OPTIMIZATION OF SINGLE-HUMP IMAGINARY POTENTIALS FOR EFFICIENT ABSORPTION OF THE WAVE FUNCTION IN NUMERICAL SOLUTION OF THE TIME-DEPENDENT SCHRÖDINGER EQUATION

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This work is devoted to the development of the imaginary potential method for efficient absorption of the wave function on the periphery of the computational domain in numerical solution of the time-dependent Schrödinger equation. The optimal relationships between the width and amplitude of single-hump imaginary potentials and the de Broglie wavelength corresponding to the maximum of absorption efficiency are determined.

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INTRODUCTION

The numerical solution of the time-dependent Schrödinger equation (TDSE) is one of the main tools for investigation of different phenomena, in particular, ionization-induced phenomena caused by ultrashort laser pulses [1-8]. In the latter case, the TDSE in the length gauge and dimensionless variables is written as

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi + V(\mathbf{r},t)\psi, \qquad (1)$$

where t is the time, $V(\mathbf{r},t)$ is the time-dependent particle potential energy, and $\mathbf{r}$ is the particle radius vector. In the mathematical formulation of the problem it is assumed that the boundaries of the computational domain are located at infinity. However, due to the finite size of the computational grid, the electronic wave function can reach the grid boundary and, depending on the method of numerical solution of the TDSE, reflect on it or move on to the opposite edge of the grid. Usually, in order to avoid reflection and transmission of the wave function, the absorbing layers are introduced near the grid boundaries [9]. The different methods of absorption are considered [6, 9 - 15], among which the simplest and most popular method uses negative imaginary potentials. The essence of this method consists in the introduction of negative imaginary potential (NIP) $U_{\mathrm{NIP}}(\mathbf{r})$ on the periphery of the computational domain [9],

$$V(\mathbf{r},t) \to V(\mathbf{r},t) + U_{\mathrm{NIP}}(\mathbf{r}). \qquad (2)$$

It is important that high efficiency of absorption is achieved in a limited range of de Broglie wavelengths. The width of this range increases with the width of the absorbing layer. However, the greater is the width of the layer, the more CPU time is required for numerical calculation. Therefore, the actual problem is the construction of compact imaginary potentials with a wide range of effective absorption.

One of the variants to construct the potential having a large range of absorption is the use of a set of smooth single-hump imaginary potentials located next to each other. Each single-hump potential will absorb in a certain range of wavelengths. The key moment is to determine the optimal parameters of single-hump potential, corresponding to the maximum absorption efficiency. In this work we investigate the reflection and transmission properties of two different single-hump imaginary potentials. We determine the dependences of the reflection and transmission coefficients on the de Broglie wavelength, as well as on the parameters of single-hump potentials. The dependences of optimal parameters of the absorbing potentials on the incident wavelength are found.

1. STATEMENT OF THE PROBLEM

Let us assume for simplicity that the boundary of the computational domain is flat and the imaginary potential depends only on the coordinate *x*, which is directed across the layer. Then the scattering of a plane wave on the imaginary potential is described by the one-dimensional stationary Schrödinger equation

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + U_{\mathrm{NIP}}(x)\psi = \frac{k^2}{2}\psi, \qquad (3)$$

where k is the *x* component of the wavenumber. The absorbing single-hump NIP is defined as

$$U_{\mathrm{NIP}}(x) = -iuf\left(x/l\right), \qquad (4)$$

where $u > 0$ and l are the amplitude and characteristic width of the potential, $f(\xi)$ is a real even bell-shaped function that defines the shape of the hump. We consider here two kinds of NIPs: *cosine-squared* potential, corresponding to

$$f(\xi) = \begin{cases} \cos^2\left(\pi\xi/2\right), & |\xi| \le 1 \\ 0, & |\xi| > 1, \end{cases} \qquad (5)$$

and *Pöschl–Teller* potential, corresponding to

$$f(\xi) = \cosh^{-2}\left(\alpha\xi\right),\ \alpha = 2\,\mathrm{acosh}\left(\sqrt{2}\right). \qquad (6)$$

The coefficient α in the last formula is introduced in such a way that width of the function $f(\xi)$ at the level of 1/2 is equal to 1, as for the function (5).

The efficiency of absorption of a plane wave is characterized by the so-called *survival probability* S, which is equal to the sum of the reflection R and transmission T coefficients [14]. Its value is less than or equal to unity due to the decrease of probability density inside the absorbing layer. The lower is S, the higher is the efficiency of the absorption. In order to find the transmission and reflection coefficients we solve Eq. (3) with the boundary conditions

$$\psi(x) = \begin{cases} e^{ikx} + re^{-ikx}, & x \to -\infty, \\ te^{ikx}, & x \to \infty, \end{cases} \qquad (7)$$

which correspond to a plane wave incident from the left. Reflection and transmission coefficients are $R = |r|^2$ and $T = |t|^2$, respectively.

The problem of scattering of a plane wave on the single-hump imaginary potential (4) has two independent parameters, namely, the normalized wavelength $\nu = \lambda/l$, where $\lambda = 2\pi/k$, and the normalized amplitude, $\varepsilon = l^2 u$. In order to optimize the parameters of imaginary potential it is necessary to find the values of ν and ε, which correspond to minimum of survival probability S.

2. RESULTS

The coefficients of reflection and transmission are calculated numerically for cosine-squared and Pöschl–Teller potentials using the reduction of Eq. (3) to the system of two equations of the first order. This system of equations is solved by the Runge-Kutta fourth order method for $l = 1$.

Fig. 1 shows the dependences of the reflection R and transmission T coefficients, as well as the survival probability S on the normalized wavelength ν for three fixed values of the normalized amplitude, $\varepsilon = 2$, 20, and 80. It can be seen that for both considered potentials there exists an optimal normalized wavelength ν_{opt} corresponding to the minimum of survival probability. When $\nu << \nu_{opt}$ or $\nu >> \nu_{opt}$ the survival probability tends to unity. It is explained by the fact that for large ν waves are mainly reflected, while for small ν they pass through the absorbing layer. The minimum value of the survival probability $S_{min} = S(\nu_{opt})$ decreases dramatically with increasing ε. In order to achieve effective absorption one should use sufficiently large values $\varepsilon \geq 20$. Also note that for the same values of ε, the minimum survival probability $S_{\min}$ for the Pöschl-Teller potential is significantly lower as compared with the cosine-squared potential. Thus, for $\varepsilon = 80$, the values of $S_{\min}$ for considered potentials differ by more than two orders of magnitude.

Fig. 2 shows the dependence of R, T, and S on the normalized amplitude ε for fixed values of normalized wavelength $\nu = 1$, 2, and 8. For both considered imaginary potentials functions $S(\varepsilon)$ first decrease to some minimum values $S_{\min} = S(\varepsilon_{opt})$ with increasing ε. Further behavior of functions $S(\varepsilon)$ is significantly different for the two considered imaginary potentials. For the cosine-squared potential S asymptotically approaches unity, while for Pöschl-Teller potential it becomes a constant, which is approximately equal to $S_{\min}$. The latter means that an increase in the amplitude of the potential do not reduce the efficiency of absorption. Note, however, that an unlimited increase in the amplitude of the Pöschl-Teller potential in the numerical solution TDSE is impossible because of the infinitely long tail of potential, which may distort the wave function in the computational domain.

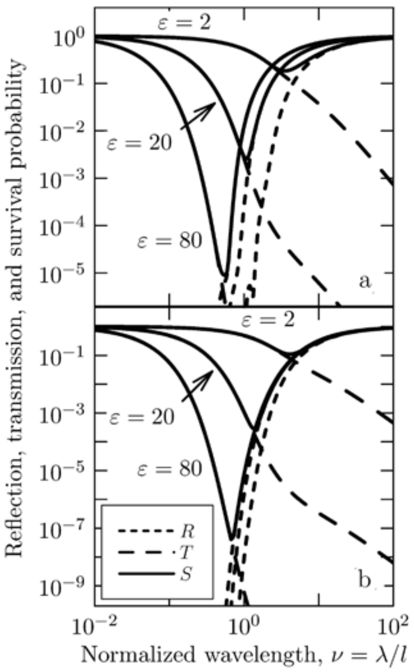

Fig. 1. Dependences of reflection (R) and transmission (T) coefficients, as well as survival probability S=R+T (short-dashed, long-dashed, and solid curves, respectively) on the normalized wavelength $\nu = \lambda/l$ for various fixed values of the normalized amplitude $\varepsilon = 2$, 20, and 80. Calculations are performed for (a) the cosine-squared potential (Eqs. (4), (5)) and (b) Pöschl-Teller potential (Eqs. (4), (6))

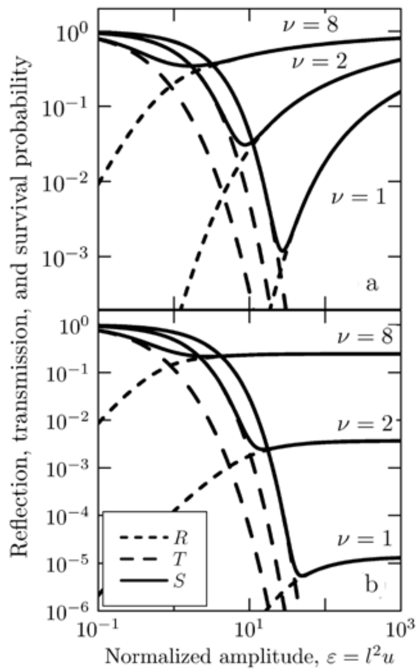

Fig. 2. Dependences of reflection (R) and transmission (T) coefficients, as well as survival probability S=R+T (short-dashed, long-dashed, and solid curves, respectively) on the normalized amplitude $\varepsilon = l^2 u$ for various fixed values of the normalized wavelength $\nu = 1$, 2 and 8. Calculations are performed for (a) the cosine-squared potential (Eqs. (4), (5)) and (b) Pöschl-Teller potential (Eqs. (4), (6))

Next, we calculated the dependence of the optimal normalized amplitude ε_{opt} on the normalized wavelength ν for the considered potentials. Quadratic interpolation of the obtained dependences using the least square method in the range of $0.5 < \nu < 2$ gives the following results. For the cosine-squared potential

$$\varepsilon_{opt} \approx 1 + 0.67\kappa^2 , \quad \kappa = 2\pi / \nu \tag{8}$$

and for the Pöschl-Teller potential,

$$\varepsilon_{opt} \approx 2 + 1.17\kappa^2 . \tag{9}$$

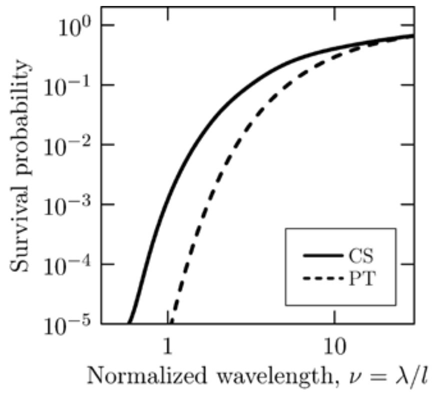

Fig. 3. Dependences of the survival probability corresponding to optimal normalized amplitude ε_{opt} on the normalized wavelength ν for the cosine-squared potential (solid curve) and Pöschl-Teller potential (dashed curve)

The results of numerical calculations of the wavelength-dependence of survival probability corresponding to the optimum amplitude are shown in Fig. 3. It can be seen that the survival probability decreases sharply with decreasing of the de Broglie wavelength. In order to find the amplitude u of the negative imaginary potential corresponding to high-efficient absorption of the de Broglie wavelength λ one should use the relation

$$u_{opt} = \varepsilon_{opt}(\lambda/l)/l^2 , \tag{10}$$

with the use of Eq. (8) or Eq. (9).

CONCLUSIONS

To conclude, in this work we have calculated the coefficients of transmission and reflection of the plane wave on the two different single-hump negative imaginary potentials (NIPs) for wide range of the potential parameters and de Broglie wavelengths. It is shown that the Pöschl-Teller potential (Eqs. (4), (6)) provides more efficient absorption of the entire range of de Broglie wavelengths than the cosine-squared potential (Eqs. (4), (5)). At the same time the advantage of using the cosine-squared potential in numerical calculations is the finite interval of its location, as opposed to Pöschl-Teller potential.

The relationships between the width and the amplitude of the considered potentials and the de Broglie wavelength corresponding to the maximum of absorption efficiency are determined. The obtained optimal parameters of NIPs can be used to construct the absorbing potential containing several humps of different width and amplitude for high-efficient absorption in wide range of de Broglie wavelengths.

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ОПТИМИЗАЦИЯ ПАРАМЕТРОВ КОЛОКОЛООБРАЗНЫХ МНИМЫХ ПОТЕНЦИАЛОВ ДЛЯ ЭФФЕКТИВНОГО ПОГЛОЩЕНИЯ ВОЛНОВОЙ ФУНКЦИИ ПРИ ЧИСЛЕННОМ РЕШЕНИИ НЕСТАЦИОНАРНОГО УРАВНЕНИЯ ШРЁДИНГЕРА

А.А. Силаев, Н.В. Введенский

Работа посвящена развитию метода мнимого потенциала для поглощения волновой функции на периферии расчётной области при численном решении нестационарного уравнения Шрёдингера. Найдены оптимальные соотношения между шириной и амплитудой мнимого потенциала и длиной волны де Бройля, соответствующие максимальной эффективности поглощения.

ОПТИМІЗАЦІЯ ПАРАМЕТРІВ ДЗВОНОВИДНИХ УЯВНИХ ПОТЕНЦІАЛІВ ДЛЯ ЕФЕКТИВНОГО ПОГЛИНАННЯ ХВИЛЬОВОЇ ФУНКЦІЇ ПРИ ЧИСЕЛЬНОМУ РОЗВ'ЯЗАННІ НЕСТАЦІОНАРНОГО РІВНЯННЯ ШРЬОДІНГЕРА

О.А. Силаєв, М.В. Введенський

Робота присвячена розвитку методу уявного потенціалу для поглинання хвильової функції на периферії розрахункової області при чисельному розв'язанні нестаціонарного рівняння Шрьодінгера. Знайдено оптимальні співвідношення між шириною і амплітудою уявного потенціалу та довжиною хвилі де Бройля, які відповідають максимальній ефективності поглинання.