Wave functions of channeling electrons in regular and chaotic cases

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Abstract. The spectral method applicability to the problem of the charged particles axial channeling is studied. The quantum state characteristics for the electron motion near the atomic string [110] direction of the silicon crystal are obtained using this method of Schrödinger equation numerical solution. The full set of eigenenergies and eigenfunctions for the electron with longitudinal energy of 5 MeV is computed. The results obtained illustrate the difference in the wave function morphology for regular and chaotic cases.

1. Introduction

The fast charged particles incident onto the crystal under a small angle to any crystallographic axis densely packed with atoms can perform the finite motion in the transverse plane; such motion is known as the axial channeling [1]–[3]. The particle motion in the axial channeling mode could be described with a good accuracy as the one in continuous potential of the atomic string, i.e. in the potential of atoms averaged along the string axis. During motion in this potential the longitudinal particle momentum $p_{\|}$ is conserved, so the motion description is reduced to two-dimensional problem of motion in the transversal plane. This transverse motion could be substantially quantum [1].

From the viewpoint of the dynamical systems theory, the channeling problem is interesting because the particle's motion could be both regular and chaotic. The wave functions of the stationary quantum states in the situations of regular and chaotic motion in the classical limit are computed in the present paper. The qualitative difference between them illustrates the basic statements of the quantum chaos theory [4]–[8].

2. Method

The electron transversal motion in the atomic string continuous potential is described by the two-dimensional Schrödinger equation

$$\hat{H}\Psi(x,y,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,y,t) \tag{1}$$

with Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2E_\parallel/c^2}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right] + U(x,y) \tag{2}$$

and the value $E_\parallel/c^2$ (here $E_\parallel = (m^2c^4 + p_\parallel^2 c^2)^{1/2}$) instead of the particle mass [1].

The Hamiltonian eigenfunctions have been found numerically as well as the transverse energy eigenvalues using the so-called spectral method [9]. For the channeling problem it has been applied for the first time in [10].

The spectral method idea is the following. Every solution of the time-dependent Schrödinger equation could be expressed as the superposition

$$\Psi(x,y,t) = \sum_{n,j} A_{n,j}\psi_{n,j}(x,y)\exp(-iE_n t/\hbar) \tag{3}$$

of the Hamiltonian eigenfunctions $\psi_{n,j}(x,y)$,

$$\hat{H}\psi_{n,j}(x,y) = E_n\psi_{n,j}(x,y) \quad ,$$

where the j index is used to distinguish the degenerate states corresponding to the energy E_n. Computation of the correlation function

$$P(t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Psi^*(x,y,0)\Psi(x,y,t)\,dxdy \tag{4}$$

for the wave function of the form (3) gives

$$P(t) = \sum_{n,n',j,j'} \exp(-iE_{n'}t/\hbar)A^*_{n,j}A_{n',j'}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} u^*_{n,j}(x,y)\psi_{n',j'}(x,y)dxdy =$$

$$= \sum_{n,n',j,j'} \exp(-iE_{n'}t/\hbar)A^*_{n,j}A_{n',j'}\delta_{nn'}\delta_{jj'} = \sum_{n,j}|A_{n,j}|^2\exp(-iE_n t/\hbar) \quad . \tag{5}$$

Fourier transformation of (5) leads to the expression

$$P_E = \int_{-\infty}^{\infty} P(t)\exp(iEt/\hbar)\,dt = 2\pi\hbar\sum_{n,j}|A_{n,j}|^2\,\delta(E-E_n) \quad . \tag{6}$$

We see the Fourier transform of the correlation function looks like a series of δ-form peaks, whose positions indicate the energy eigenvalues. So, the method is based on the numerical simulation of the time evolution of initial wave function $\Psi(x,y,0)$ according to time-dependent Schrödinger equation.

Of course, the numerical integration of (1) could be performed for the finite time interval T only, so the Fourier transform of the correlation function takes the form

$$P(E) = \int_0^T P(t)\exp\left(\frac{i}{\hbar}Et\right)dt = \sum_{n,j}|A_{n,j}|^2\,\frac{\sin\left[(E_n - E'_n)T/2\hbar\right]}{(E_n-E'_n)/2\hbar}\exp\left[\frac{i}{2\hbar}(E-E_n)T\right] \quad . \tag{7}$$

The $\sin(xT)/x$ function in the right part of (7) has the main maximum at $x = 0$, whose magnitude is increased and width is narrowed with T interval increasing. Its other maxima and minima at both sides from the main maximum have the lower magnitudes. So, instead of δ-like peaks set we have the superposition of maxima, whose widths are inverse proportional to

T. The required resolution of the computation dictates the T value, while the expected minimal distance ΔE between the neighbor energy levels dictates the resolution, and condition for T is

$$T > 2\pi\hbar/\Delta E \quad . \tag{8}$$

To avoid the superposition of side maxima of $\sin(xT)/x$ function from neighbor energy levels this requirement should be enhanced. In our calculations we use

$$T = 16\pi\hbar/\Delta E \quad . \tag{9}$$

The numerical procedure based on these ideas has been developed and successfully used for transverse energy levels search with high precision in [11]–[13].

The stationary wave functions could be obtained with the spectral method also [9, 10]. The superposition (3) multiplied by $\exp(iE_nt/\hbar)$ and integrated over the time interval T provides the eigenfunctions $\psi_{n,j}(x,y)$ of the eigenvalue E_n:

$$\int_0^T \Psi(x,y,t)\exp\left(\frac{i}{\hbar}E_nt\right)dt = \sum_{n',j} A_{n',j}\,\psi_{n',j}(x,y)\int_0^T \exp\left[\frac{i}{\hbar}(E_n - E'_n)t\right]dt = \tag{10}$$

$$= \sum_{n',j} A_{n'}\,\psi_{n',j}(x,y)\,\frac{\sin\left[(E_n - E'_n)T/2\hbar\right]}{(E_n - E'_n)/2\hbar}\exp\left[\frac{i}{2\hbar}(E_n - E'_n)T\right] \quad .$$

For the large enough T the left part integral in (10) is proportional to either eigenfunction $\psi_n(x,y)$ (without state degeneration), or $\psi_{n,j}(x,y)$ superposition (if n-th energy level is degenerated) with a good accuracy.

3. Wave functions in the regular case

The field of single atomic string has the axial symmetry $U(x,y) = U(r)$, if the neighbor strings influence is neglected. This symmetry allows us to classify the electron quantum states. In the polar coordinates

$$\hat{H} = -\frac{\hbar^2}{2E_\parallel/c^2}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right] + U(r) \quad . \tag{11}$$

The equation for the eigenfunctions and eigenvalues of the operator (11)

$$-\frac{\hbar^2}{2E_\parallel/c^2}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right]\psi(r,\varphi) + U(r)\psi(r,\varphi) = E_\perp\psi(r,\varphi) \tag{12}$$

allows us to separate the variables, and their solutions are

$$\psi_{n_r,m}(r,\varphi) = \frac{1}{\sqrt{2\pi}}\,e^{im\varphi}\rho_{n_r,|m|}(r) \quad , \tag{13}$$

where the $\rho_{n_r,|m|}(r)$ function is the solution of

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\right)\rho_{n_r,|m|}(r) + \frac{2E_\parallel/c^2}{\hbar^2}\left(E_\perp - U(r) - \frac{\hbar^2}{2E_\parallel/c^2}\frac{m^2}{r^2}\right)\rho_{n_r,|m|}(r) = 0 \quad . \tag{14}$$

The particle quantum states in the potential $U(r)$ with axial symmetry are characterized by two quantum numbers: the radial one n_r and projection m of the orbital momentum to the symmetry axis of the field. The n_r is equal to the number of zeroes of the function $\rho_{n_r,|m|}(r)$ at finite r

(except the possible zero at $r = 0$). The states with $m = 0$ are non-degenerated, while ones with non-zero m are doubly degenerated by the signum of m. The eigenvalues of Hamiltonian (11), i.e. the eigenvalues of the transversal motion energy of the channeling electron, depend in general on both quantum numbers: $E_\perp = E_{n_r,|m|}$.

First of all let's consider the low energy ($E_\parallel = 5$ MeV) electron's motion near direction of the atomic string [110] of the Si crystal. The continuous potential could be represented by the modified Lindhard potential [1]

$$U_1(x,y) = -U_0 \ln\left(1 + \frac{\beta R^2}{x^2 + y^2 + \alpha R^2}\right) \quad , \tag{15}$$

where $U_0 = 60$ eV, $\alpha = 0.37$, $\beta = 3.5$, $R = 0.194$ Å (Thomas–Fermi radius).

In the upper left plot in figure 1 the wave function of the ground state is shown. It has single maximum in center ($r = 0$) and has not zeroes at all (except the asymptotic zero at $r = \infty$).

The other wave functions are represented by black (for $\psi(x,y) < 0$) and white (for $\psi(x,y) > 0$) regions on the plane (x,y) (see figure 1). The irregularity on the periphery of some plots is due to numerical uncertainties. This representation allows us to classify the wave functions using the quantum numbers n_r and m easily, by the wave function zeroes counting.

Indeed, at the $m = 0$ (upper row in figure 1) the wave functions $\psi_{n_r,0}(r,\varphi)$ depend on radial coordinate r only, so the $\psi(x,y) = 0$ zero lines are concentric circles.

Each next solution $\rho_{n_r,0}(r)$ of the equation (14) at $m = 0$ in the solution sequence, where the corresponding eigenenergy is increased, has more zeroes than previous by exactly one. So we can enumerate the corresponding quantum eigenstates by the quantum number n_r which is equal to the number of zeroes of the radial wave function $\rho_{n_r,0}(r)$. Practically n_r is equal to number of borders between the concentric regions.

For the $m \neq 0$ case the situation is analogous. The degeneration by signum of m means the our method provides for each $E_\perp$ eigenvalue the superposition of $\psi_{n_r,m}(r,\varphi)$ and $\psi_{n_r,-m}(r,\varphi)$ functions with equal weights instead of eigenfunction (13). This superposition looks as follows:

$$\rho_{n_r,|m|}(r)\cos\left[|m|\varphi + \alpha_m\right] \quad . \tag{16}$$

So, the m value for calculated wave function equals to number of white (or black) sectors on the plot in figure 1. The energy levels of the considered system classified by quantum numbers n_r and m are presented in figure 2.

The character feature of the calculated stationary wave functions is the crossing of $\psi(x,y) = 0$ lines, which forms the chessboard-like picture. The counting of these zero lines allows us to find the quantum number values easily. The crossings presence is due to the considered system integrability. Indeed, this two-dimensional system has two degrees of freedom and two integrals of motion — transversal energy $E_\perp$ and projection m of orbital momentum to the field symmetry axis. So, the variables separation is possible in the motion equation, which appears integrable in quadratures. The presence of the zero lines (surfaces for dimensions number more than two) crossings (or thin quasicrossings) appears a general property of quantum systems, whose classical counterparts demonstrate the regular dynamic [4]–[7].

4. Wave functions in the chaotic case

The qualitatively different picture is observed for the non-integrable systems, for example, the electron motion in the field of two neighbor atomic strings [110] of Si crystal. This field (the contribution from other atomic string pairs could be neglected) could be written as

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

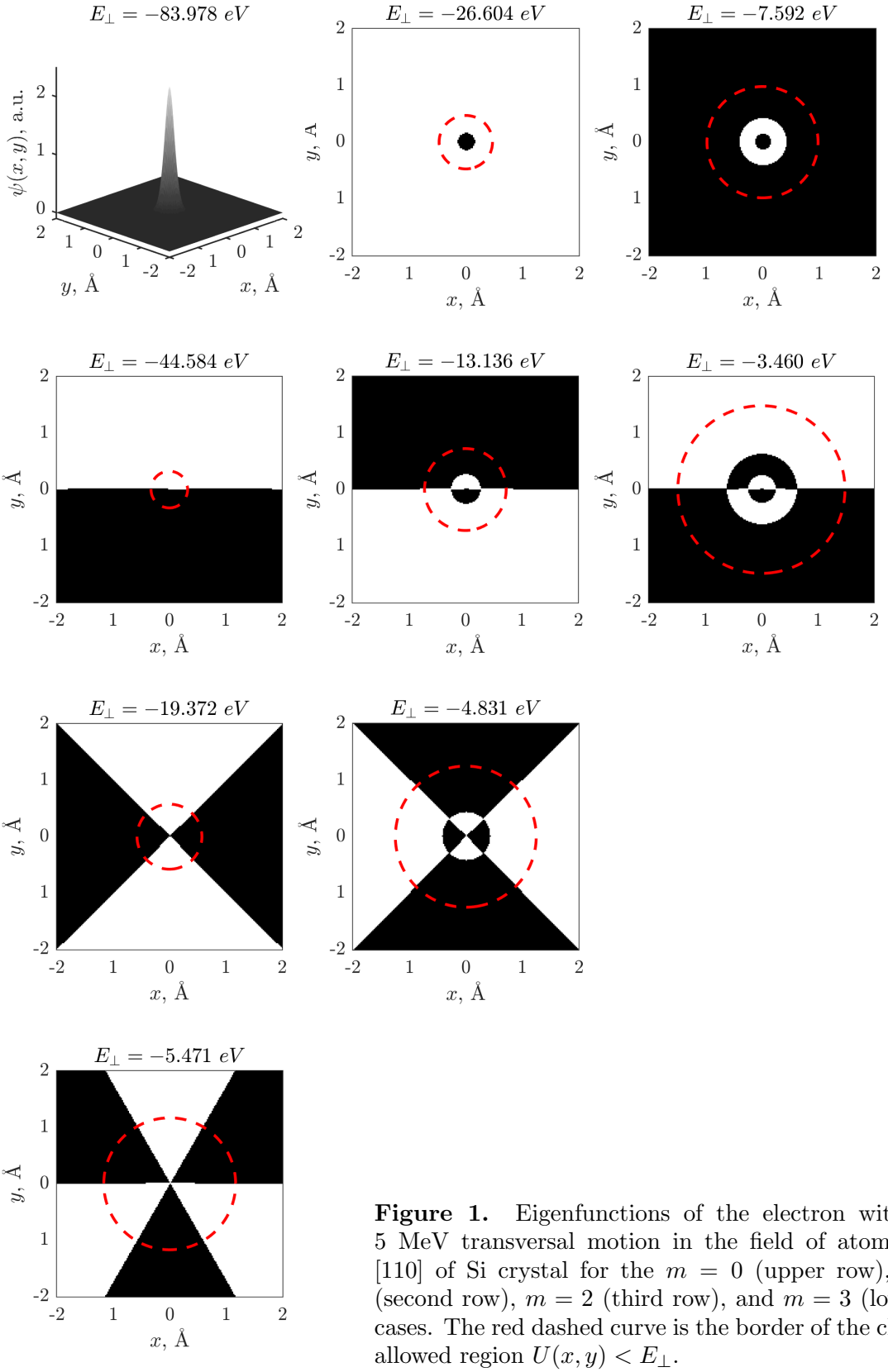

Figure 1. Eigenfunctions of the electron with $E_\parallel = 5$ MeV transversal motion in the field of atomic string [110] of Si crystal for the $m = 0$ (upper row), $m = 1$ (second row), $m = 2$ (third row), and $m = 3$ (lower row) cases. The red dashed curve is the border of the classically allowed region $U(x, y) < E_\perp$.

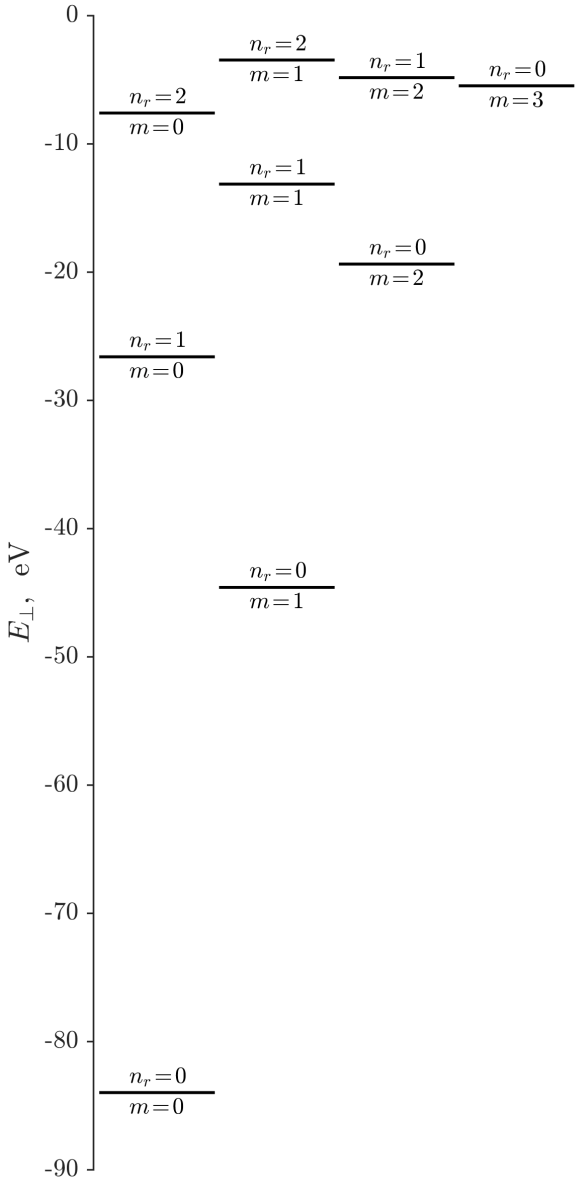

Figure 2. The energy levels classification of the electron with $E_\parallel = 5$ MeV transversal motion in the field of atomic string [110] of Si crystal.

$E_\perp$, eV	n_r	m
−83.978	0	0
−44.5838	0	1
−26.604	1	0
−19.3717	0	2
−13.136	1	1
−7.59175	2	0
−5.4715	0	3
−4.83075	1	2
−3.46025	2	1

where $a = 5.431$ Å is the lattice period. Some calculated eigenfunctions of the electron with longitudinal energy $E_\parallel = 5$ MeV channeling in this field are shown in figure 3, while all the eigenvalues — in table 1. Without the field axial symmetry the single integral of motion (energy $E_\perp$) still exists for two-dimensional system. This leads to dramatical change of the wave functions nature: the zero lines $\psi(x, y) = 0$ have not crossings. However the low energy $E_\parallel = 5$ MeV case not allows us to see this change clearly, so some wave functions of the electron channeling with $E_\parallel = 500$ MeV are presented in figure 4. The latter energy is high enough to ensure big total number of energy levels and small inter-level distances [12]. Namely this situation, similar to one in the classical mechanics with its continuous energy spectra, is needed for the quantum chaos manifestation studies [5, 6, 8]. We can see bizarre picture of black and white "islands" (see figure 4) instead of chessboard-like one for the axially symmetrical field. This behavior is general for the non-integrable systems [4]–[7].

In the classical mechanics the integrability (or not) of the system is closely related with regularity (or chaoticity) of motion of this system [5, 6]. The dynamical chaos in the classical case is the essential sensitivity of the system motion to the initial conditions, which leads to

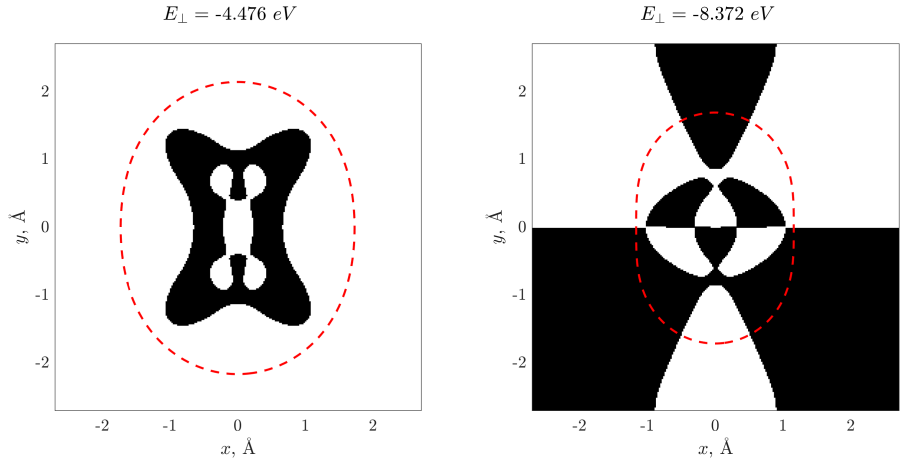

Figure 3. The eigenfunction samples for the electron with longitudinal energy of $E_\parallel = 5$ MeV channeling in the field of two neighbor atomic strings [110] of Si crystal.

Table 1. Full set of eigenenergies $E_\perp$ (eV) of the electron with $E_\parallel = 5$ MeV in the field of two neighbor atomic strings for each of four symmetry classes of the eigenfunction.

$\Psi(-x,y)=\Psi(x,y)$ $\Psi(x,-y)=\Psi(x,y)$	$\Psi(-x,y)=\Psi(x,y)$ $\Psi(x,-y)=-\Psi(x,y)$	$\Psi(-x,y)=-\Psi(x,y)$ $\Psi(x,-y)=\Psi(x,y)$	$\Psi(-x,y)=-\Psi(x,y)$ $\Psi(x,-y)=-\Psi(x,y)$
−49.0303	−48.7077	−48.711	−48.982
−31.6285	−23.7033	−24.3553	−30.8612
−24.894	−16.7748	−17.8317	−23.529
−19.98	−8.5155	−12.2515	−16.036
−12.3253	−6.3875	−9.101	−9.967
−11.214	−4.696	−6.39	−8.37175
−7.95275		−3.583	−6.071
−5.254		−3.22625	−3.36075
−4.4755			
−3.25275			
−2.84325			

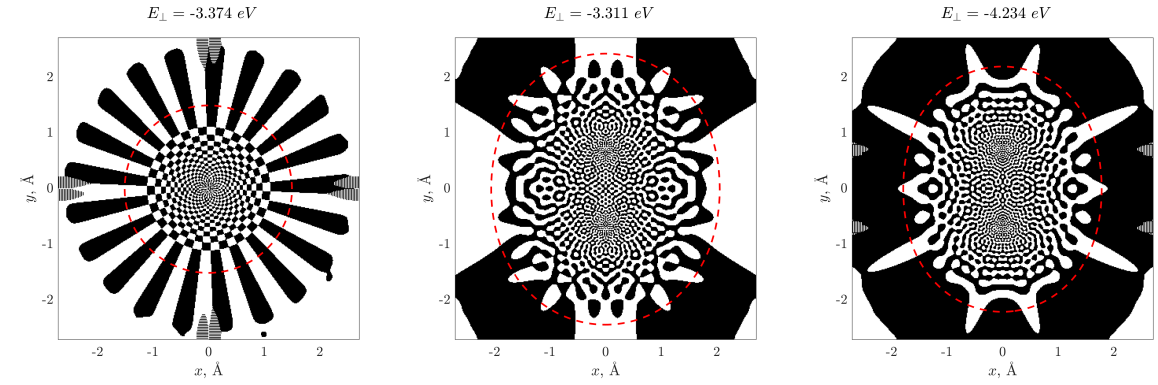

Figure 4. The eigenfunction samples for the electron with longitudinal energy of $E_\parallel = 500$ MeV channeling in the field of one (left plot) and two neighbor (center and right plots) atomic strings [110] of Si crystal.

exponential divergence of the initially close trajectories. The trajectories still deterministic (because the noise or accidental forces are assumed absent in the system) however appear very like to random ones.

Table 2. The spectral method algorithm parameters.

longitudinal energy $E_\parallel$, MeV	space lattice	time step value dt, eV^{-1}	number of time steps N_t	energy step value dE, eV
5	256×256	9.2×10^{-5}	27324375	2.5×10^{-4}
500	384×384	9.2×10^{-5}	136621875	5.0×10^{-5}

In the quantum mechanics case the exponential dependence on the initial conditions is absent. However the behavior of systems, which are regular and chaotic in the classical limit, is qualitatively different by the number of features. The search and investigation of these differences is the quantum chaos topic contents [8]. The observed difference of the wave functions structure, namely, zero lines $\psi(x, y) = 0$ picture of these functions is the one of manifestations of the quantum chaos.

5. Conclusion

The quantum mechanical problem of the fast electron motion in the axially-symmetric field of single atomic string [110] and the field of two neighbor ones of Si crystal is considered. The spectral method suitability for numerical solving, i.e. obtaining the eigenfunctions and energy eigenvalues, of the Schrödinger equation for this system in the axial channeling mode is demonstrated. This approach could be used for investigation of the quantum chaos manifestations in the electron axial channeling through the crystal.

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Appendix

First of all the spectral method algorithm was implemented on the MATLAB for debugging. After the code quality was proven the algorithm was implemented on C language using FFTW (for fast Fourier transforms) and GSL (for complex values calculations) libraries, because the MATLAB FFT performance and memory constraints appear unsatisfactory. The production calculations were performed under UNIX–like operating systems on computers of `amd64` multi-processor architecture. The same algorithm with minor changes allows us to calculate both energy levels and (in the separate run) eigenfunctions of the considered system. The algorithm parameters for present data calculations at $E_\parallel = 5$ and 500 MeV are summarized in table 2. For field of both single and two neighbor atomic strings the full set of eigenenergies and eigenfunctions at $E_\parallel = 5$ MeV was computed.

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