

# Parametrization of complex absorbing potentials for time-dependent quantum dynamics using multi-step potentials†

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In this work, the reflection and transmission of plane waves are examined from a ‘true’ complex potential. In our previous paper a simple and exact numerical procedure was proposed for treating the absorbing potential problem. The comparison of this multi-step potential method with the time-dependent wavepacket approach gave very good agreement, so our present aim is to examine an appropriate polynomial form of negative complex potentials (NCPs) using the step potential method. Calculations have been presented that optimize the coefficients and exponents of the power functions so as to get a minimal value for the sum of the reflection and transmission coefficients as a function of the kinetic energy and the absorbing length.

## 1. Introduction

Complex absorbing or optical potentials (CAP) have a very long history in time-dependent and time-independent quantum dynamics. Several different approaches have been developed<sup>1–3</sup> in this field since 1989 when Neuhauser and Baer<sup>1</sup> introduced their first negative linear potential (NIP) in the scattering theory. These kinds of potentials play an important role in the calculations because they can absorb the wavepacket near to the edge of the grid avoiding the spurious boundary effects.‡ Finding the most efficient and effective shape and the parametrization of these potentials is essential, because the absorption of the wavepacket depends strongly upon these quantities.

After the first pioneering work of Neuhauser and Baer<sup>1–3</sup> and Child,<sup>4</sup> several other forms of the NIPs have been discussed. One of us with Balint-Kurti<sup>5,6</sup> performed one-dimensional wavepacket and semi-classical Jeffreys–Wentzel–Kramers–Brillouin (JWKB) calculations to study the polynomial and exponential forms of NIPs. We have also derived an important scaling procedure and a parametrization of the Schrödinger equation so that if an optimal form of the NIP is determined for a particular reduced mass and energy, then, through the scaling relationship, the best parameters applicable to another physical situation can be derived easily from the previous ones. In 1994 Macias *et al.* optimized and compared different forms of NIPs and pointed out that the addition of a negative real part to the imaginary absorbing potential (“true” negative complex potential (NCP)) can improve the absorption.<sup>12</sup> Other essential works on the optimization of NIPs were developed by Seideman and Miller<sup>7</sup> and Riss and Meyer.<sup>16</sup> They also used the semi-classical JWKB approximation to examine the reflection and transmis-

sion properties of different NIPs. In 1998 Ge and Zhang<sup>19</sup> also published very interesting results in this field. They performed exact numerical calculations to show the ability of the NCPs, especially in the case of low energy scattering when the de Broglie wavelength is larger than the length of absorbing potential.

Recently,<sup>23</sup> we have proposed a new, but very simple and exact numerical procedure to treat the absorbing potential problem. Using a multi-step potential function any kind of analytical complex absorbing potential form can be modelled and both the reflection and the transmission coefficients can be calculated exactly. Comparing the step potential method and the grid-based time-dependent wavepacket approach the results are very close to each other. This step potential scheme works fast, produces accurate numbers and performs in good agreement with the grid-based wavepacket approach. So, applying the step potential method our present aim is to examine an appropriate polynomial form of NCPs and optimize their coefficients and the exponents of the power functions so as to get a minimal value for the sum of the reflection and transmission coefficients as a function of the kinetic energy and the absorbing length.

In the next section, we give a short description of the theoretical methods used in the calculations. In Section 3 we display and discuss the numerical results which are presented both in graphical and in tabular form. Section 4 summarizes the calculations and contains our conclusions.

## 2. Theory

In the grid based methods the absorbing potential can be given as a discrete representation:

$$V_j = V(j\Delta x) \quad (1)$$

where  $\Delta x$  is the spatial density of the grid. However this approach can give the same representation for several different analytical functions.

† Electronic Supplementary Information available. See <http://www.rsc.org/suppdata/cp/b1/b101900g/>

‡ Transmission and reflection appear if one uses periodic boundary conditions. Applying infinite barrier boundary conditions the transmission will automatically be zero.

Choosing an appropriate CAP form and using grid representation this leads to an exactly solvable one-dimensional scattering problem with step potential. Where the potential is built up from  $n_s$  step barriers with a width of  $\Delta x$  and height of  $V_j$  for the  $j$ th barrier:

$$V_s(x) = \begin{cases} 0 & \text{if } x < X_0 = \Delta x/2 \text{ or } (n_s + \frac{1}{2})\Delta x = X_{n_s} \leq x \\ V_j & \text{if } (j - \frac{1}{2})\Delta x = X_{j-1} \leq x < X_j = (j + \frac{1}{2})\Delta x \quad j = 1, \dots, n_s. \end{cases} \quad (2)$$

Determining the transmission and reflection coefficients one has to solve the time-independent Schrödinger equation. There are several well-known methods for solving this simple one-dimensional scattering problem.<sup>24,25</sup> The following scheme could be considered as a generalization of the method described in ref. 25 for complex potentials and an arbitrary number of step barriers. In this case the eigenfunction can be defined from barrier to barrier in the form

$$\Psi_j(x) = A_j \exp(ik_j x) + B_j \exp(-ik_j x) \quad (3)$$

where  $k_j = \sqrt{(2m/\hbar^2)(E_0 - V_j)}$  is the wavenumber. The continuity conditions at the border of the  $j$ th and  $(j + 1)$ th barrier for the wavefunctions and their first derivatives are

$$\Psi_j(X_j) = \Psi_{j+1}(X_j) \quad (4)$$

$$\frac{\partial}{\partial x} \Psi_j|_{x=X_j} = \frac{\partial}{\partial x} \Psi_{j+1}|_{x=X_j}. \quad (5)$$

So, the expression for  $A_j$

$$A_j = \left\{ A_{j+1} \left( 1 + \frac{k_{j+1}}{k_j} \right) \exp(ik_{j+1} X_j) + B_{j+1} \left( 1 - \frac{k_{j+1}}{k_j} \right) \exp(-ik_{j+1} X_j) \right\} \exp(ik_j X_j) / 2 \quad (6)$$

and also for  $B_j$

$$B_j = \left\{ A_{j+1} \left( 1 - \frac{k_{j+1}}{k_j} \right) \exp(ik_{j+1} X_j) + B_{j+1} \left( 1 + \frac{k_{j+1}}{k_j} \right) \exp(-ik_{j+1} X_j) \right\} \exp(ik_j X_j) / 2 \quad (7)$$

can be expressed by the coefficients of  $A_{j+1}$  and  $B_{j+1}$ . If there are  $n_s$  barriers in the absorbing region then for the  $\Psi_{n_s+1}$  we can assume

$$\begin{aligned} B_{n_s+1} &= 0 \\ A_{n_s+1} &= 1 \end{aligned} \quad (8)$$

that is, there is no incident wave at this side of the absorbing region. Applying eqn. (6) and (7) repeatedly one can easily determine the coefficients  $A_0$  and  $B_0$ . Now the reflection coefficient can be obtained as

$$R = \left| \frac{B_0}{A_0} \right|^2 \quad (9)$$

and the transmission coefficient as

$$T = \left| \frac{A_{n_s+1}}{A_0} \right|^2 = \left| \frac{1}{A_0} \right|^2. \quad (10)$$

Using these two expressions the survival probability can be defined as

$$S = R + T \quad (11)$$

### 3. Results and analysis

In this work we assume the following form§ for the CAP

$$V(x) = \begin{cases} U_r(x) + iU_i(x) & \text{if } 0 < x \leq L \\ 0 & \text{otherwise} \end{cases} \quad (12)$$

where

$$U_r(x) = E_0 \left\{ p_1 \left( \frac{x}{L} \right)^{p_2} + p_3 \right\} \quad (13)$$

and

$$U_i(x) = E_0 \left\{ q_1 \left( \frac{x}{L} \right)^{q_2} \right\}. \quad (14)$$

Here  $U_r(x)$  and  $U_i(x)$  are the real and imaginary parts of the CAP and  $L$  is the absorbing length. The width of the individual potential steps,  $\Delta x$ , is related to the absorbing length by  $\Delta x = L/n_s$ .  $E_0 = \sqrt{E_{\min} E_{\max}}$  is the central kinetic energy where  $E_{\min}$  and  $E_{\max}$  are the lowest and highest energies of the proposed absorbing range.  $p_1$ ;  $p_2$ ;  $p_3$ ;  $q_1$ ;  $q_2$  are parameters which were optimized with the multi-step potential approach so as to give a minimum value for the survival probability.

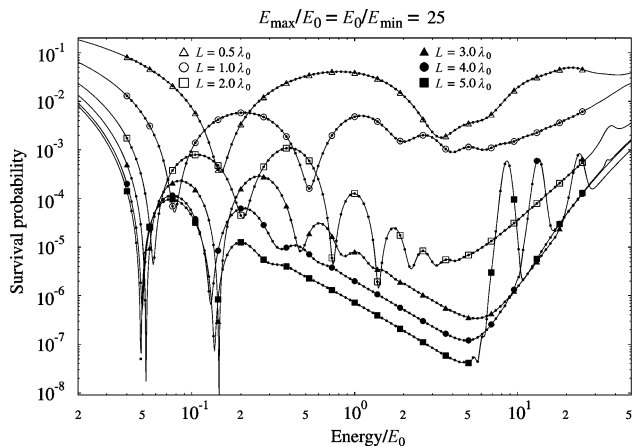
In the calculations the central kinetic energy and the mass were chosen as  $E_0 = 0.001$  au,  $m = \frac{1234}{\sqrt{2mE_0}}$  au, respectively, so the central wavelength is  $\lambda_0 = h/\sqrt{2mE_0} = 4.00$  au. For the sake of formality we give the numerical values of the energy, mass and wavelength, but it has to be emphasized that from the point of view of the results only the size of the energy interval ( $E_{\max}/E_{\min}$ ), the ratio of the absorbing length and the wavelength ( $L/\lambda_0$ ) and the number of steps in the absorbing region ( $n_s$ ) are essential. One can shift the whole energy interval and can also change the length of the absorbing region without having any effect on the values of the reflection and transmission<sup>5</sup> if the essential quantities ( $E_{\max}/E_{\min}$ ,  $L/\lambda_0$ ,  $n_s$ ) remain the same.

In the optimizations the downhill simplex method was used.<sup>26,27</sup> We chose an appropriate energy interval in which the sample points have been logarithmically evenly spaced. The initial values of the  $p_1$ ,  $p_2$ ,  $p_3$ ,  $q_1$  and  $q_2$  parameters were chosen at random with different numbers of potential steps in the absorbing region ( $n_s = 5, 10, 15, 20, 25, 30$ ), and the best results of several minimizations were eventually selected. The individual minimizations were first performed for the quadratic mean value of survival probability at 21 energy sample points, and this was followed by a new minimization with 101 sample points.¶ We also present numerical calculations with wall and without wall, the calculations with wall are presented as Electronic Supplementary Information.† ‘With wall’ means that an extra potential barrier was placed at the end of the absorbing region in order to eliminate the transmission perfectly. The width of the wall applied was that multiple of the step size which is the nearest to the value of 0.15 au and the integral of the potential function under the wall was always equal to 5.00 au. In these cases we never got transmission probability values greater than  $10^{-30}$ .

The results in Fig. 1 show the survival probability as a function of kinetic energy for the optimized values of the  $p_1$ ,  $p_2$ ,  $p_3$ ,  $q_1$  and  $q_2$  parameters. Each figure contains 6 curves which correspond to 6 different absorbing lengths: 2, 4, 8, 12, 16 and

§ The shape of the CAP proposed here is a generalized form of the widely used power function, where in order to get better results the exponent was also chosen as a parameter. It was also showed in our preliminary calculations that the survival probability can be decreased significantly by adding a small constant value to the real part of the CAP.

¶ In the figure markers and dots correspond to the sample points of the first and final optimization, respectively.



**Fig. 1** The survival probability ( $S$ ) (eqn. (11), (12) and (13)) obtained with six different values of absorbing lengths ( $L_1 = 0.5\lambda_0$ ,  $L_2 = \lambda_0$ ,  $L_3 = 2\lambda_0$ ,  $L_4 = 3\lambda_0$ ,  $L_5 = 4\lambda_0$  and  $5\lambda_0$ ) without wall as a function of the energy. Here  $\lambda_0$  the wavelength = 4.00 au. The absorbing energy range was chosen between  $E_0/25$  and  $25E_0$  where  $E_0$  is the reference kinetic energy. In the calculations the values of the optimized parameters were taken from Table 1.

20 au. In Table 1 we present the optimized values of the coefficients and exponents for the polynomial complex absorbing potential and also give the average and maximum values of the survival probability. The former was calculated as a quadratic mean of the survival probabilities at the 101 sample points of the optimization.

**Table 1** Optimized coefficients ( $p_1, q_1, p_3$ ) and exponents ( $p_2, q_2$ ) for polynomial complex absorbing potential (eqn. (14)) for five different energy ranges.  $E_0$  is the reference kinetic energy. The first and second columns contain the absorbing length ( $L$ ) expressed in terms of reference wavelength ( $\lambda_0$ ) and the number of steps ( $n_s$ ), respectively. The following 5 columns list the optimized values of the coefficients and powers, while the last two columns give the average and maximum values of the survival probability ( $S$ ), respectively

$L/\lambda_0$	$n_s$	$q_1$	$q_2$	$p_1$	$p_2$	$p_3$	$S_{ave}$	$S_{max}$
$E_{max}/E_0 = E_0/E_{min} = 2$								
0.5	10	-4.996	2.049	50.000	20.089	$-4.58 \times 10^{-1}$	$6.68 \times 10^{-4}$	$1.62 \times 10^{-3}$
1.0	10	-35.193	5.965	-9.930	3.085	$-5.05 \times 10^{-2}$	$3.21 \times 10^{-5}$	$8.61 \times 10^{-5}$
2.0	15	-27.611	6.996	-10.023	4.226	$1.40 \times 10^{-3}$	$2.46 \times 10^{-7}$	$5.48 \times 10^{-7}$
3.0	30	-32.758	7.148	-12.522	4.449	$9.91 \times 10^{-5}$	$2.89 \times 10^{-10}$	$6.37 \times 10^{-10}$
4.0	30	-24.063	7.108	-11.594	4.682	$2.19 \times 10^{-5}$	$2.25 \times 10^{-11}$	$5.54 \times 10^{-11}$
5.0	30	-14.755	6.076	-7.170	4.371	$7.64 \times 10^{-6}$	$6.31 \times 10^{-12}$	$1.67 \times 10^{-11}$
$E_{max}/E_0 = E_0/E_{min} = 4$								
0.5	5	-50.000	11.002	-10.054	4.164	$-2.09 \times 10^{-1}$	$2.74 \times 10^{-3}$	$7.39 \times 10^{-3}$
1.0	10	-39.198	7.228	-9.250	3.538	$-6.87 \times 10^{-2}$	$1.87 \times 10^{-4}$	$6.24 \times 10^{-4}$
2.0	15	-14.144	4.882	-3.921	2.725	$-9.55 \times 10^{-3}$	$4.89 \times 10^{-6}$	$1.45 \times 10^{-5}$
3.0	25	-17.276	6.718	-5.950	4.120	$7.21 \times 10^{-4}$	$1.55 \times 10^{-7}$	$5.29 \times 10^{-7}$
4.0	30	-18.338	7.005	-6.794	4.373	$6.34 \times 10^{-5}$	$9.90 \times 10^{-10}$	$3.72 \times 10^{-9}$
5.0	30	-11.417	5.943	-4.450	3.938	$3.67 \times 10^{-5}$	$1.63 \times 10^{-9}$	$7.51 \times 10^{-9}$
$E_{max}/E_0 = E_0/E_{min} = 9$								
0.5	5	-50.000	10.883	-8.909	4.242	$-2.59 \times 10^{-1}$	$9.55 \times 10^{-3}$	$2.77 \times 10^{-2}$
1.0	10	-39.733	10.064	-8.434	4.541	$-7.43 \times 10^{-2}$	$8.70 \times 10^{-4}$	$2.67 \times 10^{-3}$
2.0	20	-16.459	5.927	-3.303	2.992	$-1.72 \times 10^{-2}$	$6.00 \times 10^{-5}$	$1.86 \times 10^{-4}$
3.0	25	-10.938	4.883	-2.324	2.652	$-6.18 \times 10^{-3}$	$7.61 \times 10^{-6}$	$2.36 \times 10^{-5}$
4.0	30	-8.468	4.334	-2.024	2.532	$-2.89 \times 10^{-3}$	$1.41 \times 10^{-6}$	$4.18 \times 10^{-6}$
5.0	25	-0.944	1.355	14.848	11.717	$-2.09 \times 10^{-2}$	$7.34 \times 10^{-5}$	$2.61 \times 10^{-4}$
$E_{max}/E_0 = E_0/E_{min} = 16$								
0.5	5	-40.485	9.792	-7.053	4.037	$-2.97 \times 10^{-1}$	$2.03 \times 10^{-2}$	$5.48 \times 10^{-2}$
1.0	15	-50.000	12.402	-9.522	5.421	$-7.76 \times 10^{-2}$	$2.24 \times 10^{-3}$	$6.40 \times 10^{-3}$
2.0	20	-20.552	7.261	-3.427	3.503	$-2.10 \times 10^{-2}$	$2.24 \times 10^{-4}$	$7.31 \times 10^{-4}$
3.0	30	-13.414	5.696	-2.163	2.888	$-8.81 \times 10^{-3}$	$4.37 \times 10^{-5}$	$1.42 \times 10^{-4}$
4.0	30	-7.732	4.094	-1.427	2.257	$-4.97 \times 10^{-3}$	$7.54 \times 10^{-5}$	$5.20 \times 10^{-4}$
5.0	30	-4.839	3.283	-0.863	1.859	$-2.38 \times 10^{-3}$	$7.28 \times 10^{-5}$	$4.36 \times 10^{-4}$
$E_{max}/E_0 = E_0/E_{min} = 25$								
0.5	5	-39.051	9.715	-6.881	4.375	$-3.38 \times 10^{-1}$	$3.03 \times 10^{-2}$	$8.08 \times 10^{-2}$
1.0	15	-50.000	13.930	-9.134	5.975	$7.50 \times 10^{-2}$	$4.50 \times 10^{-3}$	$1.29 \times 10^{-2}$
2.0	25	-26.353	8.594	-3.710	4.009	$-2.26 \times 10^{-2}$	$5.22 \times 10^{-4}$	$1.74 \times 10^{-3}$
3.0	30	-17.598	6.521	-2.294	3.193	$-1.07 \times 10^{-2}$	$1.57 \times 10^{-4}$	$7.72 \times 10^{-4}$
4.0	30	-10.439	5.266	-1.527	2.717	$-5.79 \times 10^{-3}$	$1.07 \times 10^{-4}$	$5.93 \times 10^{-4}$
5.0	30	-7.111	4.332	-1.133	2.351	$-3.54 \times 10^{-3}$	$9.59 \times 10^{-5}$	$5.13 \times 10^{-4}$

Concerning our results the following remarks can be made: In order to get reasonable absorption one needs to use an absorbing length which is at least half the length of the maximum wavelength in the studied absorbing energy region. On the other hand, the survival probability increases rapidly if the widths of the potential steps are greater than half the minimum wavelength in the absorbing energy region (rows corresponding to the longest absorbing regions in Table 1 reflect this effect significantly). Combining these two effects for the case of absorption over a fairly wide energy range it turns out that one needs to use a large number of steps because the high energy part of the spectra requires a small step size whereas the low energy part needs a long absorbing region. As we mentioned before, in the calculations 6 different widths of potential steps were used and among them the shortest one was 1/30th of the absorbing length. Applying a larger number of potential steps in the fixed length absorbing region one can improve the effectiveness of the absorbing potential. Fig. 1 also displays the effect of the too-long potential steps in the form of large amplitude oscillations at the high energy part of the curves. It has to be mentioned that in many cases the optimized values of the exponents for the real and imaginary part of the potential function are often relatively close to the values of 4 and 7, respectively. Based on this observation we repeated all the calculations with the only difference being that instead of using many random configurations for the optimization parameters the individual optimizations were started from the point of  $p_1 = -5$ ,  $p_2 = 4$ ,  $p_3 = 0$ ,  $q_1 = -10$  and  $q_2 = 7$ . Except for a few cases the same local minimum places were found with this simplified procedure as for the earlier results presented in Table 1.

## 4. Summary

This paper has studied the survival probability of plane waves from a 'true' complex potential. In our previous paper a simple and exact numerical procedure (multi-step potential method) was proposed for treating the absorbing potential problem. The comparison of this method with the time-dependent wavepacket approach gave very good agreement, thus encouraging us to examine an appropriate polynomial form of negative complex potentials (NCPs) using this step potential method. Calculations have been presented that optimize the coefficients and exponents of the power functions so as to get a minimal value for the sum of the reflection and transmission coefficients as a functions of kinetic energy and the absorbing length. The most important results of the paper are presented in Table 1. This table lists the optimized potential parameters for all five different energy ranges considered.

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