Chapter 4

Two-particle states and interactions

In this chapter simple symmetry considerations for two-particle states are considered in order to clarify the consequences of the Pauli principle when such states are coupled to good total angular momentum or isospin. In Sec. 4.1 this will be done for free particles and a transformation to total and relative momentum will be considered. By first considering antisymmetric two-particle states for nucleons it is possible to simplify to other systems with smaller degeneracies like two electrons or two $^3$He atoms. It is also possible to exhibit the consequences of dealing with two free identical bosons. These considerations can be generalized to two particles (holes) outside closed shells and several examples are discussed in Sec. 4.2. In Sec. 4.3 some general considerations are collected on the subject of two-body interactions. Examples of relevant interactions for various systems are presented in Sec. 4.4.

4.1 Symmetry considerations for two-particle states

It is important to consider the consequences of the symmetry of two-particle states beyond the obvious ones discussed so far. In particular, it is frequently practical or necessary in dealing with the scattering of two particles to consider the problem in an angular momentum basis. This is particularly practical in the case of short-range interactions where the influence of the interaction is limited to a finite number of angular momentum states. The relevant transformation proceeds from plane waves to spherical waves and is usually treated at the sp level. The consequences of symmetry are substantial, however, and will be illustrated first for two nucleons in free space. It will become clear that these results can then be simplified for other identical fermion systems.
Quantum Theory of Many-Particle Systems

As discussed in Ch. 3, an appropriate one-nucleon state can be labeled by momentum, spin \( \frac{1}{2} \), spin projection, isospin \( \frac{1}{2} \), and isospin projection

\[
| p \ s = \frac{1}{2} m_s \ t = \frac{1}{2} m_t \rangle \equiv | p m_s m_t \rangle. \tag{4.1}
\]

Antisymmetry for two nucleons requires the two-body state to be constructed as follows

\[
| p_1 m_{s_1} m_{t_1}; p_2 m_{s_2} m_{t_2} \rangle = \frac{1}{\sqrt{2}} \left\{ | p_1 m_{s_1} m_{t_1} \rangle | p_2 m_{s_2} m_{t_2} \rangle - | p_2 m_{s_2} m_{t_2} \rangle | p_1 m_{s_1} m_{t_1} \rangle \right\} = \frac{1}{\sqrt{2}} \sum_{S M_S \ T M_T} \left\{ \langle \frac{1}{2} m_{s_1} \frac{1}{2} m_{s_2} | S M_S \rangle \langle \frac{1}{2} m_{t_1} \frac{1}{2} m_{t_2} | T M_T \rangle \times | p_1 p_2 S M_S T M_T \rangle \right. \\
\left. - \langle \frac{1}{2} m_{s_2} \frac{1}{2} m_{s_1} | S M_S \rangle \langle \frac{1}{2} m_{t_2} \frac{1}{2} m_{t_1} | T M_T \rangle \times | p_2 p_1 S M_S T M_T \rangle \right\},
\]

where the individual spins and isospins have been coupled to total spin and isospin in the second equality. Since the dynamics is related to the relative motion of the particles, it is appropriate to switch to a basis involving the center of mass (total) and relative momentum

\[
P = p_1 + p_2
\]

\[
p = \frac{1}{2} (p_1 - p_2). \tag{4.4}
\]

The states in the last line of Eq. (4.2) then both have the same total momentum but opposite relative momentum, \( p \) and \( -p \), respectively. The transformation of the relative momentum quantum number to the basis with the magnitude of this momentum, orbital angular momentum, and its projection for these two cases is given by

\[
| p \rangle = \sum_{L M_L} | p L M_L \rangle \langle L M_L | \hat{p} \rangle = \sum_{L M_L} | p L M_L \rangle Y_{L M_L}^\ast (\hat{p}) \tag{4.5}
\]

\[
| -p \rangle = \sum_{L M_L} | p L M_L \rangle \langle L M_L | -\hat{p} \rangle = \sum_{L M_L} | p L M_L \rangle (-1)^L Y_{L M_L}^\ast (\hat{p}), \tag{4.6}
\]

where the following property of the spherical harmonics has been used in the last equation

\[
Y_{L M_L}^\ast (-\hat{p}) = Y_{L M_L}^\ast (\pi - \theta_p, \phi_p + \pi) = (-1)^L Y_{L M_L}^\ast (\hat{p}). \tag{4.7}
\]
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One may now use the symmetry properties of the Clebsch-Gordan coefficients

\[
\begin{align*}
\left( \alpha m_{s_2} \beta m_{s_1} \mid S M_S \right) &= (-1)^{S+T} \left( \alpha m_{s_1} \beta m_{s_2} \mid S M_S \right) \\
\left( \alpha m_{m_2} \beta m_{m_1} \mid T M_T \right) &= (-1)^{S+T} \left( \alpha m_{m_1} \beta m_{m_2} \mid T M_T \right),
\end{align*}
\]

(4.8)
to write Eq. (4.2) as

\[
\begin{align*}
| p_1 m_{s_1} m_{l_1}; p_2 m_{s_2} m_{l_2} \rangle &= \\
&= \frac{1}{\sqrt{2}} \sum_{S M_S, T M_T, L M_L} \left( \alpha m_{s_1} \beta m_{s_2} \mid S M_S \right) \left( \alpha m_{l_1} \beta m_{l_2} \mid T M_T \right) Y_{LM_L}^* (\hat{p}) \\
&\quad \times [1 - (-1)^{L+S+T}] | P p \ L M_L S M_S T M_T \rangle, \quad (4.9)
\end{align*}
\]

where the coupling to total angular momentum has been performed after the last equality sign. The main point of Eq. (4.9) is the appearance of the factor \([1 - (-1)^{L+S+T}]\). Its presence demonstrates that only when \(L + S + T\) is odd a physical antisymmetric state can occur. Consider the possibilities of an \(S\)-wave interaction. In this case \(L = 0\) and therefore only two possibilities exist: either \(S = 0\) and \(T = 1\) or \(S = 1\) and \(T = 0\) and the two other combinations of spin and isospin are excluded. The spectroscopic notation for the different channels is given by \(2S+1L_J\) where the actual values of \(S\) and \(J\) are inserted and the letter notation for \(L\) is used (\(L = 0\) corresponds to \(S, L = 1\) to \(P, L = 2\) to \(D\) etc.). So the two \(S\)-wave channels for nucleons are denoted by \(^1S_0\) and \(^3S_1\). Since the strong interaction conserves parity and is a scalar with respect to rotations generated by \(J\) and \(T\), the total angular momentum and total isospin, the couplings between different channels must keep the same \(J\) and \(T\) and can change the \(L\)-value by at most 2 (due to the fact that the particles have spin \(1/2\)). This implies that the \(^1S_0\) two-proton channel is uncoupled whereas the proton-neutron channel allows a coupling between the \(^3S_1\) and \(^3D_1\) channels. The latter coupling is realized in nature due to the presence of the so-called tensor force which is instrumental in binding the deuteron and giving it its quadrupole moment. For this reason the coupling to total angular momentum in Eq. (4.9) is necessary for nucleons.
If we now turn to antisymmetric two-particle states for electrons or $^3\text{He}$ atoms which have spin $\frac{1}{2}$, one can use the above results and simply remove all referral to isospin. The corresponding factor that decides which partial wave channels are physically allowed then becomes $[1 + (-1)^{L+S}]$. This shows that an $S$-wave interaction implies a total spin of zero, whereas a $P$-wave requires a total spin of one, etc. Since for these systems one does not need to consider tensor forces, one may forego the coupling to total angular momentum states. In case there is only one spin projection of the species available, the consequences of the Pauli principle are even more dramatic. The Pauli factor now becomes $[1 - (-1)^L]$ showing that there can be no $S$-wave interaction. Recent efforts to cool fermionic atoms to temperatures substantially below the Fermi temperature have to deal with this lack of $S$-wave interaction when cooling these systems in magnetic and optical traps. For spinless bosons a similar analysis shows that only states with even $L$ survive consistent with the experimental observations discussed in Sec. 1.4.

4.2 Two particles outside closed shells

In finite systems with spherical symmetry one may also consider the coupling of angular momentum states for two particles. The consequences of the Pauli principle are also striking here. One can illustrate this example by using second quantized notation. Consider two particles added to a closed-shell nucleus such as discussed in Sect. 3.3. For the moment assume that these two particles are either two protons or two neutrons and that they are added in the same sp shell characterized by sp angular momentum $j$. Such a state can be written as

$$|\Phi_{jm,jm'}\rangle = a_{jm}^\dagger a_{jm'}^\dagger |\Phi_0\rangle. \quad (4.10)$$

It is immediately clear that a total angular momentum of $J = 2j$ is not possible since this would require both particles to have the same maximal projection of the angular momentum. The allowed total angular momentum states can be obtained by coupling the sp angular momenta and using the symmetry property of the Clebsch-Gordan coefficients, and the anti-commutation relation of the particle addition operators as follows

$$|\Phi_{jj,JM}\rangle = \sum_{mm'} (j \ m \ j \ m' \ |J \ M\rangle |\Phi_{jm,jm'}\rangle$$

$$= \sum_{mm'} (j \ m' \ j \ m \ |J \ M\rangle |\Phi_{jm',jm}\rangle$$
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\[
= \sum_{mm'} (-1)^{2j-J} \left( j \ m \ j' \ M \right)\left( -1 \right) \Phi_{jm,jm'}
\]

\[
= (-1)^J \sum_{mm'} \left( j \ m \ j' \ M \right) |\Phi_{jm,jm'}\rangle
\]

\[
= (-1)^J \left[ \Phi_{jj,JM} \right],
\]

(4.11)

where a change of dummy indices was used in the first equality. The factor \((-1)^J\) ensures that only even values of \(J\) yield physical states. To include isospin one proceeds in a similar fashion. Denoting the uncoupled states by

\[
|\Phi_{jmmu,jm'm'u'}\rangle = a_{jmmu}^\dagger a_{jm'm'u'}^\dagger |\Phi_0\rangle,
\]

(4.12)

one obtains

\[
|\Phi_{jj,JMTM'}\rangle = \sum_{mm'mu,m'm'u'} \left( j \ m \ j' \ M \right) |\Phi_{jmmu,jm'm'u'}\rangle
\]

\[
= (-1)^{J+T+1} |\Phi_{jj,JMTM'}\rangle.
\]

(4.13)

In this case \(J + T\) must be odd. This result is consistent with the previous one since for two protons or two neutrons the total isospin must be one. It is useful to determine the normalization of the states considered above. An illustration of these results is given in Fig.

For electrons in atoms one can apply the same strategy. In this case the uncoupled states can be denoted by

\[
|\Phi_{\ell mm_s,\ell m'_s}\rangle = a_{\ell mm_s}^\dagger a_{\ell m'_s}^\dagger |\Phi_0\rangle,
\]

(4.14)

one obtains

\[
|\Phi_{\ell,LMs,MS}\rangle = \sum_{m_m,m'_s} \left( \ell \ m_\ell \ |L M_L\rangle |\ell m_s\rangle \right) |\Phi_{\ell mm_s,\ell m'_s}\rangle
\]

\[
= (-1)^{L+S} |\Phi_{\ell,LMs,MS}\rangle.
\]

(4.15)

In this case \(L + S\) must be even which is illustrated in Fig. for the lowest states in C.

4.3 General discussion of two-body interactions

The main problem in dealing with a many-particle system is to properly deal with the basic interaction between the constituent particles. Before
giving some explicit examples of these interactions, it is useful to put this discussion in a wider perspective. All interactions between the particles of the Standard Model of the Electroweak and Strong Interactions take place by the exchange of spin-1 bosons between spin-$\frac{1}{2}$ fermions. These fermions include all the quarks which come in three colors and six flavors, and all the leptons which include the electron, the muon, and the tau together with their corresponding neutrino’s. The exchanged bosons include the photon of Quantum Electrodynamics (QED), the the gluons of Quantum Chromo Dynamics (QCD), and the $W^\pm$ and $Z$ bosons complementing the Electroweak interaction.

In general, interactions between particles in any setting can be considered in terms of a generalized exchange mechanism. Depending on the circumstances the “particle” that is exchanged between the constituent fermions may be a low-energy bosonic excitation (of any integer spin) of the medium. For example, electrons in a solid can exchange the lattice vibrations (phonons) of the core atoms. It will be useful to keep this exchange mechanism in mind even though it is not always obvious that it is at work. An example of such a case is provided by the instantaneous Coulomb repulsion between two electrons which does originate from the one-photon exchange mechanism [Sakurai (1967)].

Apart from their obvious thermodynamic relevance, one cannot overemphasize the importance of the low-energy excitations of a many-particle system. Their excitation energy provides a new energy scale which is not present in the vacuum. This can be illustrated at several levels by considering nuclei. The nucleons making up the nucleus are themselves composite objects made up of quarks in such a way that no explicit color is present. A nucleon can thus be considered as the lowest bound state of three quarks with total angular momentum and isospin $\frac{1}{2}$. Experimentally, it has been impossible to isolate individual quarks up to now and one can therefore say that the energy scale associated with generating individual quarks is infinite for all practical purposes, although QCD in the high-energy and experimentally accessible domain describes a weakly interacting system of massless quarks predominantly interacting by the exchange of single massless gluons. In the low-energy domain, where non-perturbative effects and confinement dominate, the lowest excited states of QCD are found at excitation energies of the order of hundreds of MeV. A particularly important example is the $\Delta$-isobar at 1232 MeV which has spin and isospin $\frac{3}{2}$. The energy difference between the nucleon and the $\Delta$ provides a new energy scale. In addition there are bosonic excitation modes of QCD which can
be interpreted in terms of quark-antiquark states. The lowest-energy state is the pion with angular momentum 0 and isospin 1 which also has opposite parity from the nucleon and the $\Delta$. The energy of the pion is about 140 MeV. One consequence of the low energy of the pion and the experimental result that it couples strongly to the nucleon is that the exchange mechanism discussed above is very important. This means that part of the interaction between two nucleons is represented by the exchange of individual pions. Since pions are the lowest-mass mesons, their exchange provides that part of the interaction which has the longest range illustrating the connection between the mass (energy) of the exchanged particle and the range of the interaction. The idea of a meson-exchange mechanism to describe the strong interaction dates back to [Yukawa (1935)]. Exchange mechanisms of higher-energy mesons with other quantum numbers can then be used to describe the interaction between two nucleons at shorter range. The energy scale which involves the explicit excitation of other QCD states therefore starts at 140 MeV with an additional important state (the $\Delta$) at 300 MeV.

This first example demonstrates that the elementary excitations of the QCD field theory are subject to a different energy scale compared to the non-interacting free field theory in which the quarks and gluons have no mass. In the interacting theory the colorless bound states dominate at low energy and explicit single quark and gluon degrees of freedom with color are effectively at infinite excitation energy. Depending on the objectives one must therefore make a choice which are the relevant degrees of freedom that most efficiently describe the properties of the system under study. In the case of one nucleon one may attempt a solution of QCD on the lattice while in the case of many nucleons it is more fruitful to start from nucleons which interact by means of the above outlined meson-exchange mechanism using input from experimental data. This approach certainly makes sense on account of the overwhelming experimental evidence that nucleons maintain much of their identity when they are brought together with other nucleons in nuclei.

In general, one can say that the experimentally observed low-lying excitations of a system themselves play an important role in understanding the physics of the many-particle system. Sometimes these excitations are referred to as elementary modes of excitation or quasiparticles. To understand the physics it may be important to treat the interaction between these modes. In liquid $^4$He one finds single-particle-like excitations, which are usually called quasiparticles, but also bosonic collective excitations like phonons and rotons. One level of understanding is achieved by describing
the liquid in terms of atoms interacting with each other, another level is achieved by working with phonons and rotons [Nozières and Pines (1990)]. Whereas the latter mode of description has certainly not yet been completely successful in bringing about a microscopic understanding of rotons, the former description mode is restricted by its inherent phenomenological character. Indeed, even if one can numerically calculate certain properties of the system microscopically, this does not imply that one understands the physics very well at the same time.

In the case of a nucleus one cannot even think of abandoning the nucleon description before one can solve QCD with an accuracy better than the lowest energy scale that is relevant for the system under study. In a nucleus the lowest excitation modes have energies of the order of MeV’s in light nuclei, but in heavy nuclei the lowest excited state (of boson character) may be at about 50 keV. Again, one is dealing with an energy scales that is introduced because nucleons are brought together in a nucleus. The nucleons, because they experience an overall attractive interaction with each other, clump together to form a self-bound system with a size dictated by the effective interactions (interactions in the nuclear medium) between the nucleons. This size in turn introduces a thin new energy scale in a self-consistent sense. One can understand this from a sp point of view in which the nucleons find themselves bound in the average attractive field of the other nucleons. This potential is obviously of the size of the nucleus and as a consequence the new energy scale related to the sp energies of this potential is introduced. An empirical potential of this kind was presented in Sec. 3.3. Associated with this new energy scale one encounters collective behavior of nuclei that are best understood in terms of nucleons moving coherently between these sp levels. It is therefore profitable to use the elementary mode of excitation description which can be applied to any many-particle system.

In a similar vein it is hard to conceive that one would be interested in understanding the Helium liquids in terms of a Hamiltonian at the level of the Coulomb interactions between the electrons, the alpha particles, and the electrons and the alpha particles (or $^3$He nuclei). Instead, many-particle theory attempts to explain the properties associated with the relevant energy scales of the liquid, which is in degrees Kelvin (again a new energy scale associated with the many-particle nature of the system), in terms of Helium atoms which experience an "effective" interaction characterizing the behavior of isolated atoms in free space. This interaction takes into account both the polarization effect of the electron cloud of one atom on
the cloud of another, representing the long-range part of the interaction, as well as simulates the effect of the Pauli principle between the electrons in the different atoms. The latter effect becomes very important when the atoms are brought close together and results in a strongly repulsive effective interaction between the atoms at short distances. This Lennard-Jones type interaction is therefore used to simulate effects that are associated with degrees of freedom that are important at higher energy scales. A helpful feature that facilitates this approach is the neat separation of electronic excitation energies that exceed those in the liquid by four to five orders of magnitude.

A similar simplification must be made in the case of electrons in a molecule or solid. The original Hamiltonian describing the Coulomb interaction between nuclei, nuclei and electrons, and electrons and electrons is too general to provide a realistic starting point for the description of the solid state. Instead, the nuclei are first considered to be localized in a lattice which most of the atomic electrons still tightly bound to these nuclei. Only those electrons that become delocalized form the relevant electronic degrees of freedom that are subject to a periodic potential that leads to the observed band structure. In this context it is good to repeat some basic questions associated with the physics of solids which were formulated in [Anderson (1963); Anderson (1984)] (without attempting any answers at this time):

(1) Why is a solid?
(2) How does one describe a solid from a truly fundamental point of view in which atomic nuclei as well as the electrons are treated truly quantummechanically?
(3) How and why does a solid hold itself together?

4.4 Examples of relevant two-body interactions

After this general perspective it is helpful to present some relevant examples of interactions used in many-particle theory. In addition, we will consider the evaluation of the relevant two-body matrix elements that appear in the Fock-space two-body operator given e.g. in Eq. (2.41). Often an interaction is grounded in theory but in some cases a certain amount of phenomenology (constrained by experiment) is involved. Such contraints may involve an accurate description of the corresponding fermion-fermion scattering in free space. In many systems the basic interaction only depends on the relative
distance between the particles and no explicit spin (or isospin) dependence needs to be considered. Spherical symmetry reduces this dependence further to the magnitude of this relative distance. For such an interaction two-body matrix elements in coordinate space yield (suppressing discrete quantum numbers)

\[
\langle r_1 r_2 | V(r_{op}) | r_3 r_4 \rangle = \langle R r | V(r_{op}) | R' r' \rangle \\
= \delta(R - R') (r | V(r_{op}) | r') = \delta(R - R') \delta(r - r') V(r),
\]

(4.16)

where a transformation to center-of-mass and relative coordinates has been used

\[
R = \frac{1}{2} (r_1 + r_2) \\
r = r_1 - r_2,
\]

(4.17)

(4.18)

and similarly for the primed coordinates. An interaction with such matrix elements in coordinate space is called a local interaction since it is diagonal in the relative coordinate. Not all interactions are local but an important example of a local one is the Coulomb interaction between charges \(q_1 e\) and \(q_2 e\)

\[
V_C(r) = \frac{q_1 q_2 e^2}{r}
\]

(4.19)

Another useful interaction is the socalled Yukawa interaction given by

\[
V_Y(r) = V_0 \frac{e^{-mr}}{\mu r}.
\]

(4.20)

In the case of nucleons, a considerable amount of operators is required to describe the interaction accurately. The simplest of these involves the spin-spin interaction which is usually written as

\[
V_{spin} = V_S(r) \sigma_1 \cdot \sigma_2,
\]

(4.21)

where the dot product involves the Pauli spin matrices of the two particles. Since \(\sigma_1 \cdot \sigma_2\) corresponds to \(4s_1 \cdot s_2 / \hbar^2\) one requires two-particle states coupled to good total spin for the eigenstates of this operator. Using the identity

\[
2s_1 \cdot s_2 = S^2 - s_1^2 - s_2^2,
\]

(4.22)

where \(S = s_1 + s_2\), one obtains

\[
\langle S'M' | \sigma_1 \cdot \sigma_2 | S M \rangle = (2S + 1 - 3) \delta_{S,S'} \delta_{M,M'},
\]

(4.23)
which yields -3 for $S = 0$ and 1 for $S = 1$. Spin-spin interactions are not present in the basic interaction between electrons or $^3$He atoms but do appear in an effective form when the interaction between these fermions is considered inside the medium. Nuclear interactions also carry an explicit isospin dependence which leads to

$$V_{\text{isospin}} = V'(r) \tau_1 \cdot \tau_2,$$

where the $\tau$ matrices are the isospin equivalent of the Pauli spin matrices. The result corresponding to Eq. (4.23) reads in this case

$$\langle T' M' | \tau_1 \cdot \tau_2 | TM \rangle = (2T(T+1) - 3) \delta_{T',T} \delta_{M,M'},$$

showing that states with good total isospin need to be considered. In addition to the spin/isospin dependent terms with their own radial dependence additional operators are required. It is possible to give an accurate account of the scattering of two nucleons up to the threshold of pion production by considering an interaction of the following form [Wiringa et al. (1984)]:

$$v^{14}(1,2) = \sum_{p=1,14} \left[ v_p^e(r) + v_p^f(r) + v_p^s(r) \right] \mathcal{O}_{12}^p. \quad (4.26)$$

The local radial dependence ($r = |r_1 - r_2|$) is governed by a long-range pion-exchange term, $v_p^e$, an intermediate-range part $v_p^f$, and a short-range contribution, $v_p^s$. Fourteen operators $\mathcal{O}_{12}^p$ need to be considered

$$\begin{align*}
1 & \quad \tau_1 \cdot \tau_2 & \quad \sigma_1 \cdot \sigma_2 & \quad \sigma_1 \cdot \sigma_2 \cdot \tau_1 \cdot \tau_2 \\
S_{12} & \quad \sigma_1 \cdot \tau_2 & \quad L \cdot S & \quad L \cdot S \cdot \tau_1 \cdot \tau_2 \\
L^2 & \quad \tau_1 \cdot \tau_2 & \quad L^2 \cdot \sigma_1 \cdot \sigma_2 & \quad L^2 \cdot \sigma_1 \cdot \sigma_2 \cdot \tau_1 \cdot \tau_2 \\
(L \cdot S)^2 & \quad (L \cdot S)^2 & \quad \tau_1 \cdot \tau_2
\end{align*} \quad (4.27)$$

This set of operators contains the usual Pauli spin and isospin matrices, the tensor operator

$$S_{12} = 3 (\sigma_1 \cdot \hat{r}) (\sigma_2 \cdot \hat{r}) - \sigma_1 \cdot \sigma_2,$$

the relative orbital angular momentum $L$, and the total spin $S$ of the pair. Employing a partial-wave basis one can use standard angular momentum techniques to determine the matrix elements of these operators [Sakurai (1994); Messiah (1999)]. Clearly it is necessary to include a coupling to total angular momentum to keep such calculations manageable. The coupling to such state was outlines in Sec. 4.1.
Matrix elements of interactions in momentum space are needed when considering scattering problems or large homogeneous systems. Using the transformation to total and relative momenta considered in Eqs. (4.3) and (4.4), one obtains for a central spin and isospin independent interaction (suppressing these discrete quantum numbers)

$$\langle p_1 p_2 | V(r_{op}) | p_3 p_4 \rangle = \langle P p | V(r_{op}) | P' p' \rangle = \delta_{P, P'} \langle p | V(r_{op}) | p' \rangle.$$  \hspace{1cm} (4.29)

One may also use wave vectors for the matrix element for the relative motion. Using this basis one needs to calculate

$$\langle k | V(r) | k' \rangle = \frac{1}{V} \int d^3 r \exp \{i(k' - k) \cdot r \} V(r). \hspace{1cm} (4.30)$$

This matrix element can be manipulated further by using the standard expansion

$$\exp \{i \mathbf{q} \cdot \mathbf{r} \} = 4\pi \sum_{\ell m} i^\ell Y_{\ell m}^*(\hat{r}) Y_{\ell m}(\hat{q}) j_\ell(qr), \hspace{1cm} (4.31)$$

where \( j_\ell \) is the spherical Bessel function. Inserting this result in Eq. (4.30) and performing the angular integration one obtains

$$\langle k | V(r) | k' \rangle = \frac{4\pi}{V} \int dr \ r^2 j_0(qr)V(r), \hspace{1cm} (4.32)$$

with \( q = |k - k'| \). For the case of the Yukawa interaction of Eq. (4.20) this last integral can e.g. be found in [Gradshtein and Ryzhik (1980)] with the result

$$\langle k | V_Y(r) | k' \rangle = \frac{4\pi V_0}{V} \frac{1}{\mu \mu' + (k' - k)'^2}. \hspace{1cm} (4.33)$$

This result can also be used to obtain the matrix element of the Coulomb interaction

$$\langle k | V_C(r) | k' \rangle = \frac{4\pi q_1 q_2 e^2}{V (k' - k)^2}, \hspace{1cm} (4.34)$$

where the case \( k = k' \) requires special consideration but can usually be omitted on account of cancellations as in the case of the homogeneous electron gas [Fetter and Walecka (1971); Mahan (1990); Gross et al. (1991); Mattuck (1992)] as discussed in Sec. 5.2.
Another type of interaction that may be useful to consider is of the following form

$$V(r) = A e^{-ar}.$$  \hspace{1cm} (4.35)

Such an interaction may be used to describe the short-range part of the atom-atom repulsion [Aziz et al. (1979)] allowing Fourier transformation unlike the Lennard-Jones type interactions. Noting that the relevant momentum space matrix element only depends on the magnitude of the transferred momentum \( q = |q| = |k' - k| \) between the particles in the case of a local interaction, one can show that for the interaction of Eq. (4.35) one obtains

$$\langle k | V(r) | k' \rangle = V(q) = -\frac{4\pi A}{V} \frac{d}{dx} \frac{1}{\sqrt{\alpha^2 + q^2}}.$$  \hspace{1cm} (4.36)

This form is useful also when one is interested in obtaining matrix elements in a partial-wave basis.

In a partial-wave basis one is looking for matrix elements of the form

$$\langle kLM_L | V | k'L'M'_L \rangle = \int d\hat{k} \langle LM_L | \hat{k} \rangle \int d\hat{k}' \langle \hat{k}' | L'M'_L \rangle \langle k | V(r) | k' \rangle.$$  \hspace{1cm} (4.37)

In the case of a Yukawa interaction one may now proceed by rewriting Eq. (4.33) in the following form

$$\langle k | V_Y(r) | k' \rangle = -\frac{4\pi V_0}{V} \frac{1}{\mu} \frac{1}{2kk'} \frac{1}{\mu^2 + k^2 + k'^2}.$$  \hspace{1cm} (4.38)

This last fraction may be expanded using the following relation involving Legendre function \( Q_\ell \) and Legendre polynomials \( P_\ell \)

$$\frac{1}{\mu^2 + k^2 + k'^2} = \sum_{\ell=0}^\infty \frac{(2\ell + 1)}{2kk'} \frac{1}{\mu^2 + k^2 + k'^2}$$

$$= \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell 4\pi Q_\ell \left( \frac{\mu^2 + k^2 + k'^2}{2kk'} \right) P_\ell(\cos \theta_{kk'})$$

$$\times Y^*_{\ell m}(\hat{k})Y_{\ell m}(\hat{k'}).$$  \hspace{1cm} (4.39)

In the last equality the addition theorem for spherical harmonics was used. Note that the argument of the Legendre function must be larger than 1 while the argument of the Legendre polynomial must be less than 1. Inserting these results into Eq. (4.37) one finally obtains after performing the
angular integrations

\[
\langle kLM_L | V | k' L' M_L' \rangle = \delta_{LL'} \delta_{M_L M_L'} \frac{(4\pi)^2 V_0}{\sqrt{\mu 2k k'}} Q_L \left( \frac{\mu^2 + k^2 + k'^2}{2kk'} \right). \tag{4.40}
\]

The first three Legendre functions are given by

\[
Q_0(z) = \frac{1}{2} \ln \left( \frac{z + 1}{z - 1} \right)
\]

\[
Q_1(z) = \frac{z}{2} \ln \left( \frac{z + 1}{z - 1} \right) - 1
\]

\[
Q_2(z) = \frac{3z^2 - 1}{4} \ln \left( \frac{z + 1}{z - 1} \right) - \frac{3}{2} z. \tag{4.41}
\]

4.5 Exercises

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