Couplings in coupled channel calculation(FRESCO)

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Chapter 1

Coupled Channel equations

1.1 Model space wave function

Let us denote the model space wave function of scattering system as

$$|\Psi\rangle = \sum_{\alpha} |\phi_\alpha\rangle \psi_\alpha(R_\alpha) \tag{1.1}$$

where α includes quantum numbers of partitions, $|\alpha\rangle \equiv |xpt; (LI_p)J_p, I_t; J_{tot}M_{tot}\rangle$ where (xpt) represents partition of projectile and target, L is a orbital angular momentum between projectile and target, I_p is a spin of projectile, $\boldsymbol{J}_p = \boldsymbol{L} + \boldsymbol{I}_p$, I_t is a spin of target, $J_{tot}M_{tot}$ is a total angular momentum of system and its projection and R_α is a coordinates between projectile and target.

In other words, more explicit form of $|\phi_\alpha\rangle$ is [1]

$$|\phi_\alpha\rangle \;=\; \left[\left[i^L Y_L(\hat{R}_x) \otimes \phi^{xp}_{I_p}(\xi_p)\right]_{J_p} \otimes \phi^{xt}_{I_t}(\xi_t)\right]_{J_{tot}M_{tot}}, \tag{1.2}$$

where $\phi^{xp}_{I_p}(\xi_p)$ and $\phi^{xt}_{I_t}(\xi_t)$ are bound state wave functions of projectile and target with ξ_p and ξ_t as internal coordinates of projectile and target.

- For a system with specific total angular momentum, wave function becomes

$$\begin{aligned}
\Psi^{M_{tot}}_{x,J_{tot}}(R_x, \xi_p, \xi_t) &= \sum_{\alpha} \left[\left[i^L Y_L(\hat{R}_x) \otimes \phi^{xp}_{I_p}(\xi_p)\right]_{J_p} \otimes \phi^{xt}_{I_t}(\xi_t)\right]_{J_{tot}M_{tot}} \frac{1}{R_x} f^{J_{tot}}_{\alpha}(R_x) \\
&= \sum_{\alpha} |xpt : (LI_p)J_p, I_t; J_{tot}M_{tot}\rangle \frac{f^{J_{tot}}_{\alpha}(R_x)}{R_x} \\
&= \sum_{\alpha} |\alpha; J_{tot}M_{tot}\rangle \frac{f^{J_{tot}}_{\alpha}(R_x)}{R_x}
\end{aligned} \tag{1.3}$$

  where $\alpha = (x, p, t, L, I_p, J_p, I_t)$.

- For a wave function from initial plane wave with momentum $\boldsymbol{k}_i$ and spin projections of μ_{p_i} and μ_{t_i} can be written as

$$\Psi^{\mu_{p_i}\mu_{t_i}}_{x_i p_i t_i}(R_x, \xi_p, \xi_t; \boldsymbol{k}_i) = \sum_{J_{tot}M_{tot}} \sum_{\alpha\alpha_i} |\alpha; J_{tot}M_{tot}\rangle \frac{f^{J_{tot}}_{\alpha\alpha_i}(R_x)}{R_x} A^{J_{tot}M_{tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i, \boldsymbol{k}_i) \tag{1.4}$$

[1] This expression follows the convention in Thompson's textbook.

where, "incoming coefficient" is defined as

$$A^{J_{tot}M_{tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i,\boldsymbol{k}_i) = \frac{4\pi}{k_i}\sum_{M_i m_i} Y^*_{L_iM_i}(\boldsymbol{k}_i)\langle L_iM_i, I_{p_i}\mu_{p_i}|J_{p_i}m_i\rangle\langle J_{p_i}m_i, I_{t_i}\mu_{t_i}|J_{tot}M_{tot}\rangle. \quad (1.5)$$

with asymptotic normalization is

$$f_{\alpha\alpha_i}(R_x) \to \frac{i}{2}[H^{(-)}_\alpha(\eta_\alpha, k_\alpha R_\alpha)\delta_{\alpha\alpha_i} - S_{\alpha\alpha_i}(k_\alpha)H^{(+)}_\alpha(\eta_\alpha, k_\alpha R_\alpha)] \quad (1.6)$$

where $H^{\pm}$ are Coulomb Hankel functions.

1.2 Coupled channel equations

One can group full Hamiltonian as

$$H = H_{xt}(\boldsymbol{\xi}_t) + H_{xp}(\boldsymbol{\xi}_p) + \hat{T}_x(\boldsymbol{R}_x) + \mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p). \quad (1.7)$$

where

$$\begin{aligned} H_{xp}(\boldsymbol{\xi}_p)\phi^{xp}_{I_p}(\boldsymbol{\xi}_p) &= \epsilon_{xp}\phi^{xp}_{I_p}(\boldsymbol{\xi}_p), \\ H_{xt}(\boldsymbol{\xi}_t)\phi^{xt}_{I_t}(\boldsymbol{\xi}_t) &= \epsilon_{xt}\phi^{xt}_{I_t}(\boldsymbol{\xi}_t), \end{aligned} \quad (1.8)$$

relative kinetic term and interaction between target and projectile becomes

$$\begin{aligned} \hat{T}_x(\boldsymbol{R}_x) &= -\frac{\hbar^2}{2\mu_x}\nabla^2_{R_x}, \\ \mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p) &= \sum_{i\in p, j\in t} V_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j). \end{aligned} \quad (1.9)$$

with reduced mass $\mu_x = \frac{m_{xp}m_{xt}}{m_{xp}+m_{xt}}$.
Assume the Model space Wave function Ψ satisfies,

$$0 = [\mathcal{H} - E]|\Psi\rangle = [\mathcal{H} - E]|\phi_i\rangle\psi_i + [\mathcal{H} - E]\sum_{j\neq i}|\phi_j\rangle\psi_j \quad (1.10)$$

If we multiply $\langle\phi_i|$ on the left hand side, for each channel i,

$$\langle\phi_i|E - \mathcal{H}|\phi_i\rangle\psi_i = -\sum_{j\neq i}\langle\phi_i|E - \mathcal{H}|\phi_j\rangle\psi_j. \quad (1.11)$$

The left hand side can be simplified by

$$\begin{aligned} \langle\phi_i|E - \mathcal{H}|\phi_i\rangle\psi_i &= \langle\phi_i|[E - H^{bd}_i - T_i - V_i]|\phi_i\rangle\psi_i = \langle\phi_i|[E_i - T_i - V_i]|\phi_i\rangle\psi_i \\ &= (E_i - T_i(R_i) - \langle\phi_i|V_i|\phi_i\rangle(R_i))\psi_i(R_i) \end{aligned} \quad (1.12)$$

where $V_i = \mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p)$, $\langle\phi_i|V_i|\phi_i\rangle(R_i)$ implies integration over projectile and target bound state internal coordinates ξ_p, ξ_t.

For the right-hand side, we may use two different ways, in post form

$$-\langle\phi_i|E - \mathcal{H}|\phi_j\rangle\psi_j = \langle\phi_i|T_i - E_i + V_i|\phi_j\rangle\psi_j = (T_i - E_i)\langle\phi_i|\phi_j\rangle\psi_j + \langle\phi_i|V_i|\phi_j\rangle\psi_j \quad (1.13)$$

or in prior form

$$-\langle\phi_i|E-\mathcal{H}|\phi_j\rangle\psi_j = \langle\phi_i|T_j-E_j+V_j|\phi_j\rangle\psi_j = \langle\phi_i|\phi_j\rangle(T_j-E_j)\psi_j + \langle\phi_i|V_j|\phi_j\rangle\psi_j \quad (1.14)$$

For the same partition, $x'=x$, we may normalize $\hat{N}_{\alpha'\alpha} = \langle\phi_{\alpha'}|\phi_\alpha\rangle = \delta_{\alpha'\alpha}$. However, in general $\langle\phi_i|\phi_j\rangle$ are non-orthogonal and may not commute with $(T_i - E_i)$.

Thus, we get

$$\begin{aligned}(E_i - T_i(R_i) - \langle\phi_i|V_i|\phi_i\rangle(R_i))\psi_i(R_i) &= \sum_{j\neq i}\left[(T_i-E_i)\langle\phi_i|\phi_j\rangle\psi_j + \langle\phi_i|V_i|\phi_j\rangle\psi_j\right], \\ &= \sum_{j\neq i}\left[\langle\phi_i|\phi_j\rangle(T_j-E_j)\psi_j + \langle\phi_i|V_j|\phi_j\rangle\psi_j\right] \quad (1.15)\end{aligned}$$

If we introduce auxiliary optical potential U_i, we may rearrange in "post form"

$$\begin{aligned}(E_i - T_i - U_i)\psi_i &= \left(\sum_{j\neq i}\langle\phi_i|V_i|\phi_j\rangle\psi_j\right) + ([\langle\phi_i|V_i|\phi_i\rangle - U_i]\psi_i) \\ &\quad + \left(\sum_{j\neq i}(T_j-E_j)\langle\phi_i|\phi_j\rangle\psi_j\right) \quad (1.16)\end{aligned}$$

Or, in "prior form",

$$\begin{aligned}(E_i - T_i - U_i)\psi_i &= \left(\sum_{j\neq i}\langle\phi_i|V_j|\phi_j\rangle\psi_j\right) + ([\langle\phi_i|V_i|\phi_i\rangle(R_i) - U_i]\psi_i) \\ &\quad + \left(\sum_{j\neq i}\langle\phi_i|\phi_j\rangle(T_j-E_j)\psi_j\right), \quad (1.17)\end{aligned}$$

Let us denote

$$V^{prior}(R_i,R_j) = \langle\phi_i|V_j|\phi_j\rangle, \quad V^{post}(R_i,R_j) = \langle\phi_i|V_i|\phi_j\rangle, \quad (1.18)$$

If we define $U_i(R_i) = \langle\phi_i|V_i|\phi_i\rangle$, diagonal term in the right hand side would vanish.

For radial wave function $\psi_\alpha = f_\alpha/R$ in a prior form for rearrangement, while separating inelastic scattering and rearrangements counplings, [2]

$$\begin{aligned}&(E_{xpt} - T_{xL}(R_x) - U_x(R_x))f_\alpha(R_x) \\ &= \langle\phi_\alpha|V_x - U_x|\phi_\alpha\rangle(R_x)f_\alpha(R_x) + \left(\sum_{\alpha'\neq\alpha}V_{\alpha\alpha'}(R_x)f_{\alpha'}(R_x)\right) \\ &+ \left(\sum_{x\neq x',\alpha'}\int dR_{x'}V^{prior}_{\alpha\alpha'}(R_x,R_{x'})f_{\alpha'}(R_{x'})\right) \\ &+ \left(\sum_{\alpha\neq\alpha'}\int dR_{x'}N_{\alpha\alpha'}(T_{x'L'} - E_{x'p't'})f_{\alpha'}(R_{x'})\right) \quad (1.19)\end{aligned}$$

[2]Compared to the coupled channel equation given in FRESCO document, (1) we have additional non-orthogonal terms (2) diagonal term in the right side can be ignored (3) We have not expanded in multipole of couplings yet (4) $i^{L-L'}$ factor are hidden in the definition of $|\phi_\alpha\rangle$.

where

$$\begin{aligned}
T_{xL}(R) &= -\frac{\hbar^2}{2\mu_x}\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2}\right), \\
V_{\alpha\alpha'}(R_x) &= \langle\phi_\alpha|V_x(R_x,\xi)|\phi_{\alpha'}\rangle, \\
V^{prior}_{\alpha\alpha'}(R_x,R_{x'}) &= R_x\langle\phi_\alpha|V^{prior}(R_{x'},\xi)|\phi_{\alpha'}\rangle\frac{1}{R_{x'}}, \\
N_{\alpha\alpha'}(R_x,R_{x'}) &= R_x\langle\phi_\alpha|\phi_{\alpha'}\rangle\frac{1}{R_{x'}}.
\end{aligned} \tag{1.20}$$

The actual form of couplings requires explicit form of potentials in a certain model. For example, inelastic channel coupling which have the same partition,

$$V_{\alpha\alpha'}(R_x) = \int d\xi_p d\xi_t \langle i^L[Y_L(\hat{R}_x)\otimes\phi_p(\xi_p)]\phi_t(\xi_t)|V_x(R_x,\xi_p,\xi_t)|i^{L'}[Y_{L'}(\hat{R}_x)\otimes\phi_{p'}(\xi_{p'})]\phi_{t'}(\xi_{t'})\rangle \tag{1.21}$$

can be described as an collective model or single particle excitation models for the integration over internal coordinates.

Also, one may further multipole expand the couplings in terms of transferred angular momentums, $\Delta L, \Delta S, \Delta J$.

Chapter 2

Couplings, Interactions

2.1 Multipole expansion of interaction

In general, the reaction occurs through the interaction between target and projectile,

$$\mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p) \quad = \sum_{i\in p, j\in t} V_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j). \tag{2.1}$$

In coupled reaction channel calculation, we need to compute (if there is no rearrangement),

$$V_{\alpha,\alpha'}(R_x) = \langle \alpha | \mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p) | \alpha' \rangle \tag{2.2}$$

where integration over internal coordinates and angular integration of $\boldsymbol{R}_x$ is implied. By factoring out factor $i^{L-L'}$, we can write

$$V_{\alpha\alpha'}(R_x) = \int d\Omega_R d\xi_p d\xi_t \left\langle [Y_L(\hat{R}_x) \otimes \phi_p(\xi_p)]_{J_p} \otimes \phi_t(\xi_t) \right| V_x(\boldsymbol{R}_x, \xi_p, \xi_t) \left| [Y_{L'}(\hat{R}_x) \otimes \phi_{p'}(\xi_{p'})] \otimes \phi_{t'}(\xi_{t'}) \right\rangle \tag{2.3}$$

By tensor decompose of the potential, we may write[1]

$$\mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p) = \sqrt{4\pi} \sum_{\lambda\mu} V_\lambda(R) Y_{\lambda\mu}(\hat{R}) T_{\lambda-\mu}(\boldsymbol{\xi}_t, \boldsymbol{\xi}_p) \tag{2.4}$$

Then, the matrix elements for states $\langle \alpha' |$ and $| \alpha \rangle$ can be expressed in terms of the product of form factor and reduced matrix elements , $V_\lambda(R) \langle \alpha || T_\lambda(\boldsymbol{\xi}_t, \boldsymbol{\xi}_p) || \alpha' \rangle$, and other all coefficients related with shuffling states and tensor decomposition of potential.

In FRESCO, the potential operators are decomposed into multipoles and the matrix elements related with orbital angular momentums are computed by FRESCO so that one only have to give inputs for reduced matrix elements and form factors of the coupling $V_\lambda(R) \langle \alpha || T_\lambda(\boldsymbol{\xi}_t, \boldsymbol{\xi}_p) || \alpha' \rangle$. In some special model, even the reduced matrix elements or form factors will be computed automatically.

This is explained in the manual of FRESCO and the textbook of I.J. Thompson. However, there is some convention difference between two.

[1] I suppose one would have $T_{\lambda-\mu}(R, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p)$ in general, instead of $V_\lambda(R) T_{\lambda-\mu}(\boldsymbol{\xi}_t, \boldsymbol{\xi}_p)$.

2.2 Example of double folding model

From now on, I am going to describe how to obtain coupling interaction but exact factors should be checked carefully later. (Thus, this is just for rough idea).

Suppose we have a scalar folding potential $v(\boldsymbol{r}_i - \boldsymbol{r}_j)$, and full interaction between projectile and target becomes[2]

$$\begin{aligned} \mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p) &= \sum_{i\in p, j\in t} v(\boldsymbol{R} + \boldsymbol{r}_i - \boldsymbol{r}_j) \\ &= \int d\boldsymbol{r}_t d\boldsymbol{r}_p v(\boldsymbol{R} + \boldsymbol{r}_p - \boldsymbol{r}_t) \sum_{i\in p, j\in t} \delta^{(3)}(\boldsymbol{r}_p - \boldsymbol{r}_i)\delta^{(3)}(\boldsymbol{r}_t - \boldsymbol{r}_j). \end{aligned} \tag{2.5}$$

We can decompose the channel state as

$$\Big|[Y_{L'}(\hat{R}_x) \otimes \phi_{p'}(\xi_{p'})] \otimes \phi_{t'}(\xi_{t'})\Big\rangle = \sum_M C_{\alpha,M} Y_{L'}(\hat{R})\phi_{I_p}(\xi_p)\phi_{I_t}(\xi_t) \tag{2.6}$$

where $C_{\alpha,M}$ is a collection of Wigner coefficients with projections $M = \{L_z, I_{pz}, I_{tz}, J_z\}$. Then,

$$\begin{aligned} V_{\alpha,\alpha'}(R) &= \langle\alpha|\mathcal{V}_{xtp}(\boldsymbol{R}_x, \boldsymbol{\xi}_t, \boldsymbol{\xi}_p)|\alpha'\rangle \\ &= \sum_{M,M'} C_{\alpha,M}C_{\alpha',M'} \int d\boldsymbol{r}_t d\boldsymbol{r}_p \langle Y_{L'}(\hat{R})|v(\boldsymbol{R} + \boldsymbol{r}_p - \boldsymbol{r}_t)|Y_L(\hat{R})\rangle \\ &\qquad \times\langle\phi_{I_p}|\sum_i \delta^{(3)}(\boldsymbol{r}_p - \boldsymbol{r}_i)|\phi_{I_p'}\rangle\langle\phi_{I_t}|\sum_j \delta^{(3)}(\boldsymbol{r}_t - \boldsymbol{r}_j)|\phi_{I_t'}\rangle \end{aligned} \tag{2.7}$$

Suppose we can obtain the density (or transition density) from

$$\rho_{II'}(\boldsymbol{r}) = \langle\phi_I|\sum_i \delta^{(3)}(\boldsymbol{r} - \boldsymbol{r}_i)|\phi_{I'}\rangle. \tag{2.8}$$

It will corresponds to density for elastic process if $I = I'$, or to transition density for inelastic process if $I \neq I'$.

We may use Fourier transformation for $v(\boldsymbol{r})$,

$$v(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3k e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\tilde{v}(\boldsymbol{k}), \tag{2.9}$$

then,

$$\begin{aligned} V_{\alpha,\alpha'}(R) &= \sum_{M,M'} C_{\alpha,M}C_{\alpha',M'} \int d\boldsymbol{r}_t d\boldsymbol{r}_p \langle Y_{L'}(\hat{R})|v(\boldsymbol{R} + \boldsymbol{r}_p - \boldsymbol{r}_t)|Y_L(\hat{R})\rangle\rho_{I_pI_p'}(\boldsymbol{r}_p)\rho_{I_tI_t'}(\boldsymbol{r}_t) \\ &= \sum_{M,M'} C_{\alpha,M}C_{\alpha',M'} \int d\boldsymbol{r}_t d\boldsymbol{r}_p \frac{1}{(2\pi)^3}\int d^3k\langle Y_{L'}(\hat{R})|\tilde{v}(\boldsymbol{k})e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{r}_p-\boldsymbol{r}_t)}|Y_L(\hat{R})\rangle\rho_{I_pI_p'}(\boldsymbol{r}_p)\rho_{I_tI_t'}(\boldsymbol{r}_t) \\ &= \sum_{M,M'} C_{\alpha,M}C_{\alpha',M'} \frac{1}{(2\pi)^3}\int d^3k\langle Y_{L'}(\hat{R})|e^{i\boldsymbol{k}\cdot\boldsymbol{R}}|Y_L(\hat{R})\rangle \times \tilde{v}(\boldsymbol{k})\tilde{\rho}_{I_pI_p'}(-\boldsymbol{k})\tilde{\rho}_{I_tI_t'}(\boldsymbol{k}) \end{aligned} \tag{2.10}$$

[2] We assumed simple separation of wave function into projectile, target and orbital while ignoring anti-symmetrization of full wave function of the system.

where the Fourier transformation of density are introduced. Then, by the partial wave expansion of plane wave, we get

$$\begin{aligned} V_{\alpha,\alpha'}(R) &= \sum_{\Delta L}\sum_{M,M'}\sum_{L_z} C_{\alpha,M}C_{\alpha',M'}\frac{\sqrt{4\pi}}{(2\pi)^3} i^{\Delta L}\int dk k^2 j_{\Delta L}(kR) \times \langle Y_{L'}|Y_{\Delta L}(\hat{R})|Y_L\rangle \\ &\quad \times \int d\Omega_k \left(\tilde{v}(\boldsymbol{k})\tilde{\rho}_{I_p I_p'}(-\boldsymbol{k})\tilde{\rho}_{I_t I_t'}(\boldsymbol{k})Y^*_{\Delta L}(\hat{k})\right) \\ &= \sum_{\Delta L}\sum_{M,M'}\sum_{L_z} C_{\alpha,M}C_{\alpha',M'}V^{\Delta L}_{\alpha,\alpha'}(R)\langle Y_{L'}|Y_{\Delta L}(\hat{R})|Y_L\rangle \end{aligned} \tag{2.11}$$

In the last line, we defined a coupling Form factor $V^{\Delta L}_{\alpha,\alpha'}(R)$ which includes all integration over internal degrees of freedom.

By comparing this equation with the expression for the general spin transfer coupling in FRESCO manual will gives us the exact expression for the input to the FRESCO.

More careful analysis of the equation would be necessary.

2.2.1 Spin/Isospin dependent folding potential

If the folding potential have additional dependence on spin or isospin,

$$v_{12} = v_0(r_{12}) + v_1(r_{12})\tau_1\cdot\tau_2 + v_2(r_{12})\sigma_1\cdot\sigma_2 + \cdots \tag{2.12}$$

If the isospin does not change during the process we can simply replace, $\tau_1\cdot\tau_2 \to \tau_1^z\tau_2^z$ and

$$\langle\phi_I|\sum_i \delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}_i)\tau_i^z|\phi_{I'}\rangle = \rho^p_{II'}(\boldsymbol{r}) - \rho^n_{II'}(\boldsymbol{r}). \tag{2.13}$$

In a very special case, $\rho_n = \frac{N}{Z}\rho_p = \frac{N}{A}\rho$, this corresponds to

$$\langle\phi_I|\sum_i \delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}_i)\tau_i^z|\phi_{I'}\rangle = \frac{Z-N}{A}\rho(\boldsymbol{r}) \tag{2.14}$$

For spin, we would get vector spin density

$$\langle\phi_I|\sum_i \delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}_i)\boldsymbol{\sigma}_i|\phi_{I'}\rangle = \vec{\rho}_{II'}(\boldsymbol{r}) \tag{2.15}$$