The finite element calculations for some problems of nuclear physics

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Outline

- What is Finite Element Method?
- 1D problem statement
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- Conclusion

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International School on Nuclear Methods and Applied Research in Environmental, Material and Life Sciences (NUMAR-GOBI)

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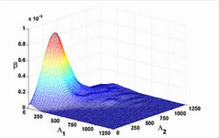
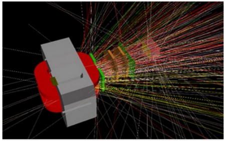
Research Areas



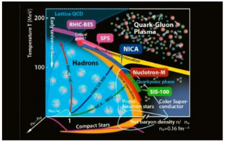
Modeling & Simulation

Development and use of mathematical and computer methods for modeling new experimental facilities, accelerator complexes and their elements, nuclear-physical processes, complex physical systems.



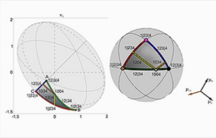
Methods & Algorithms

Development of new mathematical methods for extracting significant information from data obtained in experiments conducted with the participation of JINR; algorithms and software complexes for solving problems in high energy physics, nuclear physics, condensed matter physics, including the LHC, NICA, FAIR accelerator complexes, as well as the experimental facilities of the JINR neutrino program.



Numerical Computing

Development and support of the information-computing environment of the heterogeneous platform HybriLIT including installation and maintenance of specialized libraries and application software packages



Algebraic & Quantum Computation

Development of computer algebra-based methods, symbolic – numeric algorithms and software to solve scientific and technical problems arising in research conducted at JINR and its member states.

References

- O.C. Zienkiewicz. The finite element method in engineering science. MCgraw-hill. London, 1971.
- W. G. Strang, G. J. Fix, An analysis of the finite element method. Prentice-Hall, 1973.
- P.Ciarlet The Finite Element Method for Elliptic Problems. North-Holland Publ., 1978.
- K. J. Bathe: Finite Element Procedures In Engineering Analysis. Prentice-Hall Inc, Englewood Cliffs, New Jersey 1982.
- V.V. Shaidurov, Multigrid Methods for Finite Elements, Springer, 1995.
- ...

Discrete & Continuous Models
& Applied Computational Science

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Research article

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The volume integral equation method in magnetostatic problem

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In the presented work the main aspects of applying this approach to magnetic systems modelling are discussed on the example of linear approximation of unknown variables: discretisation of initial equations, decomposition of the calculation area to elements, calculation of discretised system matrix elements, solving the resulting non-linear equation system. In the framework of finite element method the calculation area is divided into a set of tetrahedrons. At the beginning the initial area is approximated

Key words and phrases: finite element method, magnetostatics, volume integral equations, systems of nonlinear equations, cubature formulae, iterative process

5. Magnet system modelling

The method of volume integral equations with the linear approximation of magnetization has been used for modelling the dipole and quadrupole magnets. The model of a variant of the projected dipole magnet for CBM experiment (GSI, Darmstadt) is shown In Figure 2a. A splitting of the magnet into the tetrahedrons has been done with the help of the generator **3DFEMMesh**. In the process of modelling the dipole symmetry of magnetic field has been taken into account, that allowed to reduce the number of unknown parameters by 8 times. One eighth of the magnet has been divided into 5264 tetrahedrons. There are 1363 vertexes in all tetrahedrons. In Figure 2b the distribution of the magnet field module inside the magnet is shown.The results given in Figure 2c show agreement of the present method with the famous code **TOSCA** [6] which is based on solving partial differential equations.

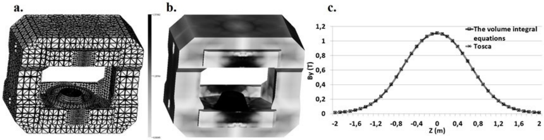


Figure 2. 3D modelling of dipole magnet CBM

The proposed approach has been also applied to the modelling of the **BOOSTER** quadrupole magnet of the projected accelerating complex **NICA** (JINR, Dubna).

The statement of the problem

A self-adjoint elliptic PDE in the region $z = (z_1, ..., z_d) \in \Omega \subset \mathcal{R}^d$ (Ω is polyhedra)

$$\left(-\frac{1}{g_0(z)} \sum_{ij=1}^{d} \frac{\partial}{\partial z_i} g_{ij}(z) \frac{\partial}{\partial z_j} + V(z) - E \right) \Phi(z) = 0, \quad g_0(z) > 0, \quad g_{ji}(z) = g_{ij}(z).$$

Boundary conditions

$$\begin{aligned}
\text{(Dirichlet)}: \quad & \Phi(z)|_S = 0, \\
\text{(Neumann)}: \quad & \left.\frac{\partial \Phi(z)}{\partial n_D}\right|_S = 0, \quad \frac{\partial \Phi(z)}{\partial n_D} = \sum_{ij=1}^{d} (\hat{n}, \hat{e}_i) g_{ij}(z) \frac{\partial \Phi(z)}{\partial z_j}, \\
\text{(Robin)}: \quad & \left.\frac{\partial \Phi(z)}{\partial n_D}\right|_S + \sigma(s) \Phi(z)\Big|_S = 0,
\end{aligned}$$

$\frac{\partial \Phi_m(z)}{\partial n_D}$ is the derivative along the conormal direction
$\hat{n}$ is the outer normal to the boundary of the domain $\partial\Omega$.

Ladyzhenskaya, O. A., The Boundary Value Problems of Mathematical Physics, Applied Mathematical Sciences, 49, (Berlin, Springer, 1985).
Shaidurov, V.V. Multigrid Methods for Finite Elements (Springer, 1995).

The statement of the problem

Conditions of normalization and orthogonality (for discrete spectrum problem)

$$\langle \Phi_m(z) | \Phi_{m'}(z) \rangle = \int\limits_{\Omega} dz g_0(z) \Phi_m(z) \Phi_{m'}(z) = \delta_{mm'}, \quad dz = dz_1 \ldots dz_d.$$

The FEM solution of the BVP is reduced to the determination of stationary points of the variational functional

$$\Xi(\Phi_m, E_m, z) \equiv \int\limits_{\Omega} dz g_0(z) \Phi_m(z) \left(D - E_m \right) \Phi(z) = \Pi(\Phi_m, E_m, z) - \oint_S \Phi_m(z) \frac{\partial \Phi_m(z)}{\partial n_D},$$

$$\Pi(\Phi_m, E_m, z) = \int\limits_{\Omega} dz \left[\sum_{ij=1}^{d} g_{ij}(z) \frac{\partial \Phi_m(z)}{\partial z_i} \frac{\partial \Phi_m(z)}{\partial z_j} + g_0(z) \Phi_m(z) (V(z) - E_m) \Phi_m(z) \right].$$

Strang, G., Fix, G.J.: An Analysis of the Finite Element Method, Prentice-Hall, Englewood Cliffs, New York (1973)

The expansion of the solution in the basis of piecewise polynomial functions $N_l^{p'}$

$$\Phi_m^h(z) = \sum_{l=1}^{L} N_l^{p'}(z)\Phi_{lm}^h,$$

Algebraic (eigenvalue) problem

$$(\mathbf{A} - \mathbf{B}E_m^h)\Phi_m^h = 0, \tag{1}$$

$$A_{ll'}^{p'} = \sum_{i,j=1}^{d} \int_\Omega \frac{\partial N_l^{p'}(z)}{\partial z_i} \frac{\partial N_{l'}^{p'}(z)}{\partial z_j} g_{ij}(z)dz - \oint_S N_l^{p'}(z)\frac{\partial N_{l'}^{p'}(z)}{\partial n_D} ds$$

$$+ \int_\Omega N_l^{p'}(z)N_{l'}^{p'}(z)U(z)\, g_0(z)dz,$$

$$B_{ll'}^{p'} = \int_\Omega N_l^{p'}(z)N_{l'}^{p'}(z)g_0(z)dz. \tag{2}$$

$${\Phi_m^h}^T \mathbf{B}\Phi_{m'}^h = \delta_{mm'}, \quad \text{(for discrete spectrum problem)} \tag{3}$$

Construction of basis of one dimensional local functions $N_{\mu}^{g}(z)$

A non-uniform Finite Element grid on interval $\Omega = [z_{\min} \equiv z_0, z_{\max} \equiv z_{q^{\max}}]$

$$\Delta_q = [z_{q-1}, z_q], \quad q = 1, ..., q^{\max}, \quad \Omega = \bigcup_{q=1}^{q^{\max}} \Delta_q = [z_{\min} \equiv z_0, z_{\max} \equiv z_{q^{\max}}]$$

Shape functions

are one-dimensional LIPs or HIPs $\varphi_{rq}(x) \equiv \varphi_{r'q}^{\kappa_{r'}}(x)$, $r = 1, ..., r^{\max}$ with nodes $r' = 0, ..., \rho$ of different multiplicities $\kappa_{r'}^{\max}$ satisfying the relations

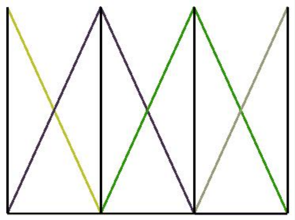
$$\varphi_{r'q}^{\kappa}(x_{r''}) = \delta_{r'r''}\delta_{\kappa 0}, \quad \left.\frac{d^{\kappa'}\varphi_{r'q}^{\kappa}(x)}{dx^{\kappa'}}\right|_{x=x_{r''}} = \delta_{r'r''}\delta_{\kappa\kappa'}$$

and ordered by r', and for equal r' by κ.

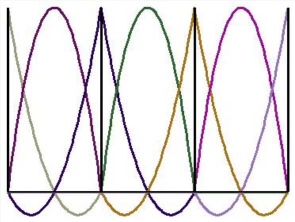
In our implementation of the FEM $\kappa_0^{\max} = \kappa_{\rho}^{\max}$ and there is a number s such that $\varphi_{rq}(x) \equiv \varphi_{0q}^{\kappa_{r'}}(x)$, $\varphi_{r+sq}(x) \equiv \varphi_{\rho q}^{\kappa_{r'}}(x)$.

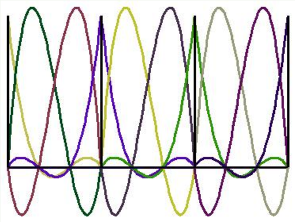
Construction of basis of one dimensional local functions $N^g_\mu(z)$

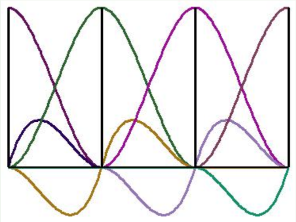
The local functions $N^g_\mu(z)$ are obtained by matching of shape functions



$$N_l(x) = \sum_{s'=0,1} \{\varphi_{r+ss',q-s'}(z), x \in \Delta_{q-s'}\}.$$





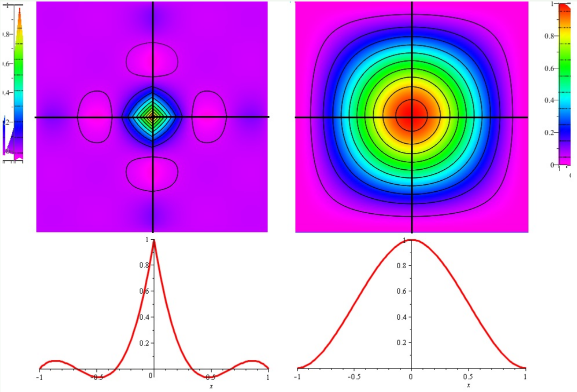


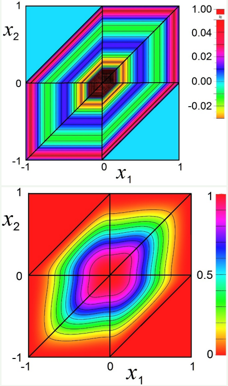
In the FEM, the polyhedral domain $\bar{\Omega}$ is divided into subdomains Δ_q, called finite elements $\bar{\Omega} = \bar{\Omega}_h(x) = \bigcup_{q=1}^{Q} \Delta_q, \quad \bar{\Omega} \subset \mathcal{R}^d$.

The shape functions , LIPs or HIPs are introduced: $\hat{\varphi}^{\kappa}_{rq}(x), \quad x \in \Delta_q$.

The piecewise polynomial functions (PPFs) constructed by joining the polynomials $\hat{\varphi}^{\kappa p'}_{rq}(x)$ on the finite elements $\Delta_q \in \bar{\Omega}_h(x)$

$$N_l(x) = \bigcup_{q=1}^{Q} \{\hat{\varphi}^{\kappa}_{rq}(x) | x \in \Delta_q\}. \qquad (4)$$





Construction of basis of multidimensional local functions $N^g_\mu(z)$

A non-uniform Finite Element grid with rectangular cells in a complex domain

$$\Delta_q \equiv \Delta_{q_1,\ldots,q_d} = [x_{1;q_1-1}, x_{1;q_1}] \otimes \cdots \otimes [x_{d;q_d-1}, x_{d;q_d}], \quad q_i = 1, \ldots, q_i^{\max},$$
$$q \equiv q(q_1, \ldots, q_d), \quad \text{is global number of the FE}$$

Shape functions are products of one-dimensional LIPs or HIPs

$$\varphi_{rq}(x) \equiv \varphi_{r_1\ldots r_d q_1\ldots q_d}(x) = \varphi_{r_1 q_1}(x_1) \times \ldots \times \varphi_{r_d q_d}(x_d) = \varphi^{\kappa_{r'_1}}_{r'_1 q_1}(x_1) \times \ldots \times \varphi^{\kappa_{r'_d}}_{r'_d q_d}(x_d)$$

The local functions $N^g_\mu(z)$

$$N_l(x) = \sum_{s_1,\ldots,s_d=0,1}^{\prime} \{\varphi_{r_1+ss_1\ldots r_d+ss_d, q_1-s_1\ldots q_d-s_d}(x), x \in \Delta_{q_1-s_1\ldots q_d-s_d}\}$$

where the summation is taken over those $s_1, \ldots, s_d$ for which the shape functions $\varphi_{r_1\ldots r_d q_1\ldots q_d}(x)$ and the cell $\Delta_{q_1-s_1\ldots q_d-s_d} \subset \Delta$ are defined.

To reduce the dim of AEP we drop $N_l(x)$ with $\kappa_{r'_1} + \ldots + \kappa_{r'_d} \geq \check{\kappa}$

Theoretical estimations of the order of the FEM schemes

In the FEM, the estimates of the approximate solution E_m^h, $\Phi_m^h(x) \in \mathcal{H}_2^{\kappa^c+1\geq 1}(\Omega_h)$ with respect to the exact solution E_m, $\Phi_m(x) \in \mathcal{H}_2^2(\Omega)$, are as follows [a]:

$$\left|E_m - E_m^h\right| \leq c_1 h^{2p}, \quad \left\|\Phi_m(x) - \Phi_m^h(x)\right\|_0 \leq c_2 h^{p+1}, \tag{5}$$

where h is the maximum size of a finite element Δ_q, p is the FEM scheme order, $c_1 > 0$ and $c_2 > 0$ are coefficients, independent of h

$$\|\Phi_m(x)\|_0^2 = \int_\Omega g_0(x)\,\Phi_m(x)\Phi_m(x)\,dx. \tag{6}$$

[a] Bathe, K. J.: Finite Element Procedures In Engineering Analysis, Prentice-Hall Inc, Englewood Cliffs, New Jersey (1982).

Finite Element Method

- BVP $\rightarrow$ minimization of quadratic functional
- Finite Element Mesh (Simplex Mesh, Parallelepiped Mesh, ...)
- Construction of shape functions
  - Lagrange Interpolation Polynomials
  - Hermite Interpolation Polynomials
  - ...
- Construction of piecewise polynomials by joining the shape functions
- Calculations of the integrals (of the order $2p$ for FEM scheme of the order p).
  - Gaussian quadratures
  - ...
- Solving of Algebraic Eigenvalue Problem

‘

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:

$$\text{(I)}: \qquad \Phi(z^t) = 0, \quad t = \min \text{ and/or} \max,$$

$$\text{(II)}: \qquad \lim_{z \to z^t} f_A(z)\left(\mathbf{I}\frac{d}{dz} - \mathbf{Q}(z)\right)\Phi(z) = 0, \quad t = \min \text{ and/or} \max,$$

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

Problem 1. For bound states

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

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

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

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

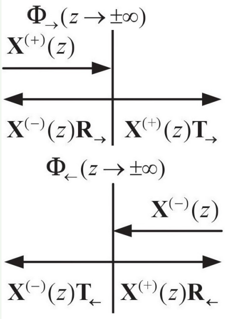
$$(\Phi_m | \Phi_{m'}) = \int_{z^{\min}}^{z^{\max}} f_B(z) (\Phi^{(m)}(z))^{T} \Phi^{(m')}(z) dz = \delta_{mm'}.$$

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

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

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

For real-valued potentials

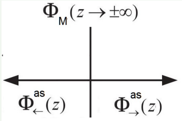
$$\mathbf{T}_{\to}^{\dagger}\mathbf{T}_{\to} + \mathbf{R}_{\to}^{\dagger}\mathbf{R}_{\to} = \mathbf{I}_{oo}, \quad \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{R}_{\leftarrow} = \mathbf{I}_{oo},$$
$$\mathbf{T}_{\to}^{\dagger}\mathbf{R}_{\leftarrow} + \mathbf{R}_{\to}^{\dagger}\mathbf{T}_{\leftarrow} = \mathbf{0}, \quad \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{T}_{\to} + \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{R}_{\to} = \mathbf{0},$$
$$\mathbf{T}_{\to}^{T} = \mathbf{T}_{\leftarrow}, \quad \mathbf{R}_{\to}^{T} = \mathbf{R}_{\to}, \quad \mathbf{R}_{\leftarrow}^{T} = \mathbf{R}_{\leftarrow}.$$

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

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

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

Asymptotic form



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

Robin (Siegert) BC

(III) :

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

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

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

- Harmonic oscillator
- Pöschl-Teller potential and Scarf complex potential
- Morse potential
- Coulomb potential
- Helmholtz problem on equilateral triangle, hypersphere, ...
- System of piecewise constant potentials
- ...

Test example (ODE System with Piecewise Constant Potentials)

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

Matching the Fundamental Solutions

$$\left(-\mathbf{I}\frac{d^2}{dz^2}+\mathbf{V}_m-E\,\mathbf{I}\right)\Phi_m(z)=0,\quad z\in(z_{m-1},z_m],\quad m=1,...,k,$$

$$\Rightarrow\quad \Phi_m(z)=\sum_{i=1}^{N}\left(A_i^{(m)}\exp(-\sqrt{\lambda_i^{(m)}-E}z)\Psi_i^{(m)}+B_i^{(m)}\exp(\sqrt{\lambda_i^{(m)}-E}z)\Psi_i^{(m)}\right),$$

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

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

$$\lim_{z\to z_{m-1}}\Phi_{m-1}(z)-\Phi_m(z)=0,\quad \lim_{z\to z_{m-1}}\frac{\Phi_{m-1}(z)}{dz}-\frac{\Phi_m(z)}{dz}=0,\quad m=2,...,k$$

$\Rightarrow 2N(k-1)$ linear eqs. with $2N(k-1)$ unknowns.

Problem 2. The scattering problem. Example of asymptotic solutions

ODE in asymptotic regions $z \to \pm\infty$

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

Asymptotic solutions

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

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

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

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

Here $\lambda_i^{L,R}$ and $\Psi_{i_c}^{L,R}$ 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. $E=\Re E+\imath\Im E$:

Example of asymptotic solutions

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

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

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

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

Robin BC

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

$$\mathbf{F}^{L,R}=\mathrm{diag}(...,\pm\sqrt{\lambda_{i_c}^{L,R}-E},...,\mp\imath\sqrt{E-\lambda_{i_o}^{L,R}},...)$$

Continuous analog of Newton method

The problem

$$\begin{cases} \left(\mathbf{A} - \lambda^h \mathbf{B}\right) \Phi^h = 0, \quad \lambda = 2E^h, \\ \left(\Phi^h, \mathbf{B}\Phi^h\right) - 1 = 0. \end{cases} \tag{7}$$

The equation of continues analog of Newton Method

$$\begin{cases} (\mathbf{A} - \lambda \mathbf{B}) \frac{d\Phi}{dt} - \frac{d\lambda}{dt} \mathbf{B}\Phi = -(\mathbf{A} - \lambda \mathbf{B}) \Phi, \\ 2\left(\frac{d\Phi}{dt}, \mathbf{B}\Phi\right) = 1 - (\Phi, \mathbf{B}\Phi), \end{cases} \tag{8}$$

where $\lambda_0 = \lambda(0)$ and $\Phi_0 = \Phi(0)$ are initial approximation to the eigenvalue and the eigenvector.

Discrete representation of derivatives

$$\left.\frac{d\Phi}{dt}\right|_{t_k} \approx \frac{\Phi_{k+1} - \Phi_k}{\tau_k} = \mathbf{v}_k \ , \quad \left.\frac{d\lambda}{dt}\right|_{t_k} \approx \frac{\lambda_{k+1} - \lambda_k}{\tau_k} = \mu_k, \quad t_{k+1} = t_k + \tau_k. \tag{9}$$

Continuous analog of Newton method

The modifed problem

$$\begin{cases} (\mathbf{A} - \lambda_k \mathbf{B})\,\mathbf{v}_k - \mu_k \mathbf{B}\Phi_k = -\mathbf{r}_k, \\ 2\,(\mathbf{v}_k, \mathbf{B}\Phi_k) = 1 - (\Phi_k, \mathbf{B}\Phi_k)\,. \end{cases} \tag{10}$$

$$\mathbf{r}_k = (\mathbf{A} - \lambda_k \mathbf{B})\,\Phi_k, \quad \mathbf{v}_k = -\Phi_k + \mu_k \Theta_k. \tag{11}$$

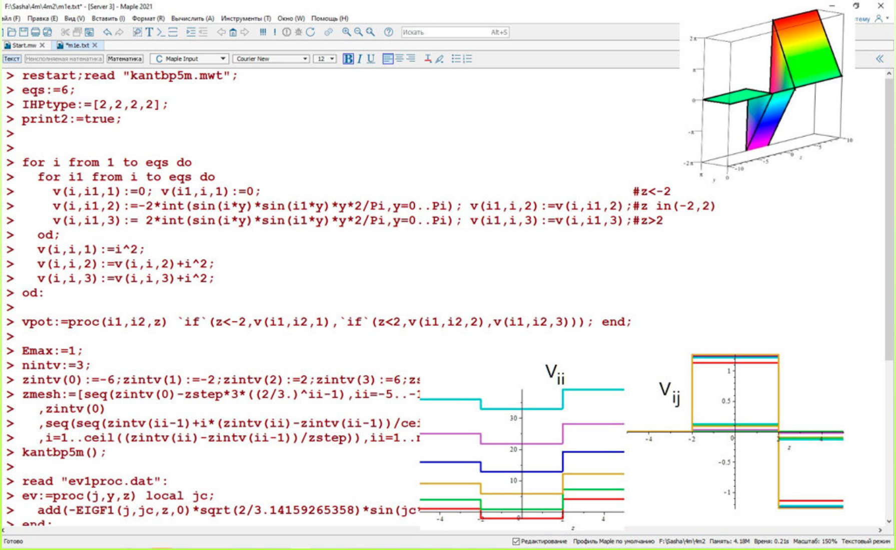
The iteration corrections Θ_k and μ_k to the eigenvector Φ_k and to the eigenvalue λ_k are calculated from the algebraic problem

$$\begin{cases} (\mathbf{A} - \lambda_k \mathbf{B})\,\Theta_k = \mathbf{B}\Phi_k, \\ 2\mu_k\,(\Theta_k, \mathbf{B}\Phi_k) = 1 + (\Phi_k, \mathbf{B}\Phi_k)\,, \end{cases} \tag{12}$$

Transition from Φ_k, λ_k at k-th step to Φ_{k+1}, λ_{k+1} at $k+1$-th step

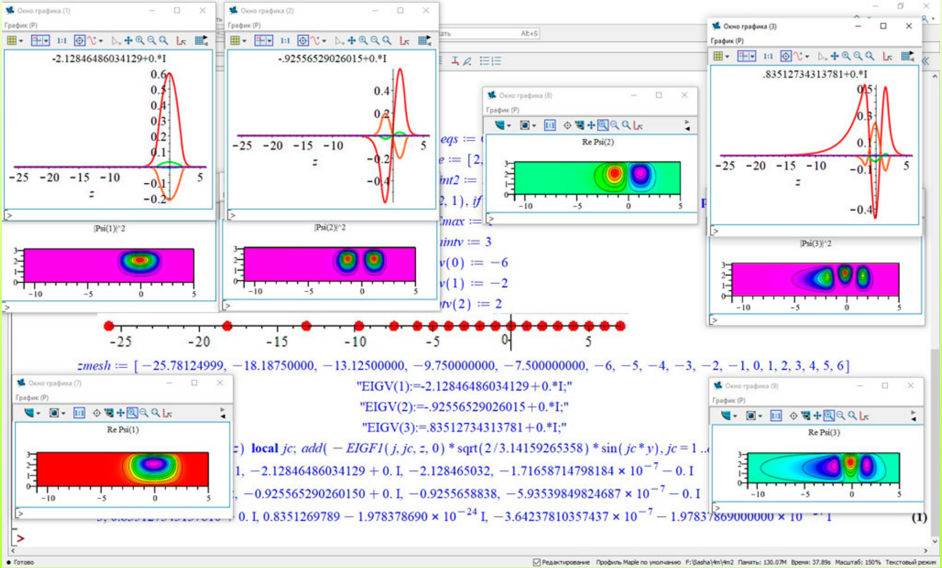
$$\begin{cases} \Phi_{k+1} = \Phi_k + \tau_k \mathbf{v}_k = (1 - \tau_k)\Phi_k + \tau_k \mu_k \blacksquare_k, \\ \lambda_{k+1} = \lambda_k + \tau_k \mu_k. \end{cases} \tag{13}$$

The piecewise constant potentials

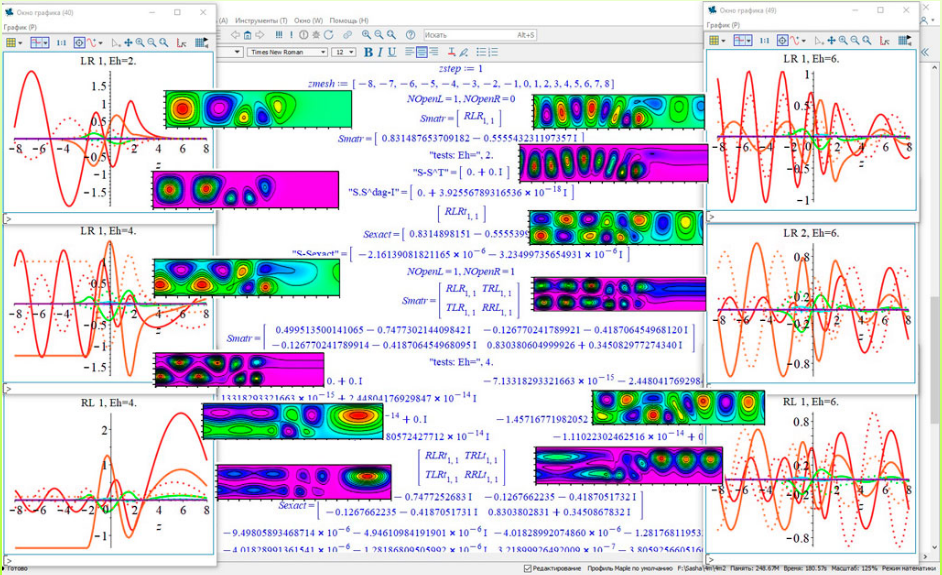


A. Gusev, S. Vinitsky, V. Gerdt, O. Chuluunbaatar, G. Chuluunbaatar, L. Le Hai, E. Zima, A Maple implementation of the finite element method for solving boundary problems of the systems of ordinary second order differential equations. Maple Conference, Waterloo Maple Inc., Canada 2020

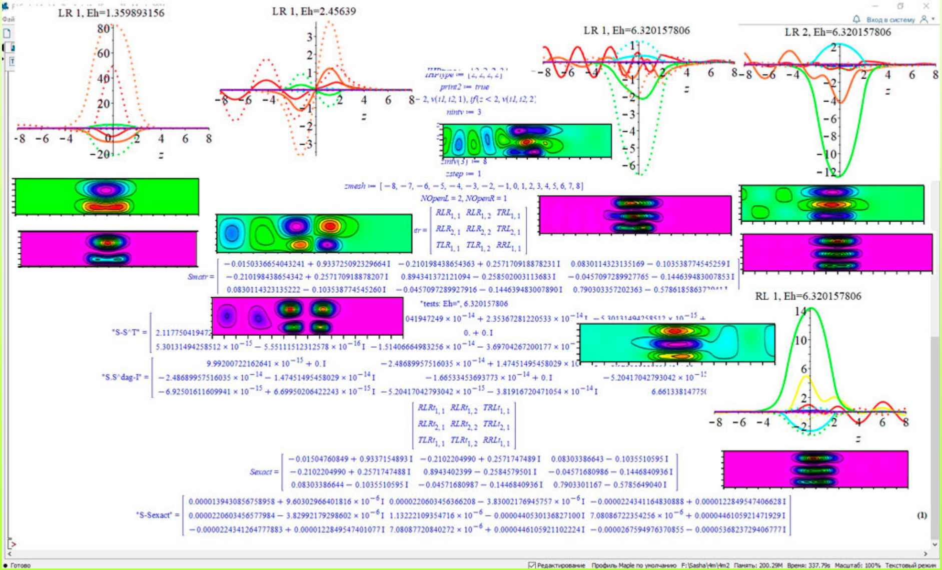
The piecewise constant potentials (eigenvalue problem)



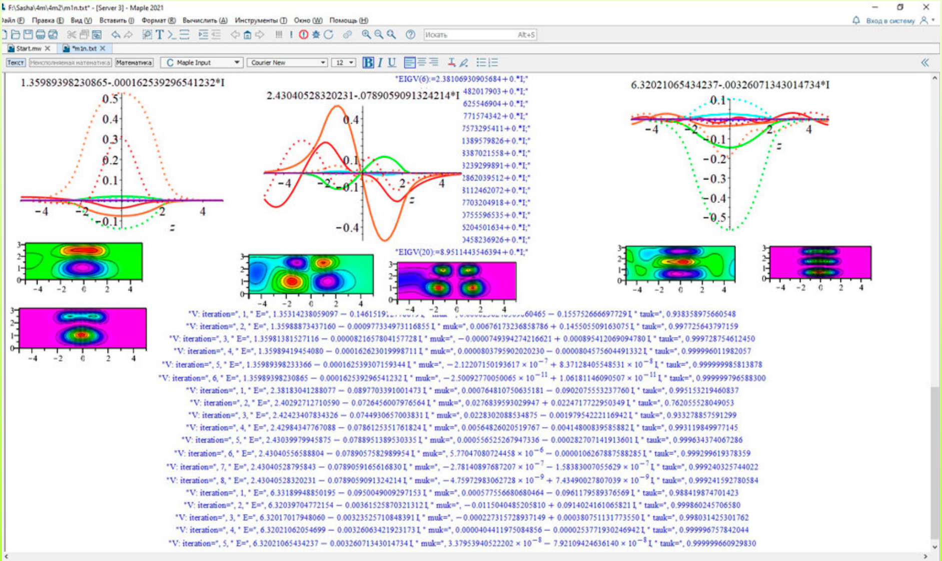
The piecewise constant potentials (multichannel scattering problem)



The piecewise constant potentials (resonance scattering states)



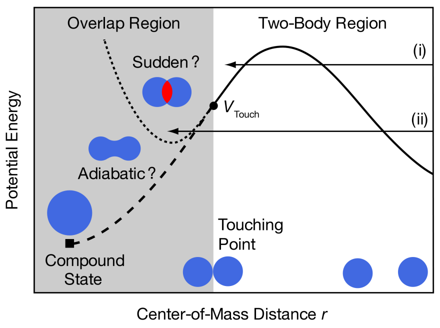
The piecewise constant potentials (metastable state problem)



Applications: Deep sub-barrier fusion

The coupled-channels Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}+V_{nn}^{(N)}(r)+\frac{Z_P Z_T e^2}{r}-E\right]\psi_n+\sum_{n'=1}^{N}V_{nn'}^{(N)}(r)\psi_{n'}(r)=0, \qquad (14)$$



The Akyüz-Winther (AW) type Woods-Saxon potential

$$V^{(N)}(r) = -\frac{V_0}{1+\exp((r-R_0)/a_0)} \qquad (15)$$

T. Ichikawa, K. Hagino and A. Iwamoto, Phys Rev C 75, 064612 (2007); Phys Rev Lett 103, 202701 (2009); T. Ichikawa, Phys Rev C 92 (6), 064604 (2015). K. Hagino, A. B. Balantekin, N. W. Lwin et al, Phys Rev C 97, 034623 (2018).

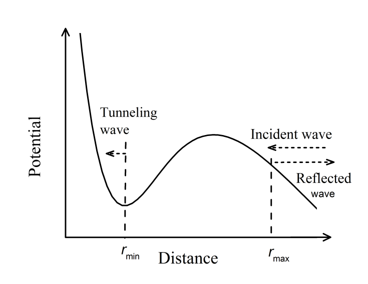
The incoming wave boundary condition

The incoming wave boundary conditions (IWBC)

$$\psi_n(r) = \begin{cases} T_n \exp\left(-ik_n(r_{\min})r\right), & r \le r_{\min} \\ H_l^-(k_n r)\delta_{n,0} - R_n H_l^+(k_n r), & r \ge r_{\max} \end{cases}$$

Here $k_n = k_n(r \to +\infty)$, and $k_n(r)$ is the local wave number for n-th channel

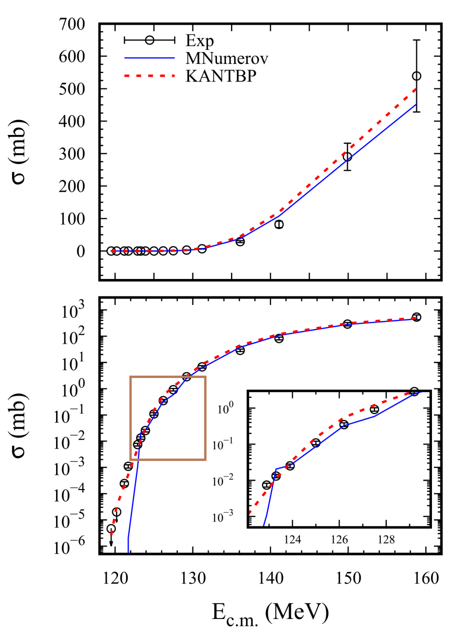
$$k_n(r) = \sqrt{\frac{2\mu}{\hbar^2}\left(E - \epsilon_n - \frac{l(l+1)\hbar^2}{2\mu r^2} - V_N^{(0)}(r) - \frac{Z_P Z_T e^2}{r} - V_{nn}(r)\right)}$$

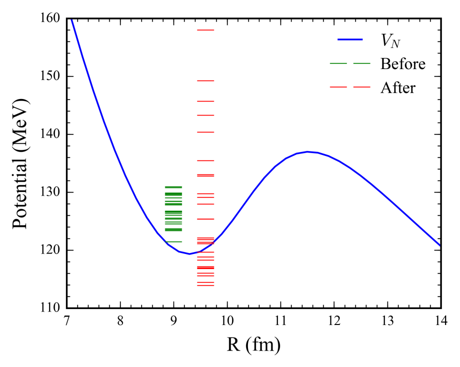


- The plane wave boundary condition at the left boundary $r_{\min}$ involves only the diagonal part. This requires that the off-diagonal matrix elements tend to zero.
- However, at $r_{\min}$, the distance between two nuclei is so short that the off-diagonal matrix elements are usually not zero.

V.V. Samarin, V.I. Zagrebaev, 2004 NPA 734 E9; V.I. Zagrebaev, V.V. Samarin, 2004 Phys. Atom. Nucl. 67 1462;

^{64}Ni+^{100}Mo: Deep sub-barrier fusion





New calculations are more stable and agree with experimental data better

The Kantorovich method (coupled-channel method, Born-Oppenheimer approximation, adiabatic approximation,...)

Boundary value problem(BVP)

$$\left(\hat{H}(x_f x_s) - E\right)\Psi(x_f, x_s) = 0 \quad + \text{boundary and orthonormality conditions},$$

$$\hat{H}(x_f x_s) = \frac{1}{g_{3s}(x_s)}\hat{H}_2(x_f; x_s) + \hat{H}_1(x_s) + \hat{V}_{fs}(x_f, x_s),$$

$$\hat{H}_f(x_f; x_s) = -\frac{1}{g_{1f}(x_f)}\frac{\partial}{\partial x_f} g_{2f}(x_f)\frac{\partial}{\partial x_f} + \hat{V}_f(x_f; x_s),$$

$$\hat{H}_s(x_s) = -\frac{1}{g_{1s}(x_s)}\frac{\partial}{\partial x_s} g_{2s}(x_s)\frac{\partial}{\partial x_s} + \hat{V}_s(x_s), .$$

$\hat{H}_f(x_f; x_s)$ and $\hat{H}_s(x_s)$ are the Hamiltonians of the fast and slow subsystems, $V_{fs}(x_f, x_s)$ is an interaction potential.

The Kantorovich method

The Kantorovich expansion

of the approximated solution $\Psi(x_f, x_s) \in W_2^1(\Omega)$ of the BVP over known parametric basis functions[a] $\Phi_j(x_f; x_s)$

$$\Psi(x_f, x_s) = \sum_{j=1}^{j_{\max}} \Phi_j(x_f; x_s)\chi_j(x_s)$$

[a] L. V. Kantorovich and V. I. Krylov, Approximate Methods of Higher Analysis (Wiley, New York, 1964)

BVP for fast subsystem

The SODE for the basis functions of the fast variable x_f and the potential curves $\mathcal{E}_i(x_s)$ continuously depended on the slow variable x_s as a parameter

$$\left\{\hat{H}_2(x_f; x_s) - \mathcal{E}_i(x_s)\right\}\Phi_i(x_f; x_s) = 0,$$

+ boundary conditions and the orthogonality and normalization conditions

$$\langle\Phi_i|\Phi_j\rangle = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\Phi_j(x_f; x_s) g_{1f}(x_f) dx_f = \delta_{ij}.$$

BVP for slow subsystem

The set of the coupled-channel SODEs for the slow subsystem

$$\mathbf{H}(\mathbf{x_s})\chi^{(i)}(x_s) = E_i\,\mathbf{I}\chi^{(i)}(x_s), \quad +\text{the boundary conditions}$$

$$\mathbf{H}(\mathbf{x_s}) = -\frac{1}{g_{1s}(x_s)}\mathbf{I}\frac{d}{dx_s}g_{2s}(x_s)\frac{d}{dx_s} + \hat{V}_s(x_s)\mathbf{I} + \mathbf{U}(x_s)$$
$$+\frac{g_{2s}(x_s)}{g_{1s}(x_s)}\mathbf{Q}(x_s)\frac{d}{dx_s} + \frac{1}{g_{1s}(x_s)}\frac{dg_{2s}(x_s)\mathbf{Q}(x_s)}{dx_s},$$

The effective potential matrices of dimension $j_{\max} \times j_{\max}$

$$U_{ij}(x_s) = \frac{1}{g_{3s}(x_s)}\mathcal{E}_i\delta_{ij}(x_s) + \frac{g_{2s}(x_s)}{g_{1s}(x_s)}W_{ij}(x_s) + V_{ij}(x_s),$$

$$V_{ij}(x_s) = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f;x_s)V_{fs}(x_f,x_s)\Phi_j(x_f;x_s)g_{1f}(x_f)dx_f,$$

$$W_{ij}(x_s) = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \frac{\partial\Phi_i(x_f;x_s)}{\partial x_s}\frac{\partial\Phi_j(x_f;x_s)}{\partial x_s}g_{1f}(x_f)dx_f,$$

$$Q_{ij}(x_s) = -\int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f;x_s)\frac{\partial\Phi_j(x_f;x_s)}{\partial x_s}g_{1f}(x_f)dx_f.$$

5DBVP for five-dimensional quadrupole Hamiltonian

AEP

$$(\mathbf{A} - \mathbf{B}E^h)\Phi^h = 0, \quad {\Phi^h}^T \mathbf{B}\Phi^h = 1, \tag{16}$$

its derivative

$$(\mathbf{A} - E^h\mathbf{B})\frac{\partial \Phi^h}{\partial x_s} = -\left(\frac{\partial \mathbf{A}}{\partial x_s} - \frac{\partial E^h}{\partial x_s}\mathbf{B}\right)\Phi^h, \quad \left(\frac{\partial \Phi^h}{\partial x_s}\right)^T \mathbf{B}^p \Phi^h = 0. \tag{17}$$

$$\frac{\partial E^h}{\partial x_s} = \left(\Phi^h\right)^T \frac{\partial \mathbf{A}^p}{\partial x_s}\Phi^h. \tag{18}$$

Then the potential matrix elements $H^h_{ij}(x_s)$ and $Q^h_{ij}(x_s)$

$$H^h_{ij}(x_s) = \left(\frac{\partial \Phi^h_i}{\partial x_s}\right)^T \mathbf{B}^p \frac{\partial \Phi^h_j}{\partial x_s}, \quad Q^h_{ij}(x_s) = -\left(\Phi^h_i\right)^T \mathbf{B}^p \frac{\partial \Phi^h_j}{\partial x_s}. \tag{19}$$

5DBVP for five-dimensional quadrupole Hamiltonian

The 5D Hamiltonian in the intrinsic frame parameterized by two internal variables $x_1 = \beta, x_2 = \gamma$ and three Euler angles $x_i = \theta_{i-2}$, $i = 3, 4, 5$ has the form

$$\hat{H} = \frac{\hbar^2}{2}(\hat{T}_{\rm vib}(x_1, x_2) + \hat{T}_{\rm rot}(x)) + V(x_1, x_2), \quad x{=}(x_1, \ldots, x_5){\in}\bar{\Omega}_5{=}\Omega_5{\cup}\partial\Omega_5{\in}\mathcal{R}^5. \tag{20}$$

Here $V = V(x_1, x_2)$ is the potential energy, $\hat{T}_{\rm vib} = \hat{T}_{\rm vib}(x_1, x_2)$ is the vibrational kinetic energy, and $\hat{T}_{\rm rot} = \hat{T}_{\rm rot}(x)$ is the rotational kinetic energy:

$$\begin{aligned}
&\hat{T}_{\rm vib}(x_1, x_2) = -\frac{1}{g_0(x_1, x_2)}\sum_{i,j=1}^{2}\frac{\partial}{\partial x_i}g_{ij}(x_1, x_2)\frac{\partial}{\partial x_j}, \quad \hat{T}_{\rm rot}(x) = \frac{\hat{I}_1^2}{J_1} + \frac{\hat{I}_2^2}{J_2} + \frac{\hat{I}_3^2}{J_3},\\
&g_0(x_1, x_2) = BB_J\beta^4\sin(3\gamma) = \frac{1}{2}\beta B|J_1J_2J_3|^{1/2}, \quad B = \sqrt{|B_{\beta\beta}B_{\gamma\gamma} - B_{\beta\gamma}^2|}\\
&g_{11}(x_1, x_2) = \frac{B_J}{B}\beta^4\sin(3\gamma)B_{\gamma\gamma} = \frac{\beta B_{\gamma\gamma}|J_1J_2J_3|^{1/2}}{2B},\\
&g_{22}(x_1, x_2) = \frac{B_J}{B}\beta^2\sin(3\gamma)B_{\beta\beta} = \frac{B_{\beta\beta}|J_1J_2J_3|^{1/2}}{2\beta B},\\
&g_{12}(x_1, x_2) = g_{21}(x_1, x_2) = -\frac{B_J}{B}\beta^3\sin(3\gamma)B_{\beta\gamma} = -\frac{B_{\beta\gamma}|J_1J_2J_3|^{1/2}}{2B}.
\end{aligned} \tag{21}$$

Here $B_J = \sqrt{B_1B_2B_3}$, moments of inertia $J_k \equiv J_k(\beta, \gamma)$ of the intrinsic frame

$$J_k(x_1, x_2) = J_k(\beta, \gamma) = 4B_k(\beta, \gamma)\beta^2\sin^2(\gamma - 2\pi k/3), \;\; k = 1, 2, 3. \tag{22}$$

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

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

$$\frac{2}{\hbar^2}(\hat{H} - E_{nI})\Psi_{nIM} = \left(\hat{T}_{\rm vib} + \hat{T}_{\rm rot} + \frac{2}{\hbar^2}(V - E_{nI})\right)\Psi_{nIM} = 0. \quad (23)$$

orthogonality and normalization conditions

$$\int_{\Omega_5} \Psi_{nIM}\Psi_{n'I'M'}\, g_0(\beta,\gamma)\, d\beta d\gamma \sin\vartheta_2 d\vartheta_1 d\vartheta_2 d\vartheta_3 = \delta_{nn'}\delta_{II'}\delta_{MM'}. \quad (24)$$

The eigenfunction Ψ_{nIM} in the representation of the angular momentum I and its projections K and M on the third axes of the intrinsic and laboratory frames

$$\Psi_{nIM}(\beta,\gamma,\vartheta_i) = \sum_{K\geq 0, even}^{I} \mathcal{D}^{I*}_{MK}(\vartheta_i)\Phi_{nIK}(\beta,\gamma), \quad (25)$$

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

$$\mathcal{D}^{I*}_{MK}(\vartheta_i) = \sqrt{\frac{2I+1}{8\pi^2}}\frac{(D^{I*}_{MK}(\vartheta_i) + \hat{\pi}(-1)^I D^{I*}_{M-K}(\vartheta_i))}{\sqrt{2(1+\delta_{K0})}}. \quad (26)$$

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

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

$$\left[\hat{T}_{\rm vib} + T^l_{KK} + \frac{2}{\hbar^2}\left(V - E_{nl}\right)\right]\Phi_{nlK} + T^l_{KK+2}\Phi_{nlK+2} + T^l_{KK-2}\Phi_{nlK-2} = 0,$$

$$\hat{T}_{\rm vib}(x_1,x_2) = -\frac{1}{g_0(x_1,x_2)}\sum_{i,j=1}^{2}\frac{\partial}{\partial x_i}g_{ij}(x_1,x_2)\frac{\partial}{\partial x_j},$$

$$T^l_{KK} = (l(l+1)-K^2)\left(\frac{1}{2J_1}+\frac{1}{2J_2}\right)+\frac{K^2}{J_3},\ T^l_{KK\pm 2} = \left(\frac{1}{4J_1}-\frac{1}{4J_2}\right)C^l_{KK\pm 2},$$

$$C^l_{KK+2} = C^l_{K+2K} = (1+\delta_{K0})^{1/2}[(l-K)(l+K+1)(l-K-1)(l+K+2)]^{1/2},$$

$$J_k(x_1,x_2) = J_k(\beta,\gamma) = 4B_k(\beta,\gamma)\beta^2\sin^2(\gamma - 2\pi k/3). \tag{27}$$

The components Φ_{nlK} are subject to Neumann or Dirichlet boundary conditions at the boundary $\partial\Omega_2$ of the domain Ω_2 and the orhtogonality and normalization conditions

$$\int_0^{\beta_{\max}}\int_0^{\pi/3} g_0(\beta,\gamma)d\beta d\gamma \sum_{K\geq 0, even}^{l_{\max}} \Phi_{nlK}(\beta,\gamma)\Phi_{n'lK}(\beta,\gamma) = \delta_{nn'}. \tag{28}$$

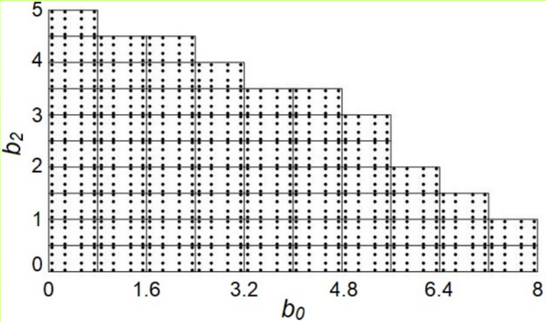
Exact solvable 5D harmonic oscillator (5DHO)

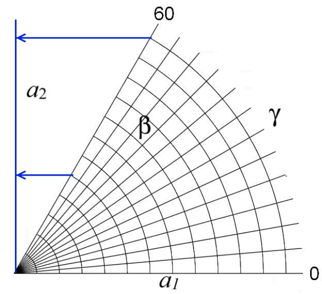
$$V(\beta,\gamma) = (C_2/2)\beta^2, \quad B_{\beta\beta} = B_{\gamma\gamma} = B_1 = B_2 = B_3 = B_0, \quad B_{\beta\gamma} = B_{\gamma\beta} = 0,$$

$$g_0(\beta,\gamma) = B_0 g_{11}(\beta,\gamma) = B_0\beta^2 g_{22}(\beta,\gamma) = B_0^{5/2}\beta^4 \sin(3\gamma), \quad g_{12}(\beta,\gamma) = g_{21}(\beta,\gamma) = 0.$$

Internal (a_0, a_2) and affine (b_0, b_2) coordinates

$$a_0 = \beta\cos(\gamma) = b_0 + \sqrt{\frac{2}{3}}b_2, \quad a_2 = \frac{1}{\sqrt{2}}\beta\sin(\gamma) = b_2.$$



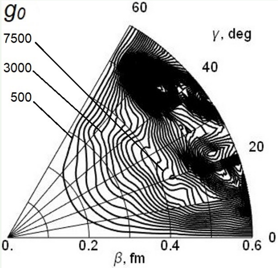


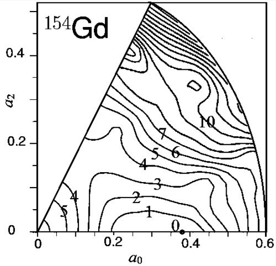
Rectangular grid of finite elements for the 5D harmonic oscillator. The Gaussian nodes are marked by circles.

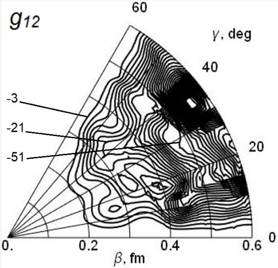
In grid Ω_{b_0,b_2} the cells Δ_q for which $\min_{(b_0,b_2)\in\Delta_q} V(b_0,b_2) > 30$ are dropped.

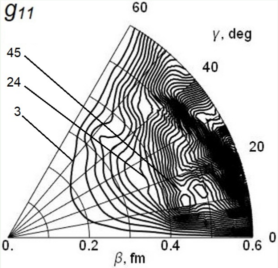
Benchmark calculations of ^{154}Gd in the RMF model

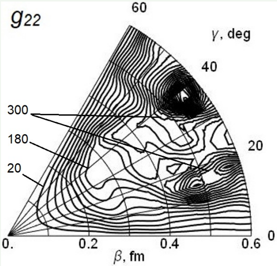
Spectrum E, isolines of $V(\beta,\gamma)$ counted from the minimum of $V(\beta{=}0.3875,\gamma{=}0)$ $=-1270.6$MeV, $g_0(\beta,\gamma)$ and $g_{ij}(\beta,\gamma)$ of ^{154}Gd calculated in PC-F1 of RMF model[a]











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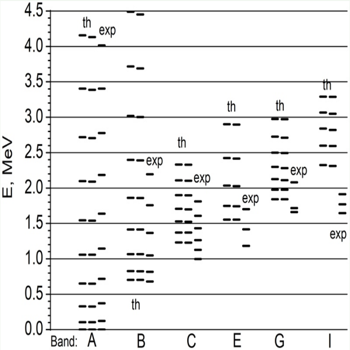
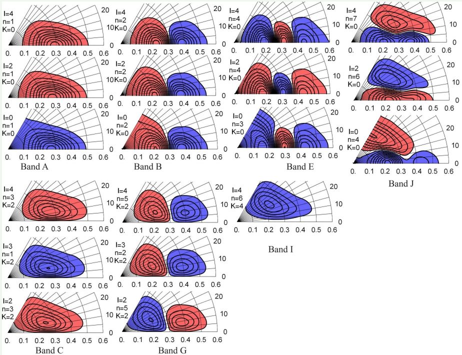
[a] T.Niksic, Z.P.Li,B. D.Vretenar, L.Prochniak, J.Meng, P.Ring, Beyond the relativistic mean-field approximation. III. Collective Hamiltonian in five dimensions, Phys.Rev.C 79, 034303(2009)

Energy spectrum of ^{154}Gd

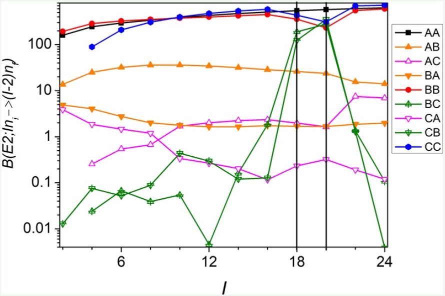




Energy spectrum of ^{154}Gd. For each state of the bands A, B, E, C, G, and I, three short bars correspond to the diagonal approximation (left), nondiagonal one (middle), and experiment (right)[http://www.nndc.bnl.gov/ensdf/].

Band(A) is the $K^\pi = 0+$ ground state band;
Band(B): the first excited $K^\pi = 0^+$ (β-vibrational) band;
Band(E), Band(J), Band(K): the second, third and forth excited $K^\pi = 0+$ bands;
Band(C): the $K^\pi = 2^+$ (γ-vibrational) band;
Band(G): the second excited $K^\pi = 2^+$ ($\beta\gamma$-vibrational) band;
Band(I): the $K^\pi = 4^+$ band.

Calculated intraband and interband transitions



$B(E2)$	ndiag	diag	exp	bands
$2_1 \to 0_1$	160	159	157	AA
$4_1 \to 2_1$	244	243	245	
$6_1 \to 4_1$	294	293	285	
$8_1 \to 6_1$	341	339	312	
$10_1 \to 8_1$	387	385	360	
$2_2 \to 0_2$	194	193	97.0	BB
$0_2 \to 2_1$	68.5	69.2	52.0	BA
$2_2 \to 4_1$	45.0	45.5	19.6	
$2_3 \to 4_1$	0.460	0.248	1.72	CA
$2_3 \to 0_1$	3.89	4.14	5.70	

Calculated intraband and interband $B(E2; In_i \to (I-2)n_f)$ transitions between A, B and C bands in Weisskopf units (W.u.) in the nondiagonal approximation (nondiag) for ^{154}Gd.

Thank you for your attention!