

# SPECTRAL METHOD IN THE QUANTUM THEORY OF AXIAL CHANNELING

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The quantization of the transverse motion energy in the continuous potentials of atomic strings and planes can take place under passage of fast charged particles through crystals. The energy levels for electron moving in axial channeling regime in a system of parallel [110] atomic strings of a silicon crystal are found for the electron energy of order of several hundreds of MeV, when a total number of energy levels becomes large. High resolution of the spectral method permits its usage for investigation of quantum chaos problem.

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## 1. INTRODUCTION

The motion of a fast charged particle in a crystal near one of crystallographic axes or planes is determined mainly by the uniform potential that is the potential of the crystal lattice averaged along the axis or plane near which the motion takes the place. The longitudinal component of the particle's momentum  $p_{\parallel}$  parallel to the crystallographic axis or plane is conserved in such field. So, the problem on the particle's motion in the crystal is reduced to the two-dimensional problem of its motion in the transverse plane. The finite motion in the potential wells formed by the uniform potentials of the atomic axes and planes is known as the axial or planar channeling, respectively (see [1, 2] and references therein). The quantum effects can manifest themselves during such motion. Particularly, the quantization of the transverse motion energy can take the place. The potential wells formed by the uniform string or plane potentials have the complicated shape that does not permit the analytical integration of the Schrödinger equation and makes necessary the development of numerical methods for searching the transverse motion energy levels and other quantum characteristics of the particle's motion in the uniform potentials of the atomic planes and strings of the crystal.

In the present article we apply the so-called spectral method [3] to the search of energy eigenvalues in the two-dimensional case of axial channeling (for [110] strings of the silicon crystal as an example). This method had been successfully used earlier in the one-dimensional problem concerning planar channeling [4].

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## 2. SPECTRAL METHOD

The spectral method of searching the energy eigenvalues of the quantum system [3] is based on the computation of correlation function for the time dependent wave functions of the system at the initial and current time momenta,  $\Psi(x, y, 0)$  and  $\Psi(x, y, t)$ :

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

Fourier transform of this correlation function,

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

contains information about the energy eigenvalues. Indeed, every solution of the time-dependent Schrödinger equation

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

could be expressed as the superposition

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

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

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

where the index  $j$  is used to distinguish the degenerate states corresponding to the energy  $E_n$ . Computation of the correlation function (1) for the wave function of the form (4) gives

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

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

Fourier transformation of (5) leads to the expression

$$P_E = 2\pi\hbar \sum_{n,j} |A_{n,j}|^2 \delta(E - E_n). \quad (6)$$

We see that the Fourier transformation of the correlation function looks like a series of  $\delta$ -form peaks, positions of which indicate the energy eigenvalues.

So, the computation of the energy levels for the given system consists of the following steps:

1. Choosing the arbitrary initial wave function  $\Psi(x, y, 0)$ . The only conditions of the choice are:

— tendency to zero under  $x, y \rightarrow \pm\infty$ , necessary for every bound state;

— wide spectrum that covers the depth of the potential well;

— absence of any symmetry which could lead to the lack of some eigenfunctions in the superposition (4).

Asymmetric Gaussian waveform would be a good choice for the most cases.

2. Numerical integration of the time-dependent Schrödinger equation (3) with the initial value  $\Psi(x, y, 0)$  for the discrete series of the time momenta; the value of the time step  $\Delta t$  as well as other computational details are discussed in [3, 4, 5, 6].

3. Computation of the integral (1) for every discrete time momentum from  $t = 0$  to some maximal  $t = T$ . Subsequent integration of the obtained correlation function  $P(t)$  with the exponent in (2) is carried out over the finite time interval:

$$P_E = \int_0^T P(t) \exp(iEt/\hbar) dt. \quad (7)$$

As a result, we obtain a series of peaks of finite width (inverse proportional to  $T$ ) instead of infinitely narrow  $\delta$ -like peaks (6).

### 3. STATISTICAL PROPERTIES OF THE ENERGY LEVELS

The motion of the fast charged particle in a crystal under small angle  $\psi$  to the crystallographic axis densely packed with atoms could be (with good accuracy) described as a motion in the uniform string potential (e.g. the potential of the atomic string averaged along its axis) [1, 2]. The longitudinal (e.g. parallel to the string axis) component of the particle's momentum  $p_{\parallel}$  is conserved in such a field. The motion in the transverse plane will be described in this

case by the two-dimensional analog of Schrödinger equation [1, Ch. 7, §53]

$$\begin{aligned}
\left\{ -\frac{\hbar^2}{2E_{\parallel}/c^2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U(x, y) \right\} \Psi(x, y, t) = \\
= i\hbar \frac{\partial}{\partial t} \Psi(x, y, t), \quad (8)
\end{aligned}$$

in which the value  $E_{\parallel}/c^2$  plays the role of the particle's mass (where  $E_{\parallel} = \sqrt{m^2 c^4 + p_{\parallel}^2 c^2}$ ).

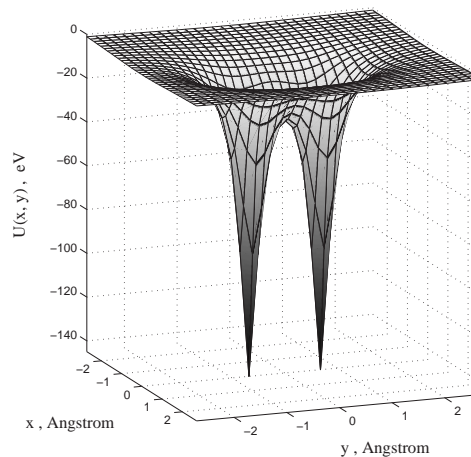
The uniform string potential could be approximated by the formula [1, Ch. 6, §41]

$$U_1(x, y) = -U_0 \ln \left( 1 + \frac{\beta R^2}{x^2 + y^2 + \alpha R^2} \right), \quad (9)$$

where for the [110] string of silicon  $U_0 = 60.0$  eV,  $\alpha = 0.37$ ,  $\beta = 3.5$ ,  $R = 0.194$  Å (Thomas-Fermi radius); the least distance between two parallel strings is  $a/4 = 5.431/4$  Å (where  $a$  is the lattice period). So, the uniform potential, in which the electron's transverse motion takes the place, will be described by the two-well function (Fig. 1)

$$U(x, y) = U_1(x, y + a/8) + U_1(x, y - a/8) \quad (10)$$

(neglecting the influence of far-away strings). The finite motion of the electron in such potential (corresponding to negative values of the transverse motion energy  $E_{\perp}$ ) is known as axial channeling [1].



**Fig.1.** Potential energy (10) of the electron in the field of uniform potentials of two neighboring atomic strings [110] of a silicon crystal

Classical motion of the particle in the axial symmetric potential (9) of the single string is regular because of the presence of two integrals of motion: transverse energy and angular momentum. The classical motion in the potential (10) for the particle with the transverse energy above the potential saddle point is chaotic [1].

The studying of quantum chaos means investigation of the behavior of quantum systems, which classical analogs allow the dynamical chaos [7]. One of the signatures of the quantum chaos phenomenon are

the statistical properties of the large massive of the energy levels of the system in the semiclassical domain, where the levels lie densely to each other.

As it stated in [7], for regular motion the different energy levels do not interact with each other, that leads to the random distribution of the distances  $s$  between neighboring energy levels with the exponential distribution function

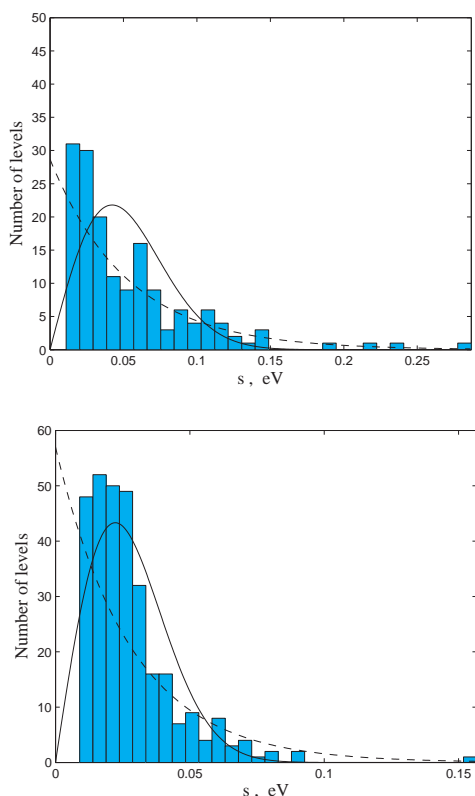
$$p(s) = \frac{1}{D} \exp(-s/D), \quad (11)$$

where  $D$  is the average distance between neighboring energy levels on the spectral interval under consideration. For the chaotic motion the phenomenon of repulsion of levels takes the place, that in typical cases leads to Wigner distribution

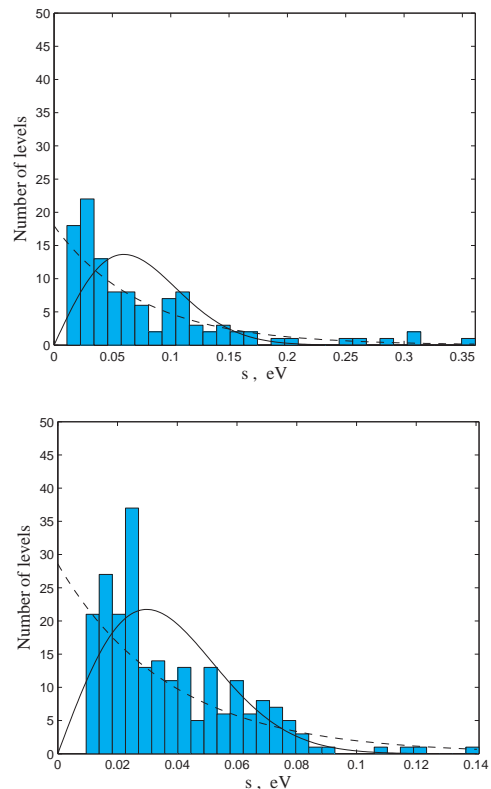
$$p(s) = \frac{\pi s}{2D^2} \exp(-\pi s^2/4D^2). \quad (12)$$

Such behavior has been observed for the particle in billiard with mirror walls and for excited states of some nuclei.

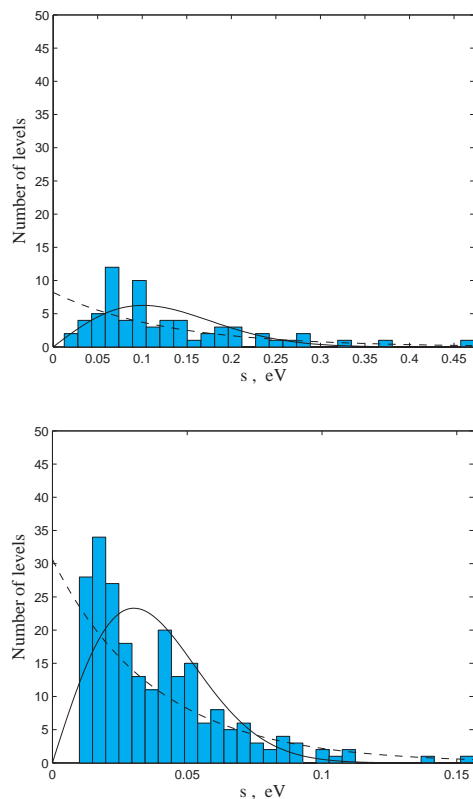
The distributions of inter-level distances for single (9) and double (10) string potentials are presented on Fig.2. We see that the behavior of levels corresponds on a certain extent to the predictions (11) and (12).



**Fig.2.** Distributions of the distances between neighboring levels in the single (upper plot) and double (lower plot) potential wells on the interval  $-11 \leq E_{\perp} \leq 2.5$  eV for the electron's longitudinal energy  $E_{\parallel} = 200$  MeV, in comparison with the exponential (11) (dashed line) and Wigner (12) (solid line) distribution functions. The resolution of levels is not worse than  $s = 0.02$  eV



**Fig.3.** The same as on Fig.2 for even states



**Fig.4.** The same as on Fig.2 for odd states

However, it is emphasized in [7] that only the levels corresponding the eigenstates with the same symmetry could interact with each other. The distribu-

tions of inter-level distances for the states with positive and negative parity are plotted on Figs. 3 and 4. We see that the obtained distributions are rather far from the predictions (11) and (12).

## 6. CONCLUSIONS

The distributions of inter-level distances between levels of the transverse motion energy for the axial channeling electron in the uniform potential of the single [110] atomic string of silicon crystal as well as the potential of two neighboring strings are calculated using the spectral method of the energy levels searching. The results demonstrate that statistical properties of the massive of energy levels in this case do not agree to the predictions of [7] for regular and chaotic motion.

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## References

1. A.I. Akhiezer, N.F. Shul'ga. *High-Energy Electrodynamics in Matter*. Amsterdam, Gordon and Breach, 1996.
2. U.I. Uggerhøj. *Rev. Mod. Phys.* 2005, v.77, p.1131.
3. M.D. Feit, J.A. Fleck, Jr. A. Steiger // *J. Comput. Phys.* 1982, v. 47, p. 412.
4. A.V. Kozlov, N.F. Shul'ga, V.A. Cherkaskiy // *Phys. Lett.* 2010, v. A374, p. 4690.
5. N.F. Shul'ga, V.V. Syshchenko, V.S. Neryabova // *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques.* 2013, v. 7, N2, p. 279.
6. N.F. Shul'ga, V.V. Syshchenko, V.S. Neryabova // *Nucl. Instr. and Meth.* 2013.
7. Yu.L. Bolotin, V.A. Cherkaskiy. Energetic spectra: from heroic past to chaotic present // *Problems of Contemporary Physics: Collected papers / N.F. Shul'ga (Ed.), Kharkov, NSC KIPT, 2008, 416 p. (in Russian).*

## СПЕКТРАЛЬНИЙ МЕТОД В КВАНТОВОЙ ТЕОРИИ АКСИАЛЬНОГО КАНАЛИРОВАНИЯ

*Н. Ф. Шул'га, В. В. Сыщенко, В. С. Нерябова*

При прохождении быстрых заряженных частиц через кристалл может иметь место квантование энергии поперечного движения в непрерывных потенциалах атомных цепочек и плоскостей. Найдены уровни энергии электрона, движущегося в режиме аксиального каналирования в системе параллельных цепочек [110] кристалла кремния, для случая электрона с энергией порядка нескольких сотен МэВ, когда число уровней энергии становится велико. Высокая разрешающая способность метода позволяет использовать его для исследования проблемы квантового хаоса.

## СПЕКТРАЛЬНИЙ МЕТОД В КВАНТОВІЙ ТЕОРІЇ АКСІАЛЬНОГО КАНАЛЮВАННЯ

*М. Ф. Шул'га, В. В. Сищенко, В. С. Нерябова*

При проходженні швидких заряджених часток крізь кристал може бути наявним квантування енергії поперечного руху в неперервних потенціалах атомних ланцюжків та площин. Виявлено рівні енергії електрона, що рухається у режимі аксіального каналювання у системі паралельних ланцюжків [110] кристала кремнію, для випадка електрона з енергією близько кількох сотень МеВ, коли число рівнів енергії стає великим. Висока роздільна здатність методу дозволяє використовувати його для дослідження проблеми квантового хаосу.