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Chapter 1

Introduction

1.1 Relative and centre of mass coordinates

Let us define the relative position \mathbf{x} , the relative momentum \mathbf{k} , the centre of mass position \mathbf{X} , and the centre of mass momentum \mathbf{K} as

$$\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2, \quad \mathbf{X} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2), \quad (1.1)$$

$$\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2), \quad \mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2, \quad (1.2)$$

where \mathbf{x}_i and \mathbf{k}_i are the position and momentum, respectively, of particle $i = 1, 2$ (figure?). Here we have assumed that the two nucleons have equal mass m , so that the reduced mass $m_r = \frac{1}{2}m$ and the total mass $M = 2m$. From Eqs. (1.2) we get the relation

$$k^2 + \frac{1}{4}K^2 = \frac{1}{2}(k_1^2 + k_2^2), \quad (1.3)$$

where the k , K , k_1 , and k_2 are the absolute values of the corresponding vectors denoted in boldface.

1.2 First-order perturbation theory

As single-particle eigenfunctions we use the plane waves

$$\phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{x}}, \quad (1.4)$$

which are normalized eigenstates in a cubic box potential, defined for a discrete set of momentum values \mathbf{k} . According to first-order perturbation theory,

the total energy of a system is

$$E = \langle \Phi | \hat{H} | \Phi \rangle, \quad (1.5)$$

where $|\Phi\rangle$ is the normalized ground state of a noninteracting Fermi gas. The Hamiltonian of the infinite nuclear matter system can be written in second quantization as

$$\begin{aligned} \hat{H} = & \sum_{\mathbf{k}\lambda\rho} \sum_{\mathbf{k}'\lambda'\rho'} \langle \mathbf{k}\lambda\rho | \hat{T} | \mathbf{k}'\lambda'\rho' \rangle a_{\mathbf{k}\lambda\rho}^\dagger a_{\mathbf{k}'\lambda'\rho'} + \frac{1}{2} \sum_{\mathbf{k}_1\lambda_1\rho_1} \cdots \sum_{\mathbf{k}_4\lambda_4\rho_4} \\ & \times \langle \mathbf{k}_1\lambda_1\rho_1, \mathbf{k}_2\lambda_2\rho_2 | V | \mathbf{k}_3\lambda_3\rho_3, \mathbf{k}_4\lambda_4\rho_4 \rangle a_{\mathbf{k}_1\lambda_1\rho_1}^\dagger a_{\mathbf{k}_2\lambda_2\rho_2}^\dagger a_{\mathbf{k}_4\lambda_4\rho_4} a_{\mathbf{k}_3\lambda_3\rho_3}. \end{aligned} \quad (1.6)$$

By substituting the Hamiltonian, we get for the ground state energy the approximation

$$\begin{aligned} E_{PT1} = & 4 \sum_{\mathbf{k}}^{k_F} \frac{\hbar^2 k^2}{2m} + \frac{1}{2} \sum_{\mathbf{k}_1\lambda_1\rho_1} \cdots \sum_{\mathbf{k}_4\lambda_4\rho_4} \langle \mathbf{k}_1\lambda_1\rho_1, \mathbf{k}_2\lambda_2\rho_2 | V | \mathbf{k}_3\lambda_3\rho_3, \mathbf{k}_4\lambda_4\rho_4 \rangle \\ & \times \langle \Phi | a_{\mathbf{k}_1\lambda_1\rho_1}^\dagger a_{\mathbf{k}_2\lambda_2\rho_2}^\dagger a_{\mathbf{k}_4\lambda_4\rho_4} a_{\mathbf{k}_3\lambda_3\rho_3} | \Phi \rangle. \end{aligned} \quad (1.7)$$

Evaluating the matrix elements with creation and annihilation operators, we get

$$\begin{aligned} E_{PT1} = & 4 \sum_{\mathbf{k}}^{k_F} \frac{\hbar^2 k^2}{2m} + \frac{1}{2} \sum_{\mathbf{k}\lambda\rho}^{k_F} \sum_{\mathbf{k}'\lambda'\rho'}^{k_F} \\ & \times \{ \langle \mathbf{k}\lambda\rho, \mathbf{k}'\lambda'\rho' | V | \mathbf{k}\lambda\rho, \mathbf{k}'\lambda'\rho' \rangle - \langle \mathbf{k}\lambda\rho, \mathbf{k}'\lambda'\rho' | V | \mathbf{k}'\lambda'\rho', \mathbf{k}\lambda\rho \rangle \}. \end{aligned} \quad (1.8)$$

If we have a continuum of plane wave states, we can change the summations to integrals and express the first-order energy as

$$\begin{aligned} E_{PT1} = & 4 \frac{V}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk \left(\frac{\hbar^2 k^2}{2m} \right) \\ & + \frac{1}{2} (4\pi)^2 \left(\frac{V}{(2\pi)^3} \right)^2 \sum_{\substack{\lambda\lambda' \\ \rho\rho'}} \int_0^{k_F} dk k^2 \int_0^{k_F} dk' k'^2 \\ & \times \{ \langle \mathbf{k}\lambda\rho, \mathbf{k}'\lambda'\rho' | V | \mathbf{k}\lambda\rho, \mathbf{k}'\lambda'\rho' \rangle - \langle \mathbf{k}\lambda\rho, \mathbf{k}'\lambda'\rho' | V | \mathbf{k}'\lambda'\rho', \mathbf{k}\lambda\rho \rangle \}. \end{aligned} \quad (1.9)$$

Observe that $\langle \mathbf{k}\mathbf{k}' | V | \mathbf{k}\mathbf{k}' \rangle \propto 1/V^2$ in the box potential plane wave basis.

1.3 Angular momentum representation

In the problems we are considering it will be useful to have the matrix elements in a coupled angular momentum representation. Assume for a while that we have the continuous plane wave basis

$$\psi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (1.10)$$

instead of the discrete box potential plane wave basis of Eq. (1.4). The bra vector $\langle \mathbf{k}_1 \mathbf{k}_2 |$ can be expanded as [3]

$$\langle \mathbf{k}_1 \mathbf{k}_2 | = \sum_{l_1 l_2 \lambda \mu} \langle k_1 l_1 k_2 l_2, \lambda \mu | \left[Y^{l_1}(\hat{\mathbf{k}}_1) Y^{l_2}(\hat{\mathbf{k}}_2) \right]_{\mu}^{\lambda}, \quad (1.11)$$

where the functions $Y^l(\hat{\mathbf{k}})$ are spherical harmonics, l_1 and l_2 are angular momenta of the two particles, λ is the total angular momentum, and μ its projection in the z direction. Observe that we use for radial wave functions the definition

$$\varphi_{\alpha lm}(k, \theta, \phi) = P_{\alpha l}(k) Y_m^l(\theta, \phi), \quad (1.12)$$

instead of

$$\varphi_{\alpha lm}(k, \theta, \phi) = \frac{1}{k} P'_{\alpha l}(k) Y_m^l(\theta, \phi), \quad (1.13)$$

as used in Ref. [3]. This is the reason why Eq. (1.11) has not the $(k_1 k_2)^{-1}$ factor present in the expression of Wong and Clement. Let us name the definition used by Wong and Clement 1 and the other definition 2. When using definition 1, the radial ket $|klm\rangle$ has the orthogonality property

$$\langle klm | k'l'm' \rangle = \delta_{ll'} \delta_{mm'} \delta(k - k'), \quad (1.14)$$

and for definition 2 we have the relation

$$\langle klm | k'l'm' \rangle = \delta_{ll'} \delta_{mm'} \delta(k - k') \frac{1}{kk'}. \quad (1.15)$$

Below we have used only the definition 2.

The bracket expression with two spherical harmonics is the $\lambda - \mu$ coupled tensor operator [5]

$$\left[Y^l(\hat{\mathbf{k}}) Y^{l'}(\hat{\mathbf{k}}') \right]_{\mu}^{\lambda} = \sum_{mm'} (ll'mm' | \lambda \mu) Y_m^l(\hat{\mathbf{k}}) Y_{m'}^{l'}(\hat{\mathbf{k}}'), \quad (1.16)$$

where the factor in front of the spherical harmonics functions is a Clebsch-Gordan coefficient. The spherical harmonics $Y_m^l(\hat{\mathbf{k}}) = \langle \hat{\mathbf{k}} | lm \rangle$ are eigenstates of the angular momentum operator \hat{L}^2 , given in the momentum representation.

We can now include the spin and isospin degrees of freedom and do the recouplings of angular momenta

$$\begin{aligned}
& (l_1 m_{l_1} s_1 m_{s_1})(t_1 m_{t_1})(l_2 m_{l_2} s_2 m_{s_2})(t_2 m_{t_2}) \\
& \longrightarrow (j_1 m_{j_1} l_1 s_1)(j_2 m_{j_2} l_2 s_2)(t_1 m_{t_1} t_2 m_{t_2}) \\
& = (j_1 m_{j_1} j_2 m_{j_2})(l_1 s_1 l_2 s_2)(t_1 m_{t_1} t_2 m_{t_2}) \\
& \longrightarrow (JM_J j_1 j_2)(l_1 s_1 l_2 s_2)(t_1 m_{t_1} t_2 m_{t_2}) \\
& = (j_1 l_1 s_1)(j_2 l_2 s_2)(JM_J)(t_1 m_{t_1} t_2 m_{t_2}). \tag{1.17}
\end{aligned}$$

The brackets are there only to emphasize which quantum numbers are recoupled. The bra vector can then be written in a new basis as (def. 2)

$$\begin{aligned}
& \sum_{m_{s_1} m_{s_2}} \sum_{m_{t_1} m_{t_2}} \langle \mathbf{k}_1 \mathbf{k}_2 | \langle m_{s_1} m_{s_2} | \langle m_{t_1} m_{t_2} | \\
& = \sum_{\substack{l_1 l_2 \\ m_{l_1} m_{l_2}}} \sum_{\substack{m_{s_1} m_{s_2} \\ m_{t_1} m_{t_2}}} \sum_{\substack{j_1 j_2 \\ m_{j_1} m_{j_2}}} \sum_{JM_J} \\
& \times (l_1 s_1 m_{l_1} m_{s_1} | j_1 m_{j_1})(l_2 s_2 m_{l_2} m_{s_2} | j_2 m_{j_2})(j_1 j_2 m_{j_1} m_{j_2} | JM_J) \\
& \times \langle k_1 j_1 l_1, k_2 j_2 l_2; JM_J | \langle m_{t_1} m_{t_2} | Y_{m_{l_1}}^{l_1}(\hat{\mathbf{k}}_1) Y_{m_{l_2}}^{l_2}(\hat{\mathbf{k}}_2), \tag{1.18}
\end{aligned}$$

where the one-particle spin and isospin quantum numbers $s_1 = s_2 = t_1 = t_2 = \frac{1}{2}$ have been suppressed from the bra vectors.

As shown in Ref. [5], p. 208–212, the nuclear two-body interaction is a tensor operator of rank 0. Given a tensor operator of rank 0, Q_{00} , it follows from the Wigner-Eckart theorem that the matrix element $\langle JM_J | Q_{00} | J' M_J' \rangle$ is independent of M_J and M_J' . Thus, the interaction is rotationally invariant with respect to the total angular momentum J . If we substitute the angular momentum expansion (1.18) into the last term of the energy expression (1.9), use the orthogonality of spherical harmonics, use the relation [5]

$$\sum_{m_1 m_2} (j_1 j_2 m_1 m_2 | JM_J)(j_1 j_2 m_1 m_2 | J' M_J') = \delta_{JJ'} \delta_{M_J M_J'} \tag{1.19}$$

for Clebsch-Gordan coefficients, utilize the rotational invariance with respect to the total angular momentum, and use a factor $(2\pi)^3/V$ to convert $|\mathbf{k}_1 \mathbf{k}_2\rangle$

from the continous basis (1.10) to the discrete basis (1.4), we get the expression

$$\begin{aligned}
E_{PT1} = & \frac{V}{5\pi^2} \frac{\hbar^2 k_F^5}{m} + \frac{1}{2} \int_0^{k_F} k_1^2 dk_1 \int_0^{k_F} k_2^2 dk_2 \\
& \times \sum_{\substack{l_1 l_2 \\ j_1 j_2}} \sum_J \sum_{m_{t_1} m_{t_2}} (2J+1) \\
& \times \langle k_1 j_1 l_1, k_2 j_2 l_2; J m_{t_1} m_{t_2} | \tilde{v} | k_1 j_1 l_1, k_2 j_2 l_2; J m_{t_1} m_{t_2} \rangle
\end{aligned} \tag{1.20}$$

for the total energy according to first order perturbation theory. Here we have defined the potential \tilde{v} such that

$$\langle k_i k_j | \tilde{v} | k_i k_j \rangle = \langle k_i k_j | v | k_i k_j \rangle - \langle k_i k_j | v | k_j k_i \rangle. \tag{1.21}$$

In our first order perturbation theory calculations we use the energy expression of Eq. (1.20).

1.4 Transformation from lab to RCM coordinates

Radial ket vectors can be transformed between the lab and the relative and centre-of-mass (RCM) coordinate systems using the relation [3] (def. 2)

$$|k_1 l_1 k_2 l_2, \lambda \mu\rangle = \int k^2 dk \int K^2 dK \sum_{lL} |klKL, \lambda \mu\rangle \langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle, \quad (1.22)$$

where the transformation coefficient $\langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle$ is called a *vector bracket*. The vector bracket can be written

$$\langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle = (4\pi)^2 \delta(u) \theta(1 - v^2) A(v), \quad (1.23)$$

where (def. 2)

$$A(v) = \frac{1}{(2\lambda + 1)} \frac{1}{k_1 k_2 k K} \sum_{\mu} \left[Y^l(\hat{\mathbf{k}}) \times Y^L(\hat{\mathbf{K}}) \right]_{\mu}^{\lambda*} \times \left[Y^{l_1}(\hat{\mathbf{k}}_1) \times Y^{l_2}(\hat{\mathbf{k}}_2) \right]_{\mu}^{\lambda}, \quad (1.24)$$

as formulated by Balian and Brezin [7] (OBS! Check $1/k$ terms. In addition, what about the $(4\pi)^2$ in Wong and $4\pi^2$ in Kung?), and

$$u = k^2 + \frac{1}{4}K^2 - \frac{1}{2}(k_1^2 + k_2^2), \quad (1.25)$$

$$v = (k_1^2 - k^2 - \frac{1}{4}K^2)/kK. \quad (1.26)$$

The delta function imposes conservation of the kinetic energy in the transition from RCM coordinates to the lab frame. The variable v is the cosine of the angle between \mathbf{k} and \mathbf{K} , and the step function $\theta(1 - v^2)$ gives therefore a necessary geometric restriction.

Now we want to write a vector $|(k_1 l_1 j_1)(k_2 l_2 j_2)(JM_J)\rangle$ as a linear combination of vectors $|klKL(\mathcal{J})SJM_J\rangle$. This kind of transformation can be obtained in the following way: First we do a recoupling from the $j-j$ scheme to the $L-S$ scheme, as in Eq. (4.13) in Ref. [5]. Further, we do the recoupling $JM_J \lambda S \longrightarrow \lambda \mu S M_S$, and get

$$\begin{aligned} |(k_1 l_1 j_1)(k_2 l_2 j_2)(JM_J)\rangle &= \sum_{\lambda S} \sum_{\mu M_S} \hat{j}_1 \hat{j}_2 \hat{\lambda} \hat{S} \left\{ \begin{matrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ \lambda & S & J \end{matrix} \right\} \\ &\times (\lambda S \mu M_S | JM_J) |k_1 l_1 k_2 l_2, \lambda \mu\rangle |SM_S\rangle, \end{aligned} \quad (1.27)$$

where we have used the definition $\hat{x} = \sqrt{2x+1}$. If we now use the lab to RCM transformation (1.22), do the recoupling $\lambda\mu SM_S \rightarrow JM_J\lambda S$, and use the $9j$ coefficient relation (A4.27) in Ref. [5], we get

$$\begin{aligned} |(k_1 l_1 j_1)(k_2 l_2 j_2)(JM_J)\rangle &= \sum_{\lambda S} \sum_{lL} \int k^2 dk \int K^2 dK \hat{j}_1 \hat{j}_2 \hat{\lambda} \hat{S} \left\{ \begin{matrix} l_1 & l_2 & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_1 & j_2 & J \end{matrix} \right\} \\ &\times \langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle |klKL(\lambda)SJM_J\rangle. \end{aligned} \quad (1.28)$$

To get the desired basis on the right hand side, we must further do the recoupling of three angular momenta $lL(\lambda)SJM_J \rightarrow lL(\mathcal{J})SJM_J$, diagrammatically sketched as [5]

$$\begin{array}{c} \text{Diagram 1: A triangle with vertices } S \text{ (top), } L \text{ (bottom right), and } (JM_J) \text{ (bottom left). A line from } S \text{ to } L \text{ is labeled } l. \text{ A line from } S \text{ to } (JM_J) \text{ is labeled } \lambda. \end{array} = \sum_{\mathcal{J}} \hat{\mathcal{J}} \hat{\lambda} W(SlJL; \mathcal{J}\lambda) \times \begin{array}{c} \text{Diagram 2: A triangle with vertices } S \text{ (top), } L \text{ (bottom right), and } (JM_J) \text{ (bottom left). A line from } S \text{ to } L \text{ is labeled } l. \text{ A line from } S \text{ to } (JM_J) \text{ is labeled } \mathcal{J}. \end{array}$$

where $W(SlJL; \mathcal{J}\lambda)$ is a *Racah coefficient* [6]. When we apply this recoupling, we get the expression

$$\begin{aligned} |(k_1 l_1 j_1)(k_2 l_2 j_2)(JM_J)\rangle &= \sum_{\lambda S} \sum_{lL} \sum_{\mathcal{J}} \int k^2 dk \int K^2 dK \hat{j}_1 \hat{j}_2 \hat{\lambda}^2 \hat{S} \hat{\mathcal{J}} \left\{ \begin{matrix} l_1 & l_2 & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_1 & j_2 & J \end{matrix} \right\} \\ &\times \langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle W(LlJS; \lambda\mathcal{J}) \\ &\times |klKL(\mathcal{J})SJM_J\rangle. \end{aligned} \quad (1.29)$$

Here we have used some symmetry relations for Racah coefficients. If we now use the relation between Racah coefficients and $6j$ symbols, and include the isospin degree of freedom, we obtain

$$\begin{aligned} |(k_1 l_1 j_1)(k_2 l_2 j_2)(JM_J m_{t_1} m_{t_2})\rangle &= \sum_{\lambda S} \sum_{lL} \sum_{\mathcal{J}} \int k^2 dk \int K^2 dK \hat{j}_1 \hat{j}_2 \hat{\lambda}^2 \hat{S} \hat{\mathcal{J}} \\ &\times (-1)^{L+l+J+S} \left\{ \begin{matrix} l_1 & l_2 & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_1 & j_2 & J \end{matrix} \right\} \\ &\times \langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle \left\{ \begin{matrix} L & l & \lambda \\ S & J & \mathcal{J} \end{matrix} \right\} \\ &\times |klKL(\mathcal{J})SJM_J m_{t_1} m_{t_2}\rangle. \end{aligned} \quad (1.30)$$

This vector is still not antisymmetrized.

Let $P(1, 2)$ be an operator that changes the order of coordinates 1 and 2. Then we have for the $A(v)$ function of the vector bracket the property

$$\begin{aligned}
P(1, 2)A(v) &= \frac{1}{(2\lambda + 1)} \frac{1}{k_1 k_2 k K} \sum_{\mu} \left[Y^l(-\hat{\mathbf{k}}) \times Y^L(\hat{\mathbf{K}}) \right]_{\mu}^{\lambda*} \\
&\quad \times \left[Y^{l_2}(\hat{\mathbf{k}}_2) \times Y^{l_1}(\hat{\mathbf{k}}_1) \right]_{\mu}^{\lambda} \\
&= \frac{1}{(2\lambda + 1)} \frac{1}{k_1 k_2 k K} (-1)^l (-1)^{\lambda - l_1 - l_2} \sum_{\mu} \left[Y^l(\hat{\mathbf{k}}) \times Y^L(\hat{\mathbf{K}}) \right]_{\mu}^{\lambda*} \\
&\quad \times \left[Y^{l_1}(\hat{\mathbf{k}}_1) \times Y^{l_2}(\hat{\mathbf{k}}_2) \right]_{\mu}^{\lambda}. \tag{1.31}
\end{aligned}$$

Here we have used Eq. (1.16), the Clebsch-Gordan property (A.11), and the property of spherical harmonics (A.13). We thus get that the vector bracket transforms as

$$\begin{aligned}
P(1, 2) \langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle &= (-1)^l (-1)^{\lambda - l_1 - l_2} \\
&\quad \times \langle klKL, \lambda | k_1 l_1 k_2 l_2, \lambda \rangle. \tag{1.32}
\end{aligned}$$

Do we get a different antisymmetrisation factor than in the harmonic oscillator case??

1.5 Calculation of matrix element

Assume our two-particle interaction is given in relative and center-of-mass coordinates. Then we can do a transformation as shown in Ref. [1], and write a matrix element as (assumption: $a \neq b$ and $c \neq d$? Otherwise the antisymmetrisation factor would be different)

$$\begin{aligned}
& \langle k_a l_a j_a k_b l_b j_b J T M_T | V | k_c l_c j_c k_d l_d j_d J T M_T \rangle \\
&= \sum_{l \lambda S \mathcal{J}} \int k^2 dk \int K^2 dK \left(\frac{1 - (-1)^{l+S+T}}{\sqrt{2}} \right) \left\{ \begin{matrix} l_a & l_b & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_a & j_b & J \end{matrix} \right\} \\
&\times (-1)^{\lambda+\mathcal{J}-L-S} \hat{\mathcal{J}} \hat{\lambda}^2 \hat{j}_a \hat{j}_b \hat{S} \left\{ \begin{matrix} L & l & \lambda \\ S & J & \mathcal{J} \end{matrix} \right\} 4\pi^2 \delta \left(k^2 + \frac{1}{4} K^2 - \frac{1}{2} (k_a^2 + k_b^2) \right) \\
&\times \theta \left(1 - \frac{(k_a^2 - k^2 - \frac{1}{4} K^2)^2}{k^2 K^2} \right) A \left(\frac{k_a^2 - k^2 - \frac{1}{4} K^2}{k K} \right) \\
&\times \sum_{l' \lambda'} \int k'^2 dk' \int K'^2 dK' \left(\frac{1 - (-1)^{l'+S+T'}}{\sqrt{2}} \right) \left\{ \begin{matrix} l_c & l_d & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_c & j_d & J \end{matrix} \right\} \\
&\times (-1)^{\lambda'+\mathcal{J}-L-S} \hat{\mathcal{J}} \hat{\lambda}'^2 \hat{j}_c \hat{j}_d \hat{S} \left\{ \begin{matrix} L & l' & \lambda' \\ S & J & \mathcal{J} \end{matrix} \right\} 4\pi^2 \delta \left(k'^2 + \frac{1}{4} K'^2 - \frac{1}{2} (k_c^2 + k_d^2) \right) \\
&\times \theta \left(1 - \frac{(k_c^2 - k'^2 - \frac{1}{4} K'^2)^2}{k'^2 K'^2} \right) A \left(\frac{k_c^2 - k'^2 - \frac{1}{4} K'^2}{k' K'} \right) \\
&\times \langle k l K L(\mathcal{J}) S J T M_T | V | k' l' K' L(\mathcal{J}) S J T M_T \rangle. \tag{1.33}
\end{aligned}$$

Here we have written the vector brackets explicitly, using Eq. (1.23). Observe also that we use only the continuous plane wave basis (1.10) when calculating this integral.

Now we first want to express the last bracket in Eq. (1.33) in terms of $\langle k l m_l | v | k' l' m_l' \rangle$. By using the Racah coupling relation

$$\begin{array}{c} \begin{array}{c} l \\ \diagup \quad \diagdown \\ S \quad L \\ \diagdown \quad \diagup \\ \mathcal{J} \\ \diagup \quad \diagdown \\ (J M_J) \end{array} \end{array} = \sum_{\lambda} \hat{\mathcal{J}} \hat{\lambda} W(S l J L; \mathcal{J} \lambda) \times \begin{array}{c} \begin{array}{c} l \\ \diagup \quad \diagdown \\ S \quad L \\ \diagdown \quad \diagup \\ \lambda \\ \diagup \quad \diagdown \\ (J M_J) \end{array} \end{array}$$

and doing the recouplings $J M_J \lambda S \rightarrow \lambda \mu S M_S$ and $\lambda \mu l L \rightarrow l m_l L m_L$, we may

write

$$\begin{aligned}
|klKL(\mathcal{J})SJM_J\rangle &= \sum_{\lambda} \sum_{\mu M_S} \sum_{m_l m_L} \hat{\mathcal{J}} \hat{\lambda} W(SlJL; \mathcal{J}\lambda) (\lambda S \mu M_S | JM_J) \\
&\times (lL m_l m_L | \lambda \mu) |klm_l\rangle |KLm_L\rangle |SM_S JM_J\rangle. \quad (1.34)
\end{aligned}$$

From this, we get the matrix element

$$\begin{aligned}
&\langle klKL(\mathcal{J})SJM_J | V | k'l'K'L(\mathcal{J})SJM_J \rangle \\
&= \sum_{\lambda\lambda'} \sum_{\substack{\mu\mu' \\ M_S}} \sum_{\substack{m_l m_L \\ m'_l}} \hat{\mathcal{J}}^2 \hat{\lambda} \hat{\lambda'} W(SlJL; \mathcal{J}\lambda) W(Sl'JL; \mathcal{J}\lambda') \\
&\times (\lambda' S \mu' M_S | JM_J) (\lambda S \mu M_S | JM_J) (l' L m'_l m_L | \lambda' \mu') \\
&\times (lL m_l m_L | \lambda \mu) \langle klm_l | V | k'l'm'_l \rangle \delta(K - K') / KK'. \quad (1.35)
\end{aligned}$$

Here we have used the normalisation relation (1.15).

Given that $\langle klm_l | V | k'l'm'_l \rangle$ is diagonal with respect to l and m_l , and that this matrix element is otherwise independent of m_l , we may use the relation for Clebsch-Gordan coefficients (A.12) and the relation for Racah coefficients [5]

$$\sum_K (2J+1)(2K+1) W(j_1 j_2 j_4 j_3; JK) W(j_1 j_2 j_4 j_3; J'K) = \delta_{JJ'}, \quad (1.36)$$

and straightforwardly show that

$$\begin{aligned}
&\langle klKL(\mathcal{J})SJM_J | V | k'l'K'L(\mathcal{J})SJM_J \rangle \\
&= \langle klm_l | V | k'l'm'_l \rangle \delta_{ll'} \delta_{m_l m'_l} \delta(K - K') / KK'. \quad (1.37)
\end{aligned}$$

In the interaction matrix element of Eq. (1.33) we have the necessary condition $k_i \leq k_F$ for $i \in \{a, b, c, d\}$. Combining this restriction with Eq. (1.3), we get the condition $k^2 + \frac{1}{4}K^2 \leq k_F^2$, or

$$\begin{aligned}
0 &\leq k \leq k_F, \\
0 &\leq K \leq 2\sqrt{k_F^2 - k^2} \quad (1.38)
\end{aligned}$$

as integration limits for k and K .

If we insert the expression (1.37) into the bracket (1.33), we get (what

about the integration limits when evaluating the simple $\delta(K - K')$?)

$$\begin{aligned}
& \langle k_a l_a j_a k_b l_b j_b J T | V | k_c l_c j_c k_d l_d j_d J T \rangle \\
&= 16\pi^4 \sum_{l L \lambda S \mathcal{J}} \left(\frac{1 - (-1)^{l+S+T}}{\sqrt{2}} \right) \left\{ \begin{matrix} l_a & l_b & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_a & j_b & J \end{matrix} \right\} (-1)^{\lambda+\mathcal{J}-L-S} \\
&\times \hat{\mathcal{J}} \hat{\lambda}^2 \hat{j}_a \hat{j}_b \hat{S} \left\{ \begin{matrix} L & l & \lambda \\ S & J & \mathcal{J} \end{matrix} \right\} \sum_{l' \lambda'} \left(\frac{1 - (-1)^{l'+S+T'}}{\sqrt{2}} \right) \\
&\times \left\{ \begin{matrix} l_c & l_d & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_a & j_b & J \end{matrix} \right\} (-1)^{\lambda'+\mathcal{J}-L-S} \hat{\mathcal{J}} \hat{\lambda}'^2 \hat{j}_c \hat{j}_d \hat{S} \left\{ \begin{matrix} L & l' & \lambda' \\ S & J & \mathcal{J} \end{matrix} \right\} \\
&\times \int_0^{k_F} k^2 dk \int_0^{2\sqrt{k_F^2 - k^2}} K dK \delta \left(k^2 + \frac{1}{4} K^2 - \frac{1}{2} (k_a^2 + k_b^2) \right) \\
&\times \theta \left(1 - \frac{(k_a^2 - k^2 - \frac{1}{4} K^2)^2}{k^2 K^2} \right) A \left(\frac{k_a^2 - k^2 - \frac{1}{4} K^2}{k K} \right) \\
&\times \int_0^{k_F} k'^2 dk' \int_0^{2\sqrt{k_F^2 - k'^2}} K' dK' \delta \left(k'^2 + \frac{1}{4} K'^2 - \frac{1}{2} (k_c^2 + k_d^2) \right) \\
&\times \theta \left(1 - \frac{(k_c^2 - k'^2 - \frac{1}{4} K'^2)^2}{k'^2 K'^2} \right) A \left(\frac{k_c^2 - k'^2 - \frac{1}{4} K'^2}{k' K'} \right) \\
&\times \langle k l m_l | V | k l m_l \rangle \delta(K - K'). \tag{1.39}
\end{aligned}$$

Let us now try to simplify the integral of Eq. (1.39). We can remove the integral with respect to K' by applying the last delta function, and get the integral part of Eq. (1.39)

$$\begin{aligned}
I &= \int_0^{k_F} k^2 dk \int_0^{2\min\{\sqrt{k_F^2 - k^2}, \sqrt{k_F^2 - k'^2}\}} K^2 dK \\
&\times \delta \left(k^2 + \frac{1}{4} K^2 - \frac{1}{2} (k_a^2 + k_b^2) \right) \\
&\times \theta \left(1 - \frac{(k_a^2 - k^2 - \frac{1}{4} K^2)^2}{k^2 K^2} \right) A \left(\frac{k_a^2 - k^2 - \frac{1}{4} K^2}{k K} \right) \\
&\times \int_0^{k_F} k'^2 dk' \delta \left(k'^2 + \frac{1}{4} K^2 - \frac{1}{2} (k_c^2 + k_d^2) \right) \\
&\times \theta \left(1 - \frac{(k_c^2 - k'^2 - \frac{1}{4} K^2)^2}{k'^2 K^2} \right) A \left(\frac{k_c^2 - k'^2 - \frac{1}{4} K^2}{k' K} \right) \\
&\times \langle k l m_l | V | k l m_l \rangle. \tag{1.40}
\end{aligned}$$

To evaluate the two other delta functions, we may define the new integration variables

$$\begin{aligned} s &= \frac{1}{4}K^2 + k^2 - \frac{1}{2}(k_a^2 + k_b^2), \\ t &= k'^2 + \frac{1}{4}K^2 - \frac{1}{2}(k_c^2 + k_d^2), \end{aligned} \quad (1.41)$$

and do a change of variables, as shown in Sec. A.1. We must check that the point $(s, t) = (0, 0)$ is within the integration limits of K and k' . From the condition that k , K , and k' should be real at the point $(s, t) = (0, 0)$, we get the restrictions

$$\begin{aligned} \sqrt{\frac{1}{2}(k_{ab} - k_{cd})} \leq k \leq \sqrt{\frac{1}{2}(k_{ab})}, \quad & \text{if } (k_{ab} - k_{cd}) \geq 0 \\ 0 \leq k \leq \sqrt{\frac{1}{2}(k_{ab})}, \quad & \text{else,} \end{aligned} \quad (1.42)$$

where we have used the definition

$$k_{ij} \equiv k_i^2 + k_j^2. \quad (1.43)$$

When checking that the point $(s, t) = (0, 0)$ is within the integration limits of K and k' , we find the additional conditions

$$\begin{aligned} k \leq \sqrt{k_F^2 + \frac{1}{2}(k_{ab} - k_{cd})}, \quad & \text{if } (k_{ab} - k_{cd}) < 0, \\ \frac{1}{2}(k_{ab} - k_{cd}) + k_F^2 \geq 0, \quad & \text{always.} \end{aligned} \quad (1.44)$$

With these conditions the integral becomes

$$\begin{aligned} I &= \int_{a_1}^{b_1} dk \, k^2 \tilde{K} \tilde{k} \, \theta \left(1 - \frac{(k_a^2 - k^2 - \frac{1}{4}\tilde{K}^2)^2}{k^2 \tilde{K}^2} \right) \\ &\times A \left(\frac{k_a^2 - k^2 - \frac{1}{4}\tilde{K}^2}{k \tilde{K}} \right) \theta \left(1 - \frac{(k_c^2 - \tilde{k}^2 - \frac{1}{4}\tilde{K}^2)^2}{\tilde{k}^2 \tilde{K}^2} \right) \\ &\times A \left(\frac{k_c^2 - \tilde{k}^2 - \frac{1}{4}\tilde{K}^2}{\tilde{k} \tilde{K}} \right) \langle klm_l | V | klm_l \rangle, \end{aligned} \quad (1.45)$$

where the integration limits are

$$a_1 = \begin{cases} \sqrt{\frac{1}{2}(k_{ab} - k_{cd})}, & \text{if } (k_{ab} - k_{cd}) \geq 0, \\ 0, & \text{if } (k_{ab} - k_{cd}) < 0, \end{cases} \quad (1.46)$$

and

$$b_1 = \begin{cases} \sqrt{\frac{1}{2}(k_{ab})}, & \text{if } (k_{ab} - k_{cd}) \geq 0, \\ \sqrt{k_F^2 + \frac{1}{2}(k_{ab} - k_{cd})}, & \text{if } (k_{ab} - k_{cd}) < 0. \end{cases} \quad (1.47)$$

In addition, we have the second condition of Eq. (1.44). In the integral (1.45), the Jacobian determinant is Kk' and the variables \tilde{K} and \tilde{k} should be read as

$$\begin{aligned} \tilde{K} &= 2 \left(-k^2 + \frac{1}{2} (k_a^2 + k_b^2) \right)^{1/2}, \\ \tilde{k} &= \left(k^2 - \frac{1}{2} (k_a^2 + k_b^2 - k_c^2 - k_d^2) \right)^{1/2}. \end{aligned} \quad (1.48)$$

If we substitute the expression for \tilde{K} into the first θ -function, we get the argument function

$$f(k) = 1 - \frac{1}{16} \frac{(k_a^2 - k_b^2)^2}{k^2 \left(-k^2 + \frac{1}{2}(k_a^2 + k_b^2) \right)}. \quad (1.49)$$

Remembering that $k \geq 0$, we find the derivatives

$$\begin{aligned} \frac{df(k)}{dk} &> 0, & \text{if } k < \frac{1}{2}(k_a^2 + k_b^2)^{1/2}, \\ \frac{df(k)}{dk} &< 0, & \text{if } k > \frac{1}{2}(k_a^2 + k_b^2)^{1/2}. \end{aligned} \quad (1.50)$$

Since $f(k \rightarrow 0^+) = -\infty$, $f(k_0) = 0$ has the only solution $k_0 = \frac{1}{2}|k_a - k_b|$ such that $k_0 \geq 0$, and $f(k \rightarrow \infty) = 1$, we find that $f(k) \geq 0$ for $k_0 \geq \frac{1}{2}|k_a - k_b|$. From this we can easily find the new integration limits

$$a_2 = \begin{cases} \sqrt{\frac{1}{2}(k_{ab} - k_{cd})}, & \text{if } (k_{ab} - k_{cd}) \geq 0 \\ \text{and } \sqrt{\frac{1}{2}(k_{ab} - k_{cd})} > \frac{1}{2}|k_a - k_b|, \\ \frac{1}{2}|k_a - k_b|, & \text{else,} \end{cases} \quad (1.51)$$

and

$$b_2 = \begin{cases} \sqrt{\frac{1}{2}(k_{ab})}, & \text{if } (k_{ab} - k_{cd}) \geq 0, \\ \sqrt{k_F^2 + \frac{1}{2}(k_{ab} - k_{cd})}, & \text{if } (k_{ab} - k_{cd}) < 0. \end{cases} \quad (1.52)$$

The integral with these limits is

$$\begin{aligned}
I &= \int_{a_2}^{b_2} dk \, k^2 \tilde{K} \tilde{k} \\
&\times A \left(\frac{k_a^2 - k^2 - \frac{1}{4} \tilde{K}^2}{k \tilde{K}} \right) A \left(\frac{k_c^2 - \tilde{k}^2 - \frac{1}{4} \tilde{K}^2}{\tilde{k} \tilde{K}} \right) \\
&\times \theta \left(1 - \frac{(k_c^2 - \tilde{k}^2 - \frac{1}{4} \tilde{K}^2)^2}{\tilde{k}^2 \tilde{K}^2} \right) \langle klm_l | V | klm_l \rangle. \tag{1.53}
\end{aligned}$$

Let us next evaluate the second θ -function. The argument function here is

$$g(k) = 1 - \frac{1}{16} \frac{(k_c^2 - k_d^2)^2}{(k^2 - \frac{1}{2}(k_{ab} - k_{cd}))(-k^2 + \frac{1}{2}(k_{ab}))}, \tag{1.54}$$

and its derivative obeys the relations

$$\begin{aligned}
\frac{dg(k)}{dk} &> 0, \quad \text{if } k < \frac{1}{2}(2k_{ab} - k_{cd})^{1/2}, \\
\frac{dg(k)}{dk} &< 0, \quad \text{if } k > \frac{1}{2}(2k_{ab} - k_{cd})^{1/2}. \tag{1.55}
\end{aligned}$$

for $k \geq 0$. If $2k_{ab} - k_{cd} < 0$, then $dg/dk < 0$ for all $k > 0$. When we analyse the function $g(k)$ assuming that $2k_{ab} - k_{cd} \geq 0$ and $k \geq 0$, we find that it has the following special points:

$$\begin{aligned}
\text{denominator of } g(k) \rightarrow 0 : & \quad k_1 = (\tfrac{1}{2}(k_{ab} - k_{cd}))^{1/2}, \quad k_5 = (\tfrac{1}{2}k_{ab})^{1/2}, \\
g(k) = 0 : & \quad k_{2,4} = (\tfrac{1}{2}k_{ab} - \tfrac{1}{4}(k_c \pm k_d)^2)^{1/2}, \\
\frac{dg}{dk} = 0 : & \quad k_3 = \tfrac{1}{2}(2k_{ab} - k_{cd}).
\end{aligned}$$

We also can find the ordering of these special points

$$k_1 \leq k_2 \leq k_3 \leq k_4 \leq k_5 < \infty.$$

Furthermore, we find that

$$\begin{aligned}
g(k \rightarrow (k_1)^-) &= +\infty, \quad g(k \rightarrow (k_1)^+) = -\infty, \\
g(k_2) &= 0, \quad g(k_3) \geq 0, \quad g(k_4) = 0, \\
g(k \rightarrow (k_5)^-) &= -\infty, \quad g(k \rightarrow (k_5)^+) = +\infty, \quad g(k \rightarrow \infty) = 1.
\end{aligned}$$

The main features of a graph of $g(k)$ could now be sketched. The final integration limits can be divided into different cases: The first case is

$$\begin{aligned}
\left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c + k_d)^2 \right)^{1/2} &\leq k \leq \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2 \right)^{1/2}, \\
\text{if } k_{ab} - k_{cd} &\geq 0 \quad \text{and} \quad \left(\frac{1}{2}(k_{ab} - k_{cd}) \right)^{1/2} > \frac{1}{2}|k_a - k_b|,
\end{aligned}$$

the second is

$$\begin{aligned} & \max \left\{ \frac{1}{2}|k_a - k_b|, \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c + k_d)^2 \right)^{1/2} \right\} \\ & \leq k \leq \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2 \right)^{1/2}, \\ & \text{if } k_{ab} - k_{cd} \geq 0 \quad \text{and} \quad \left(\frac{1}{2}(k_{ab} - k_{cd}) \right)^{1/2} \leq \frac{1}{2}|k_a - k_b|, \end{aligned}$$

and the third case is

$$\begin{aligned} & \max \left\{ \frac{1}{2}|k_a - k_b|, \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c + k_d)^2 \right)^{1/2} \right\} \\ & \leq k \leq \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2 \right)^{1/2}, \\ & \text{or } \left(\frac{1}{2}k_{ab} \right)^{1/2} < k \leq \left(k_F^2 + \frac{1}{2}(k_{ab} - k_{cd}) \right)^{1/2}, \\ & \text{if } k_{ab} - k_{cd} < 0. \end{aligned}$$

We finally get the integral

$$\begin{aligned} I &= \int_a^b dk \, k^2 \tilde{K} \tilde{k} \, A \left(\frac{k_a^2 - k^2 - \frac{1}{4}\tilde{K}^2}{k\tilde{K}} \right) \\ & \times A \left(\frac{k_c^2 - \tilde{k}^2 - \frac{1}{4}\tilde{K}^2}{\tilde{k}\tilde{K}} \right) \langle klm_l | V | klm_l \rangle. \end{aligned} \quad (1.56)$$

where

$$\begin{aligned} \tilde{K} &= 2 \left(-k^2 + \frac{1}{2}(k_{ab}) \right)^{1/2}, \\ \tilde{k} &= \left(k^2 - \frac{1}{2}(k_{ab} - k_{cd}) \right)^{1/2}, \end{aligned}$$

and a and b denote integration limits according to the different cases listed above.

Above we assumed that $2k_{ab} - k_{cd} \geq 0$. If we instead assume that $2k_{ab} - k_{cd} < 0$ and $k \geq 0$, the special points become different:

$$\begin{aligned} \text{denominator of } g(k) \rightarrow 0 : & \quad k_5 = \left(\frac{1}{2}k_{ab} \right)^{1/2}, \\ g(k) = 0 : & \quad k_4 = \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2 \right)^{1/2}, \\ \frac{dg}{dk} < 0, \forall k \geq 0. & \end{aligned}$$

We then get the integration boundaries

$$a = \begin{cases} \frac{1}{2}|k_a - k_b|, & \text{if } \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2\right) < 0, \\ \min \left\{ \frac{1}{2}|k_a - k_b|, \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2\right)^{1/2} \right\} & \text{else,} \end{cases}$$

and

$$b = \left(\frac{1}{2}k_{ab} - \frac{1}{4}(k_c - k_d)^2\right)^{1/2},$$

or

$$\left(\frac{1}{2}k_{ab}\right)^{1/2} \leq k \leq \left(k_F^2 + \frac{1}{2}(k_{ab} - k_{cd})\right)^{1/2}.$$

1.6 Remarks

1.6.1 Orthogonality

When using the definition 2 defined earlier, the radial vectors $|klm\rangle$ satisfy the orthogonality condition

$$\langle klm|k'l'm'\rangle \equiv \delta_{ll'}\delta_{mm'}\delta(k-k')\frac{1}{kk'} \quad (1.57)$$

and, equally for the coupled vector $|k_1l_1k_2l_2, \lambda\mu\rangle$,

$$\langle k_1l_1k_2l_2, \lambda\mu|k'_1l'_1k'_2l'_2, \lambda'\mu'\rangle = \delta_{l_1l'_1}\delta_{l_2l'_2}\delta_{\lambda\lambda'}\delta_{\mu\mu'}\delta(k_1-k'_1)\delta(k_2-k'_2)\frac{1}{k_1^2k_2^2}. \quad (1.58)$$

1.6.2 Interaction matrix element in RCM coordinates

A two-particle operator V can be written in second quantization as [4]

$$V = \frac{1}{2} \sum_{ijkl} \langle ij|v|kl\rangle a_i^\dagger a_j^\dagger a_l a_k, \quad (1.59)$$

where

$$\langle ij|v|kl\rangle = \int dr_1 \int dr_2 \phi_i^*(r_1) \phi_j^*(r_2) v(r_1, r_2) \phi_k(r_1) \phi_l(r_2). \quad (1.60)$$

If we take the single-particle states to be eigenfunctions of a finite cubic box with volume V , i.e. the plane waves of Eq. (1.4), the matrix elements become

$$\begin{aligned} \langle \mathbf{k}_1 \mathbf{k}_2 | v | \mathbf{k}_3 \mathbf{k}_4 \rangle &= \int d^3r_1 \int d^3r_2 \phi_{\mathbf{k}_1}^*(\mathbf{r}_1) \phi_{\mathbf{k}_2}^*(\mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2) \phi_{\mathbf{k}_3}(\mathbf{r}_1) \phi_{\mathbf{k}_4}(\mathbf{r}_2) \\ &= \frac{1}{V^2} \int d^3r_1 \int d^3r_2 e^{-i\mathbf{k}_1 \cdot \mathbf{r}_1} e^{-i\mathbf{k}_2 \cdot \mathbf{r}_2} v(\mathbf{r}_1, \mathbf{r}_2) e^{i\mathbf{k}_3 \cdot \mathbf{r}_1} e^{i\mathbf{k}_4 \cdot \mathbf{r}_2}. \end{aligned} \quad (1.61)$$

If we use the definitions of Eqs. (1.1) and (1.2), and do the change of integration variables

$$\mathbf{r}_1, \mathbf{r}_2 \longrightarrow \mathbf{r}, \mathbf{R}, \quad (1.62)$$

where \mathbf{r} and \mathbf{R} are relative and centre of mass coordinates, respectively, we get the matrix element into the form

$$\begin{aligned} \langle \mathbf{k}_1 \mathbf{k}_2 | v | \mathbf{k}_3 \mathbf{k}_4 \rangle &= \left[\frac{1}{V} \int d^3 r e^{-i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} v(r) \right] \delta_{\mathbf{K}, \mathbf{K}'} \\ &\equiv v(\mathbf{k} - \mathbf{k}') \delta_{\mathbf{K}, \mathbf{K}'}. \end{aligned} \quad (1.63)$$

Here we have assumed that the interaction is central, i.e. it depends only on the absolute value r of the relative position vector.

If we instead of the single-particle basis (1.4) use the eigenfunctions of the free-particle Hamiltonian, i.e.

$$\phi_{\mathbf{k}_i}(\mathbf{r}_i) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}_i \cdot \mathbf{r}_i}, \quad (1.64)$$

the matrix element becomes

$$\begin{aligned} \langle \mathbf{k}_1 \mathbf{k}_2 | v | \mathbf{k}_3 \mathbf{k}_4 \rangle &= \left[\frac{1}{(2\pi)^3} \int d^3 r e^{-i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} v(r) \right] \delta(\mathbf{K} - \mathbf{K}') \\ &\equiv u(\mathbf{k} - \mathbf{k}') \delta(\mathbf{K} - \mathbf{K}'). \end{aligned} \quad (1.65)$$

We see that when the basis is continuous, we get a Dirac delta instead of a Kronecker delta.

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Appendix A

Some mathematical details

A.1 Coupled delta distributions

Assume we want to calculate an integral with two coupled delta distributions

$$\begin{aligned} & \iint_{\Omega(x,y)} \delta(f(x,y)) \delta(g(x,y)) h(x,y) dx dy \\ &= \iint_{\Omega(x,y)} \delta^{(2)}(f(x,y), g(x,y)) h(x,y) dx dy. \end{aligned} \quad (\text{A.1})$$

On the right hand side we have defined the two-dimensional delta distribution $\delta^{(2)}(s, t)$. This integral can be evaluated by changing to the variables

$$s = f(x, y), \quad t = g(x, y). \quad (\text{A.2})$$

The integration measure transforms accordingly as

$$dx dy \longrightarrow \left| \begin{array}{cc} \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial s} & \frac{\partial y}{\partial t} \end{array} \right| ds dt, \quad (\text{A.3})$$

where the new measure has a Jacobian determinant factor. Let the direction of integration of the new integration domain $\Omega(s, t)$ be the same as in the old domain $\Omega(x, y)$. If the initial integration domain $\Omega(x, y)$ is chosen such that there exist unique inverse mappings

$$\begin{aligned} \eta &= x(s, t), \\ \xi &= y(s, t), \end{aligned} \quad (\text{A.4})$$

we can write the integral as

$$\begin{aligned}
& \iint_{\Omega(x,y)} \delta(f(x,y)) \delta(g(x,y)) h(x,y) dx dy \\
&= \iint_{\Omega(s,t)} \delta^{(2)}(s,t) \tilde{h}(s,t) \left| \begin{array}{cc} \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial s} & \frac{\partial y}{\partial t} \end{array} \right| ds dt \\
&= \tilde{h}(s,t) \left| \frac{\partial x}{\partial s} \cdot \frac{\partial y}{\partial t} - \frac{\partial x}{\partial t} \cdot \frac{\partial y}{\partial s} \right| \Big|_{s=t=0} \\
&= \frac{\tilde{h}(s,t)}{\left| \frac{\partial s}{\partial x} \cdot \frac{\partial t}{\partial y} - \frac{\partial s}{\partial y} \cdot \frac{\partial t}{\partial x} \right|} \Big|_{s=t=0}, \tag{A.5}
\end{aligned}$$

where we have defined $\tilde{h}(s,t) \equiv h(x(s,t), y(s,t))$. In the last equality we have applied the inverse function theorem (reference?).

A.2 Step function with a function as argument

Assume we want to calculate an integral of the form

$$\int_{x_1}^{x_2} \theta(f(x)) h(x) dx, \tag{A.6}$$

where the Heavyside step function $\theta(x)$ is defined as

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ \frac{1}{2} & \text{if } x = 0 \\ 0 & \text{if } x < 0. \end{cases} \tag{A.7}$$

Let us do a change of integration variable to

$$t = f(x). \tag{A.8}$$

Assume that there exists a unique inverse function $x(t) \equiv f^{-1}(t)$ on the interval $[x_1, x_2]$. Then we get

$$\begin{aligned}
\int_{x_1}^{x_2} \theta(f(x)) h(x) dx &= \int_{f(x_1)}^{f(x_2)} \theta(t) \left(\frac{d}{dt} f^{-1}(t) \right) h(f^{-1}(t)) dt \\
&= \int_{\max(0, f(x_1))}^{\max(0, f(x_2))} \left(\frac{d}{dt} f^{-1}(t) \right) h(f^{-1}(t)) dt. \tag{A.9}
\end{aligned}$$

We may now change the integration variable back to x , and get

$$\int_{x_1}^{x_2} \theta(f(x))h(x)dx = \int_{x'_1}^{x'_2} h(x)dx. \quad (\text{A.10})$$

Here $x'_1 = x_1$, if $f(x_1) > 0$, else $x'_1 = x_0$, where x_0 is chosen such that $f(x_0) = 0$. Equally, $x'_2 = x_2$, if $f(x_2) > 0$, and else $x'_2 = x_0$.

A.3 Properties of Clebsch-Gordan coefficients

For Clabsch-Gordan coefficients we have the general properties

$$(j_1 j_2 m_{j_1} m_{j_2} | J M_J) = (-1)^{j_1 + j_2 - J} \times (j_2 j_1 m_{j_2} m_{j_1} | J M_J), \quad (\text{A.11})$$

$$\sum_{m_{j_1} m_{j_2}} (j_1 j_2 m_{j_1} m_{j_2} | J M_J) (j_1 j_2 m_{j_1} m_{j_2} | J' M'_J) = \delta_{JJ'} \delta_{M_J M'_J}. \quad (\text{A.12})$$

A.4 Properties of spherical harmonics

The spherical harmonics $Y_m^l(\hat{\mathbf{r}}) = \langle \hat{\mathbf{r}} | l m \rangle$ are eigenfunctions of the angular momentum operator \hat{L}^2 . $Y_m^l(\hat{\mathbf{r}})$ has the property (Eq. (5.35b) in [8])

$$Y_m^l(-\hat{\mathbf{r}}) = (-1)^l Y_m^l(\hat{\mathbf{r}}). \quad (\text{A.13})$$

A.5 General quantum mechanics

For the eigenvectors of the position and momentum operators, $|\mathbf{r}\rangle$ and $|\mathbf{k}\rangle$, respectively, we have the closure relation

$$\int d^3x |\mathbf{x}\rangle \langle \mathbf{x}|. \quad (\text{A.14})$$