Spectral Method in Axial Channeling Theory

N. F. Shul'ga[a], V. V. Syshchenko[b], and V. S. Neryabova[b]

[a]Akhiezer Institute for Theoretical Physics, National Science Center Kharkiv Institute of Physics and Technology, Kharkiv, 61108 Ukraine

[b]Belgorod State National Research University, Belgorod, 308015 Russia

e-mail: syshch@bsu.edu.ru, syshch@yandex.ru

Abstract—The energy quantization of transverse particle motion in continuous potentials of atomic chains and planes can occur when fast charged particles travel in crystals. In the proposed paper, the energy levels of electrons moving in the mode of axial channeling in a system of parallel atomic chains have been found (Si crystal [110] chains have been used as an example). The energy eigenvalues were determined numerically using the so-called spectral method, which shows itself to good advantage in the problem of the plane channeling of charged particles in crystals.

INTRODUCTION

The motion of fast charged particles in a crystal near one of the crystallographic axes or planes is mainly determined by the continuous potential of the crystal lattice, i.e., the crystal potential averaged along the axis or the plane near which the motion occurs. The particle-momentum component $p_{\parallel}$ that is parallel to the crystallographic axis or plane is retained in such a field. Thus, the problem of particle motion in a crystal reduces to that of its motion in the transverse plane. The finite motion in potential wells formed by the continuous potentials of atomic planes (axes) is called plane (axial) channeling [1–3]. Quantum effects can be significant in this case; in particular, the energy of the transverse particle motion can be quantized. Potential wells in the cases under consideration have rather complicated forms not permitting analytical integration of the Schrödinger equation, which requires the development of numerical methods for finding the energy levels of the transverse motion and other quantum characteristics of the particle motion in continuous potentials of crystal atomic planes and chains.

The aim of this paper is to study the capabilities of the so-called spectral method for finding the energy levels in the case of fast-electron channeling in the two-dimensional field of an atomic chain or a system of chains (Si crystal [110] chains are used as an example). This method has been successfully used previously to find the energy levels in the one-dimensional potential of an atomic plane and a system of parallel atomic planes [5].

PROCEDURE

The spectral method for finding the energy eigenvalues of a quantum system is based on calculation of the correlation function Ψ between two wave functions $\Psi(x, t)$ and $\Psi(x, 0)$ of the system at the current and initial time instants:

$$P(t) = \int_{-\infty}^{\infty} \Psi^*(x,0)\Psi(x,t)dx. \tag{1}$$

(for simplicity, we restrict ourselves to the one-dimensional case).

It turns out that such a correlation function, more precisely, its Fourier transform

$$P_E = \int_{-\infty}^{\infty} P(t)\exp(iEt/\hbar)dt, \tag{2}$$

contains information on the energy eigenvalues of the system. Indeed, any solution of the Schrödinger equation

$$\hat{H}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{3}$$

can be represented in the form of the superposition

$$\Psi(x,t) = \sum_{n,j} A_{n,j}u_{n,j}(x)\exp(-iE_n t/\hbar), \tag{4}$$

of the eigenfunctions $u_{n,j}(x)$ of the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(x) \tag{5}$$

(where ∇^2 is the Laplace operator), i.e., the functions satisfying the equation

$$-\frac{\hbar^2}{2m}\nabla^2 u_{n,j} + U(x)u_{n,j} = E_n u_{n,j}, \qquad (6)$$

where the subscript j labels the degenerate states corresponding to the energy E_n. Calculation of the correlation function (1) for the wave function in the form of (4) gives

$$P(t) = \sum_{n,n',j,j'} \exp(-iE_{n'}t/\hbar)A_{n,j}^* A_{n',j'} \int_{-\infty}^{\infty} u_{n,j}^*(x)u_{n',j'}(x)dx$$

$$= \sum_{n,n',j,j'} \exp(-iE_{n'}t/\hbar)A_{n,j}^* A_{n',j}\delta_{nn'}\delta_{jj'} \qquad (7)$$

$$= \sum_{n,j} |A_{n,j}|^2 \exp(-iE_n t/\hbar).$$

The calculation of its Fourier transform (2) leads to the expression

$$P_E = 2\pi\hbar\sum_{n,j} |A_{n,j}|^2 \delta(E - E_n). \qquad (8)$$

We see that the Fourier transform of the correlation function is a series of δ-like peaks the positions of which correspond to the eigenvalues of the Hamiltonian (5) (to the energy eigenvalues of the system).

Thus, the determination of the energy levels of the system reduces to the following steps:

(i) The initial wave function $\Psi(x, 0)$ is chosen in its arbitrary form. The only restrictions affecting the choice of it are as follows: (a) the tendency to zero as $x \to \pm\infty$, which corresponds to any coupling state; (b) a rather broad spectrum including the energy range from the bottom to the walls of the potential well, which provides the determination of all energy levels of the system in this range; and (c) the lack of symmetry, which could lead to a loss of a part of the Hamiltonian eigenfunctions. In particular, all these requirements are satisfied by the Gaussian wave packet of the form

$$\Psi(x,0) = \frac{1}{\sigma\sqrt{\pi}}\exp\left[i\frac{p_x x}{\hbar} - \frac{x^2}{2\sigma^2}\right]$$

with the appropriate width σ (we recall that the spectral width is inversely proportional to the packet width).

(ii) The values of $\Psi(x, t)$ for a discrete set of time values $t > 0$ with the step Δt are found using numerical integration of time-dependent Schrödinger equation (3) with the initial condition $\Psi(x, 0)$. The value of the time step is determined by the width of the range of energy eigenvalues (in our case, by the depth U_{max} of the potential well) in accordance with the Nyquist criterion (which is known as the Kotel'nikov theorem in Russian publications)

$$\Delta t \le \frac{\pi\hbar}{|U_{max}|}. \qquad (9)$$

In accordance with [4], good results are obtained for

$$\Delta t < \frac{\pi\hbar}{3|U_{max}|}. \qquad (10)$$

(iii) Calculation of integral (1) for each time step in the range from 0 to the maximum T gives the values of the correlation function $P(t)$, and subsequent calculation of integral (2) gives its Fourier transform. In this case, integration in (2) turns out to be limited by a finite time interval

$$P_E = \int_0^T P(t)\exp(iEt/\hbar)dt, \qquad (11)$$

as a result, instead of infinitely narrow δ-like peaks, we obtain a series of peaks with finite widths, which are inversely proportional to T. Indeed, substituting $P(t)$ in the form of (7) into (11) yields

$$P_E = \sum_{n,j} |A_{n,j}|^2 \frac{\exp[i(E - E_n)T/\hbar] - 1}{i(E - E_n)/\hbar}$$

$$= T\sum_{n,j} |A_{n,j}|^2 \exp[i(E - E_n)T/2\hbar]\frac{\sin[(E - E_n)T/2\hbar]}{(E - E_n)T/2\hbar}. \qquad (12)$$

It is easy to see that, in accordance with the Nyquist criterion, to resolve the levels spaced by the distance ΔE_{min}, it is necessary to choose the time interval T during which our wave function satisfying the inequality

$$T > \frac{2\pi\hbar}{\Delta E_{min}}. \qquad (13)$$

is generated.

The resolution of closely located levels can be complicated because of overlapping of the lateral bands of the function $\text{sinc}(x) = \sin x/x$ in (12). The resolution can be improved [4] by multiplying the correlation function $P(t)$ by the so-called normalized window Hanning function

$$\frac{w(t)}{T} = \frac{1}{T}\begin{cases} 1 - \cos(2\pi t/T), & 0 \le t \le T, \\ 0, & t > T. \end{cases} \qquad (14)$$

before calculation of the integral (11).

RESULTS AND DISCUSSION

The motion of a fast charged particle incident at a small angle ψ to a crystallographic axis densely packed with atoms in a crystal can be represented with a good accuracy as that in the continuous potential of the atomic chain, i.e., in the potential averaged along the chain axis.

The transverse component $p_\parallel$ of particle momentum (i.e., the component that is parallel to the chain axis) is retained during motion in such a potential. The motion in the transverse plane in this case is described by a two-dimensional analogue of the nonrelativistic Schrödinger equation [1]

$$\left\{ -\frac{\hbar^2}{2E_\parallel/c^2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U(x,y) \right\} \Psi(x,y,t)$$

$$= i\hbar \frac{\partial}{\partial t} \Psi(x,y,t), \tag{15}$$

which contains the quantity $E_\parallel/c^2$, where $E_\parallel = \sqrt{m^2 c^4 + p_\parallel^2 c^2}$, instead of the particle mass m (as it would be in the nonrelativistic case).

The continuous potential of the atomic chain can be approximated by the formula [1]

$$U_1(x,y) = -U_0 \ln\left(1 + \frac{\beta R^2}{x^2 + y^2 + \alpha R^2} \right), \tag{16}$$

where, in particular, $U_0 = 60$ eV, $\alpha = 0.37$, $\beta = 3.5$, and $R = 0.194$ Å (the Thomas–Fermi radius) for the [110] chain of a Si crystal; in this case, the distance between the axes of two neighboring chains is $a/4 = 5.431/4$ Å (where a is the period of the crystal lattice). Thus, the continuous potential in which the electron moves is described by the two-well function in the form

$$U(x,y) = U_1(x, y + a/8) + U_1(x, y - a/8) \tag{17}$$

the influence of distant chains is not taken into account in this case (Fig. 1). The finite electron motion in such a potential (corresponding to the negative energies $E_\perp$ of transverse motion) is called axial channeling.

To find the energy levels of transverse motion in such a potential by means of the spectral method, we chose the initial wave function of the asymmetric Gaussian form

$$\Psi(x,y,0) = \frac{1}{\pi\sigma_x\sigma_y} \exp\left[-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{(y+a/8-y_0)^2}{2\sigma_y^2} \right]$$

$$+ \frac{1}{2\pi\sigma_x\sigma_y} \exp\left[-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{(y-a/8-y_0)^2}{2\sigma_y^2} \right], \tag{18}$$

where $\sigma_x = 0.05$ Å, $\sigma_y = 0.06$ Å, $x_0 = a/35$, and $y_0 = a/45$ (the high symmetry of the initial wave function can lead to the lack of several eigenfunctions in superposition (4) and, consequently, to the loss of several energy levels).

The results of calculating the energy levels for an electron with $E_\parallel = 20$ MeV in the double potential well (17) and the single well (16) are shown in Fig. 2. The logarithm of the absolute value of the Fourier transform of the correlation function (11) is plotted on the ordinate axis, and the energy $E_\perp$ in the potential well is
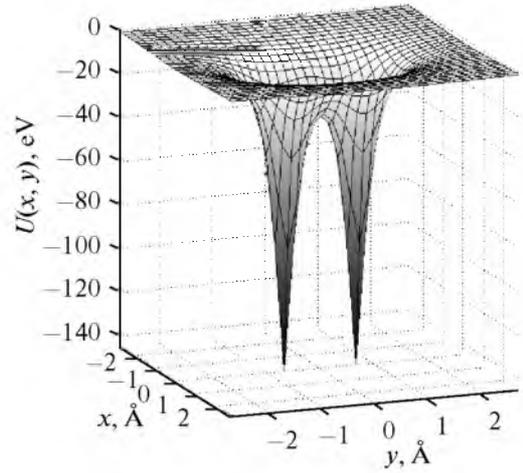
Fig. 1. Potential energy of an electron in the field of continuous potentials of two neighboring [110] chains of a Si crystal.

plotted on the abscissa axis. For convenience of comparison, these graphs corresponding to the single and double wells are located in a specular way; in this case, the negative value $U_1(0, a/4) \approx -4.111$ eV is added to the potential energy in the single well (16) in order to shift the bottom level of the single potential well to that of the double one.

It can be seen that the structure of the energy levels repeats that in the single well in the $E_\perp$ range located below the saddle point of the double-well potential; however, splitting is observed for certain levels. The reason for the splitting of deeply located levels is that the degeneracy with respect to the projection of the orbital moment on the well axis (the atomic-chain axis) is removed. Indeed, in accordance with the general principles of quantum mechanics, the states in the two-dimensional centrally symmetric field is characterized by two quantum numbers, namely, the radial one n_r (coinciding with the number of zeros of the radial wave function; zeros at zero distance and infinity from the field center are not taken into account in this case) and the projection m of the orbital momentum on the field symmetry axis (see, e.g., problem 4.7 in [6]). In this case, the states with $m = 0$ are nondegenerate, and those with $|m| \neq 0$ are doubly degenerate (the positive and negative values of m correspond to the same energy). The lower graph in Fig. 2 shows the Fourier transforms of the correlation function (11) of an electron in the single axially symmetric potential well (16) calculated with the initial wave functions in the general and axially symmetric forms. In the last case, the maxima of the correlation-function Fourier transform indicate positions of only nondegenerate energy levels corresponding to $m = 0$. Comparison with the upper graph in Fig. 2 shows that only levels corresponding to $|m| \neq 0$ are split.
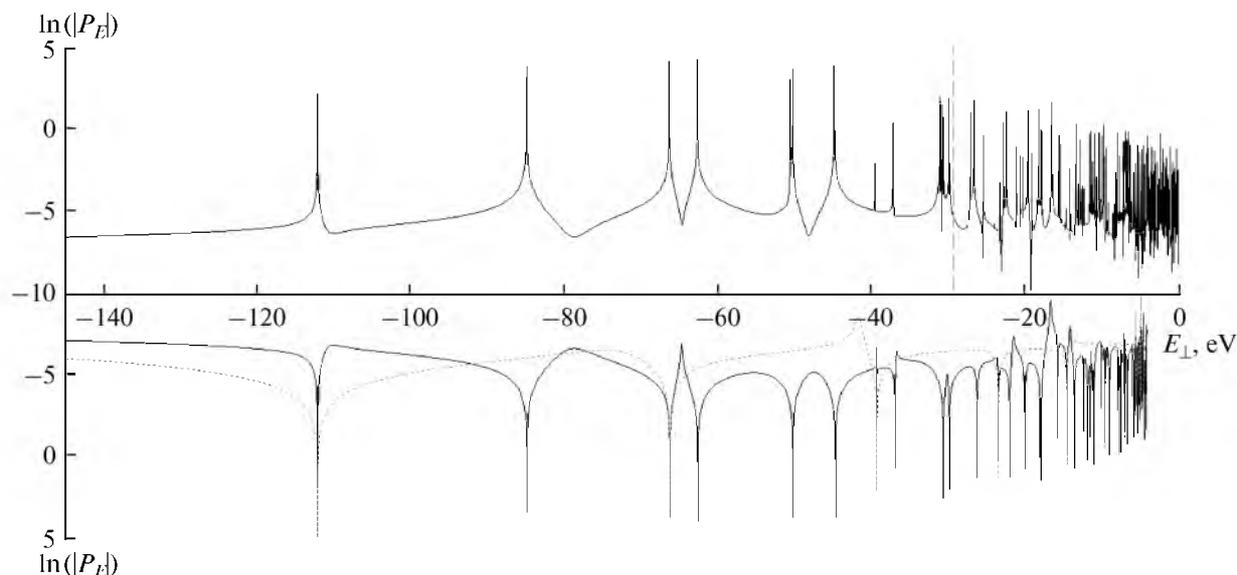
Fig. 2. Upper graph: Fourier transform (11) of the correlation function for an electron with the energy $E_\parallel = 20$ MeV in a double potential well (17) as a function of the transverse-motion energy $E_\perp$; the dashed line denotes the position of the saddle point of the potential (17). The lower graph: the Fourier transform of the correlation function for an electron in a single well (16) shifted by -4.111 eV; it was calculated for the initial wave function in the general form (the solid curve) and for the axially symmetric initial wave function (the dashed curve).

In addition, the splitting related to the tunneling effect becomes noticeable for energy levels that are close to the saddle point of the two-well potential and for which the potential barrier between the wells becomes more penetrable.

Figure 3 shows the graphs of the correlation-function Fourier transform for different $E_\parallel$. It can be seen that, as the electron energy increases, the energy levels are shifted deep into the potential well. In this case, new levels are split from the continuous spectrum ($E_\perp > 0$) and are pulled into the well so that the total number of them increases with increasing $E_\parallel$.
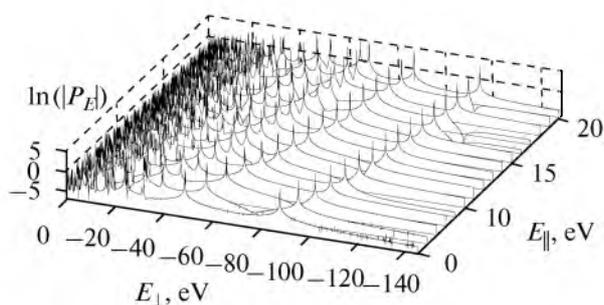
Fig. 3. Fourier transforms (11) of the correlation functions calculated for different energy values $E_\parallel$ of longitudinal electron motion in a double potential well (17). The positions of maxima indicate the eigenvalues of the transverse-motion energies $E_\perp$.

CONCLUSIONS

The conditions under which quantum effects in the interaction of particles with continuous potentials of atomic chains and planes are important can be satisfied when fast charged particles travel through oriented crystals under channeling conditions. In this paper, we considered the quantum-mechanical problem of the interaction between a particle and the continuous potential of a separate atomic chain and two adjoining chains in a crystal. We showed that the spectral method for determining Hamiltonian eigenvalues can be used in this problem. Based on this method, we have developed a procedure for calculating the energy levels of particle transverse motion, which can be used in the case of the axially symmetric potential well produced by a separate atomic chain and in the case of a potential in a more complicated form, which is formed by two parallel atomic chains of the crystal. In the last case, we demonstrated the energy-level splitting produced by the violation of axial symmetry in such a potential and also by the tunneling effect between neighboring wells. The obtained results indicate that this method can be used to analyze the formation of the band structure of energy levels of transverse motion for the axial channeling of fast particles in crystals.

ACKNOWLEDGMENTS

APPENDIX

Numerical Integration
of the Time-Dependent Schrödinger Equation

The evolution of the wave function (for simplicity, we restrict ourselves to the one-dimensional case) during the infinitesimal time interval dt is described by a well-known formula in quantum mechanics,

$$\Psi(x, t + dt) = \exp\left[-i\frac{dt}{\hbar}\hat{H}\right]\Psi(x,t). \tag{19}$$

Therefore, if the initial condition $\Psi(x, 0)$ is used, the wave function $\Psi(x, t)$ can be found at time instants $t > 0$ by means of the approximate iteration procedure:

$$\Psi(x, t + \Delta t) = \exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right]\Psi(x,t). \tag{20}$$

The Hamiltonian (5) contained in the evolution operator is the sum of the kinetic and potential terms, one of which is diagonal in the momentum representation, and the other, in the coordinate representation. In this case, it is convenient to use the so-called splitting method [7], which involves the successive implementation of the free evolution of the wave function under the action of the operator $\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{2m}\nabla^2\right]$ and of the local interaction with the potential under the action of the operator $\exp\left[-i\frac{\Delta t}{\hbar}U(x)\right]$. However, the case becomes complicated by the fact that the kinetic and potentials terms in this Hamiltonian do not switch one with another. Therefore, the evolution operator cannot be represented in the form

$$\exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right] = \exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{2m}\nabla^2\right]\exp\left[-i\frac{\Delta t}{\hbar}U(x)\right].$$

However, we can show that

$$\exp\left[\Delta t\left(\hat{A} + \hat{B}\right)\right]$$
$$= \exp\left[\frac{\Delta t}{2}\hat{A}\right]\exp\left[\Delta t\hat{B}\right]\exp\left[\frac{\Delta t}{2}\hat{A}\right]\left(1 + O\left((\Delta t)^3\right)\right),$$

therefore, in the process of numerical simulation, we act on the wave function $\Psi(x, t)$ at each iteration by the sequence of the three exponents:

$$\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\nabla^2\right]\exp\left[-i\frac{\Delta t}{\hbar}U(x)\right]\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\nabla^2\right]. \tag{21}$$

To find the result of acting on the "kinetic"-operator wave function, it is convenient to represent it in the form of the expansion in terms of eigenfunctions of the kinetic-energy operator, i.e. in the form of the Fourier integral:

$$\Psi(x, t) = \int_{-\infty}^{\infty}\Psi_k(t)\exp(ikx)\frac{dk}{2\pi}, \tag{22}$$

$$\Psi_k(t) = \int_{-\infty}^{\infty}\Psi(x,t)\exp(-ikx)dx. \tag{23}$$

The result of the "kinetic"-exponent action on the wave function written in such a way is as follows:

$$\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\nabla^2\right]\Psi(x,t)$$

$$= \int_{-\infty}^{\infty}\Psi_k(t)\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\nabla^2\right]\exp(ikx)\frac{dk}{2\pi} \tag{24}$$

$$= \int_{-\infty}^{\infty}\Psi_k(t)\exp\left[-i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}k^2\right]\exp(ikx)\frac{dk}{2\pi}.$$

The function $\Psi(x, t)$ given in the finite interval $0 \leq x \leq L$ is represented by the Fourier series rather than by the integral:

$$\Psi(x, t) = \frac{1}{\sqrt{L}}\sum_{k=-\infty}^{\infty}\Psi_k(t)\exp\left(ik\frac{2\pi}{L}x\right), \tag{25}$$

$$\Psi_k(t) = \frac{1}{\sqrt{L}}\int_0^L\Psi(x,t)\exp\left(-ik\frac{2\pi}{L}x\right)dx. \tag{26}$$

For numerical calculations, the wave function is specified at a discrete mesh with the step Δx. The corresponding relations similar to (25) and (26) have the forms

$$\Psi(x, t) = \frac{1}{\sqrt{N}}\sum_{k=-k_{max}+1}^{k_{max}}\Psi_k(t)\exp\left(ik\frac{2\pi}{L}x\right), \tag{27}$$

$$\Psi_k(t) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N}\Psi(n\Delta x, t)\exp\left(-ik\frac{2\pi}{L}n\Delta x\right), \tag{28}$$

where $N = L/\Delta x$ is the number of steps of the coordinate mesh and $k_{max} = N/2$ (it is convenient to choose the number N of steps to be even). We see that Fourier transformation (28) in this case is equivalent to multiplication of the vector of values of the wave function $\psi_n = \Psi(n\Delta x, t)$ by the unitary matrix Q_{kn} with the elements

$$Q_{kn} = \frac{1}{\sqrt{N}}\exp\left(-ik\frac{2\pi}{L}n\Delta x\right), \tag{29}$$

and inverse transformation (27) is equivalent to multiplication of the vector of the Fourier components Ψ_k by a matrix that is inverse to Q_{kn}:

$$\left(Q_{kn}\right)^{-1} = \left(Q_{kn}\right)^{+} = Q_{nk}^{*}.$$

The result of the action of the "kinetic" part of the evolution operator on the wave function (25) looks similar to (24):

$$\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\nabla^2\right]\Psi(x,t)$$

$$= \frac{1}{\sqrt{N}}\sum_{k=-k_{max}+1}^{k_{max}}\Psi_k(t)\exp\left[i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\nabla^2\right]\exp\left(ik\frac{2\pi}{L}x\right)$$

$$= \frac{1}{\sqrt{N}}\sum_{k=-k_{max}+1}^{k_{max}}\Psi_k(t)\exp\left[-i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\left(\frac{2\pi}{L}\right)^2 k^2\right]\exp\left(ik\frac{2\pi}{L}x\right).$$

Thus, one time iteration (20) can be written in the matrix form:

$$\psi_{n'''}\big|_{t+\Delta t} = Q_{n'''k'''}^{*}K_{k'''k'''}Q_{k'''n'}V_{n'n}Q_{n'k}^{*}K_{k'k}Q_{kn}\psi_n$$

or

$$\psi\big|_{t+\Delta t} = Q^{+}KQVQ^{+}KQ\psi,$$

where $K_{k'k}$ is the diagonal (in the momentum representation) matrix corresponding to the "kinetic" part of the evolution operator with the elements

$$K_{k'k} = \delta_{k'k}\exp\left[-i\frac{\Delta t}{\hbar}\frac{\hbar^2}{4m}\left(\frac{2\pi}{L}\right)^2 k^2\right],$$

and $V_{n'n}$ is diagonal (in the coordinate representation) matrix corresponding to the "potential" part of the evolution operator with the elements

$$V_{n'n} = \delta_{n'n}\exp\left[-i\frac{\Delta t}{\hbar}U(n\Delta x)\right].$$

Generalization of this algorithm to the two-dimensional case is not difficult.

The spatial mesh containing 128 × 128 elements with the step $\Delta x = 0.042$ Å was used in actual calculations. The time step was determined in accordance with criterion (10).

REFERENCES

1. A. I. Akhiezer and N. F. Shul'ga, *High Energy Electrodynamics in Matter*
2. A. I. Akhiezer, N. F. Shul'ga, V. I. Truten', et al., Phys. Usp. **38**, 1119 (1995).
3. U. I. Uggerhøj, Rev. Mod. Phys. **77**, 1131 (2005).
4. M. D. Feit, J. A. Fleck, Jr., and A. Steiger, J. Comput. Phys. **47**, 412 (1982).
5. A. V. Kozlov, N. F. Shul'ga, and V. A. Cherkaskiy, Phys. Lett. A **374**, 4690 (2010).
6. V. M. Galitskii, B. M. Karnakov, and V. I. Kogan, *Problems on Quantum Mechanics* (Nauka, Moscow, 1981) [in Russian].
7. V. V. Serov, *Numerical Methods for the Solution of Nonstationary Quantum Mechanical Problems* (Novyi veter, Saratov, 2011) [in Russian].

Translated by L. Kul'man

SPELL: 1. ok