

# Разработка схем метода конечных элементов для исследования коллективных моделей атомных ядер

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## Физ. постановка задач

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## Содержание

- Одномерные краевые задачи
  - ▶ Задача на связанные состояния
    - ★ Задача на метастабильные состояния
  - ▶ Многоканальная задача рассеяния
  - ▶ Тесты
  - ▶ Приложения к физике атомных ядер
- Многомерные краевые задачи
  - ▶ Описание коллективных моделей атомных ядер

11 октября 2024, Дубна

Осенняя Школа по информационным технологиям ОИЯИ

# Finite Element Method

## Stages:

- BVP → minimization of quadratic functional problem
- Finite Element Mesh
- Construction of shape functions
  - ▶ Interpolation Polynomials
    - ★ Lagrange Interpolation Polynomials
    - ★ Hermite Interpolation Polynomials
  - ▶ ...
- Construction of piecewise polynomial functions by joining the shape functions
- Calculations of the integrals
  - ▶ Gaussian quadratures
  - ▶ ...
- Solving of Algebraic (Eigenvalue) Problem
  - ▶ Continuous Analog of Newton Method
  - ▶ ...

## Problem statement

Self-adjoint system of  $N$  second-order ODEs for unknowns  $\Phi(z) \equiv \{\Phi^{(i)}(z)\}_{i=1}^{N_o}$ ,  
 $\Phi^{(i)}(z) = (\Phi_1^{(i)}(z), \dots, \Phi_N^{(i)}(z))^T$  by  $z$  in the region  $z \in \Omega_z = (z^{\min}, z^{\max})$

$$\left( -\frac{1}{f_B(z)} \mathbf{I} \frac{d}{dz} f_A(z) \frac{d}{dz} + \mathbf{V}(z) + \frac{f_A(z)}{f_B(z)} \mathbf{Q}(z) \frac{d}{dz} + \frac{1}{f_B(z)} \frac{d f_A(z) \mathbf{Q}(z)}{dz} - E \mathbf{I} \right) \Phi(z) = 0.$$

$f_B(z) > 0$   $f_A(z) > 0$ ,  $\mathbf{I}$  is unit matrix;  $\mathbf{V}(z)$  and  $\mathbf{Q}(z)$  are a symmetric and an antisymmetric  $N \times N$  matrices, with real or complex-valued coefficients from the Sobolev space  $\mathcal{H}_2^{s \geq 1}(\Omega)$ .

All coefficients are continuous (or piecewise continuous) functions that have derivatives up to the order of  $\kappa^{\max} - 1 \geq 1$  in the domain  $z \in \bar{\Omega}_z$ .

The boundary conditions:

$$(I) : \quad \Phi(z^t) = 0,$$

$$(II) : \quad \lim_{z \rightarrow z^t} f_A(z) \left( \mathbf{I} \frac{d}{dz} - \mathbf{Q}(z) \right) \Phi(z) = 0,$$

$$(III) : \quad \lim_{z \rightarrow z^t} \left( \mathbf{I} \frac{d}{dz} - \mathbf{Q}(z) \right) \Phi(z) = \mathbf{G}(z^t) \Phi(z^t).$$

## Problem 1. For bound or metastable states

Case of the real potentials and real eigenvalues  $E$ :  $E_1 \leq E_2 \leq \dots \leq E_{N_o}$

$$\langle \Phi_m | \Phi_{m'} \rangle = \int_{z^{\min}}^{z^{\max}} f_B(z) (\Phi^{(m)}(z))^{\dagger} \Phi^{(m')}(z) dz = \delta_{mm'}.$$

Case of the complex potentials and complex eigenvalues  $E = \Re E + i\Im E$ :  
 $\Re E_1 \leq \Re E_2 \leq \dots \leq \Re E_{N_o}$ ,

The eigenfunctions  $\Phi_m(z)$  obey the normalization and orthogonality conditions

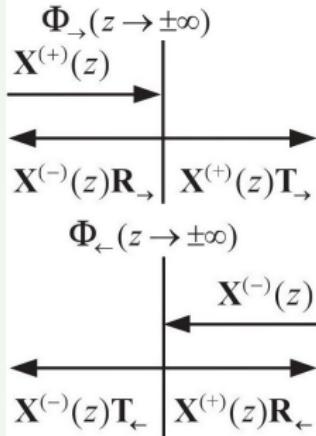
$$(\Phi_m | \Phi_{m'}) = \int_{z^{\min}}^{z^{\max}} f_B(z) (\Phi^{(m)}(z))^T \Phi^{(m')}(z) dz = \delta_{mm'}.$$

J.G. Muga, J.P. Palao, B. Navarro, I.L. Egusquiza Complex absorbing potentials  
Physics Reports 395 (2004) 357–426

A.A. Gusev et al, Symbolic-numeric solution of boundary-value problems for the Schrodinger equation using the finite element method: scattering problem and resonance states, Lecture Notes in Computer Science 9301 (2015) 182–197.

## Problem 2. The scattering problem

“incident wave + outgoing waves” asymptotic form



$$\Phi_{\rightarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}_{\min}^{(\rightarrow)}(z) + \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{R}_{\rightarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{R}_{\rightarrow}^c, & z \rightarrow -\infty \\ \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{T}_{\rightarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{T}_{\rightarrow}^c, & z \rightarrow +\infty \end{cases}$$

$$\Phi_{\leftarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{T}_{\leftarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{T}_{\leftarrow}^c, & z \rightarrow -\infty \\ \mathbf{X}_{\max}^{(\leftarrow)}(z) + \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{R}_{\leftarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{R}_{\leftarrow}^c, & z \rightarrow +\infty \end{cases}$$

$\Phi_{\rightarrow}(z)$ ,  $\Phi_{\leftarrow}(z)$  are the matrix solutions by dimension  $N \times N_o^L$ ,  $N \times N_o^R$

$N_o^L$ ,  $N_o^R$  are the numbers of open channels,

$\mathbf{X}_{\min}^{(\rightarrow)}(z)$ ,  $\mathbf{X}_{\min}^{(\leftarrow)}(z)$  are open channel asymptotic solutions at  $z \rightarrow -\infty$ , dim.  $N \times N_o^L$ ,

$\mathbf{X}_{\max}^{(\rightarrow)}(z)$ ,  $\mathbf{X}_{\max}^{(\leftarrow)}(z)$  are open channel asymptotic solutions at  $z \rightarrow +\infty$ , dim.  $N \times N_o^R$ ,

$\mathbf{X}_{\min}^{(c)}(z)$ ,  $\mathbf{X}_{\max}^{(c)}(z)$  are closed channel solutions, dim.  $N \times (N - N_o^L)$ ,  $N \times (N - N_o^R)$ ,

$\mathbf{R}_{\rightarrow}$ ,  $\mathbf{R}_{\leftarrow}$  are the reflection amplitude square matrices of dimension  $N_o^L \times N_o^L$ ,  $N_o^R \times N_o^R$ ,

$\mathbf{T}_{\rightarrow}$ ,  $\mathbf{T}_{\leftarrow}$  are the transmission amplitude rectangular mat. of dim.  $N_o^R \times N_o^L$ ,  $N_o^L \times N_o^R$ ,

$\mathbf{R}_{\rightarrow}^c$ ,  $\mathbf{T}_{\rightarrow}^c$ ,  $\mathbf{T}_{\leftarrow}^c$ ,  $\mathbf{R}_{\leftarrow}^c$  are auxiliary matrices.

## Problem 2. The scattering problem

Wronskian conditions

$$\mathbf{Wr}(\mathbf{Q}(z); \mathbf{X}^{(\mp)}(z), \mathbf{X}^{(\pm)}(z)) = \pm 2\imath I_{oo}, \quad \mathbf{Wr}(\mathbf{Q}(z); \mathbf{X}^{(\pm)}(z), \mathbf{X}^{(\pm)}(z)) = \mathbf{0}$$

$$\mathbf{Wr}(\mathbf{Q}(z); \mathbf{a}(z), \mathbf{b}(z)) = \mathbf{a}^T(z) \left( \frac{d\mathbf{b}(z)}{dz} - \mathbf{Q}(z)\mathbf{b}(z) \right) - \left( \frac{d\mathbf{a}(z)}{dz} - \mathbf{Q}(z)\mathbf{a}(z) \right)^T \mathbf{b}(z).$$

For real-valued potentials

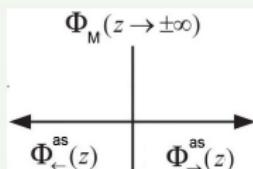
$$\begin{aligned} \mathbf{T}_{\rightarrow}^{\dagger} \mathbf{T}_{\rightarrow} + \mathbf{R}_{\rightarrow}^{\dagger} \mathbf{R}_{\rightarrow} &= \mathbf{I}_{oo}, & \mathbf{T}_{\leftarrow}^{\dagger} \mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^{\dagger} \mathbf{R}_{\leftarrow} &= \mathbf{I}_{oo}, \\ \mathbf{T}_{\rightarrow}^{\dagger} \mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^{\dagger} \mathbf{T}_{\leftarrow} &= \mathbf{0}, & \mathbf{R}_{\leftarrow}^{\dagger} \mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^{\dagger} \mathbf{R}_{\rightarrow} &= \mathbf{0}, \\ \mathbf{T}_{\rightarrow}^T &= \mathbf{T}_{\leftarrow}, & \mathbf{R}_{\rightarrow}^T &= \mathbf{R}_{\rightarrow}, & \mathbf{R}_{\leftarrow}^T &= \mathbf{R}_{\leftarrow}. \end{aligned}$$

For real-valued potentials the scattering matrix is symmetric and unitary, for complex potentials it is only symmetric

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix}, \quad \mathbf{S}^{\dagger} \mathbf{S} = \mathbf{S} \mathbf{S}^{\dagger} = \mathbf{1}.$$

Problem 3. The metastable state pr. with complex e.v.  $E = \Re E + i\Im E$ :

Asymptotic form



$$\Phi_{\rightarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{O}_{\leftarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{O}_{\leftarrow}^c, & z \rightarrow -\infty \\ \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{O}_{\rightarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{O}_{\rightarrow}^c, & z \rightarrow +\infty \end{cases}$$

Robin (Siegert) BC

$$(III) : \lim_{z \rightarrow z^t} \left( I \frac{d}{dz} - \mathbf{Q}(z) \right) \Phi(z) = \mathbf{G}(z^t) \Phi(z^t), \quad t = \min \text{ and/or } \max$$

$$\mathbf{G}(z^t) = \left( \lim_{z \rightarrow z^t} \left( I \frac{d}{dz} - \mathbf{Q}(z) \right) \left( \mathbf{X}_t^{(\leftarrow)}(z), \mathbf{X}_t^{(c)}(z) \right) \right) \left( \mathbf{X}_t^{(\leftarrow)}(z^t), \mathbf{X}_t^{(c)}(z^t) \right)^{-1}$$

Orthonormalization conditions

$$(\Phi_m | \Phi_{m'}) = \int f_B(z) (\Phi^{(m)}(z))^T \Phi^{(m')}(z) dz = \delta_{mm'}.$$

J.G. Muga, J.P. Palao, B. Navarro, I.L. Egusquiza Complex absorbing potentials  
Physics Reports 395 (2004) 357–426

## Tests:

- BP for 1 ODE
  - ▶ Morse potential
  - ▶ Pöschl-Teller potential
  - ▶ Scarf complex potential
- BP for  $N$  ODE
  - ▶ system of piecewise constant potentials
- BP for multidimensional PDE
  - ▶ Helmholtz eq. for some domains (square, equilateral triangle, ...)
  - ▶ Coulomb potential
  - ▶ Harmonic oscillator

## Test example (ODE System with Piecewise Constant Potentials)

$$\left( -\mathbf{I} \frac{d^2}{dz^2} + \mathbf{V}(z) - E \mathbf{I} \right) \Phi(z) = 0, \quad \mathbf{V}(z) = \{\mathbf{V}_1, z \leq z_1, \dots, \mathbf{V}_{k-1}, z \leq z_{k-1}, \mathbf{V}_k, z > z_{k-1}\},$$

### Matching the Fundamental Solutions

$$\begin{aligned} & \left( -\mathbf{I} \frac{d^2}{dz^2} + \mathbf{V}_m - E \mathbf{I} \right) \Phi_m(z) = 0, \quad z \in (z_{m-1}, z_m], \quad m = 1, \dots, k, \\ \Rightarrow \quad & \Phi_m(z) = \sum_{i=1}^N \left( A_i^{(m)} \exp(-\sqrt{\lambda_i^{(m)} - E} z) \Psi_i^{(m)} + B_i^{(m)} \exp(\sqrt{\lambda_i^{(m)} - E} z) \Psi_i^{(m)} \right), \end{aligned}$$

Here  $\lambda_i^{(m)}$  and  $\Psi_i^{(m)}$  are the solutions of the algebraic eigenvalue problems

$$\mathbf{V}^{L,R} \Psi_i^{(m)} = \lambda_i^{(m)} \Psi_i^{(m)}, \quad (\Psi_i^{(m)})^T \Psi_j^{(m)} = \delta_{ij}.$$

$$\begin{aligned} \lim_{z \rightarrow z_{m-1}} \Phi_{m-1}(z) - \Phi_m(z) &= 0, \quad \lim_{z \rightarrow z_{m-1}} \frac{\Phi_{m-1}(z)}{dz} - \frac{\Phi_m(z)}{dz} = 0, \quad m = 2, \dots, k \\ \Rightarrow & 2N(k-1) \text{ linear eqs. with } 2N(k-1) \text{ unknowns.} \end{aligned}$$

Problem 2. The scattering problem. Example of asymptotic solutions  
 ODE in asymptotic regions  $z \rightarrow \pm\infty$

$$\left( -\mathbf{I} \frac{d^2}{dz^2} + \mathbf{V}^{L,R} - E \mathbf{I} \right) \Phi(z) = 0, \quad \text{where } \mathbf{V}^{L,R} \text{ are constant matrices.}$$

### Asymptotic solutions

The open channel asymptotic solutions:  $i_o = 1, \dots, N_o^{L,R}$ :

$$\mathbf{X}_{i_o}^{(\leftrightarrow)}(z \rightarrow \pm\infty) \rightarrow \frac{\exp\left(\pm i\sqrt{E - \lambda_{i_o}^{L,R}} z\right)}{\sqrt[4]{E - \lambda_{i_o}^{L,R}}} \Psi_{i_o}^{L,R}, \quad \lambda_{i_o}^{L,R} < E.$$

The closed channels asymptotic solutions  $i_c = N_o^{L,R} + 1, \dots, N$ :

$$\mathbf{X}_{i_c}^{(c)}(z \rightarrow \pm\infty) \rightarrow \exp\left(-\sqrt{\lambda_{i_c}^{L,R} - E}|z|\right) \Psi_{i_c}^{L,R}, \quad \lambda_{i_c}^{L,R} \geq E.$$

Here  $\lambda_i^{L,R}$  and  $\Psi_i^{L,R}$  are the solutions of the algebraic eigenvalue problems

$$\mathbf{V}^{L,R} \Psi_i^{L,R} = \lambda_i^{L,R} \Psi_i^{L,R}, \quad (\Psi_i^{L,R})^T \Psi_j^{L,R} = \delta_{ij}.$$

Problem 3. The metastable state pr. with complex e.v.  $E = \Re E + i\Im E$ :

### Example of asymptotic solutions

The open channel asymptotic solutions:  $i_o = 1, \dots, N_o^{L,R}$ :

$$\mathbf{X}_{i_o}^{(\rightarrow)}(z \rightarrow \infty) \rightarrow \exp \left( +i\sqrt{E - \lambda_{i_o}^{L,R}}|z| \right) \Psi_{i_o}^{L,R}, \quad \lambda_{i_o}^{L,R} < \Re E, \quad i_o = 1, \dots, N_o^{L,R},$$

The closed channels asymptotic solutions  $i_c = N_o^{L,R} + 1, \dots, N$ :

$$\mathbf{X}_{i_c}^{(c)}(z \rightarrow \infty) \rightarrow \exp \left( -\sqrt{\lambda_{i_c}^{L,R} - E}|z| \right) \Psi_{i_c}^{L,R}, \quad \lambda_{i_c}^{L,R} \geq \Re E, \quad i_c = N_o^{L,R} + 1, \dots, N.$$

### Robin BC

$$\mathcal{R}(z^t) = \Psi^{L,R} \mathbf{F}^{L,R} \left( \Psi^{L,R} \right)^{-1},$$

$$\mathbf{F}^{L,R} = \text{diag}(\dots, \pm \sqrt{\lambda_{i_c}^{L,R} - E}, \dots, \mp i\sqrt{E - \lambda_{i_o}^{L,R}}, \dots)$$

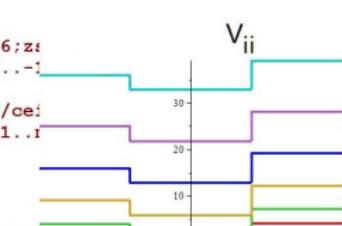
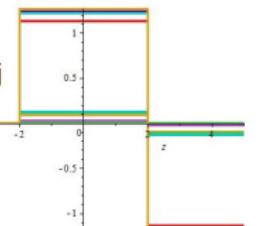
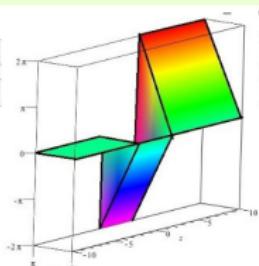
# The piecewise constant potentials

F:\Sasha\4m\4m2\m1e.txt - [Server 3] - Maple 2021

айл (F) Помощь (H) Вид (V) Вспомог (I) Формат (R) Вычислить (A) Инструменты (T) Окно (W) Помощь (H)

Start.mw X "m1e.txt X Текущий документ Maple Input Courier New 12 I U Искать Alt+S

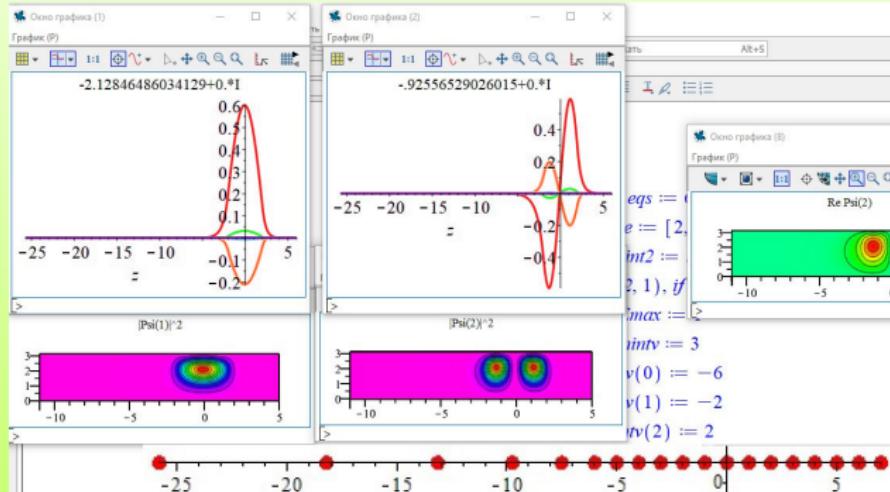
```
> restart;read "kantbp5m.mwt";
> eqs:=6;
> IHPType:=[2,2,2,2];
> print2:=true;
>
>
> for i from 1 to eqs do
>   for il from i to eqs do
>     v(i,il,1):=0; v(il,i,1):=0;
>     v(i,il,2):=-2*int(sin(i*y)*sin(il*y)*y^2/Pi,y=0..Pi); v(il,i,2):=v(i,il,2);#z in (-2,2)
>     v(i,il,3):= 2*int(sin(i*y)*sin(il*y)*y^2/Pi,y=0..Pi); v(il,i,3):=v(i,il,3);#z>2
>   od;
>   v(i,i,1):=i^2;
>   v(i,i,2):=v(i,i,2)+i^2;
>   v(i,i,3):=v(i,i,3)+i^2;
> od;
>
> vpot:=proc(il,i2,z) `if` (z<-2,v(il,i2,1),`if` (z<2,v(il,i2,2),v(il,i2,3))); end;
>
> Emax:=1;
> nintv:=3;
> zintv(0):=-6;zintv(1):=-2;zintv(2):=2;zintv(3):=6;z
> zmesh:=[seq(zintv(0)-zstep*3*((2/3.)^ii-1),ii=-5..-1
> ,zintv(0)
> ,seq(seq(zintv(ii-1)+i*(zintv(ii)-zintv(ii-1))/ce
> ,i=1..ceil((zintv(ii)-zintv(ii-1))/zstep)),ii=1..r
> kantbp5m();
>
> read "ev1proc.dat";
> ev:=proc(j,y,z) local jc;
>   add(-EIGF1(j,jc,z,0)*sqrt(2/3.14159265358)*sin(jc
> end.
```



Готово Редактирование Профили Maple по умолчанию F:\Sasha\4m\4m2 Папки: 4,08M Время: 0,23s Максимб: 150% Текстовый режим

A. Gusev, S. Vinitksy, V. Gerdt, O. Chuluunbaatar, G. Chuluunbaatar, L. Le Hai, E. Zima, A Maple implementation of the finite element method for solving boundary problems of the systems of ordinary second order differential equations. Maple

## The piecewise constant potentials (eigenvalue problem)



$\text{zmesh} := [-25.78124999, -18.18750000, -13.12500000, -9.7500000000, -7.5000000000, -6, -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6]$

```

    "EIGV(1)=-2.12846486034129+0.*I;"  

    "EIGV(2)=-.92556529026015+0.*I;"  

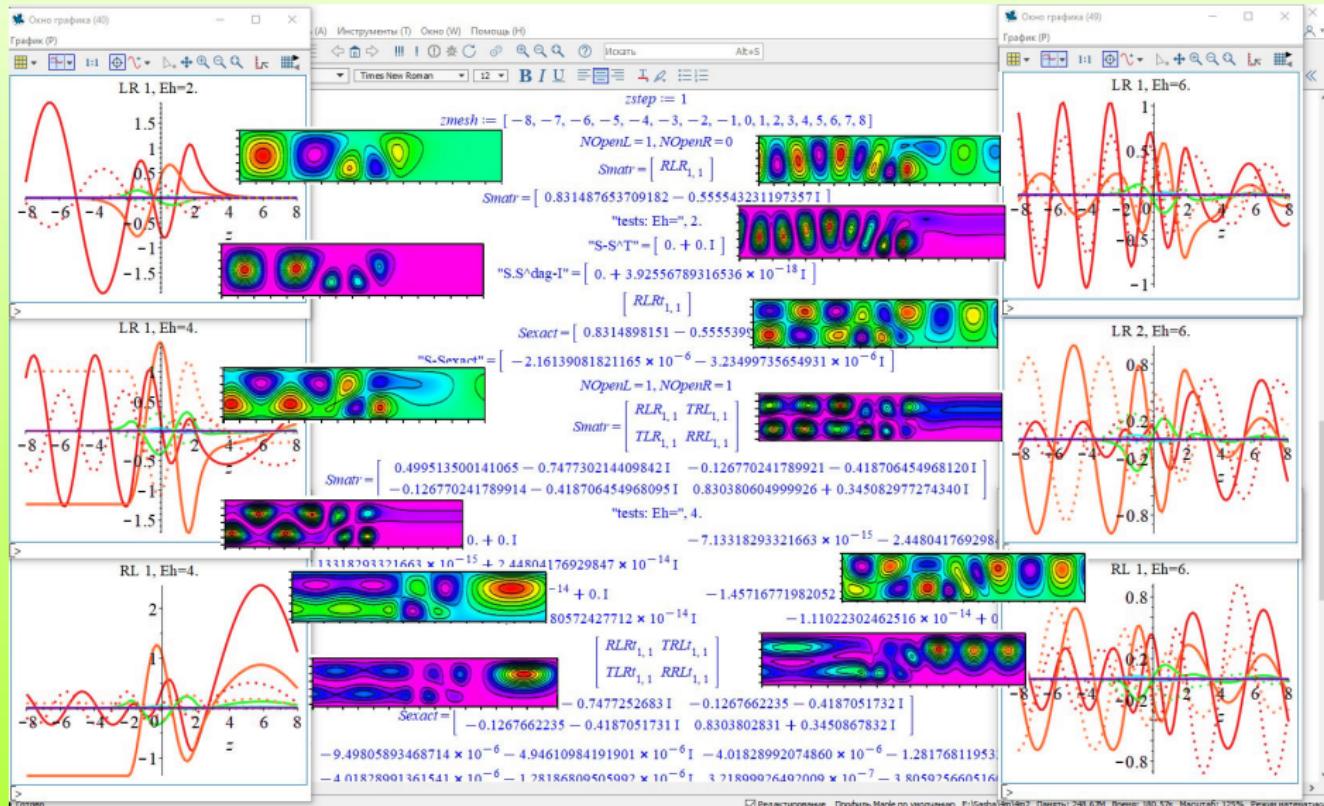
    "EIGV(3)=.83512734313781+0.*I;"  


```

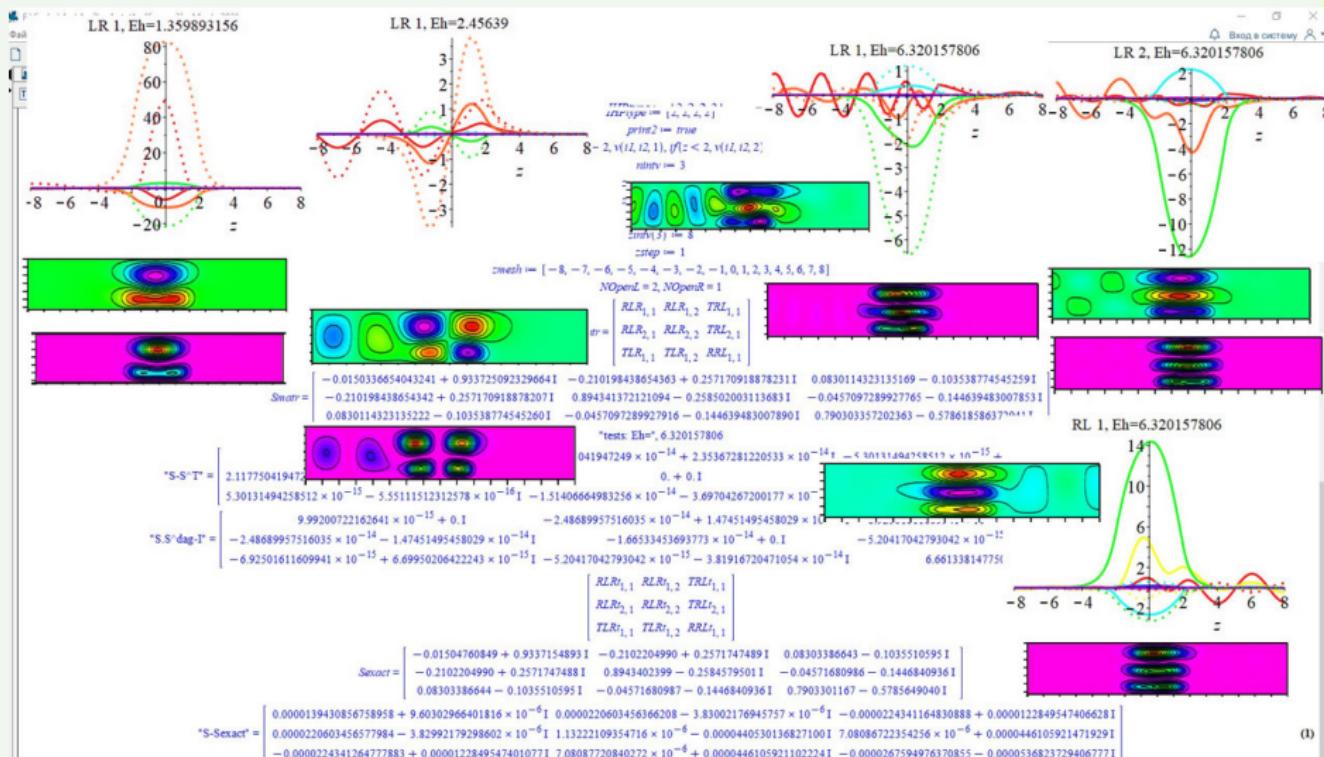
**z)** **local** jc; **add**(-EIGF1(j, jc, z, 0) \* sqrt(2/3.14159265358) \* sin(jc\*y), jc=1..  
1, -2.12846486034129 + 0. I, -2.128465032, -1.71658714798184 × 10<sup>-7</sup> - 0. I  
, -0.925565290260150 + 0. I, -0.9255658838, -5.93539849824687 × 10<sup>-7</sup> - 0. I

Редактирование Профиль Мария по умолчанию F1|[Sasha]-4m2 Пакеты: 130.07М Время: 37.89с Масштаб: 150% Текстовый режим

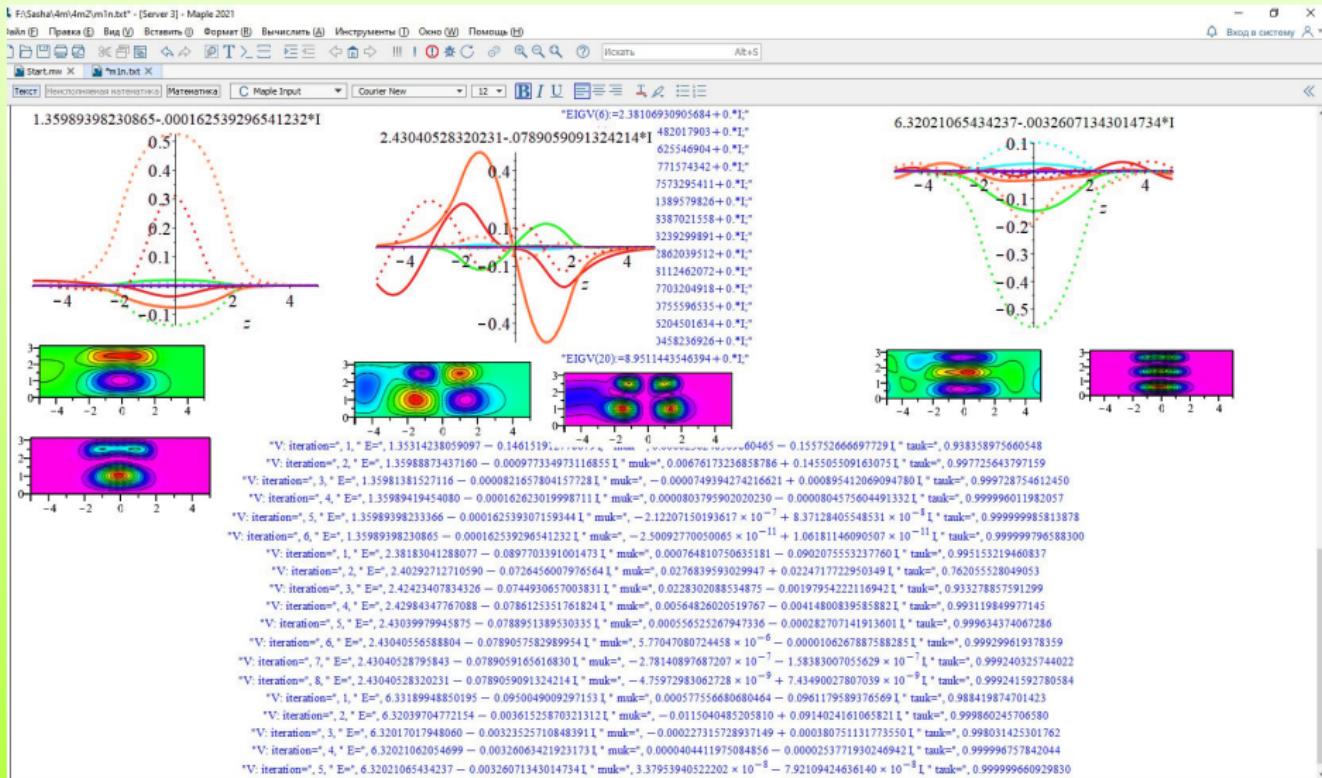
# The piecewise constant potentials (multichannel scattering problem)



# The piecewise constant potentials (resonance scattering states)



## The piecewise constant potentials (metastable state problem)



## Sub-barrier reactions of the fusion of heavy ions

The coupled-channels Schrödinger equation  $^{64}\text{Ni} + ^{100}\text{Mo}$  ( $N = 27$ )

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n - E \right] \psi_{nn_o}(r) + \sum_{n'=1}^N V_{nn'}(r) \psi_{n'n_o}(r) = 0,$$

$V_{nn'}(r)$  are mat. elem. of Coulomb and the Nuclear (Woods-Saxon,  $V_N^{(0)}(r)$ ) potentials.

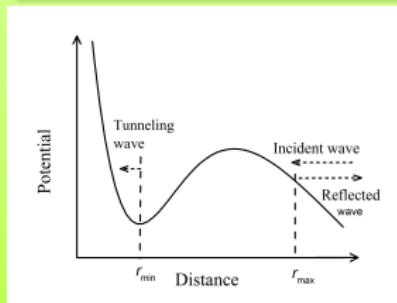
P.W. Wen, O. Chuluunbaatar, A.A. Gusev, R.G. Nazmitdinov, A.K. Nasirov, S.I. Vinitsky, C.J. Lin, and H.M. Jia, Near-barrier heavy-ion fusion: Role of boundary conditions in coupling of channels, Phys. Rev. C 101, pp. 014618 (2020).

P. W. Wen , C. J. Lin, R. G. Nazmitdinov , S. I. Vinitsky, O. Chuluunbaatar, A. A. Gusev, A. K. Nasirov, H. M. Jia, and A. Gózdź Potential roots of the deep subbarrier heavy-ion fusion hindrance phenomenon within the sudden approximation approach, Physical Review C 103, 054601 (2021)

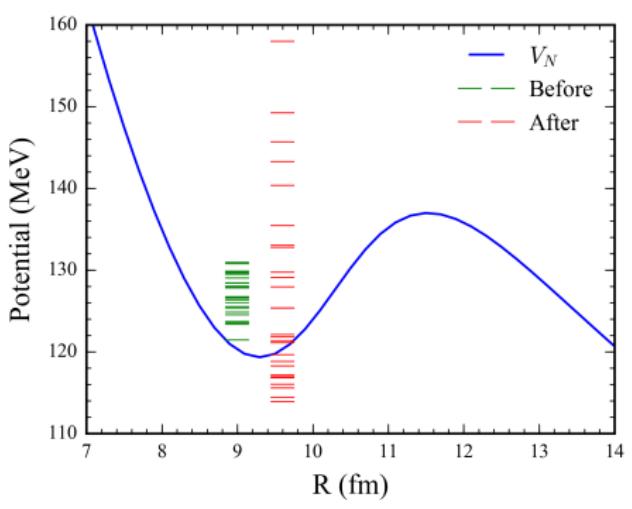
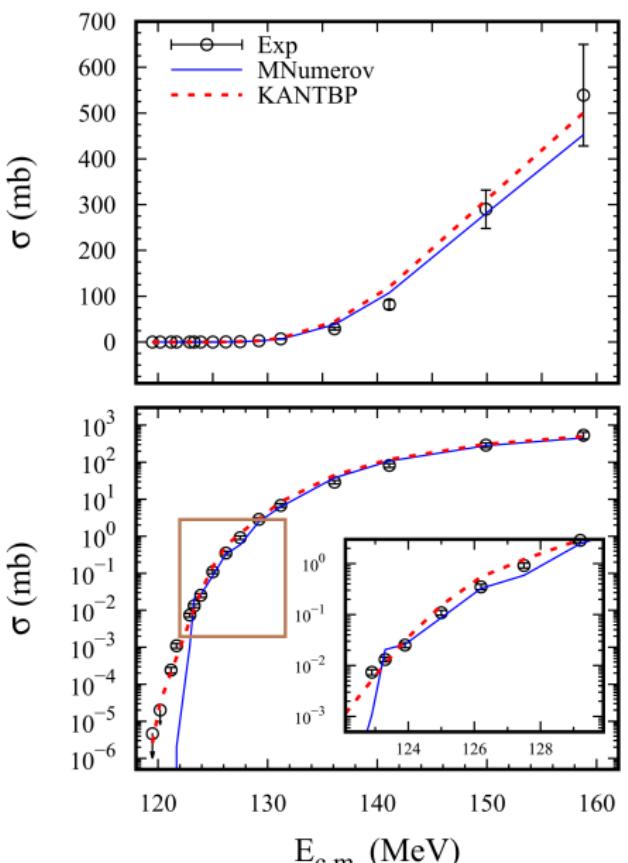
## Sub-barrier reactions of the fusion of heavy ions

$$\psi_{nn_o}^{as}(r) = \sum_{m=1}^{M_o} A_{nm} \frac{\exp(-iK_m r)}{\sqrt{K_m}} \hat{T}_{mn_o} + \sum_{m=M_o+1}^N A_{nm} \frac{\exp(|K_m|r)}{\sqrt{|K_m|}} \hat{T}_{mn_o}^c, \quad r = r_{\min},$$
$$\psi_{nn_o}^{as}(r) = \begin{cases} \hat{H}_I^-(k_n r) \delta_{n,n_o} + \hat{H}_I^+(k_n r) \hat{R}_{nn_o}, & r = r_{\max}, \\ 2|k_n|^{1/2} r \exp(-|k_n|r) U(1 + \eta_n, 2, 2|k_n|r), & r = r_{\max}. \end{cases}$$

$\hat{H}_I^\pm(k_n r)$  are Coulomb functions,  $U(1 + \eta_n, 2, 2|k_n|r)$  is Whittaker function



# $^{64}\text{Ni} + ^{100}\text{Mo}$ : Deep sub-barrier fusion



MNumerov, are the results obtained by means of CCFULL [K. Hagino, N. Rowley, and A.T. Kruppa, A FORTRAN77 program for coupled-channels calculations with all order couplings for heavy-ion fusion reactions; Comput. Phys. Comm 123 (1999) 143 - 152, also CCFULL Home Page]

## 5DBVP for the five-dimensional quarupole Hamiltonian(5DQH)

The Schrödinger equation with respect to eigenfunction  $\Psi_{nlM} \equiv \Psi_{nlM}(\beta, \gamma, \vartheta_i)$  and the corresponding eigenvalues of energy  $E_{nl}$  has the form

$$\frac{2}{\hbar^2} (\hat{H} - E_{nl}) \Psi_{nlM} = \left( \hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + \frac{2}{\hbar^2} (V - E_{nl}) \right) \Psi_{nlM} = 0. \quad (1)$$

orthogonality and normalization conditions

$$\int_{\Omega_5} \Psi_{nlM} \Psi_{n'l'M'} g_0(\beta, \gamma) d\beta d\gamma \sin \vartheta_2 d\vartheta_1 d\vartheta_2 d\vartheta_3 = \delta_{nn'} \delta_{ll'} \delta_{MM'}. \quad (2)$$

The eigenfunction  $\Psi_{nlM}$  in the representation of the angular momentum  $l$  and its projections  $K$  and  $M$  on the third axes of the intrinsic and laboratory frames

$$\Psi_{nlM}(\beta, \gamma, \vartheta_i) = \sum_{K \geq 0, \text{even}}^l D_{MK}^{l*}(\vartheta_i) \Phi_{nlK}(\beta, \gamma), \quad (3)$$

where  $D_{MK}^{l*}(\vartheta_i)$  are the normalized D-functions with the space parity  $\hat{\pi} = \pm 1$

$$D_{MK}^{l*}(\vartheta_i) = \sqrt{\frac{2l+1}{8\pi^2}} \frac{(D_{MK}^{l*}(\vartheta_i) + \hat{\pi}(-1)^l D_{M-K}^{l*}(\vartheta_i))}{\sqrt{2(1 + \delta_{K0})}}. \quad (4)$$

## 2DBVP for five-dimensional quarupole Hamiltonian(5DQH)

The unknown set of  $I_{\max}$  internal components  $\Phi_{nlK} \equiv \Phi_{nlK}(\beta, \gamma)$ , where  $K = 0, 2, \dots, I$  for even  $I$ , or  $K = 2, 4, \dots, (I - 1)$  for odd  $I$ , compose the vector eigenfunction  $\Phi_{nl}$  corresponding to the eigenvalue  $E_n^l$  (in MeV) of the BVP for a system of  $I/2 + 1$  or  $(I - 1)/2$  equations for even or odd  $I$ , respectively:

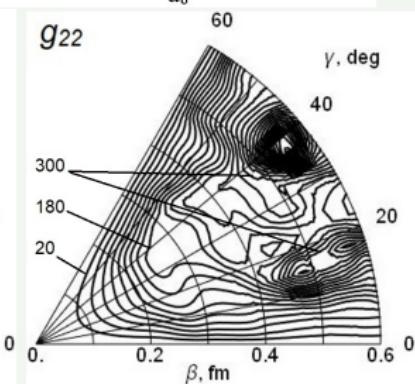
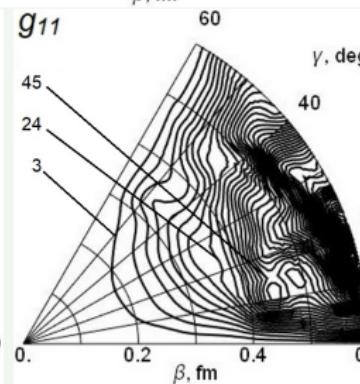
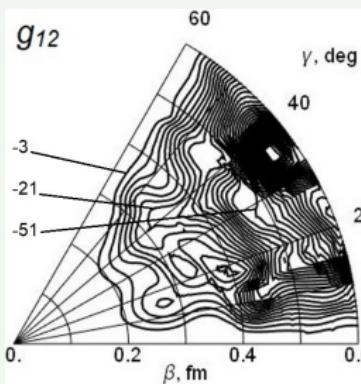
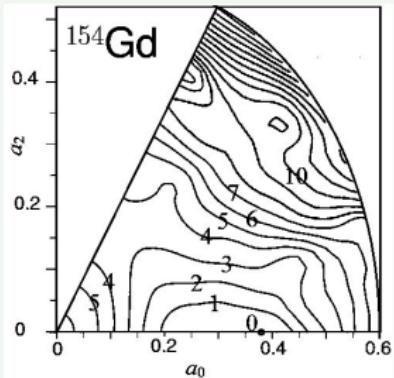
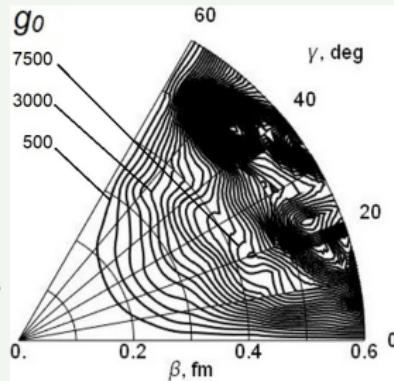
$$\begin{aligned} & \left[ \hat{T}_{\text{vib}} + T'_{KK} + \frac{2}{\hbar^2} (V - E_{nl}) \right] \Phi_{nlK} + T'_{KK+2} \Phi_{nlK+2} + T'_{KK-2} \Phi_{nlK-2} = 0, \\ & \hat{T}_{\text{vib}}(x_1, x_2) = -\frac{1}{g_0(x_1, x_2)} \sum_{i,j=1}^2 \frac{\partial}{\partial x_i} g_{ij}(x_1, x_2) \frac{\partial}{\partial x_j}, \\ & T'_{KK} = (I(I+1) - K^2) \left( \frac{1}{2J_1} + \frac{1}{2J_2} \right) + \frac{K^2}{J_3}, \quad T'_{KK\pm 2} = \left( \frac{1}{4J_1} - \frac{1}{4J_2} \right) C'_{KK\pm 2}, \\ & C'_{KK+2} = C'_{K+2K} = (1 + \delta_{K0})^{1/2} [(I - K)(I + K + 1)(I - K - 1)(I + K + 2)]^{1/2}, \\ & J_k(x_1, x_2) = J_k(\beta, \gamma) = 4B_k(\beta, \gamma)\beta^2 \sin^2(\gamma - 2\pi k/3). \end{aligned} \tag{5}$$

The components  $\Phi_{nlK}$  are subject to Neumann or Dirichlet boundary conditions at the boundary  $\partial\Omega_2$  of the domain  $\Omega_2$  and the orthogonality and normalization conditions

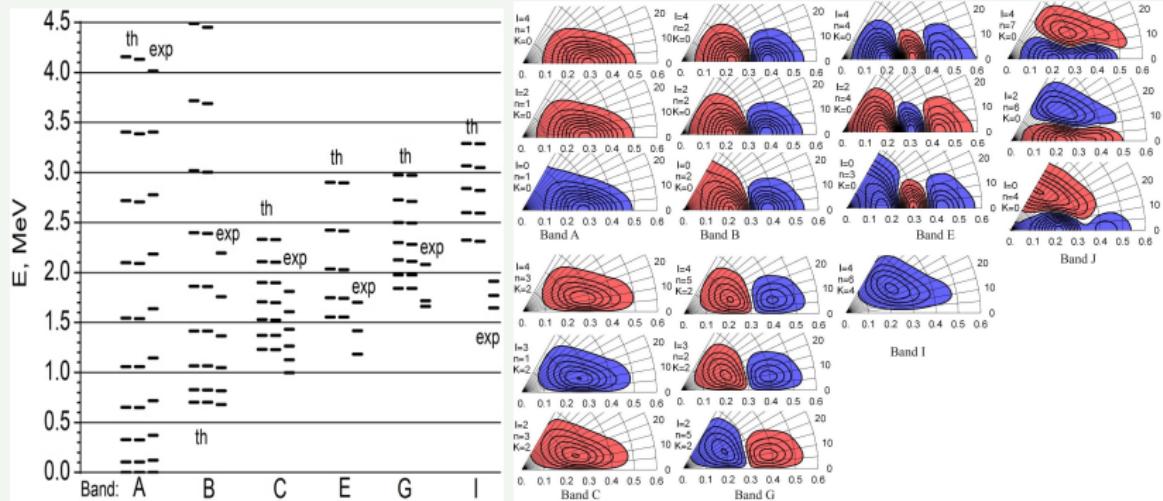
$$\int_0^{\beta_{\max}} \int_0^{\pi/3} g_0(\beta, \gamma) d\beta d\gamma \sum_{\substack{K \geq 0, \text{even}}}^{I_{\max}} \Phi_{nlK}(\beta, \gamma) \Phi_{n'l'K}(\beta, \gamma) = \delta_{nn'}. \tag{6}$$

# Benchmark calculations of $^{154}\text{Gd}$ in the RMF model

Spectrum  $E$ , isolines of  $V(\beta, \gamma)$  counted from the minimum of  $V(\beta=0.3875, \gamma=0) = -1270.6\text{ MeV}$ ,  $g_0(\beta, \gamma)$  and  $g_{ij}(\beta, \gamma)$  of  $^{154}\text{Gd}$  calculated in PC-F1 of RMF model



# Energy spectrum of $^{154}\text{Gd}$



Energy spectrum of  $^{154}\text{Gd}$ . For each state of the bands A, B, E, C, G, and I, three short bars correspond to the diagonal approximation (left), nondiagonal one (middle), and experiment (right) [<http://www.nndc.bnl.gov/ensdf/>].

Band(A) is the  $K^\pi = 0+$  ground state band;

Band(B): the first excited  $K^\pi = 0^+$  ( $\beta$ -vibrational) band;

Band(E), Band(J), Band(K): the second, third and forth excited  $K^\pi = 0^+$  bands;

Band(C): the  $K^\pi = 2^+$  ( $\gamma$ -vibrational) band;

Band(G): the second excited  $K^\pi = 2^+$  ( $\beta\gamma$ -vibrational) band;

Band(I): the  $K^\pi = 4^+$  band.

# Возможная постановка задачи для дипломных работ

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Letter

## Cluster effects on low-energy carbon burning

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### 2. Theory

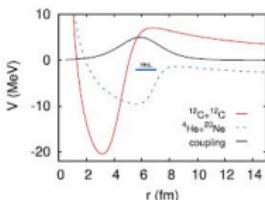
The fusion dynamics of two coupled channels involving two binary mass partitions of  $^{24}\text{Mg}$  can be described by solving the time-dependent Schrödinger equation for the radial wave functions,  $\psi_1(r, t)$  and  $\psi_2(r, t)$ , of each channel:

$$i\hbar \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \hat{T}_1 + V_1 + \epsilon_1 & V_{12} \\ V_{21} & \hat{T}_2 + V_2 + \epsilon_2 - Q_{12} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad (1)$$

where  $\hat{T}_{1,2}$  are the radial kinetic energy operators,  $\epsilon_{1,2}$  are intrinsic excitation energies,  $Q_{12}$  is the relative  $Q$ -value of the two-mass partitions,  $V_{12}(r) = V_{21}(r)$  is the real coupling potential between the partitions, and  $V_{1,2}(r)$  are the total interaction potentials in each partition. The latter are optical potentials:

$$V_{1,2}(r) = U_{1,2}(r) - iW(r), \quad (2)$$

Fig. 1. Total real potentials of the two channels problem, including the  $Q$ -value shift ( $Q_{12} = 4.62$  MeV) of the  $^4\text{He} + ^{20}\text{Ne}$  potential relative to the  $^{12}\text{C} + ^{12}\text{C}$  potential of the entrance channel. The Coulomb barrier for  $^{12}\text{C} + ^{12}\text{C}$  is approximately 7 MeV.



## Краевая задача для системы ОДУ

$$\left( -\frac{1}{f_B(z)} \frac{d}{dz} \mathbf{f}_A(z) \frac{d}{dz} + \mathbf{V}(z) + ? \frac{f_A(z)}{f_B(z)} \mathbf{Q}(z) \frac{d}{dz} + ? \frac{1}{f_B(z)} \frac{d f_A(z) \mathbf{Q}(z)}{dz} - E \mathbf{I} \right) \Phi(z) = 0.$$