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Exponential fitting method for the time-dependent Schrödinger equation

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Abstract Our purpose is to increase the accuracy of the numerical solution of the time-dependent Schrödinger equation. In particular, a modification of the standard Crank–Nicolson method by an exponential fitting Numerov formula leading to a higher order in the approximation of the second order spatial derivative along with a better description of oscillating or exponential behavior and different artificial boundary conditions aimed to reduce the reflections of the wave packet at the numerical boundaries are presented. The procedures are illustrated for the deep-tunneling case of proton emission.

Keywords Time-dependent Schrödinger equation · Crank–Nicolson method · Exponential fitted Numerov formula · Transparent boundary conditions · Proton emission

1 Introduction

In the nonrelativistic quantum mechanics the solution of the time-dependent Schrödinger equation (TDSE) is the most rigorous approach to the processes with temporal evolution like nuclear fission and fusion, nuclear and atomic collisions, quantum tunneling, laser-atom interaction. The success of this approach resides in its natural correspondence with the experiment: starting with an initial state one follows the development of the phenomena in time, which represents a modeling of the fundamental dynamical behavior. A reliable and accurate numerical determination of

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the time-dependent wave function will certainly be very useful in the description and the understanding of a variety of quantum processes. Much work has been done in this area. We cite some of the most recent published papers (see Refs. [1–5]).

In this article we propose an improved scheme of Crank–Nicolson type based on an exponential fitting formula of Numerov type combined with appropriate artificial boundary conditions. For numerical illustration, we shall treat the case of proton emission, a typical example of quantum tunneling.

2 The time-dependent Schrödinger equation

We consider the one-dimensional TDSE:

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = H\psi(r,t), \quad H \equiv \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V(r). \tag{2.1}$$

Given $\psi(r,0) \in L^2(\mathbf{R}^+)$, we search for a solution $\psi(r,t) \in L^2(\mathbf{R}^+)$ for any $t > 0$. In our study r is the radius in spherical coordinates. The boundary condition at $r = 0$ is $\psi(0,t) = 0$. The formal solution of (2.1) can be expressed by:

$$\psi(r,t+\Delta t) = \exp\left(\frac{-i\,\Delta t}{\hbar}H\right)\psi(r,t) \tag{2.2}$$

where Δt is the time step.

2.1 Approximate solution

The exponential is approximated by the Cayley transform:

$$\exp\left(\frac{-i\,\Delta t}{\hbar}H\right) = \frac{1 - i\,\Delta t\,H/2\hbar}{1 + i\,\Delta t\,H/2\hbar} + O((\Delta t)^3). \tag{2.3}$$

leading to the following propagation formula:

$$\left(1 + \frac{i\,\Delta t}{2\hbar}H\right)\psi(r,t+\Delta t) = \left(1 - \frac{i\,\Delta t}{2\hbar}H\right)\psi(r,t). \tag{2.4}$$

This approximation has the advantage of being unitary and therefore is norm-preserving and unconditionally stable.

Using an idea of Moyer (Ref. [6]), let us introduce a new function $y(r,t) \equiv \psi(r,t+\Delta t) + \psi(r,t)$. Taking into account the definition of H, we find

$$\frac{\partial^2 y}{\partial r^2} = \frac{2m}{\hbar^2}\left[V(r) - \frac{2\hbar i}{\Delta t}\right]y(r,t) + \frac{4\hbar i}{\Delta t}\frac{2m}{\hbar^2}\psi(r,t). \tag{2.5}$$

2.2 Improved Crank–Nicolson method

With respect to r, Eq. (2.5) has the form $y''(r) = g(r)y(r) + f(r)$. The Crank–Nicolson method corresponds to the standard approximation of y'':

$$h^2 y''(r) = y(r+h) - 2y(r) + y(r-h) + O(h^4) \tag{2.6}$$

We use the exponentially fitted Numerov formula, with a higher accuracy:

$$\begin{aligned} y(r+h) + a_1 y(r) + y(r-h) = h^2[b_0 y''(r+h) + b_1 y''(r) \\ + b_0 y''(r-h)] + O(h^6) \end{aligned} \tag{2.7}$$

The coefficients a_1, b_0, b_1 are determined so that Eq. (2.7) (with terms in h^6 and higher neglected) is exact for functions of the form $r^k \exp(\pm\omega r),\ k = 0, 1, 2,\ \omega \in \mathbf{C}$. With $z = \omega h, e_n^{\pm} = \exp(nz) \pm \exp(-nz), d = 3e_1^- + ze_1^+$ we have (see Ref. [7]):

$$a_1 = \frac{ze_2^+ - 3e_2^- - 6z}{d}, b_0 = \frac{ze_1^+ - e_1^-}{z^2 d}, b_1 = \frac{ze_2^+ + e_2^- - 6z}{z^2 d}. \tag{2.8}$$

The second derivatives are replaced according to Eq. (2.5). Note that other multistep formulae for such an equation do also exist and could be implemented in the scheme (see [8,9]).

For practical implementation, the numerical spatial interval $[r_0, r_{\max}]$ (finite) is divided in subintervals of the size h , resulting a grid with the mesh points $r_j = r_0 + jh,\ j = 0, \ldots, J$. We denote by ψ_j^n the solution at the time $t_n = t_0 + n\Delta t$ and the point r_j and similarly for y_j^n, g_j, f_j^n. On the basis of the Eq. (2.7) we have

$$\begin{aligned} &\left(1 - h^2 b_0 g_{j+1}\right) y_{j+1}^n + \left(a_1 - h^2 b_1 g_j\right) y_j^n + \left(1 - h^2 b_0 g_{j-1}\right) y_{j-1}^n \\ &= h^2 \left[b_0 (f_{j+1}^n + f_{j-1}^n) + b_1 f_j^n\right],\ j = 1, \ldots, J-1. \end{aligned} \tag{2.9}$$

In terms of two new functions defined as

$$d_j \equiv 1 - h^2 b_0 g_j,\ \ w_j^n \equiv d_j y_j^n - h^2 b_0 f_j^n$$

the Eq. (2.9) takes the compact form

$$w_{j+1}^n + w_{j-1}^n = \left[-a_1 + h^2(b_1 - a_1 b_0)\frac{g_j}{d_j}\right] w_j^n + h^2(b_1 - a_1 b_0)\frac{f_j^n}{d_j}.$$

This is a three-term recursion relation for the unknown w_j^n. It can be easily obtained if two initial values, say w_0^n, w_1^n, are known, but this information is not available for evolution problems. Instead, certain boundary values are assumed at the end points of the spatial interval, namely w_0^n and w_J^n $(\forall n)$. One possible choice is $w_0^n = w_J^n = 0$

corresponding to rigid-wall boundary conditions, but these usually lead to numerical difficulties, since unwanted reflections of the wave packet appear.

We shall present various alternatives of more adequate boundary conditions. The values of w_j^n at the interior points of the interval are then obtained either by solving a tridiagonal linear system or by reducing the original three-term recursion relation to a pair of two-term recursions for two new functions e_j and q_j^n. The simpler recursions result from the relation $w_{j+1}^n = e_j w_j^n + q_j^n$ introduced into the equation for w_j^n. As mentioned, for our problem $\psi_0^n = 0,\ \forall n$, which implies $w_0^n = 0$. Using this condition, one obtains the initial values e_0 and q_0^n. From these values, the two-term recursions generate e_j and q_j^n. Then, starting with a given value of w_J^n, we can use $w_{j-1}^n = (w_j^n - q_{j-1}^n)/e_{j-1}$ to construct $w_{J-1}^n, \ldots, w_1^n$. Finally,

$$\psi_j^{n+1} = -\psi_j^n + \frac{w_j^n}{d_j} + \hbar i \frac{2m}{\hbar^2} \frac{4h^2 b_0}{\Delta t} \frac{\psi_j^n}{d_j}. \tag{2.10}$$

3 Artificial boundary conditions

From mathematical point of view, TDSE is a partial differential equation, containing a temporal variable and one (or more) spatial variables. The physical spatial domain is unbounded. In order to make possible the numerical solution of the equation it should be limited to a finite one. The appropriate treatment of boundary conditions on this computational domain is decisive for the accuracy of results. The artificial boundary conditions should be consistent with the original boundary conditions on the entire space, so that the errors due to the finite approximation of the domain are avoided or at least diminished. Next, we present several such procedures. They may be incorporated into the described variant of Crank–Nicolson scheme, providing the starting value w_J^n at the right boundary.

3.1 Transparent boundary conditions (TBC)

The simplest idea is to assume near the numerical boundary $r = r_J$ the following form of the solution: $\psi = \psi_0 \exp(ikr)$, $\psi_0, k \in \mathbf{C}$. Then we have

$$\frac{\psi_J^n}{\psi_{J-1}^n} = \frac{\psi_{J-1}^n}{\psi_{J-2}^n} = \exp(ikh). \tag{3.1}$$

From the second equality it results k and then from the first equality one obtains ψ_J^n. We assume the same relation valid for the next time step, so that $\psi_J^{n+1} = \psi_{J-1}^{n+1} \exp(ikh)$. Using its definition, we then obtain w_J^n. The assumed form is valid in the hypothesis of a constant potential outside the numerical domain. However, at large r (but not too far) the potential still contains centrifugal and Coulomb terms, which cannot be considered constant. It is natural to search for boundary conditions adapted to such form of potential.

3.2 Adapted transparent boundary conditions (ATBC)

To deduce them, we suppose that near the (right) boundary the solution ψ is proportional to $O_l(\eta,\rho) = G_l(\eta,\rho) + iF_l(\eta,\rho)$, where G_l, F_l are the Coulomb functions, with the complex arguments $\rho = kr$ and η. This corresponds to a wave function of purely outgoing type. The procedure, introduced in Ref. [1] for the standard Crank–Nicolson scheme, consists in determining first k from the equation:

$$\frac{\psi^n_{J-1}}{\psi^n_{J-2}} = \frac{O_l(\eta, kr_{J-1})}{O_l(\eta, kr_{J-2})}. \tag{3.2}$$

With this value of k, which is supposed to remain the same for the next steps in space and time, we obtain the relations

$$\frac{\psi^n_J}{\psi^n_{J-1}} = \frac{\psi^{n+1}_J}{\psi^{n+1}_{J-1}} = \frac{O_l(\eta, kr_J)}{O_l(\eta, kr_{J-1})}. \tag{3.3}$$

The resulting ψ^n_J and ψ^{n+1}_J are used to generate the value of w^n_J. In order to determine k one has to solve a nonlinear complex equation $F(k) = 0$. In practice, we have used an iterative procedure with three starting points (given by the previous TBC) to calculate the pole of $f(k) = 1/F(k)$. Of course, the calculation of Coulomb functions increases the total computing time. Since we are calculating on relatively large grids ($r_J > 120$ fm), we can resort to the asymptotic series of O_l (Ref. [10]) restricted to one term:

$$O_l(\eta, kr) \approx \exp\left[i\left(kr - \eta\, ln(2kr) - l\frac{\pi}{2} + \sigma_l\right)\right]\left[1 + \frac{(i\eta + l + 1)(i\eta - l)}{2ikr}\right]. \tag{3.4}$$

By using it, we can also evaluate the flux at $r = r_J$, which has the form:

$$\Phi_J = \frac{\hbar}{m}|\psi(r_J)|^2 k_R Q(kr_J, \eta). \tag{3.5}$$

If $\Phi_J < 0$ we set $k_R = \Re(k) = 0$ which ensures a nonnegative flux, i.e. no reflected wave can enter into the numerical domain.

3.3 Discrete transparent boundary conditions (DTBC)

This procedure, formulated in Ref. [11] for the standard scheme, is based on the $\mathcal{Z}$ transform, the discrete analogue of the Laplace transformation, defined by

$$\mathcal{Z}\{\psi^n_j\} = \hat{\psi}_j(z) \equiv \sum_{n=0}^{\infty} \psi^n_j z^{-n}, \quad z \in \mathbf{C}. \tag{3.6}$$

The idea is to transform the equation for w_j^n in a difference equation only in the index j, which is exactly solved around the end point of the computational domain. To make this possible, some conditions should be assumed for the exterior region, namely: the initial wavefunction vanishes and the potential is constant, so that g_j and d_j become constants denoted by g and d. Then, the proper boundary condition is obtained by an inverse transformation.

With the notations

$$a = -\frac{a_1}{2} + (b_1 - a_1 b_0)\frac{h^2 g}{2d}, \quad \lambda = \frac{2h^2}{\Delta t},$$
$$c = 1 - \frac{2m}{\hbar^2}\lambda b_0 \frac{2\hbar i}{d}, \quad p = \frac{2m}{\hbar^2}(b_1 - a_1 b_0)\frac{2\hbar i \lambda}{d^2}.$$

by applying the $\mathcal{Z}$ transform to the equation in w_j^n near the boundary we arrive to the relation

$$\hat{\psi}_J(z) = e(z)\hat{\psi}_{J-1}(z). \tag{3.7}$$

$e(z)$ is the proper root (which gives a two-term relation) of the equation

$$e(z)^2 - \left(2a + \frac{p}{z+c}\right)e(z) + 1 = 0. \tag{3.8}$$

After some algebra, one obtains

$$(z+c)e_{\pm}(z) = az + a^* c \pm z\nu\sqrt{1 - 2\mu x + x^2}, \tag{3.9}$$
$$\nu = \sqrt{a^2 - 1}, \ \mu = \frac{1 - |a|^2}{|1 - a^2|}, \ x = \frac{\exp(-i\phi)}{z}, \ \phi = arg\left(\frac{a^2 - 1}{c}\right).$$

The inversion of the $\mathcal{Z}$ transform requires a representation of $\sqrt{1 - 2\mu x + x^2}$ in inverse powers of z. This can be obtained using the generating function for the Legendre polynomials:

$$\sqrt{1 - 2\mu x + x^2} = -\sum_0^\infty l_n z^{-n}, \tag{3.10}$$
$$l_n \equiv \frac{\exp(-in\phi)}{2n-1}\left[P_n(\mu) - P_{n-2}(\mu)\right].$$

Since the roots $e_{\pm}(z)$ are inverses, we can write Eq. (3.7) in the form $\hat{\psi}_{J-1}(z) = e_{\mp}(z)\hat{\psi}_J(z)$. With the above results, we have

$$(z+c)\hat{\psi}_{J-1}(z) = \left[az + a^* c \pm z\sqrt{a^2 - 1}\sum_0^\infty l_n z^{-n}\right]\hat{\psi}_J(z). \tag{3.11}$$

To invert the $\mathcal{Z}$ transform, we expand both sides of Eq. (3.11) in powers of $1/z$ and equate coefficients of like powers. So we find the boundary condition at the right:

$$\psi_{J-1}^{n+1} + c\psi_{J-1}^{n} = (a \mp \sqrt{a^2-1})\psi_J^{n+1} + a^* c\psi_J^n \pm \sqrt{a^2-1}\sum_{k=1}^{n} l_{n-k+1}\psi_J^k, \quad (3.12)$$

or, equivalently

$$w_{J-1}^n = \alpha w_J^n + (a^* - \alpha)d^*\psi_J^n + d(a-\alpha)\sum_{k=1}^{n} l_{n-k+1}\psi_J^k. \quad (3.13)$$

$\alpha = a \mp \sqrt{a^2-1}$ and the correct sign is that which makes $|\alpha| > 1$. Note that the relation (3.13) contains in addition to the current value ψ_J^n, the values ψ_J^k at the previous time steps, all in the point r_J. Such a relation, which takes into account the time evolution history of the wavefunction, is called non-Markovian or of memory-type. Together with $w_J^n = e_{J-1}w_{J-1}^n + q_{J-1}^n$, the above relation gives: $w_J^n = (q_{J-1}^n + \beta_J^n e_{J-1})/(1-\alpha e_{J-1})$, where

$$\beta_J^n = d^*(a^* - \alpha)\psi_J^n + d(a-\alpha)\sum_{k=1}^{n} l_{n-k+1}\psi_J^k.$$

4 Application to proton emission

From the numerical solution of TDSE we can obtain the decay rate:

$$\lambda(t) = \frac{1}{1-\rho(t)}\frac{d\rho(t)}{dt} \quad (4.1)$$

where

$$\rho(t) = \int_{r_B}^{\infty} |\psi(r,t)|^2 dr \quad (4.2)$$

represents the probability that, at time t, the particle finds beyond the nuclear border r_B, i.e., it has tunneled through the barrier. As a rule, r_B is the outer turning point and

$$\frac{d\rho(t)}{dt} = -\Phi(\infty) + \Phi(r_B) = \Phi(r_B), \quad (4.3)$$

where Φ is the flux given by

$$\Phi(r) = \frac{i\hbar}{2m}\left[\psi(r)\frac{\partial\psi^*(r)}{\partial r} - \psi^*(r)\frac{\partial\psi(r)}{\partial r}\right]. \quad (4.4)$$

As an example we have chosen the experimentally observed proton decay of ^{147}Tm ($Q_p = 1.132$ MeV)—Refs. [12,13]. The potential is a sum of several terms:

$$V(r) = V_n(r) + V_{so}(r) + V_c(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

where

– V_n is the nuclear potential of Woods–Saxon form

$$V_n(r) = -\frac{D_n}{1+\exp^{\frac{r-R_n}{a_0}}}$$

with D_n (MeV) is the depth, R_n (the radius) $= r_0 \times A_2^{1/3}$ fm, $r_0 = 1.17$, $A_2 = A - A_1 (A_1 = 1.007276$—the proton mass), a_0 (the diffuseness) $= 0.75$ fm.

– V_{so} is the spin—orbit term and has the form

$$V_{so}(r) = -\frac{D_{so}(\vec{\sigma}\ .\ \vec{l}\ )\lambda_\pi^2}{r a_{so}}\frac{\exp^{\frac{r-R_{so}}{a_{so}}}}{(1+\exp^{\frac{r-R_{so}}{a_{so}}})^2}$$

with $D_{so} = 0.2 D_n$ MeV, $\lambda_\pi^2 = 2.0$ fm^2, $a_{so} = 0.75$ fm, $R_{so} = 1.01 \times A_2^{1/3}$ fm; depending on the chosen proton state $(\vec{\sigma}\ .\ \vec{l}\ ) = l$ or $-(l+1)$.

– V_c is the Coulomb potential, defined as

$$V_c(r) = \begin{cases} \frac{Z_1 Z_2 e^2}{2R_c}[3 - (\frac{r}{R_c})^2], & r \le R_c \\ \\ \frac{Z_1 Z_2 e^2}{r}, & r > R_c. \end{cases}$$

with $Z_1 = 1$, $Z_2 = Z - Z_1$, $R_c = 1.21 \times A_2^{1/3}$ fm.

– the last term represents the centrifugal potential.

4.1 Generation of the initial wave function

The initial wave packet is produced on some interval $[0, r_{\text{init}}]$ as a bound state of a modified hamiltonian (with the potential $V(r)$ replaced by the constant $V(r_{\text{mod}}) > Q_p$ for $r \ge r_{\text{mod}}$). The bound state energy E is taken equal to the experimental one by slightly varying the depth of the nuclear potential. In fact, the energy is the eigenvalue and the initial wave function is the eigenvector of an algebraic eigenvalue problem of the form

$$\mathbf{A}\psi = E\mathbf{B}\psi \tag{4.5}$$

where the matrices $\mathbf{A}, \mathbf{B}$ have a tridiagonal structure. The solution of such a problem can be found by the package ARPACK (Ref. [14]). It allows the computation of a

selected number of eigenvalues and requires instead of storing the matrices in memory to supply only the products of matrices by a vector.

Eq. (4.5) results by discretizing the stationary Schrödinger equation

$$\frac{d^2\psi}{dr^2} + \frac{2m}{\hbar^2}[E - V_{\text{mod}}(r)]\psi(r) = 0 \tag{4.6}$$

where V_{mod} is the modified potential. The produced wave function simulates a metastable or a quasi-stationary state. To follow its time evolution we have to go back to the original hamiltonian and increase the initial grid by a factor F, so that $r_J = F \times r_{\text{init}}$. The initial wave function is set equal to zero for $r > r_{\text{init}}$.

To calculate the coefficients a_1, b_0, b_1 we take $\omega = \sqrt{\frac{2m}{\hbar^2}(\tilde{V} - E)}$, where $\tilde{V}$ is the mean value of the potential on some part of the interval. They are used both in the stationary equation, to produce the initial solution, and in the time-dependent equation. By introducing the exponentially fitted Numerov formula, one obtains a higher

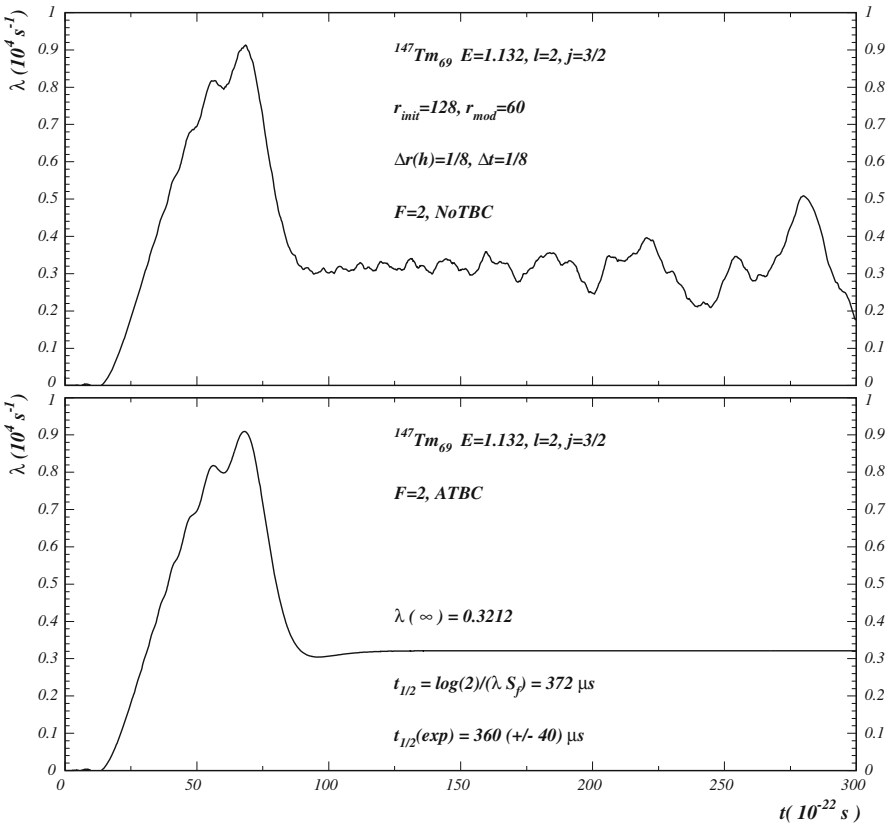

Fig. 1 Time dependent decay rate calculated for the proton decay of ^{147}Tm for a spatial grid of length 2×128 fm without and with adapted transparent boundary conditions

accuracy as well as a better description of the exponential or oscillating behavior of the solution.

4.2 Results

In Fig. 1 is shown the evolution of $\lambda(t)$ for a grid of length 2×128 fm. Without artificial boundary conditions (the upper half) the reflections make impossible to obtain a stabilized value of the decay rate. Introduction of ATBC (the lower half) leads to a stable asymptotic value λ_∞, from which the half-life can be obtained: $t_{1/2} = \log 2/(\lambda_\infty S_f)$. S_f is the so-called spectroscopic factor which represents the fragmentation probability and can be calculated in the frame of different theories (like Bardeen-Cooper-Schrieffer). We have obtained a half-life close to the experimental one. ATBC gives a better convergence compared to the other procedures (requires smaller grids). Thus, to obtain the asymptotic value $\lambda_\infty = 0.3212 \times 10^4 s^{-1}$, with ATBC is sufficient a factor $F = 2$, while for TBC and DTBC one has to use a factor $F > 2$. This situation appears since both TBC and DTBC methods are based on the assumption that $V(r \geq r_J) = constant$, which is numerically valid only at very large distances.

Also, the modified Crank–Nicolson method allows larger step size or fewer mesh points (about 4 times) for the same accuracy than the standard method. The spatial and the time steps used are indicated in the figure.

5 Conclusion

The solution of the time-dependent Schrödinger equation by an improved Crank–Nicolson method is discussed and applications to the proton emission are presented. By introducing the exponentially fitted Numerov formula for the approximation of the second spatial derivative instead of standard finite difference approximation one acquires an increase of accuracy from fourth order in the space increment h to sixth order in h with little more computational effort. Also, the exponential or oscillating behavior of the solution is better represented. This happens mainly when the wave function corresponds to higher levels, with increasing number of nodes.

To avoid unwanted reflections from the numerical boundary into the solution region, artificial boundary conditions have to be implemented. Acting only on the last point of the grid, these procedures succeed, after a certain period of time, to simulate, inside a finite domain, the motion of a wave packet that evolves in an infinite domain. Three kinds of such procedures (of TBC type) are described. An improvement of the standard TBC that takes into account the shape of the particle-nucleus interaction potential was shown to reduce the dependence of the asymptotic decay rate on the length of the numerical grid, thus allowing shorter grids to be used.

We also indicated how to produce the initial wave function as a quasi-stationary state in a modified potential, using the same Numerov-type approximation.

Finally, we have compared our time-dependent calculations with the experimental values, a good agreement being observed.

The investigated case corresponds to a deep-tunneling situation (the energy is low in comparison with the top of the potential barrier), of high physical interest.

The approach can also be applied to other problems of quantum physics or quantum chemistry requiring the solution of the time-dependent Schrödinger equation.

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