5 Angular momentum basis calculation

5.1 Definition of the channel basis and T matrix form

Define the angular momentum basis $|rlm\rangle$, which satisfies the transformation:

$$\langle rlm|\boldsymbol{r'}\rangle = \frac{\delta(r-r')}{rr'}Y_l^{m*}(\hat{r'}) \tag{77}$$

In order to describe the in and out channel, we introduce their angular momentum basis:

$$|r_{bx}r_a\alpha_{\text{in}}M\rangle = |r_{bx}r_a(l_{bx}l_a)JM\rangle \tag{78}$$

$$|r_x r_b\alpha_{\text{out}}M\rangle = |r_x r_b(l_x l_b)JM\rangle \tag{79}$$

α is short for a set of angular quantum numbers and their coupled quantum number, which is an important programming technique to include some quantum numbers into a single one. They all form a complete basis for the Hilbert space of the whole system. Their complete relations are:

$$\sum_{\alpha_{\text{in}}}\sum_{M}\int \mathrm{d}r_{bx}\mathrm{d}r_a r_{bx}^2 r_a^2|r_{bx}r_a\alpha_{in}M\rangle\langle r_{bx}r_a\alpha_{in}M| = 1 \tag{80}$$

$$\sum_{\alpha_{\text{out}}}\sum_{M}\int \mathrm{d}r_{x}\mathrm{d}r_b r_{x}^2 r_b^2|r_{x}r_b\alpha_{\text{out}}M\rangle\langle r_{x}r_b\alpha_{\text{out}}M| = 1 \tag{81}$$

insert the complete basis of the uncoupled representation, and we can obtain the transformation relation:

$$\begin{aligned}|r_{bx}r_a\alpha_{\text{in}}M\rangle &= \left(\sum_{m_{bx}m_a}|l_{bx}l_a m_{bx}m_a\rangle\langle l_{bx}l_a m_{bx}m_a|\right)|r_{bx}r_a\alpha_{in}M\rangle \\ &= \sum_{m_{bx}m_a}\langle l_{bx}l_a m_{bx}m_a|JM\rangle|r_{bx}l_{bx}m_{bx}\rangle|r_a l_a m_a\rangle\end{aligned} \tag{82}$$

$$\begin{aligned}|r_x r_b\alpha_{\text{out}}M\rangle &= \left(\sum_{m_{bx}m_a}|l_x l_b m_x m_b\rangle\langle l_x l_b m_x m_b|\right)|r_x r_b\alpha_{\text{out}}M\rangle \\ &= \sum_{m_x m_b}\langle l_x l_b m_x m_b|JM\rangle|r_x l_x m_x\rangle|r_b l_b m_b\rangle\end{aligned} \tag{83}$$

we can see that CG coefficients appear in the transformations.

With these basis the integral form of T matrix reads:

$$\begin{aligned}T_{\beta\alpha}^{M_a M_B} =&\langle\phi_B^{M_B}\chi_b^{(-)}|V_{\text{post/prior}}|\chi_a^{(+)}\phi_a^{M_a}\rangle \\ =&\sum_{\alpha_{\text{in}}\alpha_{\text{out}}}\sum_{MM'}\int r_{bx}^2 r_a^2 r_x^2 r_b^2\mathrm{d}r_{bx}\mathrm{d}r_a\mathrm{d}r_x\mathrm{d}r_b\langle\phi_B^{M_B}\chi_b^{(-)}|r_x r_b\alpha_{\text{out}}M\rangle \\ &\times\langle r_x r_b\alpha_{\text{out}}M|V_{\text{post/prior}}|r_{bx}r_a\alpha_{\text{in}}M'\rangle\langle r_{bx}r_a\alpha_{\text{in}}M'|\chi_a^{(+)}\phi_a^{M_a}\rangle\end{aligned} \tag{84}$$

5.2 Potential term

Our task in this section is to determine the potential term. Because we deal with a central potential, it doesn't depend on the orientation of the angular momentum. As a result, the inner product of M and M' turns into a Kronecker δ:

$$\langle r_x r_b\alpha_{\text{out}}M|V_{\text{post/prior}}|r_{bx}r_a\alpha_{\text{in}}M'\rangle = \langle r_x r_b\alpha_{\text{out}}|V_{\text{post/prior}}|r_{bx}r_a\alpha_{\text{in}}\rangle\delta_{MM'} \tag{85}$$

but the transformation between coupled and uncoupled basis requires the z-component. One way to deal with it is to calculate result of different Ms and then take the average:

$$\begin{aligned}&\langle r_x r_b \alpha_{\text{out}} M | V_{\text{post/prior}} | r_{bx} r_a \alpha_{\text{in}} M\rangle \\ =&\frac{1}{2J+1}\sum_{M''}\int \mathrm{d}^3\tilde{r}_x \mathrm{d}^3\tilde{r}_b \mathrm{d}^3\tilde{r}_{bx}\mathrm{d}^3\tilde{r}_a \langle r_x r_b \alpha_{out} M'' | \tilde{\boldsymbol{r}}_{\boldsymbol{x}} \tilde{\boldsymbol{r}}_{\boldsymbol{b}}\rangle \\ &\times \langle \tilde{\boldsymbol{r}}_{\boldsymbol{x}} \tilde{\boldsymbol{r}}_{\boldsymbol{b}} | V | \tilde{\boldsymbol{r}}_{\boldsymbol{bx}} \tilde{\boldsymbol{r}}_{\boldsymbol{a}}\rangle \langle \tilde{\boldsymbol{r}}_{\boldsymbol{bx}} \tilde{\boldsymbol{r}}_{\boldsymbol{a}} | r_{bx} r_a \alpha_{in} M''\rangle\end{aligned} \tag{86}$$

we have already obtained the potential in the coordinate representation:

$$\langle \tilde{\boldsymbol{r}}_{\boldsymbol{x}} \tilde{\boldsymbol{r}}_{\boldsymbol{b}} | V | \tilde{\boldsymbol{r}}_{\boldsymbol{bx}} \tilde{\boldsymbol{r}}_{\boldsymbol{a}}\rangle = V(\tilde{r_x}, \tilde{r}_{bx}, \tilde{x})\delta(\tilde{\boldsymbol{g}} - \tilde{\boldsymbol{r}}_{\boldsymbol{b}})\delta(\tilde{\boldsymbol{f}} - \tilde{\boldsymbol{r}}_{\boldsymbol{a}}) \tag{87}$$

the transformation between 3D basis and angular momentum basis reads:

$$\begin{aligned}\langle r_x r_b \alpha_{out} M'' | \tilde{\boldsymbol{r}}_{\boldsymbol{x}} \tilde{\boldsymbol{r}}_{\boldsymbol{b}}\rangle &= \sum_{m_x' m_b'} \langle r_x r_b \alpha_{out} M'' | l_x l_b m_x' m_b'\rangle \langle l_x l_b m_x' m_b' | \tilde{\boldsymbol{r}}_{\boldsymbol{x}} \tilde{\boldsymbol{r}}_{\boldsymbol{b}}\rangle \\ &= \sum_{m_x' m_b'} \langle JM'' | l_x l_b m_x' m_b'\rangle \langle r_x r_b l_x l_b m_x' m_b' | \tilde{\boldsymbol{r}}_{\boldsymbol{x}} \tilde{\boldsymbol{r}}_{\boldsymbol{b}}\rangle \\ &= \sum_{m_x' m_b'} \langle l_x l_b m_x' m_b' | JM''\rangle Y_{l_x}^{m_x' *}(\hat{\tilde{r}}_x) Y_{l_b}^{m_b' *}(\hat{\tilde{r}}_b) \frac{\delta(\tilde{r}_x - r_x)}{\tilde{r}_x r_x}\frac{\delta(\tilde{r}_b - r_b)}{\tilde{r}_b r_b}\end{aligned} \tag{88}$$

$$\begin{aligned}\langle \tilde{\boldsymbol{r}}_{\boldsymbol{bx}} \tilde{\boldsymbol{r}}_{\boldsymbol{a}} | r_{bx} r_a \alpha_{in} M''\rangle &= \sum_{m_{bx}' m_a} \langle \tilde{\boldsymbol{r}}_{\boldsymbol{bx}} \tilde{\boldsymbol{r}}_{\boldsymbol{a}} | l_{bx} l_a m_{bx}' m_a'\rangle \langle l_{bx} l_a m_{bx}' m_a' | r_{bx} r_a \alpha_{in} M''\rangle \\ &= \sum_{m_{bx}' m_a'} \langle l_{bx} l_a m_{bx}' m_a' | JM''\rangle Y_{l_{bx}}^{m_{bx}' *}(\hat{\tilde{r}}_{bx}) Y_{l_a}^{m_a' *}(\hat{\tilde{r}}_a) \frac{\delta(\tilde{r}_a - r_a)}{\tilde{r}_a r_a}\frac{\delta(\tilde{r}_{bx} - r_{bx})}{\tilde{r}_{bx} r_{bx}}\end{aligned} \tag{89}$$

carry out the integral and simplify it, we get the final form of the potential term:

$$\begin{aligned}&\frac{1}{2J+1}\sum_{M''}\int \mathrm{d}\Omega_{\tilde{x}} \mathrm{d}\Omega_{\tilde{bx}} \frac{\delta(f' - r_a)}{f' r_a}\frac{\delta(g' - r_b)}{g' r_b} V(r_x, r_{bx}, \tilde{x}) \\ &\times \sum_{m_x' m_b'} \langle l_x l_b m_x' m_b' | JM''\rangle Y_{l_x}^{m_x' *}(\hat{\tilde{r}}_x) Y_{l_b}^{m_b'}(\hat{\tilde{r}}_b) \\ &\times \sum_{m_{bx}' m_a'} \langle l_{bx} l_a m_{bx}' m_a' | JM''\rangle Y_{l_{bx}}^{m_{bx}'}(\hat{\tilde{r}}_{bx}) Y_{l_a}^{m_a'}(\hat{\tilde{r}}_a)\end{aligned} \tag{90}$$

5.3 Wave function term

Now we calculate the bound state wave function and the distorted wave funtion:

$$\begin{aligned}\langle\phi_B^{M_B}\chi_b^{(-)}|r_x r_b\alpha_{out}M\rangle &= \sum_{m_x m_b}\langle\phi_B^{M_B}\chi_b^{(-)}|l_x l_b m_x m_b\rangle\langle l_x l_b m_x m_b|r_x r_b\alpha_{out}M\rangle \\ &= \sum_{m_x m_b}\langle l_x l_b m_x m_b|JM\rangle\langle\phi_B^{M_B}|r_x l_x m_x\rangle\langle\chi_b^{(-)}|r_b l_b m_b\rangle \\ &= \sum_{m_x m_b}\langle l_x l_b m_x m_b|JM\rangle\frac{u_{l_x}(r_x)}{r_x}\delta_{M_B,m_x} \\ &\quad\times\frac{4\pi}{k_b r_b}i^{-l_b}u_{l_b}(r_b)e^{i\sigma_{l_b}}Y_{l_b}^{m_b}(\hat{k}_b) \\ &=\sum_{m_b}\langle l_x l_b M_B m_b|JM\rangle\frac{u_{l_x}(r_x)}{r_x}\times\frac{4\pi}{k_b r_b}i^{-l_b}u_{l_b}(r_b)e^{i\sigma_{l_b}}Y_{l_b}^{m_b}(\hat{k}_b) \\ &=\frac{4\pi}{k_b r_b}i^{-l_b}e^{i\sigma_{l_b}}\frac{u_{l_x}(r_x)u_{l_b}(r_b)}{r_x}\sum_{m_b}\langle l_x l_b M_B m_b|JM\rangle Y_{l_b}^{m_b}(\hat{k}_b)\end{aligned} \tag{91}$$

where we have utilized the expression:

$$\langle\chi_b^{(-)}|r_b l_b m_b\rangle = \frac{4\pi}{k_b r_b}i^{-l_b}u_{l_b}(r_b)e^{i\sigma_{l_b}}Y_{l_b}^{m_b}(\hat{k}_b) \tag{92}$$

similarly, the last term reads:

$$\begin{aligned}\langle r_{bx}r_a\alpha_{in}M'|\chi_a^{(+)}\phi_a^{M_a}\rangle &= \sum_{m_{bx}m_a}\langle l_{bx}l_a m_{bx}m_a|JM'\rangle\langle r_{bx}l_{bx}m_{bx}|\phi_a^{M_a}\rangle\langle r_a l_a m_a|\chi_a^{(+)}\rangle \\ &=\frac{4\pi}{k_a r_a}i^{l_a}e^{i\sigma_{l_a}}\frac{u_{l_{bx}}(r_{bx})u_{l_a}(r_a)}{r_{bx}}\sum_{m_a}\langle l_{bx}l_a M_a m_a|JM'\rangle Y_{l_a}^{m_a *}(\hat{k}_a)\end{aligned} \tag{93}$$

where we have utilized the expression:

$$\langle r_a l_a m_a|\chi_a^{(+)}\rangle = \frac{4\pi}{k_a r_a}i^{l_a}u_{l_a}(r_a)e^{i\sigma_{l_a}}Y_{l_a}^{m_a *}(\hat{k}_a) \tag{94}$$

5.4 Final form

Including all the expansion, we finally obtain:

$$\begin{aligned}T_{\beta\alpha}^{M_a M_B} =&\frac{(4\pi)^2}{k_a k_b}\sum_{\alpha_{\rm in}\alpha_{\rm out}}\sum_{M} i^{l_a-l_b}e^{i(\sigma_{l_a}\sigma_{l_b})} \\ &\times\int r_{bx}r_b \mathrm{d}r_{bx}\mathrm{d}r_a\mathrm{d}r_x\mathrm{d}r_b\end{aligned} \tag{95}$$