

Code CCFULL and emulator

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1 Code CCFULL

1.1 Coupled-channels equation

In heavy-ion fusion reactions, the collision process is inherently dynamic, involving strong interplay between the relative motion and the intrinsic degrees of freedom of the colliding nuclei. The total fusion probability is significantly affected by such couplings, especially at energies near and below the Coulomb barrier. Consequently, it is essential for a quantitative description of fusion to accurately incorporate the channel coupling effects. This necessitates employing a reaction Hamiltonian that explicitly accounts for these internal structures. Such Hamiltonian can be generally written as

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + V^{(0)}(r) + H_{\text{int}}(\xi) + V_{\text{coup}}(r, \xi), \quad (1)$$

where r denotes the coordinate of the relative motion between the target and the projectile nuclei, and μ is the reduced mass of the reaction system. $V^{(0)}(r)$ is the bare potential, which is the sum of the Coulomb and the nuclear potentials. $H_{\text{int}}(\xi)$ describes the intrinsic Hamiltonian that governs the excitation spectrum of the colliding nuclei, where ξ represents the internal degrees of freedom. Finally, $V_{\text{coup}}(r, \xi)$ represents the coupling potential between these intrinsic excitations and the relative motion. In conventional coupled-channels calculations, the coupling potential V_{coup} is typically constructed based on the geometrical collective model.

For each total angular momentum J , the total wave function $\Psi(r, \xi)$ is expanded as

$$\Psi(r, \xi) = \sum_n \frac{\phi_n(r)}{r} |n(\xi)\rangle, \quad (2)$$

where $|n(\xi)\rangle$ is the eigen-functions of the intrinsic Hamiltonian $H_{\text{int}}(\xi)$, satisfying $H_{\text{int}}(\xi)|n(\xi)\rangle = \epsilon_n|n(\xi)\rangle$. Here ϵ_n is the eigen-energy of the state $|n(\xi)\rangle$. Latter, I denote the $|n(\xi)\rangle$ as $|n\rangle$. For simplicity, we have used the iso-centrifugal approximation and ignored the spin of the intrinsic state $|n\rangle$. Some reference have proofed these approximations are good approximation, i recommend you can read these articles [Tan87]. The coupled-channels equations for $\phi_n(r)$ are obtained as

$$\begin{aligned} \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{J(J+1)\hbar^2}{2\mu r^2} + V^{(0)}(r) - E + \epsilon_n \right] \phi_n(r) &= - \sum_m \langle n | V_{\text{coup}}(r) | m \rangle \phi_m(r) \\ &\equiv - \sum_m V_{nm}(r) \phi_m(r), \end{aligned} \quad (3)$$

where E is the incident energy in the center of mass frame. The coupled-channels equations are solved by imposing the incoming wave boundary condition (IWBC), that is, there are only incoming waves at $r \leq r_{\text{min}}$, for which r_{min} is taken to be the minimum position of the Coulomb pocket inside the barrier. In addition, one imposes the boundary condition that there are only the outgoing waves at infinity for all the channels except for the entrance channel ($n = 1$), which has the incoming wave as well. These boundary conditions read,

$$\begin{aligned} \phi_n(r) &\rightarrow H_J^{(-)}(k_n r) \delta_{n,1} + R_n^{(J)} H_J^{(+)}(k_n r), \quad (r \rightarrow \infty), \\ &\rightarrow T_n^{(J)} \exp(-ik_n(r)r), \quad (r = r_{\text{min}}), \end{aligned} \quad (4)$$

where $k_n(r)$ is the local wave number for the n -th channel with $k_n = k_n(r = \infty)$. The local wave number $k_n(r)$ is defined as:

$$k_n(r) = \sqrt{\frac{2\mu}{\hbar^2} \left(E - \epsilon_n - \frac{J(J+1)\hbar^2}{2\mu r^2} - V_{\text{eff}}^{(n)}(r) \right)} \quad (5)$$

Here, $V_{\text{eff}}^{(n)}(r)$ represents the sum of the nuclear, Coulomb, and diagonal coupling potentials for channel n . And T_n and R_n are the transmission and the reflection coefficients for the channel n , respectively. $H_J^{(-)}$ and $H_J^{(+)}$ in Eq. (4) are the incoming and the outgoing Coulomb wave functions, respectively. The fusion cross sections $\sigma_{\text{fus}}(E)$ are then calculated as

$$\sigma_{\text{fus}}(E) = \frac{\pi}{k^2} \sum_{J=0}^{\infty} (2J+1) P_J(E) = \frac{\pi \hbar^2}{2\mu E} \sum_{J=0}^{\infty} (2J+1) P_J(E). \quad (6)$$

1.2 Coupled potential matrix

I will give explicit expressions for the coupling matrix elements V_{nm} , which includes the Coulomb component and nuclear component:

$$V_{mn}(r) = V_{mn}^C(r) + V_{mn}^N(r) \quad (7)$$

If the atomic target nucleus is deformable, we can use spherical harmonics for expansion:

$$R_T(\Omega) = R_T \left[1 + \sum_{\lambda=2}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \beta_{\lambda\mu} Y_{\lambda\mu}(\Omega) \right], \quad (8)$$

where R_T is the average radius that satisfies the volume conservation constraint. $\beta_{\lambda\mu}$ are the deformation parameters of the deformed target nucleus. Generally, we have two main collective motion modes. One is the rotational mode, the other one is the vibration mode.

1.2.1 Rotational coupling of nuclear potential

Let us first consider a rotational coupling in the target nucleus. If the target nucleus just has quadrupole, octupole, and hexadecapole deformation, we can write down the expression

$$R_0 \rightarrow R_0 + \hat{O} = R_0 + \beta_{20} R_T Y_{20} + \beta_{40} R_T Y_{40} \quad (9)$$

Where R_T is parameter as $r_{\text{couple}} A_{\text{target}}^{1/3}$, and β_{20} and β_{40} are the quadrupole and hexadecapole deformation parameters, respectively. The nuclear coupling Hamiltonian is thus given by the phenomenal Woods–Saxon potential

$$V_N(r, \hat{O}) = - \frac{V_0}{1 + \exp(r - R_0 - \hat{O})/a} \quad (10)$$

Here, $R_0 = r_0 A_{\text{target}}^{1/3}$. V_0 , r_0 , and a are the Woods–Saxon potential parameters. We need matrix elements of this coupling Hamiltonian $\langle n | V_N(r, \hat{O}) | m \rangle$. These can be easily obtained using a matrix algebra. In this algebra, one first looks for the eigenvalues and eigenvectors of the operator $\hat{O}$ which satisfies

$$\hat{O} |\alpha\rangle = \lambda_\alpha |\alpha\rangle \quad (11)$$

For the the intrinsic Hamiltonian $H_{\text{int}}(\xi)$, we use the basis function $Y_{\lambda\mu}$. if we only consider axisymmetry situation ($\mu = 0$), we can write down the matrix element $\langle I'0 | \hat{O} | I0 \rangle^1$:

$$\begin{aligned} \langle I'0 | \hat{O} | I0 \rangle &= \langle I'0 | \beta_2 R_T Y_{20} + \beta_4 R_T Y_{40} | I0 \rangle \\ &= \beta_2 R_T \sqrt{\frac{5(2I+1)(2I'+1)}{4\pi}} \begin{pmatrix} I & 2 & I' \\ 0 & 0 & 0 \end{pmatrix}^2 + \beta_4 R_T \sqrt{\frac{9(2I+1)(2I'+1)}{4\pi}} \begin{pmatrix} I & 4 & I' \\ 0 & 0 & 0 \end{pmatrix}^2 \end{aligned} \quad (12)$$

For the matrix element of the $V_N(r, \hat{O})$

$$\begin{aligned} V_{nm}^{(N)} &= \langle n | V_N(r, \hat{O}) | m \rangle \\ &= \sum_{\alpha} \sum_{\alpha'} \langle n | \alpha \rangle \langle \alpha | V_N(r, \hat{O}) | \alpha' \rangle \langle \alpha' | m \rangle \\ &= \sum_{\alpha} \sum_{\alpha'} \langle n | \alpha \rangle V_N(r, \lambda_\alpha) \delta_{\alpha\alpha'} \langle \alpha' | m \rangle \\ &= \sum_{\alpha} \langle n | \alpha \rangle \langle \alpha | m \rangle V_N(r, \lambda_\alpha) \\ &= \sum_{\alpha} c_{\alpha n} c_{\alpha m} V_N(r, \lambda_\alpha) \end{aligned} \quad (13)$$

The nuclear coupling matrix elements are then evaluated as

$$\begin{aligned} V_{nm}^{(N)} &= \langle I'0 | V_N(r, \hat{O}) | I0 \rangle - V_N^0(r) \delta_{n,m} \\ &= \sum_{\alpha} \langle I'0 | \alpha \rangle \langle \alpha | I0 \rangle V_N(r, \lambda_\alpha) - V_N^0(r) \delta_{n,m} \end{aligned} \quad (14)$$

¹ $\int Y_{j_1 m_1}(\theta, \varphi) Y_{j_2 m_2}(\theta, \varphi) Y_{j_3 m_3}(\theta, \varphi) d\Omega = \sqrt{\frac{(2j_1+1)(2j_2+1)(2j_3+1)}{4\pi}} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix}$

1.2.2 Rotational coupling of Coulomb potential

The Coulomb component of the coupling Hamiltonian is evaluated as follows.

$$V_C(r) = \int dr' \frac{Z_P Z_T e^2}{|r - r'|} \rho_T(r') \quad (15)$$

Here, ($r \gg r'$) we do a multipole expansion to $\frac{1}{|r - r'|}$,

$$\frac{1}{|r - r'|} = \sum_{\lambda} \frac{4\pi}{2\lambda + 1} \sum_{\mu=-\lambda}^{+\lambda} \frac{(r')^{\lambda}}{r^{\lambda+1}} Y_{\lambda\mu}^*(r) Y_{\lambda\mu}(r') \quad (16)$$

Therefore:

$$\begin{aligned} V_C(r) &= \int dr' \frac{Z_P Z_T e^2}{|r - r'|} \rho_T(r') \\ &= \int dr' Z_P Z_T e^2 \rho_T(r') \sum_{\lambda} \frac{4\pi}{2\lambda + 1} \sum_{\mu=-\lambda}^{+\lambda} \frac{(r')^{\lambda}}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) Y_{\lambda\mu}(\hat{r}') \\ &= \sum_{\lambda} \frac{4\pi Z_P Z_T e^2}{2\lambda + 1} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int \rho_T(r') (r')^{\lambda} Y_{\lambda\mu}(\hat{r}') dr' \\ &= \sum_{\lambda} \frac{4\pi Z_P Z_T e^2}{2\lambda + 1} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int_0^{2\pi} \int_0^{\pi} \int_0^{R_T(\theta', \phi')} \rho_T(r') (r')^{\lambda+2} Y_{\lambda\mu}(\theta', \phi') dr' d\theta' d\phi' \\ &= \sum_{\lambda} \frac{4\pi Z_P Z_T e^2}{2\lambda + 1} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int_0^{2\pi} \int_0^{\pi} \int_0^{R_T(\theta', \phi')} \frac{1}{(4\pi R_T^3/3)} (r')^{\lambda+2} Y_{\lambda\mu}(\theta', \phi') dr' d\theta' d\phi' \\ &= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda + 1)R_T^3} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int_0^{2\pi} \int_0^{\pi} \left[\int_0^{R_T(\theta', \phi')} (r')^{\lambda+2} dr' \right] Y_{\lambda\mu}(\theta', \phi') d\theta' d\phi' \\ &= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda + 1)R_T^3} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int_0^{2\pi} \int_0^{\pi} \frac{1}{\lambda + 3} R_T^{\lambda+3}(\theta', \phi') Y_{\lambda\mu}(\theta', \phi') d\theta' d\phi' \end{aligned} \quad (17)$$

If we only consider $R_T(\phi', \theta') = R_T(1 + \beta_2 Y_{20} + \beta_4 Y_{40})$ then we do the Taylor expansion to $R_T(\phi', \theta')^{\lambda+3}$

$$\begin{aligned} V_C(r, \theta) &= \frac{Z_P Z_T e^2}{r} + \frac{Z_P Z_T e^2}{r^3} R_T^2 \beta_2 Y_{20}(\theta) \\ &\quad + \frac{Z_P Z_T e^2}{r^5} R_T^4 [\beta_2^2 Y_{20}^2(\theta) + \beta_4 Y_{40}(\theta)] \\ &\quad + \frac{Z_P Z_T e^2}{r^7} R_T^6 [\beta_2^3 Y_{20}^3(\theta) + \beta_2 \beta_4 Y_{20}(\theta) Y_{40}(\theta)] \\ &\quad + \dots \end{aligned} \quad (18)$$

put the equation into the $V_C(r)$ for the situation only with the β_2 term, we get

$$\begin{aligned} V_C(r) &= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda + 1)R_T^3} \sum_{\mu=-\lambda}^{\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\theta, \phi) \\ &\quad \times \int_0^{\pi} \int_0^{2\pi} R_T^{\lambda+3} \beta_2 Y_{20}(\theta', \phi') Y_{\lambda\mu}(\theta', \phi') \sin \theta' d\phi' d\theta' \end{aligned} \quad (19)$$

for the integral, $\lambda = 2$ and $\mu = 0$ only.

$$V_C(r) = \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \beta_2 Y_{20} \quad (20)$$

for the situation only with the β_2^2 term, and we consider $\mu = 0$ we get

$$\begin{aligned}
V_C(r) &= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda+1)R_T^3} \sum_{\mu=-\lambda}^{\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\theta, \phi) \int_0^{\pi} \int_0^{2\pi} \frac{1}{\lambda+3} R_T^{\lambda+3} \frac{1}{2} (\lambda+3)(\lambda+2) \beta_2^2 Y_{20}^2(\theta', \phi') Y_{\lambda\mu}(\theta', \phi') \sin \theta' d\phi' d\theta' \\
&= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda+1)R_T^3} \cdot \frac{1}{r^{\lambda+1}} Y_{\lambda 0}^*(\theta, \phi) \cdot R_T^{\lambda+3} \cdot \frac{1}{2} (\lambda+2) \beta_2^2 \cdot \sqrt{\frac{25}{4\pi(2\lambda+1)}} \cdot \langle 2020|\lambda 0 \rangle^2
\end{aligned} \tag{21}$$

for the $\langle 2020|\lambda 0 \rangle$, λ only can take 2 or 4

$$\begin{aligned}
V_C(r) &= \frac{3Z_P Z_T e^2}{5R_T^3} \cdot \frac{Y_{20}^*(\hat{r})}{r^3} \cdot R_T^5 \beta_2^2 \sqrt{\frac{5}{\pi}} \langle 2020|20 \rangle^2 \\
&\quad + \frac{3Z_P Z_T e^2}{9R_T^3} \cdot \frac{Y_{40}^*(\hat{r})}{r^5} \cdot R_T^7 \beta_2^2 \sqrt{\frac{25}{4\pi}} \langle 2020|40 \rangle^2 \\
&= \frac{3Z_P Z_T e^2}{5} \cdot \frac{Y_{20}^*(\hat{r})}{r^3} \cdot R_T^2 \beta_2^2 \sqrt{\frac{5}{\pi}} \cdot \frac{2}{7} \\
&\quad + \frac{3Z_P Z_T e^2}{9} \cdot \frac{Y_{40}^*(\hat{r})}{r^5} \cdot R_T^4 \beta_2^2 \sqrt{\frac{1}{\pi}} \cdot \frac{5}{2} \cdot \frac{18}{35} \\
&= \frac{3Z_P Z_T e^2}{5} \cdot \frac{R_T^2}{r^3} \cdot \frac{2}{7} \sqrt{\frac{5}{\pi}} \beta_2^2 Y_{20}^*(\hat{r}) + \frac{3Z_P Z_T e^2}{9} \cdot \frac{R_T^4}{r^5} \cdot \frac{9}{7} \sqrt{\frac{1}{\pi}} \beta_2^2 Y_{40}^*(\hat{r})
\end{aligned} \tag{22}$$

for the situation only with the β_4 term, we get

$$\begin{aligned}
V_C(r) &= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda+1)R_T^3} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int_0^{\pi} \int_0^{2\pi} R_T^{\lambda+3} \beta_4 Y_{40}(\theta', \phi') Y_{\lambda\mu}(\theta', \phi') d\phi' \sin \theta' d\theta' \\
&= \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda+1)} \frac{R_T^{\lambda}}{r^{\lambda+1}} \beta_4 \sum_{\mu=-\lambda}^{+\lambda} Y_{\lambda\mu}^*(\hat{r}) \int Y_{40}(\theta', \phi') Y_{\lambda\mu}(\theta', \phi') d\Omega'
\end{aligned} \tag{23}$$

for the integral, $\lambda = 4$ and $\mu = 0$ only.

$$V_C(r) = \frac{3Z_P Z_T e^2}{9} \frac{R_T^4}{r^5} \beta_4 Y_{40} \tag{24}$$

Therefore, for the matrix element $V_{mn}(r)$

$$\begin{aligned}
\langle I'0|V^C|I0 \rangle &= \left\langle I'0 \left| \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \beta_2 Y_{20} \right| I0 \right\rangle \\
&\quad + \left\langle I'0 \left| \frac{3Z_P Z_T e^2}{9} \frac{R_T^4}{r^5} \beta_4 Y_{40} \right| I0 \right\rangle \\
&\quad + \left\langle I'0 \left| \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \cdot \frac{2}{7} \sqrt{\frac{5}{\pi}} \beta_2^2 Y_{20}^*(r) \right| I0 \right\rangle \\
&\quad + \left\langle I'0 \left| \frac{3Z_P Z_T e^2}{9} \frac{R_T^4}{r^5} \cdot \frac{9}{7} \sqrt{\frac{1}{\pi}} \beta_2^2 Y_{40}^*(r) \right| I0 \right\rangle
\end{aligned} \tag{25}$$

$$\begin{aligned}
V_{nm}^{(C)} = V_{I0, I'0}^{(C)} &= \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \sqrt{\frac{5(2I+1)(2I'+1)}{4\pi}} \left(\beta_2 + \frac{2}{7} \sqrt{\frac{5}{\pi}} \beta_2^2 \right) \begin{pmatrix} I & 2 & I' \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&\quad + \frac{3Z_P Z_T e^2}{9} \frac{R_T^4}{r^5} \sqrt{\frac{9(2I+1)(2I'+1)}{4\pi}} \left(\beta_4 + \frac{9}{7} \sqrt{\frac{1}{\pi}} \beta_2^2 \right) \begin{pmatrix} I & 4 & I' \\ 0 & 0 & 0 \end{pmatrix}^2
\end{aligned} \tag{26}$$

2 Numerical solution methods

2.1 The modified Numerov method

The modified Numerov method is a numerical technique used to solve second-order ordinary differential equations. CCFULL solves the coupled channel equations from $r = r_{\min} + \Delta r$ to $r = r_{\max}$. At first, we initially set

$$\psi_n(r_{\min}) = 1, \quad \psi_m(r_{\min}) = 0 \quad (m \neq n), \quad (27)$$

$$\frac{d}{dr}\psi_n(r_{\min}) = -ik_n(r_{\min}), \quad \frac{d}{dr}\psi_m(r_{\min}) = 0 \quad (m \neq n), \quad (28)$$

the wave functions at $r = r_{\min} + \Delta r$, Δr being the radial mesh to integrate the equations, can be determined by the Runge-Kutta method. After the wave functions at $r = r_{\min} + \Delta r$ have been thus obtained, the modified Numerov method relates the wave functions at $r_{i+1} = r_{\min} + (i+1)\Delta r$ to those at r_i and r_{i-1} as

$$\chi_{nm}^{i+1} = \left\{ \left(\frac{\Delta r^2}{\sqrt{12}} A_{nm}^i(r) + \sqrt{3} \right)^2 - 1 \right\} \chi_{nm}^i - \chi_{nm}^{i-1}, \quad (29)$$

where χ_{nm}^i is defined by

$$\chi_{nm}^i = \left(1 - \frac{\Delta r^2}{12} A_{nm}^i \right) \psi_{nm}(r), \quad (30)$$

where A_{nm}^i is defined by

$$A_{nm}^i(r) = \frac{2\mu}{\hbar^2} \left[\left(V_N^0(r) + \frac{J(J+1)\hbar^2}{2\mu r^2} + \frac{Z_P Z_T e^2}{r} + \epsilon_n - E \right) \sigma_{nm} - V_{nm}(r) \right] \quad (31)$$

At $r = r_{\max}$, $\chi_{nm}(r_{\max})$ can be expressed by a superposition of the incoming and outgoing Coulomb waves as

$$\chi_{nm}(r_{\max}) = C_{nm} H_J^{(-)}(k_m r_{\max}) + D_{nm} H_J^{(+)}(k_m r_{\max}). \quad (32)$$

The coefficients C_{nm} and D_{nm} are determined either by matching the ratio of the wave functions at $r_{\max} - \Delta r$ to those at $r_{\max} + \Delta r$. The coefficients are then obtained as

$$C_{nm} = \frac{H_{Jm}^{(+)}(k_m \cdot (r_{\max} - \Delta r)) \chi_{nm}(r_{\max} + \Delta r) - H_{Jm}^{(+)}(k_m \cdot (r_{\max} + \Delta r)) \chi_{nm}(r_{\max} - \Delta r)}{H_{Jm}^{(+)}(k_m \cdot (r_{\max} - \Delta r)) H_{Jm}^{(-)}(k_m \cdot (r_{\max} + \Delta r)) - H_{Jm}^{(+)}(k_m \cdot (r_{\max} + \Delta r)) H_{Jm}^{(-)}(k_m \cdot (r_{\max} - \Delta r))} \quad (33)$$

$$D_{nm} = \frac{H_{Jm}^{(-)}(k_m \cdot (r_{\max} - \Delta r)) \chi_{nm}(r_{\max} + \Delta r) - H_{Jm}^{(-)}(k_m \cdot (r_{\max} + \Delta r)) \chi_{nm}(r_{\max} - \Delta r)}{H_{Jm}^{(+)}(k_m \cdot (r_{\max} - \Delta r)) H_{Jm}^{(-)}(r_{\max} + \Delta r) - H_{Jm}^{(+)}(k_m \cdot (r_{\max} + \Delta r)) H_{Jm}^{(-)}(k_m \cdot (r_{\max} - \Delta r))}, \quad (34)$$

respectively.

The solution of the coupled-channel equations with the proper boundary condition is given by linear combination for χ_{nm} as

$$\psi_m(r) = \sum_n T_n \chi_{nm}(r) \quad (35)$$

At $r = r_{\max}$, the equation satisfies the boundary condition $H_J^{(-)}(k_n r) \delta_{n,0} + R H_J^{(+)}(k_n r)$, it leads to

$$\begin{aligned} \psi_m(r_{\max}) &= \sum_n T_n \chi_{nm}(r_{\max}) \\ &= \sum_n T_n (C_{nm} H_J^{(-)}(k_m r_{\max}) + D_{nm} H_J^{(+)}(k_m r_{\max})) \\ &= H_J^{(-)}(k_m \cdot r_{\max}) \delta_{n,0} + R H_J^{(+)}(k_m \cdot r_{\max}). \end{aligned} \quad (36)$$

One finds $\sum_n T_n C_{nm} = \delta_{m0}$, then $T_n = (C^{-1})_{n0}$. Taking a summation over all possible intrinsic states, the inclusive penetrability is given by

$$P(E, J) = \sum_n \frac{k_n(r_{\min})}{k_0} |T_n|^2 \quad (37)$$

2.2 The discrete basis method

The discrete basis method (DBM) generally refers to solve quantum mechanism problem by expanding a wave function $\Psi(r)$ with a set of discrete, square-integrable basis functions. A general form of the wave function $\Psi(r)$ reads

$$\Psi(r) = \sum_{i=1}^N b_i \phi_i + c \phi_H \quad (38)$$

where ϕ_i are basis functions, chosen to form a complete set within the region of interest, and b_i are the corresponding coefficients to be determined by the variation method. The last term may be added to satisfy the boundary condition for $\Psi(r)$. For the discrete basis method, $\Psi(r)$ is a scattering wave function while ϕ_i represent a delta function δ_{i,r_i} . In this formalism, the scattering problem is transformed into a matrix problem.

For the N_{ch} channel problem, we first discretize the coordinate r into N mesh points with the mesh spacing Δr . $r_1 = r_{\min}$ and $r_N = r_{\max} = r_{\min} + (N-1)\Delta r$. By applying the three-point finite difference formula for the second derivative, the coupled channels equation are transformed into matrix represnetation as:

$$\sum_{n'} \sum_{i'} (H_{ni,n'i'} - E \delta_{n,n'} \delta_{i,i'}) \phi_{n'i'} = 0. \quad (39)$$

where n and i refer to the channels and the coordinate $r_i = r_{\min} + (i-1)\Delta r$, respectively. $\phi_{n'i'}$ represents the basis function $\phi_n(r_i)$. The matrix $H_{ni,n'i'}$ is given by

$$H_{ni,n'i'} = \delta_{n,n'} (-t \delta_{i,i'+1} + 2t \delta_{i,i'} - t \delta_{i,i'-1}) + \delta_{n,n'} \delta_{i,i'} \left(\frac{J(J+1)\hbar^2}{2\mu r_i^2} + V^{(0)}(r_i) + \epsilon_n \right) + \delta_{i,i'} V_{nn'}(r_i), \quad (40)$$

if one truncates the channel number up to $N_{\text{ch}} = 3$, the corresponding coupling Hamiltonian is then given by

$$H(r) = \begin{pmatrix} 2t + \frac{J(J+1)\hbar^2}{2\mu r_i^2} + V^{(0)}(r_i) + \epsilon_1 & -t + V_{12}(r_i) & 0 \\ -t + V_{21}(r_i) & 2t + \frac{J(J+1)\hbar^2}{2\mu r_i^2} + V^{(0)}(r_i) + \epsilon_2 & -t + V_{23}(r_i) \\ 0 & -t + V_{32}(r_i) & 2t + \frac{J(J+1)\hbar^2}{2\mu r_i^2} + V^{(0)}(r_i) + \epsilon_3 \end{pmatrix}, \quad (41)$$

where t is defined as $t = \frac{\hbar^2}{2\mu r^2}$. As for the boundary condition $\phi_{n,0} = \phi_{n,1} \exp[ik_n(r_{\min})\Delta r]$, it can be easily implemented by adding a term $-t \exp[ik_n(r_{\min})\Delta r]$ to matrix element $H_{n1,n1}$. By the way, the matrix dimension is defined as $N_{\text{ch}}(N+1) \times N_{\text{ch}}(N+2)$. After modification, we define $\tilde{H}$ as

$$\tilde{H}_{ni,n'i'} = H_{ni,n'i'} - E \delta_{n,n'} \delta_{i,i'} - t e^{ik_n(r_{\min})\Delta r} \delta_{n,n'} \delta_{i,i'} \delta_{i,1}, \quad (42)$$

where i and i' run from 1 to $N+1$ and from 1 to $N+2$, respectively. Both n and n' run from 1 to N_{ch} .

For the basis function, we define the basis function matrix as

$$\psi_{sj}(n'i') = \delta_{i',j} \delta_{n',s}, \quad (1 \leq j \leq N), \quad (43)$$

$$\begin{aligned} \psi_{s,N+1}(n'i') &= \delta_{i',N+1} \delta_{n',s} H_J^{(+)}(k_n(r_{\max} + \Delta r)) \\ &\quad + \delta_{i',N+2} \delta_{n',s} H_J^{(+)}(k_n(r_{\max} + 2\Delta r)), \end{aligned} \quad (44)$$

$$\psi^{(-)}(n'i') = \delta_{n',1} (\psi_{n',N+1}(n'i'))^*, \quad (45)$$

if one truncates the channel number up to $N_{\text{ch}} = 3$, the corresponding wave functions are then given by

$$\psi_{n_1,i} = \begin{pmatrix} \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad \psi_{n_2,i} = \begin{pmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad \psi_{n_3,i} = \begin{pmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad (46)$$

Where $n_s = \{1, 2, 3\}$ and $i = \{1, \dots, N\}$. and each basis function has $(N+2)N_{\text{ch}}$ component. For the wave function $\psi_{s,N+1}(n'i')$:

$$\psi_{n_1,N+1} = \begin{pmatrix} 0 \\ \vdots \\ H_J^{(+)}(k_1(r_{\text{max}} + \Delta r)) \\ 0 \\ 0 \\ H_J^{(+)}(k_1(r_{\text{max}} + 2\Delta r)) \\ 0 \\ 0 \end{pmatrix}, \quad \psi_{n_2,N+1} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ H_J^{(+)}(k_2(r_{\text{max}} + \Delta r)) \\ 0 \\ 0 \\ H_J^{(+)}(k_2(r_{\text{max}} + 2\Delta r)) \\ 0 \end{pmatrix}, \quad \psi_{n_3,N+1} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 0 \\ H_J^{(+)}(k_3(r_{\text{max}} + \Delta r)) \\ 0 \\ 0 \\ H_J^{(+)}(k_3(r_{\text{max}} + 2\Delta r)) \end{pmatrix}, \quad (47)$$

and $\psi^{(-)}$:

$$\psi^{(-)} = \begin{pmatrix} 0 \\ \vdots \\ H_J^{(-)}(k_1(r_{\text{max}} + \Delta r)) \\ 0 \\ 0 \\ H_J^{(-)}(k_1(r_{\text{max}} + 2\Delta r)) \\ 0 \\ 0 \end{pmatrix}, \quad (48)$$

We then expand the total wave function with these basis functions as

$$\Psi(n'i') = \sum_{s=1}^{N_{\text{ch}}} \sum_{j=1}^{N+1} b_{sj} \psi_{sj}(n'i') + \psi^{(-)}(n'i'). \quad (49)$$

Notice that this form guarantees the boundary condition. By imposing $\tilde{H}'\Psi = 0$, one obtains

$$\begin{aligned} & \sum_{s=1}^{N_{\text{ch}}} \sum_{j=1}^{N+1} \left(\sum_{n'=1}^{N_{\text{ch}}} \sum_{i'=1}^{N+2} \tilde{H}_{ni,n'i'} \psi_{sj}(n'i') \right) b_{sj} \\ & + \sum_{n'=1}^{N_{\text{ch}}} \sum_{i'=1}^{N+2} \tilde{H}_{ni,n'i'} \psi^{(-)}(n'i') = 0, \end{aligned} \quad (50)$$

or

$$\sum_{s=1}^{N_{\text{ch}}} \sum_{j=1}^{N+1} (\tilde{H}\psi)_{ni,sj} b_{sj} = -(\tilde{H}\psi^{(-)})_{ni} \equiv -\tilde{\psi}_{ni}, \quad (51)$$

from which the amplitudes $\{b_{ni}\}$ can be obtained as

$$b_{ni} = - \sum_{s=1}^{N_{\text{ch}}} \sum_{j=1}^{N+1} \left[(\tilde{H}\psi)^{-1} \right]_{ni,sj} \tilde{\psi}_{sj}. \quad (52)$$

The penetrability is then computed as,

$$P_J(E) = \sum_{n=1}^{N_{\text{ch}}} \frac{k_n(r_{\text{min}})}{k} |b_{n1}|^2 = 1 - \sum_{n=1}^{N_{\text{ch}}} \frac{k_n}{k} |b_{n,N}|^2. \quad (53)$$

2.3 The modified discrete basis method

In the realistic calculation, i found the wave function is a little deviated with the exact calculation. Besides, i found the deviation is smaller when i chose a smaller coordinate interval Δr . Conversely, if Δr is too small, the dimension of the Hamiltonian matrix becomes exceptionally large, making the calculation extremely time-consuming.

In order to enhance the convergence without increasing the computational load, in this paper, we utilize the modified Numerov method for the kinetic energy operator, instead of the three-point formula. In this method, the coupled-channels equations are transformed to

$$\chi_{n,i-1} + \chi_{n,i+1} - \sum_{n'} \left\{ \left(\frac{\Delta r^2}{\sqrt{12}} \vec{A} + \sqrt{3} \cdot \vec{1} \right)^2 - \vec{1} \right\}_{ni,n'i} \chi_{n'i} = 0, \quad (54)$$

where $\vec{1}$ is the unit matrix and χ_{ni} is defined by

$$\chi_{ni} = \sum_{n'} \left(\vec{1} - \frac{\Delta r^2}{12} \vec{A} \right)_{ni,n'i} \phi_{n'i}, \quad (55)$$

with the matrix $\vec{A}$ defined as

$$A_{ni,n'i'} = \frac{2\mu}{\hbar^2} \left(\frac{J(J+1)\hbar^2}{2\mu r_i^2} + V^0(r_i) + \epsilon_n - E \right) \delta_{n,n'} \delta_{i,i'} + \frac{2\mu}{\hbar^2} V_{nn'}(r_i) \delta_{i,i'}. \quad (56)$$

Here, ϕ_{ni} is the wave function defined in the discrete basis method. With this, the Hamiltonian matrix reads,

$$H_{ni,n'i'} = \left(\delta_{n,n'} \delta_{i,i'} - \frac{\Delta r^2}{12} A_{ni,n'i'} \right) \times \left(\delta_{i,i'+1} - \left\{ \left(\frac{\Delta r^2}{\sqrt{12}} A_{ni,n'i'} + \sqrt{3} \cdot \delta_{n,n'} \right)^2 - \delta_{n,n'} \right\} \delta_{i,i'} + \delta_{i,i'-1} \right). \quad (57)$$

The modified Hamiltonian that corresponds to Eq. (42) reads,

$$\tilde{H}_{ni,n'i'} = H_{ni,n'i'} + \left(\delta_{n,n'} - \frac{\Delta r^2}{12} A_{ni,n'i'} \right) e^{ik_n(r_{\min})\Delta r} \delta_{i,i'} \delta_{i,1}. \quad (58)$$

Notice that the energy E is already included in the matrix $\mathbf{A}$. Once the Hamiltonian matrix is so constructed, all the subsequent steps remain the same as those in the discrete basis method.

2.4 The R matrix method

2.4.1 R matrix and S matrix

Now, i take one channel as an example to explain how to solve the couple channel equation by R matrix method with the complex potential. For the common Schrödinger equation $(T + V - E)\Psi = 0$, the R-matrix theory divides the coordinate space into two distinct regions separated by a channel radius r_c shown by Figure 1:

- **Internal Region** ($r < r_c$): Nuclear forces are dominant. The calculation involves solving the Schrödinger equation using a basis set expansion.
- **External Region** ($r > r_c$): Only Coulomb forces act (for charged particles). The wave functions are known analytically (Coulomb functions $H_L^{(-)}, H_L^{(+)}$).

Due to the division of the coordinate space, the Hamiltonian in the interval $(0, a)$ is not Hermitian. To restore Hermiticity within this finite domain, the Bloch operator $\mathcal{L}$ is introduced into the Schrödinger equation:

$$(T(r) + V(r) + \mathcal{L}(r) - E)\Psi = \mathcal{L}(r)\Psi, \quad (59)$$

where the Bloch operator is defined as $\mathcal{L}(r) = \frac{\hbar^2}{2\mu} \delta(r-a) \left(\frac{d}{dr} - \frac{B}{a} \right)$. For the open channel problem, we typically choose the boundary parameter $B = 0$. The kinetic energy operator is $T = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{L(L+1)\hbar^2}{2\mu r^2}$.

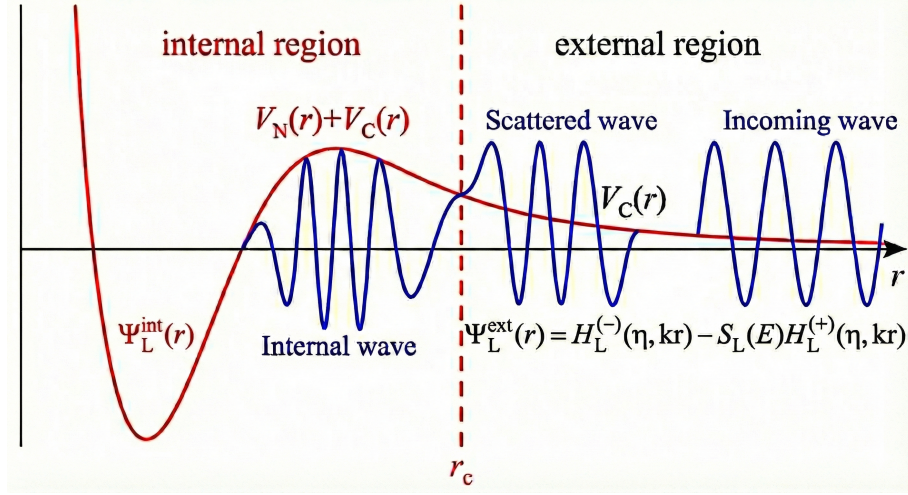


Figure 1: Schematic representation of the R-matrix division of space.

According to the continuity condition at $r = a$:

$$\Psi_L^{\text{int}}(a) = \Psi_L^{\text{ext}}(a), \quad (60)$$

the Schrödinger equation is promoted to the **Bloch-Schrödinger equation**:

$$\left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{L(L+1)\hbar^2}{2\mu r^2} + V_N(r) + V_C(r) + \mathcal{L}(r) - E \right) \Psi = \mathcal{L}(r)\Psi. \quad (61)$$

The Bloch-Schrödinger equation in could be solved by the variational method with

$$\Psi_L^{\text{int}}(r) = \sum_{n=1}^N c_n \varphi_n(r) \quad (62)$$

According to the above derivation, we can obtain

$$(T(r) + V(r) + \mathcal{L}(r) - E) \sum_{n=1}^N c_n \varphi_n(r) = \mathcal{L}(r)\Psi \quad (63)$$

To find the coefficients c_n , we need to utilize the orthogonality (or general projection) of the basis functions. We multiply both sides of the equation by $\varphi_n^*(r)$ on the left and integrate over the radial coordinates r from 0 to r_c , now we denote $r_c = a$.

$$\begin{aligned} \int_0^a \varphi_n^*(r) dr (T(r) + V(r) + \mathcal{L}(r) - E) \sum_{n=1}^N c_n \varphi_n(r) &= \int_0^a \varphi_n^*(r) dr \mathcal{L}(r) \Psi \\ \sum_{n=1}^N c_n \int_0^a \varphi_n^*(r) (T(r) + V(r) + \mathcal{L}(r) - E) \varphi_n(r) dr &= \int_0^a \varphi_n^*(r) dr \frac{\hbar^2}{2\mu} \delta(r-a) \left(\frac{d}{dr} \right) \Psi \\ \sum_{n=1}^N c_n \langle \varphi_n | T(r) + V(r) + \mathcal{L}(r) - E | \varphi_n \rangle &= \frac{\hbar^2}{2\mu a} \varphi_n^*(a) a \frac{d\Psi(a)}{dr} \end{aligned} \quad (64)$$

Let us define $\mathbf{C}$ as

$$\begin{aligned} \mathbf{C}_{nm} &= \langle \varphi_n | T(r) + V(r) + \mathcal{L}(r) - E | \varphi_m \rangle \\ c_n &= \frac{\hbar^2}{2\mu a} \sum_{m=1}^N \mathbf{C}_{nm}^{-1} \varphi_m(a) a \frac{d\Psi(a)}{dr} \end{aligned} \quad (65)$$

$$\begin{aligned}\Psi(a) &= \sum_{n=1}^N c_n \varphi_n(a) \\ \Psi(a) &= \frac{\hbar^2}{2\mu a} \sum_{n=1}^N \sum_{m=1}^N \mathbf{C}_{nm}^{-1} \varphi_m(a) \varphi_n(a) a \frac{d\Psi(a)}{dr}\end{aligned}\tag{66}$$

Here we define $\mathbf{R}$ as

$$\mathbf{R} = \frac{\hbar^2}{2\mu a} \sum_{n=1}^N \sum_{m=1}^N \mathbf{C}_{nm}^{-1} \varphi_m(a) \varphi_n(a)\tag{67}$$

$$\Psi(a) = \mathbf{R} a \frac{d\Psi(a)}{dr}\tag{68}$$

According to the continuity property on the a :

$$\begin{aligned}\Psi_L^{\text{int}}(r_c) &= \mathbf{R} a \frac{d\Psi(a)}{dr} = \Psi_L^{\text{ext}}(r_c) = H_L^{(-)} - S H_L^{(+)} \\ \mathbf{R} a \frac{d\Psi(a)}{dr} &= \mathbf{R} a (\dot{H}_L^{(-)} - S \dot{H}_L^{(+)})\end{aligned}\tag{69}$$

Here we define S as

$$S = \frac{H_L^{(-)} - \mathbf{R} a \dot{H}_L^{(-)}}{H_L^{(+)} - \mathbf{R} a \dot{H}_L^{(+)}}\tag{70}$$

For the penetration probability, one can obtain by the relation

$$P = 1 - |S|^2\tag{71}$$

2.4.2 Basis function: Lagrange basis

In the variational method $\Psi_L^{\text{int}}(r) = \sum_{n=1}^N c_n \varphi_n(r)$, the Lagrange function has been adopted. The main advantage is that, if the Gauss approximation is used for the numerical quadrature, no integral is needed for the matrix elements in the matrix $\mathbf{C}$.

The Lagrange basis functions are always associated with a Gauss quadrature. For a finite interval $[0, a]$, the N basis functions, used for all channels are defined as

$$\varphi_n(r) = (-1)^{N+n} \left(\frac{r}{ax_n}\right)^v \sqrt{ax_n(1-x_n)} \frac{P_N(2r/a-1)}{r-ax_n},\tag{72}$$

where $P_N(x)$ is the Legendre polynomial of degree N , and x_n are the zero's of

$$P_N(2x_n-1) = 0\tag{73}$$

The x_n values are therefore comprised between 0 and 1. The factor $(r/ax_n)^v$, where v is a positive integer, is aimed at regularizing the basis functions at the origin. We use $v = 1$ unless otherwise mentioned. The normalization of $\varphi_n(r)$ is chosen in such a way that the Lagrange condition

$$\varphi_n(ax_m) = \frac{1}{\sqrt{a\lambda_n}} \delta_{nm}\tag{74}$$

is satisfied. In this equation, λ_n is the weight of the Gauss-Legendre quadrature associated with the $[0, 1]$ interval. Within this approximation, the overlap and potential matrix elements read

$$\langle \varphi_n | \varphi_m \rangle = \int_0^a \varphi_n(r) \varphi_m(r) dr \approx \delta_{nm},\tag{75}$$

$$\langle \varphi_n | V | \varphi_m \rangle = \int_0^a \varphi_n(r) V(r) \varphi_m(r) dr \approx V(ax_n) \delta_{nm}\tag{76}$$

The matrix elements of the kinetic energy are available in an analytical form. Within the Gauss approximation, they read

$$\langle \varphi_n | T + \mathcal{L}(B) | \varphi_n \rangle \approx \frac{\hbar^2}{2\mu a} [\varphi_n(a)]^2 \left[\frac{(4N^2 + 4N + 3)x_n(1-x_n) - 6x_n + 1}{3x_n(1-x_n)} - B \right]\tag{77}$$

and

$$\langle \varphi_n | T + \mathcal{L}(B) | \varphi_m \rangle \approx \frac{\hbar^2}{2\mu a} \varphi_n(a) \varphi_m(a) \times [N^2 + N + 1 + \frac{x_n + x_m - 2x_n x_m}{(x_n - x_m)^2} - \frac{1}{1 - x_n} - \frac{1}{1 - x_m} - B] \quad n \neq m. \quad (78)$$

In these equations, we used $v = 1$ and $B = 0$, $\varphi_n(a)$ takes the simple form

$$\varphi_n(a) = (-1)^{N+n} \sqrt{\frac{1}{ax_n(1-x_n)}} \quad (79)$$

Consequently, all matrix elements can be computed very easily.

For problems requiring an **Incoming Wave Boundary Condition (IWBC)** or involving a region where the potential is real but separated from the origin (e.g., to define absorption), we divide the space into $[0, r_{\text{abs}}]$ (absorption), $[r_{\text{abs}}, r_c]$ (internal), and $[r_c, \infty)$ (external). The Lagrange basis functions defined on $[r_{\text{abs}}, r_c]$ with width $\Delta r = r_c - r_{\text{abs}}$ are:

$$\varphi_n(r) = (-1)^{N+n} \frac{r - r_{\text{abs}}}{\Delta r x_n} \sqrt{\Delta r x_n (1 - x_n)} \frac{P_N[(2r - r_{\text{abs}} - r_c)/\Delta r]}{r - \Delta r x_n - r_{\text{abs}}}, \quad \Delta r = r_c - r_{\text{abs}} \quad (80)$$

Within this approximation, the overlap and potential matrix elements read

$$\langle \varphi_n | V | \varphi_m \rangle = \int_{r_{\text{abs}}}^{r_c} \varphi_n(r) V(r) \varphi_m(r) dr \approx V(r_{\text{abs}} + \Delta r x_n) \delta_{nm} \quad (81)$$

Within this interval, the kinetic energy matrix elements are:

$$\langle \varphi_n | T | \varphi_n \rangle = -\frac{\hbar^2}{2\mu} \frac{1}{3\Delta r^2 x_n (1 - x_n)} [N^2 + N + 6 - \frac{2}{x_n(1 - x_n)}] \quad (82)$$

$$\langle \varphi_n | T | \varphi_m \rangle = -\frac{\hbar^2}{2\mu} \frac{(-1)^{n+m}}{\Delta r^2} \sqrt{\frac{x_m(1 - x_m)}{x_n(1 - x_n)}} \frac{2x_n x_m + 3x_n - x_m - 4x_n^2}{x_n(1 - x_n)(x_m - x_n)^2} \quad (83)$$

The Bloch operator must now account for both boundaries.

$$\langle \varphi_n | \mathcal{L}(r_{\text{abs}}) | \varphi_m \rangle = \langle \varphi_n | \delta(r - r_{\text{abs}}) \frac{d}{dr} | \varphi_m \rangle = \frac{(-1)^{n+m}}{\Delta r^2} \sqrt{\frac{x_n x_m}{(1 - x_n)(1 - x_m)}} [N(N+1) - \frac{1}{1 - x_m}] \quad (84)$$

$$\langle \varphi_n | \mathcal{L}(r_c) | \varphi_m \rangle = \langle \varphi_n | \delta(r - r_c) \frac{d}{dr} | \varphi_m \rangle = \frac{(-1)^{n+m}}{\Delta r^2} \sqrt{\frac{(1 - x_n)(1 - x_m)}{x_n x_m}} [-N(N+1) + \frac{1}{x_m}] \quad (85)$$

The final Hamiltonian matrix $\mathbf{C}$ includes contributions from kinetic energy, potential, and Bloch operators at both ends

$$\mathbf{C}_{nm} = \langle \varphi_n | T(r) + V(r) + \mathcal{L}(r_c) - \mathcal{L}(r_{\text{abs}}) - E | \varphi_m \rangle \quad (86)$$

3 Method comparison in CCFULL

I have implemented the above Four methods in the CCFULL code. And the code is available on GitHub². In this section, we will compare the accuracy, speed, and stability of these methods.

²https://github.com/murry-liao/CCFULL_progame

3.1 Accuracy

Now, we have introduced several way to solve the coupled-channel equations, and we will compare these method. Specifically, we calculated the sub-barrier fusion reaction $^{16}\text{O} + ^{144}\text{Sm}$. we consider the 3^- vibration motion of ^{144}Sm .

For the calculation parameters,

- The coupling strength $\beta_3 = 0.205$. The excitation energy of the state $3^- = 1.81\text{MeV}$.
- The energy interval ΔE is 0.18 MeV. The space interval Δr is 0.05 fm for the Numerov and DBM method. The basis number is 120 for the R matrix method.
- The Ws potential parameter $V_0 = 105.1\text{MeV}$, $r_0 = 1.1\text{fm}$, $a_0 = 0.75\text{fm}$.

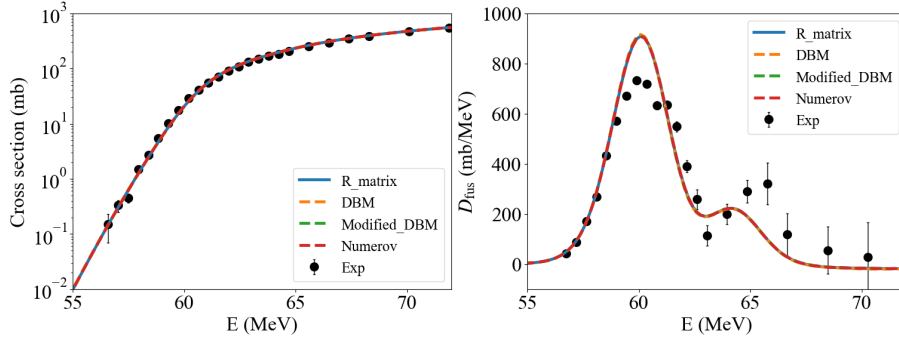


Figure 2: Comparison of experimental fusion cross sections and barrier distribution for the $^{16}\text{O} + ^{144}\text{Sm}$ system with results solved by different methods

3.2 Speed

Here I did a calculation of $^{16}\text{O} + ^{144}\text{Sm}$ system with results solved by different methods, the energy range from 55 to 75 MeV, a total of 20 energy points.

Table 1: Comparison of program execution time for different numerical methods

Method	CPU utilization	Total Time (s)
Numerov	9%	1.226
Rmatrix	79%	7.802
DBM	106%	56.466
Modified DBM	107%	56.041

Table 1 reports elapsed times for the stated 20-energy calculation. Numerov is fastest at 1.226 s, followed by the R-matrix calculation at 7.802 s. DBM and modified DBM take about 56 s each because they solve substantially larger linear systems. CPU utilization above 100% indicates threaded numerical-library activity. The 9% Numerov utilization alone is insufficient to identify an I/O bottleneck; profiling would be required for that conclusion.

3.3 Stability

Next, I calculated the fusion cross-sections of different systems. Specifically, we calculated the sub-barrier fusion reaction $^{16}\text{O}, ^{20}\text{Ne}, ^{24}\text{Mg}, ^{28}\text{Si}, ^{40}\text{Ar}, ^{40}\text{Ca}, ^{58}\text{Ni} + ^{144}\text{Sm}$. we consider the 3^- vibration motion of ^{144}Sm .

For the calculation parameters,

- The coupling strength $\beta_3 = 0.205$. The excitation energy of the state $3^- = 1.81\text{MeV}$.

- The energy interval ΔE is 1 MeV. The space interval Δr is 0.05 fm for the Numerov and DBM method. The basis number is 120 for the R matrix method.
- The W_s potential parameter we adopted the empirical form is given by:

$$V_N(r) = \frac{-V_0}{1 + \exp[(r - R_P - R_T)/a]}, \quad (87)$$

where

$$\frac{1}{a} = 1.17[1 + 0.53(A_P^{-1/3} + A_T^{-1/3})] \text{ fm}^{-1}, \quad (88)$$

$$r_0 = 1.16 \text{ fm}, \quad (89)$$

$$V_0 = 80 \text{ MeV}, \quad (90)$$

$$R_P = r_0 A_P^{-1/3}, \quad R_T = r_0 A_T^{-1/3} \quad (91)$$

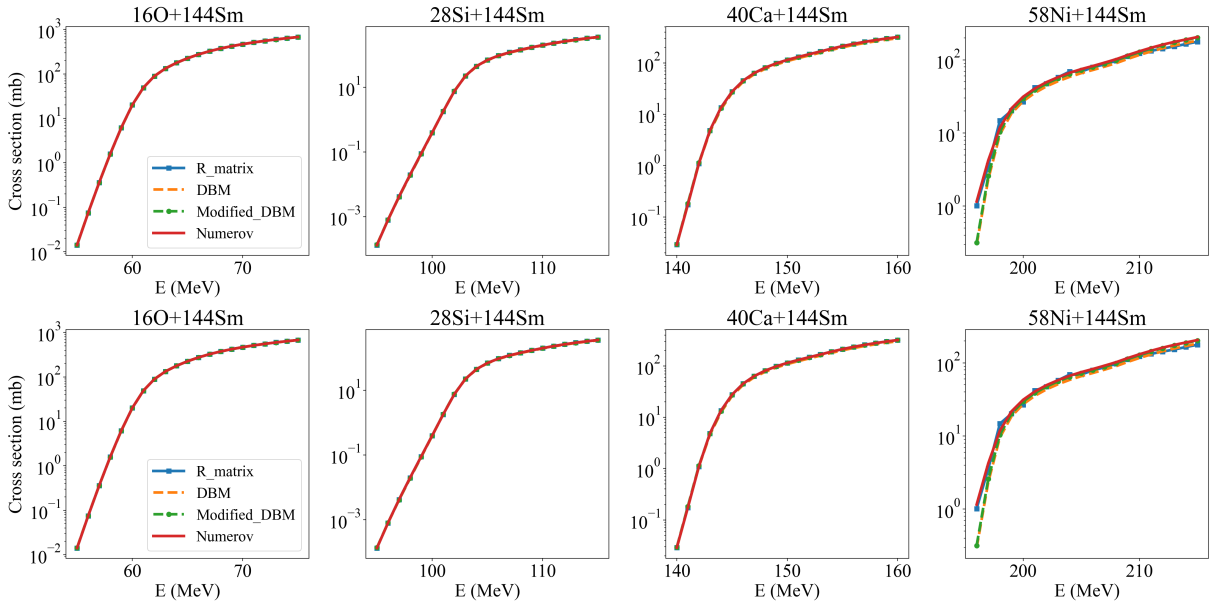


Figure 3: Comparison of fusion cross sections for the ^{16}O , ^{20}Ne , ^{24}Mg , ^{28}Si , ^{40}Ar , ^{40}Ca , $^{58}\text{Ni} + ^{144}\text{Sm}$ systems with results solved by different methods

4 Reduced-basis method and online CCFULL-ROM emulator

This section derives the reduced-order emulator used for the real-potential Numerov version of CCFULL. The main idea is to reduce the discretized coupled wave equation itself, rather than fitting the final fusion cross section. The construction combines reduced-basis projection [MDF⁺22], empirical interpolation [BMNP04], and the multipole organization of the coupled-channels reduced-order model of Catacora-Rios *et al.* [CRBLN26]. The implementation is also organized in the same offline-online manner as ROSE [O⁺24].

The derivation is arranged in the order in which the numerical model is built: first the coupled equation is discretized, then full solutions are compressed, the non-affine interaction is separated into multipoles, and finally the reduced equations and observables are assembled. Throughout this section, E and J are fixed unless they are written explicitly. A separate reduced system is trained for every (E, J) pair, because changing either quantity changes the differential operator and its boundary conditions.

4.1 Parameter vector and high-fidelity problem

For the five-dimensional application, the online parameter vector is

$$\boldsymbol{\theta} = (\beta_2, \beta_4, V_0, r_0, a_0)^T. \quad (92)$$

The first two entries control the target deformation. The last three entries control the real Woods–Saxon potential,

$$V_N(r; V_0, r_0, a_0) = -\frac{V_0}{1 + \exp[(r - R_N)/a_0]}, \quad R_N = r_0 \left(A_P^{1/3} + A_T^{1/3} \right). \quad (93)$$

All other projectile, target, excitation, charge, mesh, and convergence inputs are fixed by the selected CCFULL input file.

Let

$$\mathbf{u}(r; \boldsymbol{\theta}) = (u_1(r; \boldsymbol{\theta}) \quad \cdots \quad u_{N_{\text{ch}}}(r; \boldsymbol{\theta}))^T \quad (94)$$

be the vector of radial channel amplitudes. Equation (3) can be written as

$$-\frac{\hbar^2}{2\mu} \mathbf{u}''(r) + [\mathbf{W}(r; J, \boldsymbol{\theta}) - E\mathbf{I}] \mathbf{u}(r) = \mathbf{0}, \quad (95)$$

where

$$\mathbf{W}(r; J, \boldsymbol{\theta}) = \left[V_N(r) + V_C(r) + \frac{\hbar^2 J(J+1)}{2\mu r^2} \right] \mathbf{I} + \boldsymbol{\epsilon} + \mathbf{V}_{\text{coup}}(r; \boldsymbol{\theta}). \quad (96)$$

Here $\boldsymbol{\epsilon} = \text{diag}(\epsilon_1, \dots, \epsilon_{N_{\text{ch}}})$, and the coupling matrix contains the nuclear and Coulomb couplings. Multiplication of Eq. (95) by $-2\mu/\hbar^2$ gives the form used by Numerov,

$$\mathbf{u}''(r) = \mathbf{Q}(r; E, J, \boldsymbol{\theta}) \mathbf{u}(r), \quad \mathbf{Q} = \frac{2\mu}{\hbar^2} [\mathbf{W} - E\mathbf{I}]. \quad (97)$$

The unchanged Numerov calculation that solves this equation with IWBC is called the high-fidelity or exact model below. “Exact” therefore means exact with respect to the emulator; it does not remove the physical and numerical approximations already present in CCFULL.

4.2 Derivation of the coupled Numerov residual

Choose a uniform radial mesh $r_n = r_{\text{min}} + nh$ and write $\mathbf{u}_n = \mathbf{u}(r_n)$. Taylor expansion around r_n gives

$$\mathbf{u}_{n+1} - 2\mathbf{u}_n + \mathbf{u}_{n-1} = h^2 \mathbf{u}_n'' + \frac{h^4}{12} \mathbf{u}_n^{(4)} + \mathcal{O}(h^6), \quad (98)$$

$$\mathbf{u}_{n+1}'' + 10\mathbf{u}_n'' + \mathbf{u}_{n-1}'' = 12\mathbf{u}_n'' + h^2 \mathbf{u}_n^{(4)} + \mathcal{O}(h^4). \quad (99)$$

Eliminating the fourth derivative between these two equations yields

$$\mathbf{u}_{n+1} - 2\mathbf{u}_n + \mathbf{u}_{n-1} = \frac{h^2}{12} (\mathbf{u}_{n+1}'' + 10\mathbf{u}_n'' + \mathbf{u}_{n-1}'') + \mathcal{O}(h^6). \quad (100)$$

Substitution of $\mathbf{u}_n'' = \mathbf{Q}_n \mathbf{u}_n$ then gives the coupled Numerov stencil

$$\begin{aligned} \left(\mathbf{I} - \frac{h^2}{12} \mathbf{Q}_{n+1} \right) \mathbf{u}_{n+1} - 2 \left(\mathbf{I} + \frac{5h^2}{12} \mathbf{Q}_n \right) \mathbf{u}_n \\ + \left(\mathbf{I} - \frac{h^2}{12} \mathbf{Q}_{n-1} \right) \mathbf{u}_{n-1} = \mathbf{0}. \end{aligned} \quad (101)$$

This equation is sixth-order accurate locally for a sufficiently smooth matrix field. Its important structural property for model reduction is that it is linear in the wave function, even though its matrix coefficients are nonlinear functions of $\boldsymbol{\theta}$.

The interior stencil does not yet determine a scattering solution. At the inner radius, the IWBC logarithmic derivative is diagonal in the channel basis,

$$\mathbf{u}'(r_{\min}) = \mathbf{D}_{\text{in}} \mathbf{u}(r_{\min}), \quad (D_{\text{in}})_{cc} = \begin{cases} -ik_c(r_{\min}), & E_c(r_{\min}) > 0, \\ +\kappa_c(r_{\min}), & E_c(r_{\min}) \leq 0, \end{cases} \quad (102)$$

where

$$k_c = \sqrt{\frac{2\mu E_c}{\hbar^2}}, \quad \kappa_c = \sqrt{\frac{2\mu |E_c|}{\hbar^2}}. \quad (103)$$

The high-fidelity code takes one Runge–Kutta step from this logarithmic derivative. Denoting that step by the channel matrix $\mathbf{M}_{\text{in}}$ gives the first boundary residual

$$\mathbf{u}_1 - \mathbf{M}_{\text{in}}(\boldsymbol{\theta}) \mathbf{u}_0 = \mathbf{0}. \quad (104)$$

At the outer boundary, each open channel is matched to Coulomb functions. Let $r_a = r_{N-2}$ and $r_b = r_N$. The outgoing ratio is

$$(R_{\text{out}})_{cc} = \frac{H_J^{(+)}(\eta_c, k_c r_b)}{H_J^{(+)}(\eta_c, k_c r_a)}. \quad (105)$$

Only the entrance channel has an incoming source. Thus

$$\mathbf{u}_N - \mathbf{R}_{\text{out}} \mathbf{u}_{N-2} = \mathbf{s}_{\text{out}}, \quad (106)$$

$$(s_{\text{out}})_c = \delta_{c0} \left[H_J^{(-)}(\eta_0, k_0 r_b) - (R_{\text{out}})_{00} H_J^{(-)}(\eta_0, k_0 r_a) \right]. \quad (107)$$

For a closed outer channel, the corresponding ratio is replaced by the exponentially decaying solution.

Stacking every channel at every radial point,

$$\boldsymbol{\psi}^{EJ}(\boldsymbol{\theta}) = \text{vec}[\mathbf{u}_0, \mathbf{u}_1, \dots, \mathbf{u}_N], \quad (108)$$

turns the interior equations and the two boundary residuals into one linear system,

$$\mathbf{A}^{EJ}(\boldsymbol{\theta}) \boldsymbol{\psi}^{EJ}(\boldsymbol{\theta}) = \mathbf{b}^{EJ}(\boldsymbol{\theta}). \quad (109)$$

The dimension of $\mathbf{A}^{EJ}$ scales as the number of radial points times the number of channels. This full system is the object reduced by the emulator.

4.3 Wave-function snapshots and proper orthogonal decomposition

Map a unit-cube design point $\mathbf{x} \in [0, 1]^d$ to the physical parameter box by

$$\theta_a = \theta_{a,\min} + x_a(\theta_{a,\max} - \theta_{a,\min}). \quad (110)$$

A Latin-hypercube design provides N_s well-spread points $\{\boldsymbol{\theta}_s\}_{s=1}^{N_s}$. The high-fidelity solver produces one complex multichannel solution for the fixed entrance condition at each point. These solutions form the snapshot matrix

$$\mathbf{C}^{EJ} = [\boldsymbol{\psi}^{EJ}(\boldsymbol{\theta}_1) \quad \dots \quad \boldsymbol{\psi}^{EJ}(\boldsymbol{\theta}_{N_s})]. \quad (111)$$

Each column contains all channels and all radial mesh points. Therefore one basis vector represents a correlated change of the complete coupled wave function, rather than an independent basis for each channel.

The complex singular-value decomposition is

$$\mathbf{C}^{EJ} = \mathbf{X}^{EJ} \boldsymbol{\Sigma}^{EJ} (\mathbf{W}^{EJ})^\dagger, \quad \sigma_1 \geq \sigma_2 \geq \dots \geq 0. \quad (112)$$

Retaining the first N_b left singular vectors gives

$$\mathbf{X}_b^{EJ} = [\mathbf{x}_1 \quad \dots \quad \mathbf{x}_{N_b}], \quad (\mathbf{X}_b^{EJ})^\dagger \mathbf{X}_b^{EJ} = \mathbf{I}_{N_b}. \quad (113)$$

The Eckart–Young property gives a useful interpretation of the truncation:

$$\left\| \mathbf{C}^{EJ} - \mathbf{X}_b^{EJ} (\mathbf{X}_b^{EJ})^\dagger \mathbf{C}^{EJ} \right\|_F^2 = \sum_{q > N_b} \sigma_q^2. \quad (114)$$

Thus the discarded snapshot energy is known before any online calculation. A common rank diagnostic is

$$\epsilon_{\text{POD}}^2(N_b) = \frac{\sum_{q > N_b} \sigma_q^2}{\sum_q \sigma_q^2}. \quad (115)$$

The online wave function is approximated as

$$\hat{\psi}^{EJ}(\boldsymbol{\theta}) = \mathbf{X}_b^{EJ} \mathbf{d}^{EJ}(\boldsymbol{\theta}), \quad (116)$$

where only the N_b complex coefficients in $\mathbf{d}^{EJ}$ remain unknown. The exported IWBC solution fixes the normalization and phase of the snapshots. If a different solver produced arbitrary global phases, each snapshot would first have to be aligned to a reference by multiplying it by $\exp[-i \arg \langle \psi_{\text{ref}} | \psi_s \rangle]$.

4.4 Multipole decomposition of the non-affine interaction

Projection alone is not sufficient for a fast online model. Directly forming $\mathbf{A}(\boldsymbol{\theta})$ on the full radial mesh would preserve the high-dimensional cost. An affine or approximately affine representation is therefore required.

For an axial rotor, the deformation operator in the truncated intrinsic basis is

$$\hat{O} = R_T (\beta_2 Y_{20} + \beta_4 Y_{40}). \quad (117)$$

CCFULL diagonalizes this matrix,

$$\hat{O} \mathbf{S} = \mathbf{S} \text{diag}(\lambda_1, \dots, \lambda_{N_{\text{ch}}}), \quad (118)$$

and applies the nonlinear Woods–Saxon function to every eigenvalue,

$$\mathbf{V}_N(r; \boldsymbol{\theta}) = \mathbf{S} \text{diag} \left[-\frac{V_0}{1 + \exp[(r - R_N - \lambda_\alpha)/a_0]} \right] \mathbf{S}^T. \quad (119)$$

This all-order operation generates effective even multipoles beyond the input values $\lambda = 2$ and 4.

In a finite rotor space, the channel geometry for multipolarity ω is fixed,

$$G_{II'}^\omega = \sqrt{\frac{(2I+1)(2\omega+1)(2I'+1)}{4\pi}} \begin{pmatrix} I & \omega & I' \\ 0 & 0 & 0 \end{pmatrix}^2. \quad (120)$$

The complete interaction field is represented as

$$\mathbf{V}_{\text{field}}(r; \boldsymbol{\theta}) \simeq \mathbf{V}_{\text{static}}(r) + \sum_{\omega \in \Omega} \mathbf{G}^\omega f^\omega(r; \boldsymbol{\theta}). \quad (121)$$

Here the matrices $\mathbf{G}^\omega$ contain only angular-momentum geometry; the scalar functions f^ω contain all radial and parameter dependence. At a fixed radius, the scalar factors can be extracted by a small least-squares projection. Defining

$$\mathbf{g} = [\text{vec } \mathbf{G}^{\omega_1} \quad \dots \quad \text{vec } \mathbf{G}^{\omega_M}], \quad (122)$$

the factor vector is

$$\mathbf{f}(r; \boldsymbol{\theta}) = \mathbf{g}^+ \text{vec} [\mathbf{V}_{\text{field}}(r; \boldsymbol{\theta}) - \mathbf{V}_{\text{static}}(r)], \quad (123)$$

where $\mathbf{g}^+$ is the Moore–Penrose inverse. The residual of this finite multipole decomposition is measured separately from the radial EIM error and the reduced-wave error.

For the seven-channel target rotor $I = 0, 2, 4, 6, 8, 10, 12$, the retained finite geometry is

$$\Omega = \{0, 2, 4, \dots, 24\}. \quad (124)$$

The upper value $24 = 2I_{\text{max}}$ follows from the angular-momentum triangle rule. Keeping only $\omega = 0, 2, 4$ would discard multipoles induced by the nonlinear all-order Woods–Saxon transformation and would therefore change the physical model.

4.5 Empirical interpolation for each multipole

The radial factors in Eq. (121) remain non-affine. They are compressed with a separate interaction-only design $\{\boldsymbol{\vartheta}_s\}_{s=1}^{N_U}$. No wave equation is solved for these inexpensive points. For each ω , form

$$\mathbf{F}^\omega = [\mathbf{f}^\omega(\boldsymbol{\vartheta}_1) \quad \cdots \quad \mathbf{f}^\omega(\boldsymbol{\vartheta}_{N_U})], \quad (125)$$

where the column $\mathbf{f}^\omega$ contains the values of $f^\omega(r)$ on the radial mesh. Its SVD is

$$\mathbf{F}^\omega = \mathbf{U}^\omega \boldsymbol{\Sigma}^\omega (\mathbf{B}^\omega)^\dagger. \quad (126)$$

The retained rank M_ω obeys

$$\sigma_m^\omega > \epsilon_U \sigma_1^\omega, \quad m = 1, \dots, M_\omega, \quad (127)$$

subject to a declared maximum rank.

Let $\mathbf{U}_M^\omega$ contain the retained columns. MaxVol chooses M_ω radial rows whose square submatrix has large volume. A selection matrix $\mathbf{P}^\omega$ extracts these rows. Assume

$$\mathbf{f}^\omega(\boldsymbol{\theta}) \simeq \mathbf{U}_M^\omega \mathbf{e}^\omega(\boldsymbol{\theta}). \quad (128)$$

Requiring equality at the selected nodes gives

$$(\mathbf{P}^\omega)^\top \mathbf{f}^\omega = (\mathbf{P}^\omega)^\top \mathbf{U}_M^\omega \mathbf{e}^\omega. \quad (129)$$

Solving this small system gives the EIM coefficients,

$$\mathbf{e}^\omega(\boldsymbol{\theta}) = [(\mathbf{P}^\omega)^\top \mathbf{U}_M^\omega]^{-1} (\mathbf{P}^\omega)^\top \mathbf{f}^\omega(\boldsymbol{\theta}). \quad (130)$$

Substitution into Eq. (121) yields

$$\mathbf{V}_{\text{field}}(r; \boldsymbol{\theta}) \simeq \mathbf{V}_{\text{static}}(r) + \sum_{\omega \in \Omega} \sum_{m=1}^{M_\omega} e_m^\omega(\boldsymbol{\theta}) \mathbf{G}^\omega u_m^\omega(r). \quad (131)$$

The interpolation is exact at the selected nodes for any field represented by the retained radial space. Online work now requires only $\sum_\omega M_\omega$ scalar node values instead of the complete channel matrix at every radial point.

4.6 Galerkin projection and the online reduced equation

Insert the reduced expansion (116) into the full residual (109):

$$\mathbf{r} = \mathbf{A}(\boldsymbol{\theta}) \mathbf{X}_b \mathbf{d} - \mathbf{b}(\boldsymbol{\theta}). \quad (132)$$

The Hermitian Galerkin condition requires the residual to be orthogonal to the trial space,

$$\mathbf{X}_b^\dagger \mathbf{r} = \mathbf{0}. \quad (133)$$

Therefore

$$\mathbf{A}_b(\boldsymbol{\theta}) \mathbf{d}(\boldsymbol{\theta}) = \mathbf{b}_b(\boldsymbol{\theta}), \quad (134)$$

$$\mathbf{A}_b = \mathbf{X}_b^\dagger \mathbf{A} \mathbf{X}_b, \quad \mathbf{b}_b = \mathbf{X}_b^\dagger \mathbf{b}. \quad (135)$$

The reduced matrix has dimension $N_b \times N_b$, independent of the radial mesh size.

Because the Numerov residual is linear in the interaction field, Eq. (131) leads to

$$\mathbf{A}_b(\boldsymbol{\theta}) = \mathbf{A}_{b,0} + \sum_{\omega \in \Omega} \sum_{m=1}^{M_\omega} e_m^\omega(\boldsymbol{\theta}) \mathbf{G}_{b,m}^{EJ,\omega} + \mathbf{A}_{b,\text{bnd}}(\boldsymbol{\theta}), \quad (136)$$

where

$$\mathbf{G}_{b,m}^{EJ,\omega} = \mathbf{X}_b^\dagger \mathbf{A}^{EJ} [\mathbf{G}^\omega u_m^\omega] \mathbf{X}_b. \quad (137)$$

Every large radial contraction in Eqs. (135) and (137) is computed offline. Only the inner and outer boundary maps remain parameter dependent in a way that is not represented by the interior affine sum. The online artifact consequently stores just four boundary slices of the basis,

$$\mathbf{X}_0, \quad \mathbf{X}_1, \quad \mathbf{X}_{N-2}, \quad \mathbf{X}_N. \quad (138)$$

For example, the inner contribution is assembled from

$$\mathbf{X}_0^\dagger (\mathbf{X}_1 - \mathbf{M}_{\text{in}} \mathbf{X}_0), \quad (139)$$

and the outer source becomes $\mathbf{X}_N^\dagger \mathbf{s}_{\text{out}}$. Thus the full radial basis can be removed from an observables-only online artifact.

At one energy, partial waves having the same reduced rank are stacked into a three-dimensional array. The program performs batched assembly and solves

$$\mathbf{A}_{b,J} \mathbf{d}_J = \mathbf{b}_{b,J} \quad (140)$$

for all such J values with one array operation. Fusion has one fixed entrance channel, so one right-hand side per (E, J) is sufficient. A full scattering matrix would require repeating the reduced solve for each independent incoming-channel boundary condition, as discussed in Ref. [CRBLN26].

4.7 Observable reconstruction

Only the inner-boundary wave amplitude is needed for fusion. It follows directly from the stored basis slice,

$$\hat{\mathbf{T}}^J = \hat{\mathbf{u}}_0 = \mathbf{X}_0 \mathbf{d}^J. \quad (141)$$

For the open channels, flux conservation gives the partial-wave penetrability

$$\hat{P}_J(E; \boldsymbol{\theta}) = \sum_{c \in \text{open}} \frac{k_c(r_{\text{min}})}{k_0} \left| \hat{T}_c^J(E; \boldsymbol{\theta}) \right|^2. \quad (142)$$

The fusion cross section is then

$$\hat{\sigma}_{\text{fus}}(E; \boldsymbol{\theta}) = 10 \frac{\pi \hbar^2}{2\mu E} \sum_{J=0}^{J_{\text{max}}} (2J+1) \hat{P}_J(E; \boldsymbol{\theta}) \quad \text{mb}, \quad (143)$$

where the factor 10 converts fm^2 to mb. The same partial-wave tail criterion as the high-fidelity code is used. No regression model for σ_{fus} appears in this calculation: the observable follows from the reduced wave solution and the original CCFULL definitions.

4.8 Offline and online algorithms

The offline stage is computationally expensive but is performed once for a chosen parameter box.

1. Choose the physical parameter limits and generate independent Latin-hypercube designs for the wave functions and the interaction.
2. At every wave-design point, run the modified export interface of the standard Numerov code for every required (E, J) block.
3. Form Eq. (111), calculate the complex SVD, and retain the block-dependent wave basis $\mathbf{X}_b^{EJ}$.
4. Evaluate interaction matrices at the inexpensive interaction-design points. Extract the multipole factors with Eq. (123).
5. For each multipole, calculate its radial SVD, select MaxVol nodes, and form Eq. (130).
6. Project the fixed Numerov operator, every multipole-EIM mode, the source, and the boundary slices. Save one restartable artifact per energy.

7. Validate on parameter points excluded from both training designs. If the error is too large, add wave snapshots near the failed region or increase the retained ranks and rebuild the affected blocks.

For a new parameter point, the online stage is

1. evaluate every scalar multipole factor only at its MaxVol nodes;
2. calculate $\mathbf{e}^\omega$ from the small interpolation systems;
3. assemble Eq. (136), including the IWBC and Coulomb boundary maps;
4. solve the reduced systems in partial-wave batches;
5. reconstruct only $\hat{\mathbf{u}}_0$, calculate $\hat{P}_J$, and perform the partial-wave sum.

The first query also loads the energy artifact from disk. Algorithmic online time and user-visible time must therefore be reported separately when the model is stored in energy shards.

4.9 Accuracy measures and parameter objective

Three errors must be distinguished. First, the emulator error measures how well the ROM reproduces its high-fidelity Numerov model,

$$\epsilon_\sigma(E, \boldsymbol{\theta}) = \frac{|\hat{\sigma}_{\text{fus}}(E, \boldsymbol{\theta}) - \sigma_{\text{fus}}^{\text{HF}}(E, \boldsymbol{\theta})|}{\max(|\sigma_{\text{fus}}^{\text{HF}}(E, \boldsymbol{\theta})|, 10^{-14} \text{ mb})}. \quad (144)$$

Second, the experimental residual measures the disagreement between the physical model and data. Third, the numerical speedup is

$$S_{\text{alg}} = \frac{t_{\text{HF, warm}}}{t_{\text{ROM, warm}}}, \quad (145)$$

where both paths use the same fixed partial waves and exclude compilation and one-time artifact loading.

For parameter optimization, let y_i and δ_i^{exp} be the measured cross section and its uncertainty. The held-out p95 emulator discrepancy is represented by a relative number δ_{ROM} . The conservative fitting uncertainty is

$$s_i^2 = (\delta_i^{\text{exp}})^2 + (\delta_{\text{ROM}} y_i)^2. \quad (146)$$

The objective minimized in the present application is

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N_E} \left[\frac{\hat{\sigma}_{\text{fus}}(E_i; \boldsymbol{\theta}) - y_i}{s_i} \right]^2. \quad (147)$$

This is a bounded maximum-likelihood fit with Gaussian errors and a uniform parameter density inside the training box. No additional informative prior is used.

The optimizer first evaluates a global Latin-hypercube design. It then uses a damped Gauss–Newton step. With normalized parameters $\mathbf{x}$, residuals $r_i = (\hat{\sigma}_i - y_i)/s_i$, and a finite-difference Jacobian $J_{ia} = \partial r_i / \partial x_a$, the local proposal solves

$$\left(\mathbf{J}^T \mathbf{J} + \lambda \mathbf{I} \right) \Delta \mathbf{x} = -\mathbf{J}^T \mathbf{r}. \quad (148)$$

A trust radius limits $\|\Delta \mathbf{x}\|_\infty$, and additional nearby points protect the search against an inaccurate local derivative. Finally, the unchanged Numerov code is run once at the best ROM point. This last calculation tests emulator accuracy at the inferred parameters; it does not reuse a training snapshot.

4.10 Case study: five-dimensional analysis of $^{16}\text{O}+^{154}\text{Sm}$

The complete case uses all 39 measured fusion cross sections between $E_{\text{c.m.}} = 52.4144$ and 99.5202 MeV. The five-dimensional training box is

$$\begin{aligned} 0.30 &\leq \beta_2 \leq 0.36, & 0.015 &\leq \beta_4 \leq 0.095, \\ 165 &\leq V_0 \leq 185 \text{ MeV}, & 0.94 &\leq r_0 \leq 0.98 \text{ fm}, \\ 0.98 &\leq a_0 \leq 1.08 \text{ fm}. \end{aligned} \tag{149}$$

Table 2 records the offline construction. The seven-channel target rotor contains $I = 0, 2, 4, 6, 8, 10, 12$. The number of active partial waves varies with energy, so the full grid contains 2114 independent (E, J) blocks.

Table 2: Offline settings for the five-dimensional $^{16}\text{O}+^{154}\text{Sm}$ CCB-ROM.

Quantity	Value
Experimental energies	39
Active J values per energy	51–65
Total (E, J) blocks	2114
Wave snapshots per block	42
Retained wave rank N_b	42
Independent interaction points	1000
Multipoles	$0, 2, \dots, 24$
Rank cap per multipole	6
Total EIM rank	78
Relative EIM singular-value threshold	10^{-5}
Offline elapsed time	1854.7 s
Generated energy-shard size	2.098 GiB

The multipole-geometry decomposition was audited at 16 independent interaction points. Its median and maximum relative closure errors were 7.58×10^{-5} and 2.78×10^{-4} . A separate 16-point parameter design, evaluated at all 39 energies, supplied 624 held-out cross-section comparisons. Table 3 shows the resulting emulator accuracy. The resident warm timing comparison used identical fixed partial waves in the Numerov and ROM calculations.

Table 3: Held-out accuracy and warm algorithmic speed for the full energy grid.

Metric	Result
Median ϵ_σ	0.136%
p90 ϵ_σ	0.521%
p95 ϵ_σ	0.636%
p99 ϵ_σ	0.911%
Maximum ϵ_σ	1.244%
Median resident exact-to-ROM speedup	$4.68\times$

For the fit, Eq. (146) used $\delta_{\text{ROM}} = 0.0063572132$, the held-out p95 value. All 39 experimental points were included, so the number of degrees of freedom after fitting five parameters was $\nu = 39 - 5 = 34$. The best point inside the trained parameter box was

$$\boxed{\begin{aligned} \beta_2 &= 0.32880884, & \beta_4 &= 0.04968356, & V_0 &= 165.0000 \text{ MeV}, \\ r_0 &= 0.94765471 \text{ fm}, & a_0 &= 1.05319268 \text{ fm} \end{aligned}} \tag{150}$$

The ROM objective at this point was

$$\chi_{\text{ROM}}^2 = 323.105, \quad \frac{\chi_{\text{ROM}}^2}{\nu} = 9.503. \tag{151}$$

A fresh standalone Numerov calculation at exactly the same parameters took 15.25 s for the 39 energies and gave

$$\chi_{\text{HF}}^2 = 333.733, \quad \frac{\chi_{\text{HF}}^2}{\nu} = 9.816. \quad (152)$$

At this optimum, the ROM–Numerov cross-section differences were 0.229% median, 0.560% at p95, and 0.677% maximum. The largest relative emulator error occurred at $E_{\text{c.m.}} = 59.6614$ MeV.

Figure 4 demonstrates that the ROM and Numerov curves are nearly indistinguishable on the scale of the fusion cross section. The large reduced χ^2 has a different meaning: the selected real-potential physical model does not reproduce the measurements within the combined experimental and emulator uncertainties. It is not evidence of a large ROM error. In addition, V_0 reaches the lower training boundary. The quoted point is therefore the optimum *inside* Eq. (149), not an unconstrained physical optimum. Testing shallower potentials requires a new offline model whose training box extends below $V_0 = 165$ MeV; extrapolating the present reduced basis is not controlled.

4.11 Relation to the reference CCB-ROM and practical limits

The present emulator and Ref. [CRBLN26] share the essential reduced-order structure: full multi-channel complex snapshots, a joint POD wave basis, Hermitian Galerkin projection, independent wave and interaction designs, one radial EIM for each fixed multipole geometry, offline projection of all large operators, and online solution for a fixed incoming channel. The main differences begin before model reduction. The reference work uses a Bloch/DBMM scattering residual with complex optical interactions, whereas the present application reduces the native Numerov stencil with real-potential IWBC fusion boundary conditions. It reconstructs penetrabilities and a partial-wave fusion sum instead of a complete elastic and inelastic scattering matrix.

The reference examples contain substantially more channels and reduce much larger dense high-fidelity systems, so speedups above $100\times$ are possible. The present seven-channel Numerov calculation is already inexpensive. EIM coefficient formation, reduced-matrix assembly, small complex solves, Python coordination, and artifact I/O therefore occupy a larger fraction of the runtime. The measured $4.68\times$ median resident speedup is consistent with this smaller high-fidelity problem. Increasing the number of physical channels would increase the cost of the Numerov reference faster than the cost of a well-compressed reduced solve, and could therefore increase the attainable speedup.

Finally, every numerical statement about the emulator is conditional on the training domain, channel truncation, radial mesh, partial-wave convergence, and observable definition. A useful verification hierarchy is

$$\boxed{\text{multipole closure} \longrightarrow \text{radial EIM} \longrightarrow \text{reduced wave} \longrightarrow \text{fusion observable} \longrightarrow \text{experiment.}} \quad (153)$$

Keeping these levels separate makes it possible to decide whether a discrepancy requires more EIM modes, more wave snapshots, a wider parameter domain, or a change in the underlying physical model.

References

- [BMNP04] M. Barrault, Y. Maday, N. C. Nguyen, and A. T. Patera. An empirical interpolation method: application to efficient reduced-basis discretization of partial differential equations. *Comptes Rendus Mathématique*, 339(9):667–672, 2004.
- [CRBLN26] M. Catacora-Rios, K. Beyer, J. Lei, and F. M. Nunes. Emulation of coupled-channels scattering for strongly deformed nuclei. *arXiv preprint arXiv:2610.03910*, 2026.
- [MDF⁺22] J. A. Melendez, C. Drischler, R. J. Furnstahl, D. R. Phillips, and X. Zhang. Model reduction methods for nuclear emulators. *Journal of Physics G: Nuclear and Particle Physics*, 49:102001, 2022.
- [O⁺24] D. Odell et al. ROSE: A reduced-order scattering emulator for optical models. *Physical Review C*, 109:044612, 2024.
- [Tan87] Osamu Tanimura. Reduction of coupled equations for heavy ion reactions. *Physical Review C*, 35(4):1600–1602, April 1987.

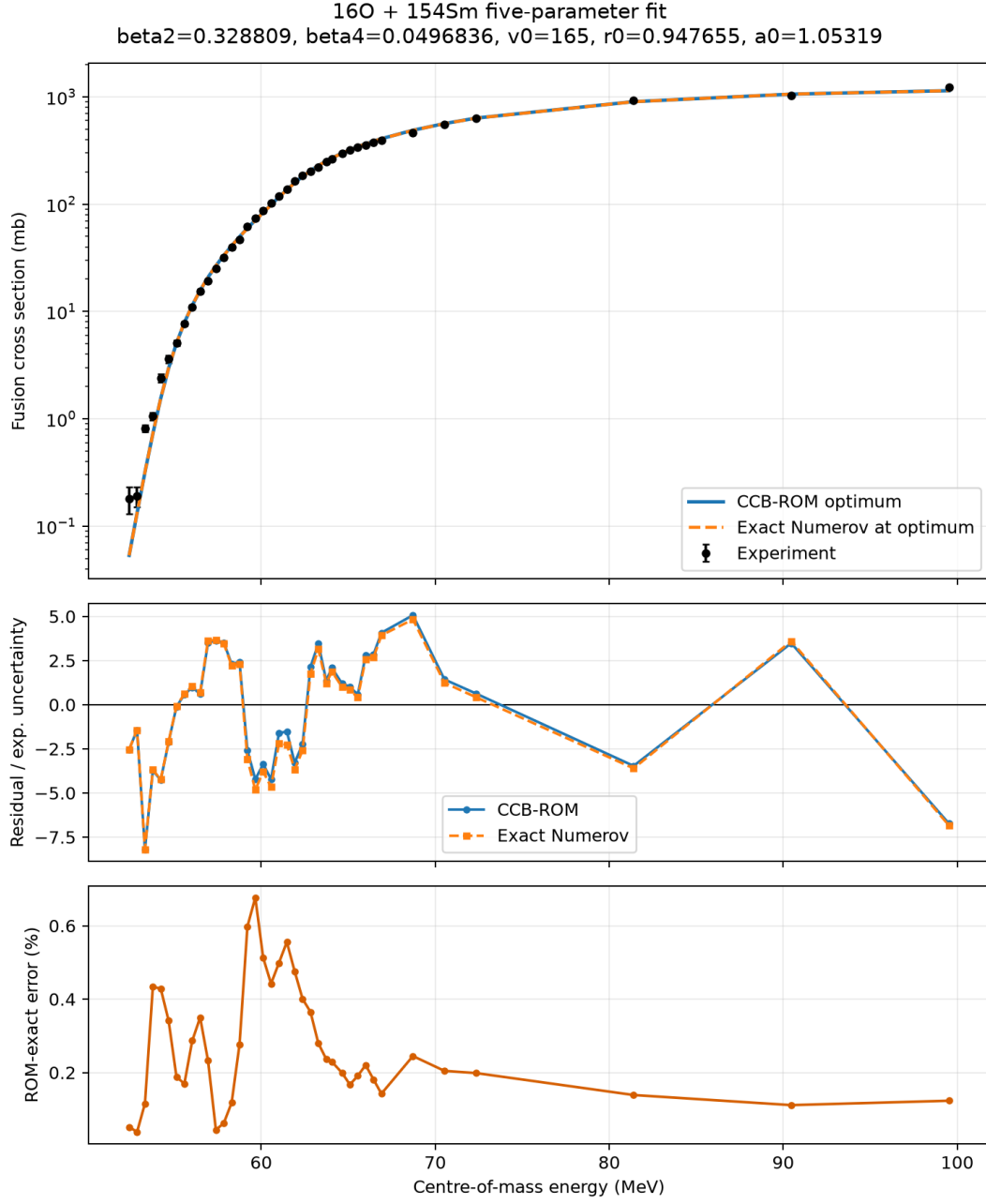


Figure 4: Five-dimensional $^{16}\text{O}+^{154}\text{Sm}$ result. The upper panel compares all experimental cross sections with the ROM optimum and an independent Numerov calculation at the same point. The middle panel shows residuals in units of the quoted experimental uncertainty. The lower panel isolates the ROM–Numerov relative difference.