

Gaussian Pairing Matrix Element Derivation

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1 Gaussian

The gaussian interaction between \vec{r} and \vec{r}' is given by,

$$g_a(\vec{r}-\vec{r}') = \frac{e^{|\vec{r}-\vec{r}'|^2/a^2}}{(a\sqrt{\pi})^3} = \frac{4}{a^3\sqrt{\pi}} e^{-\frac{r^2}{a^2}} e^{-\frac{r'^2}{a^2}} \sum_{LM} (-i)^L j_L \left(2i \frac{r r'}{a^2} \right) Y_M^{L*}(\hat{r}) Y_M^L(\hat{r}') \quad (1)$$

where we have applied the multipole expansion [3] and j_L are the bessel functions

$$j_L(ix) = x^L \left(\frac{1}{x} \frac{d}{dx} \right)^L \frac{\sinh x}{x} \quad (2)$$

2 Two-body wavefunction

One body wavefunction is generally given by

$$\phi_{nljm_j}(\vec{r}\sigma) = \mathcal{R}_{nlj}(r) \sum_{m_l} \langle lm_l, 1/2\sigma | jm_j \rangle Y_{m_l}^l(\hat{r}) \quad (3)$$

and two body Cooper pair wavefunction, so the coupled $J=0$, in a single shell

$$\Phi_{nljm_j}^{00}(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) = \frac{(-1)^{-j-m_j}}{\sqrt{2j+1}} \mathcal{R}_{nlj}(r_1) \mathcal{R}_{nlj}(r_2) \sum_{m_{l1}m_{l2}} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm_{l2}, 1/2\sigma_2 | j-m_j \rangle Y_{m_{l1}}^l(\hat{r}_1) Y_{m_{l2}}^l(\hat{r}_2) \quad (4)$$

that is already antisymmetrized since...

3 Two-body matrix element

3.1 Leading Order, no momenta terms

$$V_{LO}(\vec{r}_1, \vec{r}_2, \vec{r}'_1, \vec{r}'_2) = g_a(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_1 - \vec{r}'_1) \delta(\vec{r}_2 - \vec{r}'_2) (\delta_{\sigma_1, \sigma'_1} \delta_{\sigma_2, \sigma'_2} + x_0 P^\sigma) \quad (5)$$

where P^σ is the spin-exchange operator. We start keeping the case for general spin,

$$\begin{aligned} & \int d^3r_1 d^3r_2 d^3r'_1 d^3r'_2 \langle j^2; J=0 | r_1 r_2 \rangle \langle r_1 r_2 | \tilde{V}_{LO} | r'_1 r'_2 \rangle \langle r'_1 r'_2 | j^2; J=0 \rangle = \\ & = \int d^3r_1 d^3r_2 \frac{1}{4} \Phi_{nljm_j}^{00*}(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) g_a(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_1 - \vec{r}'_1) \delta(\vec{r}_2 - \vec{r}'_2) \Phi_{nljm'_j}^{00}(\vec{r}_1\sigma'_1, \vec{r}_2\sigma'_2) \end{aligned} \quad (6)$$

$$\begin{aligned} & \int d^3r_1 d^3r_2 \Phi_{nljm_j}^{00*}(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) g_a(\vec{r}_1 - \vec{r}_2) \Phi_{nljm'_j}^{00}(\vec{r}_1\sigma'_1, \vec{r}_2\sigma'_2) = \\ & = \int d^3r_1 d^3r_2 \frac{(-1)^{-2j-m_j-m'_j}}{2j+1} \mathcal{R}_{nlj}(r_1) \mathcal{R}_{nlj}(r_2) \sum_{m_{l1}m_{l2}} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm_{l2}, 1/2\sigma_2 | j-m_j \rangle Y_{m_{l1}}^{l*}(\hat{r}_1) Y_{m_{l2}}^{l*}(\hat{r}_2) \\ & \quad g_a(\vec{r}_1 - \vec{r}_2) \mathcal{R}_{nlj}(r_1) \mathcal{R}_{nlj}(r_2) \sum_{m'_{l1}m'_{l2}} \langle lm'_{l1}, 1/2\sigma'_1 | jm'_j \rangle \langle lm'_{l2}, 1/2\sigma'_2 | j-m'_j \rangle Y_{m'_{l1}}^l(\hat{r}_1) Y_{m'_{l2}}^l(\hat{r}_2) \\ & = \int d^3r_1 d^3r_2 \frac{(-1)^{-2j-m_j-m'_j}}{2j+1} \mathcal{R}_{nlj}^2(r_1) \mathcal{R}_{nlj}^2(r_2) \sum_{m_{l1}m_{l2}} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm_{l2}, 1/2\sigma_2 | j-m_j \rangle Y_{m_{l1}}^{l*}(\hat{r}_1) Y_{m_{l2}}^{l*}(\hat{r}_2) \\ & \quad \frac{4}{a^3\sqrt{\pi}} e^{-\frac{r_1^2}{a^2}} e^{-\frac{r_2^2}{a^2}} \sum_{LM} (-i)^L j_L \left(2i \frac{r_1 r_2}{a^2} \right) \frac{(-1)^{-2j-m_j-m'_j}}{2j+1} \sum_{m'_{l1}m'_{l2}} \langle lm'_{l1}, 1/2\sigma'_1 | jm'_j \rangle \langle lm'_{l2}, 1/2\sigma'_2 | j-m'_j \rangle Y_{m'_{l1}}^l(\hat{r}_1) Y_{m'_{l2}}^l(\hat{r}_2) \end{aligned}$$

$$\begin{aligned}
&= \frac{(-1)^{-2j-m_j-m'_j}}{2j+1} \frac{4}{a^3 \sqrt{\pi}} \sum_{LM} (-i)^L \int dr_1 dr_2 r_1^2 r_2^2 \mathcal{R}_{nlj}^2(r_1) \mathcal{R}_{nlj}^2(r_2) e^{-\frac{r_1^2}{a^2}} e^{-\frac{r_2^2}{a^2}} j_L \left(2i \frac{r_1 r_2}{a^2} \right) \\
&\quad \int d^2 \hat{r}_1 d^2 \hat{r}_2 Y_M^{L*}(\hat{r}_1) Y_M^L(\hat{r}_2) \sum_{m_{l1} m_{l2}} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm_{l2}, 1/2\sigma_2 | j-m_j \rangle Y_{m_{l1}}^{L*}(\hat{r}_1) Y_{m_{l2}}^{L*}(\hat{r}_2) \\
&\quad \sum_{m'_{l1} m'_{l2}} \langle lm'_{l1}, 1/2\sigma'_1 | jm'_j \rangle \langle lm'_{l2}, 1/2\sigma'_2 | j-m'_j \rangle Y_{m'_{l1}}^L(\hat{r}_1) Y_{m'_{l2}}^L(\hat{r}_2)
\end{aligned} \tag{7}$$

the angular part of Eq. (7) is given by

$$\begin{aligned}
&\sum_{LM, mm'} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm_{l2}, 1/2\sigma_2 | j-m_j \rangle \langle lm'_{l1}, 1/2\sigma'_1 | jm'_j \rangle \langle lm'_{l2}, 1/2\sigma'_2 | j-m'_j \rangle \\
&\int d^2 \hat{r}_1 Y_M^{L*}(\hat{r}_1) Y_{m_{l1}}^{L*}(\hat{r}_1) Y_{m'_{l1}}^L(\hat{r}_1) \int d^2 \hat{r}_2 Y_M^L(\hat{r}_2) Y_{m_{l2}}^{L*}(\hat{r}_2) Y_{m'_{l2}}^L(\hat{r}_2)
\end{aligned} \tag{8}$$

the integral of three spherical harmonics [1]

$$\begin{aligned}
&\int d^2 \hat{r}_1 Y_M^{L*}(\hat{r}_1) Y_{m_{l1}}^{L*}(\hat{r}_1) Y_{m'_{l1}}^L(\hat{r}_1) = (-1)^{m_{l1}+M} \int d^2 \hat{r}_1 Y_{-M}^L(\hat{r}_1) Y_{-m_{l1}}^L(\hat{r}_1) Y_{m'_{l1}}^L(\hat{r}_1) = \\
&\quad = (-1)^{m_{l1}+M} (2l+1) \sqrt{\frac{2L+1}{4\pi}} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & L \\ -m_{l1} & m'_{l1} & -M \end{pmatrix} \\
&\int d^2 \hat{r}_1 Y_M^L(\hat{r}_1) Y_{m_{l2}}^{L*}(\hat{r}_1) Y_{m'_{l2}}^L(\hat{r}_1) = (-1)^{m_{l2}} \int d^2 \hat{r}_1 Y_M^L(\hat{r}_1) Y_{-m_{l2}}^L(\hat{r}_1) Y_{m'_{l2}}^L(\hat{r}_1) = \\
&\quad = (-1)^{m_{l2}} (2l+1) \sqrt{\frac{2L+1}{4\pi}} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & L \\ -m_{l2} & m'_{l2} & M \end{pmatrix}
\end{aligned} \tag{9}$$

thus Eq. (8) become

$$\begin{aligned}
&\sum_{LM, mm'} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm_{l2}, 1/2\sigma_2 | j-m_j \rangle \langle lm'_{l1}, 1/2\sigma'_1 | jm'_j \rangle \langle lm'_{l2}, 1/2\sigma'_2 | j-m'_j \rangle \\
&(-1)^{m_{l1}+M} (2l+1) \sqrt{\frac{2L+1}{4\pi}} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & L \\ -m_{l1} & m'_{l1} & -M \end{pmatrix} (-1)^{m_{l2}} (2l+1) \sqrt{\frac{2L+1}{4\pi}} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & L \\ -m_{l2} & m'_{l2} & M \end{pmatrix}
\end{aligned} \tag{10}$$

using the relation between Clebsch-Gordan and Wigner 3j-symbols

$$\langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle = (-1)^{j+m_j} \sqrt{2j+1} \begin{pmatrix} l & 1/2 & j \\ m_{l1} & \sigma_1 & -m_j \end{pmatrix} \tag{11}$$

that is difficult to solve for general case of spin σ_1, σ'_1 so we start considering the term proportional to $\delta_{\sigma_1, \sigma'_1} \delta_{\sigma_2, \sigma'_2}$, thus $\sigma_1 = \sigma'_1$

$$\begin{aligned}
&\sum_{m_{l1}, m'_{l1}, \sigma_1} (-1)^{m_{l1}+M} \langle lm_{l1}, 1/2\sigma_1 | jm_j \rangle \langle lm'_{l1}, 1/2\sigma_1 | jm'_j \rangle \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & L \\ m_{l1} & -m'_{l1} & M \end{pmatrix} \\
&= (-1)^{2j} (2j+1) \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \sum_{m_{l1}, m_{l2}, \sigma_1} (-1)^{m_{l1}+M} \begin{pmatrix} l & 1/2 & j \\ m_{l1} & \sigma_1 & -m_j \end{pmatrix} \begin{pmatrix} l & 1/2 & j \\ m'_{l1} & \sigma_1 & -m'_j \end{pmatrix} \begin{pmatrix} l & l & L \\ m_{l1} & -m'_{l1} & M \end{pmatrix} \\
&= -(-1)^{2j+M+m'_j-2l-1/2} (2j+1) \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \sum_{m_{l1}, m_{l2}, \sigma_1} (-1)^{-m_{l1}-m'_{l1}-\sigma_1+2l+1/2} \\
&\quad \begin{pmatrix} l & j & 1/2 \\ -m_{l1} & m_j & -\sigma_1 \end{pmatrix} \begin{pmatrix} l & 1/2 & j \\ m'_{l1} & \sigma_1 & -m'_j \end{pmatrix} \begin{pmatrix} l & l & L \\ m_{l1} & -m'_{l1} & M \end{pmatrix} \\
&= -(-1)^{2j+M+m'_j-2l-1/2} (2j+1) \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & j & j \\ M & -m_j & m'_j \end{pmatrix} \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\}
\end{aligned} \tag{12}$$

And,

$$\begin{aligned}
& \sum_{m_{l2}, m'_{l2}, \sigma_2} (-1)^{m'_{l2}} \langle lm_{l2}, 1/2\sigma_2 | j - m_j \rangle \langle lm'_{l2}, 1/2\sigma'_2 | j - m'_j \rangle (-1)^{m_{l2}} - (2l+1) \sqrt{\frac{2L+1}{4\pi}} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & L \\ -m_{l2} & m'_{l2} & M \end{pmatrix} \\
&= (-1)^{2j} (2j+1) \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \sum_{m_{l2}, m'_{l2}, \sigma_2} (-1)^{m_{l2}} \begin{pmatrix} l & 1/2 & j \\ m_{l2} & \sigma_2 & -m_j \end{pmatrix} \begin{pmatrix} l & 1/2 & j \\ m'_{l2} & \sigma_2 & -m'_j \end{pmatrix} \begin{pmatrix} l & l & L \\ m_{l2} & -m'_{l2} & -M \end{pmatrix} \\
&= -(-1)^{2j+m'_j-2l-1/2} (2j+1) \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \sum_{m_{l2}, m'_{l2}, \sigma_1} -(-1)^{-m_{l2}-m'_{l2}-\sigma_2+2l+1/2} \\
&\quad \begin{pmatrix} l & j & 1/2 \\ -m_{l2} & m_j & -\sigma_1 \end{pmatrix} \begin{pmatrix} l & 1/2 & j \\ m'_{l2} & \sigma_1 & -m'_j \end{pmatrix} \begin{pmatrix} l & l & L \\ -m_{l2} & m'_{l2} & M \end{pmatrix} \\
&= -(-1)^{2j+m'_j-2l-1/2} (2j+1) \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & j & j \\ -M & m_j & -m'_j \end{pmatrix} \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\} \quad (13)
\end{aligned}$$

It follows that Eq. (8) becomes

$$\begin{aligned}
&= \sum_{m_j, m'_j} (-1)^{2j+m'_j-1/2} (2j+1)^2 (2l+1)^2 \frac{2L+1}{4\pi} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & j & j \\ M & -m_j & m'_j \end{pmatrix} \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\} \\
&\quad (-1)^{2j+M+m'_j-1/2} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & j & j \\ -M & m_j & -m'_j \end{pmatrix} \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\} \quad (14)
\end{aligned}$$

$2m'_j$ is odd, minus one is even. $4j$ and $2l$ are even, thus the phase is $=1$.

$$\begin{aligned}
&= (2j+1)^2 (2l+1)^2 \frac{2L+1}{4\pi} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\}^2 \sum_{m_j, m'_j} (2j+1)^2 \begin{pmatrix} L & j & j \\ -M & m_j & -m'_j \end{pmatrix} \begin{pmatrix} L & j & j \\ M & -m_j & m'_j \end{pmatrix} = \\
&= (2l+1)^2 \frac{(-1)^{2j}}{4\pi} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\}^2 \quad (15)
\end{aligned}$$

From [3] eq. (1.69) and 6j-properties

$$\begin{aligned}
&\begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} L & j & j \\ 1/2 & l & l \end{matrix} \right\} = \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} l & l & L \\ j & j & 1/2 \end{matrix} \right\} = \\
&= -\frac{1}{(2l+1)} \frac{1+(-1)^{2l+L}}{2} \begin{pmatrix} j & j & L \\ 1/2 & -1/2 & 0 \end{pmatrix} = -\frac{1}{(2l+1)} \begin{pmatrix} j & j & L \\ 1/2 & -1/2 & 0 \end{pmatrix} \quad (16)
\end{aligned}$$

with the prescription that L is even. Eq. (7) is then given by

$$\begin{aligned}
\Rightarrow (7) &= \sum_{L \text{ even}, M} (-i)^L \frac{(-1)^{-2j}}{2j+1} \frac{4}{a^3 \sqrt{\pi}} \int dr_1 dr_2 r_1^2 r_2^2 \mathcal{R}_{nlj}^2(r_1) \mathcal{R}_{nlj}^2(r_2) e^{-\frac{r_1^2}{a^2}} e^{-\frac{r_2^2}{a^2}} j_L \left(2i \frac{r_1 r_2}{a^2} \right) \\
&\quad (2j+1)^2 (2l+1)^2 \frac{(-1)^{2j}}{4\pi} \frac{1}{(2l+1)^2} \begin{pmatrix} j & j & L \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 = \\
&= \sum_{L \text{ even}, M} (-i)^L (2j+1) \begin{pmatrix} j & j & L \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 \frac{1}{a^3 \sqrt{\pi^3}} \int dr_1 dr_2 r_1^2 r_2^2 \mathcal{R}_{nlj}^2(r_1) \mathcal{R}_{nlj}^2(r_2) e^{-\frac{r_1^2}{a^2}} e^{-\frac{r_2^2}{a^2}} j_L \left(2i \frac{r_1 r_2}{a^2} \right) = \\
&= \frac{2j+1}{a^3 \sqrt{\pi^3}} \sum_{L \text{ even}} (-i)^L (2L+1) \begin{pmatrix} j & j & L \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 \int dr_1 dr_2 r_1^2 r_2^2 \mathcal{R}_{nlj}^2(r_1) \mathcal{R}_{nlj}^2(r_2) e^{-\frac{r_1^2}{a^2}} e^{-\frac{r_2^2}{a^2}} j_L \left(2i \frac{r_1 r_2}{a^2} \right) \quad (17)
\end{aligned}$$

References

- [1] <http://mathworld.wolfram.com/SphericalHarmonic.html>
- [2] <http://www.phme.it/wilt/wp-content/uploads/sites/4/2014/11/Scanned-multifunction-device.pdf>
- [3] From nucleons to nucleus, J. Suhonen, Springer