Application of the KANTBP 3.1 program and its modifications to the study of some nuclear reactions processes

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Outline

- Statement of the problem: General BVP
- The program KANTBP 3.1
- Application in nuclear physics
  - Fusion cross sections with real potential and IWBC
  - Fusion cross sections with complex potential and regular BC
- Conclusions

Statement of the problem: General BVP

The multichannel scattering problem on the whole interval $z \in (-\infty, \infty)$

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \mathbf{U}(z) + \mathbf{Q}(z)\frac{d}{dz} + \frac{d\mathbf{Q}(z)}{dz} - 2E\,\mathbf{I} \right) \chi^{(i)}(z) = 0. \qquad (1)$$

The asymptotic form of the coefficients at $z = z_\pm \to \pm\infty$

Let $\mathbf{Q}(z) = 0$, and the $\mathbf{V}(z)$ matrix is constant or weakly dependent on the variable z in the vicinity of the asymptotic regions $z \le z_{\min}$ and/or $z \ge z_{\max}$.

Matrix-solutions $\mathbf{\Phi}_v(z)$:

$$\mathbf{\Phi}_v(z) = \begin{cases} \begin{cases} \mathbf{Y}^{(+)}(z)\mathbf{T}_v, & z \ge z_{\max}, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_v, & z \le z_{\min}, \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{Y}^{(-)}(z) + \mathbf{Y}^{(+)}(z)\mathbf{R}_v, & z \ge z_{\max}, \\ \mathbf{X}^{(-)}(z)\mathbf{T}_v, & z \le z_{\min}, \end{cases} & v = \leftarrow, \end{cases} \qquad (2)$$

where $\mathbf{R}_\rightarrow$ of the dimension $N_o^L \times N_o^L$ and $\mathbf{R}_\leftarrow$ of the dimension $N_o^R \times N_o^R$ are the reflection matrices, $\mathbf{T}_\rightarrow$ of the dimension $N_o^R \times N_o^L$ and $\mathbf{T}_\leftarrow$ of dimension $N_o^L \times N_o^R$ are the transmission matrices.

Components of asymptotic boundary conditions for constant matrices

The asymptotic rectangle-matrix functions $\mathbf{X}^{(\pm)}(z)$ and $\mathbf{Y}^{(\pm)}(z)$

$$\mathbf{X}^{(\pm)}_{i_o}(z) \to \frac{\exp\left(\pm\imath p^L_{i_o} z\right)}{\sqrt{p^L_{i_o}}}\boldsymbol{\Psi}^L_{i_o}, \quad p^L_{i_o} = \sqrt{2E - \lambda^L_{i_o}}, \quad z \le z_{\min},$$

$$\mathbf{Y}^{(\pm)}_{i_o}(z) \to \frac{\exp\left(\pm\imath p^R_{i_o} z\right)}{\sqrt{p^R_{i_o}}}\boldsymbol{\Psi}^R_{i_o}, \quad p^R_{i_o} = \sqrt{2E - \lambda^R_{i_o}}, \quad z \ge z_{\max}. \tag{3}$$

Here $\lambda^{L,R}_i$ and $\boldsymbol{\Psi}^{L,R}_i = \{\Psi^{L,R}_{1i}, \ldots, \Psi^{L,R}_{Ni}\}^T$ are the solutions of algebraic eigenvalue problems with the matrices $\mathbf{V}^L = V(z_{\min})$ and $\mathbf{V}^R = V(z_{\max})$ of the dimension $N \times N$ for entangled channels

$$\mathbf{V}^{L,R}\boldsymbol{\Psi}^{L,R}_i = \lambda^{L,R}_i \boldsymbol{\Psi}^{L,R}_i, \quad (\boldsymbol{\Psi}^{L,R}_i)^T \boldsymbol{\Psi}^{L,R}_j = \delta_{ij}. \tag{4}$$

The closed channels asymptotic vector solutions at $\lambda^{L,R}_{i_c} \ge 2E$, $i = i_c = N^{L,R}_o + 1, \ldots, N$, are as follows:

$$\mathbf{X}^{(-)}_{i_c}(z) \to \exp\left(+\sqrt{\lambda^L_{i_c} - 2E}z\right)\boldsymbol{\Psi}^L_{i_c}, \quad z \le z_{\min}, \quad v = \leftarrow,$$

$$\mathbf{Y}^{(+)}_{i_c}(z) \to \exp\left(-\sqrt{\lambda^R_{i_c} - 2E}z\right)\boldsymbol{\Psi}^R_{i_c}, \quad z \ge z_{\max}, \quad v = \rightarrow. \tag{5}$$

The asymptotic boundary conditions for Coulomb potential

The asymptotic of $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ matrices

$$V_{ij}(z) = \left(\epsilon_j^L + \frac{2Z_j^L}{z}\right)\delta_{ij} + O(z^{-l}), l > 1, \quad Q_{ij}(z) = O(z^{-l}), l \geq 1, z \leq z_{\min}, \quad (6)$$

and/or

$$V_{ij}(z) = \left(\epsilon_j^R + \frac{2Z_j^R}{z}\right)\delta_{ij} + O(z^{-l}), l > 1, \quad Q_{ij}(z) = O(z^{-l}), l \geq 1, z \geq z_{\max}. \quad (7)$$

We put $V_{ij}^L = \epsilon_i^L \delta_{ij}$ and/or $V_{ij}^R = \epsilon_i^R \delta_{ij}$,

$$\mathbf{V}^{L,R}\mathbf{\Psi}_i^{L,R} = \lambda_i^{L,R}\mathbf{\Psi}_i^{L,R}, \quad (\mathbf{\Psi}_i^{L,R})^T\mathbf{\Psi}_j^{L,R} = \delta_{ij}, \quad (8)$$

and the eigenvalues λ_i^L and/or λ_i^R are ordered in ascending order of the thresholds ϵ_i^L and/or ϵ_i^R, and the corresponding eigenvectors $\mathbf{\Psi}_i^L$ and/or $\mathbf{\Psi}_i^R$ are columns of the permutated unit matrix $\mathbf{I}$.

The asymptotic boundary conditions for non constant matrices

The open and closed channel asymptotic vector solutions have the form:

$$\mathbf{X}_{i_o}^{(\pm)}(z) \to \frac{\exp\left(\pm\imath\left(p_{i_o}^L z - \frac{Z_j^L}{p_{i_o}}\ln(2p_{i_o}^L|z|)\right)\right)}{\sqrt{p_{i_o}^L}}\boldsymbol{\Psi}_{i_o}^L, \quad p_{i_o}^L = \sqrt{2E-\lambda_{i_o}^L}, \quad z \le z_{\min},$$

$$\mathbf{X}_{i_c}^{(-)}(z) \to \exp\left(+\left(p_{i_c}^L z + \frac{Z_j^L}{p_{i_c}}\ln(2p_{i_c}^L|z|)\right)\right)\boldsymbol{\Psi}_{i_c}^L, \quad p_{i_c}^L = \sqrt{\lambda_{i_c}^L - 2E}, \tag{9}$$

and/or

$$\mathbf{Y}_{i_o}^{(\pm)}(z) \to \frac{\exp\left(\pm\imath\left(p_{i_o}^R z - \frac{Z_j^R}{p_{i_o}}\ln(2p_{i_o}^R|z|)\right)\right)}{\sqrt{p_{i_o}^R}}\boldsymbol{\Psi}_{i_o}^R, \quad p_{i_o}^R = \sqrt{2E-\lambda_{i_o}^R}, \quad z \ge z_{\max},$$

$$\mathbf{Y}_{i_c}^{(+)}(z) \to \exp\left(-\left(p_{i_c}^R z + \frac{Z_j^R}{p_{i_c}}\ln(2p_{i_c}^R|z|)\right)\right)\boldsymbol{\Psi}_{i_c}^R, \quad p_{i_c}^R = \sqrt{\lambda_{i_c}^R - 2E}, \tag{10}$$

where j is the element number of the eigenvector $\boldsymbol{\Psi}_i^L$ and/or $\boldsymbol{\Psi}_i^R$, which is 1.

The program KANTBP 3.1 – KANTorovich Boundary Problem

Methods

BVP is solved on non-uniform grids using FEM and R-matrix theory. The KANTBP 3.1 program has been created.

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KANTBP 3.1: A program for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel and adiabatic approaches [☆,☆☆,☆☆☆]

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Figure 1:

Application in nuclear physics

Sub-barrier heavy ion fusion reaction [a]

[a] P.W. Wen, O. Chuluunbaatar, A.A. Gusev, et al, Near-barrier heavy-ion fusion: Role of boundary conditions in coupling of channels, Phys. Rev. C 101,014618 (2020)

$$\sum_{n'=1}^{N}\left(\left(-\frac{d^2}{dr^2}-\tilde{E}\right)\delta_{nn'}+U_{nn'}(r)\right)\psi_{n'n_o}(r)=0,\quad r\in(r_{\min},r_{\max}). \tag{11}$$

$$U_{nn'}(r)=\frac{2\mu}{\hbar^2}\left[\left(\frac{l(l+1)\hbar^2}{2\mu r^2}+V_N^{(0)}(r)+\frac{Z_P Z_T e^2}{r}+\epsilon_n\right)\delta_{nn'}+V_{nn'}(r)\right]. \tag{12}$$

Here $\tilde{E}=2\mu E/\hbar^2$ is the center-of-mass energy, $\mu=A_P A_T/(A_P+A_T)$ is the reduced mass of the target and the projectile with the masses A_T and A_P and the charges Z_T and Z_P, respectively. $V_{nn'}(r)$ are matrix elements of Coulomb and nuclear $V_N^{(0)}(r)$ (Woods-Saxon potential derived from Akyüz-Winther parameterization) potentials, $U_{nn'}(r\to\infty)=2\mu\epsilon_n/\hbar^2\delta_{nn'}$.

Application in nuclear physics

Fusion cross sections:[a] IWBC at $r_{\min} \gg 0$

[a] K. Hagino, N. Rowley, A.T. Kruppa, CCFULL..., Comput. Phys. Commun. 123 (1999) 143.

$$V_l(r) = \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\left(V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r}\right),$$

$$\tilde{E} > V_l^{\min} = V_l(r_{\min}^l)$$

$$\sigma_f(E) = \sum_{l=1}^{l_{\max}(E)} P_l,$$

$$P_l = \frac{\pi}{\tilde{E}}(2l+1)\sum_{m=1}^{N_o^L} |\mathbf{T}_{m1}^{(l)}|^2.$$

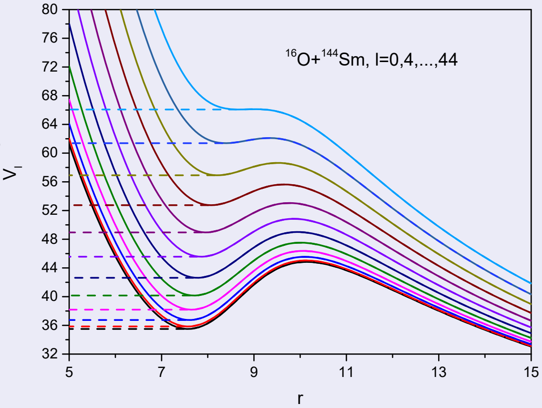


Figure 2:

Application in nuclear physics

Fusion cross sections for ^{64}Ni+^{100}Mo and ^{36}S+^{48}Ca

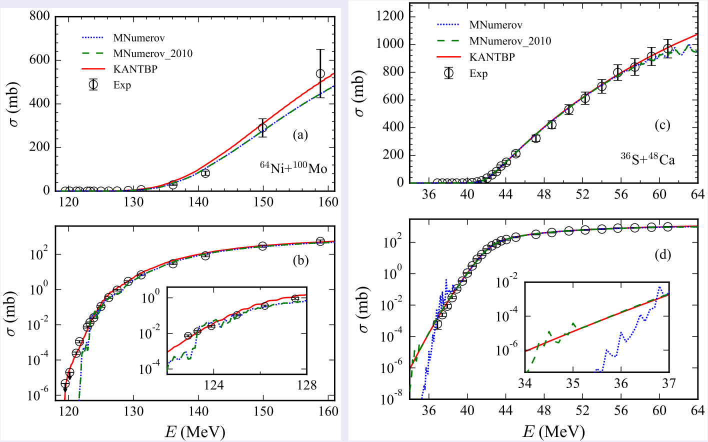


Figure 3: The modified Numerov method in CCFULL (dotted blue line), the improved Numerov method in the CCFULL (dashed green line) and KANTBP (solid red line). $N_o^R = 27$

Application in nuclear physics

Comparison of the left boundary conditions

$$\text{CCFULL:}\quad X^{(-)}_{ji_o}(r_{\min}) = \exp(-\imath q_j(r_{\min})r)\delta_{ji_o},\; q_j(r_{\min}) = \sqrt{\tilde{E} - U_{jj}(r_{\min})} \quad (13)$$

$$\text{KANTBP:}\quad \mathbf{X}^{(-)}_{i_o}(r_{\min}) = \exp\left(-\imath p^L_{i_o} r_{\min}\right) \mathbf{\Psi}^L_{i_o}, \quad p^L_{i_o} = \sqrt{2E - \lambda^L_{i_o}}, \quad (14)$$

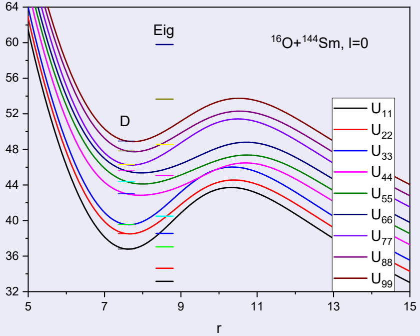


Figure 4: Lowest eigenvalues λ_m are smaller than lowest diagonal elements $U_{mm}(r_{\min})$.

Application in nuclear physics

Fission reaction $^{40}Ca+^{208}Pb$ leading to the formation of the nucleus ^{248}No

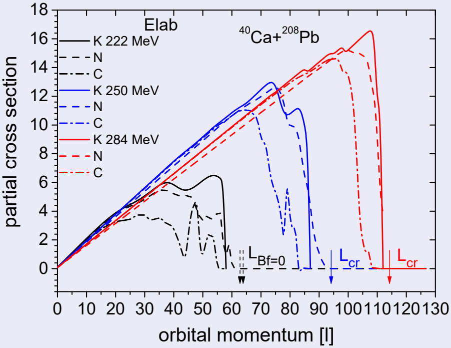
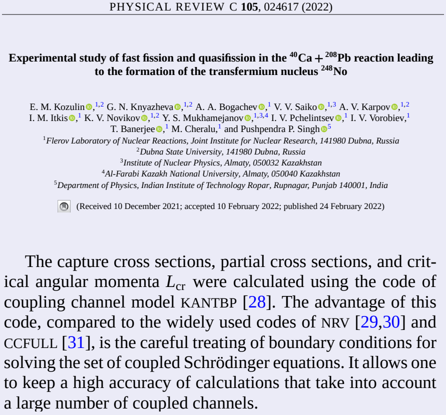


Figure 5: KANTBP (solid), NRV [http://nrv.jinr.ru/nrv] (dashed) and CCFULL (dash dotted).



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Experimental study of fast fission and quasifission in the ^{40}Ca + ^{208}Pb reaction leading to the formation of the transfermium nucleus ^{248}No

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[2]*Dubna State University, 141980 Dubna, Russia*
[3]*Institute of Nuclear Physics, Almaty, 050032 Kazakhstan*
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The capture cross sections, partial cross sections, and critical angular momenta L_{cr} were calculated using the code of coupling channel model KANTBP [28]. The advantage of this code, compared to the widely used codes of NRV [29,30] and CCFULL [31], is the careful treating of boundary conditions for solving the set of coupled Schrödinger equations. It allows one to keep a high accuracy of calculations that take into account a large number of coupled channels.

Figure 6:

Application in nuclear physics

Optical potentials and regular BC: $\psi_{nm}(r) \sim r^{l+1}$ at $r_{\min} = 0$

$$V_l(r) = \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\left(\Re \tilde{V}_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r}\right),$$

$$\tilde{E} > V_l^{\min} = V_l(r_{\min}^l)$$

$$\tilde{V}_N^{(0)}(r) = V_N^{(0)}(r) + \imath W_N^{(0)}(r) \qquad (15)$$

$$\sigma_f(E) = \sum_{l=1}^{l_{\max}(E)} P_l,$$

$$P_l = \frac{\pi}{\tilde{E}}(2l+1)\sum_{m=1}^{N_o^L}(1 - |\mathbf{R}_{m1}^{(l)}|^2), \qquad (16)$$

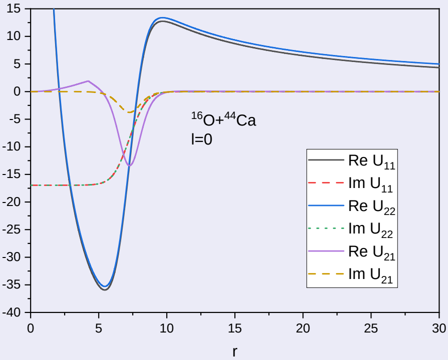

Figure 7:

Application in nuclear physics

Cross sections of light reaction ^{16}O+^{44}Ca

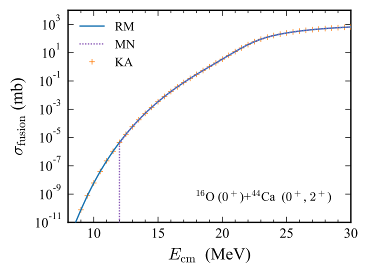

Figure 8: Fusion cross sections of ^{16}O+^{44}Ca.

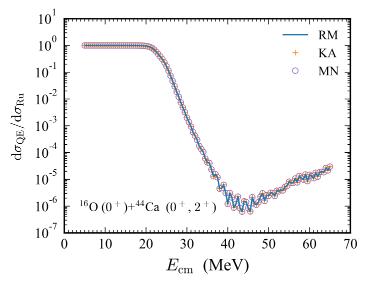

Figure 9: The back-angle QE cross section relative to the Rutherford cross section as a function of energy for ^{16}O+^{44}Ca.

R-matrix – P. Descouvemont, Comput. Phys. Commun. 200 (2016) 199.

Application in nuclear physics

Cross sections of heavy reaction $^{48}Ca+^{248}Cm$

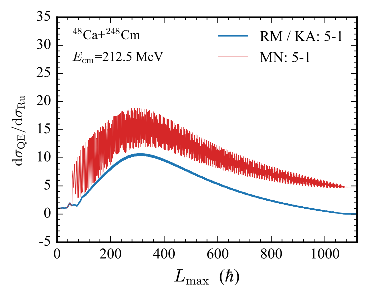

Figure 10: The back-angle quasi-elastic cross section relative to the Rutherford cross section as a function of $L_{\max}$ at deep sub-barrier energy $E_{\rm cm} = 172$ MeV.

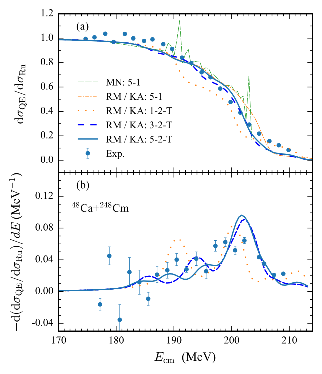

Figure 11: Upper panel: the back-angle QE cross section relative to the Rutherford cross section. Lower panel: the corresponding barrier distributions. The extra symbol '-T' denotes the extra consideration of the transfer channels in the CC calculation.

Application in nuclear physics

The Numerov method requires two initial conditions

$$\phi(r_i) = \left(1 - \frac{h^2}{12}\mathbf{A}(r_i)\right)\psi(r_i)$$

$$\phi(r_{i+1}) = \left(\left(\frac{h^2}{\sqrt{12}}\mathbf{A}(r_i) + \sqrt{3}\right)^2 - 1\right)\phi(r_i) - \phi(r_{i-1}) \quad (17)$$

$$A_{nn'}(r) = \frac{2\mu}{\hbar^2}\left[\left(\frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n - E\right)\delta_{nn'} + V_{nn'}(r)\right]$$

$$r_{i+1} = r_i + h$$

Application in nuclear physics

Numerov method in CCFULL

```
c integration of the io-th channel wave function from rmin = 0
    do 15 io=1,nlevel
      do 200 j1=1,nlevel
        psi0(j1)=0.d0
        psi1(j1)=0.d0
 200  continue
c initial conditions
      psi1(io)=1.d-6
      do 91 i0=1,nlevel
        xi1(i0,io)=(1.d0-fac/12.d0*(v(rmin+dr)-ai*w(rmin+dr)-e))*psi1(i0)
        do 92 ic=1,nlevel
          xi1(i0,io)=xi1(i0,io)
                    -fac/12.d0*(cpot(i0,ic,1)-ai*cpotw(i0,ic,1))*psi1(ic)
 92     continue
 91   continue
 15 continue
```

Application in nuclear physics

Numerov method in CCFULL

```
c integration of the io-th channel wave function from rmin = 0
    do 15 io=1,nlevel
      do 200 j1=1,nlevel
        psi0(j1)=0.d0
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c initial conditions
      psi1(io)=1.d-6
      do 91 i0=1,nlevel
        xi1(i0,io)=(1.d0-fac/12.d0*(v(rmin+dr)-ai*w(rmin+dr)-e))*psi1(i0)
        do 92 ic=1,nlevel
          xi1(i0,io)=xi1(i0,io)
                    -fac/12.d0*(cpot(i0,ic,1)-ai*cpotw(i0,ic,1))*psi1(ic)
 92     continue
 91   continue
 15 continue
```

Initial conditions in CCFULL:

$$\psi_{ij}(0) = 0 \quad \text{is correct but} \quad \psi_{ij}(h) = 10^{-6}\delta_{ij} \quad \text{is not correct} \qquad (18)$$

Conclusions

1. A FORTRAN program for calculating energy values, reflection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach are presented in Computer Physics Communications Program Library.

2. We found that the R-matrix method and the finite element method (KANTBP) are more stable for solving the multichannel scattering problem for the coupled channels equations compared to the Numerov method.

3. The programs KANTBP and R-matrix excellently confirm each other and outperform the CCFULL program.

Thank you for attention!