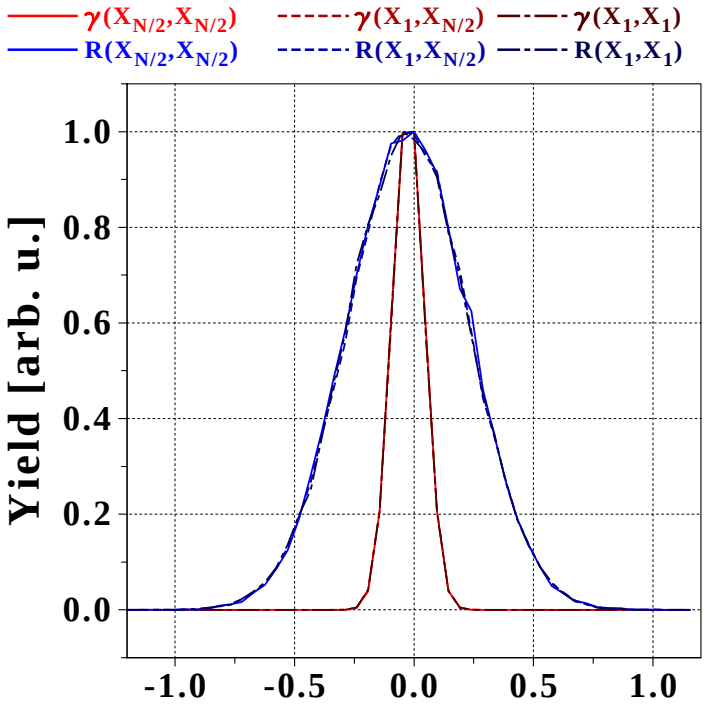


Figure F.15: Distributions of $\gamma(X_i)$ and $\mathcal{R}(X_i)$ at different positions.

Bibliography

[1] A. R. Edmonds: *Angular Momentum in Quantum Mechanics* (Princetown University Press, Princetown, NJ, 1957)

[2] D. A. Varshalovich, A. N. Moskalev and V. K. Khersonsky: *Quantum Theory of Angular Momentum: Irreducible tensors, spherical harmonics, vector coupling coefficients, 3NJ Symbols* (World Scientific, Singapore, 1988)

[3] M. Abramowitz and I. Stegun: *Handbook of Mathematical Functions* (Dover, New York, 1965)

[4] J. Winter: *Tensor spherical harmonics*. Lett. Math. Phys. **6** (1982) 91–96

[5] A. L. Goodman: *Self-consistent symmetries of the Hartree-Fock-Bogoliubov equations in a rotating frame*. Nucl. Phys. **A230** (1974) 466–476

[6] J. Dobaczewski, H. Flocard and J. Treiner: *Hartree-Fock-Bogolyubov description of nuclei near the neutron-drip line*. Nucl. Phys. **A422** (1984) 103–139

[7] C. Bloch and A. Messiah: *The canonical form of an antisymmetric tensor and its application to the theory of superconductivity*. Nucl. Phys. **39** (1962) 95–106

[8] B. Zumino: *Normal Forms of Complex Matrices*. J. Math. Phys. **3** (1962) 1055–1057

[9] J. Dobaczewski: *Generalization of the Bloch-Messiah-Zumino theorem*. Phys. Rev. C **62** (2000) 017301. arXiv:math-ph/0002034

[10] J. Escher, B. K. Jennings and H. S. Sherif: *Spectroscopic amplitudes and microscopic substructure effects in nucleon capture reactions*. Phys. Rev. C **64** (2001) 065801. arXiv:nucl-th/0107011

[11] A. E. L. Dieperink and T. de Forest, Jr.: *Center-of-mass effects in single-nucleon knock-out reactions*. Phys. Rev. C **10** (1974) 543–549

[12] B. K. Jennings: *Low energy behavior of the $^7Be(p,\gamma)^8B$ reaction*. Phys. Rev. C **62** (2002) 027602

[13] A. V. Shebeko, P. Papakonstantinou and E. Mavrommatis: *The one-body and two-body density matrices of finite nuclei with an appropriate treatment of the center-of-mass motion*. Eur. Phys. J. A **27** (2006) 143–155. arXiv:nucl-th/0602056

[14] D. Van Neck, A. E. L. Dieperink and M. Waroquier: *Natural orbitals, overlap functions, and mean-field orbitals in an exactly solvable A-body system*. Phys. Rev. C **53** (1996) 2231–2242

[15] D. Van Neck and M. Waroquier: *Single-particle properties in self-bound systems*. Phys. Rev. C **58** (1998) 3359–3367

[16] C. F. Clément: *Theory of overlap functions (I). Single particle sum rules and centre-of-mass corrections*. Nucl. Phys. **A213** (1973) 469–492

[17] C. F. Clément: *Theory of overlap functions (II). The overlap representation*. Nucl. Phys. **A213** (1973) 493–509

[18] D. Van Neck, M. Waroquier, A. E. L. Dieperink, S. C. Pieper and V. R. Pandharipande: *Center-of-mass effects on the quasi-hole spectroscopic factors in the $^{16}O(e,e'p)$ reaction*. Phys. Rev. C **57** (1998) 2308–2315. arXiv:nucl-th/9804067

[19] D. Van Neck, M. Waroquier and K. Heyde: *On the relationship between single-particle overlap functions, natural orbitals and the one-body density matrix for many-fermion systems.* Phys. Lett. B **314** (1993) 255–259

[20] A. Faessler, S. Krewald and G. J. Wagner: *Is there evidence of three-body forces from violation of the Koltun energy sum rule?* Phys. Rev. C **11** (1975) 2069–2072

[21] D. S. Koltun: *Total Binding Energies of Nuclei, and Particle-Removal Experiments.* Phys. Rev. Lett. **28** (1972) 182–185

[22] C. M. Shakin and M. S. Weiss: *Translationally invariant self-consistent field theories.* Phys. Rev C **15** (1977) 1911–1916

[23] D. Van Neck: *Priv. comm.*

[24] J. Engel: *Intrinsic-Density Functionals.* Phys. Rev. C **75** (2007) 014306. arXiv:nucl-th/0610043

[25] D. S. Lewart, V. R. Pandharipande and S. C. Pieper: *Single-particle orbitals in liquid-helium drops.* Phys. Rev. B **37** (1988) 4950–4964

[26] G. E. Brown and A. D. Jackson: *The nucleon-nucleon interaction* (North-Holland, Amsterdam, 1976)

[27] M. A. Morrison and A. N. Feldt: *Through scattering theory with gun and camera: Coping with conventions in collision theory.* Am. J. Phys. **75** (2007) 67–80

[28] B. A. Lippmann and J. Schwinger: *Variational Principles for Scattering Processes. I.* Phys. Rev. **79** (1950) 469–480

[29] L. A. L. Roriz and A. Delfino: *S-matrix pole trajectories for Yukawa potentials.* Phys. Rev. C **38** (1988) 607–610

[30] J. M. Blatt and L. C. Biedenharn: *Neutron-Proton Scattering with Spin-Orbit Coupling. I. General Expressions.* Phys. Rev. **86** (1952) 399–404

[31] H. P. Stapp, T. J. Ypsilantis and N. Metropolis: *Phase-Shift Analysis of 310-Mev Proton-Proton Scattering Experiments.* Phys. Rev. **105** (1957) 302–310

[32] G. J. M. Austen and J. J. de Swart: *An improved Coulomb potential.* Phys. Rev. Lett. **50** (1983) 2039–2042

[33] V. G. J. Stoks and J. J. De Swart: *The Magnetic moment interaction in nucleon-nucleon phase shift analyses.* Phys. Rev. C **42** (1990) 1235–1248

[34] E. A. Uehling: *Polarization effects in the positron theory.* Phys. Rev. **48** (1935) 55–63

[35] L. Durand III: *Vacuum Polarization Effects in Proton-Proton Scattering.* Phys. Rev. **108** (1957) 1597–1610

[36] E. Epelbaum, W. Glöckle and U.-G. Meißner: *The two-nucleon system at next-to-next-to-next-to-leading order.* Nucl. Phys. **A747** (2005) 362–424. arXiv:nucl-th/0405048

[37] M. J. Seaton: *Coulomb functions for attractive and repulsive potentials and for positive and negative energies.* Comp. Phys. Comm. **146** (2002) 226–249

[38] N. Michel: *Precise Coulombnext term wave functions for a wide range of complex ℓ, η and z.* Comp. Phys. Comm. **176** (2006) 232–249

[39] C. M. Vincent and S. C. Phatak: *Accurate momentum-space method for scattering by nuclear and Coulomb potentials.* Phys. Rev. C **10** (1974) 391–394

[40] M. Walzl and U.-G. Meißner: *Elastic electron deuteron scattering in chiral effective field theory.* Phys. Lett. B **513** (2001) 37–45. arXiv:nucl-th/0103020

[41] J. R. Bergervoet, P. C. van Campen, W. A. van der Sanden and J. J. de Swart: *Phase shift analysis of 0-30 MeV pp scattering data.* Phys. Rev. C **38** (1988) 15–50

[42] L. L. Foldy and E. Eriksen: *Vacuum Polarization and Proton-Proton Scattering.* Phys. Rev. **98** (1955) 775–779

[43] J. Schwinger: . Phys. Rev. **72** (1947) 742

[44] H. A. Bethe: *Theory of the Effective Range in Nuclear Scattering.* Phys. Rev. **76** (1949) 38–50

[45] G. Breit, E. U. Condon and R. D. Present: *Theory of Scattering of Protons by Protons.* Phys. Rev. **50** (1936) 825–845

[46] L. Landau: *On the energy loss of fast particles by ionization.* J. Phys. (USSR) **8** (1944) 201–205

[47] G. Breit: *Relativistic Corrections for High-Energy p-p Scattering.* Phys. Rev. **99** (1955) 1581–1596

[48] L. Heller: *Proton-Proton Effective-Range Theory with Vacuum Polarization.* Phys. Rev. **120** (1960) 627–634

[49] W. A. van der Sanden, A. H. Emmen and J. J. de Swart: *Report No. THEF-NYM-83.11, Nijmegen* (1983). Unpublished

[50] D. Gogny: In J. de Boer and H. J. Mang (Editors), *Proceedings of the International Conference on Nuclear Physics.* Madrid (North-Holland, Amsterdam, 1973) p. 48

[51] D. Gogny: In G. Ripka and M. Porneuf (Editors), *Proceedings of the International Conference on Nuclear Self-Consistent fields.* International Center for Theoretical Physics, Trieste (North-Holland, Amsterdam, 1975) p. 333

[52] J. Dechargé and D. Gogny: *Hartree-Fock-Bogolyubov calculations with the D1 effective interaction on spherical nuclei.* Phys. Rev. C **21** (1980) 1568–1593

[53] J.-F. Berger, M. Girod and D. Gogny: *Time-dependent quantum collective dynamics applied to nuclear fission.* Comp. Phys. Comm. **63** (1991) 365–374

[54] F. Chappert: *Nouvelles paramétrisations de l'interaction nucléaire effective de Gogny* (2007). Ph.D. Thesis

[55] K. DeJong: *An Analysis of the Behavior of a Class of Genetic Adaptative Systems* (1975). Ph.D. Thesis

[56] H.-P. Schwefel: *Numerical Optimization of Computer Models* (Wiley, New York, NY, 1981)

[57] Y.-W. Shang and Y.-H. Qiu: *A Note on the Extended Rosenbrock Function.* Evol. Comp. **14** (2006) 119–126

[58] H. Mühlenbein, M. Schomisch and J. Born: *The parallel genetic algorithm as function optimizer.* Parallel Comp. **17** (1991) 619–632

[59] D. H. Ackley: *A connectionist machine for genetic hillclimbing* (Kluwer Academic Publishers, Boston, MA, 1987)

[60] H. Bersini, M. Dorigo, S. Langerman, G. Geront and L. Gambardella: *Results of the First International Contest on Evolutionary Optimisation (1st ICEO).* In *Proceedings of the 2^{nd} IEEE International Conference on Evolutionary Computation* (IEEE Press, 1996) pp. 611–615

[61] J. Kowalik and J. F. Morrison: *Analysis of kinetic data for allosteric enzyme reactions as a nonlinear regression problem.* Math. Biosci. **2** (1968) 57–66

Résumé

La méthode de la fonctionnelle de la densité d'énergie (EDF) est un outil de choix pour l'étude de la structure nucléaire à basse énergie, car elle permet des calculs de noyaux finis aussi bien pour des systèmes stables connus expérimentalement dont les propriétés sont reproduites avec une bonne précision, que pour des noyaux qui ne peuvent encore être produits mais sont prédits théoriquement. Dans la première partie de cette thèse, une nouvelle méthode quantitative est introduite pour caractériser l'existence et les propriétés des halos dans les noyaux moyens et lourds, ainsi que pour étudier l'impact des corrélations d'appariement ou du choix de la fonctionnelle d'énergie sur leur formation. Il apparait que la solidité de ces résultats est limitée par le faible pouvoir prédictif des fonctionnelles utilisées jusqu'à présent qui sont ajustées sur des données expérimentales. Dans la seconde partie de ce mémoire, nous entreprenons la construction de fonctionnelles non-empiriques qui reposent sur un nouveau paradigme pour les forces nucléon-nucléon dans le vide, à savoir les interactions *low-momentum* engendrées par l'application des méthodes du groupe de renormalisation. Ces potentiels à cœur mou sont utilisés comme point de départ d'une stratégie à long terme faisant le lien entre les techniques modernes de résolution du problème à N corps et les méthodes EDF. Nous donnons ainsi des perspectives pour construire différentes réalisations d'un modèle non-empirique d'interaction $v_{\mathrm{BDRS}}^{[\mathrm{X}]}$ incluant les effets de milieu à différents niveaux d'approximation et pouvant être traité dans les codes dédiés à la structure nucléaire. Dans ce mémoire, la première étape de ce travail est initiée par l'ajustement d'une représentation opératorielle des forces *low-momentum* dans le vide réalisé au moyen d'un algorithme parallèle d'intelligence artificielle. Les premiers résultats mettent en valeur la possibilité d'incorporer la physique nécessaire à la structure de basse énergie dans ce vertex gaussien.

Abstract

The energy density functional (EDF) formalism is the tool of choice for large-scale low-energy nuclear structure calculations both for stable experimentally known nuclei whose properties are accurately reproduced and systems that are only theoretically predicted. We highlight in the present dissertation the capability of EDF methods to tackle exotic phenomena appearing at the very limits of stability, that is the formation of nuclear halos. We devise a new quantitative and model-independent method that characterizes the existence and properties of halos in medium- to heavy-mass nuclei, and quantifies the impact of pairing correlations and the choice of the energy functional on the formation of such systems. These results are found to be limited by the predictive power of currently-used EDFs that rely on fitting to known experimental data. In the second part of this dissertation, we initiate the construction of non-empirical EDFs that make use of the new paradigm for vacuum nucleon-nucleon interactions set by so-called low-momentum interactions generated through the application of renormalization group techniques. These soft-core vacuum potentials are used as a stepstone of a long-term strategy which connects modern many-body techniques and EDF methods. We provide guidelines for designing several non-empirical models $v_{\mathrm{BDRS}}^{[\mathrm{X}]}$ that include in-medium many-body effects at various levels of approximation, and can be handled in state-of-the art nuclear structure codes. In the present work, the first step is initiated through the adjustement of an operatorial representation of low-momentum vacuum interactions using a custom-designed parallel evolutionary algorithm. The first results highlight the possibility to grasp most of the relevant physics for low-energy nuclear structure using this numerically convenient gaussian vertex.