1 Minnesota potential

Antisymmetrized Minnesota potential is

$$\widetilde{V}(\vec{r}_1,\vec{r}_2) = \left[\hat{V}_R(\vec{r}_1,\vec{r}_2) + \tfrac{1}{2}(1+\hat{P}_\sigma)\hat{V}_t(\vec{r}_1,\vec{r}_2) + \tfrac{1}{2}(1-\hat{P}_\sigma)\hat{V}_s(\vec{r}_1,\vec{r}_2)\right] \times \tfrac{1}{2}(1+\hat{P}_r)(1-\hat{P}_\sigma\hat{P}_r) \tag{1}$$

where $\hat{P}_\sigma$ is spin-exchange and $\hat{P}_r$ space-exchange operator. The parts of the interaction are of gaussian type:

$$\hat{V}_R(\vec{r}_1,\vec{r}_2) = +V_{0,R}\mathrm{e}^{-\kappa_R(\vec{r}_1-\vec{r}_2)^2}, \qquad V_{0,R} = 200.00 \text{ MeV}, \qquad \kappa_R = 1.487 \text{ fm}^{-2} \tag{2a}$$

$$\hat{V}_t(\vec{r}_1,\vec{r}_2) = -V_{0,t}\mathrm{e}^{-\kappa_t(\vec{r}_1-\vec{r}_2)^2}, \qquad V_{0,t} = 178.00 \text{ MeV}, \qquad \kappa_t = 0.639 \text{ fm}^{-2} \tag{2b}$$

$$\hat{V}_s(\vec{r}_1,\vec{r}_2) = -V_{0,s}\mathrm{e}^{-\kappa_s(\vec{r}_1-\vec{r}_2)^2}, \qquad V_{0,s} = 91.85 \text{ MeV}, \qquad \kappa_s = 0.465 \text{ fm}^{-2} \tag{2c}$$

Due to antisymmetry, the space-exchange operator can be converted to spin-exchange and vice versa:

$$(1+\hat{P}_r)(1-\hat{P}_\sigma\hat{P}_r) = 1 + \hat{P}_r - \hat{P}_\sigma\hat{P}_r - \hat{P}_\sigma = (1-\hat{P}_\sigma)(1-\hat{P}_\sigma\hat{P}_r) \tag{3}$$

and because of $(1+\hat{P}_\sigma)(1-\hat{P}_\sigma) = 0$, the term $\hat{V}_t$ gives zero contribution and can be omitted. The final form is then

$$\widetilde{V}(\vec{r}_1,\vec{r}_2) = \tfrac{1}{2}\left[\hat{V}_R(\vec{r}_1,\vec{r}_2) + \hat{V}_s(\vec{r}_1,\vec{r}_2)\right](1-\hat{P}_\sigma)(1-\hat{P}_\sigma\hat{P}_r) \tag{4}$$

2 Multipolar decomposition of the Gaussian interaction

References in the following text beginnging with "V." point to the formulas from the book D. A. Varshalovich, A. N. Moskalev, V. K. Khersonskii: Quantum Theory of Angular Momentum, World Scientific Singapore 1988. Following symmetry properties of Clebsch-Gordan coefficients will be used without further reference:

$$C^{J,M}_{l,m,\lambda,\mu} = (-1)^{l+\lambda-J} C^{J,-M}_{l,-m,\lambda,-\mu} = C^{J,-M}_{\lambda,-\mu,l,-m} = (-1)^{l-m}\sqrt{\frac{2J+1}{2\lambda+1}}\, C^{\lambda,-\mu}_{l,m,J,-M} = (-1)^{\lambda+\mu}\sqrt{\frac{2J+1}{2l+1}}\, C^{l,-m}_{J,-M,\lambda,\mu} \tag{V. 8.4.10,11}$$

Since Talmi-Moshinsky transformation to center-of-mass frame is analytically difficult, I will factorize a two-body Gaussian interaction in laboratory frame as

$$\mathrm{e}^{-\mu(\vec{r}_1-\vec{r}_2)^2} = \mathrm{e}^{-\mu(r_1^2+r_2^2)}\mathrm{e}^{2\mu\vec{r}_1\cdot\vec{r}_2} \tag{5}$$

The term with scalar product can be decomposed using a well known formula

$$\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} = 4\pi\sum_{LM}\mathrm{i}^L j_L(kr) Y^*_{LM}(\hat{k}) Y_{LM}(\hat{r}) \tag{V. 5.17.14}$$

where imaginary unit is eliminated by utilizing modified spherical Bessel function $i_L(z)$ instead of spherical Bessel function $j_L(z)$:

$$(-\mathrm{i})^L j_L(iz) = i_L(z) = i_L^*(z) = \sum_{k=0}^{\infty}\frac{z^{L+2k}}{2^k k!(2L+2k+1)!!} \tag{6}$$

Desired formula is therefore

$$\mathrm{e}^{-\mu(\vec{r}_1-\vec{r}_2)^2} = \mathrm{e}^{-\mu(r_1^2+r_2^2)}4\pi\sum_{LM} i_L(2\mu r_1 r_2) Y^*_{LM}(\hat{r}_1)Y_{LM}(\hat{r}_2) = \mathrm{e}^{-\mu(r_1-r_2)^2}4\pi\sum_{LM}\frac{i_L(2\mu r_1 r_2)}{\exp(2\mu r_1 r_2)} Y^*_{LM}(\hat{r}_1)Y_{LM}(\hat{r}_2) \tag{7}$$

Last expression takes into account exponentially divergent nature of $i_L(z)$ for large z. In fact, the version of $i_L(z)$ given by the GSL library is exactly the one rescaled by an exponential.

Sometimes, only the $L = 0$ part is needed. It can be expressed analytically by well known functions ($Y_{00} = 1/\sqrt{4\pi}$):

$$i_0(z) = \frac{\mathrm{e}^z - \mathrm{e}^{-z}}{2z} \quad\rightarrow\quad \left(\mathrm{e}^{-\mu(\vec{r}_1-\vec{r}_2)^2}\right)_{L=0} = \frac{\mathrm{e}^{-\mu(r_1-r_2)^2} - \mathrm{e}^{-\mu(r_1+r_2)^2}}{4\mu r_1 r_2} 4\pi Y^*_{00}(\hat{r}_1)Y_{00}(\hat{r}_2) \tag{8}$$

3 Matrix elements of the particle-hole part (for HF)

Interaction is rewritten in second quantization as

$$\hat{V} = \tfrac{1}{4}\bar{v}_{acbd}\hat{a}^+_a\hat{a}^+_c\hat{a}_d\hat{a}_b \tag{9}$$

where the labeling was chosen to give a convenient expression for the mean-field HF hamiltonian:

$$h_{ab} = t_{ab} + \sum_{cd}\bar{v}_{acbd}\rho_{dc} \qquad \text{where } \rho_{dc} = \langle\mathrm{HF}|\hat{a}^+_c\hat{a}_d|\mathrm{HF}\rangle \tag{10}$$

Matrix element $\bar{v}_{acbd}$ is then calculated according to (4) symbolically as

$$\bar{v}_{acbd} = \left[\psi_a^\dagger(r_1\sigma_1)\psi_b(r_1\sigma_1)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_2)\right] - \left[\psi_a^\dagger(r_1\sigma_1)\psi_d(r_1\sigma_1)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_b(r_2\sigma_2)\right] \tag{11a}$$

$$- \left[\psi_a^\dagger(r_1\sigma_1)\psi_b(r_1\sigma_2)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_1)\right] + \left[\psi_a^\dagger(r_1\sigma_1)\psi_d(r_1\sigma_2)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_b(r_2\sigma_1)\right] \tag{11b}$$

where the single particle wavefunction of spherical HO with quantum numbers $a = (n_a, j_a, l_a, m_a)$ is (χ is spinor)

$$\psi_a(\vec{r}) = R_{n_a l_a}(r)\sum_\sigma C^{j_a,m_a}_{l_a,m_a-\sigma,\frac{1}{2},\sigma} Y_{l_a,m_a-\sigma}(\hat{r})\chi_\sigma \tag{12}$$

and V_{12} is a shortcut for $\frac{1}{2}V_{R,s}(\vec{r}_1,\vec{r}_2)$. Integration over $\vec{r}_1$, $\vec{r}_2$ and summation over σ_1, σ_2 is assumed in (11) without explicit notion.

The terms in (11) will not be evaluated straight away, but only after considering the summation over m of cd in (10), and will be highlighted by **[+]** and **[–]**. The point is that density matrix ρ_{cd} mixes only the states with the same (j,l,m), assuming unbroken spherical symmetry. Moreover, the density matrix is numerically the same for all m. The density matrix can be therefore broken into independent submatrices $\rho_{cd}^{(j,l)}$, where $j_c = j_d = j$, $l_c = l_d = l$ and $m_c = m_d$ is arbitrary (i.e. there are $2j+1$ identical submatrices with different m).

Analytical evaluation of $\sum_m \bar{v}_{acbd}\rho_{dc}$ for individual terms in (11) will go as follows:

1. Angular functions in $\left[\dots\right]$ will be coupled into $Y_{LM}(r_{1/2})$, which will be then eliminated by angular integration (by orthogonality of Y_{LM}) with corresponding term from V_{12}. The second bracket will be first treated by relation $Y_{L,-M} = (-1)^M Y_{LM}^*$. The form of (11a) allows the summation over $\sigma_{1,2}$ to be performed in this step as well.
2. Summation over $m_c = m_d = m$ with $\rho_{cd}^{(j,l)}$ will be applied in the second bracket. Besides forcing $j_c = j_d = j$ and $l_c = l_d = l$, this will lead to various simplification and equalities, often in a multi-step way. An important feature is the equality of LM for the first and second bracket $\left[\dots\right]$ due to (7).
3. Finally, the equalities $j_a = j_b$, $l_a = l_b$ and $m_a = m_b$ (as Kronecker deltas) will be obtained together with final expressions. The final expression will still contain radial integrals over r_1, r_2 and summation over L. Finally, the density matrix $\rho_{cd}^{(j,l)}$ can be formally factorized out from the result to obtain effective matrix elements $\bar{v}_{acbd}$.

When the coupling of spatial and spin part is not separated, spinorbitals can be directly multiplied to get

$$\left[\psi_a^\dagger(r_1\sigma_1)\psi_b(r_1\sigma_1)\right] = R_a(r_1)R_b(r_1)\sum_{LM}(-1)^{j_a+m_a+j_b+L+\frac{1}{2}}\sqrt{\frac{(2j_a+1)(2j_b+1)(2l_a+1)(2l_b+1)}{4\pi(2L+1)}}$$
$$\times \begin{Bmatrix} j_a & j_b & L \\ l_b & l_a & \frac{1}{2}\end{Bmatrix} C^{L0}_{l_a0l_b0}C^{L,M}_{j_a,-m_a,j_b,m_b}Y_{LM}(\hat{r}_1) \qquad \text{(V. 7.2.40)}$$

Summation of the second bracket with density matrix leads to

$$\sum_m \left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_2)\right]\rho_{dc}^{(j,l)} = \rho_{dc}^{(j,l)}R_c(r_2)R_d(r_2)\sum_L\left[\sum_m(-1)^{j+m}C^{L,0}_{j,-m,j,m}\right]$$
$$\times \frac{(2j+1)(2l+1)}{\sqrt{4\pi(2L+1)}}\begin{Bmatrix} j & j & L \\ l & l & \frac{1}{2}\end{Bmatrix}(-1)^{j+L+\frac{1}{2}}C^{L0}_{l0l0}Y_{L0}(\hat{r}_2) \tag{13}$$

This expression can be simplified by the following steps (orthogonality of CG coefficients etc.):

$$(-1)^{j+m} = \sqrt{2j+1}\,C^{0,0}_{j,-m,j,m}, \quad \sum_m(-1)^{j+m}C^{L,0}_{j,-m,j,m} = \sqrt{2j+1}\,\delta_{L0} \qquad \text{(V. 8.5.1, 8.7.2 or 4)}$$

$$C^{00}_{l0l0} = \frac{(-1)^l}{\sqrt{2l+1}}, \quad \begin{Bmatrix} j & j & 0 \\ l & l & \frac{1}{2}\end{Bmatrix} = \frac{(-1)^{j+l+\frac{1}{2}}}{\sqrt{(2l+1)(2j+1)}} \qquad \text{(V. 9.5.1)}$$

to get

$$\sum_m \left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_2)\right]\rho_{dc}^{(j,l)} = (2j+1)\rho_{dc}^{(j,l)}R_c(r_2)R_d(r_2)\frac{1}{\sqrt{4\pi}}Y_{00}^*(\hat{r}_2) \tag{14}$$

From $L=0$, I get $j_a = j_b$, $l_a = l_b$, and $m_a = m_b$ in (V. 7.2.40) due to Clebsch-Gordan coefficients (or $6j$ symbol), using also $C^{0,0}_{j,-m,j,m} = (-1)^{j+m}/\sqrt{2j+1}$:

$$\sum_m \left[\psi_a^\dagger(r_1\sigma_1)\psi_b(r_1\sigma_1)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_2)\right]\rho_{dc}^{(j,l)} =$$
$$= (2j+1)\rho_{dc}^{(j,l)}\int_0^\infty r_1^2\mathrm{d}r_1\int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_b(r_1)\frac{\mathrm{e}^{-\mu(r_1-r_2)^2}-\mathrm{e}^{-\mu(r_1+r_2)^2}}{4\mu r_1 r_2}R_c(r_2)R_d(r_2) \quad [+] \tag{15}$$

Exchange term in (11a) is more complicated:

$$\sum_m \left[\psi_a^\dagger(r_1\sigma_1)\psi_d(r_1\sigma_1)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_b(r_2\sigma_2)\right]\rho_{dc}^{(j,l)} =$$

$$= \rho_{dc}^{(j,l)}\int_0^\infty r_1^2\mathrm{d}r_1\int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_d(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_c(r_2)R_b(r_2)\sum_{LM}\frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1r_2)}\frac{(-1)^{j_a-j_b+m_a-m_b}}{2L+1}$$
$$\times\sqrt{(2j_a+1)(2j_b+1)(2l_a+1)(2l_b+1)}\,(2j+1)(2l+1)\begin{Bmatrix} j_a & j & L\\ l & l_a & \frac12\end{Bmatrix}\begin{Bmatrix} j & j_b & L\\ l_b & l & \frac12\end{Bmatrix}C^{L0}_{l_a0l0}C^{L0}_{l0l_b0}$$
$$\times\sum_m C^{L,M}_{j_a,-m_a,j,m}C^{L,-M}_{j,-m,j_b,m_b} \tag{16}$$

Sum over m and M in two last CG coefficients is

$$\sum_{mM}C^{L,M}_{j_a,-m_a,j,m}C^{L,-M}_{j,-m,j_b,m_b} = \frac{2L+1}{\sqrt{(2j_a+1)(2j_b+1)}}\sum_{mM}C^{j_a,m_a}_{L,-M,j,m}C^{j_b,m_b}_{L,-M,j,m} = \frac{2L+1}{2j_a+1}\delta_{j_aj_b}\delta_{m_am_b} \tag{17}$$

Then, the coefficients $C^{L0}_{l_a0l0}C^{L0}_{l0l_b0}$ imply that both l_a, l_b are either even or odd. So they are equal (due to $j=l\pm\frac12$). Final result is

$$\sum_m \left[\psi_a^\dagger(r_1\sigma_1)\psi_d(r_1\sigma_1)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_b(r_2\sigma_2)\right]\rho_{dc}^{(j,l)} =$$
$$= (2j+1)\rho_{dc}^{(j,l)}\int_0^\infty r_1^2\mathrm{d}r_1\int_0^\infty r_2^2\mathrm{d}r_2R_a(r_1)R_d(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_c(r_2)R_b(r_2)$$
$$\times(2l_a+1)(2l+1)\sum_L\frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1r_2)}\begin{Bmatrix} j_a & j & L\\ l & l_a & \frac12\end{Bmatrix}^2\left(C^{L0}_{l_a0l0}\right)^2 \qquad [-] \tag{18}$$

Terms with spin-exchanged coordinates (11b) need to be decomposed to spatial and spin part (12). Spatial part will be coupled first:

$$Y^*_{l_a,m_a-\sigma_1}(\hat r_1)Y_{l_b,m_b-\sigma_2}(\hat r_1) = \sum_{LM}(-1)^{m_a-\sigma_1}\sqrt{\frac{(2l_a+1)(2l_b+1)}{4\pi(2L+1)}}\,C^{L0}_{l_a0l_b0}C^{L,M}_{l_a,-m_a+\sigma_1,l_b,m_b-\sigma_2}Y_{LM}(\hat r_1) \tag{V. 5.6.9}$$

and spin part $\sigma_{1,2}$ will be coupled and eliminated later. Second bracket of the first term in (11b) after summation with ρ_{dc} gives:

$$\sum_m\left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_1)\right]\rho_{dc}^{(j,l)} = \rho_{dc}^{(j,l)}R_c(r_2)R_d(r_2)\sum_L\frac{2l+1}{\sqrt{4\pi(2L+1)}}C^{L0}_{l0l0}Y_{L,\sigma_2-\sigma_1}(\hat r_2)$$
$$\times\sum_m(-1)^{m-\sigma_2}C^{j,m}_{l,m-\sigma_2,\frac12,\sigma_2}C^{j,m}_{l,m-\sigma_1,\frac12,\sigma_1}C^{L,\sigma_2-\sigma_1}_{l,-m+\sigma_2,l,m-\sigma_1} \tag{19}$$

The sum of CG coefficients in the last line can be converted into a $6j$ symbol:

$$\sum_m(-1)^{m-\sigma_2}C^{L,\sigma_2-\sigma_1}_{l,-m+\sigma_2,l,m-\sigma_1}C^{j,m}_{l,m-\sigma_2,\frac12,\sigma_2}C^{j,m}_{l,m-\sigma_1,\frac12,\sigma_1} =$$
$$= (-1)^{j+\frac12}\sqrt{\frac{2L+1}{2}}\,(2j+1)C^{\frac12,\sigma_2}_{L,\sigma_2-\sigma_1,\frac12,\sigma_1}\begin{Bmatrix} l & l & L\\ \frac12 & \frac12 & j\end{Bmatrix} \tag{V. 8.7.16}$$
$$= (-1)^l\frac{2j+1}{2\sqrt{2l+1}}\delta_{\sigma_1\sigma_2} \tag{20}$$

The last equality is based on the following: Triangular inequality in the obtained CG coefficient allows an L equal to 0 or 1. So, according to C^{L0}_{l0l0} in (19), L is even, and thus $L=0$ and $\sigma_1=\sigma_2$. Then, $l_a=l_b$ follows from $C^{00}_{l_a0l_b0}$, $m_a=m_b$ follows from $C^{0,0}_{l_a,-m_a+\sigma,l_a,m_b-\sigma}$, and $j_a=j_b$ follows from

$$\sum_\sigma C^{j_a,m_a}_{l_a,m_a-\sigma,\frac12,\sigma}C^{j_b,m_a}_{l_a,m_a-\sigma,\frac12,\sigma} = \delta_{j_aj_b} \tag{V. 8.7.4}$$

Final result for the third term of (11) is then (it is half of the first term (15))

$$\sum_m\left[\psi_a^\dagger(r_1\sigma_1)\psi_b(r_1\sigma_2)\right]V_{12}\left[\psi_c^\dagger(r_2\sigma_2)\psi_d(r_2\sigma_1)\right]\rho_{dc}^{(j,l)} =$$
$$= \frac12(2j+1)\rho_{dc}^{(j,l)}\int_0^\infty r_1^2\mathrm{d}r_1\int_0^\infty r_2^2\mathrm{d}r_2R_a(r_1)R_b(r_1)\frac{\mathrm{e}^{-\mu(r_1-r_2)^2}-\mathrm{e}^{-\mu(r_1+r_2)^2}}{4\mu r_1r_2}R_c(r_2)R_d(r_2) \qquad [-] \tag{21}$$

Last term is more tricky, since simplifications are possible only when the term is written in its entirety:

$$\sum_m \big[\psi_a^\dagger(r_1\sigma_1)\psi_d(r_1\sigma_2)\big]V_{12}\big[\psi_c^\dagger(r_2\sigma_2)\psi_b(r_2\sigma_1)\big]\rho_{dc}^{(j,l)} =$$

$$= \rho_{dc}^{(j,l)}\int_0^\infty r_1^2 \mathrm{d}r_1 \int_0^\infty r_2^2 \mathrm{d}r_2 R_a(r_1)R_d(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_c(r_2)R_b(r_2) \tag{22}$$

$$\times \sum_L \frac{i_L(2\mu r_1 r_2)}{\exp(2\mu r_1 r_2)}\frac{\sqrt{(2l_a+1)(2l_b+1)}\,(2l+1)}{2L+1}C^{L0}_{l_a0l0}C^{L0}_{l0l_b0}(-1)^{m_a-m_b}$$

$$\times \sum_{mM\sigma_1\sigma_2} C^{j_a,m_a}_{l_a,m_a-\sigma_1,\frac{1}{2},\sigma_1} C^{j,m}_{l,m-\sigma_2,\frac{1}{2},\sigma_2} C^{L,M}_{l_a,-m_a+\sigma_1,l,m-\sigma_2} C^{j,m}_{l,m-\sigma_2,\frac{1}{2},\sigma_2} C^{j_b,m_b}_{l_b,m_b-\sigma_1,\frac{1}{2},\sigma_1} C^{L,-M}_{l,-m+\sigma_2,l_b,m_b-\sigma_1}$$

Last summation contains four degrees of freedom (in fact, only three degrees of freedom give nontrivial contribution) which have to be treated carefully. First I will sum over m and σ_2, keeping constant $m-\sigma_2$ (thus eliminating one degree of freedom), then over $m-\sigma_2$ and M, and finally over σ_1:

$$\sum_{m,\sigma_2}^{(1)} C^{j,m}_{l,m-\sigma_2,\frac{1}{2},\sigma_2}C^{j,m}_{l,m-\sigma_2,\frac{1}{2},\sigma_2} = \frac{2j+1}{2l+1}\sum_{m,\sigma_2}^{(1)} C^{l,-m+\sigma_2}_{j,-m,\frac{1}{2},\sigma_2}C^{l,-m+\sigma_2}_{j,-m,\frac{1}{2},\sigma_2} = \frac{2j+1}{2l+1} \tag{23a}$$

$$\sum_{m-\sigma_2,M} C^{L,M}_{l_a,-m_a+\sigma_1,l,m-\sigma_2}C^{L,-M}_{l,-m+\sigma_2,l_b,m_b-\sigma_1} = \frac{2L+1}{\sqrt{(2l_a+1)(2l_b+1)}}\sum_{m-\sigma_2,M} C^{l_a,m_a-\sigma_1}_{L,-M,l,m-\sigma_2}C^{l_b,m_b-\sigma_1}_{L,-M,l,m-\sigma_2}$$

$$= \frac{2L+1}{2l_a+1}\delta_{l_al_b}\delta_{m_am_b} \tag{23b}$$

$$\sum_{\sigma_1} C^{j_a,m_a}_{l_a,m_a-\sigma_1,\frac{1}{2},\sigma_1}C^{j_b,m_a}_{l_a,m_a-\sigma_1,\frac{1}{2},\sigma_1} = \delta_{j_aj_b} \tag{23c}$$

The fourth term of (11) is then

$$\sum_m \big[\psi_a^\dagger(r_1\sigma_1)\psi_d(r_1\sigma_2)\big]V_{12}\big[\psi_c^\dagger(r_2\sigma_2)\psi_b(r_2\sigma_1)\big]\rho_{dc}^{(j,l)} =$$

$$= (2j+1)\rho_{dc}^{(j,l)}\int_0^\infty r_1^2\mathrm{d}r_1\int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_d(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_c(r_2)R_b(r_2)\sum_L\frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1r_2)}\Big(C^{L0}_{l_a0l0}\Big)^2 \quad [+] \tag{24}$$

4 Matrix elements of the particle-particle part (for HFB)

Pairing part of the HFB mean-field is

$$\Delta_{ab} = \frac{1}{2}\sum_{cd}\bar{v}_{abcd}\kappa_{cd} \qquad \text{where } \kappa_{cd} = \langle\mathrm{HFB}|\hat{a}_d\hat{a}_c|\mathrm{HFB}\rangle \tag{25}$$

Independence of κ_{cd} on m has to be treated more carefully, it is not given a priori, also because $m_c=-m_d$. It turns out that independence on m can be implemented by using time-reversed states (I use convention $\hat{T}=\mathrm{i}\hat{\sigma}_y\hat{K}$, where $\hat{K}$ is complex conjugation):

$$\psi_{\bar{a}} = \hat{T}\psi_a = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\psi_a^* = R_{n_a,l_a}\sum_\sigma C^{j_a,m_a}_{l_a,m_a-\sigma,\frac{1}{2},\sigma}(-1)^{m_a-\sigma}Y_{l_a,-m_a+\sigma}(-1)^{\sigma+\frac{1}{2}}\chi_{-\sigma} = (-1)^{l_a+j_a+m_a}\psi_{-a} \tag{26}$$

where $-a=(n_a,j_a,l_a,-m_a)$. So an m-independent pairing tensor can be defined as

$$\kappa^{(j,l)}_{c\bar{d}} = (-1)^{l+j+m}\kappa_{c,-d} \qquad (m=m_c=m_d) \tag{27}$$

Matrix element of the interaction can be then calculated in four parts

$$\bar{v}_{a\bar{b}c\bar{d}} = \big[\psi_a^\dagger(r_1\sigma_1)\psi_c(r_1\sigma_1)\big]V_{12}\big[\psi_{\bar{b}}^\dagger(r_2\sigma_2)\psi_{\bar{d}}(r_2\sigma_2)\big] - \big[\psi_a^\dagger(r_1\sigma_1)\psi_{\bar{d}}(r_1\sigma_1)\big]V_{12}\big[\psi_{\bar{b}}^\dagger(r_2\sigma_2)\psi_c(r_2\sigma_2)\big] \tag{28a}$$

$$- \big[\psi_a^\dagger(r_1\sigma_1)\psi_c(r_1\sigma_2)\big]V_{12}\big[\psi_{\bar{b}}^\dagger(r_2\sigma_2)\psi_{\bar{d}}(r_2\sigma_1)\big] + \big[\psi_a^\dagger(r_1\sigma_1)\psi_{\bar{d}}(r_1\sigma_2)\big]V_{12}\big[\psi_{\bar{b}}^\dagger(r_2\sigma_2)\psi_c(r_2\sigma_1)\big] \tag{28b}$$

The first term is

$$\sum_m \big[\psi_a^\dagger(r_1\sigma_1)\psi_c(r_1\sigma_1)\big]V_{12}\big[\psi_{\bar{b}}^\dagger(r_2\sigma_2)\psi_{\bar{d}}(r_2\sigma_2)\big]\kappa^{(j,l)}_{c\bar{d}} =$$

$$= \kappa^{(j,l)}_{c\bar{d}}\int_0^\infty r_1^2\mathrm{d}r_1\int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_c(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_b(r_2)R_d(r_2)\sum_{LM}\frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1r_2)}\frac{(2j+1)(2l+1)}{2L+1}$$

$$\times\sqrt{(2j_a+1)(2j_b+1)(2l_a+1)(2l_b+1)}\begin{Bmatrix} j_a & j & L\\ l & l_a & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} j_b & j & L\\ l & l_b & \frac{1}{2}\end{Bmatrix}C^{L0}_{l_a0l0}C^{L0}_{l_b0l0}$$

$$\times\sum_m(-1)^{j_a-j_b+m_a+m}(-1)^{l_b+l+j_b+j+m_b+m}C^{L,M}_{j_a,-m_a,j,m}C^{L,-M}_{j_b,m_b,j,-m} \tag{29}$$

Sum over m and M is evaluated as

$$\sum_{mM} C^{L,M}_{j_a,-m_a,j,m} C^{L,-M}_{j_b,m_b,j,-m} = \frac{(-1)^{j_b+j-L}(2L+1)}{\sqrt{(2j_a+1)(2j_b+1)}} \sum_{mM} C^{j_a,m_a}_{L,-M,j,m} C^{j_b,m_b}_{L,-M,j,m} = (-1)^{j_a+j+L}\frac{2L+1}{2j_a+1}\delta_{j_aj_b}\delta_{m_am_b} \quad (30)$$

Equality $l_a = l_b$ then follows from parity in $C^{L0}_{l_a0l0}C^{L0}_{l_b0l0}$. Final result is

$$\sum_m \left[\psi^\dagger_a(r_1\sigma_1)\psi_c(r_1\sigma_1)\right] V_{12} \left[\psi^\dagger_{\bar b}(r_2\sigma_2)\psi_{\bar d}(r_2\sigma_2)\right]\kappa^{(j,l)}_{c\bar d} =$$

$$= (2j+1)\kappa^{(j,l)}_{c\bar d}\int_0^\infty r_1^2\mathrm{d}r_1 \int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_c(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_b(r_2)R_d(r_2)$$

$$\times (2l_a+1)(2l+1)\sum_L \frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1 r_2)}\begin{Bmatrix} j_a & j & L \\ l & l_a & \frac{1}{2}\end{Bmatrix}^2 \left(C^{L0}_{l_a0l0}\right)^2 \qquad [+] \quad (31)$$

The second term is

$$\sum_m \left[\psi^\dagger_a(r_1\sigma_1)\psi_{\bar d}(r_1\sigma_1)\right] V_{12} \left[\psi^\dagger_{\bar b}(r_2\sigma_2)\psi_c(r_2\sigma_2)\right]\kappa^{(j,l)}_{c\bar d} =$$

$$= \kappa^{(j,l)}_{c\bar d}\int_0^\infty r_1^2\mathrm{d}r_1 \int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_d(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_b(r_2)R_c(r_2)\sum_{LM}\frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1r_2)}\frac{(2j+1)(2l+1)}{2L+1}$$

$$\times\sqrt{(2j_a+1)(2j_b+1)(2l_a+1)(2l_b+1)}\begin{Bmatrix} j_a & j & L \\ l & l_a & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} j_b & j & L \\ l & l_b & \frac{1}{2}\end{Bmatrix} C^{L0}_{l_a0l0}C^{L0}_{l_b0l0}$$

$$\times\sum_m (-1)^{j_a-j_b+m_a-m}(-1)^{l+l_b+j+j_b+m+m_b} C^{L,M}_{j_a,-m_a,j,-m}C^{L,-M}_{j_b,m_b,j,m}$$

$$= -(2j+1)\kappa^{(j,l)}_{c\bar d}\int_0^\infty r_1^2\mathrm{d}r_1 \int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_d(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_b(r_2)R_c(r_2)$$

$$\times (2l_a+1)(2l+1)\sum_L \frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1 r_2)}\begin{Bmatrix} j_a & j & L \\ l & l_a & \frac{1}{2}\end{Bmatrix}^2 \left(C^{L0}_{l_a0l0}\right)^2 \qquad [-] \quad (32)$$

The third term is

$$\sum_m \left[\psi^\dagger_a(r_1\sigma_1)\psi_c(r_1\sigma_2)\right] V_{12} \left[\psi^\dagger_{\bar b}(r_2\sigma_2)\psi_{\bar d}(r_2\sigma_1)\right]\kappa^{(j,l)}_{c\bar d} =$$

$$= \kappa^{(j,l)}_{c\bar d}\int_0^\infty r_1^2\mathrm{d}r_1 \int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_c(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_b(r_2)R_d(r_2)\sum_{LM}\frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1r_2)}\frac{2l+1}{2L+1}$$

$$\times\sqrt{(2l_a+1)(2l_b+1)}\,C^{L0}_{l_a0l0}C^{L0}_{l_b0l0}\sum_{m\sigma_1\sigma_2}(-1)^{m_a+m+l_b+l+j_b+j+m_b+m}$$

$$\times C^{j_a,m_a}_{l_a,m_a-\sigma_1,\frac{1}{2},\sigma_1} C^{j,m}_{l,m-\sigma_2,\frac{1}{2},\sigma_2} C^{L,M}_{l_a,-m_a+\sigma_1,l,m-\sigma_2} C^{j_b,-m_b}_{l_b,-m_b-\sigma_2,\frac{1}{2},\sigma_2} C^{j,-m}_{l,-m-\sigma_1,\frac{1}{2},\sigma_1} C^{L,-M}_{l_b,m_b+\sigma_2,l,-m-\sigma_1} \quad (33)$$

The sum can be converted into a $9j$ symbol:

$$\sum_{mM\sigma_1\sigma_2} C^{L,M}_{l_a,-m_a+\sigma_1,l,m-\sigma_2} C^{j,-m}_{l,-m-\sigma_1,\frac{1}{2},\sigma_1} C^{j_a,m_a}_{l_a,m_a-\sigma_1,\frac{1}{2},\sigma_1} C^{L,-M}_{l_b,m_b+\sigma_2,l,-m-\sigma_1} C^{j,m}_{l,m-\sigma_2,\frac{1}{2},\sigma_2} C^{j_b,-m_b}_{l_b,-m_b-\sigma_2,\frac{1}{2},\sigma_2} =$$

$$= \sum_{mM\sigma_1\sigma_2}(-1)^{-\sigma_2-\sigma_1+l+\frac{1}{2}-j+l_b+l-L+\sigma_1+\sigma_2+l_b+\frac{1}{2}-j_b}\frac{(2L+1)(2j+1)}{2\sqrt{(2l_a+1)(2l_b+1)}}$$

$$\times C^{l_a,m_a-\sigma_1}_{L,-M,l,m-\sigma_2} C^{\frac{1}{2},\sigma_1}_{l,m+\sigma_1,j,-m} C^{j_a,m_a}_{l_a,m_a-\sigma_1,\frac{1}{2},\sigma_1} C^{l_b,m_b+\sigma_2}_{L,-M,l,m+\sigma_1} C^{\frac{1}{2},-\sigma_2}_{l,m-\sigma_2,j,-m} C^{j_b,m_b}_{l_b,m_b+\sigma_2,\frac{1}{2},-\sigma_2}$$

$$= (-1)^{L+j-j_b}(2L+1)(2j+1)\begin{Bmatrix} L & l & l_a \\ l & j & \frac{1}{2} \\ l_b & \frac{1}{2} & j_a\end{Bmatrix}\delta_{j_aj_b}\delta_{m_am_b} \quad \text{(V. 10.1.8)}$$

Equality $l_a = l_b$ then follows from $C^{L0}_{l_a0l0}C^{L0}_{l_b0l0}$. The final result is

$$\sum_m \left[\psi^\dagger_a(r_1\sigma_1)\psi_c(r_1\sigma_2)\right] V_{12} \left[\psi^\dagger_{\bar b}(r_2\sigma_2)\psi_{\bar d}(r_2\sigma_1)\right]\kappa^{(j,l)}_{c\bar d} =$$

$$= -(2j+1)\kappa^{(j,l)}_{c\bar d}\int_0^\infty r_1^2\mathrm{d}r_1 \int_0^\infty r_2^2\mathrm{d}r_2 R_a(r_1)R_c(r_1)\mathrm{e}^{-\mu(r_1-r_2)^2}R_b(r_2)R_d(r_2)$$

$$\times (2l_a+1)(2l+1)\sum_L \frac{i_L(2\mu r_1r_2)}{\exp(2\mu r_1 r_2)}\begin{Bmatrix} L & l & l_a \\ l & j & \frac{1}{2} \\ l_a & \frac{1}{2} & j_a\end{Bmatrix}\left(C^{L0}_{l_a0l0}\right)^2 \qquad [-] \quad (34)$$

The fourth term is similar

$$\sum_m \left[\psi_a^\dagger(r_1\sigma_1)\psi_{\bar d}(r_1\sigma_2)\right] V_{12} \left[\psi_{\bar b}^\dagger(r_2\sigma_2)\psi_c(r_2\sigma_1)\right] \kappa_{c\bar d}^{(j,l)} =$$

$$= \kappa_{c\bar d}^{(j,l)} \int_0^\infty r_1^2 \mathrm{d}r_1 \int_0^\infty r_2^2 \mathrm{d}r_2 R_a(r_1) R_d(r_1) \mathrm{e}^{-\mu(r_1-r_2)^2} R_b(r_2) R_c(r_2) \sum_{LM} \frac{i_L(2\mu r_1 r_2)}{\exp(2\mu r_1 r_2)} \frac{2l+1}{2L+1}$$
$$\times \sqrt{(2l_a+1)(2l_b+1)}\, C_{l_a0l0}^{L0} C_{l_b0l0}^{L0} \sum_{m\sigma_1\sigma_2} (-1)^{m_a-m+l+l_b+j+j_b+m+m_b}$$
$$\times C_{l_a,m_a-\sigma_1,\frac12,\sigma_1}^{j_a,m_a} C_{l,-m-\sigma_2,\frac12,\sigma_2}^{j,-m} C_{l_a,-m_a+\sigma_1,l,-m-\sigma_2}^{L,M} C_{l_b,-m_b-\sigma_2,\frac12,\sigma_2}^{j_b,-m_b} C_{l,m-\sigma_1,\frac12,\sigma_1}^{j,m} C_{l_b,m_b+\sigma_2,l,m-\sigma_1}^{L,-M}$$
$$= (2j+1)\kappa_{c\bar d}^{(j,l)} \int_0^\infty r_1^2 \mathrm{d}r_1 \int_0^\infty r_2^2 \mathrm{d}r_2 R_a(r_1) R_d(r_1) \mathrm{e}^{-\mu(r_1-r_2)^2} R_b(r_2) R_c(r_2)$$
$$\times (2l_a+1)(2l+1) \sum_L \frac{i_L(2\mu r_1 r_2)}{\exp(2\mu r_1 r_2)} \begin{Bmatrix} L & l & l_a \\ l & j & \frac12 \\ l_a & \frac12 & j_a \end{Bmatrix} \left(C_{l_a0l0}^{L0}\right)^2 \qquad [+] \tag{35}$$

5 Some considerations of HFB equations

During the solution of Hartree-Fock-Bogoliubov task, the particle creation and annihilation operators in spherical harmonic oscillator basis $\hat{a}_a^+$, $\hat{a}_a$ are transformed into quasiparticle creation and annihilation operators $\hat\beta_k^+$, $\hat\beta_k$, so that

$$\hat\beta_k|\mathrm{HFB}\rangle = 0, \qquad \hat\beta_k^+|\mathrm{HFB}\rangle = |k\rangle, \qquad \langle k|\hat H|k\rangle - \langle \mathrm{HFB}|\hat H|\mathrm{HFB}\rangle = E_k \tag{36}$$

The transformation between particles and quasiparticles is unitary

$$\begin{aligned} \hat\beta_k^+ &= \sum_a U_{ak}\hat a_a^+ + V_{ak}\hat a_a & \qquad \hat a_a^+ &= \sum_k U_{ak}^*\hat\beta_k^+ + V_{ak}\hat\beta_k \\ \hat\beta_k &= \sum_a V_{ak}^*\hat a_a^+ + U_{ak}^*\hat a_a & \qquad \hat a_a &= \sum_k V_{ak}^*\hat\beta_k^+ + U_{ak}\hat\beta_k \end{aligned} \tag{37}$$

Density matrices are then

$$\rho_{ab} = \langle \mathrm{HFB}|\hat a_b^+\hat a_a|\mathrm{HFB}\rangle = \sum_k V_{bk}V_{ak}^*, \qquad \kappa_{ab} = \langle \mathrm{HFB}|\hat a_b\hat a_a|\mathrm{HFB}\rangle = \sum_k U_{bk}V_{ak}^* \tag{38}$$

The ground state energy is

$$E_0 = \sum_{ab} t_{ab} + \frac12 \sum_{abcd} \bar v_{acbd}\rho_{ba}\rho_{dc} + \frac14 \sum_{abcd} \bar v_{abcd}\kappa_{ab}^*\kappa_{cd} \tag{39}$$

The HFB equations (with particle-number constrain) can be formulated as an eigenvalue problem

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k \tag{40}$$

Since our system has spherical symmetry, the matrices and coefficients are real and the only non-zero terms are (I consider $m_a = m_b$ in each term)

$$h_{ab} = h_{\bar a\bar b}, \quad \Delta_{a\bar b} = -\Delta_{\bar a b}, \quad U_{ak} = U_{\bar a\bar k}, \quad V_{a\bar k} = -V_{\bar a k}, \quad \rho_{ab} = \rho_{\bar a\bar b}, \quad \kappa_{a\bar b} = -\kappa_{\bar a b} \tag{41}$$

Similarly as in the previous section, I will prefer terms h_{ab}, $\Delta_{a\bar b}$, ρ_{ab}, $\kappa_{a\bar b}$ in the final expressions. So for example

$$\hat\beta_k^+ = \sum_a U_{ak}\hat a_a^+ - V_{a\bar k}\hat a_{\bar a}, \quad \rho_{ab} = \sum_k V_{a\bar k}V_{b\bar k}, \quad \kappa_{a\bar b} = \sum_k V_{a\bar k}U_{bk} \tag{42}$$

The HFB equation (40) can be separated into blocks

$$\begin{pmatrix} h_{ab}-\lambda & 0 & 0 & \Delta_{a\bar b} \\ 0 & h_{\bar a\bar b}-\lambda & \Delta_{\bar a b} & 0 \\ 0 & -\Delta_{a\bar b} & -h_{ab}+\lambda & 0 \\ -\Delta_{\bar a b} & 0 & 0 & -h_{\bar a\bar b}+\lambda \end{pmatrix} \begin{pmatrix} U_{bk} \\ 0 \\ 0 \\ V_{\bar b k} \end{pmatrix} \text{or} \begin{pmatrix} 0 \\ U_{\bar b\bar k} \\ V_{b\bar k} \\ 0 \end{pmatrix} = \begin{pmatrix} U_{ak} \\ 0 \\ 0 \\ V_{\bar a k} \end{pmatrix} \text{or} \begin{pmatrix} 0 \\ U_{\bar a\bar k} \\ V_{b\bar k} \\ 0 \end{pmatrix} E_{k,\bar k} \tag{43}$$

Its solution is numerically equivalent to the solution of

$$\begin{pmatrix} h_{ab}-\lambda & -\Delta_{a\bar b} \\ -\Delta_{a\bar b} & -h_{ab}+\lambda \end{pmatrix} \begin{pmatrix} U_{bk} \\ V_{b\bar k} \end{pmatrix} = E_k \begin{pmatrix} U_{ak} \\ V_{a\bar k} \end{pmatrix} \tag{44}$$