



Research Article

CALCULATION OF METASTABLE STATES IN SCATTERING AND EIGENVALUE PROBLEMS FOR COMPLEX POTENTIAL BARRIER

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ABSTRACT

This paper presents the computational scheme and calculation results of metastable states in scattering and eigenvalue problems for complex potential barriers. For the scattering problem, the wave functions with S -scattering matrix are calculated at fixed real-valued energy of an incident wave, and the eigenvalue problem with corresponding eigenvalues are calculated as well. Then, we consider the wave functions of metastable states in the vicinity of these resonance energies for two of these problems. The solution to the problems is performed using the authors' software package with the high-accuracy finite element method. The calculation results are shown in table and graph form.

Keywords: complex potential barrier; eigenvalue problem; KANTBP 4M program; metastable states; scattering problem

1. Introduction

In recent years, several complex potential models (symmetric versions of the harmonic oscillator, one-dimensional Coulomb-like, Scarf) have been investigated to show analysis of bound or scattering states (Znojil, 1999; Bagchi & Quesne, 2000). There are also a number of scientific works investigating and studying metastable states for these complex potential energy barriers and presenting interesting research results. Metastable states of a quantum system sometimes exist in real and complex potential energy barriers or wells (Ahmed, 2001; Jia, Lin, & Sun, 2002; Bagchi & Quesne, 2002). However, the number of such works is not much. It has been known that metastable state, in physics and chemistry, particular excited state of an atom, nucleus, or other system that has a longer lifetime than the ordinary excited states and that generally has a shorter lifetime than the lowest, often stable, energy state,

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called the ground state. The metastable state of a quantum system is an important model in quantum physics and atomic nuclear physics.

In our last work (Gusev et al., 2015), we presented a numerical scheme and algorithm to calculate resonance metastable states in scattering and eigenvalue problems containing complex potential barriers like complex rectangular and Scarf potentials. As a result, we have shown that for these complex potential barriers not only bound states but also metastable states exist. In the present work, we continue studying these problems for another complex potential barrier, the Poschl-Teller potential barrier. This barrier type plays an important role in mathematical models, describing wave propagation in smoothly irregular waveguides, tunneling and channelling of compound quantum systems through multidimensional potential barriers, photoionization, photoabsorption (Muga & Rodriguez, 2004; Cervero et al., 2004; Sevastyanov et al., 2014), and transport in atomic, molecular, and quantum-dimensional semiconductor systems (Chuluunbaatar et al., 2007; Vinitzky et al., 2013; Vinitzky et al., 2014).

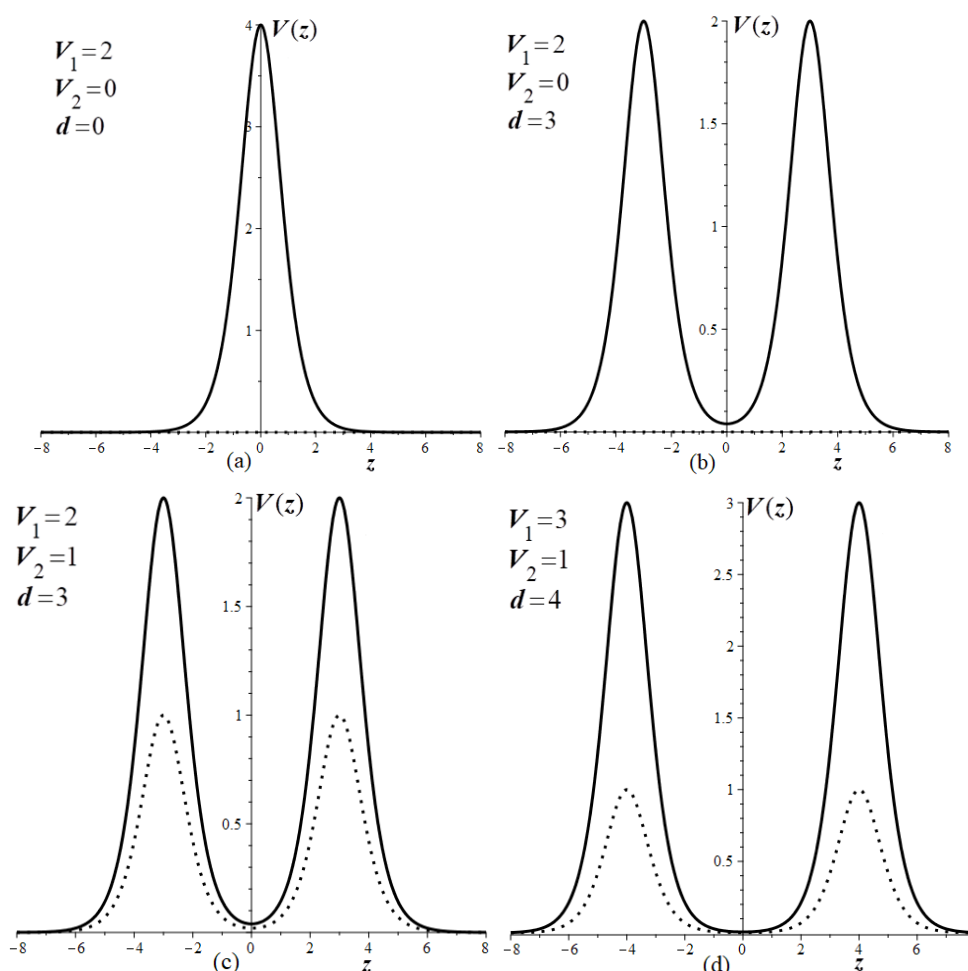


Figure 1. The system of two complex Poschl-Teller potential barriers at different values of V_1 , V_2 and d . The solid line shows the real part and the dotted line shows the imaginary part

The paper is organized as follows. In Section 2, the formulation of the boundary-value problems with the boundary conditions of the first, second, and third kind is presented. Section 3 presents the algorithm for calculating the metastable states in scattering and eigenvalue problems for complex Poschl-Teller potential barriers in KANTBP 4M program (Gusev et al., 2015). This program solves BVPs of mathematical models reduced from low-dimensional complex quantum models based on the finite element method (FEM) with Hermite interpolation polynomials (HIPs). Finally, in Section 4 by using KANTBP 4M program, the calculation results are presented in graphs and tables. In the conclusion section, we discuss further applications of the elaborated method and results.

2. Problem statement and method of research

2.1. Problem statement

The one dimensional Schrodinger equation has the form:

$$\left(-\frac{d}{dz^2} + V(z) - E_m \right) \Phi_m(z) = 0 \tag{1}$$

A complex double Poschl-Teller potential barrier is given by:

$$V(z) = \frac{V_1}{\cosh(z-d)^2} + i \frac{V_2}{\cosh(z-d)^2} + \frac{V_1}{\cosh(z+d)^2} + i \frac{V_2}{\cosh(z+d)^2} \tag{2}$$

Here d is the distance between two separated barriers. V_1, V_2 , and d are considered as parameters of potential barriers (2). Obviously, at $V_1 < 0, V_2 < 0$ we have potential well, and at $V_1 > 0, V_2 > 0$ we have a potential barrier. Figure1 shows the system of two complex Poschl-Teller potential barriers at different values of V_1, V_2 , and d . One can be seen that the complex Poschl-Teller potential barrier is symmetric. Indeed, at $d = 0, V_1 > 0, V_2 = 0$ there is one barrier only (Figure 1a), at $d > 0, V_1 > 0, V_2 = 0$ there are two symmetric barriers with separated distance d (Figure 1b) and at $d > 0, V_1 > 0, V_2 > 0$ we have two symmetric barriers with real and imaginary parts (Figure 1c and Figure 1d). We must consider possible metastable states existing in these barriers depending on different values of V_1, V_2 and d .

2.2. Method of research: Algorithm for calculating metastable states in scattering and eigenvalue problems

To solve Eq. (1) for metastable states, we consider the boundary value problem (BVP) for the system of ordinary differential equations (ODE) of the second-order with respect to the unknown functions $\Phi(z) = (\Phi_1(z), \dots, \Phi_N(z))^T$ of the independent variable $z \in (z^{\min}, z^{\max})$ (Streng & Fics, 1977):

$$\left(-\frac{1}{f_B(z)} \mathbf{I} \frac{d}{dz} f_A(z) \frac{d}{dz} + \mathbf{V}(z) + \frac{f_A(z)}{f_B(z)} \mathbf{Q}(z) \frac{d}{dz} + \frac{1}{f_B(z)} \frac{d f_A(z) \mathbf{Q}(z)}{dz} - \mathbf{E} \mathbf{I} \right) \Phi(z) = 0 \tag{3}$$

Here $f_A(z) > 0$ and $f_B(z) > 0$ are continuous or piecewise continuous positive functions, \mathbf{I} is the unit matrix, $\mathbf{V}(z)$ is a symmetric matrix ($V_{ij}(z) = V_{ji}(z)$), and $\mathbf{Q}(z)$ is an antisymmetric matrix ($Q_{ij} = -Q_{ji}$). These matrices have dimension $N \times N$, and their elements are continuous or piecewise continuous real or complex-valued coefficients from the Sobolev space $\mathcal{H}_2^{s \geq 1}(\Omega)$, providing the existence of nontrivial solutions subjected to homogeneous boundary conditions: Dirichlet (I kind) and/or Neumann (II kind) and/or third kind (III kind or the Robin condition) at the boundary points of the interval $z \in (z^{\min}, z^{\max})$ at given values of the elements of the real or complex-valued matrix $\mathcal{R}(z^t)$ of dimension $N \times N$.

$$(I): \quad \Phi(z^t) = 0, \quad t = \min \text{ and/or } \max \tag{4}$$

$$(II): \quad \lim_{z \rightarrow z^t} f_A(z) \left(\mathbf{I} \frac{d}{dz} - \mathbf{Q}(z) \right) \Phi(z) = 0, \quad t = \min \text{ and/or } \max \tag{5}$$

$$(III): \quad \left(\mathbf{I} \frac{d}{dz} - \mathbf{Q}(z) \right) \Phi(z) \Big|_{z=z^t} = R(z^t) \Phi(z^t), \quad t = \min \text{ and/or } \max \tag{6}$$

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

$$(\Phi_m | \Phi_{m'}) = \int_{z_{\min}}^{z_{\max}} f_B(\Phi_m(z))^T \Phi_{m'}(z) dz = \delta_{mm'}. \tag{7}$$

2.2.1. For the multichannel scattering problem

On the axis $z \in (-\infty, +\infty)$ at fixed energy $E = \Re E$, the desired matrix solutions $\Phi(z) \equiv \{\Phi_\nu^{(i)}(z)\}_{i=1}^N$, $\Phi_\nu^{(i)}(z) = (\Phi_{1\nu}^{(i)}(z), \dots, \Phi_{N\nu}^{(i)}(z))^T$ of the boundary problem (3) (the subscript ν means the initial direction of the incident wave from left to right \rightarrow or from right to left \leftarrow) in the interval $z \in (z^{\min}, z^{\max})$. These matrices solutions are subjected to homogeneous third kind boundary conditions (6) at the boundary points of the interval $z \in (z^{\min}, z^{\max})$ with the asymptotes of the “incident wave + outgoing waves” type in open channels $i = 1, \dots, N_o$ (Gusev et al., 2016):

$$\Phi_{\rightarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}_{\min}^{(\rightarrow)}(z) + \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{R}_{\rightarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{R}_{\rightarrow}^c, & z \rightarrow -\infty, \\ \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{T}_{\rightarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{T}_{\rightarrow}^c, & z \rightarrow +\infty, \end{cases} \tag{8}$$

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

Here $\Phi_{\rightarrow}(z), \Phi_{\leftarrow}(z)$ are matrix solutions with dimensions $N \times N_o^L, N \times N_o^R$, where 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 $z \rightarrow -\infty$, dimensions $N \times N_o^L, \mathbf{X}_{\max}^{(\rightarrow)}(z), \mathbf{X}_{\max}^{(\leftarrow)}(z)$ are open channel asymptotic solutions at $z \rightarrow +\infty$, dimensions $N \times N_o^R, \mathbf{X}_{\min}^{(c)}(z), \mathbf{X}_{\max}^{(c)}(z)$ are closed channel solutions, dimension $N \times (N - N_o^L), N \times (N - N_o^R), \mathbf{R}_{\rightarrow}, \mathbf{R}_{\leftarrow}$ 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 matrices of dimension $N_o^R \times N_o^L, N_o^L \times N_o^R, \mathbf{R}_{\rightarrow}^c, \mathbf{T}_{\rightarrow}^c, \mathbf{T}_{\leftarrow}^c, \mathbf{R}_{\leftarrow}^c$ are auxiliary matrices. For real valued potentials $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ the transmission \mathbf{T} and reflection \mathbf{R} amplitudes satisfy the relations:

$$\begin{aligned} \mathbf{T}_{\rightarrow}^+ \mathbf{T}_{\rightarrow} + \mathbf{R}_{\rightarrow}^+ \mathbf{R}_{\rightarrow} &= \mathbf{I}_{oo}, \quad \mathbf{T}_{\leftarrow}^+ \mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^+ \mathbf{R}_{\leftarrow} = \mathbf{I}_{oo}, \\ \mathbf{T}_{\rightarrow}^+ \mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^+ \mathbf{T}_{\leftarrow} &= \mathbf{0}, \quad \mathbf{R}_{\leftarrow}^+ \mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^+ \mathbf{R}_{\rightarrow} = \mathbf{0}, \\ \mathbf{T}_{\rightarrow}^T &= \mathbf{T}_{\leftarrow}, \quad \mathbf{R}_{\rightarrow}^T = \mathbf{R}_{\leftarrow}, \quad \mathbf{R}_{\leftarrow}^T = \mathbf{R}_{\rightarrow} \end{aligned} \tag{9}$$

ensuring unitarity and symmetry of the \mathbf{S} -scattering matrix:

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix}, \quad \mathbf{S}^+ \mathbf{S} = \mathbf{S} \mathbf{S}^+ = \mathbf{I}. \tag{10}$$

Here symbols $^+$ and T denote conjugate transpose and the transpose of a matrix, respectively.

2.2.2. For the eigenvalue problem

The KANTBP 4M program calculates a set of M energy eigenvalues $E: \Re E_1 \leq \Re E_2 \leq \dots \leq \Re E_M$ and the set of corresponding eigenfunctions $\Phi(z) \equiv \{\Phi^m(z)\}_{m=1}^M, \Phi^m(z) = (\Phi_1^{(m)}(z), \dots, \Phi_N^{(m)}(z))^T$ from the space \mathcal{H}_2^2 for the system (3). The solutions are subjected to the normalization and orthogonality conditions:

$$\langle \Phi^{(m)} | \Phi^{(m')} \rangle = \int_{z_{\min}}^{z_{\max}} f_B(z) (\Phi^{(m)}(z))^{\dagger} \Phi^{(m')}(z) dz = \delta_{mm'} \tag{11}$$

To solve the problem for bound states on the axis or on the semiaxis the initial problem is approximated by boundary value problem (3)–(6) on a finite interval $z \in (z^{\min}, z^{\max})$ with boundary conditions (4)–(6).

2.2.3. For the calculation of metastable states

With complex eigenvalues $E = \Re E + i \Im E, \Im E < 0: \Re E_1 \leq \Re E_2 \leq \dots$ the Robin BC follow from outgoing wave fundamental asymptotic solutions that correspond to Siegert outgoing wave BCs (Gusev et al., 2015).

For the set ODEs (1) with $f_A(z) = f_B(z) = 1, Q_{ij}(z) = 0$ and constant effective potentials $V_{ij}(z) = V_{ij}^{L,R}$ in the asymptotic region, asymptotic solutions $\mathbf{X}_i^{(*)}(z \rightarrow \pm\infty)$ are expressed by the following formulas:

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

$$\mathbf{X}_{i_c}^{(c)}(z \rightarrow \infty) \rightarrow \exp\left(-\sqrt{\lambda_{i_c}^{L,R} - E}|z|\right)\psi_{i_c}^{L,R}, \lambda_{i_c}^{L,R} \geq \Re E, i_o = N_o^{L,R} + 1, \dots, N.$$
(12)

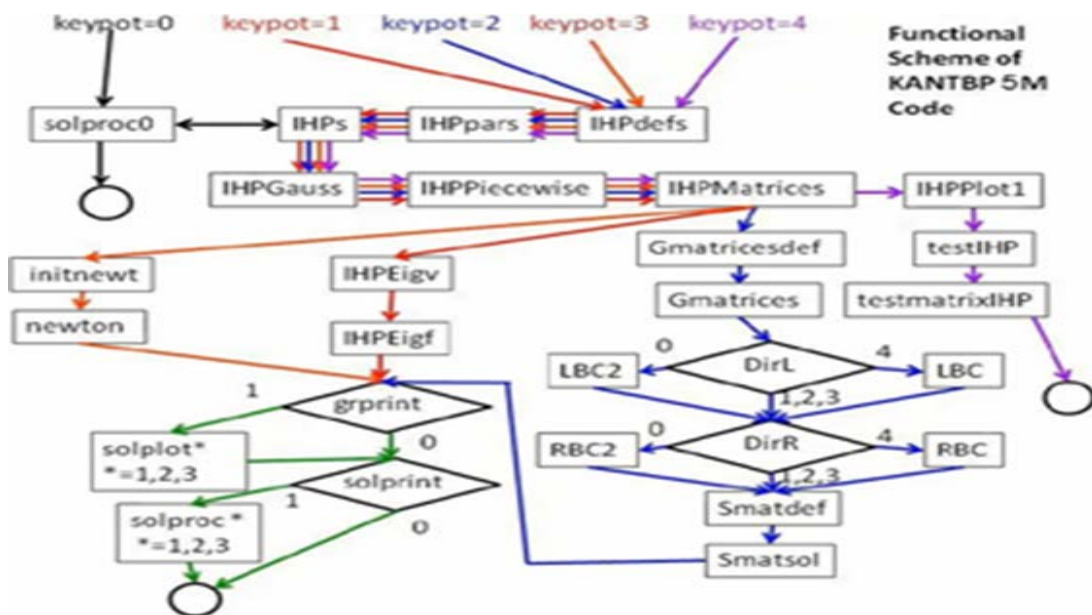


Figure 2. Functional structure of KANTBP 4M code for different types of quantum problems $keypot = 0$, approximation of function given in nodes by a continuous one in the form of a procedure.

$keypot = 1$ solution of the eigenvalue problem,

$keypot = 2$ solution of the multichannel scattering problem,

$keypot = 3$ solution of the eigenvalue problem by Newton method.

$keypot = 4$ (supplementary) calculations of errors estimation of IHP and stiffness and mass matrices elements of the algebraic problem.

DirL, DirR; boundary condition key in the left and right points of interval:

1 Dirichlet boundary condition,

2 Neumann boundary condition,

3 Robin boundary condition,

0 Robin boundary condition that determined from the asymptotic solution,

4 Robin boundary condition that determined from the asymptotic solution for the user supplied procedure.

Figure 2 shows the functional structure of the KANTBP 4M code for different types of boundary quantum problems. One can be seen that for different values of *keypot* there are different boundary problem types. For example, at *keypot* = 1, we have a solution to the eigenvalue problem, at *keypot* = 2, we have a solution to the multichannel scattering problem and at *keypot* = 3, we have a solution to the eigenvalue problem by Newton method for calculating metastable states. *DirL* and *DirR* are the boundary condition keys in the left and right points of the interval.

3. Results of calculating metastable states

3.1. For scattering problem

In this problem, by using KANTBP 4M at *keypot* = 2 and *keypot* = 3, the mesh has been chosen as $\Omega_i = [seq(0, 75.i, i = -40, 40)]$ with III kind boundary condition (Robin condition) (6). In this case, *DirL* = *DirR* = 0 for scattering problem and *DirL* = *DirR* = 3 for calculation of metastable states. The numerical calculating results are presented in Figure 3 and Figure 4. These figures show the graph of wave functions in scattering problem with fixed energy $E = \Re E$ of the incident wave and wave function of metastable state at different values of V_1, V_2 , and d . The solid line shows the real part, and the dotted line shows the imaginary part. It can be seen that for a wave from left there is one open channel, and from right there is one open channel also. The amplitude of wave functions depends on the height (V_1, V_2) of the potential barriers and the distance d between them and decreases after passing through the potential barriers (left and middle). The metastable states explicitly exist in the region between the two potential barriers (right). The lower panel shows scattering matrix **S** calculated by formula (10). All elements of scattering matrix **S** are complex.

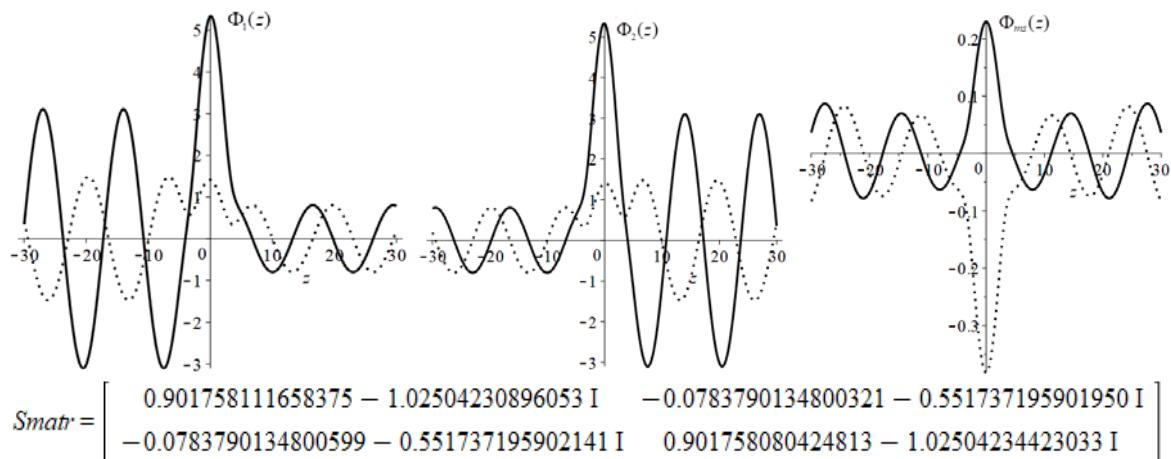


Figure 3. Upper panel shows the plot of wave functions $\Phi_m(z)$ in the scattering problem (left and middle) with fixed energy $\Re E = 0, 23456$ of the incident wave and wave function of the metastable state (right) at $V_1 = 1; V_2 = 0, 1; d = 3, 5$. The solid line shows the real part, and the dotted line shows the imaginary part. The lower panel presents scattering matrix **S**.

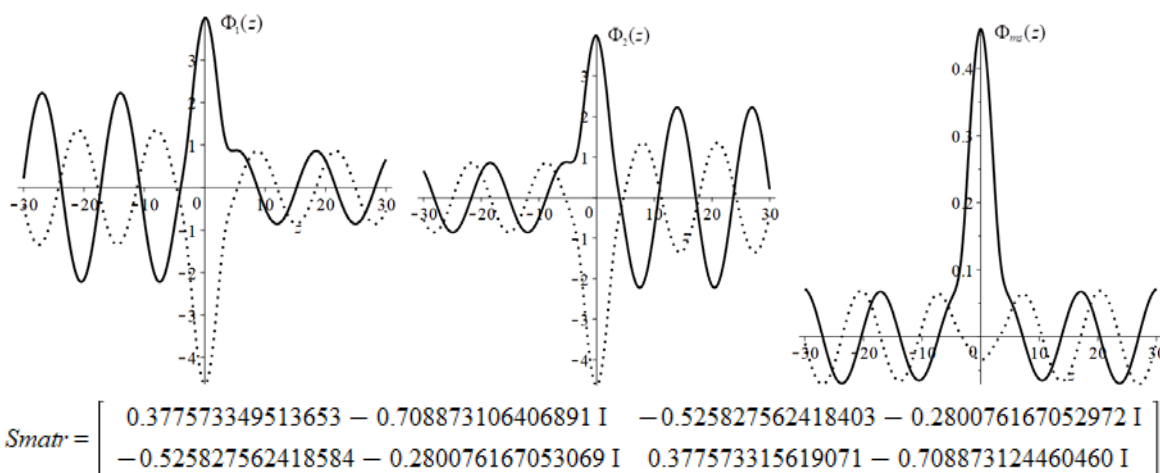


Figure 4. Upper panel shows the plot of wave functions $\Phi_m(z)$ in the scattering problem (left and middle) with fixed energy $\Re E = 0,23456$ of the incident wave and wave function of the metastable state (right) at $V_1 = 1; V_2 = 0; d = 3,5$. The solid line shows the real part, and the dotted line shows the imaginary part. The lower panel presents scattering matrix **S**.

3.2. For eigenvalue problem

In this problem, by using KANTBP 4M at *keypot* = 1 and *keypot* = 3, the mesh has been chosen as $\Omega_2 = [seq(0,75.i, i = \overline{-10,10})]$ with I kind (Dirichlet condition) (4) and III kind boundary conditions (Robin condition) (6). In this case, $DirL = DirR = 1$ for eigenvalue problem and $DirL = DirR = 3$ for calculation of metastable states. The numerical calculating results are presented in Table 1 and in Figure 5 and Figure 6.

Table 1. The first eigenvalues E_m ($m = 1,2,3,4$) and corresponding resonance energies $\Re E_{\text{res}}$ of the metastable states at different values of V_1, V_2 , and d .

Parameters of potential barrier	Eigenvalues E_m	Resonance energies $\Re E_{\text{res}}$
$V_1 = 1; V_2 = 0,3;$ $d = 3$	$E_1 = 0,300062354377042 + 0,0530851054023483.i$	0,3071
	$E_2 = 0,493225802797972 + 0,059921912036273.i$	0,4898
	$E_3 = 0,533511451371992 + 0,0373263631142993.i$	0,5042
	$E_4 = 0,993897759035974 + 0,102470325986607.i$	0,9935
$V_1 = 1,3; V_2 = 0,2;$ $d = 3$	$E_1 = 0,346182612766816 + 0,0302082273991865.i$	0,3545
	$E_2 = 0,542268506977339 + 0,0319825094259676.i$	0,5319
	$E_3 = 0,568501040007439 + 0,0228587829711715.i$	0,5697
	$E_4 = 1,09844657800175 + 0,0688183686207677.i$	1,1036

Table 1 shows the eigenvalues E_m and corresponding real-valued resonance energies $\Re E_{\text{res}}$ in the eigenvalue problem. One can be seen that at $V_2 \neq 0$ the imaginary part of eigenvalues exist and as the difference between the peaks of the two potential barriers ($V_1 - V_2$) increases, the energy eigenvalues also increase, thereby increasing the resonance energy for the metastable states.

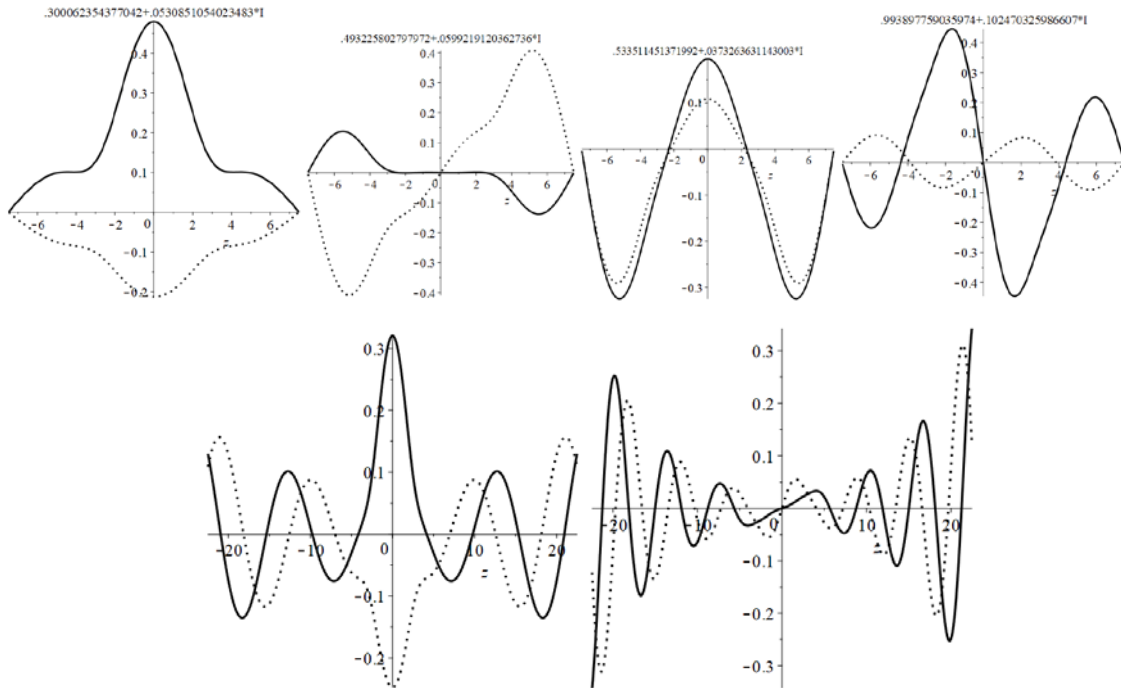
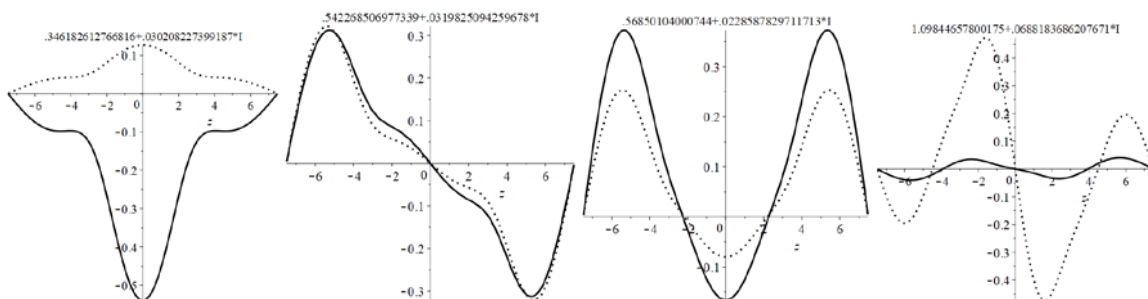


Figure 5. Upper panel: Plots of wave functions $\Phi_m(z)$ with corresponding eigenvalues E_m in eigenvalue problem at $V_1 = 1; V_2 = 0, 3; d = 3$. Lower panel: Plots of wave functions for metastable states in the vicinity of resonance energies $\Re E_{\text{res}} \approx 0,3071$ (left) and $\Re E_{\text{res}} \approx 0,9935$ (right) respectively, given in Table 1. The solid line shows the real part, and the dotted line shows the imaginary part



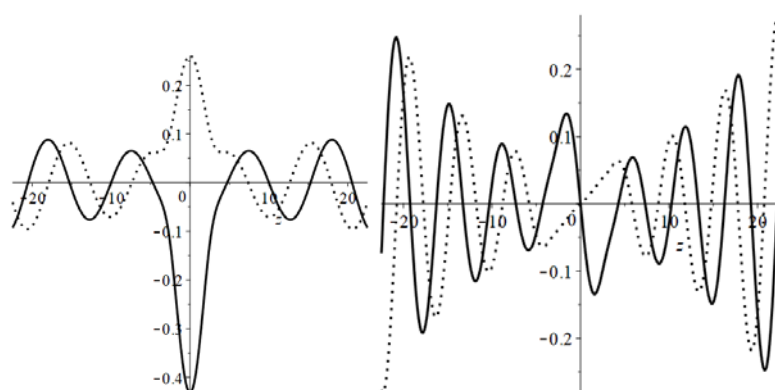


Figure 6. Upper panel: Plots of wave functions $\Phi_m(z)$ with corresponding eigenvalues E_m in eigenvalue problem at $V_1 = 1, 3; V_2 = 0, 2; d = 3$. Lower panel: Plots of wave functions for metastable states in the vicinity of resonance energies $\Re E_{\text{res}} \approx 0,3545$ (left) and $\Re E_{\text{res}} \approx 1,1036$ (right) respectively, given in Table 1. The solid line shows the real part, and the dotted line shows the imaginary part

Figure 5 and Figure 6 show the wave functions $\Phi_m(z)$ with corresponding eigenvalues E_m in the eigenvalue problem (upper panel) at different values of $V_1; V_2; d$. As can be seen that the wave functions obtained by using KANTBP 4M are similar to the ones in the analytical method (Jia, Sun & Li, 2002). That means that the program KANTBP 4M gives pretty high accuracy. The lower panel shows wave functions for metastable states in the vicinity of resonance energies $\Re E_{\text{res}}$, given in Table 1. The solid line shows the real part and the dotted line shows the imaginary part. One can be seen that as the resonance energy increases, the wave function will oscillate more strongly in the region between the two potential barriers.

4. Conclusion

This paper presented a computational scheme and calculation results of metastable states in scattering and eigenvalue problems for complex Poschl-Teller potential barriers. These two problems are considered boundary value problems on a finite interval of one independent variable. The reduced mathematical model was solved using the authors' software package with the high-accuracy finite element method. The complex Poschl-Teller potential barrier has different shapes depending on its parameters. As expected, this potential barrier has not only bound states, but also finite number of metastable states.

These results have significant importance for further experiments in studying important mathematical models, describing wave propagation in smoothly irregular waveguides, tunneling and channelling of compound quantum systems through multidimensional potential barriers, photoionization, photoabsorption, and transport in

atomic, molecular, and quantum-dimensional semiconductor systems. In the future, based on the obtained elaborated method and results, we will continue to investigate the metastable state for complex potential barriers in a more complex form, thereby constructing new numerical schemes and algorithms to investigate the physical properties of any quantum system.

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**TÍNH TOÁN CÁC TRẠNG THÁI SIÊU BỀN
TRONG BÀI TOÁN TÁN XẠ VÀ BÀI TOÁN TRỊ RIÊNG CHỨA RÀO THỂ PHỨC**
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TÓM TẮT

Trong bài báo này chúng tôi trình bày sơ đồ thuật toán và kết quả tính toán các trạng thái siêu bền trong bài toán tán xạ và bài toán trị riêng chứa rào thế năng ở dạng phức. Đối với bài toán tán xạ, các hàm sóng với ma trận tán xạ S được tính toán với năng lượng có giá trị thực xác định của sóng tới, còn đối với bài toán trị riêng, các hàm sóng cùng với các trị riêng tương ứng cũng được tính toán. Sau đó, chúng tôi khảo sát và tính toán hàm sóng của các trạng thái siêu bền trong lân cận của các giá trị năng lượng cộng hưởng cho hai bài toán này. Nghiệm của bài toán biên được tính toán bằng chương trình phần mềm được biên soạn bởi tác giả bài báo cùng các cộng sự khoa học ở Viện Liên hiệp Nghiên cứu Hạt nhân Dubna, Thành phố Dubna, Liên bang Nga. Các thuật toán của chương trình tính toán này dựa trên phương pháp phân tử hữu hạn với độ chính xác cao. Kết quả tính toán được biểu diễn dưới dạng bảng và đồ thị.

Từ khóa: rào thế năng; bài toán trị riêng; chương trình KANTBP 4M; trạng thái siêu bền; bài toán tán xạ