Convergent Close-Coupling Calculations of Positron-Helium Collisions

This thesis is presented for the degree of Doctor of Philosophy

by

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Declaration

I declare that this thesis is my own account of my research and contains as its main content, work which has not previously been submitted for a degree at any tertiary education institution.

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ABSTRACT

The Convergent Close Coupling (CCC) method is applied, for the first time, to the scattering of positrons on helium. The helium target wave functions are obtained within various configuration interaction (CI) expansions. In the full CI expansion the two electrons are treated equally and thus all electron-electron correlations are taken into account. In the frozen-core (FC) approximation the CI expansion fixes one of the electrons to be described by a pure 1s orbital of He^{+}, while maintaining the required singlet and triplet symmetries. Lastly, the multi-configuration (MC) approximation relaxes the FC approximation to allow the description of the inner electron to include several low-lying orbitals and is therefore more accurate than the FC approximation. The accuracy of the target wave functions is tested by comparing the calculated energy levels with the experimental data.

Based on positron-hydrogen scattering, comprehensive close-coupling formulas for positron-helium scattering are developed. The reduced two-centre V-matrix elements are derived in momentum space for various channels. These include direct, excitation and rearrangement channels, i.e. positronium formation.

We first consider low energy positron-helium elastic scattering for energies below the positronium formation threshold of 17.8 eV. Utilizing a single-centre expansion the elastic cross section and phase shifts have been calculated as a function of the positron incident energy. The calculations agree very well with the experimental data and the variational calculations, but not previous single-or double-centre close-coupling calculations.

We then consider energies above the first ionization threshold (24.6 eV) and calculate helium elastic, excitation, fragmentation and total cross sections within the single-centre expansion approach. Good agreement with the available experimental and other theoretical results has been obtained.

The studies have proved that a single-centre expansion, with accurate target state description, can deliver accurate data of practical value over a broad range of energies. However in the low-energy region, between the positronium formation threshold of 17.8 eV and the ionization threshold of 24.6 eV, implementation of the two-centre expansion is required. We expect this work to be undertaken in the near future, based on the derivations presented in this thesis.

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1. INTRODUCTION

One of the great successes of the twentieth century physics is the discovery of the positron, e^+, first predicted by Dirac in his relativistic theory of electrons (Dirac, 1930), subsequently discovered by Anderson (1933) and confirmed by Blackett and Occhialini (1933). The positron has the same mass and spin as the electron. It carries the same amount of charge as the electron but with the opposite sign. It is therefore the anti-particle of electron. Although the positron is a stable particle under vacuum, it will annihilate with an electron when it interacts with normal matter.

Due to the unique properties of positrons, the study of their collisions with atoms, molecules and solids is of great interest not only to the fundamental understanding of interactions between matter and antimatter, but also to the comparisons with the phenomena observed with other projectiles, such as electrons, protons and anti-protons. This can provide information about the effects on the scattering process of different masses and charges and hence offer a test of different theoretical approximations. For example, the opposite sign of the charge on the positron and electron has significant effects on the collision process. The important electron-electron exchange effect between the incident electron with the target electrons in electron-atom scattering does not exist in positron-atom scattering. The repulsive static interaction between the positron and atom has the same magnitude but opposite sign to the attractive force between the electron and the atom. However, the polarisation potential is attractive and of the same magnitude for both positrons and electrons, due to the dependence of the polarisation potential on the quadratic form of the charge of the projectile. The repulsive static and attractive polarisation interactions between the positron and atom tend to cancel each other and make the overall interaction generally less attractive than that between an electron and the atom. Consequently, at low energies, when polarisation effects are most important, total scattering cross sections are usually much smaller for positrons than for electrons, except for alkali atoms for which significant contribution from positronium formation can occur, while this process is absent for electrons. Another consequence of the partial cancellation of the static and polarisation potentials is that a positron is much less likely to be bound to an atom than an electron. The opposite sign of the static and polarisation potentials also causes the s-wave elastic scattering phaseshift to change sign with incident positron energy between 1 eV and 3 eV, where the contribution from S-wave to the total elastic scattering cross section is zero. This gives rise to the Ramsauer minimum in the cross sections for some atoms.

The absence of exchange in positron-atom scattering is also an important incentive for the study of the low energy positron scattering. It might have been expected that the absence of exchange effects between the incoming projectile and the target electrons would lead to a simpler formulation of the scattering process than is the case with electrons. Unfortunately the strong correlation between positrons and electrons due to the attractive electrostatic interaction between them, introduces even bigger challenges to the description of the collision processes. One of the consequences from this correlation is the positronium formation in which the incident positron forms a stable state by capture of one target electron. Then the collision becomes a two-centre problem in which the centres of the atom and the positronium have to be considered simultaneously. Targets with two or more electrons give rise to a further complication, namely the exchange effect with the electron in the positronium and the other electron in the ion, as well as within the target.

At sufficiently high projectile energies the polarisation and exchange interactions eventually become negligible compared with the static interaction. The same magnitude of the static interaction for positrons and electrons will result in a merging of the corresponding positron- and electron-atom scattering cross sections at sufficiently high projectile energy (Kauppila *et al*, 1981).

As in electron-atom collisions, many processes can occur during the interaction of positrons and atoms. A schematic representation of the process is shown in Figure 1.1. At low energies, elastic scattering is usually the only open channel apart from annihilation of the positron with one of the electrons of the helium atom. The annihilation process has been studied theoretically and experimentally (Van Reeth and Humberston, 1998; Laricchia and Wilkin, 1997; Kurz *et al*, 1996). The cross section for the annihilation is up to 10^{-5} smaller than that of elastic scattering so the annihilation channel can be safely neglected in scattering calculations. As the positron's energy increases, various inelastic channels become accessible, including positronium formation, target excitation and ionisation. The theoretical modelling of these processes in positron-atom collisions is much more difficult than the case of electron-atom collisions. The accurate determination of the various parameters characterising the collision processes provides a stringent test of different approximation methods. The most detailed theoretical studies have been performed for simple atoms and molecules like atomic hydrogen, helium, the alkali atoms (quasi-one-electron atoms) and molecular hydrogen. For detailed reviews, please refer to Ghosh *et al* (1982), Bransden and Noble (1994)

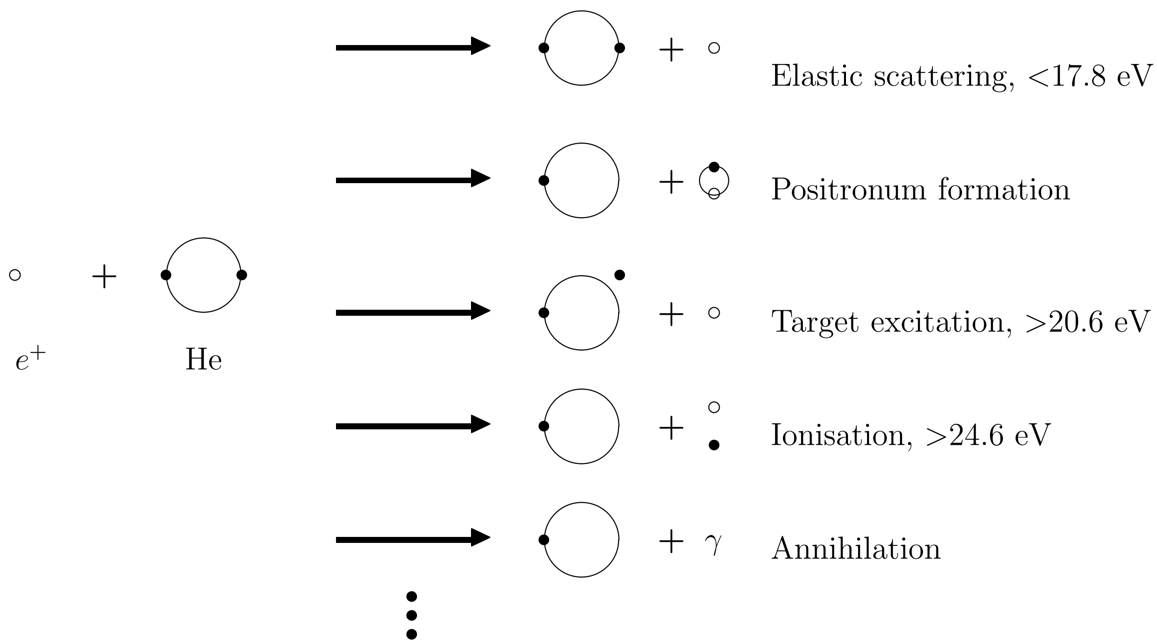

Fig. 1.1: The various positron helium interaction channels are depicted schematically.

and the recent book by Charlton and Humberston (2001).

In positron-helium collisions, elastic scattering is the only open channel for energy below 17.8 eV which is the threshold for ground state positronium formation. For energies up to 20.6 eV, the positronium formation remains the only open inelastic channel. At 20.6 eV, the excitation of the helium 2^1S state becomes possible. As the energy is increased, excitations of higher helium states and other bound states from positronium have to be considered. For energies above 24.6 eV, ionisation of the helium atom can occur. Many theoretical calculations (Parcell *et al*, 1983, 1987; Campeanu *et al*, 1996; Schultz and Olson, 1988; Campeanu *et al*, 1996; Walters *et al*, 1997; Campbell *et al*, 1998; Van Reeth and Humberston, 1999*b*; Dunn *et al*, 2000) as well as experimental measurements (Stein *et al*, 1978;

Kauppila *et al*, 1981; Fromme *et al*, 1986; Jacobsen *et al*, 1995; Moxom *et al*, 1996) have been done for the elastic scattering, excitation, positronium formation and ionisation. At even higher energies, double excitation and ionisation of the helium atom could also be possible along with all other channels.

In the following sections, a brief review of theoretical modelling of collisions between positrons and helium with various methods will be given. The methods reviewed have all been used in some form or other to provide theoretical predictions for positron-helium scattering. Some are more sophisticated than others. The experimental results will be mentioned as a comparison to theory.

1.1 Close-Coupling Approximation

The most commonly used method is the close coupling scheme. The total wave function may be formally expanded in terms of complete sets of the discrete and continuum states of the target atom and those of positronium. To avoid the double complete expansion and improve the rate of convergence, a truncated expansion involving states of both target atom and positronium is usually applied. Substituting the expansion into the Schrödinger equation, a set of coupled integro-differential equations is obtained. Numerically solving these equations will give the parameters characterising the collision processes. A detailed study of positron-hydrogen scattering was made by Kernoghan *et al* (1995) who used 18 states including 9 hydrogen and 9 positronium discrete and pseudostates.

The close-coupling approach has also been applied on the low energy positron-hydrogen scattering by Mitroy's group. In their calculations both physical states and pseudostates of hydrogen and positronium were used (Mitroy, 1993*b*,*a*; Mitroy and Stelbovics, 1994; Mitroy *et al*, 1994; Mitroy and Ratnavelu, 1995; Mitroy, 1995, 1996). The similar approach has also been used in positron-alkali atom scattering (Mitroy and Ratnavelu, 1994).

At energies below the first inelastic threshold, ie. positronium formation, a single centre expansion of the hydrogenic target states should suffice to describe the scattering. Bray and Stelbovics (1992*b*) applied a convergent close-coupling (CCC) expansion in which the projectile-target system wave functions are expanded in terms of the target atom states generated in an L^2 basis. In the CCC method, the Schrödinger equation was thus reduced to a set of close-coupling equations and which were solved numerically in momentum space rather than in configuration space. Bray and Stelbovics showed that this type of single centre expansion approach would lead to converged scattering amplitude at low energies.

For positron-helium scattering, the most comprehensive study with a close-coupling method was carried out by Campbell *et al* (1998). They used two expansions . The first one was the 27-state approximation including 24 He states (true atomic eigenstates and pseudostates) and the first 3 positronium states. The second expansion used only helium states (30-state) with extra 6 F-pseudostates added to the 24-state used in the first approximation. The problem was solved in the configuration space. Two assumptions were introduced in the modelling of helium target structures; firstly the helium ion was assumed to be left in its ground state after positronium formation and secondly the helium atomic wave functions were formed in a frozen orbital approximation. The atomic eigenstates, pseudostates and positronium states were obtained by diagonalizing the atom and positronium Hamiltonian using a Slater basis

$$\psi_{nl}(\boldsymbol{r}) = r^n e^{-\lambda r} Y_{lm}(\hat{\boldsymbol{r}}) \tag{1.1}$$

where l is the orbital angular momentum of the orbital, m is its magnetic quantum number , n is an integer with $n \geqslant l$ and λ is a parameter which needs to be the same for all basis functions (1.1).

For the 27-state approximation, only results in the energy range above the positronium (1s) formation were given. At lower energies, unsatisfactory results were obtained and it was suggested that this might be due to the lack of convergence from the use of inaccurate helium ground state wave function.

The predicted total cross sections from both 27-state and 30-state approximations agreed well with the experimental results from Stein *et al* (1978), Kauppila *et al* (1981) and Mizogawa *et al* (1985) for the energy range above the threshold of positronium formation. For lower energies, general agreement was obtained in terms of the shape and the reproduction of Ramsauer-Townsend minimum near 2 eV, while the theoretical results are significantly larger than the experimental data.

For positronium formation, the cross sections predicated by the 27-state approximation agree well with the existing experimental data of Moxom *et al* (1993) up to about 60 eV and with the data of Fornari *et al* (1983) and Diana *et al* (1986) until 90 eV. For energies above 100 eV, the theoretical results are much lower than the experimental data from Diana *et al* (1986) and Fromme *et al* (1986) and closer to the data from Overton *et al* (1993). Another close-coupling calculation by Hewitt *et al* (1992), using both helium and positronium states with a simple one-electron model for the helium atom, showed less satisfactory agreement with the experimental data. The results from Chaudhuri and Adhikari (1998), who include only 5 helium and 3 positronium states in the expansion, agree well with the experimental data of Moxom *et al* (1993) at low energies and have a better agreement with the higher energy data of Overton *et al* (1993). However, the theoretical data is much lower than the experimental data for energies corresponding to the maximum cross section.

It was predicted, with the 27-state approximation, that the helium 2^1P excitation cross section initially rose quite steeply and then became fairly flat up to 150 eV. The results are in reasonably good agreement with the experimental data of Coleman *et al* (1982) and Mori and Sueoka (1994). The excitation cross sections for helium have also been obtained using various forms of the close coupling approximation, either with or without including positronium states in the expansion of the wave function. Willis and McDowell (1982) used a 5-state CCA expansion without any positronium states. Their results for both $n = 2$ transitions are significantly larger than those obtained with the distorted wave approximation of Parcell *et al* (1983, 1987) at all energies up to 150 eV. As already mentioned Hewitt *et al* (1992) included both helium and positronium states but used a simple one-electron model for the helium atom. Despite the simplicity of the helium model used, the sum of the 2^1S and 2^1P excitation cross section from Hewitt *et al* (1992) is in reasonable agreement with the experimental results by Mori and Sueoka (1994) at energies below 36 eV but becomes 50% larger than the experimental data at higher energies.

For the ionisation of helium, the 27-state calculation of Campbell *et al* (1998) is generally in agreement with the available experimental data from Fromme *et al* (1986), Knudsen *et al* (1990), Mori and Sueoka (1994) and Ashley *et al* (1996), except that the experimental data from Fromme *et al* (1986) is much lower than the theoretical results for energies above 80 eV.

As for the total fragmentation cross section (the sum of positronium formation and ionisation), the general agreement between theoretical predictions from both 27-state and 30-state expansions and experimental data from Fromme *et al* (1986) and Moxom *et al* (1996) was found. The exceptions are the positronium formation threshold given by the 30-state approximation is higher than the experimental data and the cross section is lower than the experimental data at the peak energies (near 60.0 eV).

1.2 Kohn Variational Method

Humberston and his co-workers have developed an alternative approach to incorporate the correlations between the colliding particles into the formulation of positron-atom scattering by using a trial wave function in a variational method. The method was initially developed for calculating S-wave phaseshift in positron-hydrogen scattering (Schwartz, 1961). Subsequently it was extended to obtain higher wave phaseshifts for elastic scattering and then to calculate positronium formation cross sections (Houston and Draachman, 1971; Brown and Humberston, 1984, 1985). The method has also been used for positron-helium collisions (Humberston, 1973; Campeanu and Humberston, 1975; Humberston and and, 1980; Van Reeth and Humberston, 1995; Van Reeth *et al*, 1996).

The Kohn variational method is based on the following functional

$$K_v = \tan\ \eta_v = \tan\ \eta_t - < \Psi_t | L | \Psi_t >, \tag{1.2}$$

where $K_v = \tan\ \eta_v$, η_v is the variationally determined phaseshift; $L = 2(H - E)$; Ψ_t is the trial wave function representing the scattering process and η_t is the associated trial phaseshift.

The trial wave function is usually chosen as a combination of positron and target wave functions plus some short-range Hylleraas terms which represent the various inter-particle correlations. For example, for positron-hydrogen scattering, the trial wave function can be written as

$$\Psi_t = S + K_t C + \sum_i (c_i \phi_i), \tag{1.3}$$

where

$$K_t = \tan\ \eta_t.$$

S and C are associated with the wave function of positron and target atom and

$$\phi_i = \exp[-(\alpha r_1 + \beta r_2 + \gamma r_{12})] r_1^{k_i} r_2^{l_i} r_{12}^{m_i}$$

is the Hylleraas term and r_1, r_2 and r_{12} are the distances of the positron, the target electron and the positron-electron system with the atom assumed static at the origin of the coordinate system. The summation over i in (1.3) usually includes all the correlation terms such that

$$k_i + l_i + m_i = \omega, \tag{1.4}$$

where k_i, l_i, m_i and ω are positive integers. The parameter ω is considered as a measure of the quality of the trial wave function; larger ω requires larger numbers of Hylleraas terms.

Substituting the trial wave function into (1.2) and using the requirement that the Kohn functional K_v be stationary with respect to the variations of the linear parameters K_t and c_i $(i = 1, 2, \cdots, n)$, that is,

$$\frac{\partial K_v}{\partial K_t} = 0 \quad \text{and} \quad \frac{\partial K_v}{\partial c_i} = 0 \quad (i = 1, 2, \cdots, n) \tag{1.5}$$

we obtain a set of linear simultaneous equations which contain the unknown linear parameters of K_t and c_i which can be obtained by solving these equations. Putting these parameters back into (1.2) gives the stationary value of K_v. The optimum values of other non-linear parameters can be determined by repeating the whole calculation for a range of values for each non-linear parameter. Eventually, the accurate phaseshift can be obtained. Further details of the method and procedure can be found in the article by Armour and Humberston (1991).

The most recent and comprehensive study of positron-helium scattering with the variational method was given by Van Reeth and Humberston (1999*a*), while their preliminary studies were published earlier (Humberston, 1973, 1974; Campeanu and Humberston, 1975, 1977; Van Reeth and Humberston, 1995, 1997). Very flexible trial wave functions and a very accurate helium wave function were used in the recent calculations. In addition to the normal Kohn and inverse Kohn variational method, they have applied a third approach, called the complex Kohn method, which uses a complex trial wave function. Two improvements have been made in the trial wave function by adding explicitly two extra functions representing the effect of virtual positronium weakly bound to the residual ion near the threshold of the positronium formation and the distortion of the positronium atom by the ion, respectively.

The elastic scattering and positronium formation cross sections have been calculated for energies below the first excitation threshold (20.61 eV for 2^1S) of helium. The cross sections for the two processes were claimed to have convergence to within 5% and 10%, respectively. The calculated total cross section, both above and below the positronium formation threshold, agrees with the experimental data of Mizogawa *et al* (1985) and Stein *et al* (1978), to within 10%. The sharp increase in the total cross section at the positronium formation threshold, due to the rapid rise of S-wave cross section, was predicted. However, the calculated postronium formation cross section are about 25% lower than the experimental data by Moxom *et al* (1994), although they agree generally in the energy dependence. The angular dependence of the elastic and positronium formation cross sections has also been calculated.

1.3 The Born and Distorted-Wave Born approximations

In addition to the above-discussed methods for modelling positron-helium scattering, there are also various approximations based on the Born series developed for the theoretical description of the positron-impact collision systems. The comprehensive review can be obtained in the book by Charlton and Humberston (2001). Since the Born approximations are usually good for high energy scattering, the following discussions will be focused on the studies on excitation and ionisation processes of positron-helium scattering.

For target excitation from the ground state to a final state, the differential cross section is given by

$$\frac{d\sigma_{f0}}{d\Omega} = \left(\frac{k_0}{k_f}\right) \frac{|T_{f0}|^2}{4\pi^2} \tag{1.6}$$

where $T_{f0} = \left\langle \Phi_f | V | \Psi_0^+ \right\rangle$ is the T-matrix element. Here Ψ_0^+ is the exact total wave function of the positron-target system, and Φ_f is the product wave function for a positron with momentum $\boldsymbol{k}_f$ and the target final state wave function ϕ_f. The V is the positron-target interaction potential. The total cross section for the excitation can be obtained by integration over all directions of $\boldsymbol{k}_f$.

The First Born approximation (FBA) corresponds to the replacement of Ψ_0^+ with Φ_0 being the product wave function for a positron with momentum $\boldsymbol{k}_i$ and the target ground state wave function ϕ_0. Then the T-matrix element is given by

$$T_{f0} = \langle \Phi_f | V | \Phi_0 \rangle \tag{1.7}$$

The BA can be improved by including the second order amplitude in the series expansion and this gives the second Born approximation.

The distorted-wave Born approximation (DWBA) was developed by taking into account the distortion of the positron wave function in both the initial and the final states. In addition to the static interaction, the polarisation effect of the target atom can also be included in the interaction potentials. The partial distorted wave functions are obtained by solving the following differential equations for each channel

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V_d(r) - \frac{k^2}{2} \right) u_{lk}(r) = 0, \tag{1.8}$$

where $V_d(r)$ is the distorting potential.

Subsequently, the calculated distorted wave functions can be used to determine the T matrix elements and then the cross sections.

The earlier work by McEachran *et al* (1977) for the low energy elastic positron helium scattering agreed well with the experimental results. Parcell *et al* (1983, 1987) studied the helium 2^1S and 2^1P excitations by positrons with the DWBA in the energy range from near the threshold up to 150 eV. In their treatment, the positronium formation channel was not considered. Although the agreement with experimental data is not very good, the DWBA indicated the importance of the inclusion of the polarisation potential in the excited channel at low energies. The orientation and alignment parameters as a function of scattering angles were calculated by Madison and Winters (1983) with the DWBA. The effects from first-order or second-order transition potential with different order of distortion have been studied. Srivastava *et al* (1986) have calculated the differential and total cross sections for the excitation of helium 2^1S state with a distorted wave polarised orbital approach. As for the ionisation process, the most systematic studies with the DWBA are those carried out by Campeanu *et al* (1996, 1987). In their model, the Coulomb and plane waves were used and exchange effects were included. The realistic description of the final state of the system were applied dependent on the relative velocity of the scattered positron and ejected electron after collision. The calculated ionisation cross section agreed very well with the experimental data (Mori and Sueoka, 1994; Fromme *et al*, 1986; Knudsen *et al*, 1990; Moxom *et al*, 1996), over the energy range from near threshold to 500 eV.

1.4 Convergent Close-Coupling (CCC) method

Based on the standard close-coupling formalism, Bray and Stelbovics (1992*a*) introduced the Convergent Close-Coupling (CCC) method initially for electron-hydrogen scattering. Then this method has been extended to the calculation of electron-helium scattering (Fursa and Bray, 1995; Stelbovics and Berge, 1997; Fursa and Bray, 1997*b*; Stelbovics, 1999), electron-helium-like atoms and ions (Fursa and Bray, 1997*a*) and positron hydrogen scattering (Bray and Stelbovics, 1993*b*, 1994; Stelbovics and Berge, 1996). In the CCC theory, the target state wave functions are obtained by diagonalizing the target Hamiltonian in a complete Laguerre basis

$$\zeta_{nl}(r) = \left(\frac{\lambda_l (n-1)!}{(2l+1+n)!} \right)^{\frac{1}{2}} (\lambda_l r)^l \exp(-\lambda_l r/2) L_{n-1}^{2l+2}(\lambda_l r), \tag{1.9}$$

where $L_{n-1}^{2l+2}(\lambda r)$ are the associated Laguerre polynomials (Gradshteyn *et al*, 1994), n ranges from 1 to the basis size $N_l = N_0 - l$ for $0 \leq l \leq l_{\max}$, N_0 is N_l for $l = 0$ and λ_l is an orbital-dependent parameter. The square integrability of the Laguerre basis ensures that both the negative and positive energy target states are also square integrable. As the basis size increases, the negative energy states converge to the true eigenstates, while the positive energy states provide an increasingly dense discretisation of the target continuum. Convergence is obtained by increasing the basis parameters N_l and $l_{\max}$. Bray and Stelbovics (1993*b*) have shown that the CCC method is valid for describing positron-atom scattering problems by applying the method to positron-hydrogen scattering below the postronium formation threshold. This thesis reports on the first application of the CCC method to positron-helium collisions.

It is the objective of this thesis to provide the complete set of effective interaction potentials to describe all the reactions which can take place for positron-helium scattering. The resultant potentials are given in momentum space so that they provide the necessary input for the coupled-channel equations in momentum space upon which the CCC method is based. The helium target wave functions are constructed with configuration interaction included. Some preliminary numeric calculations for total cross section at low energies, excitation and fragmentation (positronium formation and ionisation) cross sections at intermediate to high energies with certain approximations are carried out. The comparisons with other theoretical results and available experimental data are given.

2. HELIUM ATOMIC STRUCTURE

In the close coupling treatment of positron-helium scattering, the total wave function is expanded in a set of properly constructed helium target states. In this chapter, the determination of the helium target states with a Configuration Interaction (CI) approach will be presented. Two approaches, the simpler Frozen Core (FC) approximation and a more general Multi-configuration Core (MC) approximation are discussed.

The Hamiltonian for the helium atom is given by

$$H = H_1 + H_2 + V_{12}, \tag{2.1}$$

where

$$H_i = -\frac{\hbar \bigtriangledown_i^2}{2m_i} - \frac{Z}{r_i} \qquad i = 1, 2 \tag{2.2}$$

is the one-electron Hamiltonian of the He^+ with $Z = 2$ and

$$V_{12} = \frac{1}{r_{12}}. \tag{2.3}$$

is the electron-electron potential. Atomic units are used throughout unless specified otherwise.

Generally the helium atomic wave functions are obtained by solving the following Schrödinger equation:

$$(H - \epsilon_{\alpha ls})\Psi_{\alpha lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) = 0. \tag{2.4}$$

here $\Psi_{\alpha lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2)$ denotes the wave function of the helium atom, with $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ representing the space and spin coordinate of the two electrons respectively. The l, m, s and m_s are the quantum numbers specifying the state orbital angular momentum, its projection, spin and spin projection of the state, respectively. The α represents all the quantum numbers other than l, m, s and m_s required to describe the helium state and $\epsilon_{\alpha ls}$ is the energy of helium target state.

For the helium atom, the spin-orbit interaction can be neglected. Consequently, no spin-orbit coupling terms appear in the Hamiltonian. The helium wave function can be expressed by the product of the space coordinate wave function and spin coordinate wave function:

$$\Psi_{\alpha lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2)\chi_{sm_s}(\sigma_1, \sigma_2). \tag{2.5}$$

Here $\chi_{sm_s}(\sigma_1, \sigma_2)$ represents the spin function, $\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ denotes the space coordinate wave function and $\sigma_i = \pm\frac{1}{2}, \ (i = 1, 2)$.

The Schrödinger equation can be written in terms of the space coordinate wave function as:

$$(H - \epsilon_{\alpha ls})\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) = 0. \tag{2.6}$$

In principle, the helium target state wave functions can be obtained by solving the above Schrödinger equation (2.6). Since the analytical solution of (2.6) does not exist, several approximations have been developed to solve it numerically. The configuration interaction (CI) approach, the frozen core (FC) method and the multi-configuration core (MC) method are discussed below.

2.1 CI approximation to helium structure

In the picture of CI, the helium atomic wave function is expanded in a set of antisymmetrized two-electron functions (helium configurations):

$$\Psi_{\alpha lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) \quad = \quad \sum_i C^i_{\alpha ls} \Phi^i_{lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) \tag{2.7}$$

where $\Phi^i_{lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2)$ are the helium configurations. By substituting the expansion (2.7) into (2.6), the Schrödinger equation is then converted to a matrix eigenvalue equations which can be solved numerically as will be discussed below.

2.1.1 Helium configurations

The helium configurations can be constructed from antisymmetric combinations of one-electron wave functions which are coupled together to give a two electron configuration of total orbital angular momentum l and total spin s:

$$\begin{aligned}
\Phi^{ab}_{lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \frac{1}{\sqrt{2}}(1 - P_{12}) \left\langle \boldsymbol{x}_1 \boldsymbol{x}_2 | ab(l_a l_b) lm(\frac{1}{2}\frac{1}{2}) sm_s \right\rangle \\
&= \frac{1}{\sqrt{2}} \sum_{m_a m_b \mu_a \mu_b} \langle l_a l_b m_a m_b | lm \rangle \left\langle \frac{1}{2}\frac{1}{2} \mu_a \mu_b | sm_s \right\rangle \\
&\quad \begin{vmatrix} \phi_{n_a l_a m_a \mu_a}(x_1) & \phi_{n_a l_a m_a \mu_a}(x_2) \\ \\ \phi_{n_b l_b m_b \mu_b}(x_1) & \phi_{n_b l_b m_b \mu_b}(x_2) \end{vmatrix},
\end{aligned} \tag{2.8}$$

where $\langle l_a l_b m_a m_b | lm \rangle$ and $\langle \frac{1}{2}\frac{1}{2}\mu_a\mu_b | s m_s \rangle$ are Clebsch-Gordan coefficients. The one-electron orbitals $\phi_{nlm\mu}(\boldsymbol{x})$ in (2.8) are defined by

$$\phi_{nlm\mu}(\boldsymbol{x}) = \zeta_{nl}(r) Y_{lm}(\hat{\boldsymbol{r}}) \chi_{\frac{1}{2}\mu}(\sigma)$$

with $Y_{lm}(\hat{\boldsymbol{r}})$ being a spherical harmonic and $\chi_{\frac{1}{2}\mu}(\sigma)$ the spin function of an electron. The single electron radial wave functions $\zeta_{nl}(r)$ may be Laguerre (1.9) or Slater type orbitals given by

$$\zeta_{nl}(r) = r^n e^{-\lambda_l r/2} \tag{2.9}$$

where l is the angular momentum of the state, n is an integer and λ is an orbital dependent parameter. More generally single particle orbitals may be made from linear combination of such orbitals. It is convenient if the basis can be expanded in a systematic way, for example, by using the same λ for all terms with same l, taking $n = l, l+1, \cdots, N$ and letting N increase. However, as the powers of r^n go up, this leads to numerical linear dependence problem (Walters *et al*, 1997) for the Slater type orbitals (2.9). This numerical difficulty can be overcome by adopting the square integrable orthogonal Laguerre basis (1.9). By choosing the Laguerre basis, mathematically the basis is equivalent to Slater basis formed from functions $r^m e^{-\lambda_l r/2}$ with $l \leqslant m \leqslant n + l - 1$. Numerically Laguerre polynomials can be generated from a recurrence relation. Laguerre functions are mutually orthogonal for different n although choosing different λ_l for different l will lead to non-orthogonal basis (Bray and Fursa, 1995). In the case of a non-orthogonal basis we will have to solve the generalised eigenvalue problem.

The helium configuration, equation (2.8), can be further written as (see Appendix B) in a more convenient form or a product of angular, radial and spin functions

$$\Phi^{ab}_{lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \phi^{ab}_{(l_a l_b)ls}(r_1, r_2)\mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)\chi_{sm_s}(\sigma_1, \sigma_2), \tag{2.10}$$

with

$$\phi^{ab}_{(l_a l_b)ls}(r_1, r_2) = \frac{1}{\sqrt{2}}\left[1 + (-1)^{l_a+l_b+l+s}\right]\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2), \tag{2.11}$$

and $\mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)$ is a bipolar spherical harmonic and is defined in terms of two spherical harmonics as:

$$\mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = \sum_{m_a m_b} Y_{l_a m_a}(\hat{\boldsymbol{r}}_1)Y_{l_b m_b}(\hat{\boldsymbol{r}}_2)\langle l_a l_b m_a m_b | lm\rangle \tag{2.12}$$

The bipolar harmonics are also written in a shorthand notation as $\langle\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2|(l_a l_b)lm\rangle$. They satisfy the following orthogonality property:

$$\langle l_a l_b lm | l'_a l'_b l' m'\rangle = \delta_{l_a l'_a}\delta_{l_b l'_b}\delta_{ll'}\delta_{mm'}. \tag{2.13}$$

The spin function $\chi_{sm_s}(\sigma_1, \sigma_2)$ in (2.10) consists of three symmetric functions for $s = 1$ and one antisymmetric function for $s = 0$ (Kessler, 1985):

$$\begin{cases} \chi_{1,1}(\sigma_1, \sigma_2) = \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \\ \chi_{1,0}(\sigma_1, \sigma_2) = \frac{1}{\sqrt{2}}\left(\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) + \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\right) \\ \chi_{1,-1}(\sigma_1, \sigma_2) = \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) \end{cases} \tag{2.14}$$

$$\chi_{00}(\sigma_1,\sigma_2) = \frac{1}{\sqrt{2}}\left(\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) - \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\right). \tag{2.15}$$

2.1.2 Helium target states

To obtain helium target states we expand the helium wave functions using the helium configurations by substituting equation (2.10) into the configuration expansion equation (2.7). With some algebra (see Appendix B), we can show that the expansion is only for the radial functions. The helium target states can be written as:

$$\psi_{\alpha lms}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_{l_a l_b} \psi_{\alpha(l_a l_b)ls}(r_1,r_2)\mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2), \tag{2.16}$$

where

$$\psi_{\alpha(l_a l_b)ls}(r_1,r_2) = \sum_{n_a n_b} C^{ab}_{\alpha ls}\phi^{ab}_{(l_a l_b)ls}(r_1,r_2), \tag{2.17}$$

and $\phi^{ab}_{(l_a l_b)ls}(r_1,r_2)$ is given by equation(2.11). Now we apply the CI expansion of the helium orbital wave function equation (2.16) to the helium Schrödinger equation (2.6) and get

$$(H-\epsilon_{\alpha ls})\sum_{l_a l_b}\psi_{\alpha(l_a l_b)ls}(r_1,r_2)\mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2) = 0. \tag{2.18}$$

From the completeness of the bipolar harmonics and after projecting from the left with a bipolar harmonic and integrating over angles,

$$\sum_{l_a l_b}\langle(l'_a l'_b)l'm'|H'_{l_a l_b} - \epsilon_{\alpha ls}|(l_a l_b)lm\rangle\psi_{\alpha(l_a l_b)ls}(r_1,r_2) = 0, \tag{2.19}$$

where

$$H'_{l_a l_b} = \sum_{i=1}^{2}\left[-\frac{\partial^2}{\partial r_i^2} - \frac{2}{r_i}\frac{\partial}{\partial r_i} - \frac{Z}{r_i}\right] + \frac{l_a(l_a+1)}{r_1^2} + \frac{l_b(l_b+1)}{r_2^2} + \frac{1}{r_{12}}.$$

By applying the Wigner Eckart theorem to the scalar operator $H'_{l_a l_b} - \epsilon_{\alpha ls}$ we have $l = l'$ and $m = m'$. Thus in terms of reduced matrix elements, equation (2.19) becomes

$$\sum_{l_a l_b} \langle (l'_a l'_b) l || H'_{l_a l_b} - \epsilon_{\alpha ls} || (l_a l_b) l \rangle \psi_{\alpha(l_a l_b) ls}(r_1, r_2) = 0. \tag{2.20}$$

It is easy to prove (see Appendix C) that

$$\begin{aligned}
&\langle (l'_a l'_b) l || H'_{l_a l_b} - \epsilon_{\alpha ls} || (l_a l_b) l \rangle \\
&= \left(\sum_{i=1}^{2}\left[-\frac{\partial^2}{\partial r_i^2} - \frac{2}{r_i}\frac{\partial}{\partial r_i} - \frac{Z}{r_i}\right] + \frac{l_a(l_a+1)}{r_1^2} + \frac{l_b(l_b+1)}{r_2^2} - \epsilon_\alpha\right)\delta_{l'_a l_a}\delta_{l'_b l_b} \\
&\quad + \sum_\lambda \frac{4\pi}{2\lambda+1}\frac{r_<^\lambda}{r_>^{\lambda+1}}(-1)^{l+\lambda}\hat{l}_a\hat{l}_b\hat{l}'_a\hat{l}'_b \times \begin{pmatrix} l_a & \lambda & l'_a \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_b & \lambda & l'_b \\ 0 & 0 & 0 \end{pmatrix},
\end{aligned} \tag{2.21}$$

where we use the notation $\hat{l} = \sqrt{2l+1}$.

From equation (2.20), we obtain the matrix eigenvalue equations:

$$AC = \eta BC \tag{2.22}$$

where,η is the eigenvalue corresponding to the energies of the helium target state. The partial wave Hamiltonian matrix A is given by

$$\begin{aligned}
A^{(a'b')(ab)}_{l's'ls} &= \frac{1}{2}\int dr_1 dr_2 \left[1 + (-1)^{l'_a+l'_b+l'+s'}\right]\left[1 + (-1)^{l_a+l_b+l+s}\right] \\
&\quad \zeta_{n'_a l'_a}(r_1)\zeta_{n'_b l'_b}(r_2)\langle (l'_a l'_b) l || H'_{l_a l_b} || (l_a l_b) l \rangle \zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2) \\
&= \frac{1}{2}\left[1 + (-1)^{l'_a+l'_b+l'+s'}\right]\left[1 + (-1)^{l_a+l_b+l+s}\right]
\end{aligned}$$

$$
\begin{aligned}
&\times \Biggl\{ \delta_{l'_a l_a} \delta_{l'_b l_b} \int dr_1 dr_2 \zeta_{n'_a l'_a}(r_1) \zeta_{n'_b l'_b}(r_2) \\
&\times \left(\sum_{i=1}^{2} \left[-\frac{\partial^2}{\partial r_i^2} - \frac{2}{r_i}\frac{\partial}{\partial r_i} - \frac{Z}{r_i} \right] + \frac{l_a(l_a+1)}{r_1^2} + \frac{l_b(l_b+1)}{r_2^2} \right) \\
&\times \zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) \\
&+ \int dr_1 dr_2 \zeta_{n'_a l'_a}(r_1) \zeta_{n'_b l'_b}(r_2) \zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) \\
&\times \sum_{\lambda} \frac{4\pi}{2\lambda+1} \frac{r_<^{\lambda}}{r_>^{\lambda+1}} (-1)^{l+\lambda} \hat{l}_a \hat{l}_b \hat{l}'_a \hat{l}'_b \times \begin{pmatrix} l_a & \lambda & l'_a \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_b & \lambda & l'_b \\ 0 & 0 & 0 \end{pmatrix} \Biggr\},
\end{aligned}
\tag{2.23}
$$

the overlap matrix B is given by

$$
\begin{aligned}
B_{ls}^{(a'b')(ab)} &= \delta_{l_a l'_a} \delta_{l_b l'_b} \int dr_1 dr_2 \zeta^*_{n'_a l'_a}(r_1) \zeta_{n_a l_a}(r_1) \zeta^*_{n'_b l'_b}(r_2) \zeta^*_{n_b l_b}(r_2) \\
&+(-1)^{l_a+l_b+l+s} \delta_{l_a l'_b} \delta_{l_b l'_a} \int dr_1 dr_2 \zeta^*_{n'_b l'_b}(r_1) \zeta_{n_a l_a}(r_1) \zeta^*_{n'_a l'_a}(r_2) \zeta^*_{n_b l_b}(r_2).
\end{aligned}
\tag{2.24}
$$

The eigenvector C is formed from the coupling coefficients in equation (2.17) as (ab) take on all their values and the following normalisation is satisfied:

$$
\sum_{(a'b')(ab)} C_{ls}^{*(a'b')} B_{ls}^{(a'b')(ab)} C_{ls}^{(ab)} = \delta_{n'_a n_a} \delta_{n'_b n_b}
$$

The matrix eigenvalue equations (2.22) are solved numerically. The calculations in this thesis are performed by the LAPACK routine `DSYGV` which is for real (double precision) symmetric matrices.

2.2 Helium atomic structure

The electron energy levels for a helium atom demonstrate a number of features of multi-electron atoms. The helium ground state consists of two identical 1s electrons with anti-parallel spin and is a singlet state. The ionisation energy for the first electron is 24.6 eV while that for the second electron is 54.6 eV. Figure 2.1 gives the first few negative energy levels for the S-, P-, D- and F-state parahelium and orthohelium (singlet-spin and triplet-spin helium) atom quoted from the experimental values given on the website *http://physics.nist.gov/cgi-bin/AtData/levels-form*. For those energy levels shown in figure 2.1 one electron

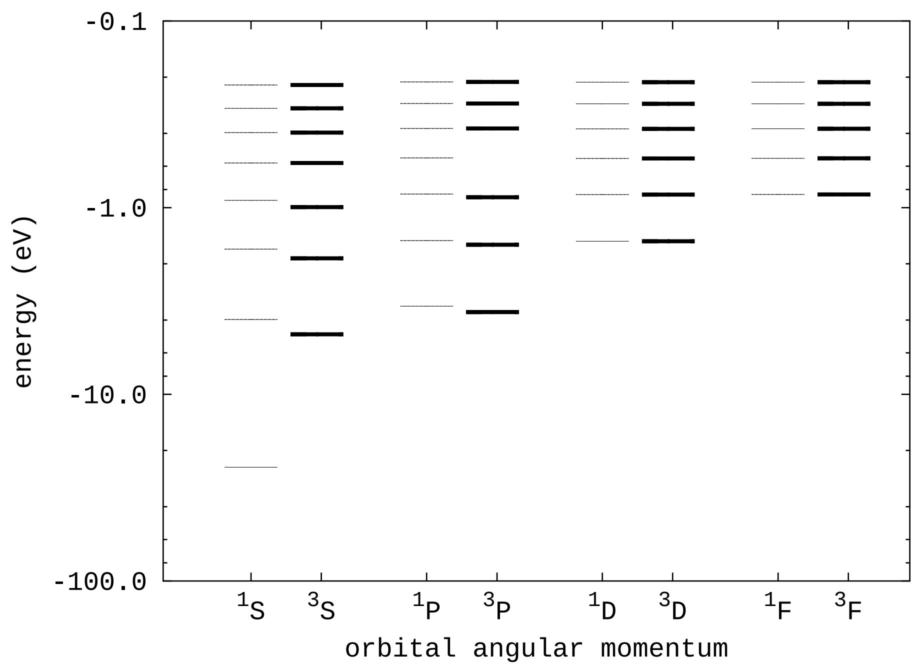

Fig. 2.1: Helium atom energy levels relative to $He^+(1S)$. The experimental values are as given on the website *http://physics.nist.gov/cgi-bin/AtData/levels-form*

of helium atom is presumed to be in the ground state, the 1s state. The other electron in the upper state can have spin anti-parallel to the ground state electron ($S = 0$, singlet state, parahelium) or parallel to the ground state electron ($S = 1$, triplet state, orthohelium). The energy levels for the helium ion differ from that of hydrogen by a factor of 4 since the hydrogen energy levels depend upon square of the nuclear charge.

In the CI approach, the wave functions and energies of the ground and low lying excited states of the helium atom can be calculated to a very high accuracy if sufficient number of configurations in the CI basis are included. We will employ two practical approximations to construct helium structure, frozen core approximation and multi-configuration core approximation. Those methods will be discussed in detail in Chapter 4. They will be used in the calculations for the elastic and inelastic helium positron scattering in Chapters 4 and 5.

It will be seen that there are some differences due to the higher quality of the MC generated wave functions, for some of the cross sections reported.

3. CLOSE COUPLING FORMALISM FOR POSITRON-HELIUM SCATTERING

In general, the Convergent Close Coupling approximation involves solving a set of coupling equations derived from the Schrödinger equation after expanding the system wave function in the basis of target states. The coupled set of differential equations are often reformulated into integral equations called the Lippmann-Schwinger equations. The momentum space Lippmann-Schwinger equations are solved to give the $\boldsymbol{K}$ matrix and the closely associated $\boldsymbol{T}$ matrix, which contain all the scattering amplitudes for various scattering processes. In the calculations of the momentum-space $\boldsymbol{K}$ or $\boldsymbol{T}$ matrix elements, the momentum-space interaction potential $\boldsymbol{V}$ matrix (Bray and Stelbovics, 1996) are the driving terms for the Lippmann-Schwinger equations. The $\boldsymbol{V}$ matrix contains all the interactions information between the projectile and target atoms.

In this chapter the general scattering formalism for positron-helium scattering system based on the close coupling method is presented. The transition matrix will be discussed in general, followed by the derivations of the effective potentials for the different scattering processes including atom-atom, Ps-Ps and rearrangement (atom-Ps) transitions.

3.1 Scattering Formalism

The coordinate system for position-helium scattering is indicated in figure 3.1. The positron-helium system wave function ψ is expanded in terms of helium and positronium atom wave functions as:

$$\begin{aligned}&\psi(\boldsymbol{r}_0, \boldsymbol{r}_1, \boldsymbol{r}_2)\\&\quad= \sum_{\alpha lms} f_{\alpha lms}(\boldsymbol{r}_0)\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) + \sum_{\beta} g_\beta(\boldsymbol{R}, \boldsymbol{r})\phi_\beta(\boldsymbol{\rho}),\end{aligned} \tag{3.1}$$

where the sum over αlms is for helium atom states and the sum over β is for positronium states, lm specify the angular momentum quantum numbers of the helium atom and s denotes the spin of the helium atom. The index 0 denotes

the incident positron space and indices 1 and 2 are for the target electron space. The index β denotes all the quantum numbers needed to describe the positronium states $\phi_\beta(\boldsymbol{\rho})$. The vector $\boldsymbol{r}$ denotes the valence electron coordinate of the helium ion. $\boldsymbol{R}$ is the vector of the centre of mass of the positronium relative to the helium nucleus and $\boldsymbol{\rho}$ is the relative vector between the positron and electron.

The helium atom wave functions are obtained by solving the helium atom Schrödinger equations numerically using Slater or Laguerre functions as discussed in detail in Chapter 2.

By adopting the hydrogen atom wave functions with reduced mass of $\frac{1}{2}$a.u. we can express the positronium wave functions as:

$$\phi_\beta(\boldsymbol{\rho}) = \zeta_{n_\beta l_\beta}(\rho) Y_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}), \tag{3.2}$$

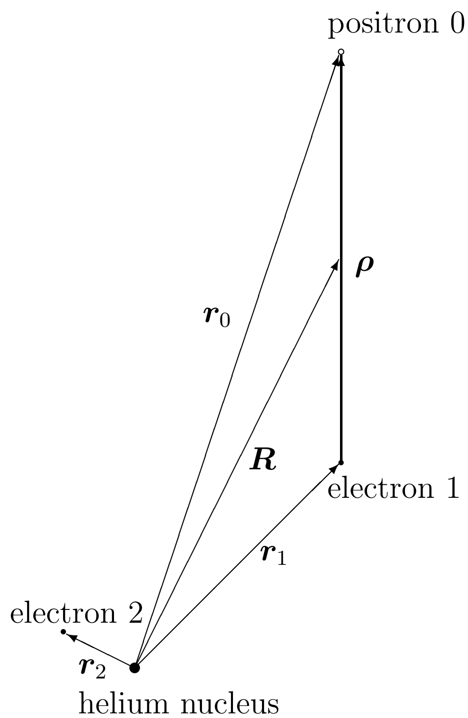

Fig. 3.1: Coordinate system for positron-helium scattering

where

$$\zeta_{n_\beta l_\beta}(\rho) = \left(\frac{\lambda(n_\beta - 1)!}{(2l_\beta + 1 + n_\beta)!} \right)^{\frac{1}{2}} (\lambda\rho)^{l_\beta} \exp(-\lambda\rho/2) L_{n_\beta - 1}^{2l_\beta+2}(\lambda\rho).$$

Here $\lambda = \frac{1}{n_\beta + l_\beta}$, $Y_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})$ is the spherical harmonics and $L_{n_\beta-1}^{2l_\beta+2}(\rho)$ is the Laguerre polynomial as defined in equation (A.10).

We should be aware that by including both the helium atom states and the positronium states in the expansion of (3.1), the required boundary conditions of bound atomic and Ps channels are incorporated, but double counting of the continuum is introduced. If the sets of states $\psi_{\alpha lms}$ and ϕ_β are complete, then either

$$\sum_{\alpha lms} f_{\alpha lms}(\boldsymbol{r}_0) \psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \tag{3.3}$$

or

$$\sum_{\beta} g_{\beta}(\boldsymbol{Rr})\phi_{\beta}(\boldsymbol{\rho}) \tag{3.4}$$

alone will give an exact expansion of the system wave function. Then the expansion in (3.1) is over complete and not necessary orthogonal between the positronium part and the atom part. This leads to numerical instabilities in the solution of the equations, as demonstrated by Stelbovics and Berge (1996). However in real calculations, such problem is usually avoided by using finite number of states in the expansion (3.1). The main concern is how fast the convergence is by using different forms of expansion (3.1),(3.3) and (3.4) as the number of states is increased. It is expected that a mixed expansion such as (3.1) will make the convergence faster as both the atom channels and positronium channels are directly represented, as indicated in Walters *et al* (1997). Two centre close coupling calculations have been extensively used in the 1990s (Hewitt *et al*, 1990; Higgins and Burke, 1991; Mitroy, 1993*a*,*b*; Mitroy and Stelbovics, 1994; Mitroy *et al*, 1994; Mitroy, 1995, 1996; Walters *et al*, 1997). The related problems have been studied thoroughly in the late 90's (Stelbovics, 1999; Stelbovics and Berge, 1997). A detailed study of convergence was given recently by Kadyrov and Bray (2002).

It should be noted that in certain restricted kinematic regimes single centre expansion will still yield very satisfactory results (Bray and Stelbovics, 1993*b*, 1994; Wu *et al*, 2004*b*,*a*).

By substituting the expansion (3.1) into the Schrödinger equation,

$$(E-H)\left(\sum_{\alpha lms} f_{\alpha lms}(\boldsymbol{r}_0)\psi_{\alpha lms}(\boldsymbol{r}_1,\boldsymbol{r}_2) + \sum_{\beta} g_{\beta}(\boldsymbol{R},\boldsymbol{r})\phi_{\beta}(\boldsymbol{\rho})\right) = 0 \tag{3.5}$$

and folding on the left side of equation (3.5) with helium atom states and positronium atom states respectively, we obtain the following coupled equations for the functions of $f_{\alpha lms}(\boldsymbol{r}_0)$ and $g_\beta(\boldsymbol{R}, \boldsymbol{r})$, which contain the scattering amplitude information:

$$\begin{aligned}
&(E + \nabla_0^2 - \epsilon_{\alpha ls}) f_{\alpha' l' m' s'}(\boldsymbol{r}_0) \\
&= \sum_{\alpha lms} \left\langle \psi_{\alpha' l' m' s'} \left| \frac{Z}{r_0} - \frac{1}{r_{01}} - \frac{1}{r_{02}} \right| \psi_{\alpha lms} \right\rangle f_{\alpha lms}(\boldsymbol{r}_0) \\
&\quad + \sum_{\beta} \langle \psi_{\alpha' l' m' s'} \left| E - H \right| \phi_\beta \rangle g_\beta(\boldsymbol{R}, \boldsymbol{r})
\end{aligned} \tag{3.6}$$

and

$$\begin{aligned}
&(E + \frac{1}{2}\nabla_{\boldsymbol{R}}^2 - \epsilon - \epsilon_\beta) g_\beta(\boldsymbol{R}, \boldsymbol{r}) \\
&= \sum_{\alpha lms} \langle \phi_{\beta'} | E - H | \psi_{\alpha lms} \rangle f_{\alpha lms}(\boldsymbol{r}_0) \\
&\quad + \sum_{\beta} \left\langle \phi_{\beta'} \left| \left(\frac{Z}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho}|} - \frac{Z}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho}|} \right. \right. \right. \\
&\quad \left. \left. \left. + \frac{1}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}|} - \frac{1}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}|} \right) \right| \phi_\beta \right\rangle g_\beta(\boldsymbol{R}, \boldsymbol{r}).
\end{aligned} \tag{3.7}$$

Here H is the Hamiltonian of the system for positron and helium atom:

$$H = -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{Z}{r_0} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - \frac{1}{r_{01}} - \frac{1}{r_{02}} \tag{3.8}$$

or in terms of the alternate coordinates for the positronium and helium ion

$$\begin{aligned}
H \;=\; & -\frac{1}{4}\nabla_{\boldsymbol{R}}^2 - \nabla_{\boldsymbol{\rho}}^2 - \frac{1}{2}\nabla^2 + \frac{Z}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho}|} - \frac{Z}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho}|} - \frac{Z}{r} \\
& + \frac{1}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}|} - \frac{1}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}|} - \frac{1}{\rho},
\end{aligned}$$

(3.9)

The helium target states $\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ satisfy the equation

$$\left(-\frac{1}{2}\bigtriangledown_1^2 - \frac{1}{2}\bigtriangledown_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - \epsilon_{\alpha ls}\right)\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) = 0, \tag{3.10}$$

where $\epsilon_{\alpha ls}$ is the eigenenergy of the helium target state. Similarly ϵ_β is the eigenenergy of the positronium state defined by equation

$$\left(-\bigtriangledown_{\boldsymbol{\rho}}^2 - \frac{1}{\rho} - \epsilon_\beta\right)\phi_\beta(\boldsymbol{\rho}) = 0. \tag{3.11}$$

Finally we also need to consider helium ion states $\psi^+_{\boldsymbol{k}}(\boldsymbol{r})$ which satisfy:

$$\left(-\frac{1}{2}\bigtriangledown^2 - \frac{Z}{r} - \epsilon\right)\psi^+_{\boldsymbol{k}}(\boldsymbol{r}) = 0, \tag{3.12}$$

where $\frac{1}{2}\boldsymbol{k} = \epsilon$.

Instead of solving the differential form of the close-coupling equations (3.6) and (3.7), we solve the integral form of Lippmann-Schwinger (LS) equation in the momentum space (Bray and Stelbovics, 1992a) for the T matrix.

To simplify our notation we introduce the index γ which ranges over all helium atom states αlms and positronium states β. The expansion (3.1) becomes

$$\psi = \sum_\gamma F_\gamma \psi_\gamma(\boldsymbol{r}_\gamma) \tag{3.13}$$

The Lippmann-Schwinger integral equations for the transition amplitudes $T_{\gamma\gamma'}$ are given by

$$T_{\gamma'\gamma}(\boldsymbol{q}_{\gamma'}, \boldsymbol{q}_\gamma) = V_{\gamma'\gamma}(\boldsymbol{q}_{\gamma'}, \boldsymbol{q}_\gamma) + \sum\!\!\!\!\!\!\int_{\gamma''} \frac{d^3\boldsymbol{q}_{\gamma''}}{(2\pi)^3} V_{\gamma'\gamma''}(\boldsymbol{q}_{\gamma'}, \boldsymbol{q}_{\gamma''}) G_{\gamma''}(q^2_{\gamma''}) T_{\gamma''\gamma}(\boldsymbol{q}_{\gamma''}, \boldsymbol{q}_\gamma),$$

where $\boldsymbol{q}_\gamma$ can be the momentum of the incident positron $\boldsymbol{k}_0$ or momentum of positronium $\boldsymbol{k}$ for Ps states. $G_{\gamma''}(q^2_{\gamma''})$ is the Green's function of the system (Kadyrov and Bray, 2002).

The effective interaction potentials for direct atom-atom, Ps-Ps and rearrangement (atom-Ps) transition are given, respectively, by

$$V_{\gamma'\gamma}(\boldsymbol{q}_{\gamma'}, \boldsymbol{q}_\gamma) = \langle \boldsymbol{q}_{\gamma'}\psi_{\gamma'}|U_{\gamma'\gamma}|\psi_\gamma \boldsymbol{q}_\gamma\rangle, \tag{3.14}$$

where

$$U_{\alpha,\alpha} = \frac{Z}{r_0} - \frac{1}{r_{01}} - \frac{1}{r_{02}}, \tag{3.15}$$

$$U_{\beta,\beta} = \frac{Z}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho}|} - \frac{Z}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho}|} + \frac{1}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}|} - \frac{1}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}|}, \tag{3.16}$$

$$U_{\alpha,\beta} = H - E. \tag{3.17}$$

3.2 Direct momentum space potential $V_{\alpha'\alpha}$

The potential matrix for the direct interaction between the positron and helium atom from an initial target state $\psi_{\alpha'l'm'}$ to a final target state $\psi_{\alpha lm}$ is given by:

$$V_{\alpha'\alpha} = \langle \boldsymbol{k}'_0\psi_{\alpha'l'm's'}|U_{\alpha,\alpha}|\psi_{\alpha lms}\boldsymbol{k}_0\rangle$$

$$
\begin{aligned}
&= (2\pi)^{-3} \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \\
&\quad \psi^*_{\alpha' l' m' s'}(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \left[\frac{Z}{r_0} - \frac{1}{r_{01}} - \frac{1}{r_{02}}\right] e^{i(\boldsymbol{k}_0 - \boldsymbol{k}_0')\cdot \boldsymbol{r}_0} \\
&= I_0 + 2I_1, \qquad (3.18)
\end{aligned}
$$

where

$$
\begin{aligned}
I_0 &= (2\pi)^{-3} \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \psi^*_{\alpha' l' m' s'}(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2)\frac{Z}{r_0} e^{i(\boldsymbol{k}_0 - \boldsymbol{k}_0')\cdot \boldsymbol{r}_0}, \\
I_1 &= (2\pi)^{-3} \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \psi^*_{\alpha' l' m' s'}(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \left[-\frac{1}{r_{01}}\right] e^{i(\boldsymbol{k}_0 - \boldsymbol{k}_0')\cdot \boldsymbol{r}_0} \\
&= -\frac{1}{2\pi^2 K^2} \int d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \psi^*_{\alpha' l' m' s'}(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) e^{i(\boldsymbol{k}_0 - \boldsymbol{k}_0')\cdot \boldsymbol{r}_1},
\end{aligned}
$$

with

$$
\boldsymbol{K} = \boldsymbol{k}_0 - \boldsymbol{k}_0'.
$$

After performing the integrations over the angles, I_0 and I_1 can be expressed as (see Appendix D.1 for details)

$$
\begin{aligned}
I_0 = &\sum_{l_0' l_1' l_0 l_1 l_2 \lambda m_0' m_1' m_0 m_1 m_2 m_\lambda} (-1)^{m_0' + m_1 + m + m' + \lambda} \langle \hat{\boldsymbol{k}}_0' | l_0' m_0' \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \hat{l}_0' \hat{l}_0 \hat{l}_1' \hat{l}_1 \hat{l}' \hat{l} \\
&\xi^0_{k_0' l_0' k_0 l_0 \alpha' (l_1' l_2') l' s' \alpha (l_1 l_2) l s \lambda} \begin{pmatrix} l_0' & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_2' & l' \\ m_1' & m_2' & -m \end{pmatrix} \\
&\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_1' & l_1 & \lambda \\ -m_1' & m_1 & -m_\lambda \end{pmatrix} \begin{pmatrix} l_0' & l_0 & \lambda \\ -m_0' & m_0 & m_\lambda \end{pmatrix}, \qquad (3.19)
\end{aligned}
$$

where

$$\xi^0_{k'_0 l'_0 k_0 l_0 \alpha'(l'_1 l'_2) l' s' \alpha(l_1 l_2) l s \lambda} = \int r_0^2 dr_0 r_1^2 dr_1 r_2^2 dr_2 \langle k'_0 l'_0 | r_0 \rangle \langle r_0 | k_0 l_0 \rangle \langle r_1 r_2 | \alpha(l_1 l_2) l s \rangle \langle \alpha'(l'_1 l'_2) l' s' | r_1 r_2 \rangle \frac{\delta_{\lambda,0}}{r_0} \tag{3.20}$$

and

$$I_1 = -\sum_{l'_0 l'_1 l_0 l_1 l_2 \lambda m'_0 m'_1 m_0 m_1 m_2 m_\lambda} (-1)^{m'_0+m_1+m+m'+\lambda} \langle \hat{\boldsymbol{k}}'_0 | l'_0 m'_0 \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \hat{l}'_0 \hat{l}_0 \hat{l}'_1 \hat{l}_1 \hat{l}' \hat{l}$$
$$\xi^1_{k'_0 l'_0 k_0 l_0 \alpha'(l'_1 l'_2) l' s' \alpha(l_1 l_2) l s \lambda} \begin{pmatrix} l'_0 & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'_1 & l'_2 & l' \\ m'_1 & m'_2 & -m \end{pmatrix}$$
$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l'_1 & l_1 & \lambda \\ -m'_1 & m_1 & -m_\lambda \end{pmatrix} \begin{pmatrix} l'_0 & l_0 & \lambda \\ -m'_0 & m_0 & m_\lambda \end{pmatrix}, \tag{3.21}$$

where

$$\xi^1_{k'_0 l'_0 k_0 l_0 \alpha'(l'_1 l'_2) l' s' \alpha(l_1 l_2) l s \lambda} = \int r_0^2 dr_0 r_1^2 dr_1 r_2^2 dr_2 \langle k'_0 l'_0 | r_0 \rangle \langle r_0 | k_0 l_0 \rangle \langle r_1 r_2 | \alpha(l_1 l_2) l s \rangle \langle \alpha'(l'_1 l'_2) l' s' | r_1 r_2 \rangle \frac{r_<^\lambda}{r_>^{\lambda+1}} \tag{3.22}$$

and $\langle r_0 | k_0 l_0 \rangle = 4\pi i^{l_0} j_{l_0}(k_0, r_0)$ is the radial wave function for the positron where $j_{l_0}(k_0, r_0)$ is the spherical Bessel function. $\langle r_1 r_2 | \alpha(l_1 l_2) l s \rangle \equiv \psi_{\alpha(l_1 l_2) l s}(r_1, r_2)$ is the radial wave function for the helium target states.

For practical computation we usually solve the partial wave form of coupled channel equations and so we make the partial wave expansion of the V matrix elements. This is done by expanding V matrix in terms of a complete set of total angular momentum states. We expressed the initial state i.e. positron plane wave function $\boldsymbol{k}_0$ and helium atom eigenstates $|\alpha lms\rangle$ into total angular momentum eignstates $|\boldsymbol{J}M_J>$:

$$\begin{aligned}
&|\boldsymbol{k}_0\alpha lms\rangle \\
&\quad= \sum_{l_0m_0l_1l_2JM_J}\langle JM_J|l_0m_0lm\rangle\langle\hat{\boldsymbol{k}}_0|l_0m_0\rangle|k_0l_0\alpha(l_1l_2)ls\rangle|J(l_0(l_1l_2)l)M_J\rangle.
\end{aligned} \tag{3.23}$$

Noticing that the potential V is a scalar operator and applying the Wigner-Eckart theorem, we have

$$\begin{aligned}
&\langle k_0'l_0'\alpha'(l_1'l_2')l's'J'(l_0'(l_1'l_2')l')M_J'|V|k_0l_0\alpha(l_1l_2)lsJ(l_0(l_1l_2)l)M_J\rangle \\
&\quad\equiv \delta_{J'J}\delta_{M_J'M_J}\langle k_0'l_0'\alpha'(l_1'l_2')l's'J'(l_0'(l_1'l_2')l')||V||k_0l_0\alpha(l_1l_2)lsJ(l_0(l_1l_2)l)\rangle \\
&\quad= \delta_{J'J}\delta_{M_J'M_J}V^J_{\alpha'\alpha}(k_0',k_0)
\end{aligned}$$

where $V^J_{\alpha'\alpha}(k_0',k_0)$ is the partial wave reduced matrix element of the direct potential and is defined as

$$\begin{aligned}
&V^J_{\alpha'\alpha}(k_0',k_0) \\
&\quad= \langle k_0'l_0'\alpha'(l_1'l_2')l's'J'(l_0'(l_1'l_2')l')||V||k_0l_0\alpha(l_1l_2)lsJ(l_0(l_1l_2)l)\rangle \\
&\quad= \int d^3\hat{\boldsymbol{k}}_0'd^3\hat{\boldsymbol{k}}_0\sum_{m_0'''m'm_0''m}\langle J'M_J'|l_0'''m_0'''l'm'\rangle\langle J'M_J'|l_0''m_0''lm\rangle \\
&\quad\quad\langle\hat{\boldsymbol{k}}_0'|l_0'''m_0'''\rangle\langle l_0''m_0''|\hat{\boldsymbol{k}}_0\rangle\langle\psi_{\alpha'l'm's'}\boldsymbol{k}_0'|V|\boldsymbol{k}_0\psi_{\alpha lms}\rangle \\
&\quad= \int d^3\hat{\boldsymbol{k}}_0'd^3\hat{\boldsymbol{k}}_0
\end{aligned}$$

$$\sum_{m_0'''m'm_0''m} \langle J'M_J'|l_0'''m_0'''l'm'\rangle\langle J'M_J'|l_0''m_0''lm\rangle\langle\hat{\boldsymbol{k}}_0'|l_0'''m_0'''\rangle\langle l_0''m_0''|\hat{\boldsymbol{k}}_0\rangle V_{\alpha'\alpha}. \tag{3.24}$$

Substituting equations (3.18), (3.19) and (3.21) into (3.24), integrating over the angular variables and simplifing the expression by contracting the three-j symbols into six-j symbols we finally have

$$\begin{aligned} & V^J_{\alpha'\alpha}(k_0', k_0) \\ = & \sum_{l_0'l_1'l_0l_1l_2\lambda} \xi_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda}(-1)^{l_2'+J'}\hat{l}_0'\hat{l}_0\hat{l}_1'\hat{l}_1\hat{l}\hat{l}' \\ & \begin{pmatrix} l_0' & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l & \lambda & l' \\ l_1' & l_2' & l_1 \end{Bmatrix}\begin{Bmatrix} l & l_0 & J' \\ l_0' & l' & \lambda \end{Bmatrix}, \end{aligned} \tag{3.25}$$

where

$$\begin{aligned} & \xi_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda} \\ = & \xi^0_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda} + 2\xi^1_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda}, \end{aligned} \tag{3.26}$$

here we use the abbreviation $\hat{l} = \sqrt{2l+1}$ and ξ^0 and ξ^1 are defined in equation (3.20) and equation (3.22). The detailed derivation for equation (3.25) can be found in Appendix D.1 (equation D.2).

3.3 Direct transition $V_{\beta'\beta}$

In this section the interaction potential matrix for Ps-Ps transition in positron-helium scattering will be given, based on considering the system consisting of positronium and helium ion which in turn is approximately treated as a proton with an effective charge Z'. The resulting effective potential takes the following form

$$U_{\beta,\beta} = \frac{Z'}{|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho}|} - \frac{Z'}{|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho}|} \tag{3.27}$$

and the potential matrix for an initial state of positronium β with momentum $\boldsymbol{k}$ going to a final positronium state β' with momentum $\boldsymbol{k}'$ is given by

$$\begin{aligned} V_{\beta'\beta} &= \langle \boldsymbol{k}'\beta'|U_{\beta,\beta}|\boldsymbol{k}\beta\rangle = \langle e^{i\boldsymbol{k}'\cdot\boldsymbol{R}}\phi_{\beta'}|U_{\beta'\beta}|e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\phi_{\beta}\rangle \\ &= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{R}d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\rho)\Phi_\beta(\rho)e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\left[\frac{Z'}{\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho}}\right]e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho})} \\ &\quad -\frac{1}{(2\pi)^3}\int d^3\boldsymbol{R}d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\rho)\Phi_\beta(\rho)e^{-\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\left[\frac{Z'}{\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho}}\right]e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho})}. \end{aligned} \tag{3.28}$$

In order to simplify this expression we use the well known identity

$$\int \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{r}d^3\boldsymbol{r} = \frac{4\pi}{k^2} \tag{3.29}$$

to obtain

$$V_{\beta'\beta} = \frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}\int d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\rho)\Phi_\beta(\rho)\left[e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}} - e^{-\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\right]. \tag{3.30}$$

Expanding in the total angular momentum space and using the Wigner-Eckart theorem we derive the following partial wave reduction for $V_{\beta'\beta}$ (see Appendix D.2):

$$\begin{aligned} &V^J_{\beta'\beta}(k',k) \\ &= \sum_{m_{\beta'}m_\beta M'M\lambda\mu\tau\mu'\lambda' m_{\lambda'}} 2\pi i^\lambda(-1)^{\tau+\lambda'+\lambda+J}\hat{\lambda}^3\hat{\lambda'}^2\hat{l}_\beta\hat{l}_{\beta'}\hat{L}\hat{L}'k^{\lambda-\tau}k'^\tau Y^{\lambda\lambda'}_{\beta'\beta}(kk') \end{aligned}$$

$$\left(\frac{(2\lambda)!}{(2\tau)!(2(\lambda-\tau))!}\right)^{1/2}\begin{pmatrix}\lambda & l_\beta & l_{\beta'}\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda' & \tau & L'\\ 0 & 0 & 0\end{pmatrix}$$
$$\begin{pmatrix}L & \lambda' & \lambda-\tau\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}\lambda & L' & L\\ \lambda' & \lambda-\tau & \tau\end{Bmatrix}\begin{Bmatrix}l_{\beta'} & L' & J\\ L & l_\beta & \lambda\end{Bmatrix} \tag{3.31}$$

3.4 Rearrangement $V_{\alpha\beta}$

The positronium formation is a rearrangement process from initial positron continuum state plus atomic ground state to a positronium state plus a residual ion state. The potential corresponding to this rearrangement process is given by

$$\begin{aligned} V = U_{\alpha\beta} &= H - E \\ &= -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{Z}{r_0} - \frac{Z}{r_1} - \frac{Z}{r_2} \\ &\quad + \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|} - E \end{aligned} \tag{3.32}$$

In the following derivations we define $\boldsymbol{\rho} = \boldsymbol{r}_0 - \boldsymbol{r}_1$, $\boldsymbol{r} = \boldsymbol{r}_2$ and $\mathbf{R} = \frac{1}{2}(\mathbf{r}_0 + \mathbf{r}_1)$. This corresponds to the case that electron 1 and the incident positron form the positronium while electron 2 stays with the helium nucleus as a helium ion (see figure 3.1). The derivation for the case corresponding to $\boldsymbol{\rho} = \boldsymbol{r}_0 - \boldsymbol{r}_2$, $\boldsymbol{r} = \boldsymbol{r}_1$ and $\mathbf{R} = \frac{1}{2}(\mathbf{r}_0 + \mathbf{r}_2)$ is the same after interchange the indices of 1 and 2.

The potential matrix $V_{\alpha\beta}$ for a transition from initial state with the target helium atom in state α and positron with momentum $\boldsymbol{k}$ to a final state with helium ion in state i and positronium atom in state β with momentum $\boldsymbol{k}'$ is given by

$$V_{\alpha\beta} =< \boldsymbol{k}'\beta i|U_{\alpha\beta}|\boldsymbol{k}\alpha lms >$$

$$= \sum_{n_1n_2l_1l_2m_1m_2} d^{\alpha(l_1l_2)l}_{n_1n_2} \langle l_1l_2m_1m_2|lm\rangle \sum_{n_i} d_{n_i} \sum_{n_\beta} d_{n_\beta} \left(I_1 + I_2 + I_3 + I_4 + I_5 + I_6\right),$$

where

$$\begin{aligned}
I_1 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
&\quad \left(\frac{1}{2}k^2 + \frac{1}{2}(\boldsymbol{k}-\boldsymbol{k}')^2 - \epsilon - E\right) \\
&\quad e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2) Y_{l_1m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2m_2}(\hat{\boldsymbol{r}}_2), \\
I_2 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
&\quad \left(\frac{Z}{r_0}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2) Y_{l_1m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2m_2}(\hat{\boldsymbol{r}}_2), \\
I_3 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
&\quad \left(\frac{Z}{r_1}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2) Y_{l_1m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2m_2}(\hat{\boldsymbol{r}}_2), \\
I_4 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_{01}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
&\quad \left(\frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2) Y_{l_1m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2m_2}(\hat{\boldsymbol{r}}_2), \\
I_5 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_{01}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
&\quad \left(-\frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_1|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2) Y_{l_1m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2m_2}(\hat{\boldsymbol{r}}_2), \\
I_6 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_{01}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
&\quad \left(-\frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_2|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2) Y_{l_1m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned} \tag{3.33}$$

and $d_{n_1 n_2}^{\alpha(l_1 l_2)l}$ is the expansion coefficient of the helium wave functions in the Laguerre basis, they are obtained by solving the target helium Schrödinger equation, so is d_{n_i} for helium and d_{n_β} for positronium atom.

Carrying out the integrations in momentum space and applying the Wigner-Eckart theorem, we can write the reduced potential matrix:

$$\begin{aligned}
&V^J_{\alpha\beta}(k'_0, k_0) \\
&= \sum_{l_1 l_2} \sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 \int d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
&\quad \langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle V_{\alpha\beta} \\
&= \sum_{l_1 l_2} \sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 \int d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
&\quad \langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
&\quad \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2)l} d_{n_i} d_{n_\beta} \left(I_1 + I_2 + I_3 + I_4 + I_5 + I_6\right) \\
&= {}_1V^J_{\alpha\beta} +_2 V^J_{\alpha\beta} +_3 V^J_{\alpha\beta} +_4 V^J_{\alpha\beta} +_5 V^J_{\alpha\beta} +_6 V^J_{\alpha\beta},
\end{aligned} \tag{3.34}$$

The details can be found in equations (D.3), (D.4) and (D.5) in Appendix D.3. The $\{{}_nV^J_{\alpha\beta}\}(n = 1, 2, \cdots 6)$ terms can be further reduced to

$$\begin{aligned}
{}_1V^J_{\alpha\beta} &= \frac{1}{4\pi} \sum_{l_1 l_2 \lambda q'_1 q_1 \tau_\beta \tau_1} i^{l_\beta + l_1} (-1)^{l_1 + l' + \tau_\beta + \tau_1} \\
&\quad \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!}\right)^{1/2} \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1 - \tau_1))!}\right)^{1/2} \\
&\quad \hat{l}^2_\beta \hat{l}^3_1 \hat{l'_R} \hat{l}_0 \hat{\lambda}^2 \hat{q}'^2 \hat{q}^2_1 \hat{J}^2 \hat{l}' \left(\frac{1}{2}\right)^{l_\beta - \tau_\beta} {}_1Z^\lambda_{\beta i}(k, k') k'^{l_\beta + l_1 - \tau_\beta - \tau_1} k^{\tau_\beta + \tau_1} \\
&\quad \sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q'_1} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q'_1} + m'_R + m_\lambda + m_{q_1} + m' + m_\beta} \\
&\quad \begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

$$\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix} \begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$
$$\begin{pmatrix} l_1-\tau_1 & \tau_1 & l_1 \\ m_1-m_{\tau_1} & m_{\tau_1} & -m_1 \end{pmatrix} \begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}$$
$$\begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1} \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1} \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$\begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1} \end{pmatrix} \begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ m_\beta-m_{\tau_\beta} & m_1-m_{\tau_1} & m_{q'_1} \end{pmatrix},$$

$$ {}_2V^J_{\alpha\beta} = \frac{1}{4\pi} \sum_{l_1 l_2 \lambda q'_1 q_1 \tau_\beta \tau_1} i^{l_\beta+l_1} (-1)^{l_1+l'+\tau_\beta+\tau_1} \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!} \right)^{1/2}$$
$$\left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!} \right)^{1/2} \hat{l}^2_\beta \hat{l}^3_1 \hat{l}'_R \hat{l}_0 \hat{\lambda}^2 \hat{q}'^2 \hat{q}^2_1 \hat{J}^2 \hat{l}' \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}$$

$$ {}_2Z^{\lambda l_0}_{\beta i}(k,k') k'^{l_\beta+l_1-\tau_\beta-\tau_1}$$
$$\sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q'_1} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q'_1}+m'_R+m_\lambda+m_{q_1}+m'+m_\beta}$$
$$\begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix} \begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$
$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_1-\tau_1 & \tau_1 & l_1 \\ m_1-m_{\tau_1} & m_{\tau_1} & -m_1 \end{pmatrix} \begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}$$
$$\begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1} \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1} \end{pmatrix}$$
$$\begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1} \end{pmatrix} \begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ m_\beta-m_{\tau_\beta} & m_1-m_{\tau_1} & m_{q'_1} \end{pmatrix},$$

$$
{}_3V^J_{\alpha\beta} = \frac{1}{4\pi}\sum_{l_1 l_2}\sum_{\lambda q_1' q_1}\sum_{\tau_\beta \tau_1} i^{l_\beta+l_1}(-1)^{l_1+l'+\tau_\beta+\tau_1}
$$

$$
\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!}\right)^{1/2}
$$

$$
\hat{l}_\beta^2\hat{l}_1^3\hat{l}_R'\hat{l}_0\hat{\lambda}^2\hat{q}'^2\hat{q}_1^2\hat{J}^2\hat{l}'\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}{}_3Z^{\lambda}_{\beta i}(k,k')k'^{l_\beta+l_1-\tau_\beta-\tau_1}k^{\tau_\beta+\tau_1}
$$

$$
\sum_{m_R' m_\beta m_0 m m_R' m' m_1 m_2 m_\lambda m_{q_1'} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q_1'}+m_R'+m_\lambda+m_{q_1}+m'+m_\beta}
$$

$$
\begin{pmatrix} l_R' & \lambda & q \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda & l_0 & q_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q_1' \\ 0 & 0 & 0 \end{pmatrix}
$$

$$
\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix}\begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix}\begin{pmatrix} l_R' & l_\beta & l' \\ m_R' & m_\beta & -m' \end{pmatrix}
$$

$$
\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} l_1-\tau_1 & \tau_1 & l_1 \\ m_1-m_{\tau_1} & m_{\tau_1} & -m_1 \end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}
$$

$$
\begin{pmatrix} l_R' & \lambda & q_1 \\ -m_R' & -m_\lambda & m_{q_1} \end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1} \end{pmatrix}
$$

$$
\begin{pmatrix} \lambda & l_0 & q_1' \\ m_\lambda & m_0 & m_{q_1'} \end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q_1' \\ m_\beta-m_{\tau_\beta} & m_1-m_{\tau_1} & m_{q_1'} \end{pmatrix},
$$

$$
{}_4V^J_{\alpha\beta} =
$$

$$
\sum_{m_R' m_\beta m_0 m m_R' m' l_1 l_2 m_1 m_2 c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6} \tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7} q_1 m_{q_1} q_2 m_{q_2} q_1' m_{q_1'} q_2' m_{q_2'}}
$$

$$
i^{c+l_\beta+l_1}(-1)^{l_1+\tau_c+l_1+\tau_\beta+l'+l}
$$

$$
(-1)^{m_i-m_\beta+m_R'+m_{\lambda_5}+m_{\lambda_7}+m_{\lambda_6}+m_{q_1}+m_{q_2}+m_{q_1'}+m_{q_2'}+m'+m}
$$

$$
\frac{1}{(4\pi)^3}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}k'^{c-\tau_c+l_\beta-\tau_\beta}k^{c_5-\tau_5+\tau_\beta}{}_4Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5\tau_5}(k,k')
$$

$$
\hat{l}_i\hat{l}_2\hat{l}_c\hat{c}\hat{c}_5\hat{\lambda}_5\hat{c}_5\hat{c}_5\hat{l}_\beta\hat{c}\hat{c}_5\hat{l}_\beta\hat{l}_0'\hat{\lambda}_5\hat{\lambda}_7\hat{q}_1^2\hat{q}_2^2\hat{l}_0\hat{\lambda}_6\hat{\lambda}_7\hat{q}_1'\hat{q}_1'\hat{q}_2'\hat{q}_2'\hat{\tau}_5\hat{\lambda}_6\hat{l}_1\hat{J}^2\hat{l}\hat{l}'
$$

$$\left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2}\left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}$$
$$\begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l'_R & c-\tau_c & q_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda_6 & \tau_\beta & q'_2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} q'_1 & q'_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} q_1 & q_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_0 & c_5-\tau_5 & q'_1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} \tau_5 & \lambda_6 & l_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix}\begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix}\begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}\begin{pmatrix} c_5-\tau_5 & \tau_5 & c_5 \\ m_{c_5}-m_{\tau_5} & m_{\tau_5} & -m_{c_5} \end{pmatrix}$$
$$\begin{pmatrix} c-\tau_c & \tau_c & c \\ m_c-m_{\tau_c} & m_{\tau_c} & -m_c \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix}\begin{pmatrix} q_1 & q_2 & \lambda_7 \\ m_{q_1} & m_{q_1} & m_{\lambda_7} \end{pmatrix}$$
$$\begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}\begin{pmatrix} l'_R & c-\tau_c & q_1 \\ -m'_R & m_c-m_{\tau_c} & m_{q_1} \end{pmatrix}$$

$$\begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2 \\ -m_{\lambda_5} & m_\beta-m_{\tau_\beta} & m_{q_2} \end{pmatrix}\begin{pmatrix} l_0 & c_5-\tau_5 & q'_1 \\ m_0 & m_{c_5}-m_{\tau_5} & m_{q'_1} \end{pmatrix}$$

$$\begin{pmatrix} \lambda_6 & \tau_\beta & q'_2 \\ m_{\lambda_6} & m_{\tau_\beta} & m_{q'_2} \end{pmatrix}\begin{pmatrix} q'_1 & q'_2 & \lambda_7 \\ m_{q'_2} & m_{q'_2} & m_{\lambda_7} \end{pmatrix}\begin{pmatrix} \tau_5 & \lambda_6 & l_1 \\ m_{\tau_5} & m_{\lambda_6} & m_1 \end{pmatrix},$$

$$ {}_5V^J_{\alpha\beta} = \frac{1}{4\pi}\sum_{l_1 l_2 \lambda q'_1 q_1 \tau_\beta \tau_1} i^{l_\beta+l_1}(-1)^{l_1+l'+\tau_\beta+\tau_1}$$
$$\frac{\sqrt{(2l_\beta)!}}{\sqrt{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}}\frac{\sqrt{(2l_1)!}}{\sqrt{(2\tau_1)!(2(l_1-\tau_1))!}}$$
$$\hat{l}^2_\beta \hat{l}^3_1 \hat{l'}_R \hat{l}_0 \hat{\lambda}^2 \hat{q}^{'2} \hat{q}^2_1 \hat{J}^2 \hat{l}' \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} {}_5Z^\lambda_{\beta i}(k,k') k'^{l_\beta+l_1-\tau_\beta-\tau_1} k^{\tau_\beta+\tau_1}$$
$$\sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q'_1} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q'_1}+m'_R+m_\lambda+m_{q_1}+m'+m_\beta}$$

$$\begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix} \begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$
$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_1 - \tau_1 & \tau_1 & l_1 \\ m_1 - m_{\tau_1} & m_{\tau_1} & -m_1 \end{pmatrix}$$
$$\begin{pmatrix} l_\beta - \tau_\beta & \tau_\beta & l_\beta \\ m_\beta - m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix} \begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1} \end{pmatrix}$$
$$\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1} \end{pmatrix} \begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1} \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ m_\beta - m_{\tau_\beta} & m_1 - m_{\tau_1} & m_{q'_1} \end{pmatrix},$$

$$_6V^J_{\alpha\beta} = \sum_{m'_R m_\beta m_0 m m'_R m' l_1 l_2 m_1 m_2} \int d^2\hat{\mathbf{k}}'_0 \int d^2\hat{\mathbf{k}}_0 \langle l'_R m'_R | \hat{\mathbf{k}}' \rangle \langle \hat{\mathbf{k}} | l_0 m_0 \rangle$$
$$(-1)^{l'-m'+l-m} \hat{J}\hat{J}\hat{l}'\hat{l} \begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix}$$
$$\begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$\sum_{c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6} \tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7}} i^{c+l_\beta+l_1} (-1)^{\tau_c+\tau_\beta+m_i-m_\beta+m'_R+m_{\lambda_5}+m_{\lambda_7}}$$
$$\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} k'^{c-\tau_c+l_\beta-\tau_\beta} k^{c_5-\tau_5} \frac{\hat{l_1}^2 \hat{l}_2 \hat{l}_c \hat{c}^2 \hat{c}_5^3 \hat{\lambda}_5^2 \hat{l}_\beta^2}{\sqrt{(2c-2\tau_c+1)(2c_5-2\tau_5+1)(2l_\beta-2\tau_\beta+1)}}$$
$$_6Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5 \tau_5}(k,k') \frac{\sqrt{(2c)!(2c_5)!(2l_\beta)!}}{\sqrt{\sqrt{(2\tau_c)!(2(c-\tau_c))!}(2\tau_5)!(2(c_5-\tau_5))!(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}}$$
$$\begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & \tau_\beta & l_\beta \\ m_\beta - m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}$$
$$\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix} \begin{pmatrix} c - \tau_c & \tau_c & c \\ m_c - m_{\tau_c} & m_{\tau_c} & -m_c \end{pmatrix}$$
$$\begin{pmatrix} c_5 - \tau_5 & \tau_5 & c_5 \\ m_{c_5} - m_{\tau_5} & m_{\tau_5} & -m_{c_5} \end{pmatrix} \begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}$$

$$\sum_{q_1 m_{q_1} q_2 m_{q_2} q'_1 m_{q'_1} q'_2 m_{q'_2}} \frac{\hat{l}'_0 (c \hat{-} \tau_c)(\hat{l_\beta - \tau_\beta})(c_5 \hat{-} \tau_5)\hat{\lambda}_6^2 \hat{\lambda}_7^2 \hat{q}_1'^2 \hat{q}_2'^2 \hat{q}_1^2 \hat{q}_2^2}{(4\pi)^3}$$
$$(-1)^{m_{q_1}+m_{q_2}+m_{\lambda_6}+m_{q'_1}+m_{q'_2}} \begin{pmatrix} l'_0 & c-\tau_c & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_5 & l_\beta - \tau_\beta & q_2 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\begin{pmatrix} q_1 & q_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_5-\tau_5 & \lambda_6 & l_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'_0 & c-\tau_c & q_1 \\ -m'_R & m_c - m_{\tau_c} & m_{q_1} \end{pmatrix}$$
$$\begin{pmatrix} \lambda_5 & l_\beta - \tau_\beta & q_2 \\ -m_{\lambda_5} & m_\beta - m_{\tau_\beta} & m_{q_2} \end{pmatrix} \begin{pmatrix} c_5-\tau_5 & \lambda_6 & l_1 \\ m_{c_5} - m_{\tau_5} & -m_{\lambda_6} & m_1 \end{pmatrix}$$
$$\begin{pmatrix} \tau_\beta & \lambda_7 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_5 & \lambda_6 & q'_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q'_1 & q'_2 & l_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & \lambda_7 \\ m_{q_1} & m_{q_1} & m_{\lambda_7} \end{pmatrix}$$
$$\begin{pmatrix} \tau_\beta & \lambda_7 & q'_1 \\ m_{\tau_b eta} & m_{\lambda_7} & m_{q'_1} \end{pmatrix} \begin{pmatrix} \tau_5 & \lambda_6 & q'_2 \\ m_{\tau_5} & m_{\lambda_6} & m_{q'_2} \end{pmatrix} \begin{pmatrix} q'_1 & q'_2 & l_1 \\ m_{q'_2} & m_{q'_2} & m_1 \end{pmatrix}.$$

This concludes the derivation of the complete set of partial-wave potentials needed for the partial-wave coupled channel equations for positron helium scattering where the positronium formation is explicitly included.

4. LOW ENERGY POSITRON-HELIUM ELASTIC SCATTERING

4.1 Introduction

For incident positron energies below the ground state positronium formation threshold (17.8 eV), the only open channel is elastic scattering in the interaction of positrons and helium atoms. There have been extensive studies both theoretically and experimentally of this process. The most comprehensive theoretical study of low energy positron-helium scattering has been performed by Van Reeth and Humberston (1999*a*) using the variational method based on their earlier work (Humberston, 1973, 1974; Van Reeth and Humberston, 1995, 1997). This system has also been studied by Campbell *et al* (1998) utilising a close-coupling method for both low and high energies, as discussed in Chapter 1.

In our aim to study positron-helium scattering by the convergent close coupling (CCC) method, we first investigate the elastic scattering process with single centre expansions which should be able to provide accurate ab-initio cross sections and phaseshifts at low energies, as pointed out by Bray and Stelbovics (1993*a*). Two approaches, frozen core (FC) and multi-configuration core (MC), are used in the construction of helium target wave functions. Following a brief discussion of the construction of the helium wave function and the presentation of the V-matrix for the positron-helium elastic scattering process, the calculated total elastic scattering cross sections and phaseshifts will be presented and discussed separately for FC and MC approximations; finally the comparison between the FC and MC results will be given. A summary of the following work has been published by Wu *et al* (2004*b*).

4.2 Helium target states

The construction of the helium target wave function was discussed in detail in Chapter 2. In the real calculation we have to use approximations so here we will present the specific calculations of helium states carried out using frozen core approximation and multi-configuration core approximation. These calculated helium states will be used later in the CCC calculations of the elastic scattering of positron off helium at low energies below the positronium formation threshold and the calculations of inelastic scattering at intermediate to high energies.

For the helium target, the dominant collision processes are associated with only one-electron excitation while the second electron remains in the $1s$ orbital to form the core state of $He^+(1s)$. Therefore it is usually a good approximation to keep the "core" electron fixed in the CI expansion, the so-called frozen core model. Then the calculations are much simpler than in the full CI calculations. The frozen-core model has been fully tested by Fursa (1995) in the studies of electron-helium scattering. The helium states calculated using FC model depend on an orbital dependent parameter λ_l and the basis size that is characterised by the maximum angular momentum $l_{\max}$ and N_l, the Laguerre basis size for each l. We will denote the set of helium target states constructed by the FC model by FC(N_0, $l_{\max}$), with $N_l = N_0 - l$. Throughout our calculation we use $\lambda_l = 4.0$ for all $l_{\max}$. This yields an exact He^+ $1s$ orbital and gives good short-ranged orbitals for describing the ground state.

Three sets of FC(12,3), FC(12,8) and FC(16,8) will be used in the CCC calculations for testing of the convergence. The basis sizes are sufficiently large so that the same helium ground state energy of -23.742 eV and dipole polarizability of 1.364 (a_0^3) were obtained with all the selected basis sets. This is very close to the experimental values of -24.586 eV and 1.38(a_0^3). Only with the use of MC wavefunctions can the theoretical binding energy be further lowered.

The other more accurate method for the construction of helium target states is the multi-configuration core (MC) approximation. In the MC model the "core" electron occupies only limited orbitals, while the other "outer" electron takes the desired orbitals as to the accuracy of the calculation demands. Six states of three s, two p and one d are used for the description of the "core" electron. The "outer" electron's basis sets are described by an orbital dependent parameter λ_l and the basis size parameter (N_0, $l_{\max}$) where $l_{\max}$ is the maximum angular momentum and N_0 is related to the l^{th} Laguerre basis size N_l by $N_l = N_0 - l$. The FC approach is adopted for all other symmetries. The helium states constructed by MC will be denoted by MC(N_0, $l_{\max}$). Three sets of basis MC(12,3), MC(12,8) and MC(16,8) with $\lambda_l = 4.0$ for all the λ_l were constructed with this approach. These selected basis sizes are large enough to generate the same helium ground state energy of -24.515 eV and dipole polarizability of 1.364 (a_0^3).

While the same value of dipole polarizability were obtained with both FC and MC approaches, a much more accurate ground state energy from MC model is obtained than with the FC model when compared with the experimental values. In table 4.1 we present the comparison of the energy levels obtained by MC(16,8) and FC(16,8) together with the experimental data from Martin (1987). The CCC calculations using FC and MC model for the study of low energy positron helium elastic scattering is carried out in Section 4.4.

Tab. 4.1: Energy levels of helium atom

	FC(16,8)	MC(16,8)	experiment
1^1S	-23.74	-24.52	-24.59
2^1S	-3.90	-3.97	-3.97
3^1S	-1.36	-1.39	-1.67
2^1P	-3.33	-3.33	-3.37
3^1P	-1.17	-1.17	-1.50
3^1D	-1.38	-1.38	-1.52

4.3 V-matrix

At energies below the ground state positronium formation, only elastic scattering channel is open. The single centre coupled channel equations only require the matrix elements of the form $V_{\alpha\alpha'}$ which were given in Chapter 3. The reduced partial wave V-matrix $V^J_{\alpha'\alpha}(k'_0, k_0)$ is given by equation (3.25).

In this particular elastic scattering case the V-matrix will be the same as electron helium scattering except for a change in sign for the charge of the projectile and the dropping of electron-electron exchange terms. That means in the single centre approach we can utilise the electron helium implementation of the CCC method by Fursa and Bray (1995) by just changing in sign for the charge of the projectile and the dropping off of exchange terms.

4.4 Results and discussions

The total elastic scattering cross section (TCS), S-, P-, D- and F-phaseshifts calculated based on the FC and MC bases are presented separately. The comparison with the available experimental and other theoretical data is included. Finally the comparison of the TCS between the FC and MC approximation is given.

4.4.1 Frozen core approach

Calculations with convergent close-coupling approximation using the three sets of FC bases, FC(12,3), FC(12,8) and FC(16,8) were carried out. The results obtained are denoted by CCC(12,3,FC), CCC(12,8,FC) and CCC(16,8,FC) respectively. The first two calculations show the influence of increasing $l_{\max}$ only while the latter two calculations test the convergence as a function of increasing N_l.

The calculation CCC(12,3,FC) includes 100 channels and couples 42 states consisting of 12^1S, 11^1P, 10^1D and 9^1F states. In the CCC(12,8,FC) calculation, 300 channels and 72 states of 12^1S, 11^1P, 10^1D, 9^1F, 8^1G, 7^1H, 6^1I, 5^1J and 4^1K states are used. The CCC(16, 8, FC) calculation has 480 channels and couples 108 states consisting of 16^1S, 15^1P, 14^1D, 13^1F, 12^1G, 11^1H, 10^1I, 9^1J and 8^1K.

The calculated total cross sections from the different basis sets are displayed in the top panel of figure 4.1 , while the result from the CCC(16,8,FC) is compared with the available experimental and other theoretical calculations, as indicated in the lower panel of the figure 4.1.

It is shown in the top panel of the figure 4.1 that the total scattering cross section from CCC(12,3,FC), dotted line, is noticeably lower than the calculations CCC(16,8,FC) and CCC(12,8,FC), indicated by the solid and dashed lines respectively, at energies around the Ramsauer minimum. This indicates the

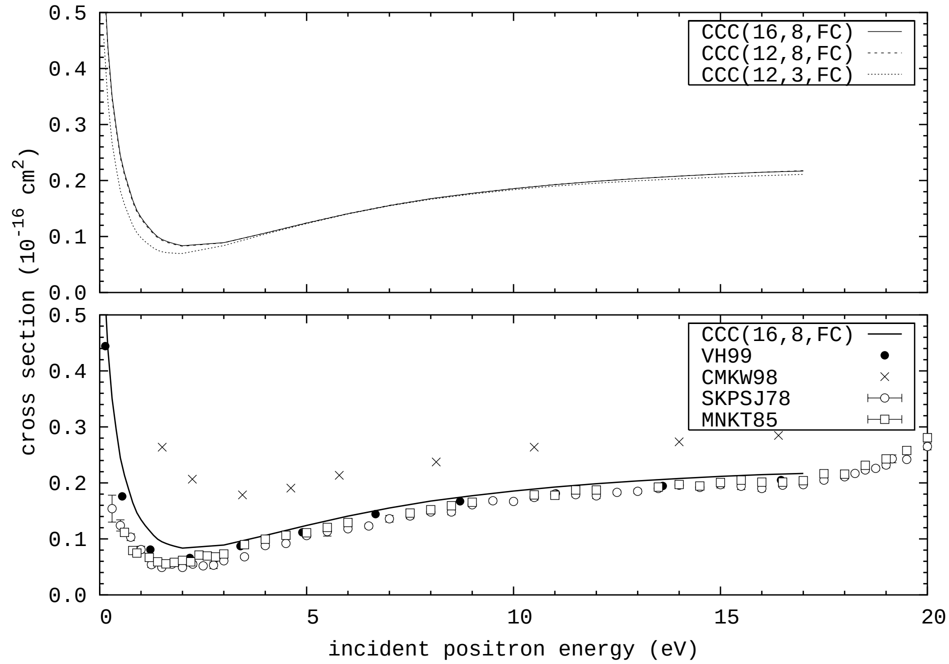

Fig. 4.1: Total (elastic) e^+ - He scattering cross sections as a function of the incident positron energy. The present frozen-core CCC calculations are denoted by CCC(16,8,FC), CCC(12,8,FC) and CCC(12,3,FC), (as described in the text). VH99 represents the theoretical results from Van Reeth and Humberston (1999*a*) with the variational method and CMKW98 represents the close-coupling calculations from Campbell *et al* (1998). The experimental data denoted by SKPSJ78 and MNKT85 are due to Stein *et al* (1978) and Mizogawa *et al* (1985) respectively.

non-convergence of the CCC(12,3,FC) calculation. However the results from CCC(12,8,FC) and CCC(16,8,FC) are almost identical. This provides a clear indication that these calculations with respect to the N_l have converged.

As demonstrated in the lower panel of the figure 4.1, the CCC(16,8,FC) result agrees reasonably well with the experimental results of Stein *et al* (1978) and Mizogawa *et al* (1985) and the variational theoretical results by Van Reeth and Humberston (1999*a*) in the energy range above the Ramsauer minimum. However the CCC(16,8,FC) result is noticeable higher than the two sets of experimental data at energies in the vicinity of the Ramsauer minimum and below. We shall see that the inaccuracy of the CCC calculations with the FC approximation in the

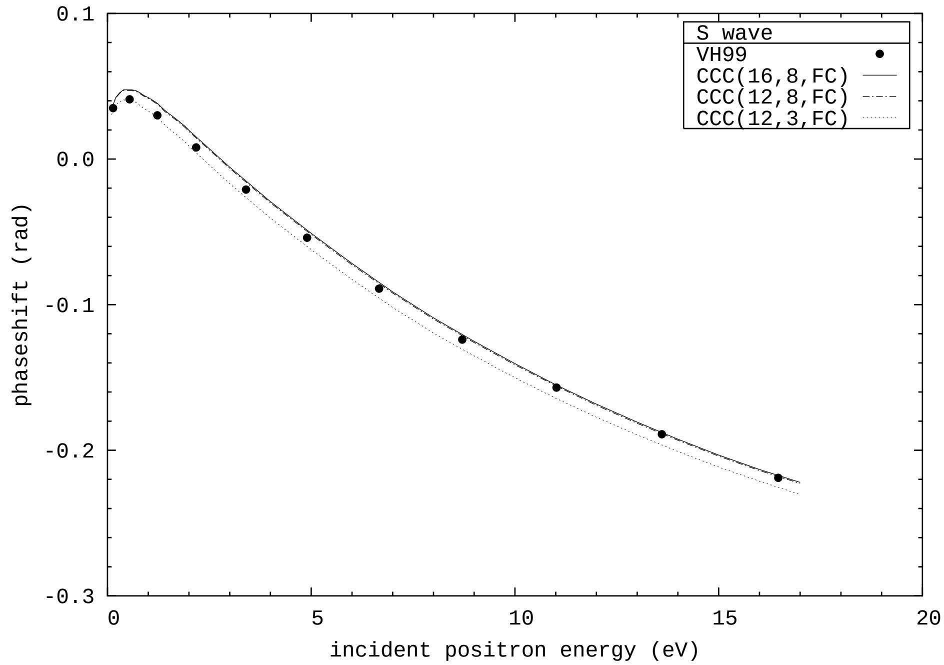

Fig. 4.2: The S-wave phaseshifts as a function of the incident positron energy below the Ps formation threshold. The present calculations are denoted by CCC(16,8,FC), CCC(12,8,FC) and CCC(12,3,FC); The variational calculation of Van Reeth and Humberston (1999*a*) is denoted by VH99.

very low energy region is due to an insufficient account of the electron-electron correlation in the target ground state. The close-coupling calculations by Campbell et al are significantly higher than all other theoretical calculations in the whole energy range considered here. It should also be noticed that the non-convergent CCC(12,3,FC) result has a better accidental agreement with the experimental data in the low energy region.

As shown in figure 4.2, the S-wave phaseshifts from the CCC(16,8,FC) and CCC(12,8,FC) agree well with the variational calculations by Van Reeth and Humberston (1999*a*). The general energy dependence including the sign changing around 2 eV for the S-wave phaseshift is reproduced by our CCC calculations. The convergence from the CCC(12,3,FC) to CCC(16,8,FC) is demonstrated in the figure too.

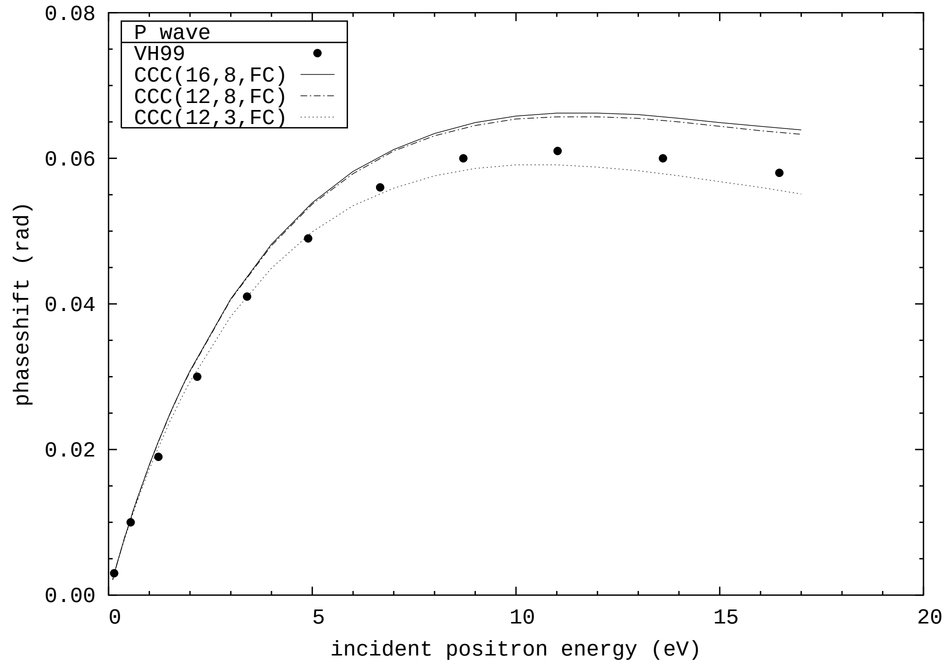

Fig. 4.3: P-wave phaseshifts. The legend is the same as for figure 4.2.

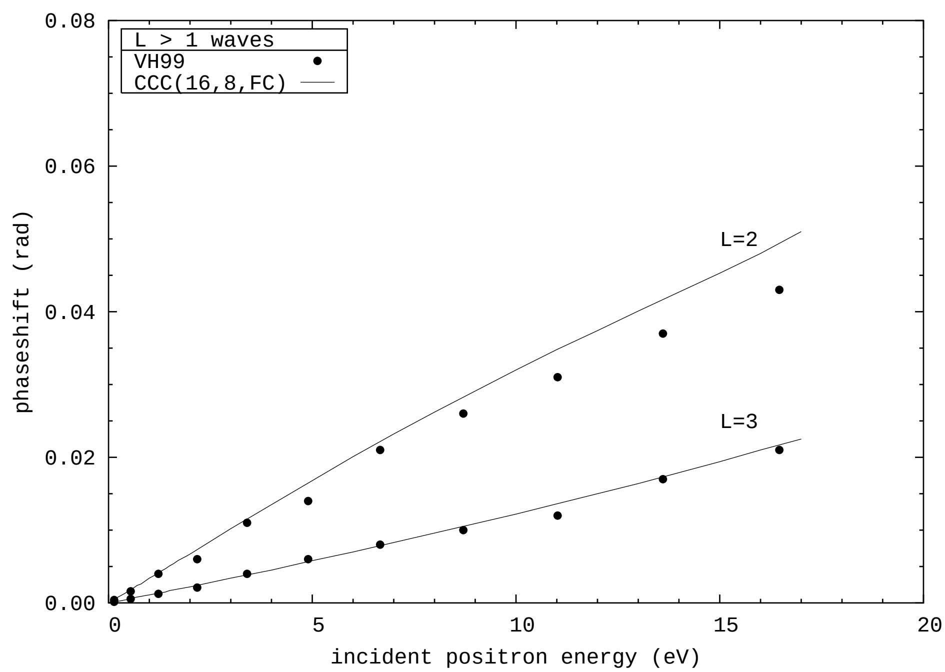

Fig. 4.4: D-wave and F-wave phaseshifts. The legend is the same as for figure 4.2.

For P-wave phaseshift, as presented in figure 4.3, the CCC results from the CCC(16,8,FC) and CCC(12,8,FC) are similar to the variational calculations for energies below 2 eV, but overshoot compared to the variational method at higher energies. The calculations from CCC(12,3,FC) gives lower values than the variational results, although the three sets of calculations converge at low energies below 2 eV.

For the D-wave phaseshift, the CCC converged results are again consistently higher than those of the variational method above 5 eV, while all the results converge at energies below 5 eV. In the case of F-wave phaseshift, good agreement has been obtained between the CCC results and the variational calculations, as shown in figure 4.4, for the whole energy range considered.

4.4.2 Multi-configuration core approach

Three calculations, denoted by CCC(12,3), CCC(12,8) and CCC(16,8) corresponding to the basis sets of MC(12,3), MC(12,8) and MC(16,8), respectively, have been carried out. Due to the frozen-core expansion of the $l > 0$ states the three CCC($N_0, l_{\max}$) calculations generate $N_0 - l$ singlet helium states of $l \leq l_{\max}$. However, for the ^1S symmetry the usage of six orbitals for the inner electrons yields many more ^1S states than necessary for describing low-energy scattering. We take sufficiently many of these for convergence, the first 44 lowest-lying states, irrespective of the basis size N_0. Consequently, the calculation of CCC(12,3) couples 74 states with 132 channels and consists of 44^1S, 11^1P, 10^1D and 9^1F states. In the CCC(12,8) calculation, 332 channels and 104 states of 44^1S, 11^1P, 10^1D, 9^1F, 8^1G, 7^1H, 6^1I, 5^1J and 4^1K states are used. The CCC(16,8) calculation has 508 channels and couples 136 states consisting of 44^1S, 15^1P, 14^1D, 13^1F, 12^1G, 11^1H, 10^1I, 9^1J and 8^1K.

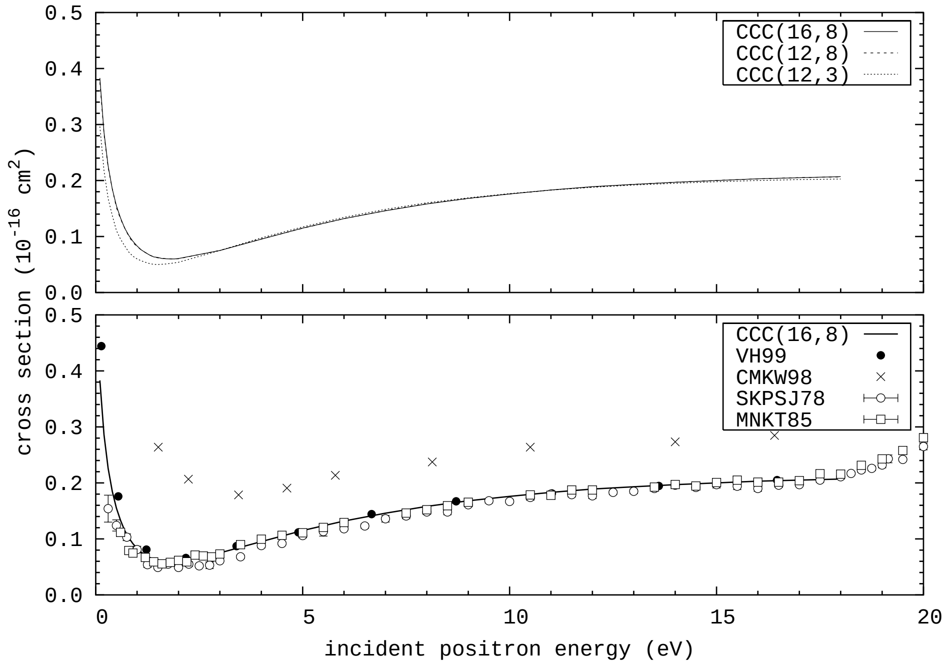

Fig. 4.5: Total scattering cross sections as a function of the incident positron energy. The present calculations are denoted by CCC(16,8), CCC(12,8) and CCC(12,3), (as also described in the text). VH99 represents the theoretical results from the variational method (Van Reeth and Humberston, 1999*a*) and CMKW98 represents the close-coupling calculations of Campbell *et al* (1998). The experimental data denoted by SKPSJ78 and MNKT85 are due to Stein *et al* (1978) and Mizogawa *et al* (1985) respectively.

As indicated in the top panel of figure 4.5, the convergence of scattering cross section with respect to the N_l has been achieved as demonstrated by the nearly identical cross section from the two calculations, CCC(16,8) and CCC(12,8). The results from the CCC(12,3) calculation, is noticeably lower than the other two calculations at energies around the Ramsauer minimum indicating the $l_{\max}$ is too small.

The lower panel of figure 4.5 presents the comparisons between the CCC(16,8) calculation with the two experimental data of Stein *et al* (1978) and Mizogawa *et al* (1985) and theoretical results from the variational method Van Reeth and Humberston (1999*a*) and the close-coupling approximation Campbell *et al* (1998).

The CCC(16, 8) result, as shown in the figure 4.5, agrees very well with the experimental data of Stein *et al* (1978) and Mizogawa *et al* (1985) for the whole energy range considered here. The discrepancy between the CCC(16,8,FC) results and the experimental data, as shown in the figure 4.1, has been removed by the CCC(16,8) calculation which has taken into account the electron-electron correlation by describing the ^{1}S state of the "core" electron in a combination of s-, p- and d-orbitals in the target structure construction. The study has demonstrated that the electron-electron correlation is important for the low energy scattering.

As indicated in the lower panel of figure 4.5, the perfect agreement between the CCC(16, 8) and the variational results is obtained. However, the discrepancy with the earlier close-coupling calculation by Campbell et al still exists. We suspect that the discrepancy are probably not due to the usage of frozen-core approximation, but rather due to the lack of convergence with N_l in their work.

The phaseshifts for $l = 0, 1, \cdots, 5$ partial waves, calculated from CCC(12, 3), CCC(12, 8) and CCC(16, 8), are shown in figures 4.6, 4.7 and 4.8 respectively, and compared with the variational calculations of Van Reeth and Humberston (1999a) and the often-used formula (O'Malley *et al*, 1962)

$$\eta_l = \frac{\pi \alpha k^2}{(2l-1)(2l+1)(2l+3))} + R \tag{4.1}$$

where the remainder term R is of order k^3 for $l = 1$ and of order k^4 for $l > 1$.

As shown in the figure 4.6, the S-wave phaseshifts from the CCC(16,8) and CCC(12, 8) agree perfectly with the variational calculations by Van Reeth and Humberston (1999a) for the whole energy range studied here. The general energy dependence including the sign changing around 2 eV for the S-wave phaseshift has been well reproduced by the CCC calculations. The result from CCC(12, 3) is considerably lower than other results, due to the non-convergence of the

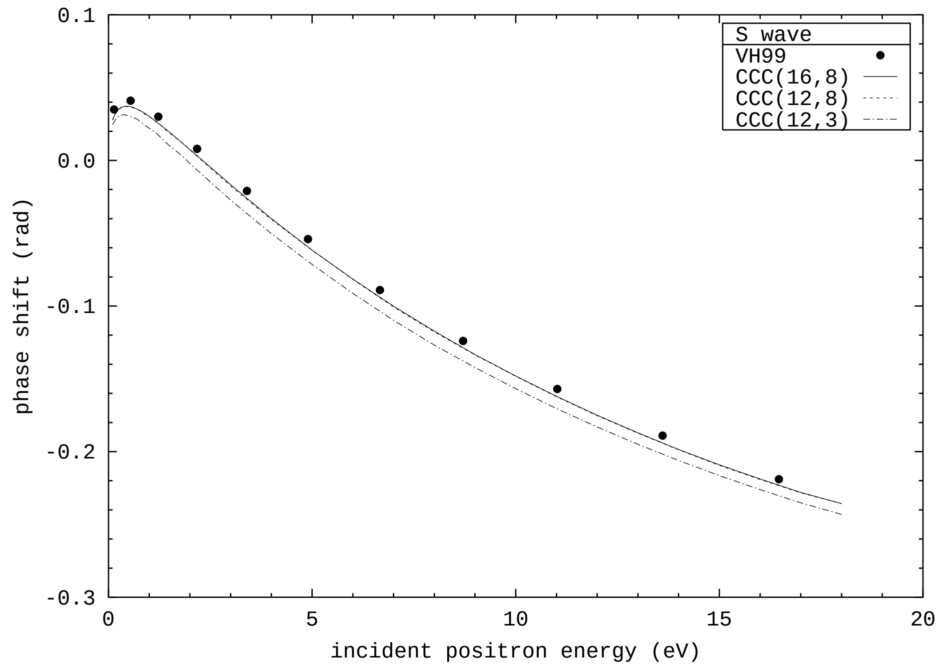

Fig. 4.6: The e^+-He S-wave phaseshifts as a function of the incident positron energy. The present calculations are denoted by CCC(16, 8), CCC(12, 8) and CCC(12, 3); Results denoted with VH99 are the variational calculations (Van Reeth and Humberston, 1999*a*).

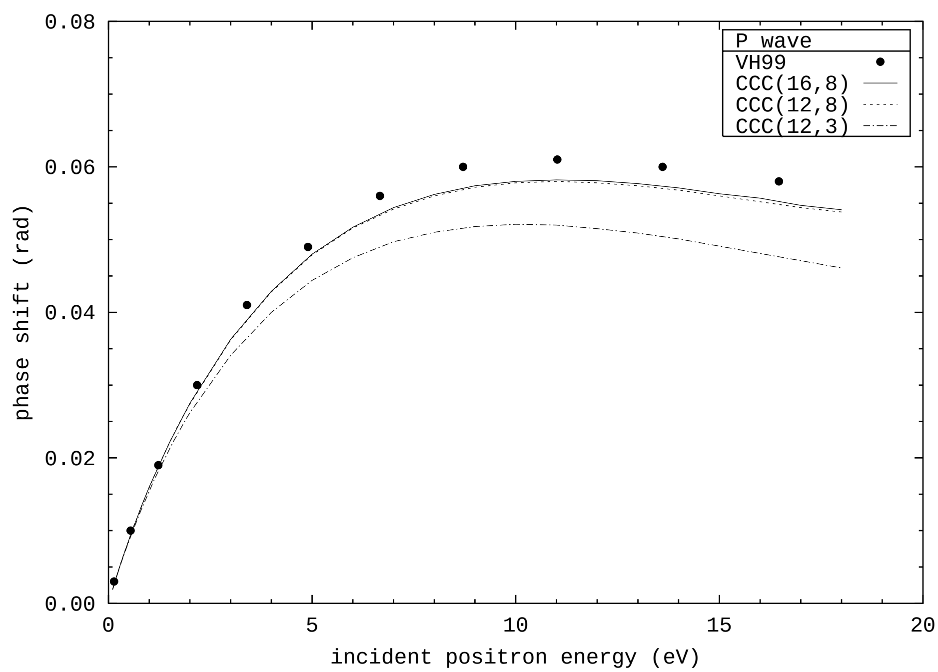

Fig. 4.7: P-wave phaseshift, the legend is the same as for figure 4.6.

calculations.

For the P-wave phaseshift, as indicated in the figure 4.7, the results from both CCC(16,8) and CCC(12,8) agree very well with the variational calculations for energies below 5 eV, while lower values than the variational data appear at higher energies. The calculations from the CCC(12,3) give much lower values than the variational results, although the three sets of calculations converge at low energies below 2 eV.

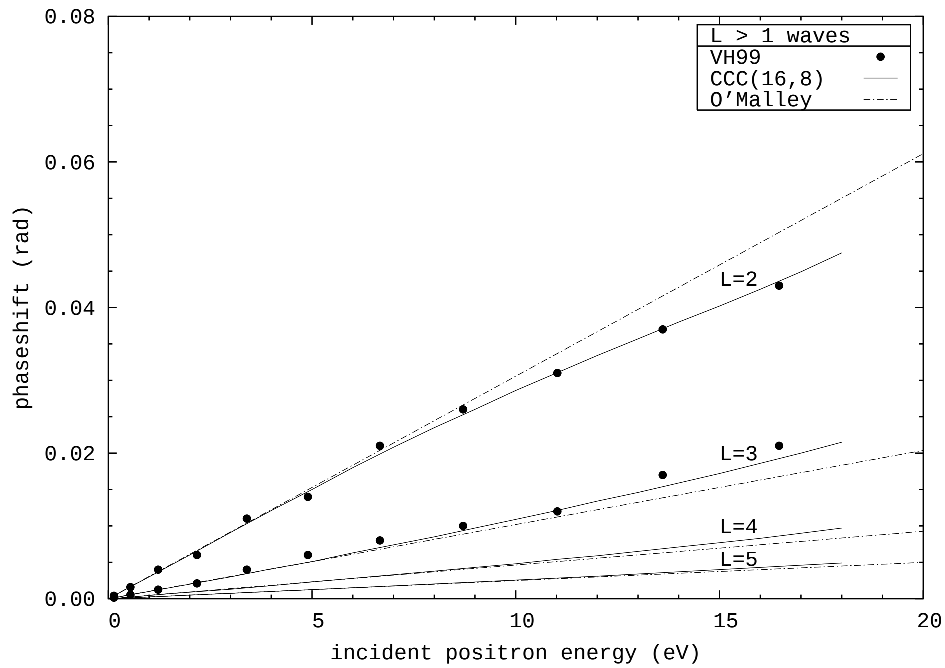

Fig. 4.8: L = 2,3,4 and 5 phaseshifts, the legend is the same as for figure 4.6 except for the CCC(16,8) only. Additionally, we give the phaseshift estimation due to O'Malley *et al* (1962).

The $2 \leqslant l \leqslant 5$ phaseshifts are given in figure 4.8. Here convergence considerations are much the same as for L =0 and 1 and are not repeated here. For D and F-wave phaseshifts, we have good agreement between CCC (16,8) and the variational calculations. The variational results fluctuate a little compared to our calculations indicating our numeries are slightly more stable. As expected, agreement with the O'Malley *et al* (1962) estimate improves with decreasing energy. For $l = 4, 5$ agreement between the ab initio CCC(16,8) calculation and the O'malley's estimate is excellent over most of the energy range.

In figure 4.6 and 4.7 there is a visible difference between the $l_{\max} = 3$ and $l_{\max} = 8$ calculations for both the s-wave and p-wave phaseshifts. However the resulting cross sections, when summed, average out the difference and yield much the same result above 2 eV, given in figure 4.5.

To summaries the results of this chapter, in figure 4.9 we compare the CCC models using FC and MC approaches for calculation of the total cross section.

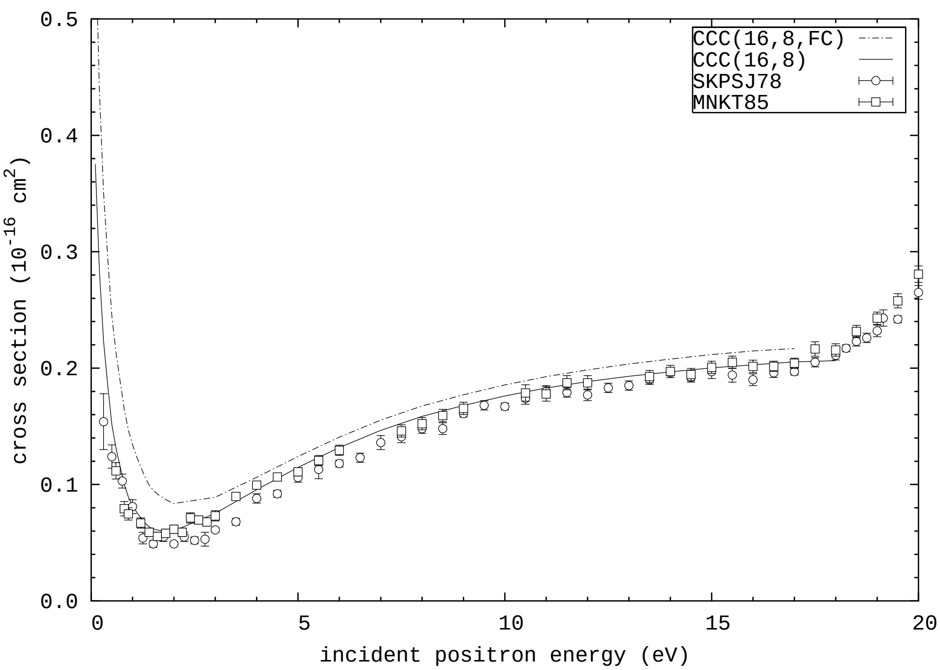

Fig. 4.9: Total scattering cross sections as a function of the incident positron energy below the positronium formation threshold. The present calculations are denoted by CCC(16,8) and CCC(16,8,FC) (as described in the text). The experimental data denoted by SKPSJ78 and MNKT85 are due to Mizogawa *et al* (1985) and Stein *et al* (1978) respectively.

The relatively simple frozen core (FC) method gives consistent higher values than the experimental data. The MC model, taking into account the electron-

electron correlations in the construction of the target wave functions and so giving a more accurate ground helium state, yields much better agreement with the experimental data. This indicates the significance of the electron-electron correlation in the low energy positron-helium scattering. Most importantly we have demonstrated that single centre target state expansions using multi-configuration interaction wave functions are necessary and sufficient to describe positron-helium atom scattering below the positronium formation threshold.

5. POSITRON-HELIUM SCATTERING AT INTERMEDIATE TO HIGH ENERGIES

5.1 Introduction

At incident positron energies above the helium first ionisation threshold of 24.6 eV, positronium formation, ionisation and target excitation processes are all possible . The fragmentation cross section is defined as the sum of the positronium formation and ionisation cross sections. Close to the ionisation threshold, the positronium formation channel is dominant while at higher energies the ionisation is the main contributor to this cross section (Moxom *et al*, 1995). At sufficiently high energies when electron exchange effects are minimal, the positron-impact ionisation cross section should merge with the corresponding electron-impact cross section allowing direct comparison between positron- and electron-atom scattering systems. The existence of the positronium formation and its interference with direct ionisation and excitation make the theoretical study of positron-helium scattering more interesting (and more complex) and challenging than for the corresponding electron-impact case.

Measurements of the total e^+-He scattering cross section have been performed by Stein *et al* (1978) at low energies and by Kauppila *et al* (1981) at intermediate to high energies. The total helium fragmentation cross section has been measured by Moxom *et al* (1995). Several measurements of positronium formation (Overton *et al*, 1993; Fromme *et al*, 1986; Fornari *et al*, 1983) and direct ionisation cross sections (Knudsen *et al*, 1990; Fromme *et al*, 1986; Diana *et al*, 1985) have also been performed. The threshold ionisation behaviour has been studied experimentally by Ashley *et al* (1996) for energies from 0.5 to 10 eV above the ionisation threshold. The total helium excitation cross section, which is dominated by the 2^1S and 2^1P cross sections, has been measured by Mori and Sueoka (1994) utilising a time-of-flight technique.

Positronium formation and ionisation cross sections have been calculated by Schultz and Olson (1988) using a Monte Carlo simulation. The sum of the two cross sections gave the total fragmentation cross section that did not agree well with the measurements of Moxom *et al* (1995). The positronium formation cross section was calculated by Mandal *et al* (1979) using a distorted-wave approximation and the agreement with the experimental data is satisfactory. As for the direct ionisation, many early theoretical studies have been reported, including a semi-empirical estimation (Griffith *et al*, 1979), distorted-wave approximations (Basu *et al*, 1985; Campeanu *et al*, 1987) and a pseudostate closed-state method (Chen, 1994). For a detailed comparison between these theories and experiments we refer the reader to Moxom *et al* (1995).

For helium 2^1S and 2^1P excitations, theoretical calculations have been carried out based on several different approaches: distorted wave approximation (Parcell *et al*, 1987), close-coupling (Willis and McDowell, 1982) and random phase approximation (Varracchio, 1990). However, the agreement between theory and experiment was not satisfactory, mainly due to the exclusion of the effects of positronium formation in these early models. Later, Hewitt *et al* (1992) developed a close-coupling approximation aiming to include fully the effects of coupling between various target channels. A single electron approximation with a model potential was used to describe the helium atom and yielded improved agreement with experiment.

The most recent close-coupling study of e^+-He scattering has been performed by Campbell *et al* (1998). While unsatisfactory results were obtained for energies below the positronium formation threshold, agreement with various measurements at the higher energies was generally satisfactory, as discussed in Chapter 1.

More recently, the quantal-semiclassical calculation of Deb and Crothers (2002) achieved excellent agreement with the absolute experimental threshold ionisation cross section of Ashley *et al* (1996).

Following on from our studies (see Chapter 4) on low-energy positron-helium scattering with the convergent close-coupling (CCC) method we now apply the CCC method at energies above the ionisation threshold through to 1 keV. At such energies positronium formation is taken into account through positive-energy pseudostates of relatively large orbital angular momentum l. Though we are not able to separate positronium formation from the ionisation channels the CCC method should yield accurate results for their combined cross sections, as well as the total, and individual discrete atomic transitions.

5.2 Calculations

Having found some minor variation between the results using the frozen-core (FC) approximation and the more accurate multi-configuration (MC) expansion at low energies (Wu *et al*, 2004*b*), we also consider both cases in the present study. In the earlier work we gave some detailed examples of convergence studies which we do not repeat here. Instead, we have checked that by taking $N_l = 16 - l$ and $l_{\max} = 8$ we have convergence with respect to increasing N_l and $l_{\max}$ to within a few percent for the cross sections presented in this work. The calculation labelled CCC(FC) couples 108 states with the ground state ionisation energy of 23.742 eV and static dipole polarisability of 1.364 a_0^3. The calculation labelled CCC(MC) couples a total of 136 states with the ground state ionisation energy of 24.515 eV with unchanged polarisability. The latter agrees satisfactorily with the corresponding data of 24.586 eV and 1.38 a_0^3 (quoted from Van Reeth and Humberston (1999*a*)). The extra accuracy of the ground state in the CCC(MC) calculation is achieved by allowing the "inner" electron to be described by $n \leq 3$ Laguerre orbitals with $\lambda = 4$. This is done only when generating ^{1}S states in the CCC(MC) calculations resulting in a more accurate ground state, as well as generating many more ^{1}S states. Otherwise the CCC(MC) and CCC(FC) are identical. For the higher energies we need to take into account more higher partial waves. In the following calculations we included partial waves up to $J = 25$.

The CCC calculations are by far the biggest, and hopefully the most accurate, single-centred approach to the problem to date. The following results have been submitted for publication (Wu *et al*, 2004*a*).

5.3 Total scattering cross section

Figure 5.1 presents the total scattering cross sections, from both the CCC(FC) and CCC(MC) calculations as a function of the excess energy (incident positron energy minus the calculated He ionisation energy). The experimental results (Stein *et al*, 1978; Kauppila *et al*, 1981) and the 30-state close-coupling calculations (Campbell *et al*, 1998) are also presented for comparison. Overall, the agreement between all theories and experiment is satisfactory, but a number of issues are worth mentioning. The CCC(FC) results agree reasonably well with the 30-state calculations of Campbell *et al* (1998), which are also based on frozen core approximation. A bigger variation is provided by an improved description of the ground state which leads to a minor, but a systematic underestimation of the experiment. We have tried to investigate this further, but have found that as we improve the target structure from the FC model the calculations (labelled CCC(MC)) move systematically through the experiment and converge a little below the measurements as shown.

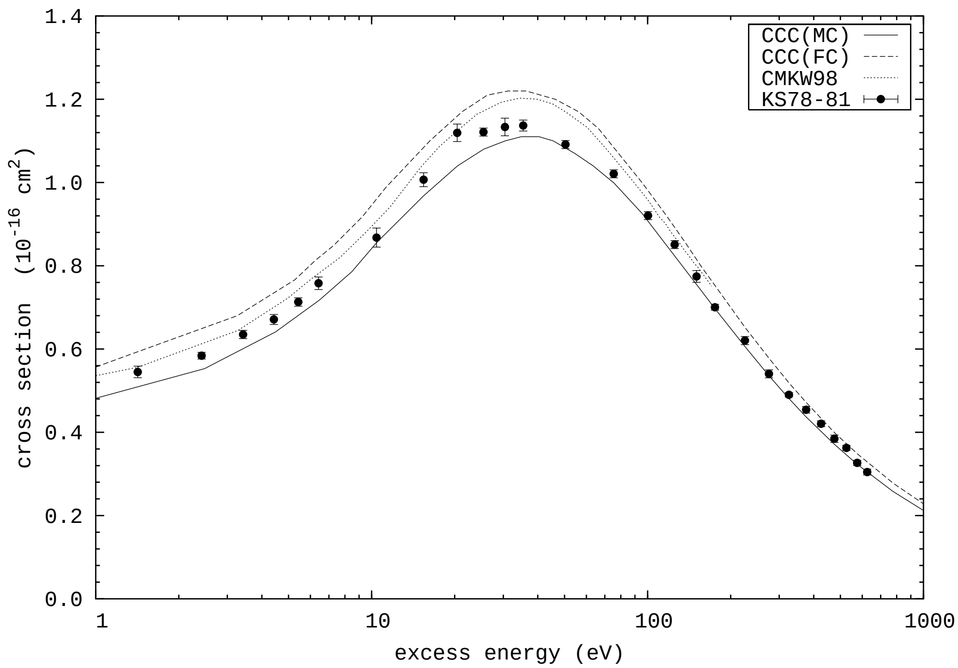

Fig. 5.1: Total positron-helium scattering cross sections as a function of energy above the He ionisation threshold. The present CCC calculations are labelled by the multi-configuration or frozen-core target structure, see text. The 30-state close-coupling results of Campbell *et al* (1998) denoted by CMKW98, and the experimental data of Stein *et al* (1978) and Kauppila *et al* (1981) denoted by KS78-81.

5.4 Fragmentation cross section

Figure 5.2 presents the fragmentation cross section, which is the sum of positronium formation and ionisation cross sections. As in figure 5.1 CCC(MC) gives generally marginally lower values than the experimental data from (Fromme *et al*, 1986; Moxom *et al*, 1995). However, unlike figure 5.1, the 30-state calculations of Campbell *et al* (1998) are now in very good agreement with the CCC(MC) calculation at sufficiently high energies, and not the CCC(FC) calculation. At

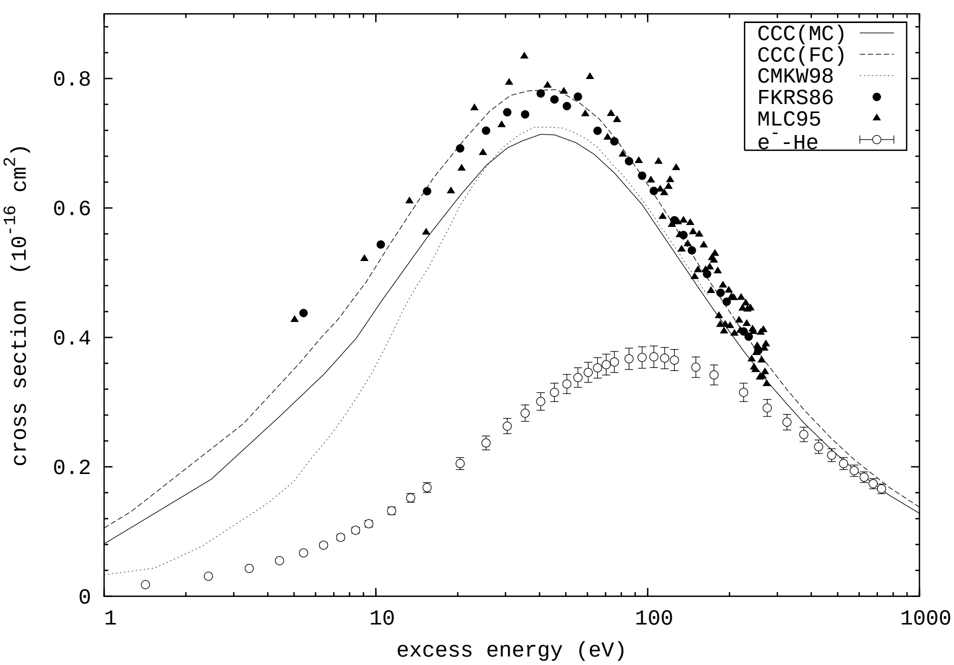

Fig. 5.2: The positron-helium fragmentation cross sections as a function of energy above the He ionisation threshold. The theory is same as in figure 5.1. The experimental data of Fromme *et al* (1986) is indicated by FKRS86. The experimental ionisation cross section for electron-helium scattering is due to Montague *et al* (1984).

the lower energies we require relatively large $l_{\max}$ to absorb the positronium flux, and hence the $l_{\max} = 3$ in the 30-state calculations of Campbell *et al* (1998) leads to a too small result. The 27-state calculation of Campbell *et al* (1998), which included explicit positronium formation yields much better agreement with experiment at the lower energies, but yields even lower cross sections at excess energies above 20 eV. The better agreement of our CCC(FC) calculation with the experimental data below 100 eV is accidental. At high energies, the positronium formation becomes a minor process compared to the ionisation channel. As expected, the ionisation cross section for positron-helium scattering merges with the corresponding electron-helium case measured by Montague *et al* (1984). There it is apparent that the better quality wave function of MC converges excellently to the high-energy experimental results whereas the FC calculation overestimates the experiment.

5.5 Elastic and excitation cross sections

The elastic cross section and He(2^1S) and He(2^1P) excitation cross sections are presented in figure 5.3 as a function of the excess energy. Previous close-coupling calculations from Campbell *et al* (1998) and Hewitt *et al* (1992) are also presented for comparison. For elastic scattering, the current CCC calculations generally predict lower values than the other two close-coupling calculations, although the results from Hewitt *et al* (1992) converge to the CCC calculations at the higher energies. It is not possible to be sure as to the origin of the discrepancy at the smaller energies. Campbell *et al* (1998) presented only the elastic results from the 27-state calculation, which yields a total cross section that is substantially too large (see their figures 13 and 14). Generally, a lack of excitation and ionisation channels in the calculations can lead to overestimated cross sections which is a feature of their calculation.

For the He(2^1P) and He(2^1S) excitation the theories are generally in better agreement. The largest discrepancy occurs around the maximum of the cross

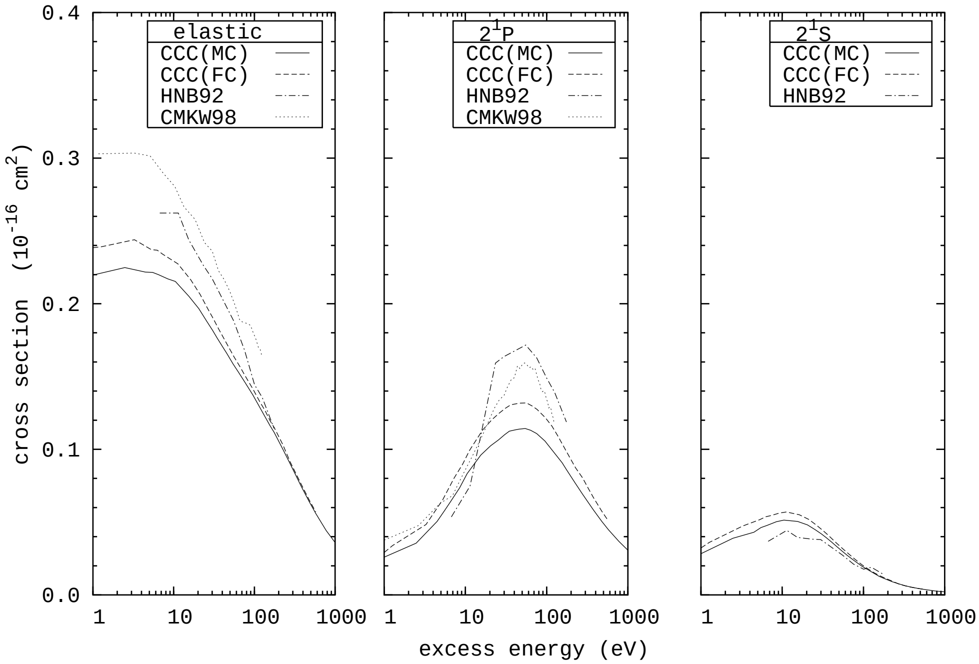

Fig. 5.3: The positron-helium elastic and He(2^1S), He(2^1P) excitation cross sections as a function of excess energy. The present calculations are represented by CCC(MC) and CCC(FC), see text. CMKW98 denotes the 27-state close-coupling calculation of Campbell *et al* (1998) and HNB92 denotes the close-coupling calculation of Hewitt *et al* (1992).

section. The systematic reduction of the cross sections by improving the target structure seems to be a systematic trend across all channels.

In figure 5.4 a comparison is presented between the current CCC calculations, and the close-coupling results of Hewitt *et al* (1992) for the combined excitations of the He(2^1S+2^1P) states. Since Campbell *et al* (1998) did not present their calculations of He(2^1S) excitation we are unable to compare with their data here. Corresponding He(2^1S+2^1P) experimental excitation data of Sueoka, as presented by Charlton and Laricchia (1990), are plotted together with the total excitation data of Mori and Sueoka (1994). The minor difference between the two sets of data indicates the dominance of the He(2^1S+2^1P) cross section in the total excitation cross section. This time the CCC(MC) results are a little higher than

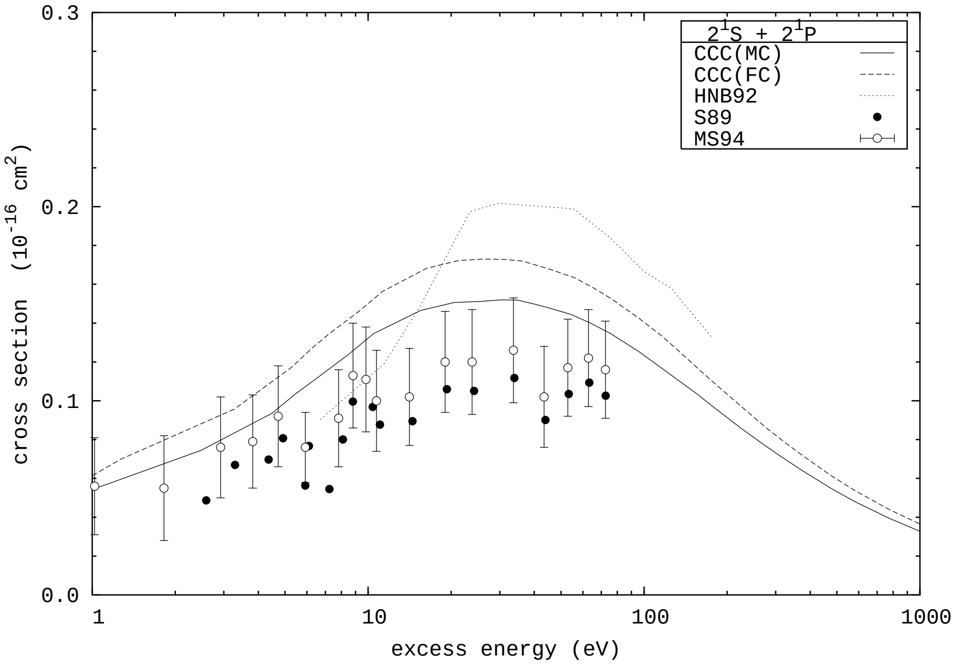

Fig. 5.4: The sum of the positron-impact excitation cross sections of He(2^1S) and He(2^1P). The theory is as for figure 5.3. The corresponding experimental data of Sueoka, as presented by Charlton and Laricchia (1990), is denoted by S89. The total excitation cross section data of Mori and Sueoka (1994) is denoted by MS94.

experiment, but are much improved on the CCC(FC) results. The dominant He(2^1P) contribution of Hewitt *et al* (1992) around the maximum, given in figure 5.3, leads to a substantial overestimate of the experimental data.

In conclusion we have applied the single-centred convergent close coupling calculations to positron-helium scattering above the ionisation threshold. We found that the often-used frozen-core approximation for the helium target yields to an overestimation of the cross sections by around 10% or so. Generally, satisfactory agreement between the CCC calculations, with the most accurate target structure, and the available experimental data has been achieved. Given the vast difference in the size of the various close-coupling calculations and the different approach to the target structure we find the similarity of the calculations to be quite remarkable. There are occasional differences, and we suggest that the present results are the most accurate on those occasions.

6. CONCLUSION

The Convergent Close Coupling (CCC) method has been applied, for the first time, to the scattering of positrons on helium. The helium target wave functions, as the basis in the expansion of the system wave functions, were obtained within various configuration interaction (CI) approximations. In the full CI approximation the two electrons are treated equally and thus all electron-electron correlation are taken into account. In the frozen-core (FC) approximation the CI expansion fixes one of the electrons to be described by a pure 1s orbital of He^+, while maintaining the required singlet and triplet symmetries. Lastly, the multi-configuration (MC) approximation relaxes the FC approximation to allow the description of the inner electron to include several low-lying orbitals. The accuracy of the target wave functions has been tested by comparing the calculated energy levels with the experimental data. The convergence of the calculations as a function of basis size in the expansion has been studied for both FC and MC expansions. The calculations performed in this thesis have been ensured to a level of a few percent convergences.

Based on positron-hydrogen scattering, comprehensive close-coupling formulas for positron-helium scattering have been developed. The reduced two-centre V-matrix elements were derived in momentum space for various channels. These include direct excitation and rearrangement channels, i.e. positronium formation. These formulas are ready for implementation in the future full two-centre CCC calculations for the positron-helium scattering.

Utilising a single-centre expansion, the low energy positron-helium elastic scattering has been studied by CCC for energies below the positronium formation threshold of 17.8 eV. The elastic cross section and phase shifts have been calculated as a function of the positron incident energy. The calculations agree very well with the experimental data and the variational calculations, but not previous single-centred calculations by Campbell *et al* (1998). It is believed that the differences are due to the lack of convergence in their calculations. Systematic comparisons between FC and MC calculations have indicated the significance of electron-electron correlation in the target wave function construction. The excellent agreement between the current CCC calculations with multi configuration (MC) and the experimental data has showed that the single-centre expansion is able to deliver accurate results for low energy positron-helium scattering.

For intermediate to high energies above the first ionisation threshold (24.6 eV), the same single-centre CCC expansion has been applied to calculate the elastic, excitation, fragmentation and total cross sections for positron-helium collisions. While the frozen core approach gave 10% overestimation of the cross sections, good agreement with the available experimental and other theoretical results has been obtained with multi core configuration (MC) approximation. At sufficiently high energies (above 300 eV), the fragmentation cross sections from both FC and MC approaches merged the ionisation cross section of electron-helium collisions.

The studies have proved that single-centre expansion, with accurate target state description, can deliver accurate data of practical value over a broad range of energies. In the small energy region, between positronium formation threshold of 17.8 eV and the ionisation threshold of 24.6 eV, implementation of the two-centre expansion is required to study explicitly the positronium formation process. Near the ionisation threshold, positronium formation is expected to have significant contribution to the fragmentation cross section. Two-centre expansion is also necessary to separate the ionisation and positronium formation processes at this energy range. We expect this work to be undertaken in the near future, based on the derivations presented in this thesis.

APPENDIX

A. PROPERTIES OF SOME SPECIAL FUNCTIONS

Some useful properties of the spherical harmonics, Legendre polynomials, Laguerre polynomials, Clebsch-Gorden coefficients, 3-j symbols and 6-j symbols are quoted mainly from Brink and Satchler (1993). Also included in this appendix are some derived properties which have been used in the derivation of the potential matrices.

A.1 Properties of Spherical Harmonics

Useful expansions

$$\begin{aligned} &|\boldsymbol{a}+\boldsymbol{b}|^l C_{l\,m}(\hat{\boldsymbol{a}+\boldsymbol{b}}) \\ &= \sum_{\lambda\mu} \left(\frac{(2l)!}{(2\lambda)!(2(l-\lambda))!} \right)^{1/2} a^{l-\lambda} b^{\lambda} C_{l-\lambda\ m-\mu}(\theta_a,\phi_a)\ C_{\lambda\,\mu}(\theta_b,\phi_b) \\ &\quad \langle l-\lambda\ \lambda\ \ m-\mu\ \ \mu | l\ m \rangle \end{aligned} \tag{A.1}$$

where

$$\hat{a} = \sqrt{2a+1},$$
$$C_{a\alpha}(\lambda,\mu) = \sqrt{\frac{4\pi}{2a+1}} Y_{a\alpha}(\lambda,\mu).$$

Combination of 2 spherical harmonics

$$Y_{a\alpha}(\theta,\phi)Y_{b\beta}(\theta,\phi) = \frac{\hat{a}\hat{b}}{\sqrt{4\pi}}\sum_c \hat{c}Y_{c\gamma}(\theta,\phi)(-1)^{\gamma}\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} \tag{A.2}$$

Integration over 3 spherical harmonics

$$\int Y_{a\alpha}(\theta,\phi)Y_{b\beta}(\theta,\phi)Y_{c\gamma}(\theta,\phi)\sin\theta d\theta d\phi = \frac{\hat{a}\hat{b}\hat{c}}{\sqrt{4\pi}}\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \tag{A.3}$$

Integration over 4 spherical harmonics

$$\begin{aligned} &\int d^2\hat{\boldsymbol{k}} Y_{l_1m_1}(\hat{\boldsymbol{k}})Y_{l_2m_2}(\hat{\boldsymbol{k}})Y_{l_3m_3}(\hat{\boldsymbol{k}})Y_{l_4m_4}(\hat{\boldsymbol{k}}) \\ &= \sum_{q_1m_{q_1}} \frac{\hat{l}_1\hat{l}_2\hat{l}_3\hat{l}_4\hat{q}_1^2}{4\pi}\begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_3 & l_4 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix}\begin{pmatrix} l_3 & l_4 & q_1 \\ m_3 & m_4 & m_{q_1} \end{pmatrix} \end{aligned} \tag{A.4}$$

Proof

$$\begin{aligned} &\int d^2\hat{\boldsymbol{k}} Y_{l_3m_3}(\hat{\boldsymbol{k}})Y_{l_4m_4}(\hat{\boldsymbol{k}})Y_{l_3m_3}(\hat{\boldsymbol{k}})Y_{l_4m_4}(\hat{\boldsymbol{k}}) \\ &= \int d^2\hat{\boldsymbol{k}} \sum_{q_1m_{q_1}} \frac{\hat{l}_1\hat{l}_2\hat{q}_1}{\sqrt{4\pi}}(-1)^{q_1}Y_{q_1m_{q_1}}(\hat{\boldsymbol{k}})\begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\ &\quad \sum_{q_2m_{q_2}} \frac{\hat{l}_1\hat{l}_2\hat{q}_1}{\sqrt{4\pi}}(-1)^{m_{q_2}}Y_{q_2m_{q_2}}(\hat{\boldsymbol{k}})\begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \end{aligned}$$

$$
\begin{aligned}
&= \sum_{q_1 m_{q_1}} \frac{\hat{l}_1 \hat{l}_2 \hat{q}_1}{\sqrt{4\pi}} (-1)^{m_{q_1}} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2 m_{q_2}} \frac{\hat{l}_3 \hat{l}_4 \hat{q}_2}{\sqrt{4\pi}} (-1)^{m_{q_2}} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&\quad \int d^2\hat{\boldsymbol{k}} Y_{q_1 m_{q_1}}(\hat{\boldsymbol{k}}) Y_{q_2 m_{q_2}}(\hat{\boldsymbol{k}}) \\
&= \sum_{q_1 m_{q_1}} \frac{\hat{l}_1 \hat{l}_2 \hat{q}_1}{\sqrt{4\pi}} (-1)^{m_{q_1}} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2 m_{q_2}} \frac{\hat{l}_3 \hat{l}_4 \hat{q}_2}{\sqrt{4\pi}} (-1)^{m_{q_2}} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&\quad \delta_{q_1 q_2} \delta_{m_{q_1} m_{q_2}} \\
&= \sum_{q_1 m_{q_1}} \frac{\hat{l}_1 \hat{l}_2 \hat{l}_3 \hat{l}_4 \hat{q}_1^2}{4\pi} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_1 \\ m_3 & m_4 & m_{q_1} \end{pmatrix}
\end{aligned}
$$

Integration over 5 spherical harmonics

$$
\begin{aligned}
&\int d^2\hat{\boldsymbol{k}} Y_{l_1 m_1}(\hat{\boldsymbol{k}}) Y_{l_2 m_2}(\hat{\boldsymbol{k}}) Y_{l_3 m_3}(\hat{\boldsymbol{k}}) Y_{l_4 m_4}(\hat{\boldsymbol{k}}) Y_{l_5 m_5}(\hat{\boldsymbol{k}}) \\
&= \sum_{q_1 m_{q_1} q_2 m_{q_2}} \frac{\hat{l}_1 \hat{l}_2 \hat{l}_3 \hat{l}_4 \hat{l}_5 \hat{q}_1^2 \hat{q}_2^2}{\left(\sqrt{4\pi}\right)^3} (-1)^{m_{q_1} + m_{q_2}} \\
&\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & l_5 \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \begin{pmatrix} q_1 & q_2 & l_5 \\ m_{q_1} & m_{q_2} & m_5 \end{pmatrix} \qquad \text{(A.5)}
\end{aligned}
$$

Proof

$$
\int d^2\hat{\boldsymbol{k}} Y_{l_3 m_3}(\hat{\boldsymbol{k}}) Y_{l_4 m_4}(\hat{\boldsymbol{k}}) Y_{l_3 m_3}(\hat{\boldsymbol{k}}) Y_{l_4 m_4}(\hat{\boldsymbol{k}}) Y_{l_5 m_5}(\hat{\boldsymbol{k}})
$$

$$
\begin{aligned}
&= \int d^2\hat{\boldsymbol{k}} Y_{l_5 m_5}(\hat{\boldsymbol{k}}) \sum_{q_1 m_{q_1}} \frac{\hat{l}_1 \hat{l}_2 \hat{q}_1}{\sqrt{4\pi}} (-1)^{m_{q_1}} Y_{q_1 m_{q_1}}(\hat{\boldsymbol{k}}) \\
&\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2 m_{q_2}} \frac{\hat{l}_1 \hat{l}_2 \hat{q}_1}{\sqrt{4\pi}} (-1)^{m_{q_2}} Y_{q_2 m_{q_2}}(\hat{\boldsymbol{k}}) \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&= \sum_{q_1 m_{q_1}} \frac{\hat{l}_1 \hat{l}_2 \hat{q}_1}{\sqrt{4\pi}} (-1)^{m_{q_1}} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2 m_{q_2}} \frac{\hat{l}_3 \hat{l}_4 \hat{q}_2}{\sqrt{4\pi}} (-1)^{m_{q_2}} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&\quad \int d^2\hat{\boldsymbol{k}} Y_{q_1 m_{q_1}}(\hat{\boldsymbol{k}}) Y_{q_2 m_{q_2}}(\hat{\boldsymbol{k}}) Y_{l_5 m_5}(\hat{\boldsymbol{k}}) \\
&= \sum_{q_1 m_{q_1}} \frac{\hat{l}_1 \hat{l}_2 \hat{q}_1}{\sqrt{4\pi}} (-1)^{m_{q_1}} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2 m_{q_2}} \frac{\hat{l}_3 \hat{l}_4 \hat{q}_2}{\sqrt{4\pi}} (-1)^{m_{q_2}} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&\quad \frac{\hat{q}_1 \hat{q}_2 \hat{l}_5}{\sqrt{4\pi}} \begin{pmatrix} q_1 & q_2 & l_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & l_5 \\ m_{q_1} & m_{q_2} & m_5 \end{pmatrix} \\
&= \sum_{q_1 m_{q_1} q_2 m_{q_2}} \frac{\hat{l}_1 \hat{l}_2 \hat{l}_3 \hat{l}_4 \hat{l}_5 \hat{q}_1^2 \hat{q}_2^2}{\left(\sqrt{4\pi}\right)^3} (-1)^{m_{q_1} + m_{q_2}} \\
&\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & l_5 \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \begin{pmatrix} q_1 & q_2 & l_5 \\ m_{q_1} & m_{q_2} & m_5 \end{pmatrix}
\end{aligned}
$$

Integration over 6 spherical harmonics

$$
\begin{aligned}
&\int d^2\hat{\boldsymbol{k}} Y_{l_1 m_1}(\hat{\boldsymbol{k}}) Y_{l_2 m_2}(\hat{\boldsymbol{k}}) Y_{l_3 m_3}(\hat{\boldsymbol{k}}) Y_{l_4 m_4}(\hat{\boldsymbol{k}}) Y_{l_5 m_5}(\hat{\boldsymbol{k}}) Y_{l_6 m_6}(\hat{\boldsymbol{k}}) \\
&= \sum_{q_1 m_{q_1} q_2 m_{q_2} q_3 m_{q_3}} \frac{\hat{l}_1 \hat{l}_2 \hat{l}_3 \hat{l}_4 \hat{l}_5 \hat{l}_6 \hat{q}_1^2 \hat{q}_2^2 \hat{q}_3^2}{\left(\sqrt{4\pi}\right)^3} (-1)^{m_{q_1} + m_{q_2} + m_{q_3}}
\end{aligned}
$$

$$\begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_5 & l_6 & q_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & q_3 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix}$$
$$\begin{pmatrix} l_5 & l_6 & q_3 \\ m_5 & m_6 & m_{q_3} \end{pmatrix} \begin{pmatrix} q_1 & q_2 & q_3 \\ m_{q_1} & m_{q_2} & m_{q_3} \end{pmatrix} \tag{A.6}$$

Proof

$$\begin{aligned}
&\int d^2\hat{\boldsymbol{k}} Y_{l_3m_3}(\hat{\boldsymbol{k}})Y_{l_4m_4}(\hat{\boldsymbol{k}})Y_{l_3m_3}(\hat{\boldsymbol{k}})Y_{l_4m_4}(\hat{\boldsymbol{k}})Y_{l_5m_5}(\hat{\boldsymbol{k}})Y_{l_6m_6}(\hat{\boldsymbol{k}}) \\
&= \int d^2\hat{\boldsymbol{k}} \sum_{q_1m_{q_1}} \frac{\hat{l}_1\hat{l}_2\hat{q}_1}{\sqrt{4\pi}}(-1)^{m_{q_1}} Y_{q_1m_{q_1}}(\hat{\boldsymbol{k}}) \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2m_{q_2}} \frac{\hat{l}_1\hat{l}_2\hat{q}_1}{\sqrt{4\pi}}(-1)^{m_{q_2}} Y_{q_2m_{q_2}}(\hat{\boldsymbol{k}}) \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&\quad \sum_{q_3m_{q_3}} \frac{\hat{l}_5\hat{l}_6\hat{q}_3}{\sqrt{4\pi}}(-1)^{m_{q_3}} Y_{q_3m_{q_3}}(\hat{\boldsymbol{k}}) \begin{pmatrix} l_5 & l_6 & q_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_5 & l_6 & q_3 \\ m_5 & m_6 & m_{q_3} \end{pmatrix} \\
&= \sum_{q_1m_{q_1}} \frac{\hat{l}_1\hat{l}_2\hat{q}_1}{\sqrt{4\pi}}(-1)^{m_{q_1}} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2m_{q_2}} \frac{\hat{l}_3\hat{l}_4\hat{q}_2}{\sqrt{4\pi}}(-1)^{m_{q_2}} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix} \\
&\quad \sum_{q_3m_{q_3}} \frac{\hat{l}_5\hat{l}_6\hat{q}_3}{\sqrt{4\pi}}(-1)^{m_{q_3}} \begin{pmatrix} l_5 & l_6 & q_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_5 & l_6 & q_3 \\ m_5 & m_6 & m_{q_3} \end{pmatrix} \\
&\quad \int d^2\hat{\boldsymbol{k}} Y_{q_1m_{q_1}}(\hat{\boldsymbol{k}})Y_{q_2m_{q_2}}(\hat{\boldsymbol{k}})Y_{q_3m_{q_3}}(\hat{\boldsymbol{k}}) \\
&= \sum_{q_1m_{q_1}} \frac{\hat{l}_1\hat{l}_2\hat{q}_1}{\sqrt{4\pi}}(-1)^{m_{q_1}} \begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \\
&\quad \sum_{q_2m_{q_2}} \frac{\hat{l}_3\hat{l}_4\hat{q}_2}{\sqrt{4\pi}}(-1)^{m_{q_2}} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix}
\end{aligned}$$

$$\sum_{q_3 m_{q_3}} \frac{\hat{l}_5\hat{l}_6\hat{q}_3}{\sqrt{4\pi}}(-1)^{m_{q_3}} \begin{pmatrix} l_5 & l_6 & q_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_5 & l_6 & q_3 \\ m_5 & m_6 & m_{q_3} \end{pmatrix}$$

$$\frac{\hat{q}_1\hat{q}_2\hat{q}_3}{\sqrt{4\pi}} \begin{pmatrix} q_1 & q_2 & q_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & q_3 \\ m_{q_1} & m_{q_2} & m_{q_3} \end{pmatrix}$$

$$= \sum_{q_1 m_{q_1} q_2 m_{q_2} q_3 m_{q_3}} \frac{\hat{l}_1\hat{l}_2\hat{l}_3\hat{l}_4\hat{l}_5\hat{l}_6\hat{q}_1^2\hat{q}_2^2\hat{q}_3^2}{\left(\sqrt{4\pi}\right)^3}(-1)^{m_{q_1}+m_{q_2}+m_{q_3}}$$

$$\begin{pmatrix} l_1 & l_2 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_5 & l_6 & q_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & q_3 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} l_1 & l_2 & q_1 \\ m_1 & m_2 & m_{q_1} \end{pmatrix} \begin{pmatrix} l_3 & l_4 & q_2 \\ m_3 & m_4 & m_{q_2} \end{pmatrix}$$

$$\begin{pmatrix} l_5 & l_6 & q_3 \\ m_5 & m_6 & m_{q_3} \end{pmatrix} \begin{pmatrix} q_1 & q_2 & q_3 \\ m_{q_1} & m_{q_2} & m_{q_3} \end{pmatrix}$$

A.2 Some properties of Legendre Polynomials

The associated Legendre Polynomial is defined as (Landau and Lifshitz, 1977)

$$P_l^{|m|}(\cos\theta) = \frac{\sin^{|m|}\theta}{2^l l!}\frac{d^{l+|m|}}{d\cos\theta^{l+|m|}}(\cos^2\theta - 1)^l. \tag{A.7}$$

The Legendre Polynomials (the associated Polynomials with $m = 0$) are orthogonal and normalised to $\frac{2}{2l+1}$

$$\int_{-1}^{1} P_l(x)P_m(x)dx = \delta_{lm}\frac{2}{2l+1}. \tag{A.8}$$

The Legendre Polynomials are also expressed in terms of spherical harmonics via the addition theorem:

$$P_l(\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}}') = \frac{4\pi}{2l+1}\sum_{m=-l}^{m=l} Y^*_{lm}(\hat{\boldsymbol{n}}')Y_{lm}(\hat{\boldsymbol{n}}). \tag{A.9}$$

A.3 A property of Laguerre Polynomial

The Laguerre polynomial is given explicitly by the expansion

$$L_{n+l}^{2l+1}(\rho) = -[(n+l)!]^2 \sum_{k=0}^{n-l-1} \frac{(-\rho)^k}{k!(n-l-1-k)!(2l+1+k)!}, \tag{A.10}$$

which we find useful in calculating some of the integrals.

A.4 Identities involving plane waves

Plan wave can be expanded as functions of spherical harmonics (Brink and Satchler, 1993),

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = 4\pi \sum_{\lambda\mu} i^{\lambda} j_{\lambda}(kr) Y_{\lambda\mu}^{*}(\hat{\boldsymbol{k}}) Y_{\lambda\mu}(\hat{\boldsymbol{r}}) \tag{A.11}$$

$$\int d^3\boldsymbol{r}_0 \frac{e^{i(\boldsymbol{k}_0-\boldsymbol{k}_0')\cdot\boldsymbol{r}_0}}{r_0} = \frac{4\pi}{|\boldsymbol{k}_0-\boldsymbol{k}_0'|^2} \tag{A.12}$$

$$\int d^3\boldsymbol{r}_0 \frac{e^{i(\boldsymbol{k}_0-\boldsymbol{k}_0')\cdot\boldsymbol{r}_0}}{r_{01}} = \frac{4\pi e^{i(\boldsymbol{k}_0-\boldsymbol{k}_0')\cdot\boldsymbol{r}_1}}{|\boldsymbol{k}_0-\boldsymbol{k}_0'|^2} \tag{A.13}$$

A.5 Contraction of 3-j symbols

We make extensive use in the thesis derivations for the potentials of the following two identities:

$$\sum_{\alpha\beta\gamma}(-1)^{A+B+C+\alpha+\beta+\gamma}\begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix}\begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix}\begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix}$$
$$= \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma' \end{pmatrix}\begin{Bmatrix} a & b & c \\ A & B & C \end{Bmatrix}, \tag{A.14}$$

$$\sum_{\alpha\beta\gamma\alpha'\beta'}(-1)^{A+B+C+\alpha+\beta+\gamma}$$
$$\begin{pmatrix} A & B & c \\ \alpha & -\beta & \gamma' \end{pmatrix}\begin{pmatrix} B & C & a \\ \beta & -\gamma & \alpha' \end{pmatrix}\begin{pmatrix} C & A & b \\ \gamma & -\alpha & \beta' \end{pmatrix}\begin{pmatrix} a & b & c_1 \\ \alpha' & \beta' & \gamma'_1 \end{pmatrix}$$
$$= \frac{1}{2c+1}\delta_{cc_1}\delta_{\gamma'\gamma'_1}\begin{Bmatrix} a & b & c \\ A & B & C \end{Bmatrix}. \tag{A.15}$$

B. DERIVATION OF EXPRESSION (2.10)

The purpose of this Appendix is to derive the helium wave function in the format of equation (2.10) from the general Configuration Interaction expansion format, equation (2.7). We start from analysis the singlet- and triplet-spin functions. Then we will apply these functions to the CI expansion (2.7) and demonstrate that we obtain the expression (2.5).

B.1 Expressions (2.10)

In the configuration interaction expansion of the helium wave function, equation (2.7), the helium wave function is expanded in helium configurations which are the linear combination of a series of products of 2-single electron orbital and spin functions. These expansions can be reorganised into product of helium angular, radial and spin functions. The angular helium wave function is described by the bipolar spherical harmonics. The radial wave function consists of the coupled product of two Laguerre functions. The coupling coefficients will be solved numerically. The spin function can be found in Kessler (1985). Its derivation will be given in the following section.

B.1.1 Triplet Spin $s = 1, \mu = -1, 0, 1$

For the triplet spin we have $\mu = -1, 0, 1$.

For $s = 1, \mu = 1$:

$\mu_a = \frac{1}{2}, \mu_b = \frac{1}{2}$ and $\left\langle \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}|11\right\rangle = 1$

$$\begin{aligned}
\Phi^{ab}_{lm11}(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \frac{1}{\sqrt{2}}(1 - P_{12}) \left\langle \boldsymbol{x}_1\boldsymbol{x}_2|ab(l_al_b)lm(\frac{1}{2}\frac{1}{2})11 \right\rangle \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b\mu_a\mu_b} \langle l_al_bm_am_b|lm\rangle \left\langle \frac{1}{2}\frac{1}{2}\mu_a\mu_b|s\mu \right\rangle \\
&\times \Big(\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \\
&\quad -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\Big) \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \left[\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\right. \\
&\quad \left. -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\right] \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1) \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \left[\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\right. \\
&\quad \left. -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\right] \chi_{1,1}(\sigma_1, \sigma_2),
\end{aligned}$$

where we used equation (2.14).

For $s = 1, \mu = -1$:

$\mu_a = -\frac{1}{2}, \mu_b = -\frac{1}{2}$ and $\left\langle \frac{1}{2}\frac{1}{2} - \frac{1}{2} - \frac{1}{2}|1 - 1\right\rangle = 1$

$$\begin{aligned}
\Phi^{ab}_{lm1-1}(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \frac{1}{\sqrt{2}}(1 - P_{12}) \left\langle \boldsymbol{x}_1\boldsymbol{x}_2|ab(l_al_b)lm(\frac{1}{2}\frac{1}{2})1-1 \right\rangle \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b\mu_a\mu_b} \langle l_al_bm_am_b|lm\rangle \left\langle \frac{1}{2}\frac{1}{2}\mu_a\mu_b|s\mu \right\rangle \\
&\times \Big[\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) \\
&\quad - \zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\Big] \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \left[\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\right. \\
&\quad \left. - \zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\right] \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)
\end{aligned}$$

$$
\begin{aligned}
= \quad & \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \left[\zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \right. \\
& \left. - \zeta_{n_a l_a}(r_2) \zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \right] \chi_{1,-1}(\sigma_1, \sigma_2),
\end{aligned}
$$

again using equation (2.14).

For $s = 1, \mu = 0$:

$\mu_a = \frac{1}{2},\ \mu_b = -\frac{1}{2}$ or $\mu_a = -\frac{1}{2},\ \mu_b = \frac{1}{2}$, $\left\langle \frac{1}{2} \frac{1}{2} \frac{1}{2} - \frac{1}{2} | 10 \right\rangle = \frac{1}{\sqrt{2}}$

and $\left\langle \frac{1}{2} \frac{1}{2} - \frac{1}{2} \frac{1}{2} | 10 \right\rangle = \frac{1}{\sqrt{2}}$, we have

$$
\begin{aligned}
\Phi^{ab}_{lm10}(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \frac{1}{\sqrt{2}} (1 - P_{12}) \left\langle \boldsymbol{x}_1 \boldsymbol{x}_2 | ab(l_a l_b) lm (\frac{1}{2} \frac{1}{2}) 10 \right\rangle \\
= \quad & \frac{1}{\sqrt{2}} \sum_{m_a m_b \mu_a \mu_b} \langle l_a l_b m_a m_b | lm \rangle \left\langle \frac{1}{2} \frac{1}{2} \mu_a \mu_b | 10 \right\rangle \\
& \times \Big(\zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \chi_{\frac{1}{2}\mu_a}(\sigma_1) \chi_{\frac{1}{2}\mu_b}(\sigma_2) \\
& -\zeta_{n_a l_a}(r_2) \zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \chi_{\frac{1}{2}\mu_a}(\sigma_2) \chi_{\frac{1}{2}\mu_b}(\sigma_1) \Big) \\
= \quad & \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \left\langle \frac{1}{2} \frac{1}{2} \frac{1}{2} - \frac{1}{2} | 10 \right\rangle \\
& \times \Big(\zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) \\
& -\zeta_{n_a l_a}(r_2) \zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1) \Big) \\
& + \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \left\langle \frac{1}{2} \frac{1}{2} - \frac{1}{2} \frac{1}{2} | 10 \right\rangle \\
& \times \Big(\zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \\
& -\zeta_{n_a l_a}(r_2) \zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1) \Big) \\
= \quad & \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \frac{1}{\sqrt{2}} \\
& \times \Big(\zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) \\
& -\zeta_{n_a l_a}(r_2) \zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1) \\
& + \zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1) \chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)
\end{aligned}
$$

$$
\begin{aligned}
&\quad -\zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1)Y_{l_a m_a}(\hat{\boldsymbol{r}}_2)Y_{l_b m_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\Big) \\
&= \frac{1}{\sqrt{2}}\sum_{m_a m_b}\langle l_a l_b m_a m_b|lm\rangle \\
&\quad \times[\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2)Y_{l_a m_a}(\hat{\boldsymbol{r}}_1)Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \\
&\quad -\zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1)Y_{l_a m_a}(\hat{\boldsymbol{r}}_2)Y_{l_b m_b}(\hat{\boldsymbol{r}}_1)] \\
&\quad \times\frac{1}{\sqrt{2}}\left(\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2)+\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\right) \\
&= \frac{1}{\sqrt{2}}\sum_{m_a m_b}\langle l_a l_b m_a m_b|lm\rangle\left[\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2)Y_{l_a m_a}(\hat{\boldsymbol{r}}_1)Y_{l_b m_b}(\hat{\boldsymbol{r}}_2)\right. \\
&\quad \left. -\zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1)Y_{l_a m_a}(\hat{\boldsymbol{r}}_2)Y_{l_b m_b}(\hat{\boldsymbol{r}}_1)\right]\chi_{1,0}(\sigma_1,\sigma_2)
\end{aligned}
$$

from equation (2.14).

Thus the wave functions of the system with spin 1 states are given by

$$
\Phi^{ab}_{lm1\mu}(\boldsymbol{x}_1,\boldsymbol{x}_2)=\phi^{ab}_{lm1}(\boldsymbol{r}_1,\boldsymbol{r}_2)\chi_{1\mu}(\sigma_1,\sigma_2) \tag{B.1}
$$

where $\chi_{1\mu}$ denotes the triplet spin symmetric wave functions defined in equation (2.14) and $\phi^{ab}_{lm1}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is the antisymmetric orbital helium wave function

$$
\begin{aligned}
&\phi^{ab}_{lm1}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\
&\quad = \frac{1}{\sqrt{2}}\sum_{m_a m_b}\langle l_a l_b m_a m_b|lm\rangle\left[\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2)Y_{l_a m_a}(\hat{\boldsymbol{r}}_1)Y_{l_b m_b}(\hat{\boldsymbol{r}}_2)\right. \\
&\quad\quad \left. -\zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1)Y_{l_a m_a}(\hat{\boldsymbol{r}}_2)Y_{l_b m_b}(\hat{\boldsymbol{r}}_1)\right]
\end{aligned}
$$

B.1.2 Singlet spin $s = 0, \mu = 0$

Since $\mu_a = \frac{1}{2}, \mu_b = -\frac{1}{2}$ *or* $\mu_a = -\frac{1}{2}, \mu_b = \frac{1}{2}$, $\left\langle \frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2}|00\right\rangle = \frac{1}{\sqrt{2}}$

and $\left\langle \frac{1}{2}\frac{1}{2} - \frac{1}{2}\frac{1}{2}|00\right\rangle = -\frac{1}{\sqrt{2}}$, we have

$$\begin{aligned}
\Phi^{ab}_{lm00}(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \frac{1}{\sqrt{2}}(1 - P_{12}) \left\langle \boldsymbol{x}_1\boldsymbol{x}_2|ab(l_al_b)lm(\frac{1}{2}\frac{1}{2})00 \right\rangle \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b\mu_a\mu_b} \langle l_al_bm_am_b|lm\rangle \left\langle \frac{1}{2}\frac{1}{2}\mu_a\mu_b|00\right\rangle \\
&\quad \times \Big(\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi_{\frac{1}{2}\mu_a}(\sigma_1)\chi_{\frac{1}{2}\mu_b}(\sigma_2) \\
&\qquad -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}\mu_a}(\sigma_2)\chi_{\frac{1}{2}\mu_b}(\sigma_1)\Big) \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \left\langle \frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2}|00\right\rangle \\
&\quad \times \Big(\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) \\
&\qquad -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\Big) \\
&\quad +\frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \left\langle \frac{1}{2}\frac{1}{2} - \frac{1}{2}\frac{1}{2}|00\right\rangle \\
&\quad \times \Big(\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \\
&\qquad -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\Big) \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \frac{1}{\sqrt{2}} \\
&\quad \times \Big(\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi^{(\sigma_1)}_{\frac{1}{2}\frac{1}{2}}\chi^{(\sigma_2)}_{\frac{1}{2}-\frac{1}{2}} \\
&\qquad -\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1) \\
&\quad - \zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \\
&\qquad +\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\Big) \\
&= \frac{1}{\sqrt{2}} \sum_{m_am_b} \langle l_al_bm_am_b|lm\rangle \, [\zeta_{n_al_a}(r_1)\zeta_{n_bl_b}(r_2)Y_{l_am_a}(\hat{\boldsymbol{r}}_1)Y_{l_bm_b}(\hat{\boldsymbol{r}}_2) \\
&\quad +\zeta_{n_al_a}(r_2)\zeta_{n_bl_b}(r_1)Y_{l_am_a}(\hat{\boldsymbol{r}}_2)Y_{l_bm_b}(\hat{\boldsymbol{r}}_1)]
\end{aligned}$$

$$
\begin{aligned}
& \times \frac{1}{\sqrt{2}} \Big(\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_2) - \chi_{\frac{1}{2}-\frac{1}{2}}(\sigma_1)\chi_{\frac{1}{2}\frac{1}{2}}(\sigma_2) \Big) \\
= \ & \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \left[\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \right. \\
& \left. + \zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \right] \times \chi_{00}(\sigma_1 \sigma_2) \\
= \ & \phi^{ab}_{lm0}(\boldsymbol{r}_1, \boldsymbol{r}_2) \chi_{00}(\sigma_1, \sigma_2)
\end{aligned}
$$

where $\chi_{00}(\sigma_1, \sigma_2)$ is given by equation (2.15) and $\phi^{ab}_{lm0}(\boldsymbol{r}_1, \boldsymbol{r}_2)$, the symmetric radial and angular part, is given by

$$
\begin{aligned}
\phi^{ab}_{lm0}(\boldsymbol{r}_1, \boldsymbol{r}_2) \ = \ & \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \left[\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \right. \\
& \left. + (-1)^s \zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \right].
\end{aligned}
$$

Thus

$$
\Phi^{ab}_{lm00}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \phi^{ab}_{lm0}(\boldsymbol{r}_1, \boldsymbol{r}_2) \chi_{00}(\sigma_1, \sigma_2) \tag{B.2}
$$

B.1.3 Expressions (2.10)

From the previous subsections we may write

$$
\Phi^{ab}_{lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \phi^{ab}_{lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \chi_{sm_s}(\sigma_1, \sigma_2) \tag{B.3}
$$

here

$$
\begin{aligned}
\phi^{ab}_{lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \ = \ & \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle l_a l_b m_a m_b | lm \rangle \left[\zeta_{n_a l_a}(r_1)\zeta_{n_b l_b}(r_2) Y_{l_a m_a}(\hat{\boldsymbol{r}}_1) Y_{l_b m_b}(\hat{\boldsymbol{r}}_2) \right. \\
& \left. + (-1)^s \zeta_{n_a l_a}(r_2)\zeta_{n_b l_b}(r_1) Y_{l_a m_a}(\hat{\boldsymbol{r}}_2) Y_{l_b m_b}(\hat{\boldsymbol{r}}_1) \right]
\end{aligned}
$$

and $\chi_{sm_s}(\sigma_1, \sigma_2)$ are the spin wave functions given by (2.14) and (2.15). Interchanging the indices (a, b) for the second item in the above expression and noting

$$\langle l_a l_b m_a m_b | lm \rangle = (-1)^{l_a+l_b+l} \langle l_b l_a m_b m_a | lm \rangle$$

we have

$$\begin{aligned} \phi^{ab}_{lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) &= \frac{1}{\sqrt{2}} \left[1 + (-1)^{l_a+l_b+l+s}\right] \zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2) \mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) \\ &= \phi^{(ab)}_{(l_a l_b)lms}(r_1, r_2) \mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2), \end{aligned} \tag{B.4}$$

with

$$\phi^{(ab)}_{(l_a l_b)lms}(r_1, r_2) = \frac{1}{\sqrt{2}} \left[1 + (-1)^{l_a+l_b+l+s}\right] \zeta_{n_a l_a}(r_1) \zeta_{n_b l_b}(r_2)$$

and the $\mathcal{Y}_{(l_a l_b)lm}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)$ are bipolar spheric harmonics defined in (2.12). (B.3) and (B.4) together give the expression (2.10).

Finally we note that equation (2.5) giving the general factorisation of the helium wave function into a product of a space coordinate part and spin part follows from the above equations.

Applying the (B.3) and (B.4) to the general MCI helium wave function equation (2.7), we have

$$\Psi_{\alpha lms}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sum_{(ab)} C^{ab}_{\alpha lms} \Phi^{ab}_{lmsm_s}(\boldsymbol{x}_1, \boldsymbol{x}_2)$$

$$
\begin{aligned}
&= \left(\sum_{(ab)} C^{ab}_{\alpha lms} \phi^{ab}_{lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \right) \chi_{sm_s}(\sigma_1, \sigma_2) \\
&= \psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \chi_{sm_s}(\sigma_1, \sigma_2)
\end{aligned}
$$

with

$$
\psi_{\alpha lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{(ab)} C^{(ab)}_{\alpha lms} \phi^{(ab)}_{lms}(\boldsymbol{r}_1, \boldsymbol{r}_2) \tag{B.5}
$$

C. FORMULAS AND MATRIX ELEMENTS INVOLVING $\frac{1}{R_{12}}$

The followings are derivations for the equation (2.21) for the helium target structure calculation.

C.1 Expansion of $\frac{1}{r_{12}}$

A generating function for the Legendre polynomials is (Landau and Lifshitz, 1977)

$$\frac{1}{(1+2xt+t^2)^{\frac{1}{2}}} = \sum_{l=0}^{\infty} P_l(x)t^l, \qquad |t| < 1.$$

By definition

$$\begin{aligned}\frac{1}{r_{12}} &= \frac{1}{(r_1^2 - 2r_1 r_2 \cos(\theta) + r_2^2)^{\frac{1}{2}}} \\ &= \frac{1}{(r_<^2 - 2r_< r_> \cos(\theta) + r_>^2)^{\frac{1}{2}}} \\ &= \frac{1}{r_>(1 - 2(\frac{r_<}{r_>})\cos(\theta) + (\frac{r_<}{r_>})^2)^{\frac{1}{2}}}\end{aligned}$$

where $\theta = \hat{\boldsymbol{r}}_1 \cdot \hat{\boldsymbol{r}}_2$ and $r_{<(>)} = \min(\max)(r_1, r_2)$.

If we take $t = \frac{r_<}{r_>}$ $x = \cos(\theta)$ and use the addition theorem (A.9) we get the following useful formula

$$\frac{1}{r_{12}} = \sum_{\lambda m_\lambda} \frac{4\pi}{2\lambda+1} \frac{r_<^\lambda}{r_>^{\lambda+1}} Y_{\lambda m}(\hat{\boldsymbol{r}}_1) Y_{\lambda m}^\star(\hat{\boldsymbol{r}}_2). \tag{C.1}$$

C.2 The matrix element $\langle l'_1 l'_2 m'_1 m'_2 \left| \frac{1}{r_{12}} \right| l_1 l_2 m_1 m_2 \rangle$

$$
\begin{aligned}
&\langle l'_1 l'_2 m'_1 m'_2 \left| \frac{1}{r_{12}} \right| l_1 l_2 m_1 m_2 \rangle \\
&= \sum_{\lambda m_\lambda} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{m'_1+m'_2+m_\lambda} \hat{l}'_1 \hat{l}_1 \hat{l}'_2 \hat{l}_2 \\
&\quad \begin{pmatrix} l_1 & \lambda & l'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & \lambda & l'_1 \\ m_1 & m_\lambda & -m'_1 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ m_2 & -m_\lambda & -m'_2 \end{pmatrix}
\end{aligned} \tag{C.2}
$$

Proof

$$
\begin{aligned}
&\langle l'_1 l'_2 m'_1 m'_2 \left| \frac{1}{r_{12}} \right| l_1 l_2 m_1 m_2 \rangle \\
&= \int d\hat{\boldsymbol{r}}_1 d\hat{\boldsymbol{r}}_2 \langle l'_1 l'_2 m'_1 m'_2 | \hat{\boldsymbol{r}}_1 \hat{\boldsymbol{r}}_2 \rangle \langle \hat{\boldsymbol{r}}_1 \hat{\boldsymbol{r}}_2 | \frac{1}{r_{12}} | l_1 l_2 m_1 m_2 \rangle \\
&= \int d\hat{\boldsymbol{r}}_1 d\hat{\boldsymbol{r}}_2 \langle l'_1 l'_2 m'_1 m'_2 | \hat{\boldsymbol{r}}_1 \hat{\boldsymbol{r}}_2 \rangle \frac{1}{r_{12}} \langle \hat{\boldsymbol{r}}_1 \hat{\boldsymbol{r}}_2 | l_1 l_2 m_1 m_2 \rangle \\
&= \int d\hat{\boldsymbol{r}}_1 d\hat{\boldsymbol{r}}_2 Y^*_{l'_1 m'_1}(\hat{\boldsymbol{r}}_1) Y^*_{l'_2 m'_2}(\hat{\boldsymbol{r}}_2) \frac{1}{r_{12}} Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}
$$

$$
\begin{aligned}
&= \int d\hat{\boldsymbol{r}}_1 d\hat{\boldsymbol{r}}_2 Y^*_{l'_1 m'_1}(\hat{\boldsymbol{r}}_1) Y^*_{l'_2 m'_2}(\hat{\boldsymbol{r}}_2) Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&\quad \sum_{\lambda m_\lambda} \frac{4\pi}{2\lambda+1} \frac{r_<^\lambda}{r_>^{\lambda+1}} Y_{\lambda m_\lambda}(\hat{\boldsymbol{r}}_1) Y^\star_{\lambda m_\lambda}(\hat{\boldsymbol{r}}_2)
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{\lambda m_\lambda} \frac{4\pi}{2\lambda+1} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{m'_1+m'_2+m_\lambda} \\
&\quad \times \int d\hat{\boldsymbol{r}}_1 Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{\lambda m_\lambda}(\hat{\boldsymbol{r}}_1) Y_{l'_1 -m'_1}(\hat{\boldsymbol{r}}_1) \\
&\quad \int d\hat{\boldsymbol{r}}_2 Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) Y_{\lambda\, -m_\lambda}(\hat{\boldsymbol{r}}_2) Y_{l'_2 -m'_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{\lambda m_\lambda} \frac{4\pi}{2\lambda+1} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{m_1'+m_2'+m_\lambda} (4\pi)^2 \\
&\quad \times \left[\frac{(2l_1+1)}{4\pi}\frac{(2\lambda+1)}{4\pi}\frac{(2l_1'+1)}{4\pi}\right]^{\frac{1}{2}} \begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & \lambda & l_1' \\ m_1 & m_\lambda & -m_1' \end{pmatrix} \\
&\quad \times \left[\frac{(2l_2+1)}{4\pi}\frac{(2\lambda+1)}{4\pi}\frac{(2l_2'+1)}{4\pi}\right]^{\frac{1}{2}} \begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l_2' \\ m_2 & -m_\lambda & -m_2' \end{pmatrix} \\
&= \sum_{\lambda m_\lambda} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{m_1'+m_2'+m_\lambda} \hat{l}_1'\hat{l}_1\hat{l}_2'\hat{l}_2 \times \begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \begin{pmatrix} l_1 & \lambda & l_1' \\ m_1 & m_\lambda & -m_1' \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l_2' \\ m_2 & -m_\lambda & -m_2' \end{pmatrix}.
\end{aligned}
$$

C.3 The matrix element $\langle (l'_1 l'_2) l' m' | \frac{1}{r_{12}} | (l_1 l_2) l m \rangle$

Noting that

$$
\begin{aligned}
|(l_1 l_2) l m\rangle &= \sum_{m_1 m_2} |l_1 l_2 m_1 m_2\rangle \langle l_1 l_2 m_1 m_2 | (l_1 l_2) l m\rangle \\
&= \sum_{m_1 m_2} (-1)^{l_1 - l_2 - m} \hat{l} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} |l_1 l_2 m_1 m_2\rangle
\end{aligned}
$$

we have

$$
\begin{aligned}
&\langle (l'_1 l'_2) l' m' \left| \frac{1}{r_{12}} \right| (l_1 l_2) l m \rangle \\
&= \sum_{\lambda} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{l+\lambda} \hat{l}_1'\hat{l}_1\hat{l}_2'\hat{l}_2 \delta_{ll'} \delta_{mm'} \\
&\quad \begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_1 & l_1' & \lambda \\ l_2' & l_2 & l \end{Bmatrix} \\
&. \qquad \text{(C.3)}
\end{aligned}
$$

Proof

$$
\begin{aligned}
&\langle (l'_1 l'_2) l' m' \left| \frac{1}{r_{12}} \right| (l_1 l_2) l m \rangle \\
= &\sum_{m'_1 m'_2 m_1 m_2} (-1)^{l'_1 - l'_2 - m'} (-1)^{l_1 - l_2 - m} \hat{l}' \hat{l} \\
&\begin{pmatrix} l'_1 & l'_2 & l' \\ m'_1 & m'_2 & -m' \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \langle l'_1 l'_2 m'_1 m'_2 \left| \frac{1}{r_{12}} \right| l_1 l_2 m_1 m_2 \rangle \\
= &\sum_{m'_1 m'_2 m_1 m_2} (-1)^{l'_1 - l'_2 - m'} (-1)^{l_1 - l_2 - m} \hat{l}' \hat{l} \\
&\begin{pmatrix} l'_1 & l'_2 & l' \\ m'_1 & m'_2 & -m' \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \\
&\sum_{\lambda m_\lambda} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{m'_1 + m'_2 + m_\lambda} \hat{l}'_1 \hat{l}_1 \hat{l}'_2 \hat{l}_2 \times \begin{pmatrix} l_1 & \lambda & l'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ 0 & 0 & 0 \end{pmatrix} \\
&\begin{pmatrix} l_1 & \lambda & l'_1 \\ m_1 & m_\lambda & -m'_1 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ m_2 & -m_\lambda & -m'_2 \end{pmatrix} \\
= &\sum_\lambda (-1)^{l'_1 - l'_2 - m'} (-1)^{l_1 - l_2 - m} \frac{r_<^\lambda}{r_>^{\lambda+1}} \hat{l}'_1 \hat{l}_1 \hat{l}'_2 \hat{l}_2 \hat{l} \hat{l}' \begin{pmatrix} l_1 & \lambda & l'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \sum_{m'_1 m'_2 m_1 m_2 m_\lambda} (-1)^{m'_1 + m'_2 + m_\lambda} \begin{pmatrix} l'_1 & l'_2 & l' \\ m'_1 & m'_2 & -m' \end{pmatrix} \\
&\times \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_1 & \lambda & l'_1 \\ m_1 & m_\lambda & -m'_1 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ m_2 & -m_\lambda & -m'_2 \end{pmatrix} \\
= &\sum_\lambda (-1)^{l'_1 - l'_2 - m'} (-1)^{l_1 - l_2 - m} \frac{r_<^\lambda}{r_>^{\lambda+1}} \hat{l}'_1 \hat{l}_1 \hat{l}'_2 \hat{l}_2 \hat{l} \hat{l}' \begin{pmatrix} l_1 & \lambda & l'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \sum_{m'_1 m'_2 m_1 m_2 m_\lambda} (-1)^{m'_1 + m'_2 + m_\lambda} (-1)^{l'_1 + l'_2 + l'} (-1)^{l_1 + \lambda + l'_1} \\
&\begin{pmatrix} l'_2 & l'_1 & l' \\ m'_2 & m'_1 & -m' \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \\
&\begin{pmatrix} \lambda & l_1 & l'_1 \\ m_\lambda & m_1 & -m'_1 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ m_2 & -m_\lambda & -m'_2 \end{pmatrix} \\
= &\sum_\lambda (-1)^{l'_1 - l'_2 - m'} (-1)^{l'_1 + l'_2 + l'} (-1)^{l_1 + \lambda + l'_1}
\end{aligned}
$$

$$
\begin{aligned}
& \times(-1)^{l_1-l_2-m}\frac{r_<^\lambda}{r_>^{\lambda+1}}\hat{l}_1'\hat{l}_1\hat{l}_2'\hat{l}_2\hat{l}\hat{l}'\begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \\
& \times\sum_{m_1'm_2'm_1m_2m_\lambda}(-1)^{m_1'+m_2'+m_\lambda}(-1)^{l_2+\lambda+l_2'}(-1)^{l_1+l_1'+\lambda} \\
& \begin{pmatrix} l_2' & l_1' & l' \\ m_2' & m_1' & -m' \end{pmatrix}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \\
& \begin{pmatrix} \lambda & l_1 & l_1' \\ -m_\lambda & -m_1 & m_1' \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ -m_2 & m_\lambda & m_2' \end{pmatrix} \\
= & \sum_\lambda\frac{r_<^\lambda}{r_>^{\lambda+1}}(-1)^{l+\lambda+m+m'}\hat{l}_1'\hat{l}_1\hat{l}_2'\hat{l}_2\hat{l}\hat{l}'\begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \\
& \times\sum_{m_1'm_2'm_1m_2m_\lambda}(-1)^{l_1+l_2+\lambda+m_1'+m_2'+m_\lambda} \\
& \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ -m_2 & m_\lambda & m_2' \end{pmatrix} \\
& \begin{pmatrix} \lambda & l_1 & l_1' \\ -m_\lambda & -m_1 & m_1' \end{pmatrix}\begin{pmatrix} l_2' & l_1' & l' \\ m_2' & m_1' & -m' \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
= & \sum_\lambda\frac{r_<^\lambda}{r_>^{\lambda+1}}(-1)^{l+\lambda}\hat{l}_1'\hat{l}_1\hat{l}_2'\hat{l}_2\hat{l}\hat{l}'\begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \\
& \times(-1)^{m+m'}\frac{1}{2l+1}\delta_{ll'}\delta_{mm'}\begin{Bmatrix} l_2' & l_1' & l \\ l_1 & l_2 & \lambda \end{Bmatrix} \\
= & \delta_{ll'}\delta_{mm'}\sum_\lambda\frac{r_<^\lambda}{r_>^{\lambda+1}}(-1)^{l+\lambda}\hat{l}_1'\hat{l}_1\hat{l}_2'\hat{l}_2 \\
& \begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l_1 & l_1' & \lambda \\ l_2' & l_2 & l \end{Bmatrix}
\end{aligned}
$$

C.4 The reduced matrix element $\langle (l'_1 l'_2) l' || \frac{1}{r_{12}} || (l_1 l_2) l \rangle$

The Wigner-Eckart theorem (Brink and Satchler, 1993) states that the matrix elements of tensor operators with respect to angular momentum eigenstates satisfy

$$\langle \alpha JM | T_{kq} | \alpha' J' M' \rangle = (-1)^{2k} \langle JM | J' k M' q \rangle \langle \alpha J || T_k || \alpha' J' \rangle . \tag{C.4}$$

Since $\frac{1}{r_{12}}$ is a scalar, using the Wigner-Eckart theorem with $(k = 0, q = 0)$ we have

$$\langle (l'_1 l'_2) l m' \left| \frac{1}{r_{12}} \right| ((l_1 l_2) l m \rangle = \delta_{ll'} \delta m m' \langle (l'_1 l'_2) l \left|\left| \frac{1}{r_{12}} \right|\right| ((l_1 l_2) l \rangle . \tag{C.5}$$

Comparing the above equation with the matrix elements of $\langle (l'_1 l'_2) l' m' | \frac{1}{r_{12}} | (l_1 l_2) l m \rangle$ in Eq. (C.3), we have

$$\begin{aligned} & \langle (l'_1 l'_2) l \left|\left| \frac{1}{r_{12}} \right|\right| ((l_1 l_2) l \rangle \\ = & \sum_{\lambda m_\lambda} \frac{r_<^\lambda}{r_>^{\lambda+1}} (-1)^{l+\lambda} \hat{l}_1 \hat{l}_2 \hat{l}'_1 \hat{l}'_2 \begin{pmatrix} l_1 & \lambda & l'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l'_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_1 & l'_1 & \lambda \\ l'_2 & l_2 & l \end{Bmatrix} . \end{aligned} \tag{C.6}$$

D. APPENDIX TO CHAPTER 3

D.1 Derivation of (3.25)

In (3.18) the direct momentum space potential $V_{\alpha'\alpha}$ is written as:

$$V_{\alpha'\alpha}(k_0', k_0) = I_0 + 2I_1,$$

where

$$\begin{aligned}
I_1 = & \\
& \langle \boldsymbol{k}_0'\alpha' l' m' s' \left| -\frac{1}{r_{01}} \right| \boldsymbol{k}_0 \alpha l m s\rangle \sum_{l_0' m_0' l_1' l_2' l_0 m_0 l_1 l_2} \langle l_0' m_0' | \langle (l_1' l_2') l' m' | \langle l_0' m_0' | \hat{\boldsymbol{k}}_0' \rangle \\
& \times \langle k_0' l_0' | \langle \alpha' (l_1' l_2') l' s' | \left(-\frac{1}{r_{01}} \right) | l_0 m_0 \rangle | (l_1 l_2) l m \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle | k_0 l_0 \rangle | \alpha (l_1 l_2) l s \rangle \\
= & - \sum_{l_0' m_0' l_1' l_2' l_0 m_0 l_1 l_2} \langle l_0' m_0' | \hat{\boldsymbol{k}}_0' \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \\
& \times \langle l_0' m_0' | \langle (l_1' l_2') l' m' | \langle k_0' l_0' | \langle \alpha' (l_1' l_2') l' s' | \\
& \left(\frac{1}{r_{01}} \right) | l_0 m_0 \rangle | (l_1 l_2) l m \rangle | k_0 l_0 \ \rangle | \alpha (l_1 l_2) l s \rangle \\
= & - \sum_{l_0' m_0' l_1' l_2' l_0 m_0 l_1 l_2} \langle l_0' m_0' | \hat{\boldsymbol{k}}_0' \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \int d^3\boldsymbol{r}_0' d^3\boldsymbol{r}_1' d^3\boldsymbol{r}_2' d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \\
& \times \langle l_0' m_0' | \hat{\boldsymbol{r}'}_0 \rangle \langle (l_1' l_2') l' m' | \hat{\boldsymbol{r}'}_1 \hat{\boldsymbol{r}'}_2 \rangle \langle k_0' l_0' | r_0' \rangle \langle \alpha' (l_1' l_2') l' s' | r_1' r_2' \rangle \\
& \left(\langle \boldsymbol{r'}_0 \boldsymbol{r'}_1 \boldsymbol{r'}_2 | \frac{1}{r_{01}} | \boldsymbol{r}_0 \boldsymbol{r}_1 \boldsymbol{r}_2 \rangle \right) \\
& \times \langle \hat{\boldsymbol{r}}_0 | l_0 m_0 \rangle \langle \hat{\boldsymbol{r}}_1 \hat{\boldsymbol{r}}_2 | (l_1 l_2) l m \rangle \langle r_0 | k_0 l_0 \rangle \langle r_1 r_2 | \alpha (l_1 l_2) l s \rangle
\end{aligned}$$

$$
\begin{aligned}
&= -\sum_{l_0'm_0'l_1'l_2'l_0m_0l_1l_2}\langle l_0'm_0'|\hat{\boldsymbol{k}}_0'\rangle\langle\hat{\boldsymbol{k}}_0|l_0m_0\rangle\int d^3\boldsymbol{r}_0'd^3\boldsymbol{r}_1'd^3\boldsymbol{r}_2'd^3\boldsymbol{r}_0d^3\boldsymbol{r}_1d^3\boldsymbol{r}_2\\
&\quad\times\langle l_0'm_0'|\hat{\boldsymbol{r}'}_0\rangle\langle(l_1'l_2')l'm'|\hat{\boldsymbol{r}'}_1\hat{\boldsymbol{r}'}_2\rangle\langle k_0'l_0'|r_0'\rangle\langle\alpha'(l_1'l_2')l's'|r_1'r_2'\rangle\\
&\quad\times\left(\delta(\boldsymbol{r'}_0-\boldsymbol{r}_0)\delta(\boldsymbol{r'}_1-\boldsymbol{r}_1)\delta(\boldsymbol{r'}_2-\boldsymbol{r}_2)\frac{1}{r_{01}}\right)\\
&\quad\times\langle\hat{\boldsymbol{r}}_0|l_0m_0\rangle\langle\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2|(l_1l_2)lm\rangle\langle r_0|k_0l_0\rangle\langle r_1r_2|\alpha(l_1l_2)ls\rangle\\
&= -\sum_{l_0'm_0'l_1'l_2'l_0m_0l_1l_2}\langle l_0'm_0'|\hat{\boldsymbol{k}}_0'\rangle\langle\hat{\boldsymbol{k}}_0|l_0m_0\rangle\int d^3\boldsymbol{r}_0d^3\boldsymbol{r}_1d^3\boldsymbol{r}_2\\
&\quad\times\langle l_0'm_0'|\hat{\boldsymbol{r}}_0\rangle\langle(l_1'l_2')l'm'|\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2\rangle\langle k_0'l_0'|r_0\rangle\langle\alpha'(l_1'l_2')l's'|r_1r_2\rangle\\
&\quad\times\sum_{\lambda m_\lambda}\frac{4\pi}{2\lambda+1}\frac{r_<^\lambda}{r_>^{\lambda+1}}\langle\lambda m_\lambda|\hat{r}_1\rangle\langle\hat{r}_0|\lambda m_\lambda\rangle\\
&\quad\times\langle\hat{\boldsymbol{r}}_0|l_0m_0\rangle\langle\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2|(l_1l_2)lm\rangle\langle r_0|k_0l_0\rangle\langle r_1r_2|\alpha(l_1l_2)ls\rangle\\
&= -\sum_{l_0'm_0'l_1'l_2'l_0m_0l_1l_2}\langle l_0'm_0'|\hat{\boldsymbol{k}}_0'\rangle\langle\hat{\boldsymbol{k}}_0|l_0m_0\rangle\\
&\quad\sum_{\lambda m_\lambda}\frac{4\pi}{2\lambda+1}\int d\hat{\boldsymbol{r}}_0\langle l_0'm_0'|\hat{\boldsymbol{r}}_0\rangle\langle\hat{\boldsymbol{r}}_0|l_0m_0\rangle\langle\hat{r}_0|\lambda m_\lambda\rangle\\
&\quad\times\int d\hat{\boldsymbol{r}}_1d\hat{\boldsymbol{r}}_2\langle(l_1'l_2')l'm'|\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2\rangle\langle\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2|(l_1l_2)lm\rangle\langle\lambda m_\lambda|\hat{r}_1\rangle\\
&\quad\times\int dr_0dr_1dr_2r_0^2r_1^2r_2^2\langle k_0'l_0'|r_0\rangle\langle r_0|k_0l_0\rangle\\
&\quad\times\langle r_1r_2|\alpha(l_1l_2)ls\rangle\langle\alpha'(l_1'l_2')l's'|r_1r_2\rangle\frac{r_<^\lambda}{r_>^{\lambda+1}}.
\end{aligned}
$$

Note that

$$
\begin{aligned}
&\langle(l_1'l_2')l'm'|\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2\rangle\\
&= \mathcal{Y}^*{}_{(l_1'l_2')l'm'}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2)=\sum_{m_1'm_2'}\langle l_1'm_1'|\hat{\boldsymbol{r}}_1\rangle\langle l_2'm_2'|\hat{\boldsymbol{r}}_2\rangle\langle l_1'l_2'm_1'm_2'|l'm'\rangle,
\end{aligned}
$$

$$
\begin{aligned}
&\langle\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2|(l_1l_2)lm\rangle\\
&= \mathcal{Y}_{(l_1l_2)lm}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2)=\sum_{m_1m_2}\langle\hat{\boldsymbol{r}}_1|l_1m_1\rangle\langle\hat{\boldsymbol{r}}_2|l_2m_2\rangle\langle l_1l_2m_1m_2|lm\rangle,
\end{aligned}
$$

$$\begin{aligned}
&\int d\hat{\boldsymbol{r}}_1 \langle l_1' m_1' | \hat{\boldsymbol{r}}_1 \rangle \langle \hat{\boldsymbol{r}}_1 | l_1 m_1 \rangle \langle \lambda m_\lambda | \hat{\boldsymbol{r}}_1 \rangle \\
&= \frac{(-1)^{m_1} \hat{l}_0' \hat{l}_0 \hat{\lambda}}{\sqrt{4\pi}} \begin{pmatrix} l_1' & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_1 & \lambda \\ -m_1' & m_1 & -m_\lambda \end{pmatrix},
\end{aligned}$$

$$\begin{aligned}
&\int d\hat{\boldsymbol{r}}_0 \langle l_0' m_0' | \hat{\boldsymbol{r}}_0 \rangle \langle \hat{\boldsymbol{r}}_0 | l_0 m_0 \rangle \langle \hat{\boldsymbol{r}}_0 | \lambda m_\lambda \rangle \\
&= \frac{(-1)^{m_0'} \hat{l}_0' \hat{l}_0 \hat{\lambda}}{\sqrt{4\pi}} \begin{pmatrix} l_0' & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_0' & l_0 & \lambda \\ -m_0' & m_0 & m_\lambda \end{pmatrix},
\end{aligned}$$

and

$$\int d\hat{\boldsymbol{r}}_2 \langle l_2' m_2' | \hat{\boldsymbol{r}}_2 \rangle \langle \hat{\boldsymbol{r}}_2 | l_2 m_2 \rangle = \delta_{l_2' l_2} \delta_{m_2' m_2}.$$

Combining these relations we have:

$$\begin{aligned}
I_1 &= - \sum_{l_0' m_0' l_1' l_2' l_0 m_0 l_1 l_2} i \langle l_0' m_0' | \hat{\boldsymbol{k}}_0' \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \sum_{\lambda m_\lambda} \frac{4\pi}{2\lambda + 1} \\
&\quad \times \sum_{m_1' m_2' m_1 m_2} \langle l_1' l_2' m_1' m_2' | l' m' \rangle \langle l_1 l_2 m_1 m_2 | l m \rangle \\
&\quad \times \int d\hat{\boldsymbol{r}}_0 \langle l_0' m_0' | \hat{\boldsymbol{r}}_0 \rangle \langle \hat{\boldsymbol{r}}_0 | l_0 m_0 \rangle \langle \hat{\boldsymbol{r}}_0 | \lambda m_\lambda \rangle \int d\hat{\boldsymbol{r}}_1 \langle l_1' m_1' | \hat{\boldsymbol{r}}_1 \rangle \langle \hat{\boldsymbol{r}}_1 | l_1 m_1 \rangle \langle \lambda m_\lambda | \hat{\boldsymbol{r}}_1 \rangle \\
&\quad \times \int d\hat{\boldsymbol{r}}_2 \langle l_2' m_2' | \hat{\boldsymbol{r}}_2 \rangle \langle \hat{\boldsymbol{r}}_2 | l_2 m_2 \rangle \xi^1_{k_0' l_0' k_0 l_0 \alpha' l' (l_1' l_2') s' \alpha l (l_1 l_2) s \lambda} \\
&= - \sum_{l_0' m_0' l_1' m_1' l_0 m_0 l_1 m_1 l_2 m_2 \lambda m_\lambda} (-1)^{m_0' + m_1 + m + m' + \lambda} \langle \hat{\boldsymbol{k}}_0' | l_0' m_0' \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \\
&\quad \times \xi^1_{k_0' l_0' k_0 l_0 \alpha' (l_1' l_2') l' s' \alpha (l_1 l_2) l s \lambda} \hat{l}_0' \hat{l}_0 \hat{l}_1' \hat{l}_1 \hat{l}' \hat{l} \begin{pmatrix} l_0' & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \begin{pmatrix} l_1' & l_2' & l' \\ m_1' & m_2' & -m \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \\
&\quad \begin{pmatrix} l_1' & l_1 & \lambda \\ -m_1' & m_1 & -m_\lambda \end{pmatrix} \begin{pmatrix} l_0' & l_0 & \lambda \\ -m_0' & m_0 & m_\lambda \end{pmatrix},
\end{aligned} \tag{D.1}$$

where ξ^1 is defined in equation (3.22).

By performing the similar algebra as we did for I_1, we have

$$\begin{aligned}
I_0 &= \sum_{l'_0 m'_0 l'_1 m'_1 l_0 m_0 l_1 m_1 l_2 m_2 \lambda m_\lambda} (-1)^{m'_0+m_1+m+m'+\lambda} \langle \hat{\boldsymbol{k}}'_0 | l'_0 m'_0 \rangle \langle \hat{\boldsymbol{k}}_0 | l_0 m_0 \rangle \hat{l}'_0 \hat{l}_0 \hat{l}'_1 \hat{l}_1 \hat{l}' \hat{l} \\
&\times \xi^0_{k'_0 l'_0 k_0 l_0 \alpha' (l'_1 l'_2) l' s' \alpha (l_1 l_2) l s \lambda} \begin{pmatrix} l'_0 & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\begin{pmatrix} l'_1 & l'_2 & l' \\ m'_1 & m'_2 & -m \end{pmatrix} \times \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \\
&\begin{pmatrix} l'_1 & l_1 & \lambda \\ -m'_1 & m_1 & -m_\lambda \end{pmatrix} \begin{pmatrix} l'_0 & l_0 & \lambda \\ -m'_0 & m_0 & m_\lambda \end{pmatrix},
\end{aligned}$$

where ξ^0 is defined in equation (3.20).

Using equations (3.18), (3.19), (3.21) and (3.24) and the above expression for I_0 and I_1, we get the partial wave reduction for $V_{\alpha'\alpha}$.

$$\begin{aligned}
&V^J_{\alpha\alpha}(k'_0, k_0) \\
&= \int d^3\hat{\boldsymbol{k}}'_0 d^3\hat{\boldsymbol{k}}_0 \sum_{m'''_0 m' m''_0 m} \langle J' M'_J | l'''_0 m'''_0 l' m' \rangle \langle J' M'_J | l''_0 m''_0 l m \rangle \\
&\quad \langle \hat{\boldsymbol{k}}'_0 | l'''_0 m'''_0 \rangle \langle l''_0 m''_0 | \hat{\boldsymbol{k}}_0 \rangle V_{\alpha'\alpha} \\
&= \int d^3\hat{\boldsymbol{k}}'_0 d^3\hat{\boldsymbol{k}}_0 \sum_{m'''_0 m' m''_0 m} \langle J' M'_J | l'''_0 m'''_0 l' m' \rangle \langle J' M'_J | l''_0 m''_0 l m \rangle \\
&\quad \times \langle \hat{\boldsymbol{k}}'_0 | l'''_0 m'''_0 \rangle \langle l''_0 m''_0 | \hat{\boldsymbol{k}}_0 \rangle (I_0 + 2I_1) \\
&= \sum_{l'_0 l'_1 l_0 l_1 l_2} (-1)^{l+l'+\lambda} \xi_{k'_0 l'_0 k_0 l_0 \alpha' l' (l'_1 l'_2) s' \alpha l (l_1 l_2) s \lambda} \hat{l}'_0 \hat{l}_0 \hat{l}'_1 \hat{l}_1 \hat{l} \hat{l} \hat{l}' \hat{L} \hat{L}' \\
&\quad \begin{pmatrix} l'_0 & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

$$
\begin{aligned}
&\times \sum_{m'mm_0'm_1'm_0m_1m_2\lambda m_\lambda} (-1)^{m_0'+m_1+m+m'} \begin{pmatrix} l_0' & l' & L' \\ m_0' & m' & -M' \end{pmatrix} \\
&\begin{pmatrix} l_0 & l & L' \\ m_0 & m & -M' \end{pmatrix} \begin{pmatrix} l_1' & l_2' & l' \\ m_1' & m_2' & -m \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \\
&\begin{pmatrix} l_1' & l_1 & \lambda \\ -m_1' & m_1 & -m_\lambda \end{pmatrix} \begin{pmatrix} l_0' & l_0 & \lambda \\ -m_0' & m_0 & m_\lambda \end{pmatrix} \\
= &\sum_{l_0'l_1'l_0l_1l_2\lambda} (-1)^{l+l'} \xi_{k_0'l_0'k_0l_0\alpha'l'(l_1'l_2')s'\alpha l(l_1l_2)s\lambda} \hat{l}_0'\hat{l}_0\hat{l}_1'\hat{l}_1\hat{l}\hat{l}'\hat{J}\hat{J}' \\
&\begin{pmatrix} l_0' & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \sum_{mm'm_0m_0'm_\lambda} (-1)^{m_0'} \begin{pmatrix} l_0' & l' & J' \\ m_0' & m' & -M_J' \end{pmatrix} \begin{pmatrix} l_0 & l & J' \\ m_0 & m & -M_J' \end{pmatrix} \\
&\begin{pmatrix} l_0' & l_0 & \lambda \\ -m_0' & m_0 & m_\lambda \end{pmatrix} \times (-1)^{l_2'+\lambda+m'} \begin{pmatrix} \lambda & l & l' \\ m_\lambda & m & m' \end{pmatrix} \begin{Bmatrix} l & \lambda & l' \\ l_1' & l_2' & l_1 \end{Bmatrix} \\
= &\sum_{l_0'l_1'l_0l_1l_2\lambda} \xi_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha l(l_1l_2)s\lambda} (-1)^{l_2'+J'} \hat{l}_0'\hat{l}_0\hat{l}_1'\hat{l}_1\hat{l}\hat{l}' \\
&\times \begin{pmatrix} l_0' & l_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l & \lambda & l' \\ l_1' & l_2' & l_1 \end{Bmatrix} \begin{Bmatrix} l & l_0 & J' \\ l_0' & l' & \lambda \end{Bmatrix}, \qquad \text{(D.2)}
\end{aligned}
$$

where

$$
\xi_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda} = \xi^0_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda} + 2\xi^1_{k_0'l_0'k_0l_0\alpha'(l_1'l_2')l's'\alpha(l_1l_2)ls\lambda},
$$

and ξ^0 and ξ^1 are as defined in equations (3.20) and (3.22).

D.2 Expansion of $V_{\beta'\beta}$

The potential matrix for the direct interaction for positrium-helium-ion is described in equation(3.28).

$$\begin{aligned}
V_{\beta'\beta} &= \langle \boldsymbol{k}'\beta' \,|U_{\beta,\beta}|\, \boldsymbol{k}\beta\rangle \\
&= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{R} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\left[\frac{1}{\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho}} - \frac{1}{\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho}}\right] e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\Phi_\beta(\boldsymbol{\rho}) \\
&= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{R} d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\left[\frac{1}{\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho}}\right] e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho})} \\
&\quad -\frac{1}{(2\pi)^3}\int d^3\boldsymbol{R} d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{-\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\left[\frac{1}{\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho}}\right] e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho})}.
\end{aligned}$$

Let $\boldsymbol{r} = \boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho}$, note that $d^3\boldsymbol{r}d^3\boldsymbol{\rho} = d^3\boldsymbol{R}d^3\boldsymbol{\rho}$ and $\int \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{r} d^3\boldsymbol{r} = \frac{4\pi}{k^2}$, the first term of $V_{\beta'\beta}$ may be rewritten as

$$\begin{aligned}
&\frac{1}{(2\pi)^3}\int d^3\boldsymbol{R} d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\left(\frac{1}{\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho}}\right) e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}-\frac{1}{2}\boldsymbol{\rho})} \\
&= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\int d^3\boldsymbol{r}\frac{1}{\boldsymbol{r}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \\
&= \frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}\int d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}.
\end{aligned}$$

Similar for the second term of $V_{\beta'\beta}$, we have

$$\begin{aligned}
&\frac{1}{(2\pi)^3}\int d^3\boldsymbol{R}\int d^3\boldsymbol{\rho}\;\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{-\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\left[\frac{1}{\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho}}\right] e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}+\frac{1}{2}\boldsymbol{\rho})} \\
&= \frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}\int d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho}) e^{-\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}.
\end{aligned}$$

Finally we rewrite $V_{\beta'\beta}$ as

$$
\begin{aligned}
V_{\beta'\beta} &= \frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}\int d^3\boldsymbol{\rho}\Phi^*_{\beta'}(\boldsymbol{\rho})\Phi_\beta(\boldsymbol{\rho})\left[e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}} - e^{-\frac{i}{2}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\rho}}\right] \\
&= \frac{1}{2\pi^2 K^2}\sum_{\lambda\mu}\left[1-(-1)^\lambda\right] i^\lambda(-1)^{m_{\beta'}+\mu} \\
&\quad \times Y^\lambda_{\beta'\beta}(K)c^\lambda_{-\mu}(\hat{\boldsymbol{K}})\hat{l_\beta}\hat{l_{\beta'}}\hat{\lambda}^2\begin{pmatrix} l_\beta & \lambda & l_{\beta'} \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'}\end{pmatrix}
\end{aligned}
$$

where

$$
Y^\lambda_{\beta'\beta}(K) = \int_0^\infty d\rho\rho^2\phi_\beta(\rho)\phi^*_{\beta'}(\rho)j_\lambda(\frac{K}{2}\rho).
$$

Now we derive the partial wave reduction for $V_{\beta'\beta}$:

$$
\begin{aligned}
V^J_{\beta'\beta}(k',k) = &\sum_{m_{\beta'}m_\beta M'M}\int d\hat{\boldsymbol{k}}'d\hat{\boldsymbol{k}}Y^*_{L'M'}(\hat{\boldsymbol{k}}')Y_{LM}(\hat{\boldsymbol{k}}) < \boldsymbol{k}'\beta'|V|\beta\boldsymbol{k} > \\
&\times < L'M'l_{\beta'}\ m_{\beta'}|JM_J >< LMl_\beta m_\beta|JM_J > \\
= &\sum_{m_{\beta'}m_\beta M'M\lambda\mu}\int d\hat{\boldsymbol{k}}'d\hat{\boldsymbol{k}}Y^*_{L'M'}(\hat{\boldsymbol{k}}')Y_{LM}(\hat{\boldsymbol{k}}) \\
&< L'M'l_{\beta'}m_{\beta'}|JM_J >< LMl_\beta m_\beta|JM_J > \\
&\times\frac{i^\lambda(-1)^{m_{\beta'}+\mu}}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'}\end{pmatrix} \\
&Y^\lambda_{\beta'\beta}(|\boldsymbol{k}-\boldsymbol{k}'|)C_{\lambda\,-\mu}(\widehat{\boldsymbol{k}-\boldsymbol{k}'})\hat{l}_\beta\hat{l}_{\beta'}\hat{\lambda}^2 \\
= &\sum_{m_{\beta'}m_\beta M'M\lambda\mu}\int d\hat{\boldsymbol{k}}'d\hat{\boldsymbol{k}}i^\lambda(-1)^{m_{\beta'}+\mu}\hat{l}_\beta\hat{l}_{\beta'}\hat{\lambda}^2 Y^*_{L'M'}(\hat{\boldsymbol{k}}')Y_{LM}(\hat{\boldsymbol{k}})C_{\lambda-\mu}(\widehat{\boldsymbol{k}-\boldsymbol{k}'}) \\
&\times\frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}Y^\lambda_{\beta'\beta}(|\boldsymbol{k}-\boldsymbol{k}'|) < L'M'l_{\beta'}m_{\beta'}|JM_J >< LMl_\beta m_\beta|JM_J > \\
&\times\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'}\end{pmatrix} \\
= &\sum_{m_{\beta'}m_\beta M'M\lambda\mu}\int d\hat{\boldsymbol{k}}'d\hat{\boldsymbol{k}}i^\lambda(-1)^{m_{\beta'}+\mu}\hat{l}_\beta\hat{l}_{\beta'}\hat{\lambda}^2\frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^2}Y^\lambda_{\beta'\beta}(|\boldsymbol{k}-\boldsymbol{k}'|)
\end{aligned}
$$

$$\times < L'M'l_{\beta'}m_{\beta'}|JM_J >< LMl_\beta m_\beta|JM_J >$$
$$\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'} \end{pmatrix} \frac{1}{|\boldsymbol{k}-\boldsymbol{k}'|^\lambda}$$
$$\times \sum_{\tau\mu'} (-1)^{M'+\tau} k^{\lambda-\tau} k'^\tau \frac{4\pi\sqrt{(2\lambda)!}}{\sqrt{(2(\lambda-\tau)+1)(2\tau+1)(2\tau)!(2(\lambda-\tau))!}}$$
$$\times \langle \lambda-\tau \;\; \tau \;\; -\mu-\mu' \;\; \mu' | \lambda \;\; -\mu \rangle$$
$$Y_{L'-M'}(\hat{\boldsymbol{k}}')Y_{L\,M}(\hat{\boldsymbol{k}})Y_{\lambda-\tau \;\; -\mu-\mu'}(\hat{\boldsymbol{k}})Y_{\tau-\mu'}(\hat{\boldsymbol{k}}')$$
$$= \sum_{m_{\beta'}m_\beta M'M\lambda\mu\tau\mu'} \int d\hat{\boldsymbol{k}}' d\hat{\boldsymbol{k}} i^\lambda (-1)^{m_{\beta'}+\mu+M'+\tau} \hat{l}_\beta \hat{l}_{\beta'} \hat{\lambda}^2 k^{\lambda-\tau} k'^\tau$$
$$\times < L'M'l_{\beta'}m_{\beta'}|JM_J >< LMl_\beta \; m_\beta|JM_J >$$
$$\langle \lambda-\tau \;\; \tau \;\; -\mu-\mu' \;\; \mu' | \lambda \;\; -\mu \rangle$$
$$\times \frac{4\pi(2\lambda)!}{\sqrt{(2(\lambda-\tau)+1)(2\tau+1)(2\tau)!(2(\lambda-\tau))!}}$$
$$\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'} \end{pmatrix}$$
$$\times Y_{L'-M'}(\hat{\boldsymbol{k}}')Y_{LM}(\hat{\boldsymbol{k}})Y_{\lambda-\tau \;\; -\mu-\mu'}(\hat{\boldsymbol{k}})Y_{\tau-\mu'}(\hat{\boldsymbol{k}}')$$
$$\frac{1}{2\pi^2|\boldsymbol{k}-\boldsymbol{k}'|^{\lambda+2}} Y^\lambda_{\beta'\beta}(|\boldsymbol{k}-\boldsymbol{k}'|)$$
$$= \sum_{m_{\beta'}m_\beta M'M\lambda\mu\tau\mu'} \int d\hat{\boldsymbol{k}}' d\hat{\boldsymbol{k}} i^\lambda (-1)^{m_{\beta'}+\mu+M'+\tau} \hat{l}_\beta \hat{l}_{\beta'} \hat{\lambda}^2 k^{\lambda-\tau} k'^\tau$$
$$\times < L'M'l_{\beta'}m_{\beta'}|JM_J >< LMl_\beta m_\beta|JM_J >$$
$$\langle \lambda-\tau \;\; \tau \;\; -\mu-\mu' \;\; \mu' | \lambda \;\; -\mu \rangle$$
$$\times \frac{4\pi(2\lambda)!}{\sqrt{(2(\lambda-\tau)+1)(2\tau+1)(2\tau)!(2(\lambda-\tau))!}}$$
$$\begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'} \end{pmatrix}$$
$$\times Y_{L'-M'}(\hat{\boldsymbol{k}}')Y_{LM}(\hat{\boldsymbol{k}})Y_{\lambda-\tau \;\; -\mu-\mu'}(\hat{\boldsymbol{k}})Y_{\tau \;\; -\mu'}(\hat{\boldsymbol{k}}')$$
$$\times 2\pi \sum_{\lambda' m_{\lambda'}} (-1)^{m_{\lambda'}} Y_{\lambda' \, -m_{\lambda'}}(\hat{\boldsymbol{k}}') Y_{\lambda' \, m_{\lambda'}}(\hat{\boldsymbol{k}}) Y^{\lambda\lambda'}_{\beta'\beta}(kk')$$
$$= \sum_{m_{\beta'}m_\beta M'M\lambda\mu\tau\mu'\lambda' m_{\lambda'}} 2\pi i^\lambda (-1)^{m_{\beta'}+\mu+M'+\tau+m_{\lambda'}} \hat{l}_\beta \hat{l}_{\beta'} \hat{\lambda}^2 k^{\lambda-\tau} k'^\tau Y^{\lambda\lambda'}_{\beta'\beta}(kk')$$
$$\times < L'M'l_{\beta'}m_{\beta'}|JM_J >< LMl_\beta m_\beta|JM_J >$$

$$
\begin{aligned}
& \langle \lambda-\tau \;\; \tau \;\; -\mu-\mu' \;\; \mu' | \lambda \;\; -\mu \rangle \\
& \times \frac{4\pi(2\lambda)!}{\sqrt{(2(\lambda-\tau)+1)(2\tau+1)(2\tau)!(2(\lambda-\tau))!}} \\
& \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ \mu & m_\beta & -m_{\beta'} \end{pmatrix} \\
& \times \int d\hat{\boldsymbol{k}}' Y_{L' \; -M'}(\hat{\boldsymbol{k}}') Y_{\tau \; -\mu'}(\hat{\boldsymbol{k}}') Y_{\lambda' \; -m_{\lambda'}}(\hat{\boldsymbol{k}}') \\
& \times \int d\hat{\boldsymbol{k}} Y_{L\,M}(\hat{\boldsymbol{k}}) Y_{\lambda \; -\tau-\mu-\mu'}(\hat{\boldsymbol{k}}) Y_{\lambda' \, m_{\lambda'}}(\hat{\boldsymbol{k}}) \\
= & \sum_{m_{\beta'} m_\beta M' M \lambda \mu \tau \mu' \lambda' m_{\lambda'}} 2\pi i^\lambda (-1)^{\tau+\lambda'+\lambda+J} \\
& \times \hat{\lambda}^3 \hat{\lambda'}^2 \hat{l}_\beta \hat{l}_{\beta'} \hat{L} \hat{L}' \hat{J}^2 k^{\lambda-\tau} k'^\tau Y^{\lambda\lambda'}_{\beta'\beta}(k,k') \left(\frac{(2\lambda)!}{(2\tau)!(2(\lambda-\tau))!} \right)^{1/2} \\
& \times \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda' & \tau & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & \lambda' & \lambda-\tau \\ 0 & 0 & 0 \end{pmatrix} \\
& \times (-1)^{\lambda'+\lambda+m_{\lambda'}+\mu} \\
& \times \begin{pmatrix} \lambda' & \lambda-\tau & L \\ m_{\lambda'} & -\mu-\mu' & M \end{pmatrix} \begin{pmatrix} \lambda-\tau & \tau & \lambda \\ \mu+\mu' & -\mu' & -\mu \end{pmatrix} \begin{pmatrix} \tau & \lambda' & L' \\ \mu' & -m_{\lambda'} & -M' \end{pmatrix} \\
& \times (-1)^{L+l_\beta+\lambda-M+m_\beta-\mu} \\
& \times \begin{pmatrix} L & l_\beta & J \\ -M & -m_\beta & M_J \end{pmatrix} \begin{pmatrix} l_\beta & \lambda & l_{\beta'} \\ m_\beta & \mu & -m_{\beta'} \end{pmatrix} \begin{pmatrix} l_{\beta'} & L' & J \\ -m_{\beta'} & -M' & M_J \end{pmatrix} \\
= & \sum_{m_{\beta'} m_\beta M' M \lambda \mu \tau \mu' \lambda' m_{\lambda'}} 2\pi i^\lambda (-1)^{\tau+\lambda'+\lambda+J} \hat{\lambda}^3 \hat{\lambda'}^2 \hat{l}_\beta \hat{l}_{\beta'} \hat{L} \hat{L}' k^{\lambda-\tau} k'^\tau Y^{\lambda\lambda'}_{\beta'\beta}(k,k') \\
& \times \left(\frac{(2\lambda)!}{(2\tau)!(2(\lambda-\tau))!} \right)^{1/2} \begin{pmatrix} \lambda & l_\beta & l_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda' & \tau & L' \\ 0 & 0 & 0 \end{pmatrix} \\
& \begin{pmatrix} L & \lambda' & \lambda-\tau \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \lambda & L' & L \\ \lambda' & \lambda-\tau & \tau \end{Bmatrix} \begin{Bmatrix} l_{\beta'} & L' & J \\ L & l_\beta & \lambda \end{Bmatrix}
\end{aligned}
$$

The last step is reached by using the properties of the contraction of 3-j symbols (A.14) and (A.15).

D.3 Expansion of $V_{\alpha\beta}$

The Hamiltonian for the positronium formation channel is

$$
\begin{aligned}
H &= H_0 + H_1 + H_2 + V_{12} + V_{01} + V_{02} \\
&= -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{Z}{r_0} - \frac{Z}{r_1} - \frac{Z}{r_2} \\
&\quad + \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_2|} \\
&= -\nabla_{\boldsymbol{\rho}}^2 - \frac{1}{4}\nabla_{\boldsymbol{R}}^2 - \frac{1}{2}\nabla^2 + \frac{Z}{|\boldsymbol{R} + \frac{\boldsymbol{\rho}}{2}|} - \frac{Z}{|\boldsymbol{R} - \frac{\boldsymbol{\rho}}{2}|} - \frac{Z}{r} \\
&\quad + \frac{1}{|\boldsymbol{R} - \frac{\boldsymbol{\rho}}{2} + \boldsymbol{r}|} - \frac{1}{\rho} - \frac{1}{|\boldsymbol{R} + \frac{\boldsymbol{\rho}}{2} + \boldsymbol{r}|}
\end{aligned}
$$

where $\boldsymbol{\rho}$ is relative coordinate for positron and electron of the positronium and $\boldsymbol{R}$ is the coordinate of the positronium centre of mass. The relations between $(\boldsymbol{\rho}, \boldsymbol{R}, \boldsymbol{r})$ and $(\boldsymbol{r}_0, \boldsymbol{r}_1, \boldsymbol{r}_2)$ can be either :

$$
\left\{
\begin{aligned}
\boldsymbol{r} &= \boldsymbol{r}_2 \\
\boldsymbol{\rho} &= \boldsymbol{r}_0 - \boldsymbol{r}_1 \\
\boldsymbol{R} &= \tfrac{1}{2}(\boldsymbol{r}_0 + \boldsymbol{r}_1)
\end{aligned}
\right.
$$

or

$$
\left\{
\begin{aligned}
\boldsymbol{r} &= \boldsymbol{r}_1 \\
\boldsymbol{\rho} &= \boldsymbol{r}_0 - \boldsymbol{r}_2 \\
\boldsymbol{R} &= \tfrac{1}{2}(\boldsymbol{r}_0 + \boldsymbol{r}_2)
\end{aligned}
\right.
$$

and

$$
d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 = d^3\boldsymbol{\rho} d^3\boldsymbol{R}.
$$

Folding on the left of the Schrödinger equation with the positronium states and doing the integration,

$$
\begin{aligned}
&< \boldsymbol{k}'\beta i|H-E|\boldsymbol{k}\alpha lms > \\
&= \int d^3\boldsymbol{\rho} d^3\boldsymbol{R} d^3\boldsymbol{r}' \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r} < \boldsymbol{k}'\beta i|\boldsymbol{\rho}\boldsymbol{R}\boldsymbol{r}_2' > \\
&\quad \times < \boldsymbol{\rho}\boldsymbol{R}\boldsymbol{r}'|H-E|\boldsymbol{r}_0\boldsymbol{r}_1\boldsymbol{r}_2 >< \boldsymbol{r}_0\boldsymbol{r}_1\boldsymbol{r}_2|\boldsymbol{k}\alpha lms > \\
&= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 < \boldsymbol{k}'\beta i|\boldsymbol{\rho}\boldsymbol{R}\boldsymbol{r}' > \\
&\quad \times \left(-\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{Z}{r_0} - \frac{Z}{r_1} - \frac{Z}{r_2}\right. \\
&\quad \left. + \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|} - E\right) < \boldsymbol{r}_0\boldsymbol{r}_1\boldsymbol{r}_2|\boldsymbol{k}\alpha lms > \\
&= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \phi_\beta^*(\rho)\psi_i^{+*}(\boldsymbol{r}) \\
&\quad \times \left(-\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{Z}{r_0} - \frac{Z}{r_1} - \frac{Z}{r_2}\right. \\
&\quad \left. + \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|} - E\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\psi_{\alpha lms}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\
&= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \phi_\beta^*(\rho)\psi_i^{+*}(\boldsymbol{r}) \\
&\quad \times \left(-\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \epsilon_i + \frac{Z}{r_0} - \frac{Z}{r_1}\right. \\
&\quad \left. + \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|} - E\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\psi_{\alpha lms}(\boldsymbol{r}_1\boldsymbol{r}_2) \\
&= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \phi_\beta^*(\rho)\psi_i^{+*}(\boldsymbol{r}) \\
&\quad \times \left(\frac{1}{2}k^2 + \frac{1}{2}(\boldsymbol{k}-\boldsymbol{k}')^2 - \epsilon_i - E + \frac{Z}{r_0} - \frac{Z}{r_1}\right. \\
&\quad \left. + \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\psi_{\alpha lms}(\boldsymbol{r}_1,\boldsymbol{r}_2)
\end{aligned}
$$

Expanding the wave functions of the helium atom $\psi_{\alpha lmS}(\boldsymbol{r}_1,\boldsymbol{r}_2)$, positrium atom

$\phi_\beta(\boldsymbol{\rho})$ and helium ion $\psi_i^+(\boldsymbol{r}_2)$ in the square integrable Laguerre basis $\zeta_{nl}(r)$ as

$$\begin{aligned}&\psi_{\alpha lms}(\boldsymbol{r}_1,\boldsymbol{r}_2)\\ &\quad= \sum_{n_1n_2l_1l_2m_1m_2} d^{\alpha(l_1l_2)l}_{n_1n_2}\langle l_1l_2m_1m_2|lm\rangle\,\zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2)Y_{l_1m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2m_2}(\hat{\boldsymbol{r}}_2)\end{aligned} \tag{D.3}$$

$$\psi_i^+(\boldsymbol{r}_2) = \sum_{n_i} d_{n_i}\zeta_{n_il_i}(r_2)Y_{l_im_i}(\hat{\boldsymbol{r}}_2) \tag{D.4}$$

$$\phi_\beta(\boldsymbol{\rho}) = \sum_{n_\beta} d_{n_\beta}\zeta_{n_\beta l_\beta}(\rho)Y_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \tag{D.5}$$

$$\begin{aligned}&< \boldsymbol{k}'\beta i|H-E|\boldsymbol{k}\alpha lms >\\
&\quad= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\phi^*_\beta(\rho)\psi_i^{+*}(\boldsymbol{r})\\
&\qquad\times\left(\frac{1}{2}k^2+\frac{1}{2}(\boldsymbol{k}-\boldsymbol{k}')^2-\epsilon_i-E+\frac{Z}{r_0}-\frac{Z}{r_1}\right.\\
&\qquad\quad\left.+\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|}-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\psi_{\alpha lmS}(\boldsymbol{r}_1,\boldsymbol{r}_2)\\
&\quad= \sum_{n_1n_2l_1l_2m_1m_2} d^{\alpha(l_1l_2)l}_{n_1n_2}\langle l_1l_2m_1m_2|lm\rangle\sum_{n_i}d_{n_i}\sum_{n_\beta}d_{n_\beta}\\
&\qquad\times\int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_il_i}(r_2)Y^*_{l_im_i}(\hat{\boldsymbol{r}})\\
&\qquad\times\left(\frac{1}{2}k^2+\frac{1}{2}(\boldsymbol{k}-\boldsymbol{k}')^2-\epsilon_i-E+\frac{Z}{r_0}-\frac{Z}{r_1}\right.\\
&\qquad\quad\left.+\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|}-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|}\right)\\
&\qquad\times e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\zeta_{n_1l_1}(r_1)\zeta_{n_2l_2}(r_2)Y_{l_1m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2m_2}(\hat{\boldsymbol{r}}_2)\\
&\quad= \sum_{n_1n_2l_1l_2m_1m_2} d^{\alpha(l_1l_2)l}_{n_1n_2}\langle l_1l_2m_1m_2|lm\rangle\\
&\qquad\sum_{n_i}d_{n_i}\sum_{n_\beta}d_{n_\beta}\left(I_1+I_2+I_3+I_4+I_5+I_6\right)\end{aligned}$$

where I_1, I_2, I_3, I_4, I_5 and I_6 are integrations given by (3.33). These integrations are most conveniently done in momentum space.

D.3.1 Potential matrix in momentum space

Expansion of I_1 in momentum space

$$\begin{aligned}
I_1 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r)Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\quad\times\left(\frac{1}{2}k^2+\frac{1}{2}(\boldsymbol{k}-\boldsymbol{k}')^2-\epsilon_i-E\right) \\
&\quad\times e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&= \int d^3\boldsymbol{\rho} e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\rho}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\int d^3\boldsymbol{r}_1 e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}_1}Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)\zeta_{n_1 l_1}(r_1) \\
&\quad\times\int d^3\boldsymbol{r}_2\zeta^*_{n_i l_i}(r)\zeta_{n_2 l_2}(r_2)Y^*_{l_i m_i}(\hat{\boldsymbol{r}})Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&\quad\times\left(\frac{1}{2}k^2+\frac{1}{2}(\boldsymbol{k}'-\boldsymbol{k})^2-\epsilon_i-E\right)
\end{aligned}$$

Expansion of I_2 in momentum space

$$\begin{aligned}
I_2 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r)Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\quad\times\left(\frac{Z}{r_0}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r)Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\quad\times(Z)\,(2\pi)^{-3}\int d^3\boldsymbol{q}\frac{4\pi}{|\boldsymbol{k}-\boldsymbol{q}|^2}e^{i\boldsymbol{q}\cdot\boldsymbol{r}_0}\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}$$

$$\begin{aligned}
&= \frac{Z}{2\pi^2}\int d^3\boldsymbol{q}\frac{1}{|\boldsymbol{k}-\boldsymbol{q}|^2} \\
&\times \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r_2)Y^*_{l_i m_i}(\hat{\boldsymbol{r}})e^{i\boldsymbol{q}\cdot\boldsymbol{r}_0} \\
&\times \zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}$$

Expansion of I_3 in momentum space

$$\begin{aligned}
I_3 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r_2)Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\times \left(-\frac{Z}{r_1}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&= \int d^3\boldsymbol{\rho} e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\rho}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \\
&\times \int d^3\boldsymbol{r}_1 e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}_1}Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)\left(-\frac{Z}{r_1}\right)\zeta_{n_1 l_1}(r_1) \\
&\times \int d^3\boldsymbol{r}_2 \zeta^*_{n_i l_i}(r)\zeta_{n_2 l_2}(r_2)Y^*_{l_i m_i}(\hat{\boldsymbol{r}})Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}$$

Expansion of I_4 in momentum space

$$\begin{aligned}
I_4 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r)Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\times \left(\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0}\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}\left(\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\right) \\
&\times e^{i(\boldsymbol{k}-\frac{1}{2}\boldsymbol{k}')\cdot(\boldsymbol{r}_0-\boldsymbol{r}_1)}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_2}\zeta^*_{n_i l_i}(r)\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2) \\
&= \left(\frac{1}{2\pi^2}\right)\int d^3q\frac{1}{|\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}|^2}
\end{aligned}$$

$$\times \int d^3\boldsymbol{\rho} e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot(\boldsymbol{r}_0-\boldsymbol{r}_1)} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})$$
$$\times \int d^3\boldsymbol{r}_1 Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) \zeta_{n_1 l_1}(r_1) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_1}$$
$$\times \int d^3\boldsymbol{r}_2 Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \zeta^*_{n_i l_i}(r) \zeta_{n_2 l_2}(r_2) e^{-i(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{r}_2}$$

Expansion of I_5 in momentum space

$$\begin{aligned}
I_5 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\quad \times \left(-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1 l_1}(r_1) \zeta_{n_2 l_2}(r_2) Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&= -\int d^3\boldsymbol{\rho} \frac{e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\rho}}}{\rho} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \\
&\quad \times \int d^3\boldsymbol{r}_1 e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}_1} Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) \zeta_{n_1 l_1}(r_1) \\
&\quad \times \int d^3\boldsymbol{r}_2 \zeta^*_{n_i l_i}(r) \zeta_{n_2 l_2}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}$$

Expansion of I_6 in momentum space

$$\begin{aligned}
I_6 &= \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) \\
&\quad \times \left(-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1 l_1}(r_1) \zeta_{n_2 l_2}(r_2) Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
&= -\int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_0-\boldsymbol{r}_2)} \frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|} \\
&\quad \times e^{-i\frac{1}{2}\boldsymbol{k}'\cdot(\boldsymbol{r}_0-\boldsymbol{r}_1)} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_2} \zeta^*_{n_i l_i}(r) \zeta_{n_1 l_1}(r_1) \zeta_{n_2 l_2}(r_2) \\
&= -\left(\frac{1}{2\pi^2}\right) \int d^3q \frac{1}{|\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}|^2} \\
&\quad \int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)
\end{aligned}$$

$$
\begin{aligned}
& \times e^{-i\frac{1}{2}\boldsymbol{k}'\cdot(\boldsymbol{r}_0-\boldsymbol{r}_1)}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \\
& \times e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_2}\zeta^*_{n_i l_i}(r_2)\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_0-\boldsymbol{r}_2)} \\
= & -\left(\frac{1}{2\pi^2}\right)\int d^3q\frac{1}{|\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}|^2}\int d^3\boldsymbol{\rho}_{01}e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{q})\cdot\boldsymbol{\rho}}\zeta^*_{n_\beta l_\beta}(\rho_{01})Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \\
& \times\int d^3\boldsymbol{r}_2 Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)\zeta^*_{n_i l_i}(r_2)\zeta_{n_2 l_2}(r_2)e^{-i(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{r}_2} \\
& \times\int d^3\boldsymbol{r}_1 Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)\zeta_{n_1 l_1}(r_1)e^{i\boldsymbol{q}\cdot\boldsymbol{r}_1}
\end{aligned}
$$

.

D.3.2 Partial wave reductions for $V_{\alpha\beta}$

Derivation of ${}_1V^J_{\alpha\beta}$

$$
\begin{aligned}
{}_1V^J_{\alpha\beta} = & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2}\int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0\langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} I_1 \\
= & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2}\int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0\langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} \\
& \times\int d^3\boldsymbol{\rho}e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\rho}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\int d^3\boldsymbol{r}_1 e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}_1}Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)\zeta_{n_1 l_1}(r_1) \\
& \times\int d^3\boldsymbol{r}_2\zeta^*_{n_i l_i}(r)\zeta_{n_2 l_2}(r_2)Y^*_{l_i m_i}(\hat{\boldsymbol{r}})Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2)\left(\frac{1}{2}k^2+\frac{1}{2}(\boldsymbol{k}'-\boldsymbol{k})^2-\epsilon_i-E\right) \\
= & \sum_{m'_0 m_\beta m_0 m m'_0 m' l_1 l_2 m_1 m_2}\int d^2\hat{\boldsymbol{k}}' d^2\hat{\boldsymbol{k}}\langle l'_0 m'_0|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_0 m'_0 l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle
\end{aligned}
$$

$$
\begin{aligned}
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta} \delta_{n_i n_2} \delta_{l_i l_2} \delta_{m_i m_2} \left(\frac{1}{2} k^2 + \frac{1}{2} (\boldsymbol{k}' - \boldsymbol{k})^2 - \epsilon_i - E \right) \\
&\times i^{l_\beta + l_1} (-1)^{l_\beta + l_1} \eta_{n_\beta l_\beta}(K_1) \eta_{n_1 l_1}(K_2) \\
&\times \sum_{\tau_\beta m_{\tau_\beta}} \frac{(4\pi)^{1/2} \hat{l}_\beta}{(2l_\beta - 2\tau_\beta + 1)^{1/2} \hat{\tau}_\beta} \frac{1}{K_1^{l_\beta}} \\
&\times (-1)^{\tau_\beta} \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!} \right)^{1/2} \left(\frac{k'}{2} \right)^{l_\beta - \tau_\beta} k^{\tau_\beta} \\
&\times Y_{l_\beta - \tau_\beta \;\; m_\beta - m_{\tau_\beta}}(\hat{\boldsymbol{k}}) \, Y_{\tau_\beta \; m_{\tau_\beta}}(\hat{\boldsymbol{k}}') \langle l_\beta - \tau_\beta \; \tau_\beta \;\; m_\beta - m_{\tau_\beta} \;\; m_{\tau_\beta} | l_\beta \; m_\beta \rangle \\
&\times \sum_{\tau_1 m_{\tau_1}} \frac{(4\pi)^{1/2} \hat{l}_1}{(2l_1 - 2\tau_1 + 1)^{1/2} \hat{\tau}_1} \frac{1}{K_2^{l_1}} (-1)^{\tau_1} \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1 - \tau_1))!} \right)^{1/2} k'^{l_1 - \tau_1} k^{\tau_1} \\
&\times Y_{l_1 - \tau_1 \;\; m_1 - m_{\tau_1}}(\hat{\boldsymbol{k}}) \, Y_{\tau_1 \; m_{\tau_1}}(\hat{\boldsymbol{k}}') \langle l_1 - \tau_1 \; \tau_1 \;\; m_1 - m_{\tau_1} \;\; m_{\tau_1} | l_1 \; m_1 \rangle \\
= & \sum_{m_0' m_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2} i^{l_\beta + l_1} (-1)^{l_\beta + l_1} \\
&\times \langle J M_J | l_0 m_0 l m \rangle \langle J M_J | l' m' l_i m_i \rangle \langle l' m' | l_0' m_0' l_\beta m_\beta \rangle \langle l_1 l_2 m_1 m_2 | l m \rangle \\
&\times \sum_{\tau_\beta m_{\tau_\beta} \tau_1 m_{\tau_1}} \frac{4\pi \hat{l}_\beta \hat{l}_1}{(2l_\beta - 2\tau_\beta + 1)^{1/2} \hat{\tau}_\beta (2l_1 - 2\tau_1 + 1)^{1/2} \hat{\tau}_1} \\
&\times (-1)^{\tau_\beta + \tau_1} \left(\frac{1}{2} \right)^{l_\beta - \tau_\beta} k'^{l_\beta + l_1 - \tau_\beta - \tau_1} k^{\tau_\beta + \tau_1} \\
&\times \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!} \right)^{1/2} \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1 - \tau_1))!} \right)^{1/2} \\
&\times \langle l_\beta - \tau_\beta \; \tau_\beta \;\; m_\beta - m_{\tau_\beta} \;\; m_{\tau_\beta} | l_\beta \; m_\beta \rangle \langle l_1 - \tau_1 \; \tau_1 \;\; m_1 - m_{\tau_1} \;\; m_{\tau_1} | l_1 \; m_1 \rangle \\
&\times \int d^2 \hat{\boldsymbol{k}}' Y^*_{l_0' m_0'}(\hat{\boldsymbol{k}}') Y_{\tau_\beta \; m_{\tau_\beta}}(\hat{\boldsymbol{k}}') Y_{\tau_1 \; m_{\tau_1}}(\hat{\boldsymbol{k}}') \\
&\times \int d^2 \hat{\boldsymbol{k}} Y_{l_0 m_0}(\hat{\boldsymbol{k}}) Y_{l_\beta - \tau_\beta \;\; m_\beta - m_{\tau_\beta}}(\hat{\boldsymbol{k}}) Y_{l_1 - \tau_1 \;\; m_1 - m_{\tau_1}}(\hat{\boldsymbol{k}}) \\
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta} \eta_{n_\beta l_\beta}(K_1) \eta_{n_1 l_1}(K_2) \frac{1}{K_1^{l_\beta}} \frac{1}{K_2^{l_1}} \\
&\times \delta_{n_i n_2} \delta_{l_i l_2} \delta_{m_i m_2} \left(\frac{1}{2} k^2 + \frac{1}{2} (\boldsymbol{k}' - \boldsymbol{k})^2 - \epsilon_i - E \right) \\
= & \sum_{m_0' m_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2} i^{l_\beta + l_1} (-1)^{l_\beta + l_1} \\
&\times \langle J M_J | l_0 m_0 l m \rangle \langle J M_J | l' m' l_i m_i \rangle \langle l' m' | l_0' m_0' l_\beta m_\beta \rangle \langle l_1 l_2 m_1 m_2 | l m \rangle
\end{aligned}
$$

$$
\begin{aligned}
& \times \sum_{\tau_\beta m_{\tau_\beta}} \sum_{\tau_1 m_{\tau_1}} \frac{4\pi \hat{l}_\beta \hat{l}_1}{(2l_\beta - 2\tau_\beta + 1)^{1/2} \hat{\tau}_\beta (2l_1 - 2\tau_1 + 1)^{1/2} \hat{\tau}_1} \\
& \times (-1)^{\tau_\beta + \tau_1} \left(\frac{1}{2}\right)^{l_\beta - \tau_\beta} k'^{l_\beta + l_1 - \tau_\beta - \tau_1} k^{\tau_\beta + \tau_1} \\
& \times \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!}\right)^{1/2} \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1 - \tau_1))!}\right)^{1/2} \\
& \times \langle l_\beta - \tau_\beta \; \tau_\beta \;\; m_\beta - m_{\tau_\beta} \;\; m_{\tau_\beta} | l_\beta \; m_\beta \rangle \langle l_1 - \tau_1 \; \tau_1 \;\; m_1 - m_{\tau_1} \;\; m_{\tau_1} | l_1 \; m_1 \rangle \\
& \times \int d^2 \hat{\boldsymbol{k}}' Y^*_{l'_0 m'_0}(\hat{\boldsymbol{k}}') Y_{\tau_\beta \, m_{\tau_\beta}}(\hat{\boldsymbol{k}}') Y_{\tau_1 \, m_{\tau_1}}(\hat{\boldsymbol{k}}') \\
& \times \int d^2 \hat{\boldsymbol{k}} Y_{l_0 m_0}(\hat{\boldsymbol{k}}) Y_{l_\beta - \tau_\beta \;\; m_\beta - m_{\tau_\beta}}(\hat{\boldsymbol{k}}) Y_{l_1 - \tau_1 \;\; m_1 - m_{\tau_1}}(\hat{\boldsymbol{k}}) \\
& \times \sum_{\lambda m_\lambda} {}_1 Z^\lambda_{\beta i}(k k') Y_{\lambda m_\lambda}(\hat{\boldsymbol{k}}) Y^*_{\lambda m_\lambda}(\hat{\boldsymbol{k}}') \\
= & \sum_{m'_0 m_\beta m_0 m m'_0 m' l_1 l_2 m_1 m_2} i^{l_\beta + l_1} (-1)^{l_\beta + l_1} \\
& \times \sum_{\tau_\beta m_{\tau_\beta} \tau_1 m_{\tau_1} \lambda m_\lambda} \frac{4\pi \hat{l}_\beta \hat{l}_1}{(2l_\beta - 2\tau_\beta + 1)^{1/2} \hat{\tau}_\beta (2l_1 - 2\tau_1 + 1)^{1/2} \hat{\tau}_1} \\
& \times (-1)^{\tau_\beta + \tau_1} \left(\frac{}{2}\right)^{l_\beta - \tau_\beta} \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!}\right)^{1/2} \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1 - \tau_1))!}\right)^{1/2} \\
& \times {}_1 Z^\lambda_{\beta i}(k, k') k'^{l_\beta + l_1 - \tau_\beta - \tau_1} k^{\tau_\beta + \tau_1} \\
& \times \langle J M_J | l_0 m_0 l m \rangle \langle J M_J | l' m' l_i m_i \rangle \langle l' m' | l'_0 m'_0 l_\beta m_\beta \rangle \langle l_1 l_2 m_1 m_2 | l m \rangle \\
& \times \langle l_\beta - \tau_\beta \; \tau_\beta \;\; m_\beta - m_{\tau_\beta} \;\; m_{\tau_\beta} | l_\beta \; m_\beta \rangle \langle l_1 - \tau_1 \; \tau_1 \;\; m_1 - m_{\tau_1} \;\; m_{\tau_1} | l_1 \; m_1 \rangle \\
& \times \int d^2 \hat{\boldsymbol{k}}' Y^*_{l'_0 m'_0}(\hat{\boldsymbol{k}}') Y^*_{\lambda m_\lambda}(\hat{\boldsymbol{k}}') Y_{\tau_\beta \, m_{\tau_\beta}}(\hat{\boldsymbol{k}}') Y_{\tau_1 \, m_{\tau_1}}(\hat{\boldsymbol{k}}') \\
& \times \int d^2 \hat{\boldsymbol{k}} Y_{l_0 m_0}(\hat{\boldsymbol{k}}) Y_{\lambda m_\lambda}(\hat{\boldsymbol{k}}) Y_{l_\beta - \tau_\beta \;\; m_\beta - m_{\tau_\beta}}(\hat{\boldsymbol{k}}) Y_{l_1 - \tau_1 \;\; m_1 - m_{\tau_1}}(\hat{\boldsymbol{k}}) \\
= & \frac{1}{4\pi} \sum_{l_1 l_2 \lambda q'_1 q_1 \tau_\beta \tau_1} i^{l_\beta + l_1} (-1)^{l_1 + l' + \tau_\beta + \tau_1} \\
& \times \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!}\right)^{1/2} \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1 - \tau_1))!}\right)^{1/2} \\
& \times \hat{l}_\beta^2 \hat{l}_1^3 \hat{l}'_R \hat{l}_0 \hat{\lambda}^2 \hat{q}'^2 \hat{q}_1^2 \hat{J}^2 \hat{l}' \left(\frac{1}{2}\right)^{l_\beta - \tau_\beta} {}_1 Z^\lambda_{\beta i}(k, k') k'^{l_\beta + l_1 - \tau_\beta - \tau_1} k^{\tau_\beta + \tau_1} \\
& \times \sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q'_1} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q'_1} + m'_R + m_\lambda + m_{q_1} + m' + m_\beta}
\end{aligned}
$$

$$\times \begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix} \begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$
$$\times \begin{pmatrix} l_1 - \tau_1 & \tau_1 & l_1 \\ m_1 - m_{\tau_1} & m_{\tau_1} & -m_1 \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & \tau_\beta & l_\beta \\ m_\beta - m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}$$
$$\times \begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1} \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1} \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$\times \begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1} \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ m_\beta - m_{\tau_\beta} & m_1 - m_{\tau_1} & m_{q'_1} \end{pmatrix},$$

where

$$\begin{aligned} {}_1Z^{\lambda}_{\beta i}(k,k') &= 2\pi \int_{-1}^{1} \sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2) l}_{n_1 n_2} d_{n_i} d_{n_\beta} \left(\frac{1}{2}k^2 + \frac{1}{2}K_2^2 - \epsilon_i - E \right) \\ &\quad \times \delta_{n_i n_2} \delta_{l_i l_2} \delta_{m_i m_2} \eta_{n_\beta l_\beta}(K_1) \eta_{n_1 l_1}(K_2) \frac{1}{K_1^{l_\beta}} \frac{1}{K_2^{l_1}} P_\lambda(u) du \end{aligned}$$

and where

$$\begin{cases} \boldsymbol{K}_1 = \frac{1}{2}\boldsymbol{k}' - \boldsymbol{k}, \quad \boldsymbol{K}_2 = \boldsymbol{k}' - \boldsymbol{k}, \\ u = \hat{\mathbf{k}}' \cdot \hat{\mathbf{k}} \\ K_1^2 = \left(\frac{1}{2}k'\right)^2 + k^2 - k'ku \qquad K_2^2 = k'^2 + k^2 - 2k'ku, \end{cases} \tag{D.6}$$

$$\eta_{n_\beta l_\beta}(K_1) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty dr r^2 \zeta_{n_\beta l_\beta}(r) j_{l_\beta}(K_1 r), \tag{D.7}$$

$$\eta_{r,n_1 l_1}(K_2) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty dr r^2 \frac{\zeta_{n_1 l_1}(r)}{r} j_{l_1}(K_2 r). \tag{D.8}$$

.**Derivation of** ${}_2V^J_{\alpha\beta}$

$$
\begin{aligned}
{}_2V^J_{\alpha\beta} = & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} I_2 \\
= & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} \frac{1}{\pi^2}\int d^3\boldsymbol{q}\frac{1}{|\boldsymbol{k}-\boldsymbol{q}|^2} \\
& \times\int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})\zeta^*_{n_i l_i}(r_2)Y^*_{l_i m_i}(\hat{\boldsymbol{r}})e^{i\boldsymbol{q}\cdot\boldsymbol{r}_0} \\
& \times\zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2)Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
= & \sum_{m'_0 m_\beta m_0 m m'_0 m' l_1 l_2 m_1 m_2} i^{l_\beta+l_1}(-1)^{l_\beta+l_1} \\
& \times\sum_{\tau_\beta m_{\tau_\beta}\tau_1 m_{\tau_1}\lambda m_\lambda \lambda_2 m_{\lambda_2}} \frac{4\pi\hat{l}_\beta\hat{l}_1}{(2l_\beta-2\tau_\beta+1)^{1/2}\hat{\tau}_\beta(2l_1-2\tau_1+1)^{1/2}\hat{\tau}_1} \\
& \times(-1)^{\tau_\beta+\tau_1}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!}\right)^{1/2} \\
& \times k'^{l_\beta+l_1-\tau_\beta-\tau_1}\int_0^\infty dq q^2 \;\; {}_2Z^\lambda_{\beta i}(q,k')q^{\tau_\beta+\tau_1}Z_{\lambda_2}(k,q) \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_0 m'_0 l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\langle l_\beta-\tau_\beta\;\tau_\beta\;\; m_\beta-m_{\tau_\beta}\;\; m_{\tau_\beta}|l_\beta\; m_\beta\rangle\langle l_1-\tau_1\;\tau_1\;\; m_1-m_{\tau_1}\;\; m_{\tau_1}|l_1\; m_1\rangle \\
& \times\int d^2\hat{\boldsymbol{k}}' Y^*_{l'_0 m'_0}(\hat{\boldsymbol{k}}')Y^*_{\lambda m_\lambda}(\hat{\boldsymbol{k}}')Y_{\tau_\beta\, m_{\tau_\beta}}(\hat{\boldsymbol{k}}')Y_{\tau_1\, m_{\tau_1}}(\hat{\boldsymbol{k}}') \\
& \times\int d^2\hat{\boldsymbol{k}} Y_{l_0 m_0}(\hat{\boldsymbol{k}})Y^*_{\lambda_2 m_{\lambda_2}}(\hat{\boldsymbol{k}}) \\
& \times\int d^2\hat{\boldsymbol{q}} Y_{\lambda_2 m_{\lambda_2}}(\hat{\boldsymbol{q}})Y_{\lambda m_\lambda}(\hat{\boldsymbol{q}})Y_{l_\beta-\tau_\beta\;\; m_\beta-m_{\tau_\beta}}(\hat{\boldsymbol{q}})Y_{l_1-\tau_1\;\; m_1-m_{\tau_1}}(\hat{\boldsymbol{q}}) \\
= & \sum_{m'_0 m_\beta m_0 m m'_0 m' l_1 l_2 m_1 m_2} i^{l_\beta+l_1}(-1)^{l_\beta+l_1}
\end{aligned}
$$

$$
\begin{aligned}
&\times \sum_{\tau_\beta m_{\tau_\beta}\tau_1 m_{\tau_1}\lambda m_\lambda} \frac{4\pi \hat{l}_\beta \hat{l}_1}{(2l_\beta - 2\tau_\beta + 1)^{1/2}\hat{\tau}_\beta (2l_1 - 2\tau_1 + 1)^{1/2}\hat{\tau}_1} \\
&\times (-1)^{\tau_\beta+\tau_1}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!}\right)^{1/2} \\
&\times k'^{l_\beta+l_1-\tau_\beta-\tau_1}\,{}_2Z^{\lambda l_0}_{\beta i}(k,k') \\
&\times \langle JM_J|l_0m_0lm\rangle\langle JM_J|l'm'l_im_i\rangle\langle l'm'|l'_0m'_0l_\beta m_\beta\rangle\langle l_1l_2m_1m_2|lm\rangle \\
&\times \langle l_\beta-\tau_\beta\;\tau_\beta\;\; m_\beta - m_{\tau_\beta}\;\; m_{\tau_\beta}|l_\beta\; m_\beta\rangle\langle l_1-\tau_1\;\tau_1\;\; m_1-m_{\tau_1}\;\; m_{\tau_1}|l_1\; m_1\rangle \\
&\times \int d^2\hat{\boldsymbol{k}}' Y^*_{l'_0m'_0}(\hat{\boldsymbol{k}}')Y^*_{\lambda m_\lambda}(\hat{\boldsymbol{k}}')Y_{\tau_\beta\, m_{\tau_\beta}}(\hat{\boldsymbol{k}}')Y_{\tau_1\, m_{\tau_1}}(\hat{\boldsymbol{k}}') \\
&\times \int d^2\hat{\boldsymbol{q}} Y_{l_0m_0}(\hat{\boldsymbol{q}})Y_{\lambda m_\lambda}(\hat{\boldsymbol{q}})Y_{l_\beta-\tau_\beta\;\; m_\beta-m_{\tau_\beta}}(\hat{\boldsymbol{q}})Y_{l_1-\tau_1\;\; m_1-m_{\tau_1}}(\hat{\boldsymbol{q}}) \\
= \;& \frac{1}{4\pi}\sum_{l_1l_2\lambda q'_1q_1\tau_\beta\tau_1} i^{l_\beta+l_1}(-1)^{l_\beta+l_1+\tau_\beta+\tau_1}\hat{l}_\beta\hat{l}_1\hat{l}'_0\hat{l}_0\hat{\lambda}^2\hat{q}'^2\hat{q}_1^2 k'^{l_\beta+l_1-\tau_\beta-\tau_1} \\
&\times \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}{}_2Z^{\lambda l_0}_{\beta i}(k,k')\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!}\right)^{1/2} \\
&\times \sum_{m'_0m_\beta m_0mm'_0m'm_1m_2m_\lambda m_{q'_1}m_{q_1}m_{\tau_\beta}m_{\tau_1}} (-1)^{m_{q'_1}+m'_0+m_\lambda+m_{q_1}} \\
&\times \begin{pmatrix} l'_0 & \lambda & q \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ 0 & 0 & 0\end{pmatrix} \\
&\times \langle JM_J|l_0m_0lm\rangle\langle JM_J|l'm'l_im_i\rangle\langle l'm'|l'_0m'_0l_\beta m_\beta\rangle\langle l_1l_2m_1m_2|lm\rangle \\
&\times \langle l_\beta-\tau_\beta\;\tau_\beta\;\; m_\beta - m_{\tau_\beta}\;\; m_{\tau_\beta}|l_\beta\; m_\beta\rangle\langle l_1-\tau_1\;\tau_1\;\; m_1-m_{\tau_1}\;\; m_{\tau_1}|l_1\; m_1\rangle \\
&\times \begin{pmatrix} l'_0 & \lambda & q_1 \\ -m'_0 & -m_\lambda & m_{q_1}\end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1}\end{pmatrix} \\
&\times \begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1}\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ m_\beta-m_{\tau_\beta} & m_1-m_{\tau_1} & m_{q'_1}\end{pmatrix} \\
= \;& \frac{1}{4\pi}\sum_{l_1l_2\lambda q'_1q_1\tau_\beta\tau_1} i^{l_\beta+l_1}(-1)^{l_1+l'+\tau_\beta+\tau_1}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2} \\
&\times \left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!}\right)^{1/2}\hat{l}_\beta^2\hat{l}_1^3\hat{l}'_R\hat{l}_0\hat{\lambda}^2\hat{q}'^2\hat{q}_1^2\hat{J}^2\hat{l}' \\
&\times \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}{}_2Z^{\lambda l_0}_{\beta i}(k,k')k'^{l_\beta+l_1-\tau_\beta-\tau_1}
\end{aligned}
$$

$$\times \sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q'_1} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q'_1}+m'_R+m_\lambda+m_{q_1}+m'+m_\beta}$$
$$\times \begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix} \begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$
$$\times \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_1 - \tau_1 & \tau_1 & l_1 \\ m_1 - m_{\tau_1} & m_{\tau_1} & -m_1 \end{pmatrix} \begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1} \end{pmatrix}$$
$$\times \begin{pmatrix} l_\beta - \tau_\beta & \tau_\beta & l_\beta \\ m_\beta - m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix} \begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1} \end{pmatrix}$$
$$\times \begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1} \end{pmatrix} \begin{pmatrix} l_\beta - \tau_\beta & l_1 - \tau_1 & q'_1 \\ m_\beta - m_{\tau_\beta} & m_1 - m_{\tau_1} & m_{q'_1} \end{pmatrix},$$

where

$$ {}_2Z_{\beta i}^{\lambda l_0}(k,k') \;=\; \int_0^\infty dq q^2 \;\; {}_2Z_{\beta i}^{\lambda}(q,k') q^{\tau_\beta+\tau_1} Z_{\lambda_2}(k,q),$$

and where

$$ {}_2Z_{\beta i}^{\lambda}(q,k') \;=\; 2\pi \int_{-1}^{1} \sum_{n_1 n_2} \sum_{n_\beta} \sum_{n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta} \left(\frac{1}{\pi^2}\right)$$
$$\times \delta_{n_i n_2} \delta_{l_i l_2} \delta_{m_i m_2} \eta_{n_\beta l_\beta}(K_3) \eta_{n_1 l_1}(K_4) \frac{1}{K_3^{l_\beta}} \frac{1}{K_4^{l_1}} P_\lambda(u) du,$$

and where

$$\begin{cases} \boldsymbol{K}_3 = \frac{1}{2}\boldsymbol{k}' - \boldsymbol{q}, \quad \boldsymbol{K}_4 = \boldsymbol{k}' - \boldsymbol{q}, \\ u = \hat{\mathbf{k}}' \cdot \hat{\mathbf{q}}, \\ K_3^2 = \left(\frac{1}{2}k'\right)^2 + q^2 - k'qu, \qquad K_4^2 = k'^2 + q^2 - 2k'qu, \end{cases} \tag{D.9}$$

while $\eta_{n_\beta l_\beta}(K_3)$ and $\eta_{n_1 l_1}(K_4)$ are given by:

$$\eta_{n_\beta l_\beta}(K_3) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty drr^2 \zeta_{n_\beta l_\beta}(r) j_{l_\beta}(K_3 r), \tag{D.10}$$

$$\eta_{n_1 l_1}(K_4) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty drr^2 \frac{\zeta_{n_1 l_1}(r)}{r} j_{l_1}(K_4 r); \tag{D.11}$$

and

$$Z_{\lambda_2}(k,q) \;\; = \;\; 2\pi \int_{-1}^{1} P_{\lambda_2}(u') \frac{1}{|\mathbf{k}-\mathbf{q}|^2} du'.$$

.**Derivation of** ${}_3V^J_{\alpha\beta}$

$$\begin{aligned}
{}_3V^J_{\alpha\beta} = & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times \langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times \sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} I_3 \\
= & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times \langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times \sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} \int d^3\boldsymbol{\rho} e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\rho}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \\
& \times \int d^3\boldsymbol{r}_1 e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}_1} Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) \left(-\frac{Z}{r_1}\right) \zeta_{n_1 l_1}(r_1) \\
& \times \int d^3\boldsymbol{r}_2 \zeta^*_{n_i l_i}(r) \zeta_{n_2 l_2}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
= & \frac{1}{4\pi} \sum_{l_1 l_2 \lambda q'_1 q_1 \tau_\beta \tau_1} i^{l_\beta + l_1} (-1)^{l_1 + l' + \tau_\beta + \tau_1}
\end{aligned}$$

$$\times\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\left(\frac{(2l_1)!}{(2\tau_1)!(2(l_1-\tau_1))!}\right)^{1/2}$$
$$\times\hat{l}_\beta^2\hat{l}_1^3\hat{l}'_R\hat{l}_0\hat{\lambda}^2\hat{q}'^2\hat{q}_1^2\hat{J}^2\hat{l}'\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}{}_3Z^\lambda_{\beta i}(k,k')k'^{l_\beta+l_1-\tau_\beta-\tau_1}k^{\tau_\beta+\tau_1}$$
$$\times\sum_{m'_R m_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q'_1} m_{q_1} m_{\tau_\beta} m_{\tau_1}}(-1)^{m_{q'_1}+m'_R+m_\lambda+m_{q_1}+m'+m_\beta}$$
$$\times\begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & l_0 & q'_1 \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ 0 & 0 & 0\end{pmatrix}$$
$$\times\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J\end{pmatrix}\begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J\end{pmatrix}\begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m'\end{pmatrix}$$
$$\times\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m\end{pmatrix}\begin{pmatrix} l_1-\tau_1 & \tau_1 & l_1 \\ m_1-m_{\tau_1} & m_{\tau_1} & -m_1\end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1}\end{pmatrix}$$
$$\times\begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta\end{pmatrix}\begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1}\end{pmatrix}$$
$$\times\begin{pmatrix} \lambda & l_0 & q'_1 \\ m_\lambda & m_0 & m_{q'_1}\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q'_1 \\ m_\beta-m_{\tau_\beta} & m_1-m_{\tau_1} & m_{q'_1}\end{pmatrix},$$

where

$$\begin{aligned}{}_3Z^\lambda_{\beta i}(k,k') &= -4\pi\int_{-1}^{1}\sum_{n_1n_2n_\beta n_i} d^{\alpha(l_1l_2)l}_{n_1n_2}d_{n_i}d_{n_\beta}\\ &\quad\times\delta_{n_in_2}\delta_{l_il_2}\delta_{m_im_2}\eta_{n_\beta l_\beta}(K_1)\eta_{r,n_1l_1}(K_2)\frac{1}{K_1^{l_\beta}}\frac{1}{K_2^{l_1}}P_\lambda(u)du\end{aligned}$$

and where $\boldsymbol{K}_1$, $\boldsymbol{K}_2$ and u are given by equation (D.6) and $\eta_{n_\beta l_\beta}(K_1)$, $\eta_{r,n_1l_1}(K_2)$ are given by equations (D.7) and (D.8).

Derivation of ${}_4V^J_{\alpha\beta}$

$$\begin{aligned}{}_4V^J_{\alpha\beta} = &\sum_{l_1l_2m'_Rm_\beta m_0mm'_Rm'm_1m_2}\int d^2\hat{\boldsymbol{k}}'_0d^2\hat{\boldsymbol{k}}_0\langle l'_Rm'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0m_0\rangle\\ &\times\langle JM_J|l_0m_0lm\rangle\langle JM_J|l'm'l_im_i\rangle\langle l'm'|l'_Rm'_Rl_\beta m_\beta\rangle\langle l_1l_2m_1m_2|lm\rangle\end{aligned}$$

$$
\begin{aligned}
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta} I_4 \\
= & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2 \hat{\boldsymbol{k}}'_0 d^2 \hat{\boldsymbol{k}}_0 \langle l'_R m'_R | \hat{\boldsymbol{k}}' \rangle \langle \hat{\boldsymbol{k}} | l_0 m_0 \rangle \\
&\times \langle J M_J | l_0 m_0 l m \rangle \langle J M_J | l' m' l_i m_i \rangle \langle l' m' | l'_R m'_R l_\beta m_\beta \rangle \langle l_1 l_2 m_1 m_2 | l m \rangle \\
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta} \left(\frac{1}{2\pi^2} \right) \int d^3 q \frac{1}{|\boldsymbol{k}' - \boldsymbol{k} + \boldsymbol{q}|^2} \\
&\times \int d^3 \boldsymbol{\rho} e^{-i(\frac{1}{2}\boldsymbol{k}' - \boldsymbol{k}) \cdot (\boldsymbol{r}_0 - \boldsymbol{r}_1)} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \int d^3 \boldsymbol{r}_1 Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) \zeta_{n_1 l_1}(r_1) e^{i \boldsymbol{q} \cdot \boldsymbol{r}_1} \\
&\times \int d^3 \boldsymbol{r}_2 Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \zeta^*_{n_i l_i}(r) \zeta_{n_2 l_2}(r_2) e^{-i(\boldsymbol{k}' - \boldsymbol{k} + \boldsymbol{q}) \cdot \boldsymbol{r}_2} \\
= & \sum_{m'_0 m_\beta m_0 m m'_0 m' l_1 l_2 m_1 m_2} \int d^2 \hat{\boldsymbol{k}}'_0 d^2 \hat{\boldsymbol{k}}_0 \langle l'_0 m'_0 | \hat{\boldsymbol{k}}' \rangle \langle \hat{\boldsymbol{k}} | l_0 m_0 \rangle \\
&\times \langle J M_J | l_0 m_0 l m \rangle \langle J M_J | l' m' l_i m_i \rangle \langle l' m' | l'_0 m'_0 l_\beta m_\beta \rangle \langle l_1 l_2 m_1 m_2 | l m \rangle \\
&\times \sum_{c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6}} i^c (-1)^{l_1 + c + c_5 + \tau_c} (-1)^{m_i + m_c + m_{c_5}} k'^{c - \tau_c} k^{c_5 - \tau_5} \\
&\times \frac{\hat{l}_i \hat{l}_2 \hat{l}_c \hat{c} \hat{c}_5 \hat{\lambda}_5 \hat{c}_5 \hat{c}_5}{\hat{\tau}_5 (2c - 2\tau_c + 1)^{1/2} (2c_5 - 2\tau_5 + 1)^{1/2}} \left(\frac{(2c)!}{(2\tau_c)!(2(c - \tau_c))!} \right)^{1/2} \\
&\times \left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5 - \tau_5))!} \right)^{1/2} \begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix} \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix} \\
&\times \langle c - \tau_c \; \tau_c \;\; m_c - m_{\tau_c} \;\; m_{\tau_c} | c \; m_c \rangle \langle c_5 - \tau_5 \; \tau_5 \;\; m_{c_5} - m_{\tau_5} \;\; m_{\tau_5} | c_5 \; m_{c_5} \rangle \\
&\times Y_{c - \tau_c \;\; m_c - m_{\tau_c}}(\hat{\boldsymbol{k}}') Y^*_{\lambda_5 m_{\lambda_5}}(\hat{\boldsymbol{k}}') Y_{c_5 - \tau_5 \;\; m_{c_5} - m_{\tau_5}}(\hat{\boldsymbol{k}}) Y^*_{\lambda_6 m_{\lambda_6}}(\hat{\boldsymbol{k}}) \\
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l \pi s} d_{n_i} d_{n_\beta} \left(\frac{1}{2\pi^2} \right) \\
&\times \int d^3 \boldsymbol{q} q^{\tau_5} Z^{\lambda_5, \lambda_6}_{4, c \tau_c c_5 n_i l_i n_2 l_2}(k' k q) Y_{\tau_5 \; m_{\tau_5}}(\hat{\boldsymbol{q}}) Y_{\lambda_6 m_{\lambda_6}}(\hat{\boldsymbol{q}}) \\
&\times \sum_{\tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7}} i^{l_\beta + l_1} (-1)^{l_\beta + l_1 + \tau_\beta} Z^{\lambda_7}_{4, n_\beta l_\beta n_1 l_1}(k k' q) k^{\tau_\beta} \left(\frac{k'}{2} \right)^{l_\beta - \tau_\beta} \\
&\times \langle l_\beta - \tau_\beta \; \tau_\beta \;\; m_\beta - m_{\tau_\beta} \;\; m_{\tau_\beta} | l_\beta \; m_\beta \rangle \\
&\times \frac{(4\pi)^{1/2} \hat{l}_\beta}{(2l_\beta - 2\tau_\beta + 1)^{1/2} \hat{\tau}_\beta} \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta - \tau_\beta))!} \right)^{1/2}
\end{aligned}
$$

$$
\begin{aligned}
&\times Y_{l_\beta-\tau_\beta\;\; m_\beta-m_{\tau_\beta}}(\hat{\boldsymbol{k}}')\; Y_{\tau_\beta\; m_{\tau_\beta}}(\hat{\boldsymbol{k}}) Y^*_{\lambda_7 m_{\lambda_7}}(\hat{\boldsymbol{k}}') Y_{\lambda_7 m_{\lambda_7}}(\hat{\boldsymbol{k}}) Y_{l_1 m_1}(\hat{\boldsymbol{q}})\\
= &\sum_{m_0' m_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2} \langle JM_J|l_0 m_0 l m\rangle \langle JM_J|l'm'l_i m_i\rangle \langle l'm'|l_0' m_0' l_\beta m_\beta\rangle\\
&\times \langle l_1 l_2 m_1 m_2|lm\rangle \sum_{c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6} \tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7}} i^{c+l_\beta+l_1}\\
&\times (-1)^{l_1+c+c_5+\tau_c+l_\beta+l_1+\tau_\beta} (-1)^{m_i+m_c+m_{c_5}} \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} k'^{c-\tau_c+l_\beta-\tau_\beta} k^{c_5-\tau_5+\tau_\beta}\\
&\times \frac{\hat{l}_i \hat{l}_2 \hat{l}_c \hat{c} \hat{c}_5 \hat{\lambda}_5 \hat{c}_5 \hat{c}_5}{\hat{\tau}_5 (2c-2\tau_c+1)^{1/2} (2c_5-2\tau_5+1)^{1/2}} \left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2}\\
&\times \frac{(4\pi)^{1/2} \hat{l}_\beta}{(2l_\beta-2\tau_\beta+1)^{1/2} \hat{\tau}_\beta} \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2} \left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2}\\
&\times \begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix} \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix}\\
&\times \langle c-\tau_c\; \tau_c\;\; m_c-m_{\tau_c}\;\; m_{\tau_c}|c\; m_c\rangle \langle c_5-\tau_5\; \tau_5\;\; m_{c_5}-m_{\tau_5}\;\; m_{\tau_5}|c_5\; m_{c_5}\rangle\\
&\times \langle l_\beta-\tau_\beta\; \tau_\beta\;\; m_\beta-m_{\tau_\beta}\;\; m_{\tau_\beta}|l_\beta\; m_\beta\rangle\\
&\times \int d^2\hat{\boldsymbol{k}}' Y^*_{l_0' m_0'}(\hat{\boldsymbol{k}}') Y_{c-\tau_c\;\; m_c-m_{\tau_c}}(\hat{\boldsymbol{k}}') Y^*_{\lambda_5 m_{\lambda_5}}(\hat{\boldsymbol{k}}') Y_{l_\beta-\tau_\beta\;\; m_\beta-m_{\tau_\beta}}(\hat{\boldsymbol{k}}') Y^*_{\lambda_7 m_{\lambda_7}}(\hat{\boldsymbol{k}}')\\
&\times \int d^2\hat{\boldsymbol{k}} Y_{l_0 m_0}(\hat{\boldsymbol{k}}) Y_{c_5-\tau_5\;\; m_{c_5}-m_{\tau_5}}(\hat{\boldsymbol{k}}) Y^*_{\lambda_6 m_{\lambda_6}}(\hat{\boldsymbol{k}}) Y_{\tau_\beta\; m_{\tau_\beta}}(\hat{\boldsymbol{k}}) Y_{\lambda_7 m_{\lambda_7}}(\hat{\boldsymbol{k}})\\
&\times \sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2) l\pi s}_{n_1 n_2} d_{n_i} d_{n_\beta}\\
&\times \left(\frac{1}{2\pi^2}\right) \int_0^\infty dq q^2 q^{\tau_5} Z^{\lambda_5,\lambda_6}_{4,c\tau_c c_5 n_i l_i n_2 l_2}(k'kq) Z^{\lambda_7}_{4,n_\beta l_\beta n_1 l_1}(kk'q)\\
&\times \int d^2\hat{\boldsymbol{q}} Y_{\tau_5\; m_{\tau_5}}(\hat{\boldsymbol{q}}) Y_{\lambda_6 m_{\lambda_6}}(\hat{\boldsymbol{q}}) Y_{l_1 m_1}(\hat{\boldsymbol{q}})\\
= &\sum_{m_0' m_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2} \langle JM_J|l_0 m_0 l m\rangle\\
&\times \langle JM_J|l'm'l_i m_i\rangle \langle l'm'|l_0' m_0' l_\beta m_\beta\rangle \langle l_1 l_2 m_1 m_2|lm\rangle\\
&\times \sum_{c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6} \tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7}} i^{c+l_\beta+l_1} (-1)^{l_1+c+c_5+\tau_c+l_\beta+l_1+\tau_\beta}\\
&\times (-1)^{m_i+m_c+m_{c_5}} \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} k'^{c-\tau_c+l_\beta-\tau_\beta} k^{c_5-\tau_5+\tau_\beta} {}_4Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5 \tau_5}(k,k')\\
&\times \frac{\hat{l}_i \hat{l}_2 \hat{l}_c \hat{c} \hat{c}_5 \hat{\lambda}_5 \hat{c}_5 \hat{c}_5}{\hat{\tau}_5 (2c-2\tau_c+1)^{1/2} (2c_5-2\tau_5+1)^{1/2}} \left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2}
\end{aligned}
$$

$$\times\left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2}\frac{(4\pi)^{1/2}\hat{l}_\beta}{(2l_\beta-2\tau_\beta+1)^{1/2}\hat{\tau}_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}$$
$$\times\begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix}$$
$$\times\langle c-\tau_c\ \tau_c\ \ m_c-m_{\tau_c}\ \ m_{\tau_c}|c\ m_c\rangle\langle c_5-\tau_5\ \tau_5\ \ m_{c_5}-m_{\tau_5}\ \ m_{\tau_5}|c_5\ m_{c_5}\rangle$$
$$\times\langle l_\beta-\tau_\beta\ \tau_\beta\ \ m_\beta-m_{\tau_\beta}\ \ m_{\tau_\beta}|l_\beta\ m_\beta\rangle$$
$$\times\int d^2\hat{\boldsymbol{k}}' Y^*_{l_0'm_0'}(\hat{\boldsymbol{k}}')Y_{c-\tau_c\ \ m_c-m_{\tau_c}}(\hat{\boldsymbol{k}}')Y^*_{\lambda_5 m_{\lambda_5}}(\hat{\boldsymbol{k}}')Y_{l_\beta-\tau_\beta\ \ m_\beta-m_{\tau_\beta}}(\hat{\boldsymbol{k}}')Y^*_{\lambda_7 m_{\lambda_7}}(\hat{\boldsymbol{k}}')$$
$$\times\int d^2\hat{\boldsymbol{k}} Y_{l_0m_0}(\hat{\boldsymbol{k}})Y_{c_5-\tau_5\ \ m_{c_5}-m_{\tau_5}}(\hat{\boldsymbol{k}})Y^*_{\lambda_6 m_{\lambda_6}}(\hat{\boldsymbol{k}})Y_{\tau_\beta\ m_{\tau_\beta}}(\hat{\boldsymbol{k}})Y_{\lambda_7 m_{\lambda_7}}(\hat{\boldsymbol{k}})$$
$$\times\int d^2\hat{\boldsymbol{q}} Y_{\tau_5\ m_{\tau_5}}(\hat{\boldsymbol{q}})Y_{\lambda_6 m_{\lambda_6}}(\hat{\boldsymbol{q}})Y_{l_1m_1}(\hat{\boldsymbol{q}})$$
$$=\sum_{m_0'm_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2}\hat{J}^2\begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix}\begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix}$$
$$\times(-1)^{l'-m'}\hat{l}'\begin{pmatrix} l_0' & l_\beta & l' \\ m_0' & m_\beta & -m' \end{pmatrix}(-1)^{l-m}\hat{l}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$\times\sum_{cm_c\tau_c m_{\tau_c}\lambda_5 m_{\lambda_5}\tau_5 m_{\tau_5}c_5 m_{c_5}\lambda_6 m_{\lambda_6}\tau_\beta m_{\tau_\beta}\lambda_7 m_{\lambda_7}} i^{c+l_\beta+l_1}(-1)^{l_1+c+c_5+\tau_c+l_\beta+l_1+\tau_\beta}$$
$$\times(-1)^{m_i+m_c+m_{c_5}}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}k'^{c-\tau_c+l_\beta-\tau_\beta}k^{c_5-\tau_5+\tau_\beta}\,{}_4Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5\tau_5}(k,k')$$
$$\times\frac{\hat{l}_i\hat{l}_2\hat{l}_c\hat{c}\hat{c}_5\hat{\lambda}_5\hat{c}_5\hat{c}_5}{\hat{\tau}_5(2c-2\tau_c+1)^{1/2}(2c_5-2\tau_5+1)^{1/2}}\left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2}$$
$$\times\frac{(4\pi)^{1/2}\hat{l}_\beta}{(2l_\beta-2\tau_\beta+1)^{1/2}\hat{\tau}_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2}$$
$$\times\begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix}$$
$$\times(-1)^{c-m_c+c_5-m_{c_5}+l_\beta-m_\beta}\hat{c}\hat{c}_5\hat{l}_\beta\begin{pmatrix} c-\tau_c & \tau_c & c \\ m_c-m_{\tau_c} & m_{\tau_c} & -m_c \end{pmatrix}$$
$$\times\begin{pmatrix} c_5-\tau_5 & \tau_5 & c_5 \\ m_{c_5}-m_{\tau_5} & m_{\tau_5} & -m_{c_5} \end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}$$
$$\times(-1)^{m_0'+m_{\lambda_5}+m_{\lambda_7}}\sum_{q_1m_{q_1}q_2m_{q_2}}\frac{\hat{l}_0'c\hat{-}\tau_c\hat{\lambda}_5 l_\beta\hat{-}\tau_\beta\hat{\lambda}_7\hat{q}_1^2\hat{q}_2^2}{(\sqrt{4\pi})^3}(-1)^{m_{q_1}+m_{q_2}}$$

$$\times \begin{pmatrix} l'_0 & c-\tau_c & q_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 & q_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l'_0 & c-\tau_c & q_1 \\ -m'_0 & m_c-m_{\tau_c} & m_{q_1} \end{pmatrix} \begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2 \\ -m_{\lambda_5} & m_\beta-m_{\tau_\beta} & m_{q_2} \end{pmatrix}$$

$$\times \begin{pmatrix} q_1 & q_2 & \lambda_7 \\ m_{q_1} & m_{q_1} & m_{\lambda_7} \end{pmatrix}$$

$$\times(-1)^{m_{\lambda_6}} \sum_{q'_1 m_{q'_1} q'_2 m_{q'_2}} \frac{\hat{l}_0 c_5 \hat{-} \tau_5 \hat{\lambda}_6 \hat{\tau}_\beta \hat{\lambda}_7 \hat{q}'_1 \hat{q}'_1 \hat{q}'_2 \hat{q}'_2}{(\sqrt{4\pi})^3} (-1)^{m_{q'_1}+m_{q'_2}}$$

$$\times \begin{pmatrix} l_0 & c_5-\tau_5 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_6 & \tau_\beta & q'_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q'_1 & q'_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_0 & c_5-\tau_5 & q'_1 \\ m_0 & m_{c_5}-m_{\tau_5} & m_{q'_1} \end{pmatrix} \begin{pmatrix} \lambda_6 & \tau_\beta & q'_2 \\ m_{\lambda_6} & m_{\tau_\beta} & m_{q'_2} \end{pmatrix} \begin{pmatrix} q'_1 & q'_2 & \lambda_7 \\ m_{q'_2} & m_{q'_2} & m_{\lambda_7} \end{pmatrix}$$

$$\times \frac{\hat{\tau}_5 \hat{\lambda}_6 \hat{l}_1}{\sqrt{4\pi}} \begin{pmatrix} \tau_5 & \lambda_6 & l_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_5 & \lambda_6 & l_1 \\ m_{\tau_5} & m_{\lambda_6} & m_1 \end{pmatrix}$$

$$= \sum_{m'_R m_\beta m_0 m m'_R m' l_1 l_2 m_1 m_2 c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5}}$$

$$\sum_{\lambda_6 m_{\lambda_6} \tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7} q_1 m_{q_1} q_2 m_{q_2} q'_1 m_{q'_1} q'_2 m_{q'_2}}$$

$$\times i^{c+l_\beta+l_1} (-1)^{l_1+\tau_c+l_1+\tau_\beta+l'+l}$$

$$\times(-1)^{m_i-m_\beta+m'_R+m_{\lambda_5}+m_{\lambda_7}+m_{\lambda_6}+m_{q_1}+m_{q_2}+m_{q'_1}+m_{q'_2}+m'+m}$$

$$\times \frac{1}{(4\pi)^3} \left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} k'^{c-\tau_c+l_\beta-\tau_\beta} k^{c_5-\tau_5+\tau_\beta} Z^{\lambda_5\lambda_6\lambda_7}_{4,c\tau_c c_5 \tau_5}(kk')$$

$$\times \hat{l}_i \hat{l}_2 \hat{l}_c \hat{c} \hat{c}_5 \hat{\lambda}_5 \hat{c}_5 \hat{c}_5 \hat{l}_\beta \hat{c} \hat{c}_5 \hat{l}_\beta \hat{l}'_0 \hat{\lambda}_5 \hat{\lambda}_7 \hat{q}_1^2 \hat{q}_2^2 \hat{l}_0 \hat{\lambda}_6 \hat{\lambda}_7 \hat{q}'_1 \hat{q}'_1 \hat{q}'_2 \hat{q}'_2 \hat{\tau}_5 \hat{\lambda}_6 \hat{l}_1 \hat{J}^2 \hat{l} \hat{l}'$$

$$\times \left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2} \left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2} \left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}$$

$$\times \begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'_R & c-\tau_c & q_1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \lambda_6 & \tau_\beta & q'_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q'_1 & q'_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} q_1 & q_2 & \lambda_7 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_0 & c_5-\tau_5 & q'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_5 & \lambda_6 & l_1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J \end{pmatrix} \begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J \end{pmatrix} \begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m' \end{pmatrix}$$
$$\times \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}$$
$$\times \begin{pmatrix} c_5-\tau_5 & \tau_5 & c_5 \\ m_{c_5}-m_{\tau_5} & m_{\tau_5} & -m_{c_5} \end{pmatrix} \begin{pmatrix} c-\tau_c & \tau_c & c \\ m_c-m_{\tau_c} & m_{\tau_c} & -m_c \end{pmatrix}$$
$$\times \begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix} \begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta \end{pmatrix}$$
$$\times \begin{pmatrix} l'_R & c-\tau_c & q_1 \\ -m'_R & m_c-m_{\tau_c} & m_{q_1} \end{pmatrix} \begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2 \\ -m_{\lambda_5} & m_\beta-m_{\tau_\beta} & m_{q_2} \end{pmatrix}$$
$$\times \begin{pmatrix} q_1 & q_2 & \lambda_7 \\ m_{q_1} & m_{q_1} & m_{\lambda_7} \end{pmatrix} \begin{pmatrix} l_0 & c_5-\tau_5 & q'_1 \\ m_0 & m_{c_5}-m_{\tau_5} & m_{q'_1} \end{pmatrix}$$

$$\times \begin{pmatrix} \lambda_6 & \tau_\beta & q'_2 \\ m_{\lambda_6} & m_{\tau_\beta} & m_{q'_2} \end{pmatrix} \begin{pmatrix} q'_1 & q'_2 & \lambda_7 \\ m_{q'_2} & m_{q'_2} & m_{\lambda_7} \end{pmatrix} \begin{pmatrix} \tau_5 & \lambda_6 & l_1 \\ m_{\tau_5} & m_{\lambda_6} & m_1 \end{pmatrix},$$

where

$$\begin{aligned} & {}_4Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5\tau_5}(k,k') \\ &= \sum_{n_1n_2n_\beta n_i} d^{\alpha(l_1l_2)l}_{n_1n_2} d_{n_i} d_{n_\beta} \left(\frac{1}{2\pi^2}\right) \\ &\quad \times \int_0^\infty dq q^2 q^{\tau_5}\, {}_4Z^{\lambda_5\lambda_6}_{c\tau_c c_5 n_i l_i n_2 l_2}(k',k,q) \;\; {}_4Z^{\lambda_7}_{n_\beta l_\beta n_1 l_1}(k,k',q), \end{aligned}$$

$${}_4Z^{\lambda_5\lambda_6}_{c\tau_c c_5 n_i l_i n_2 l_2}(k',k,q) \;=\; 2\pi \int_{-1}^{1} {}_4Z^{\lambda_5}_{c n_i l_i n_2 l_2}(k',K_6) K_6^{\tau_c - c_5} P_{\lambda_6}(u) du, \quad \text{(D.12)}$$

$$\begin{aligned} & {}_4Z^{\lambda_5}_{c n_i l_i n_2 l_2 c}(k',K_6) \\ &= \sqrt{8\pi} \int_{-1}^{1} du_1 \int_0^\infty dr_2 r_2^2 \zeta^*_{n_i l_i}(r_2) \zeta_{n_2 l_2}(r_2) j_{l_\beta}(K_5 r_2) \frac{1}{K_5^{2+c}} P_{\lambda_5}(u_1), \end{aligned} \quad \text{(D.13)}$$

and where

$$\boldsymbol{K}_5 = \boldsymbol{k}' - \boldsymbol{k} + \boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{K}_6, \quad ; \quad \boldsymbol{K}_6 = \boldsymbol{k} - \boldsymbol{q},$$

$$u_1 = \hat{\boldsymbol{k}}' \cdot \hat{\boldsymbol{K}}_6, \quad ; \quad u = \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{q}},$$

$$K_5^2 = k'^2 + {K_6}^2 - k'K_6u_1. \quad ; \quad K_6^2 = k^2 + q^2 - kqu.$$

Also

$$_4Z^{\lambda_7}_{n_\beta l_\beta n_1 l_1}(k,k',q) \;=\; 2\pi \int_{-1}^{1} \eta_{n_\beta l_\beta}(K_1)\eta_{n_1 l_1}(q)\frac{1}{K_1^{l_\beta}} P_{\lambda_7}(u_2)du_2, \tag{D.14}$$

$$\times u_2 = \hat{\boldsymbol{k}}' \cdot \hat{\boldsymbol{k}} \qquad {K_1}^2 = \left(\frac{k'}{2}\right)^2 + k^2 - \frac{1}{2}k'ku_2$$

where $\eta_{n_\beta l_\beta}(K_1)$ and $\eta_{r,n_1 l_1}(K_2)$ are given by (D.7) and (D.8).

Derivation of II_5

$$\begin{aligned}
_5V^J_{\alpha\beta} = & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times \sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} I_2 \\
= & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times \sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} - \int d^3\boldsymbol{\rho}\frac{e^{-i(\frac{1}{2}\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\rho}}}{\rho}\zeta^*_{n_\beta l_\beta}(\rho)Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}})
\end{aligned}$$

$$
\begin{aligned}
& \times \int d^3\boldsymbol{r}_1 e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}_1} Y_{l_1m_1}(\hat{\boldsymbol{r}}_1)\zeta_{n_1l_1}(r_1) \\
& \times \int d^3\boldsymbol{r}_2 \zeta^*_{n_il_i}(r)\zeta_{n_2l_2}(r_2)Y^*_{l_im_i}(\hat{\boldsymbol{r}})Y_{l_2m_2}(\hat{\boldsymbol{r}}_2) \\
= \; & \frac{1}{4\pi}\sum_{l_1l_2\lambda q_1' q_1\tau_\beta\tau_1} i^{l_\beta+l_1}(-1)^{l_1+l'+\tau_\beta+\tau_1} \\
& \times \frac{\sqrt{(2l_\beta)!}}{\sqrt{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}}\frac{\sqrt{(2l_1)!}}{\sqrt{(2\tau_1)!(2(l_1-\tau_1))!}} \\
& \times \hat{l}_\beta^2\hat{l}_1^3\hat{l}'_R\hat{l}_0\hat{\lambda}^2\hat{q}'^2\hat{q}_1^2\hat{J}^2\hat{l}'\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} {}_5Z^\lambda_{\beta i}(k,k')k'^{l_\beta+l_1-\tau_\beta-\tau_1}k^{\tau_\beta+\tau_1} \\
& \times \sum_{m'_Rm_\beta m_0 m m'_R m' m_1 m_2 m_\lambda m_{q_1'} m_{q_1} m_{\tau_\beta} m_{\tau_1}} (-1)^{m_{q_1'}+m'_R+m_\lambda+m_{q_1}+m'+m_\beta} \\
& \times \begin{pmatrix} l'_R & \lambda & q \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & l_0 & q_1' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q_1' \\ 0 & 0 & 0\end{pmatrix} \\
& \times \begin{pmatrix} l_0 & l & J \\ m_0 & m & -M_J\end{pmatrix}\begin{pmatrix} l' & l_i & J \\ m' & m_i & -M_J\end{pmatrix}\begin{pmatrix} l'_R & l_\beta & l' \\ m'_R & m_\beta & -m'\end{pmatrix} \\
& \times \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m\end{pmatrix}\begin{pmatrix} l_1-\tau_1 & \tau_1 & l_1 \\ m_1-m_{\tau_1} & m_{\tau_1} & -m_1\end{pmatrix}\begin{pmatrix} \tau_\beta & \tau_1 & q_1 \\ m_{\tau_\beta} & m_{\tau_1} & m_{q_1}\end{pmatrix} \\
& \times \begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta \\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta\end{pmatrix}\begin{pmatrix} l'_R & \lambda & q_1 \\ -m'_R & -m_\lambda & m_{q_1}\end{pmatrix} \\
& \times \begin{pmatrix} \lambda & l_0 & q_1' \\ m_\lambda & m_0 & m_{q_1'}\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & l_1-\tau_1 & q_1' \\ m_\beta-m_{\tau_\beta} & m_1-m_{\tau_1} & m_{q_1'}\end{pmatrix},
\end{aligned}
$$

where

$$
\begin{aligned}
{}_5Z^\lambda_{\beta i}(k,k') \;=\; & 2\pi\int_{-1}^{1}\sum_{n_1n_2n_\beta n_i} d^{\alpha(l_1l_2)l}_{n_1n_2}d_{n_i}d_{n_\beta} \\
& \times\delta_{n_in_2}\delta_{l_il_2}\delta_{m_im_2}\eta_{\rho,n_\beta l_\beta}(K_1)\eta_{r,n_1l_1}(K_2)\frac{1}{K_1^{l_\beta}}\frac{1}{K_2^{l_1}}P_\lambda(u)du
\end{aligned}
$$

and K_1, K_2 and u are given by equation (D.6).

Derivation of ${}_6V^J_{\alpha\beta}$

The derivation of ${}_6V^J_{\alpha\beta}$ is quite similiar to that of ${}_4V^J_{\alpha\beta}$. Following the same steps in derivation of ${}_4V^J_{\alpha\beta}$, we have

$$
\begin{aligned}
{}_6V^J_{\alpha\beta} = & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} I_6 \\
= & \sum_{l_1 l_2 m'_R m_\beta m_0 m m'_R m' m_1 m_2} \int d^2\hat{\boldsymbol{k}}'_0 d^2\hat{\boldsymbol{k}}_0 \langle l'_R m'_R|\hat{\boldsymbol{k}}'\rangle\langle\hat{\boldsymbol{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_R m'_R l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{n_1 n_2 n_\beta n_i} d^{\alpha(l_1 l_2)l}_{n_1 n_2} d_{n_i} d_{n_\beta} \\
& \times\int d^3\boldsymbol{r}_0 d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_{01}} \zeta^*_{n_\beta l_\beta}(\rho) Y^*_{l_\beta m_\beta}(\hat{\boldsymbol{\rho}}) \zeta^*_{n_i l_i}(r_2) Y^*_{l_i m_i}(\hat{\boldsymbol{r}}_2) \\
& \times\left(-\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_2|}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_0} \zeta_{n_1 l_1}(r_1)\zeta_{n_2 l_2}(r_2) Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \\
= & \sum_{m'_0 m_\beta m_0 m m'_0 m' l_1 l_2 m_1 m_2} \int d^2\hat{\mathbf{k}}'_0 d^2\hat{\mathbf{k}}_0 \langle l'_0 m'_0|\hat{\mathbf{k}}'\rangle\langle\hat{\mathbf{k}}|l_0 m_0\rangle \\
& \times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l'_0 m'_0 l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
& \times\sum_{c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6}} i^c(-1)^{l_1+c+c_5+\tau_c}(-1)^{m_i+m_c+m_{c_5}} k'^{c-\tau_c} k^{c_5-\tau_5} \\
& \times\frac{\hat{l}_i\hat{l}_2\hat{l}_c\hat{c}\hat{c}_5\hat{\lambda}_5\hat{c}_5\hat{c}_5}{\hat{\tau}_5(2c-2\tau_c+1)^{1/2}(2c_5-2\tau_5+1)^{1/2}} \\
& \times\left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2}\left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2} \\
& \times\begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix} \\
& \times\langle c-\tau_c\ \tau_c\ \ m_c-m_{\tau_c}\ \ m_{\tau_c}|c\ m_c\rangle\langle c_5-\tau_5\ \tau_5\ \ m_{c_5}-m_{\tau_5}\ \ m_{\tau_5}|c_5\ m_{c_5}\rangle \\
& \times Y_{c-\tau_c\ \ m_c-m_{\tau_c}}(\hat{\mathbf{k}}') Y^*_{\lambda_5 m_{\lambda_5}}(\hat{\mathbf{k}}') Y_{c_5-\tau_5\ \ m_{c_5}-m_{\tau_5}}(\hat{\mathbf{k}}) Y^*_{\lambda_6 m_{\lambda_6}}(\hat{\mathbf{k}})
\end{aligned}
$$

$$
\begin{aligned}
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta} \\
&\times \left(\frac{1}{2\pi^2}\right) \int d^3\mathbf{q} q^{\tau_5}\,{}_4Z^{\lambda_5,\lambda_6}_{c\tau_c c_5 n_i l_i n_2 l_2}(k',k,q) Y_{\tau_5\, m_{\tau_5}}(\hat{\mathbf{q}}) Y_{\lambda_6 m_{\lambda_6}}(\hat{\mathbf{q}}) \\
&\times \sum_{\tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7}} i^{l_\beta+l_1}(-1)^{l_\beta+l_1+\tau_\beta}\,{}_4Z^{\lambda_7}_{n_\beta l_\beta n_1 l_1}(k,k',q) q^{\tau_\beta}\left(\frac{k'}{2}\right)^{l_\beta-\tau_\beta} \\
&\times \langle l_\beta-\tau_\beta\;\tau_\beta\;\; m_\beta-m_{\tau_\beta}\;\; m_{\tau_\beta}|l_\beta\; m_\beta\rangle \\
&\times \frac{(4\pi)^{1/2}\hat{l}_\beta}{(2l_\beta-2\tau_\beta+1)^{1/2}\hat{\tau}_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2} \\
&\times Y_{l_\beta-\tau_\beta\;\; m_\beta-m_{\tau_\beta}}(\hat{\mathbf{k}}')\; Y_{\tau_\beta\, m_{\tau_\beta}}(\hat{\mathbf{q}}) Y^*_{\lambda_7 m_{\lambda_7}}(\hat{\mathbf{k}}') Y_{\lambda_7 m_{\lambda_7}}(\hat{\mathbf{q}}) Y_{l_1 m_1}(\hat{\mathbf{q}}) \\
= &\sum_{m_0' m_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2} \int d^2\hat{\mathbf{k}}_0' d^2\hat{\mathbf{k}}_0 \langle l_0' m_0'|\hat{\mathbf{k}}'\rangle\langle\hat{\mathbf{k}}|l_0 m_0\rangle \\
&\times \langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l_0'm_0'l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle \\
&\times \sum_{c m_c \tau_c m_{\tau_c} \lambda_5 m_{\lambda_5} \tau_5 m_{\tau_5} c_5 m_{c_5} \lambda_6 m_{\lambda_6} \tau_\beta m_{\tau_\beta} \lambda_7 m_{\lambda_7}} k'^{c-\tau_c+l_\beta-\tau_\beta} k^{c_5-\tau_5} \\
&\times i^{c+l_\beta+l_1}(-1)^{l_1+c+c_5+\tau_c+l_\beta+l_1+\tau_\beta}(-1)^{m_i+m_c+m_{c_5}}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} \\
&\times \frac{\hat{l}_i\hat{l}_2\hat{l}_c\hat{c}\hat{c}_5\hat{\lambda}_5\hat{c}_5\hat{c}_5}{\hat{\tau}_5(2c-2\tau_c+1)^{1/2}(2c_5-2\tau_5+1)^{1/2}}\left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2} \\
&\times \left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2}\frac{(4\pi)^{1/2}\hat{l}_\beta}{(2l_\beta-2\tau_\beta+1)^{1/2}\hat{\tau}_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2} \\
&\times \begin{pmatrix} l_i & l_2 & c \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_i & l_2 & c \\ -m_i & m_2 & m_c \end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5 \\ m_{\tau_c} & m_{\lambda_5} & m_{c_5} \end{pmatrix} \\
&\times \langle c-\tau_c\;\tau_c\;\; m_c-m_{\tau_c}\;\; m_{\tau_c}|c\; m_c\rangle\langle c_5-\tau_5\;\tau_5\;\; m_{c_5}-m_{\tau_5}\;\; m_{\tau_5}|c_5\; m_{c_5}\rangle \\
&\times \langle l_\beta-\tau_\beta\;\tau_\beta\;\; m_\beta-m_{\tau_\beta}\;\; m_{\tau_\beta}|l_\beta\; m_\beta\rangle \\
&\times \int d^2\hat{\mathbf{k}}' Y^*_{l_0'm_0'}(\hat{\mathbf{k}}') Y_{c-\tau_c\;\; m_c-m_{\tau_c}}(\hat{\mathbf{k}}') Y^*_{\lambda_5 m_{\lambda_5}}(\hat{\mathbf{k}}') Y_{l_\beta-\tau_\beta\;\; m_\beta-m_{\tau_\beta}}(\hat{\mathbf{k}}') Y^*_{\lambda_7 m_{\lambda_7}}(\hat{\mathbf{k}}') \\
&\times \int d^2\hat{\mathbf{k}} Y_{l_0 m_0}(\hat{\mathbf{k}}) Y_{c_5-\tau_5\;\; m_{c_5}-m_{\tau_5}}(\hat{\mathbf{k}}) Y^*_{\lambda_6 m_{\lambda_6}}(\hat{\mathbf{k}}) \\
&\times \int d^2\hat{\mathbf{q}} Y_{\tau_\beta\, m_{\tau_\beta}}(\hat{\mathbf{q}}) Y_{\lambda_7 m_{\lambda_7}}(\hat{\mathbf{q}}) Y_{l_1 m_1}(\hat{\mathbf{q}}) Y_{\tau_5\, m_{\tau_5}}(\hat{\mathbf{q}}) Y_{\lambda_6 m_{\lambda_6}}(\hat{\mathbf{q}}) \\
&\times \sum_{n_1 n_2 n_\beta n_i} d_{n_1 n_2}^{\alpha(l_1 l_2) l} d_{n_i} d_{n_\beta}
\end{aligned}
$$

$$
\begin{aligned}
&\left(\frac{1}{2\pi^2}\right)\int_0^\infty dq q^2 q^{\tau_5+\tau_\beta}{}_4Z^{\lambda_5,\lambda_6}_{c\tau_c c_5 n_i l_i n_2 l_2}(k',k,q){}_4Z^{\lambda_7}_{n_\beta l_\beta n_1 l_1}(k,k',q)\\
=&\sum_{m_0' m_\beta m_0 m m_0' m' l_1 l_2 m_1 m_2}\int d^2\hat{\mathbf{k}}_0' d^2\hat{\mathbf{k}}_0\langle l_0' m_0'|\hat{\mathbf{k}}'\rangle\langle\hat{\mathbf{k}}|l_0 m_0\rangle\\
&\times\langle JM_J|l_0 m_0 l m\rangle\langle JM_J|l'm'l_i m_i\rangle\langle l'm'|l_0'm_0'l_\beta m_\beta\rangle\langle l_1 l_2 m_1 m_2|lm\rangle\\
&\times\sum_{c m_c \tau_c m_{\tau_c}\lambda_5 m_{\lambda_5}\tau_5 m_{\tau_5} c_5 m_{c_5}\lambda_6 m_{\lambda_6}\tau_\beta m_{\tau_\beta}\lambda_7 m_{\lambda_7}} k'^{c-\tau_c+l_\beta-\tau_\beta}k^{c_5-\tau_5}{}_6Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5\tau_5}(k,k')\\
&\times i^{c+l_\beta+l_1}(-1)^{l_1+c+c_5+\tau_c+l_\beta+l_1+\tau_\beta}(-1)^{m_i+m_c+m_{c_5}}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}\\
&\times\frac{\hat{l}_i\hat{l}_2\hat{l}_c\hat{c}\hat{c}_5\hat{\lambda}_5\hat{c}_5\hat{c}_5}{\hat{\tau}_5(2c-2\tau_c+1)^{1/2}(2c_5-2\tau_5+1)^{1/2}}\left(\frac{(2c)!}{(2\tau_c)!(2(c-\tau_c))!}\right)^{1/2}\\
&\times\left(\frac{(2c_5)!}{(2\tau_5)!(2(c_5-\tau_5))!}\right)^{1/2}\frac{(4\pi)^{1/2}\hat{l}_\beta}{(2l_\beta-2\tau_\beta+1)^{1/2}\hat{\tau}_\beta}\left(\frac{(2l_\beta)!}{(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}\right)^{1/2}\\
&\times\begin{pmatrix} l_i & l_2 & c\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_i & l_2 & c\\ -m_i & m_2 & m_c\end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5\\ m_{\tau_c} & m_{\lambda_5} & m_{c_5}\end{pmatrix}\\
&\times\langle c-\tau_c\ \tau_c\ \ m_c-m_{\tau_c}\ \ m_{\tau_c}|c\ m_c\rangle\langle c_5-\tau_5\ \tau_5\ \ m_{c_5}-m_{\tau_5}\ \ m_{\tau_5}|c_5\ m_{c_5}\rangle\\
&\times\langle l_\beta-\tau_\beta\ \tau_\beta\ \ m_\beta-m_{\tau_\beta}\ \ m_{\tau_\beta}|l_\beta\ m_\beta\rangle\\
&\times\int d^2\hat{\mathbf{k}}' Y^*_{l_0'm_0'}(\hat{\mathbf{k}}')Y_{c-\tau_c\ \ m_c-m_{\tau_c}}(\hat{\mathbf{k}}')Y^*_{\lambda_5 m_{\lambda_5}}(\hat{\mathbf{k}}')Y_{l_\beta-\tau_\beta\ \ m_\beta-m_{\tau_\beta}}(\hat{\mathbf{k}}')Y^*_{\lambda_7 m_{\lambda_7}}(\hat{\mathbf{k}}')\\
&\times\int d^2\hat{\mathbf{k}} Y_{l_0 m_0}(\hat{\mathbf{k}})Y_{c_5-\tau_5\ \ m_{c_5}-m_{\tau_5}}(\hat{\mathbf{k}})Y^*_{\lambda_6 m_{\lambda_6}}(\hat{\mathbf{k}})\\
&\times\int d^2\hat{\mathbf{q}} Y_{\tau_\beta\ m_{\tau_\beta}}(\hat{\mathbf{q}})Y_{\lambda_7 m_{\lambda_7}}(\hat{\mathbf{q}})Y_{l_1 m_1}(\hat{\mathbf{q}})Y_{\tau_5\ m_{\tau_5}}(\hat{\mathbf{q}})Y_{\lambda_6 m_{\lambda_6}}(\hat{\mathbf{q}})\\
=&\sum_{m_R' m_\beta m_0 m m_R' m' l_1 l_2 m_1 m_2}\\
&\times\int d^2\hat{\mathbf{k}}_0'\int d^2\hat{\mathbf{k}}_0\langle l_R' m_R'|\hat{\mathbf{k}}'\rangle\langle\hat{\mathbf{k}}|l_0 m_0\rangle(-1)^{l'-m'+l-m}\hat{J}\hat{J}\hat{l}'\hat{l}\\
&\times\begin{pmatrix} l_0 & l & J\\ m_0 & m & -M_J\end{pmatrix}\begin{pmatrix} l' & l_i & J\\ m' & m_i & -M_J\end{pmatrix}\\
&\times\begin{pmatrix} l_R' & l_\beta & l'\\ m_R' & m_\beta & -m'\end{pmatrix}\begin{pmatrix} l_1 & l_2 & l\\ m_1 & m_2 & -m\end{pmatrix}\\
&\times\sum_{c m_c \tau_c m_{\tau_c}\lambda_5 m_{\lambda_5}\tau_5 m_{\tau_5} c_5 m_{c_5}\lambda_6 m_{\lambda_6}\tau_\beta m_{\tau_\beta}\lambda_7 m_{\lambda_7}} i^{c+l_\beta+l_1}\\
&\times(-1)^{\tau_c+\tau_\beta+m_i-m_\beta+m_R'+m_{\lambda_5}+m_{\lambda_7}}
\end{aligned}
$$

$$
\begin{aligned}
&\times\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta} {}_6Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5\tau_5}(k,k')k'^{c-\tau_c+l_\beta-\tau_\beta}k^{c_5-\tau_5}\\
&\times\frac{\hat{l_1}^2\hat{l}_2\hat{l}_c\hat{c}^2\hat{c}_5^3\hat{\lambda}_5^2\hat{l}_\beta^2}{\sqrt{(2c-2\tau_c+1)(2c_5-2\tau_5+1)(2l_\beta-2\tau_\beta+1)}}\\
&\times\frac{\sqrt{(2c)!(2c_5)!(2l_\beta)!}}{\sqrt{\sqrt{(2\tau_c)!(2(c-\tau_c))!}(2\tau_5)!(2(c_5-\tau_5))!(2\tau_\beta)!(2(l_\beta-\tau_\beta))!}}\\
&\times\begin{pmatrix} l_i & l_2 & c\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \tau_c & \lambda_5 & c_5\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_\beta-\tau_\beta & \tau_\beta & l_\beta\\ m_\beta-m_{\tau_\beta} & m_{\tau_\beta} & -m_\beta\end{pmatrix}\\
&\times\begin{pmatrix} \tau_c & \lambda_5 & c_5\\ m_{\tau_c} & m_{\lambda_5} & m_{c_5}\end{pmatrix}\begin{pmatrix} c-\tau_c & \tau_c & c\\ m_c-m_{\tau_c} & m_{\tau_c} & -m_c\end{pmatrix}\\
&\times\begin{pmatrix} c_5-\tau_5 & \tau_5 & c_5\\ m_{c_5}-m_{\tau_5} & m_{\tau_5} & -m_{c_5}\end{pmatrix}\begin{pmatrix} l_i & l_2 & c\\ -m_i & m_2 & m_c\end{pmatrix}\\
&\times\sum_{q_1m_{q_1}q_2m_{q_2}q'_1m_{q'_1}q'_2m_{q'_2}}\frac{\hat{l}'_0(c\hat{-}\tau_c)(\hat{l_\beta-\tau_\beta})(c_5\hat{-}\tau_5)\hat{\lambda}_6^2\hat{\lambda}_7^2\hat{q}_1'^2\hat{q}_2'^2\hat{q}_1^2\hat{q}_2^2}{(4\pi)^3}\\
&\times(-1)^{m_{q_1}+m_{q_2}+m_{\lambda_6}+m_{q'_1}+m_{q'_2}}\begin{pmatrix} l'_0 & c-\tau_c & q_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2\\ 0 & 0 & 0\end{pmatrix}\\
&\times\begin{pmatrix} q_1 & q_2 & \lambda_7\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} c_5-\tau_5 & \lambda_6 & l_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l'_0 & c-\tau_c & q_1\\ -m'_R & m_c-m_{\tau_c} & m_{q_1}\end{pmatrix}\\
&\times\begin{pmatrix} \lambda_5 & l_\beta-\tau_\beta & q_2\\ -m_{\lambda_5} & m_\beta-m_{\tau_\beta} & m_{q_2}\end{pmatrix}\begin{pmatrix} c_5-\tau_5 & \lambda_6 & l_1\\ m_{c_5}-m_{\tau_5} & -m_{\lambda_6} & m_1\end{pmatrix}\\
&\times\begin{pmatrix} \tau_\beta & \lambda_7 & q'_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \tau_5 & \lambda_6 & q'_2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} q'_1 & q'_2 & l_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} q_1 & q_2 & \lambda_7\\ m_{q_1} & m_{q_1} & m_{\lambda_7}\end{pmatrix}\\
&\times\begin{pmatrix} \tau_\beta & \lambda_7 & q'_1\\ m_{\tau_beta} & m_{\lambda_7} & m_{q'_1}\end{pmatrix}\begin{pmatrix} \tau_5 & \lambda_6 & q'_2\\ m_{\tau_5} & m_{\lambda_6} & m_{q'_2}\end{pmatrix}\begin{pmatrix} q'_1 & q'_2 & l_1\\ m_{q'_2} & m_{q'_2} & m_1\end{pmatrix}
\end{aligned}
$$

where

$$
\begin{aligned}
{}_6Z^{\lambda_5\lambda_6\lambda_7}_{c\tau_c c_5\tau_5}(k,k') = &\sum_{n_1n_2n_\beta n_i} d^{\alpha(l_1l_2)l}_{n_1n_2}d_{n_i}d_{n_\beta}\\
&\times\left(\frac{1}{2\pi^2}\right)\int_0^\infty dqq^2q^{\tau_5+\tau_\beta}{}_4Z^{\lambda_5,\lambda_6}_{c\tau_c c_5n_il_in_2l_2}(k',k,q){}_4Z^{\lambda_7}_{n_\beta l_\beta n_1l_1}(k,k',q)
\end{aligned}
$$

and where ${}_4Z^{\lambda_5,\lambda_6}_{c\tau_c c_5 n_i l_i n_2 l_2}(k', k, q)$ and ${}_4Z^{\lambda_7}_{n_\beta l_\beta n_1 l_1}(k, k', q)$ are given by equations (D.12) and (D.14).

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