CHAPTER 3

Coupled-Channel Optical Method (CCOM)

In this chapter, the formalism of the CCOM for positron-H scattering is presented. This formalism is based on the work of electron-H scattering by McCarthy and Stelbovics (1983a) and positron-H scattering by Ratnavelu and Rajagopal (1999). This method was also extended to positron scattering by alkali atoms (Natchimuthu and Ratnavelu 2001 and Ratnavelu and Ng 2006). Here, we outline the basics of the formalism.

3.1 Optical Potential Formalism

For the derivation of the optical potential, the Schrodinger equation is rewritten as:

$$E - K - v = 0 \tag{3.1}$$

where $v = v_1 + v_2 + v_3$ and $K = K_1 + K_2$. v represents the potential operator while K stands for kinetic energy. The subscripts 1, 2 and 3 are the electron 1-core, electron 2-core and electron 1-electron 2 subsystem, respectively.

The Schrodinger equation is decomposed using Feshbach projection operators, P and Q. After the decomposition, the whole space of target wavefunction is decomposed into 2 subspaces which are P space and Q space. P space is a finite set including the ground state and Q space describes the continuum states. Following Ratnavelu and Ng (2006), both P and Q can be divided again into orthogonal subspaces P_1, P_2, Q_1 and Q_2, with subscripts 1 and 2 representing the atomic and Ps channels respectively:

$$P = P_1 + P_2 = \sum_{a \in P_1} |\psi_a\rangle\langle\psi_a| + \sum_{b \in P_2} |\phi_b\rangle\langle\phi_b| \tag{3.2a}$$

$$Q = Q_1 + Q_2 = \sum_{c \in Q_1} |\psi_c\rangle\langle\psi_c| + \sum_{d \in Q_2} |\phi_d\rangle\langle\phi_d| \tag{3.2b}$$

The term ψ_a and ϕ_b are the asymptotic 'free' state vectors that describe the target system and the Ps in the state 'a' and 'b' in a particular atomic and Ps entrance channels, respectively. The state 'c' and 'd' represents the neglected discrete and continuum channels in the atomic target and Ps, respectively. However, in the present work, the optical potential approach is only allowed for the discrete and continuum states of the H atom. With this approximation, the labels P represents P_1 and Q represents Q_1 in the analysis below. By using the following properties of projection operator:

$$Q = 1 - P \qquad Q^{-1}Q = 1 \qquad PQ = QP = 0 \qquad P^2 = P \qquad Q^2 = Q \tag{3.3}$$

It can be shown that:

$$\sum_\alpha \langle\psi_\alpha|(E - K - v)(P + Q)|\psi_{\alpha'}\rangle F_{\alpha'} = 0$$

$$\Rightarrow \begin{cases} \sum_{\alpha'}\langle\psi_\alpha|P(E - K - v)(P + Q)|\psi_{\alpha'}\rangle F_{\alpha'} = 0 \\ \sum_{\alpha'}\langle\psi_\alpha|P(E - K - v)(P + Q)|\psi_{\alpha'}\rangle F_{\alpha'} = 0 \end{cases}$$

$$\Rightarrow \begin{cases} \sum_{\alpha'}\langle\psi_\alpha|P(E - K - v)P|\psi_{\alpha'}\rangle F_{\alpha'} + \langle\psi_\alpha|P(E - K - v)Q|\psi_{\alpha'}\rangle F_{\alpha'} = 0 \\ \sum_{\alpha'}\langle\psi_\alpha|Q(E - K - v)P|\psi_{\alpha'}\rangle F_{\alpha'} + \langle\psi_\alpha|Q(E - K - v)Q|\psi_{\alpha'}\rangle F_{\alpha'} = 0 \end{cases}$$

$$\Rightarrow \begin{cases} \sum_{\alpha'}\langle\psi_\alpha|P(E - K - v)P|\psi_{\alpha'}\rangle F_{\alpha'} + \langle\psi_\alpha|P(E - K)Q|\psi_{\alpha'}\rangle F_{\alpha'} = \langle\psi_\alpha|PvQ|\psi_{\alpha'}\rangle F_{\alpha'} \\ \sum_{\alpha'}\langle\psi_\alpha|Q(E - K)P|\psi_{\alpha'}\rangle F_{\alpha'} + \langle\psi_\alpha|Q(E - K - v)Q|\psi_{\alpha'}\rangle F_{\alpha'} = \langle\psi_\alpha|QvP|\psi_{\alpha'}\rangle F_{\alpha'} \end{cases}$$

$$\tag{3.4}$$

Since P and Q spaces are orthogonal, the following relationship can be established:

$$\langle\psi_\alpha|P(E - K)Q|\psi_{\alpha'}\rangle = 0 \tag{3.5a}$$

$$\langle\psi_\alpha|Q(E - K)P|\psi_{\alpha'}\rangle = 0 \tag{3.5b}$$

So, it can be shown that:

$$\Rightarrow \quad \begin{cases} \sum_{\alpha'} \langle \psi_\alpha | P(E - K - v)P | \psi_{\alpha'} \rangle F_{\alpha'} = \langle \psi_\alpha | PvQ | \psi_{\alpha'} \rangle F_{\alpha'} & \text{(3.6a)} \\ \sum_{\alpha'} \langle \psi_\alpha | Q(E - K - v)Q | \psi_{\alpha'} \rangle F_{\alpha'} = \langle \psi_\alpha | QvP | \psi_{\alpha'} \rangle F_{\alpha'} & \text{(3.6b)} \end{cases}$$

$$\Rightarrow \quad \begin{cases} P(E - K - v)P = PvQ & \text{(3.7a)} \\ Q(E - K - v)Q = QvP & \text{(3.7b)} \end{cases}$$

Multiplying both sides of equation (3.7b) with $Q \frac{1}{Q(E-K-v)Q}$ the following equation can

be shown:

$$Q\psi_{\alpha'} = Q \frac{1}{Q(E-K-v)Q} QvP\psi_{\alpha'} \tag{3.8}$$

Substituting equation (3.8) into equation (3.7a):

$$P(E - K - v)P\psi_{\alpha'} = PvQ \frac{1}{Q(E-K-v)Q} QvP\psi_{\alpha'} \tag{3.9}$$

Since v_2 does not connect the P and Q, equation (3.9) can be written as:

$$P(E - K - v_1 - v_2 - v_3)P\psi_{\alpha'} = P(v_1 + v_3)Q \frac{1}{Q(E-K-v)Q} Q(v_1 + v_3)vP\psi_{\alpha'} \tag{3.10a}$$

$$P(E - K - v_2)P\psi_{\alpha'} = P(v_1 + v_3)P\psi_{\alpha'} + P(v_1 + v_3)Q \frac{1}{Q(E - K - v)Q} Q(v_1 + v_3)vP\psi_{\alpha'}$$

$$\tag{3.10b}$$

The optical potential, $V^{(Q)}$ can then be defined as :

$$V^{(Q)} = (v_1 + v_3) + (v_1 + v_3)Q \frac{1}{Q(E-k-v)Q} Q(v_1 + v_3) \tag{3.11}$$

Equation (3.11) can be also written as:

$$V^{(Q)} = V + W^{(Q)} \tag{3.12}$$

where the first and second terms of equation (3.12) are known as the static-exchange

potential and the complex polarization term, respectively.

Following Faddeev (1965), the Green's function in the spherical representation is defined as:

$$\frac{1}{Q(E^{(+)}-K-V)Q} = Q \sum_l \left|\Psi_l^{(-)}\right\rangle \frac{1}{E^{(+)}-E_l} \left\langle\Psi_l^{(-)}(q)\right|Q \tag{3.13}$$

The spectral index l is a discrete notation for the continuum. It defines the asymptotic partition of the 3-body system into the bound or ionized states as well as specifying the momentum and quantum number within each partition. The Green's function is diagonal in Q space, provided that v_3 is diagonal in the Q space.

Defining $Q = \sum_{m \in Q} |\phi_m\rangle\langle\phi_m|$ and substituting equation (3.13) into equation (3.11):

$$V^{(Q)} = (v_1 + v_3) + \sum_l \sum_{m \in Q} (v_1 + v_3) |\phi_m\rangle\langle\phi_m|\Psi_l^{(-)}(q)\rangle \frac{1}{E^{(+)} - E_l}$$

$$\times \langle\Psi_l^{(-)}(q)|\phi_m\rangle\langle\phi_m|(v_1 + v_3) \tag{3.14}$$

The momentum-space representation of the optical potential connecting channels α and α' in P space is written as:

$$V_{\alpha\alpha'}^{(Q)}(k, k') = \left\langle k\phi_\alpha\left|V^{(Q)}\right|\phi_{\alpha'} k'\right\rangle \tag{3.15}$$

Following Ratnavelu and Rajagopal (1999), the polarization term in momentum-space representation is:

$$W_{\alpha\alpha'}(k, k') = \int dq \sum_l \sum_{m,m' \in Q} \langle k\phi_\alpha|(v_1 + v_3)|\phi_m\rangle\langle\phi_m|\Psi_l^{(-)}(q)\rangle \frac{1}{E^{(+)} - E_l}$$

$$\times \langle\Psi_l^{(-)}(q)|\phi_{m'}\rangle\langle\phi_{m'}|v_1 + v_3|\alpha'k'\rangle \tag{3.16}$$

Following the weak-coupling approximation from McCarthy and Stelbovics (1980), the partial overlap term, $\langle\phi_m|\Psi_l^{(-)}(q)\rangle$ is a distorted wave in the space of electron 1:

$$\langle \phi_m | \Psi_l^{(-)} \rangle \equiv | \mathcal{X}_n^{(-)}(q) \rangle \qquad\qquad n \equiv ml \qquad\qquad (3.17)$$

So, after substituting equation (3.17) into equation (3.14):

$$V^{(Q)} = (v_1 + v_3) + \sum_{n \in Q}(v_1 + v_3)\left|\phi_m \mathcal{X}_n^{(-)}(q)\right\rangle \frac{1}{E^{(+)} - E_n} \langle \phi_m \mathcal{X}_n^{(-)}(q)|(v_1 + v_3) \text{ (3.18)}$$

Following Ratnavelu and Rajagopal (1999), the polarization term in momentum-space representation can be rewritten as:

$$W_{\alpha\alpha'}(k, k') = \int dq \sum_{n \in Q}\left\langle k\alpha\left|(v_1 + v_3)\right|\phi_m \mathcal{X}_n^{(-)}(q)\right\rangle \frac{1}{E - \varepsilon - \frac{1}{2}q^2}$$

$$\times \left\langle \mathcal{X}_n^{(-)}(q)\phi_m\left|(v_1 + v_3)\right|\alpha'k'\right\rangle \qquad\qquad (3.19)$$

Equation (3.19) can be separated into Hermitian and anti-Hermitian parts:

$$W_{\alpha\alpha'}(k, k') = U_R + iU_I \qquad\qquad (3.20)$$

where U_R and U_I is the real and imaginary parts of the Green's function respectively. U represents the real polarization term involving the off-energy-shell excitation into Q space while W is the absorptive term involving the on-shell excitation.

Following Ratnavelu and Rajagopal (1999), the summation $\sum_{n \in Q}$ in equation (3.19) is replaced by $\int dq'$, defining q' as the momentum of the ionized electron. The orthogonalized Born-Oppenheimer (OBO) is used to calculate the ionization cross sections. Considering 2 particles moving at different speed: the slower particle is described by the full Coulomb wave while the faster particle is described by a plane wave orthogonalized to the ground state of the atom. This is represented by:

$$|\phi_m\rangle = |\psi^{(-)}(q')\rangle \qquad\qquad |\mathcal{X}_n^{(-)}\rangle = |q\rangle \qquad\qquad q \geq q' \qquad (3.21a)$$

$$|\phi_m\rangle = |q'\rangle \qquad\qquad |\mathcal{X}_n^{(-)}(q)\rangle = |\psi^{(-)}q\rangle \qquad\qquad q < q' \qquad (3.21b)$$

Substituting equations (3.21) into equation (3.19) yields:

$$W_c = \int dq \int dq' \langle k'\phi_{\alpha'}|v_3|\psi^{(-)}(q_<)q_>\rangle \frac{1}{E^{(+)} - \frac{1}{2}(q^2 + q'^2)}$$

$$\times \langle q_>\psi^{(-)}(q_<)|v_3|\phi_\alpha k\rangle \tag{3.22}$$

Separating equation (3.22) into Hermitian and anti-Hermitian parts:

$$W_c = Z_R + iZ_I \tag{3.23}$$

where Z_R and Z_I are the real and imaginary parts of the polarization potential, respectively. $Z_I(0)$ is obtained when $|k_i| = |k_f|$.

So, the total ionization cross section is defined as:

$$\sigma_{ion} = \left(\frac{2}{k}\right)(2\pi)^3 Z_I(0) \tag{3.24}$$

After obtaining the optical potential, the T-matrix of the positron-Rb scattering can be rewritten as:

$$\langle k'\Psi_{\alpha'}|T|k\Psi_\alpha\rangle = \langle k'\Psi_{\alpha'}|V^{(Q)}|k\Psi_\alpha\rangle$$

$$+ \sum_{\alpha''} \int d^3k'' \left(\frac{\langle k'\Psi_{\alpha'}|V^{(Q)}|k''\Psi_{\alpha''}\rangle}{E^{(+)} - \frac{1}{2}k''^2 - \epsilon_{\alpha''} - \epsilon_{core}}\right)\langle k''\Psi_{\alpha''}|T|k\Psi_\alpha\rangle$$

$$+ \sum_{\beta''\gamma''} \int d^3k'' \left(\frac{\langle k'\Psi_{\alpha'}|V|k''\Phi_{\beta''}\Omega_{\gamma''}\rangle}{E^{(+)} - \frac{1}{4}k''^2 - \epsilon_{\beta''} - \epsilon_{core}}\right)\langle k''\Phi_{\beta''}\Omega_{\gamma''}|T|k\Psi_\alpha\rangle$$

$$\tag{3.25a}$$

$$\langle k'\Phi_{\beta'}\Omega_{\gamma'}|T|k\Psi_\alpha\rangle = \langle k'\Phi_{\beta'}\Omega_{\gamma'}|V|k\Psi_\alpha\rangle$$

$$+ \sum_{\alpha''} \int d^3k'' \left(\frac{\langle k'\Phi_{\beta'}\Omega_{\gamma'}|V|k''\Psi_{\alpha''}\rangle}{E^{(+)} - \frac{1}{2}k''^2 - \epsilon_{\alpha''} - \epsilon_{core}}\right)\langle k''\Psi_{\alpha''}|T|k\Psi_\alpha\rangle$$

$$+ \sum_{\beta'' \, \gamma''} \int d^3 k'' \left(\frac{\langle k' \Phi_{\beta'} \Omega_{\gamma'} |V| k'' \Phi_{\beta''} \Omega_{\gamma''} \rangle}{E^{(+)} - \frac{1}{4} k''^2 - \epsilon_{\beta''} - \epsilon_{core}} \right) \langle k'' \Phi_{\beta''} \Omega_{\gamma''} |T| k \Psi_\alpha \rangle$$

$$(3.25b)$$

Due to the reason that in this thesis we also report the CCOM calculations for electron-Rb scattering, the LS equation for the electron-Rb scattering is written as:

$$\langle k' \psi_{\alpha'} |T| k \psi_\alpha \rangle = \langle k' \psi_{\alpha'} |V^{(Q)}| k \psi_\alpha \rangle + \sum_{\alpha''} \int d^3 k'' \frac{\langle k' \psi_{\alpha'} |V^{(Q)}| k'' \psi_{\alpha''} \rangle \langle k'' \psi_{\alpha''} |T| k \psi_\alpha \rangle}{\left(E^{(+)} - \varepsilon_{\alpha''} - \frac{1}{2} k''^2 \right)}$$

$$(3.26)$$

3.2   Computational Details of the Optical Potentials

Following McCarthy and Stelbovics (1980), by using the equivalent local potential, equation (3.22) can be written as:

$$W_{LC} = \frac{1}{2} \int_{-1}^{1} du \int dq_1 \int dq_2 \, f^*(k, q_1, q_2) \frac{1}{(E-K)} f(k', q_1, q_2) \qquad (3.27)$$

as equation (3.22) is a non-local continuum polarization potential. $f(k, q_1, q_2)$ is the direct breakup matrix element. By using the Gaussian hypergeometric series, the analytical expression in the integrals of $f(k, q_1, q_2)$ can be obtained. In order to integrate equation (3.27), we need to partition the Green's function into principal value and imaginary parts. Firstly, we define some of the terms in hyperspherical forms:

$$q_1 = \sigma \cos \alpha \qquad\qquad q_2 = \sigma \sin \alpha \qquad\qquad q_1^2 + q_2^2 = \sigma^2$$

$$q_2^2 dq_2^2 q_1^2 dq_1^2 = \sigma^5 (\cos \alpha \sin \alpha)^2 d\alpha d\sigma \qquad (3.28)$$

where $0 \leq \alpha \leq \frac{\pi}{4}$ and $0 \leq \sigma \leq \infty$.

Rewriting equation (3.27) as:

$$W_{LC} = \frac{1}{2} \int_{-1}^{1} du \int d\hat{q}_1 \int d\hat{q}_2 \int_{0}^{\frac{\pi}{4}} d\alpha \left[P \int_{0}^{\infty} d\sigma \frac{JF(k,k^{'},q_1,q_2)}{\left(\mu - \frac{1}{2}\sigma^2\right)} \right.$$

$$\left. -i\pi F_{on}(k,k^{'},\sigma_\mu,\sigma_\mu)J_\alpha \mu^2 \right] \tag{3.29}$$

where:

$$J_\alpha = (\sin \alpha \cos \alpha)^2 \qquad F_{on} = F(k,k^{'},\sigma_W,\sigma_W) \qquad J = \sigma^5 J_\alpha$$

$$W = 2E \qquad \sigma_W = (2E)^{\frac{1}{2}} \tag{3.30}$$

The term, F, is the product of $f(k^{'},q_1,q_2)$ and $f^*(k,q_1,q_2)$. Following McCarthy and Stelbovics (1980), the imaginary part of F is omitted while the real part is retained in order to satisfy the requirements of Hermiticity for the two components of W_c.

The principal value integral can be transformed into a regular integral by using the identity:

$$P \int_{0}^{\infty} \frac{d\sigma}{E - \frac{1}{2}\sigma^2} = 0 \tag{3.31}$$

Subtracting the on-shell values of the integrand, the following integrals can be obtained:

$$ReW_{LC} = \int d\hat{q}_1 \int d\hat{q}_2 \int_{0}^{\infty} d\sigma \int_{0}^{\frac{\pi}{4}} d\alpha J_\alpha \left(\frac{\sigma^4 F - W^2 F_{on}}{W - \sigma^2} \right) \tag{3.32a}$$

$$ImW_{LC} = -\pi \int d\hat{q}_1 \int d\hat{q}_2 \int_{0}^{\infty} d\sigma \int_{0}^{\frac{\pi}{4}} d\alpha J_\alpha W^2 F_{on} \tag{3.32b}$$

These integrals are integrated using the Diophantine method. Expressing some of the terms in equation (3.32) in Diophantine variables $(x_1, x_2, x_3, x_4, x_5, x_6, x_7)$:

$$\phi = 2\pi x_2 \qquad \phi' = 2\pi x_4 \qquad c = 2x_1 - 1 \qquad c^{'} = 2x_3 - 1$$

$$\alpha = \frac{\pi}{4} x_5 \qquad \sigma = \frac{\alpha x_6}{1 - x_6} \qquad u = 2x_7 - 1$$

$$\int_{-1}^{1} dc = 2 \int_{0}^{1} dx_1 \qquad\qquad\qquad \int_{-1}^{1} dc' = 2 \int_{0}^{1} dx_3$$

$$\int_{0}^{2\pi} d\phi = 2\pi \int_{0}^{1} dx_2 \qquad\qquad \int_{0}^{2\pi} d\phi' = 2\pi \int_{0}^{1} dx_4$$

$$\int_{0}^{\frac{\pi}{4}} d\alpha = \frac{\pi}{4} \int_{0}^{1} dx_5 \qquad\qquad \int_{0}^{\infty} d\sigma = \int_{0}^{1} \frac{\alpha}{(1-x_6)^2} dx_6$$

$$\int_{-1}^{1} du = 2 \int_{0}^{1} dx_7$$

$$\int d\hat{q}_1 = \int_{-1}^{1} dc \int_{0}^{2\pi} d\phi \qquad \int d\hat{q}_2 = \int_{-1}^{1} dc' \int_{0}^{2\pi} d\phi' \tag{3.33}$$

Substituting equation (3.30) and equation (3.33) into equation (3.32b):

$$ImW_{LC} = -8\pi^4 \int_{0}^{1} dx_1 \int_{0}^{1} dx_2 \int_{0}^{1} dx_3 \int_{0}^{1} dx_4 \int_{0}^{1} dx_5 \int_{0}^{1} dx_7 \, F_{on} E_p^2$$

$$\left[\cos\left(\frac{\pi}{4}x_5\right) \sin\left(\frac{\pi}{4}x_5\right) \right]^2 \tag{3.34}$$

Equation (3.34) can be computed using the Diophantine multidimensional integration method. (Refer to Appendix V for the summary of Diophantine method)

Table 3.1 shows the convergence of the continuum optical potential for 5s-5s coupling for various momentum transfers at selected energies. Generally, the imaginary part of W_{LC} has better convergence compared to the real part. The real part converged slowly because of the Green's function. In order to obtain good convergence for the optical potential, large number of quadrature points are needed. For our convergence test, we used up to 800000 qudrature points and we are able to obtain decent convergence.

The details of the coupled-channel optical method for electron and positron scattering can be found in the works by McCarthy and Stelbovics (1980, 1983a) and Ratnavelu and Rajagopal (1999).

Table 3.1 : Convergence of the continuum polarization potential for 5s-5s coupling for various momentum transfers and incident energies.

P=0.0 a.u	E = 10eV		E = 50eV		E = 100eV	
Quad.	Real	Imag	Real	Imag	Real	Imag
8000	-2.630	-0.500	1.857	-1.783	0.105	-1.802
20000	-2.488	-0.501	-1.798	-1.262	0.262	-1.275
60000	-2.697	-0.509	-0.957	-1.327	-1.885	-1.144
120000	-2.636	-0.509	-0.488	-1.304	-11.180	-1.194
200000	-2.553	-0.506	-0.934	-1.403	-0.726	-1.196
400000	-2.618	-0.507	-1.159	-1.317	-0.188	-1.217
800000	-2.668	-0.508	-1.158	-1.324	-1.843	-1.199

P=0.5 a.u	E = 10eV		E = 50eV		E = 100eV	
Quad.	Real	Imag	Real	Imag	Real	Imag
8000	-0.907	-0.080	-0.211	-0.390	-0.065	-0.388
20000	-0.697	-0.094	-0.200	-0.402	0.038	-0.395
60000	-0.813	-0.096	-0.401	-0.409	-0.096	-0.362
120000	-0.692	-0.102	-0.308	-0.413	-0.575	-0.420
200000	-0.773	-0.097	-0.323	-0.380	-0.173	-0.355
400000	-0.780	-0.102	-0.337	-0.401	-0.088	-0.374
800000	-0.789	-0.113	-0.280	-0.395	-0.329	-0.370

P=1.0 a.u	E = 10eV		E = 50eV		E = 100eV	
Quad.	Real	Imag	Real	Imag	Real	Imag
8000	-0.153	0.108	-0.060	-0.080	-0.120	-0.084
20000	-0.131	0.067	-0.107	-0.067	-0.099	-0.080
60000	-0.164	0.105	-0.072	-0.060	-0.018	-0.069
120000	-0.175	0.100	-0.073	-0.060	-0.054	-0.077
200000	-0.160	0.102	-0.080	-0.062	-0.034	-0.067
400000	-0.157	0.095	-0.066	-0.061	-0.039	-0.073
800000	-0.158	0.097	-0.070	-0.061	-0.049	-0.074