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Computational method for the long time propagation of quantum channeled particles in crystals and carbon nanotubes

M. Ćosić [a,b,*], S. Petrović [a], N. Nešković [a]

[a] Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia
[b] School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, Belgrade 11120, Serbia

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ABSTRACT

This work reports on the computational method for the long time propagation of the quantum channeled particles in infinite and finite harmonic interaction wells and in a realistic carbon nanotube interaction potential well. This method is based on the Chebyshev global propagation method for solving of the corresponding time dependent Schrödinger equation. For comparison, the computational method based on the Crank–Nicolson propagation method is also presented. In the case of quantum particle motion in infinite harmonic potential well, when the analytical solution of the corresponding time-dependent Schrödinger equation exists, we show that the obtained propagation method is efficient, very accurate and numerically stable. It is superior with respect to the method based on the Crank–Nicolson propagation method. A detailed study of the long time quantum particle motion in the finite harmonic interaction potential well shows that the obtained computational method based on the Chebyshev global propagation method can be successfully applied for following of the channeled quantum particle in crystals and carbon nanotubes. This is demonstrated in the case of quantum particle motion in a realistic carbon nanotube interaction potential well.

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1. Introduction

Channeling effect of positive charged particle in crystals [1] and carbon nanotubes [2,3] occurs when the particle's velocity vector with respect to the crystal's and nanotube's axes remains small during its motion through crystals and carbon nanotubes, respectively. The ion channeling effect in crystals was discovered in a computer simulation of Robinson and Oen [4]. It can be shown that the classical treatment of the particle channeling motion is adequate for heavy particles – ions [1]. However, for a light particle (e.g. positron) the quantum treatment must be implemented [5].

Recently, the strong spatial focusing of the channeled protons along the axis of the ⟨100⟩ silicon crystal, which was named the superfocusing effect, was proposed [6]. In that study, the analytical solution of the time-dependent Schrödinger equation for the quantum particle motion in the infinite harmonic interaction potential well, assuming initially centered Gaussian wave packet, was used to demonstrate the focusing of the wave packet at the subatomic dimension. It has been shown that the superfocusing effect is a consequence of the crystal rainbow effect [7,8]. Petrović et al. have presented the possibility for development of a measurement technique with the picometer resolution – the rainbow subatomic microscopy, which is based on the superfocusing effect [9].

In this work we investigate the computational method for the long time propagation of quantum particle in a finite harmonic interaction potential well. The aim of this work is to develop efficient and accurate method that can be used for following of the channeled quantum particle in crystals and carbon nanotubes.

2. Physical model

The time-dependent Schrödinger equation is basic equation of quantum mechanics. Its most general form is given with the expression:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\hat{H}(\hat{\mathbf{p}},\hat{\mathbf{r}},t)\psi(\mathbf{r},t), \tag{1}$$

where $\psi(\mathbf{r},t)$ is the coordinate representation of quantum state, with $\mathbf{r}$ and t being its position vector and time, respectively, $\hat{H}(\hat{\mathbf{p}},\hat{\mathbf{r}},t)$ is the operator representation of total energy, i.e. Hamiltonian of system, which could be an explicit function of time t, with $\hat{\mathbf{r}}$

* Corresponding author at: Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia. Tel.: +381 11 6447700.
E-mail address: mcosic@vinca.rs (M. Ćosić).
URL: http://www.vinca-at.org (M. Ćosić).

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and $\hat{\mathbf{p}}$ being the operators of its position and momentum vectors, respectively, and $\hbar$ is the reduced Planck constant.

We consider here motion of positively charged quantum particle in a finite harmonic interaction potential well. Finite harmonic interaction potential is a good qualitative approximation of the continuum crystal and carbon nanotube interaction potentials. As we have already mentioned, the infinite harmonic interaction potential have been already applied for studding of the superfocusing effect of the channeled particles in the silicon crystal [6]. Also, the harmonic interaction potential approximation of the continuum carbon nanotube interaction potential was used to demonstrate how the particle channeling in carbon nanotubes could be applied as a new source of hard X-ray radiation [10].

Finite harmonic interaction potential V_{FH} is defined by the following expressions:

$$V_{FH}(r) = \begin{cases} \frac{1}{2} m_o \omega_o^2 r^2, & \text{for } r \leqslant R \\ 0, & \text{for } r > R \end{cases}, \tag{2}$$

where ω_o is characteristic angular frequency of quantum particle motion, $r = (x^2 + y^2)^{1/2}$ is distance from the center of the potential well; x and y are coordinates of the transverse motion of quantum particle, and R radius of the potential well. It is depicted in Fig. 1(a). Since the interaction potential V_{FH} is not an explicit function of time, the formal solution of Eq. (1) is given by:

$$\psi(\mathbf{r}, t) = \hat{U}(t)\psi(\mathbf{r}, 0) = \exp(-i\hat{H}t/\hbar)\psi(\mathbf{r}, 0), \tag{3}$$

where $\hat{U}(t)$ is the evolution operator and $\hat{H} = \hat{\mathbf{p}}^2/(2m_o) + \hat{V}_{FH}$ is the Hamiltonian of the system.

Initially, the quantum particle is represented with the wave function in the form of a Gaussian wave packet of some known standard deviation, with the impact parameter corresponding to the center of the wave packet. Numerical integration of Eq. (1) gives the time evolution of the wave function $\psi(\mathbf{r}, t)$. Knowing this all physical quantities for the system under the consideration can be obtained. However, from the numerical point of view, the potential given by the expressions (2) is undesirable because it is discontinuous and its derivatives are discontinuous at the potential well edges. Therefore, the Lorentzian and exponential functions are used to smooth the well edges. This smoothing is schematically shown in Fig. 1(b). The obtained interaction potential is given by the following expressions:

$$V(r) = \begin{cases} \frac{1}{2} m_o \omega_o^2 r^2, & \text{for } r \leqslant R \\ \frac{V_0}{1+\left(\frac{r-r_1}{r_0}\right)^2}, & \text{for } R < r \leqslant r_2 \\ V_1 e^{-\frac{r-r_2}{r_3}}, & \text{for } r > r_2 \end{cases}, \tag{4}$$

where V_0, V_1, r_0, r_1 and r_2 are the fitting parameters. Four of them, V_0, V_1, r_0, r_1, were determined through the imposed conditions of continuity of the interaction potential and its first derivative at the $r = R$ and $r = r_2$. Therefore, this procedure leaves only one free parameter, r_2, and let us denote the obtained potential with $V(r, r_2)$. Optimal value for the parameter r_2 can be obtained from the requirement that the difference between $V(r, r_2)$ and $V_{FH}(r)$ should be less than some predetermined small quantity ε:

$$||V(r, r_2) - V_{FH}(r)||^2 \leqslant \varepsilon, \tag{5}$$

where $||V(r, r_2) - V_{FH}(r)||$ represents the functional norm. We solved this problem using Trust-Region-Reflective algorithm [11] for the least-square nonlinear curve fitting with ε as the stopping criteria. In the case under the consideration here the parameter ε was set to be 10^{-6}.

3. Numerical methods

In this work, for simplicity, we investigate the numerical methods for solving 1D time dependent Schrödinger equation (1) for the finite harmonic interaction potential (4). This simplifications is not crucial, since the application of the numerical methods in the 2D case is straightforward and all the conclusions from the obtained results will hold in the 2D case as well. In the literature devoted to the numerical mathematics one can find various methods for integration of time-dependent Schrödinger equation [12,13]. Computational complexity and efficiency practically limit area of application of certain numerical integration method. Optimal numerical solver for the particle channeling in crystals and nanotubes should be efficient i.e. reasonably fast to be used in the long time particle propagation and unconditionally stable, because it should be used for different initial wave packets corresponding to different impact parameters of the channeled particles.

For the numerical integration of Eq. (1) using the interaction potential defined by the expressions (4), we have considered the Chebyshev global propagation method, which was adopted by us for the problem under the consideration and, for the comparison, the Crank–Nicolson propagation method. Both of them are grid methods using the space discretization of the continuous function $\psi(x, t)$. The discretization grid is finite in size and is kept fixed during the calculations. It should be noted here that in both of the numerical methods only the values of the interaction potential on the fixed grid are required. This fact was important in our choice of the possible numerical methods for solving of the time-dependent Schrödinger equation, since the chosen methods can be easily

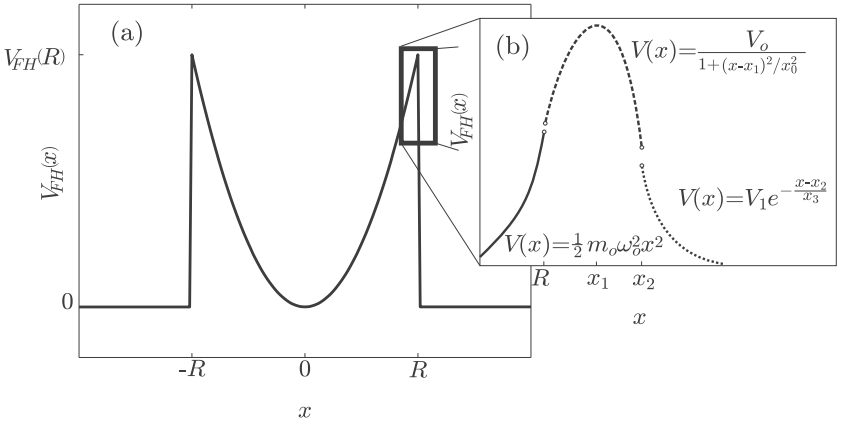

Fig. 1. (a) The slice through the axially symmetric interaction potential $V_{FH}(r)$ for $y = 0$, where R is radius of the potential well and $V_{FH}(R)$ is the value of the interaction potential at the well edges. (b) Enlarged schematically presented smoothed part of the slice around the potential well edge. Full line represent its parabolic part, dashed line its Lorentzian part, and doted line its exponential part.

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