A Maple implementation of KANTBP code for solving problems in coupled channel method

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In collaboration with

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Outline

- Problem statement (Finite Element Method)
  - Eigenvalue problem
    - Metastable state problem
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    - Sub-barrier reactions of the fusion of heavy ions (PRC, 2020, 2021)

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Problem statement

Self-adjoint system of N second-order ODEs for unknowns $\Phi(z) \equiv \{\Phi^{(i)}(z)\}_{i=1}^{N_o}$, $\Phi^{(i)}(z) = (\Phi_1^{(i)}(z), \ldots, \Phi_N^{(i)}(z))^T$ 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:

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

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

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

Problem 1. For bound or metastable states

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

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

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

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

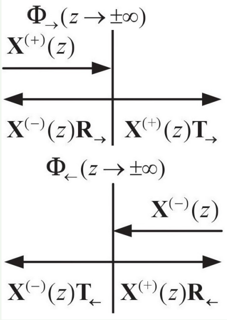
$$(\Phi_m | \Phi_{m'}) = \int_{z^{\min}}^{z^{\max}} f_B(z) (\Phi^{(m)}(z))^T \Phi^{(m')}(z) dz = \delta_{mm'}.$$

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



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

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

$\Phi_{\rightarrow}(z)$, $\Phi_{\leftarrow}(z)$ 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,

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

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

$\mathbf{X}^{(c)}_{\min}(z)$, $\mathbf{X}^{(c)}_{\max}(z)$ 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. $N_o^R\times N_o^L$, $N_o^L\times N_o^R$,

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

Problem 2. The scattering problem

Wronskian conditions

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

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

For real-valued potentials

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

$$\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{T}_{\leftarrow} = \mathbf{0}, \quad \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{0},$$

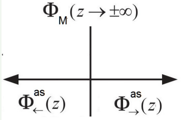
$$\mathbf{T}_{\rightarrow}^{T} = \mathbf{T}_{\leftarrow}, \quad \mathbf{R}_{\rightarrow}^{T} = \mathbf{R}_{\rightarrow}, \quad \mathbf{R}_{\leftarrow}^{T} = \mathbf{R}_{\leftarrow}.$$

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

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

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

Test example 1 (Scarf potential)

SE with the complex Scarf potential

$$\left(-\frac{d^2}{dz^2}+V_{Scarf}(z)-E\right)\Phi(z)=0,\ V_{Scarf}(z)=\frac{V_1}{\cosh^2 z}+\imath\frac{V_2\sinh z}{\cosh^2 z},\ z\in(-\infty,+\infty).$$

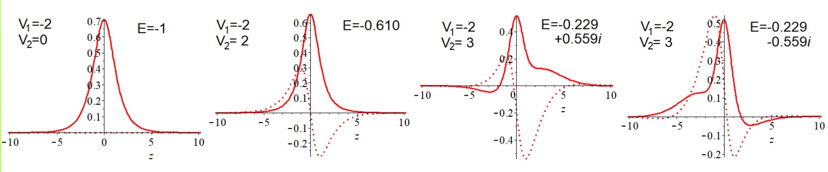
BP for $V_1<0$ and $V_2^2\in\mathcal{R}$

At $|V_2|<1/4-V_1$ the eigenvalues are essentially complex conjugate pairs:

$$E_n^{+}=-\left(n-(g_+^*+\imath g_-^*-1)/2\right)^2,\ g_\pm^*=\sqrt{1/4-V_1\mp V_2},\ n=0,1,...<(g_+^*-1)/2.$$

At $|V_2|\geq 1/4-V_1$ (or when V_2 is imaginary) the eigenvalues are real:

$$E_n=-\left(n-(g_+^*+g_-^*-1)/2\right)^2,\quad n=0,1,...<(g_+^*+g_-^*-1)/2.$$



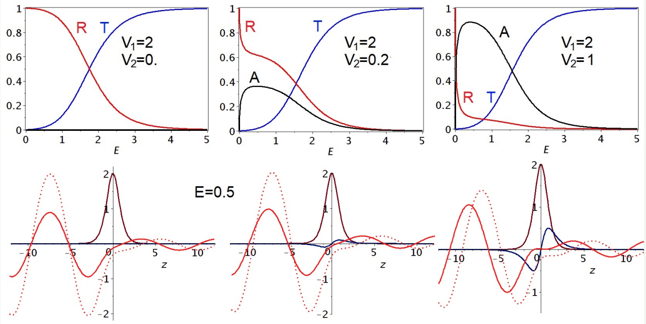
Ahmed, Z.: Real and complex discrete eigenvalues in an exactly solvable one-dimensional complex PT -invariant potential. Phys. Lett. A 282 (2001) 343–348

Test example 1 (Scarf potential)

Scattering problem

$$|R_\rightarrow|^2 + |T_\rightarrow|^2 = 1 - A_\rightarrow, \quad |R_\leftarrow|^2 + |T_\leftarrow|^2 = 1 - A_\leftarrow, \quad T_\rightarrow = T_\leftarrow \equiv T$$

$$A_\rightarrow = \frac{s_+ s_- - s_-^2}{1 + s_+ s_-}, \quad A_\leftarrow = \frac{s_+ s_- - s_+^2}{1 + s_+ s_-}, \quad s_\pm = \frac{\cosh(\pi g_+) e^{\pm \pi k} + \cosh(\pi g_-) e^{\mp \pi k}}{\sinh(2\pi k)}.$$



Here we consider only positive values $A_\rightarrow > 0$ (or $A_\leftarrow > 0$), commonly interpreted as the probability of absorption.

Ahmed, Z.: Schrödinger transmission through one-dimensional complex potentials. Phys. Rev. A 64 (2001) 042716

Cerveró, J.M., Rodríguez, A.: Absorption in atomic wires. Phys. Rev. A 70 (2004) 052705

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 $i_c = N_o^{L,R} + 1, \ldots, N$:

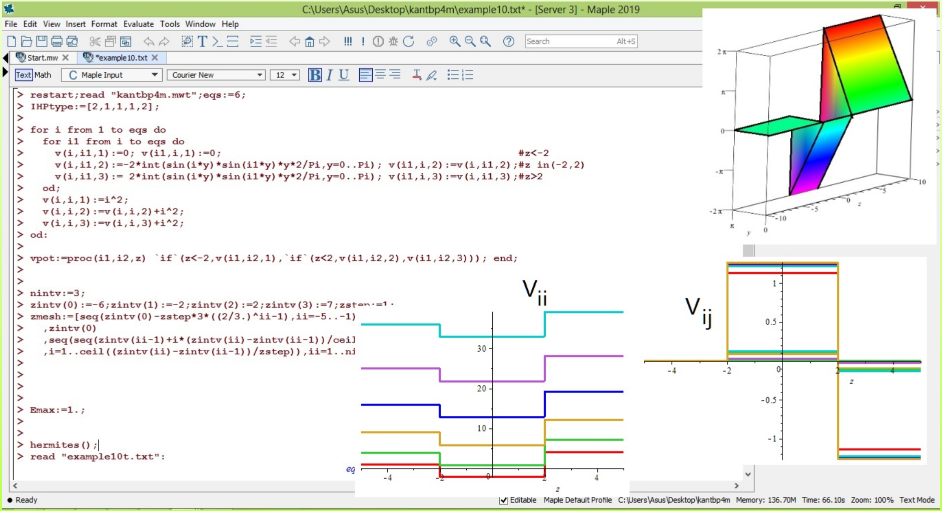
$$\mathbf{X}_{i_c}^{(c)}(z\to\infty)\to\exp\left(-\sqrt{\lambda_{i_c}^{L,R}-E}|z|\right)\Psi_{i_c}^{L,R}, \quad \lambda_{i_c}^{L,R}\geq\Re E, \quad i_c=N_o^{L,R}+1,\ldots,N.$$

Robin BC

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

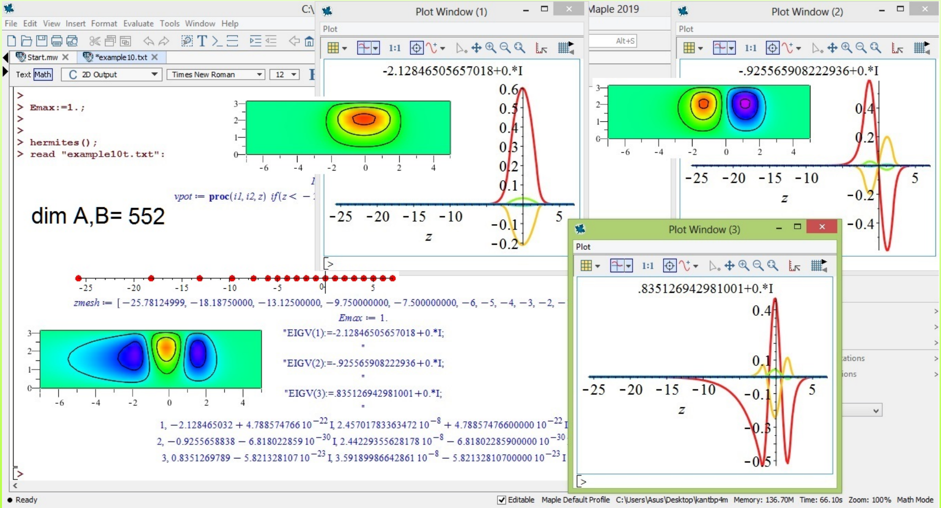
$$\mathbf{F}^{L,R}=\mathrm{diag}(...,\pm\sqrt{\lambda_{i_c}^{L,R}-E},...,\mp\imath\sqrt{E-\lambda_{i_o}^{L,R}},...)$$

The piecewise constant potentials

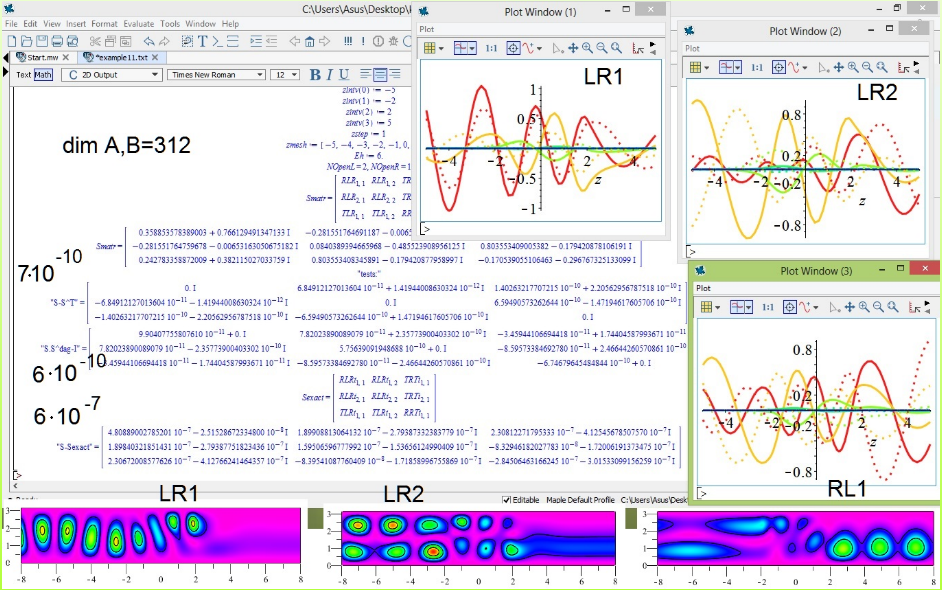


A. Gusev, S. Vinitsky, V. Gerdt, O. Chuluunbaatar, G. Chuluunbaatar, L. Le Hai, E. Zima, A Maple implementation of the finite element method for solving boundary problems of the systems of ordinary second order differential equations. Maple Conference, Waterloo Maple Inc., Canada 2020

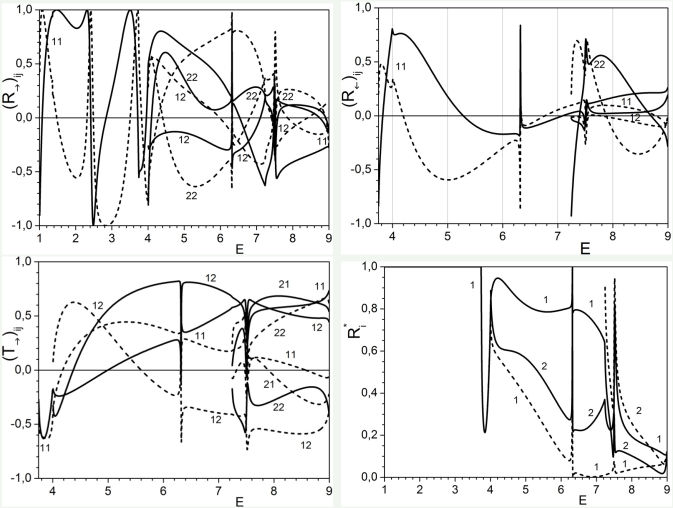
The piecewise constant potentials (eigenvalue problem)



The piecewise constant potentials (multichannel scattering problem)

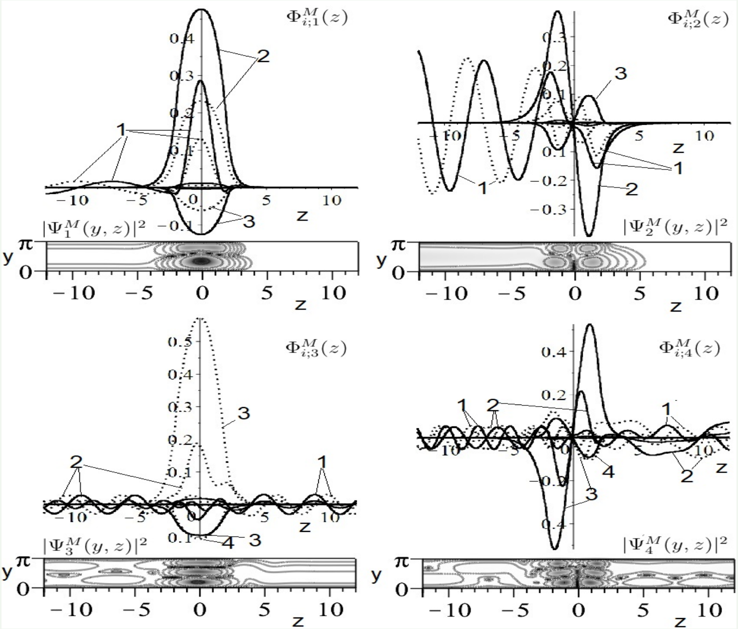


The piecewise constant potentials (multichannel scattering problem)

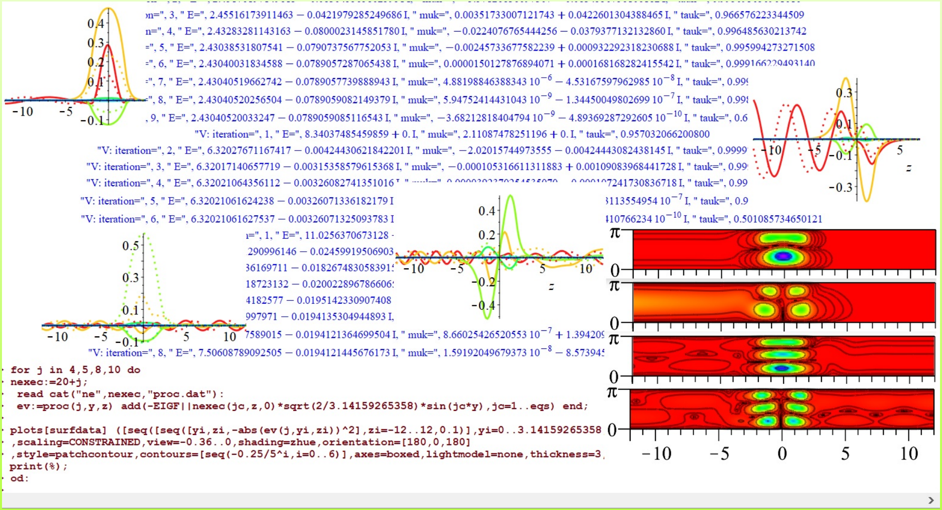


Real (solid curves) and imaginary (dashed curves) parts of elements $(R_\rightarrow)_{ij}$, $(R_\leftarrow)_{ij}$, $(T_\rightarrow)_{ij} = (T_\leftarrow)_{ji}$ of reflection $\mathbf{R}_\rightarrow$, $\mathbf{R}_\leftarrow$ and transmission $\mathbf{T}_\rightarrow$, $\mathbf{T}_\leftarrow$ amplitudes, and reflection coefficients $R^*_i = (\mathbf{R}^\dagger_* \mathbf{R}_*)_{ii}$ at $* =\rightarrow$ (solid curves) and $* =\leftarrow$ (dashed curves) as functions of scattering energy E.

The piecewise constant potentials (resonance scattering states)



The piecewise constant potentials (metastable state problem)



Spectrum of vibrational-rotational bound and metastable states of beryllium dimer

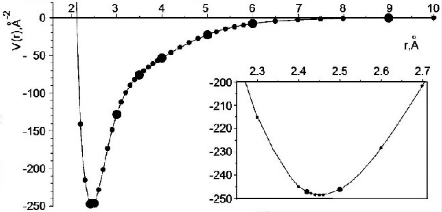
C:\Users\Asus\Desktop\kantbp4m\example23.txt* - [Server 3] - Maple 2019

$$\left(-\frac{1}{z^2}\frac{d}{dz}z^2\frac{d}{dz}+V(z)-E_i\right)\Phi_i(z)=0,$$

$$V(z)=\{V_{\rm grid}, z<z_{as}; V_{as}, z\geq z_{as}\}+\frac{L(L+1)}{z^2}.$$

$$\left.\frac{d\Phi(z)}{dz}\right|_{z=z_{\min}}=0,\quad \left.\frac{d\Phi(z)}{dz}\right|_{z=z_{\max}}=\mathcal{R}(E)\Phi(z_{\max})$$

```
> restart;read "kantbp4m.mwt";
> nexec:=100;keypot:=0;pmax:=5;
> fgrid:=[[ 1.50,0.1118807175059 ],[ 1.60,0.0739898922057 ],[ 1.70,0.0466443312944 ],[ 1.80,0.02
  ...
  [42.00,-0.000000023785252],[44.00,-0.000000013564164],[46.00,-0.000000012564136],[48.00,-0.0000
> hermites();
> sc1:=58664.99239;sc2:=1/0.2672973729;
>
> zmax:=15.0;fa:=proc(z) z^2*sc2; end;fb:=proc(z) z^2; end;
> read "ap100proc.dat":
> vpotas:=proc(z) 214/z^6+10230/z^8+504300/z^10; end;
> vpotsc:=sc1*APPR100(zmax,0)/vpotas(zmax/sc2);
> vpot:=proc(z)
> (`if`(z<zmax,sc1*APPR100(z,0),vpotsc*vpotas(z/sc2))+L*(L+1)/z^2)*sc2;
> end;
> zmesh1:=[1.90,2.00,2.15,2.30,2.42,2.50,2.62,2.80,seq(3+0.25*i,i=0..11),seq(
>
> L :=11;
> for i from nops(zmesh1)-1 to 2 by -1 do
> if(vpot(zmesh1[i])>vpot(zmesh1[i+1]) and vpot(zmesh1[i])>vpot(zmesh1[i-1]))
> if(vpot(zmesh1[i])<vpot(zmesh1[i+1]) and vpot(zmesh1[i])<vpot(zmesh1[i-1]))
> od;
> Emin:=max(0,vpot(zmin1));Emax:=vpot(zmax1);
> nexec:=99;
> keypot:=1;IHPtype:=[3,3];zmesh:=zmesh1[1..imax];DirR:=3;RBoundR:=-0.001*I;hermites();
> read "ev99proc.dat":
> for j from 1 to Ecur99 do
>   keypot:=3;  nexec:=1000+10*L+j;  zmesh:=zmesh1;
>   DirR:=3;  RBoundR:=sqrt(-EEh/sc2);
>   Eh:=EIGV99[j];
>   EIGFinit:=proc(z,ndiff) EIGF99(j,z,ndiff) end:
>   hermites();
> od:
```



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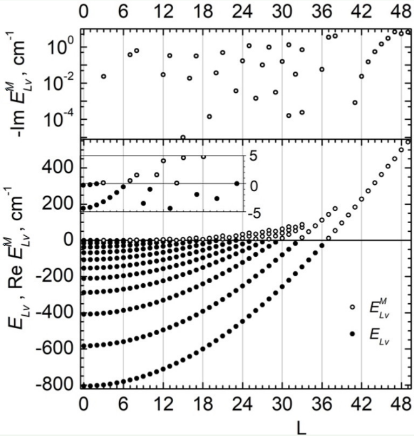
V.L.Derbov, G.Chuluunbaatar, A.A.Gusev, O.Chuluunbaatar, S.I.Vinitsky, A.Góźdź, P.M.Krassovitskiy, I.Filikhin, A.V. Mitin, Spectrum of beryllium dimer in ground $X^1\Sigma_g^+$ state, Journal of Quantitative Spectroscopy and Radiative Transfer Volume 262, 107529 (2021)

Spectrum of vibrational-rotational bound and metastable states of beryllium dimer

Comparison of the vibrational spectra $E_{v=0,L=0} - E_{vL=0}$ (in cm^{-1}) for the $X^1\Sigma_g^+$ state of the beryllium dimer.

v	STO	FEM STO	FEM MEMO	MEMO	EMO	Exp
r_e	2.4344	2.447	2.4534	2.4534	2.4535	2.4536
D_e	934.6	934.4	929.804	929.74	929.74	929.7±2
D_0	807.7	807.7	806.07	806.48	806.5	807.4
1	223.4	223.5	222.50	222.16	222.7	222.6
2	400.1	398.2	397.34	397.6	397.8	397.1
3	517.3	519.3	517.71	517.87	518.2	518.1
4	595.1	595.7	594.89	595.06	595.4	594.8
5	651.7	652.2	651.91	652.10	652.4	651.5
6	698.7	699.3	698.92	699.14	699.4	698.8
7	738.0	738.1	737.72	737.97	738.2	737.7
8	769.3	768.6	768.27	768.56	768.8	768.2
9	790.1	790.1	789.74	790.05	790.7	789.9
10	802.6	802.6	801.66	802.08	803.4	802.6
11	807.5	807.2	805.74	806.21		
rms	1.0	0.7	0.4	0.4	0.6	



Eigenenergies E_{vL} of bound states and real part $\Re E^M_{Lv}$ and imaginary part $-\Im E^M_{Lv}$ of complex eigenenergies of metastable states.

Sub-barrier reactions of the fusion of heavy ions

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

$V_{nn'}(r)$ are matrix elements of Coulomb and the Nuclear (Woods-Saxon potential derived from Akyüz-Winther parameterization) $V_N^{(0)}(r)$ potentials.

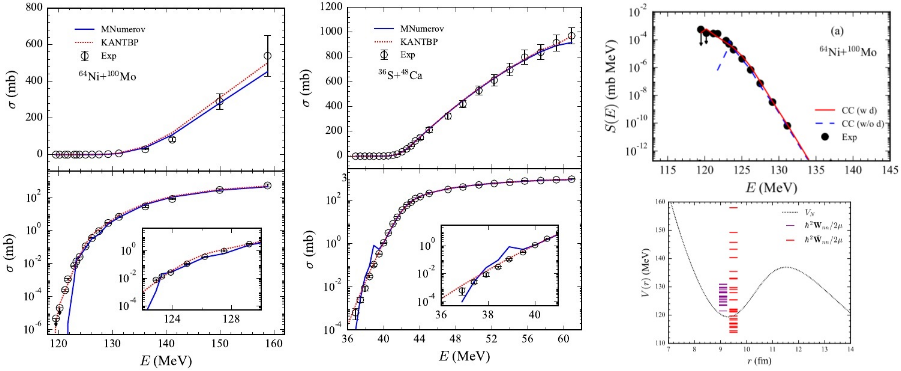
$$\psi^{as}_{nn_o}(r)=\sum_{m=1}^{M_o}A_{nm}\frac{\exp(-iK_m r)}{\sqrt{K_m}}\hat{T}_{mn_o}+\sum_{m=M_o+1}^{N}A_{nm}\frac{\exp(|K_m|r)}{\sqrt{|K_m|}}\hat{T}^c_{mn_o},\quad r=r_{\min},$$

$$\psi^{as}_{nn_o}(r)=\begin{cases}\hat{H}^-_l(k_n r)\delta_{n,n_o}+\hat{H}^+_l(k_n r)\hat{R}_{nn_o}, & r=r_{\max},\\ 2|k_n|^{1/2+l}r^{1+l}\exp(-|k_n|r)U(1+l+\eta_n,2,2+2l|k_n|r), & r=r_{\max}.\end{cases}$$

$\hat{H}^{\pm}_l(...)$ are Coulomb functions, $U(...)$ is Whittaker function

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. Góźdź 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



Fusion cross sections $\sigma_f(E) = \pi/k_{no}^2 \sum_{l=1}^{l_{\max}(E)} (2l+1) \sum_{m=1}^{M_o} |\mathbf{T}^{(l)}|^2_{mn_o}$ for ^{64}Ni+^{100}Mo and ^{36}S+^{48}Ca.

solid line (MNumerov), are the results obtained by means of CCFULL [a]

dotted line are the results obtained by means of KANTBP.

The astrophysical $S(E)$ factor $S(E) = E\sigma_f(E)\exp(2\pi(\eta - \eta_0))$ for the reaction ^{64}Ni+^{100}Mo calculated with (solid) and without (dashed line) taking into account non-diagonal elements, where $\eta_n = k_n Z_P Z_T e^2/(2E_n)$ is the Sommerfeld parameter, $E_n = E - \epsilon_n$, $\eta_0 = 105.74$. The potential, diagonal matrix elements and eigenvalues of matrix of potentials.

Conclusion

- The KANTBP 5M program [G. Chuluunbaatar, A. Gusev et al Communications in Computer and Information Science 1414, pp. 152–166 (2021)] (the upgrade of KANTBP 4M by A.A. Gusev et al, JINRLIB [https://wwwinfo.jinr.ru/programs/jinrlib/kantbp4m/indexe.html]) implemented in MAPLE for solutions to a given accuracy of multichannel scattering and eigenvalue problems for the system of ODEs of the second order with continuous or piecewise continuous real or complex-valued coefficients.
- Discretization of the boundary problems are implemented by the FEM with the interpolation Hermite polynomials preserves the property of continuity of derivatives of the desired solutions.
- For the reduction of the scattering problem with a different number of open channels in the two (left and right) asymptotic regions to the boundary problems on a finite interval, the asymptotic boundary conditions are approximated homogeneous Robin (or third-type) boundary conditions (RBC).
- For the calculation of metastable states with complex eigenvalues, or to solve the problem for bound states with RBC depending on the spectral parameter the Newtonian iteration scheme is implemented.
- Code of the KANTBP 5M and test examples will be present in program library JINRLIB.

Thank you for your attention