# Updates of KANTBP code and their applications for solving problems in atomic, molecular and nuclear physics

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- Statement of the problem: General BVP
- The code KANTBP 1.0
- The code KANTBP 2.0
- The code KANTBP 3.0
- Applications
- The code KANTBP 3.1
- App. in nuclear physics
- Conclusion

# Statement of the problem: General BVP

## Multidimensional elliptic equation

In many cases the solution of a multi-dimensional quantum mechanical problem is reduced to a solution of the $d > 1$ dimensional elliptic equation for wave function $\Psi(z,\Omega)$

$$\left(-\frac{1}{g_1(z)}\frac{\partial}{\partial z}g_2(z)\frac{\partial}{\partial z}+\frac{1}{g_3(z)}\left(-\hat{\Lambda}_\Omega^2+V(z,\Omega)\right)\right)\Psi(z,\Omega)=2E\Psi(z,\Omega), \quad (1)$$

$$a\frac{\partial\Psi(z,\Omega)}{\partial \mathbf{n}}-b\Psi(z,\Omega)=0, \quad \Omega\in\partial\hat{X}, \quad z\in[z_{\min},z_{\max}], \quad (2)$$

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$$a\frac{\partial\Psi(z,\Omega)}{\partial \mathbf{n}} - b\Psi(z,\Omega) = 0, \quad \Omega \in \partial\hat{X}, \quad z \in [z_{\min}, z_{\max}], \quad (2)$$

$$\mu_1 \frac{\partial\Psi(z,\Omega)}{\partial z} - \lambda_1 \Psi(z,\Omega) = 0, \quad z = z_{\min}, \quad \Omega \in \partial\hat{X} \cup \hat{X}; \quad (3)$$

$$\mu_2 \frac{\partial\Psi(z,\Omega)}{\partial z} - \lambda_2 \Psi(z,\Omega) = 0, \quad z = z_{\max}, \quad \Omega \in \partial\hat{X} \cup \hat{X}; \quad (4)$$

Here $\Omega = \{\Omega_j\}_{j=1}^{d-1} \in \hat{X} \subset \mathbf{R}^{d-1}$ are fast variables (or fast subsystem),
$z \in (z_{\min}, z_{\max}) \in B \subset \mathbf{R}^1$ is slow variable (or slow subsystem),

$g_1(z) > 0,\ g_2(z) > 0,\ g_3(z) > 0,$

$L(\Omega; z) = -\hat{\Lambda}^2_\Omega + V(z,\Omega)$ has only discrete spectrum.

# Statement of the problem: General BVP

## Standard projection method – Coupled channels method

$$\Psi(z,\Omega) = \sum_{j=1}^{N} B_j(\Omega)\chi_j(z). \tag{5}$$

$$\left(-\hat{\Lambda}^2_\Omega + \tilde{U}(z_{\rm fix},\Omega)\right) B_j(\Omega) = \varepsilon_j B_j(\Omega), \tag{6}$$

$$a\frac{\partial B_j(\Omega)}{\partial \mathbf{n}} - bB_j(\Omega) = 0, \quad \Omega \in \partial\hat{X}, \quad z_{\rm fix} \in [z_{\rm min}, z_{\rm max}], \tag{7}$$

with

$$\int B_i(\Omega)B_j(\Omega)d\Omega = \delta_{ij}. \tag{8}$$

# Statement of the problem: BVP for slow subsystem

## Standard projection method – Coupled channels method

$$\left(-\frac{1}{g_1(z)}\mathbf{I}\frac{d}{dz}g_2(z)\frac{d}{dz}+\frac{1}{g_3(z)}\mathbf{U}(z)-2E\,\mathbf{I}\right)\chi(z)=0, \quad (9)$$

$$\mu_1\frac{d}{dz}\chi(z)-\lambda_1\chi(z)=0, \quad z=z_{\min}, \quad (10)$$

$$\mu_2\frac{d}{dz}\chi(z)-\lambda_2\chi(z)=0, \quad z=z_{\max}. \quad (11)$$

Here $\mathbf{I}$ and $\mathbf{U}(z)$ are matrices of dimension $N\times N$:

$$I_{ij}=\delta_{ij},$$

$$U_{ij}(z)=U_{ji}(z)=\frac{\varepsilon_i+\varepsilon_j}{2}\delta_{ij}+\int B_i(\Omega)[U(z,\Omega)-\tilde{U}(z_{\rm fix},\Omega)]B_j(\Omega)d\Omega, \quad (12)$$

# Statement of the problem: General BVP

## Kantorovich method

$$\Psi_i(z,\Omega) = \sum_{j=1}^{N} B_j(\Omega;z)\chi_j(z). \qquad (13)$$

$$L(\Omega;z)B_j(\Omega;z) = \left(-\hat{\Lambda}^2_\Omega + U(z,\Omega)\right) B_j(\Omega;z) = \varepsilon_j(z)B_j(\Omega;z), \qquad (14)$$

$$a\frac{\partial B_j(\Omega;z)}{\partial \mathbf{n}} - bB_j(\Omega;z) = 0, \quad \Omega \in \partial\hat{X}, \quad z \in [z_{\min}, z_{\max}], \qquad (15)$$

with

$$\int B_i(\Omega;z)B_j(\Omega;z)d\Omega = \delta_{ij}. \qquad (16)$$

# Statement of the problem: BVP for slow subsystem

## The system differential equation for the slow subsystem

$$\left(-\frac{1}{g_1(z)}\mathbf{I}\frac{d}{dz}g_2(z)\frac{d}{dz}+\mathbf{U}(z)\right.$$
$$\left.+\frac{g_2(z)}{g_1(z)}\mathbf{Q}(z)\frac{d}{dz}+\frac{1}{g_1(z)}\frac{dg_2(z)\mathbf{Q}(z)}{dz}-2E\,\mathbf{I}\right)\chi(z)=0, \qquad (17)$$

$$\mu_1\left(\mathbf{I}\frac{d}{dz}-\mathbf{Q}(z)\right)\chi(z)-\lambda_1\chi(z)=0, \quad z=z_{\min}, \qquad (18)$$

$$\mu_2\left(\mathbf{I}\frac{d}{dz}-\mathbf{Q}(z)\right)\chi(z)-\lambda_2\chi(z)=0, \quad z=z_{\max}. \qquad (19)$$

Here $\mathbf{U}(z)$ and $\mathbf{Q}(z)$ are matrices of dimension $N\times N$:

$$U_{ij}(z)=U_{ji}(z)=\frac{\varepsilon_i(z)+\varepsilon_j(z)}{2g_3(z)}\delta_{ij}+\frac{g_2(z)}{g_1(z)}\int\frac{\partial B_i(\Omega;z)}{\partial z}\frac{\partial B_j(\Omega;z)}{\partial z}d\Omega, \qquad (20)$$

$$Q_{ij}(z)=-Q_{ji}(z)=-\int B_i(\Omega;z)\frac{\partial B_j(\Omega;z)}{\partial z}d\Omega.$$

# The code KANTBP 1.0 – KANTorovich Boundary Problem

## BVP

$$\left(-\frac{1}{r^{d-1}}\mathbf{I}\frac{d}{dr}r^{d-1}\frac{d}{dr}+\mathbf{U}(r)+\mathbf{Q}(r)\frac{d}{dr}+\frac{1}{r^{d-1}}\frac{dr^{d-1}\mathbf{Q}(r)}{dr}-2E\,\mathbf{I}\right)\chi(r)=0, \quad (21)$$

## Bound state problem

$$\left(\mathbf{I}\frac{d}{dr}-\mathbf{Q}(r)\right)\chi(r)=0 \quad \text{or} \quad \chi(r)=0, \quad r=r_{\min}, \quad r_{\max}. \quad (22)$$

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## Multichannel scattering problem on the semi-axis $r \in (r_{\min}=0, r_{\max}) \subset (0,\infty)$

$$\lim_{r\to 0} r^{d-1}\left(\mathbf{I}\frac{d}{dr}-\mathbf{Q}(r)\right)\chi(r)=0 \quad \text{or} \quad \chi(0)=0, \qquad (23)$$

# The code KANTBP 1.0

### Multichannel scattering problem on the semi-axis $r \in (r_{\min} = 0, r_{\max}) \subset (0, \infty)$

Let matrix potentials $\mathbf{V}(r)$ and $\mathbf{Q}(r)$ satisfy the following asymptotic behaviour at large $r$

$$V_{jj}(r) = \epsilon_j - \frac{2Z_j}{r} + O(r^{-2}), \quad V_{ij}(r) = O(r^{-2}), \quad Q_{ij}(r) = O(r^{-1}), \qquad (24)$$

where $\epsilon_1 \leq \ldots \leq \epsilon_N$ are the threshold energy values. RWF $\mathbf{\Phi}(r) = \{\chi^{(i)}(r)\}_{i=1}^{N_o}$:

$$\mathbf{\Phi}(r) \to \mathbf{\Phi}^{reg}(r) + \mathbf{\Phi}^{irr}(r)\mathbf{K}, \qquad (25)$$

$$\Phi^{reg}_{ji_o}(r) \to \frac{\sin(w_j(r))}{\sqrt{k_j r^{d-1}}}\delta_{ji_o}, \quad \Phi^{irr}_{ji_o}(r) \to \frac{\cos(w_j(r))}{\sqrt{k_j r^{d-1}}}\delta_{ji_o}, \ i_o = \overline{1, N_o},$$

$$w_j(r) = k_j r + \frac{Z_j}{k_j}\ln(2k_j r), \quad k_j = \sqrt{2E - \epsilon_j}. \qquad (26)$$

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$$\mathbf{Wr}(\mathbf{Q}(r); \mathbf{\Phi}_{\rm irr}(r), \mathbf{\Phi}_{\rm reg}(r)) = \mathbf{I}_{oo}, \qquad (27)$$

$$\mathbf{Wr}(\bullet; \mathbf{a}(r), \mathbf{b}(r)) = r^{d-1}\left[\mathbf{a}^T(r)\left(\frac{d\mathbf{b}(r)}{dr} - \bullet\mathbf{b}(r)\right) - \left(\frac{d\mathbf{a}(r)}{dr} - \bullet\mathbf{a}(r)\right)^T \mathbf{b}(r)\right].$$

# The code KANTBP 1.0

## FEM

The system of equations is solved using high-order accuracy approximations of the finite-element method on non-uniform grids.

## Calculation accuracy:

Then the following estimations are valid[a]

$$|\, E_m^h - E_m \,| \leq c_1\, h^{2p}, \quad \left\| \chi_m^h(r) - \chi_m(r) \right\|_0 \leq c_2\, h^{p+1}, \tag{28}$$

where $h$ is the maximal step of the finite-element grid;

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where $h$ is the maximal step of the finite-element grid;

$$|\, (\lambda^{(i)})^h - \lambda^{(i)} \,| \leq c_1\, h^{2p}, \quad \left\| (\chi^{(i)}(r))^h - (\chi^{(i)}(r)) \right\|_0 \leq c_2\, h^{p+1}, \tag{29}$$

where $\lambda^{(i)}$ are the eigenvalues of the reaction matrix **K**.

[a] G. Strang et al, An analysis of the finite element method, Prentice-Hall, EC, NY, 1973.


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KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach ☆

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# The code KANTBP 2.0

## Multichannel scattering problem on the semi-axis $r \in (r_{\min} \neq 0, r_{\max}) \subset (0, \infty)$

$$\frac{d\chi(r)}{dr} = \mathcal{R}(r)\chi(r), \quad r = r_{\min}, \tag{30}$$

where $\mathcal{R}(r)$ is a unknown $N \times N$ matrix-function, $\mathbf{G}(r) = \mathcal{R}(r) - \mathbf{Q}(r)$ should be symmetric according to the conventual **R**-matrix theory.

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$$\chi(r) = \chi_{reg}(r)\mathbf{C}, \tag{31}$$

$$\mathcal{R}(r) = \frac{d\chi(r)}{dr}\chi^{-1}(r) = \frac{d\chi_{reg}(r)}{dr}\underbrace{\mathbf{C}\mathbf{C}^{-1}}_{\mathbf{I}}\chi_{reg}^{-1}(r) = \frac{d\chi_{reg}(r)}{dr}\chi_{reg}^{-1}(r), \tag{32}$$

where $\chi_{reg}(r)$ is the $N \times N$ regular solution of equation, $\mathbf{C}$ is the unknown nonzero constant matrix of dimension $N \times N_o$.

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# The code KANTBP 3.0

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

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \mathbf{U}(z) + \mathbf{Q}(z)\frac{d}{dz} + \frac{d\mathbf{Q}(z)}{dz} - 2E\,\mathbf{I}\right)\chi^{(i)}(z) = 0. \qquad (33)$$

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

$$U_{ij}(z_{\pm}) = \left(\epsilon_j + \frac{2Z_j^{\pm}}{z_{\pm}}\right)\delta_{ij} + O(z_{\pm}^{-2}), \quad Q_{ij}(z_{\pm}) = O(z_{\pm}^{-1}), \qquad (34)$$

where $\epsilon_1 \leq \ldots \leq \epsilon_N$ are the threshold energy values.

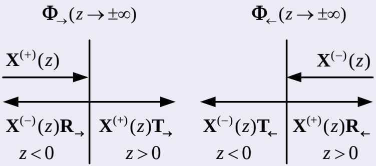
## The boundary conditions at $z = z_{\min} \to -\infty$ and $z = z_{\max} \to +\infty$:

$$\left.\frac{d\mathbf{\Phi}(z)}{dz}\right|_{z=z_{\min}} = \mathcal{R}(z_{\min})\mathbf{\Phi}(z_{\min}), \quad \left.\frac{d\mathbf{\Phi}(z)}{dz}\right|_{z=z_{\max}} = \mathcal{R}(z_{\max})\mathbf{\Phi}(z_{\max}), \qquad (35)$$

$\mathbf{\Phi}(z) = \{\chi^{(j)}(z)\}_{j=1}^{N_o}$ is the required $N \times N_o$ matrix-solution and $N_o$ is the number of open channels, $N_o = \max_{2E \geq \epsilon_j} j \leq N$.

# The code KANTBP 3.0

## Schematic diagrams of the continuum spectrum waves having the asymptotic form: "incident wave + outgoing waves":




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

$$\mathbf{\Phi}_v(z \to \pm\infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z)\mathbf{T}_v, & z > 0, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_v, & z < 0, \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\mathbf{R}_v, & z > 0, \\ \mathbf{X}^{(-)}(z)\mathbf{T}_v, & z < 0, \end{cases} & v = \leftarrow, \end{cases} \qquad (36)$$

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the reflection and transmission $N_o \times N_o$ matrices, $v = \rightarrow$ and $v = \leftarrow$ denote the initial direction of the particle motion along the $z$ axis.

# The asymptotic boundary conditions

**The leading term of the asymptotic matrix functions $\mathbf{X}^{(\pm)}(z)$ has the form**

$$X_{ij}^{(\pm)}(z) \to p_j^{-1/2} \exp\left(\pm\imath\left(p_j z - \frac{Z_j}{p_j}\ln(2p_j|z|)\right)\right)\delta_{ij}, \qquad (37)$$

$$p_j = \sqrt{2E - \epsilon_j} \quad i = 1, \ldots, N, \quad j = 1, \ldots, N_o,$$

where $Z_j = Z_j^+$ at $z > 0$ and $Z_j = Z_j^-$ at $z < 0$.

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$$X_{ij}^{(\mp)}(z) \to q_j^{-1/2} \exp\left(\pm\left(q_j z + \frac{Z_j^{\mp}}{q_j}\ln(2q_j|z|)\right)\right)\delta_{ij}, \quad (38)$$

$$q_j = \sqrt{\epsilon_j - 2E}, \quad i = 1, \ldots, N, \quad j = N_o + 1, \ldots, N.$$

**Generalized Wronskian with a long derivative**

$$\mathbf{Wr}(\mathbf{Q}(z); \mathbf{X}^{(\mp)}(z), \mathbf{X}^{(\pm)}(z)) = \pm 2\imath \mathbf{I}_{oo}, \quad (39)$$

$$\mathbf{Wr}(\bullet; \mathbf{a}(z), \mathbf{b}(z)) = \mathbf{a}^T(z)\left(\frac{d\mathbf{b}(z)}{dz} - \bullet\mathbf{b}(z)\right) - \left(\frac{d\mathbf{a}(z)}{dz} - \bullet\mathbf{a}(z)\right)^T \mathbf{b}(z). \quad (40)$$

# The code KANTBP 3.0

## Scattering matrix

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix} \tag{41}$$

The reflection and transmission matrices having the following properties

$$\begin{aligned} &\mathbf{T}^{\dagger}_{\rightarrow}\mathbf{T}_{\rightarrow} + \mathbf{R}^{\dagger}_{\rightarrow}\mathbf{R}_{\rightarrow} = \mathbf{I}_{oo} = \mathbf{T}^{\dagger}_{\leftarrow}\mathbf{T}_{\leftarrow} + \mathbf{R}^{\dagger}_{\leftarrow}\mathbf{R}_{\leftarrow}, \\ &\mathbf{T}^{\dagger}_{\rightarrow}\mathbf{R}_{\leftarrow} + \mathbf{R}^{\dagger}_{\rightarrow}\mathbf{T}_{\leftarrow} = \mathbf{0} = \mathbf{R}^{\dagger}_{\leftarrow}\mathbf{T}_{\rightarrow} + \mathbf{T}^{\dagger}_{\leftarrow}\mathbf{R}_{\rightarrow}, \\ &\mathbf{T}^{T}_{\rightarrow} = \mathbf{T}_{\leftarrow}, \quad \mathbf{R}^{T}_{\rightarrow} = \mathbf{R}_{\rightarrow}, \quad \mathbf{R}^{T}_{\leftarrow} = \mathbf{R}_{\leftarrow}. \end{aligned} \tag{42}$$

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KANTBP 3.0: New version of a program for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel adiabatic approach[☆]

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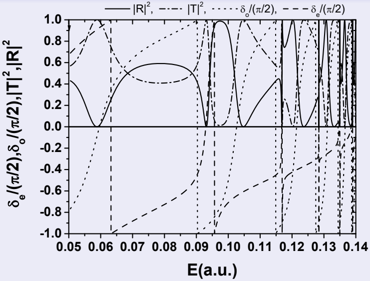
[a] Joint Institute for Nuclear Research, Dubna, 141980 Moscow region, Russia
[b] National University of Mongolia, Ulaanbaatar, Mongolia
[c] IBM Toronto Lab, 8200 Warden Avenue, Markham, ON L6G 1C7, Canada

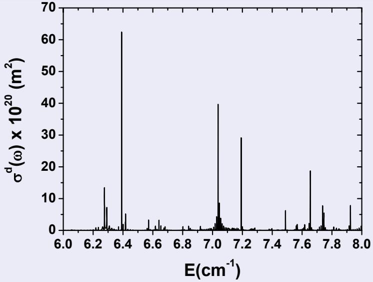
# Applications of KANTBP 1.0

## Calculation of a hydrogen atom photoionization in a strong magnetic field[a]:

[a]O. Chuluunbaatar, A.A. Gusev, . . . , S.I. Vinitsky, J. Phys. **A 40**, pp. 11485–11524 (2007).




(a)




(b)

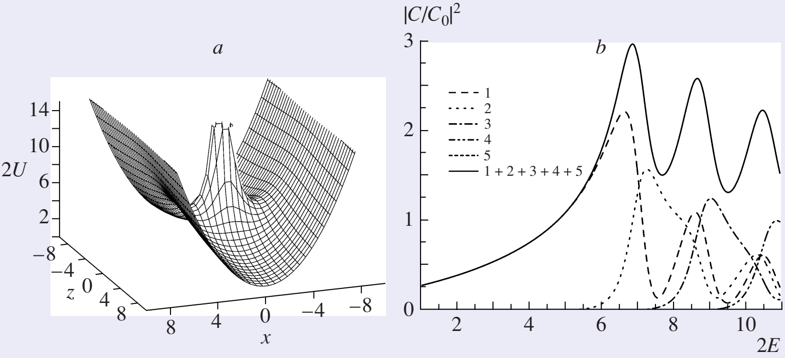
(a) Transmission $|\mathbf{T}|^2$ and reflection $|\mathbf{R}|^2$ coefficients, even $\delta_e$ and odd $\delta_o$ phase shifts at $Z=1$, $m=0$ and $B_0 = 2.35\times10^4$ T. (b) The cross section of photoionization from the state $3s_0$ for the final state $\sigma=-1$ at $B_0 = 6.10$ T and $Z=1$.

$$\mathbf{T} = \frac{1}{2}\left(-\mathbf{S}_e + \mathbf{S}_o\right), \mathbf{R} = \frac{1}{2}\left(-\mathbf{S}_e - \mathbf{S}_o\right), \mathbf{S}_{e,o} = (\mathbf{I}_{oo} + \imath\mathbf{K}_{e,o})(\mathbf{I}_{oo} - \imath\mathbf{K}_{e,o})^{-1} \quad (43)$$

# Applications of KANTBP 2.0

## Channeling problem for charged particles produced by confining environment[a]:

[a]O.Chuluunbaatar, A.A.Gusev, . . . , P.M.Krassovitskiy, S.I.Vinitsky, Phys. Atom. Nucl. 72, 768 (2009).

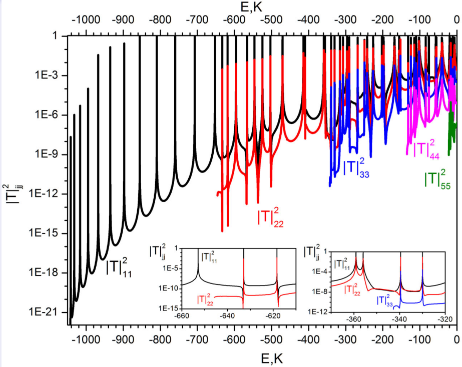



(a) Effective potential $2U = 2Z/\sqrt{\rho^2 + z^2} + \gamma^2\rho^2/4$ in the $z, x$ plane for the effective charge $Z = +6$ and $\gamma = 1$; (b) The full enhancement coefficient (solid line) and partial enhancement coefficients in each open channel ($i = 1 - 5$) versus the energy $2E$.

# Applications of KANTBP 3.0

## Adiabatic representation for atomic dimers in collinear configuration[a]:

[a] A.A. Gusev, S.I. Vinitsky, O. Chuluunbaatar, . . . , P. M. Krassovitskiy, Phys. Atom. Nucl. 81, 945 (2018).




The total probability $|T|^2_{ii}(E) = \sum_{j=1}^{N_o} T^*_{ij} T_{ji}$ (lines) of penetration of the dimer $Be_2$ for the initial states $i$ through the repulsive Gaussian potential barriers versus the total energy $E$. The values of the threshold energies $\epsilon_i, i = 1, \ldots, 5$ corresponding to the energies of ground and excited initial states are shown by arrows.

**Bound state problem for a system of differential equations:**

- dimension of the system of differential equations – 280;
- dimensions of stiffness and mass matrices – $\sim 300\,000 \times 300\,000$;
- the order of approximation of the FEM – 10;
- maximum block width – 3079;
- relative accuracy of calculation of the eigenvalues $\sim 10^{-14}$.

**Scattering problem for a system of differential equations:**

- dimension of the system of differential equations – 40;
- dimensions of stiffness matrix – $\sim 900\,000 \times 900\,000$;
- the order of approximation of the FEM – 10;
- maximum block width – 439;
- maximal number of the open channels – 16;
- relative accuracy of calculation of reaction matrix (transmission and reflection matrices) $\sim 10^{-12}$.

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## Премии ОИЯИ за 2015 год

Новости, 24 сентября 2016

### III. В области научно-методических исследований

**Первая премия**

***«Создание кинематического сепаратора (фильтра скоростей) SHELS»***
*Авторы: А.В.Еремин, А.Г.Попеко, О.Н.Малышев, А.Лопез-Мартенс, К.Хошильд, О.Дорво, В.И.Чепигин, А.И.Свирихин, А.В.Исаев, М.Л.Челноков*

**Вторые премии**

1. ***«Проблемно-ориентированный комплекс программ для решения краевых задач динамики малочастичных квантовых систем»***
*Авторы: О.Чулуунбаатар, А.А.Гусев, С.И.Виницкий, В.П.Герд, В.А.Ростовцев, А.Г. Абрашкевич, В.Л.Дербов, А.Гужд, П.М.Красовицкий, Э.М.Казарян*

# The code KANTBP 3.1

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

$$\left(-\mathbf{I}\frac{d^2}{dz^2} + \mathbf{U}(z) + \mathbf{Q}(z)\frac{d}{dz} + \frac{d\mathbf{Q}(z)}{dz} - 2E\,\mathbf{I}\right)\chi^{(i)}(z) = 0. \qquad (44)$$

## 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 $z \leq z_{\min}$ and $z \geq z_{\max}$.

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

$$\mathbf{\Phi}_v(z) = \begin{cases} \begin{cases} \mathbf{Y}^{(+)}(z)\mathbf{T}_v, & z \geq z_{\max}, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_v, & z \leq z_{\min}, \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{Y}^{(-)}(z) + \mathbf{Y}^{(+)}(z)\mathbf{R}_v, & z \geq z_{\max}, \\ \mathbf{X}^{(-)}(z)\mathbf{T}_v, & z \leq z_{\min}, \end{cases} & v = \leftarrow, \end{cases} \qquad (45)$$

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.

# The asymptotic boundary conditions

## The leading term of the asymptotic rectangle-matrix functions $\mathbf{X}^{(\pm)}(z)$ and $\mathbf{Y}^{(\pm)}(z)$

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

$$\mathbf{Y}_{i_o}^{(\pm)}(z) \to \frac{\exp\left(\pm\imath p_{i_o}^{R} z\right)}{\sqrt{p_{i_o}^{R}}}\boldsymbol{\Psi}_{i_o}^{R}, \quad p_{i_o}^{R} = \sqrt{2E - \lambda_{i_o}^{R}}, \quad z \ge z_{\max}. \tag{46}$$

Here $\lambda_i^{L,R}$ and $\boldsymbol{\Psi}_i^{L,R} = \{\Psi_{1i}^{L,R}, \ldots, \Psi_{Ni}^{L,R}\}^T$ 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

$$\mathbf{V}^{L,R}\boldsymbol{\Psi}_i^{L,R} = \lambda_i^{L,R}\boldsymbol{\Psi}_i^{L,R}, \quad (\boldsymbol{\Psi}_i^{L,R})^T\boldsymbol{\Psi}_j^{L,R} = \delta_{ij}. \tag{47}$$

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$$\mathbf{Y}_{i_o}^{(\pm)}(z) \to \frac{\exp\left(\pm\imath p_{i_o}^R z\right)}{\sqrt{p_{i_o}^R}}\mathbf{\Psi}_{i_o}^R, \quad p_{i_o}^R = \sqrt{2E-\lambda_{i_o}^R}, \quad z \ge z_{\max}. \qquad (46)$$

Here $\lambda_i^{L,R}$ and $\mathbf{\Psi}_i^{L,R} = \{\Psi_{1i}^{L,R},\ldots,\Psi_{Ni}^{L,R}\}^T$ 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

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

$$\mathbf{X}_{i_c}^{(-)}(z) \to \exp\left(+\sqrt{\lambda_{i_c}^L - 2E}z\right)\mathbf{\Psi}_{i_c}^L, \quad z \le z_{\min}, \quad v = \leftarrow,$$
$$\mathbf{Y}_{i_c}^{(+)}(z) \to \exp\left(-\sqrt{\lambda_{i_c}^R - 2E}z\right)\mathbf{\Psi}_{i_c}^R, \quad z \ge z_{\max}, \quad v = \rightarrow. \qquad (48)$$

# The asymptotic boundary conditions

## Properties

In addition, it should be noted that the open channel asymptotic vector solutions $\mathbf{X}^{(\pm)}(z)$ and $\mathbf{Y}^{(\pm)}(z)$ satisfy the relations

$$\mathbf{Wr}(\mathbf{Q}(z); \mathbf{X}^{(\mp)}(z), \mathbf{X}^{(\pm)}(z)) = \pm 2\imath \mathbf{I}_{oo}^{L},$$
$$\mathbf{Wr}(\mathbf{Q}(z); \mathbf{Y}^{(\mp)}(z), \mathbf{Y}^{(\pm)}(z)) = \pm 2\imath \mathbf{I}_{oo}^{R}. \qquad (49)$$

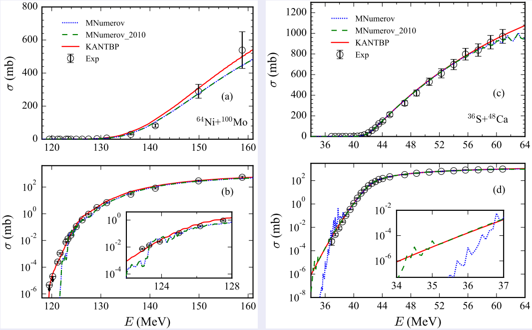
Then the following properties of the reflection and transmission matrices are held:

$$\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{I}_{oo}^{L}, \quad \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{R}_{\leftarrow} = \mathbf{I}_{oo}^{R},$$
$$\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{T}_{\leftarrow} = \mathbf{0}_{oo}^{L}, \quad \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{0}_{oo}^{R}, \qquad (50)$$
$$\mathbf{T}_{\rightarrow}^{T} = \mathbf{T}_{\leftarrow}, \quad \mathbf{R}_{\rightarrow}^{T} = \mathbf{R}_{\rightarrow}, \quad \mathbf{R}_{\leftarrow}^{T} = \mathbf{R}_{\leftarrow}.$$

Here $\mathbf{I}_{oo}^{L,R}$ is the unit $N_o^{L,R} \times N_o^{L,R}$ matrix, and $\mathbf{0}_{oo}^{L,R}$ is the zero $N_o^{L,R} \times N_o^{R,L}$ matrix.

# Nuclear physics

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




The modified Numerov method in CCFULL[a] (dotted blue line), the improved Numerov method in the CCFULL[b] (dashed green line) and KANTBP (solid red line).

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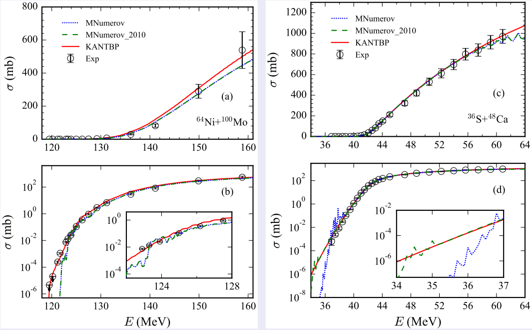



The modified Numerov method in CCFULL[a] (dotted blue line), the improved Numerov method in the CCFULL[b] (dashed green line) and KANTBP (solid red line).

$$X^{(-)}_{ji_o}(z_{\min}) = \exp(-\imath q_j(z_{\min})r)\delta_{ji_o}, \quad q_j(z_{\min}) = \sqrt{2E - U_{jj}(z_{\min})} > 0. \tag{51}$$

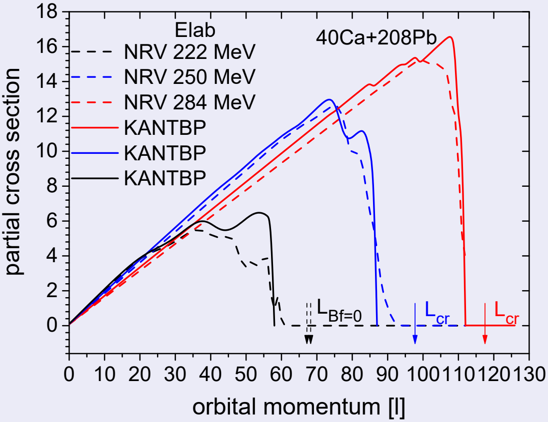
Lowest eigenvalues $\lambda_m$ are smaller than lowest diagonal elements $U_{mm}(z_{\min})$.

[a] K. Hagino, N. Rowley, A.T. Kruppa, Comput. Phys. Commun. 123 (1999) 143–152.
[b] K. Hagino, www2.yukawa.kyoto-u.ac.jp/~kouichi.hagino/ccfull/ccfull.f

# Nuclear physics

## Fission in the $^{40}$Ca+$^{208}$Pb reaction leading to the formation of the nucleus $^{248}$No[a]

[a]E.M. Kozulin, et al, V.V. Saiko, A.V. Karpov, et al, Phys. Rev. C 105 (2022) 024617.




The results are obtained using NRV[a] (dashed line), and KANTBP (solid line).

[a]http://nrv.jinr.ru/nrv

# Conclusion

A FORTRAN programs for calculating energy values, reflection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach are presented (transferred) in Comput. Phys. Commun. Program Library.

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Thank you for attention!