

STATISTICAL PROPERTIES OF THE ENERGY LEVELS IN THE AXIAL CHANNELING QUANTUM THEORY

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The energy of transversal motion of relativistic charged particles in the uniform potential of atomic strings of a crystal could be quantized. The energy levels of electrons axially channeled in the system of parallel [110] atomic strings of silicon crystal are obtained. The distribution of distances between neighbor energy levels in the quasi-classical region, where the levels density is high, is agreed with quantum chaos theory predictions.

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1. INTRODUCTION

Axial channeling of fast electrons in crystal is a rather simple example of the situation where the classical dynamics could be both regular and chaotic. Particularly, the motion in the uniform potential of two neighboring [110] atomic strings of the diamond-like crystal (Fig. 1) above the saddle of the potential will be predominantly chaotic [1].

One of the main statements of the quantum chaos theory [2] is that the statistical properties of the energy level arrays for regular and chaotic (in classical limit) systems are dramatically different. Particularly, the eigenenergies of the quantum system, which classical counterpart demonstrates the chaotic behavior, have a tendency to mutual repulsion. This behavior leads to Wigner distribution of the distances s between each two successive eigenenergies:

$$p(s) = \frac{\pi s}{2D^2} \exp\left(-\frac{\pi s^2}{4D^2}\right), \quad (1)$$

where D is the average inter-level distance for considered energy range. For the regular motion this correlation between energy levels is absent that leads to exponential form of nearest-neighbor distribution (NND) of eigenenergies:

$$p(s) = \frac{1}{D} \exp\left(-\frac{s}{D}\right). \quad (2)$$

The goal of the present paper is to test that statement as applied to the problem of axial channeling in the field described below.

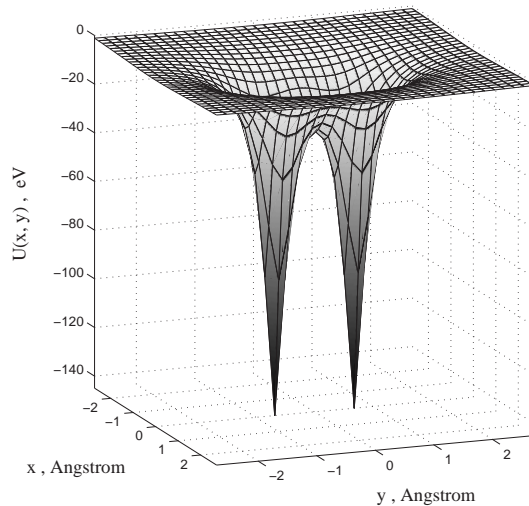


Fig.1. Electron potential energy in the field of uniform potentials of the two neighbor [110] atomic strings of the silicon crystal

2. RESULTS AND DISCUSSION

The uniform string potential could be approximated [1] as follows

$$U_1(x, y) = -U_0 \ln\left(1 + \frac{\beta R^2}{x^2 + y^2 + \alpha R^2}\right), \quad (3)$$

where for the [110] atomic string of silicon $U_0 = 60$ eV, $\alpha = 0.37$, $\beta = 3.5$, $R = 0.194$ Å (Thomas-Fermi radius); the least distance between two parallel strings $a/4 = 5.431/4$ Å (where a is the lattice

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period). So, the uniform potential, in which the electron's transverse motion takes a place, will be described by the two-well function (see Fig. 1)

$$U(x, y) = U_1(x, y + a/8) + U_1(x, y - a/8) \quad (4)$$

(we neglect the far-away strings influence). The electron finite motion in this field is known as axial channeling [1].

Conservation of the electron's momentum component parallel to atomic strings p_{\parallel} leads to reduction of quantum description of the axial channeling to the solution of two-dimensional Schrödinger equation in which the parameter E_{\parallel}/c^2 (where $E_{\parallel} = \sqrt{m^2c^4 + p_{\parallel}^2c^2}$ is the energy of longitudinal motion) plays the role of the particle's mass.

To find the transverse motion energy levels in the potential well (4) we use the spectral method [3]-[5], which has been successfully tested for the channeling problem in [6], [7].

The potential well (4) has two planes of mirror symmetry: $x = 0$ and $y = 0$. Hence, every eigenstate of the electron in the potential (4) belongs to one of four classes of wave function (WF) symmetry:

$$\begin{cases} \Psi_{++}(-x, y) = \Psi_{++}(x, y), \\ \Psi_{++}(x, -y) = \Psi_{++}(x, y), \end{cases} \quad (5)$$

$$\begin{cases} \Psi_{+-}(-x, y) = \Psi_{+-}(x, y), \\ \Psi_{+-}(x, -y) = -\Psi_{+-}(x, y), \end{cases} \quad (6)$$

$$\begin{cases} \Psi_{-+}(-x, y) = -\Psi_{-+}(x, y), \\ \Psi_{-+}(x, -y) = \Psi_{-+}(x, y), \end{cases} \quad (7)$$

$$\begin{cases} \Psi_{--}(-x, y) = -\Psi_{--}(x, y), \\ \Psi_{--}(x, -y) = -\Psi_{--}(x, y). \end{cases} \quad (8)$$

The statistical properties of transverse motion eigenenergies should be investigated separately for each of these four classes [2].

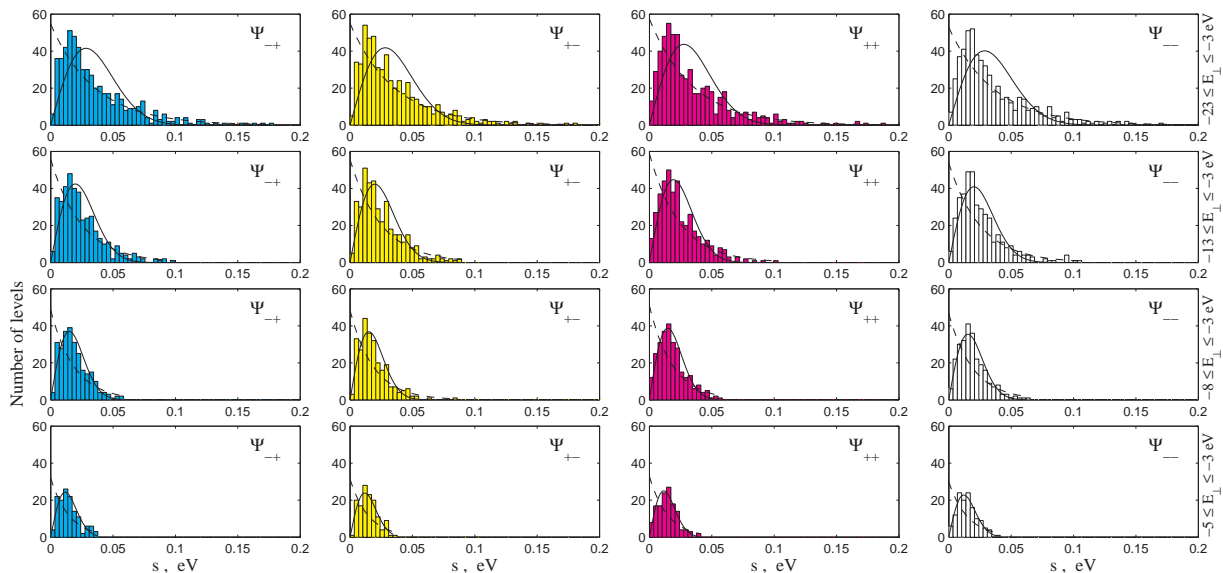


Fig. 2. NND for four different subranges of $-23 \leq E_{\perp} \leq -3$ eV range ($-23..-3$, $-13..-3$, $-8..-3$, and $-5..-3$ eV from upper to lower rows, respectively) and four WF symmetries (Ψ_{+-} , Ψ_{+-} , Ψ_{++} , and Ψ_{--} from left to right columns, respectively). The solid curves are Wigner distributions (1) with D values calculated for the corresponding subrange, the dashed curves are exponential (2) ones

Below we will discuss the properties of energy levels E_{\perp} of transversal electron motion with longitudinal energy $E_{\parallel} = 500$ MeV for $-23 \leq E_{\perp} \leq -3$ eV energy range where the quantum chaos should manifest itself. The corresponding calculation algorithm had been designed in MATLAB [8] environment, however further it had been ported into Unix environment using C language and GSL [9], FFTW [10] libraries. We had been forced to do that because Unix FFTW implementation is up to date, so uses fast instruction sets SSE2 and AVX. This allows us to reach the energy level resolution better than 0.004 eV during yet reasonable calculation time (approximately 65 days per 10 eV range per WF symmetry class using

384×384 coordinate lattice for $E_{\parallel} = 500$ MeV on the single core of Intel Core i7-2600 3.4 GHz processor with AVX).

First of all we plot the NND for the whole calculated range (Fig. 2, upper row).

As we can see, the distribution has maximum as expected according to (1), however its parameters are differ from the theoretically predicted ones. This is because the average inter-level distance D is increased linearly with falling into potential well (Fig. 3). This increase is fast enough to substantially raise the contribution of big s . Consequently the variance of D is too big to assume the inter-level spacing is described correctly by the only one parameter.

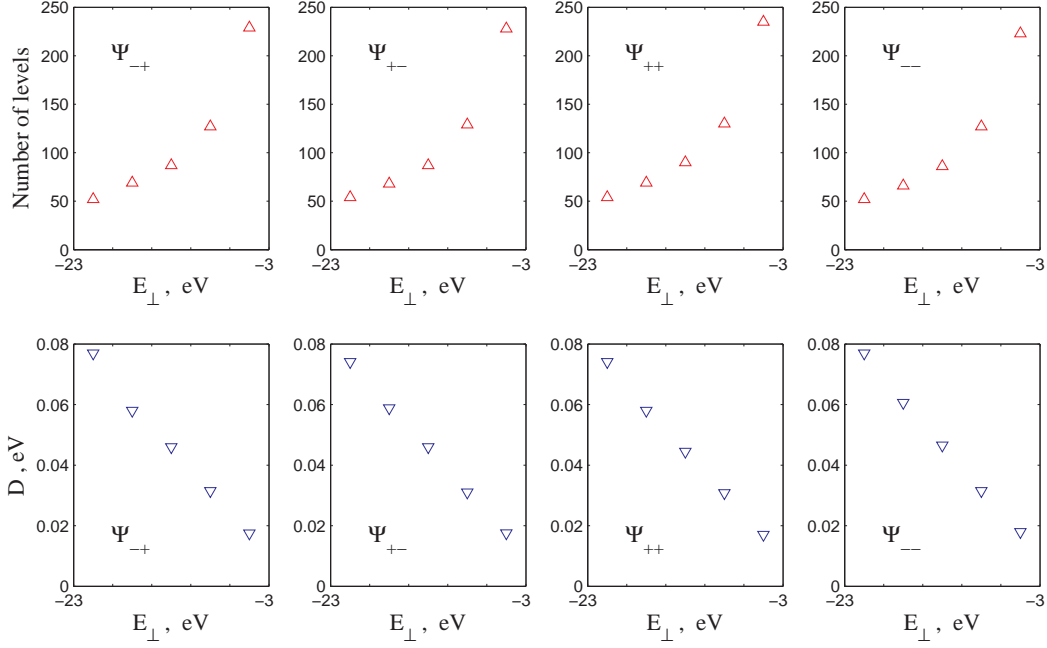


Fig.3. Energy levels number (upper row) and average inter-level distance D (lower row) for four WF symmetries: Ψ_{-+} , Ψ_{+-} , Ψ_{++} , and Ψ_{--} (from left to right columns)

However the agreement of calculated data and Wigner distribution is increased at narrowing the considered energy range (see Fig. 2). For $-5 \leq E_{\perp} \leq -3$ eV energy range the agreement is confirmed by fit of the calculated NND data using the maximum like-

lihood method by the Wigner distribution with D as a free parameter (Fig. 4). The D values derived from the calculated data and obtained as a free parameter of the data fit (as well as χ^2 values for both cases) are summarized in table.

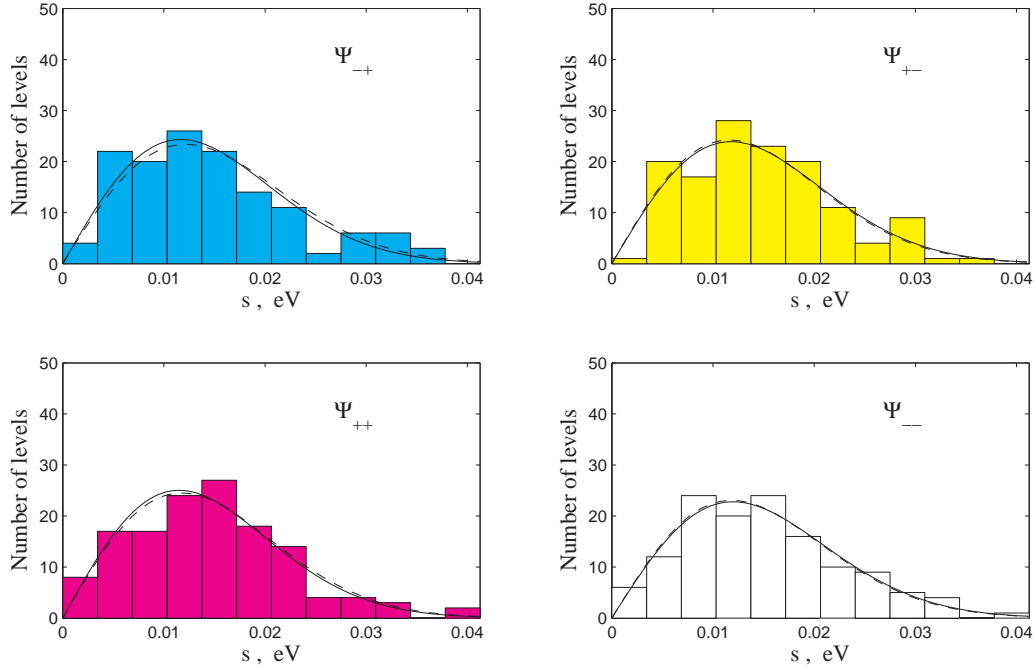


Fig.4. Inter-level distances distribution on the $-5 \leq E_{\perp} \leq -3$ eV range (histograms), Wigner distribution with actual D values (solid curves), Wigner data fit by maximum likelihood method (dashed curves) for four WF symmetries

WF symmetry	χ_t^2	D_t , eV	χ_f^2	D_f , eV
Ψ_{-+}	19.3802	0.0146	17.0507	0.0152
Ψ_{+-}	15.4161	0.0148	15.6688	0.0146
Ψ_{++}	9.6547	0.0144	8.7188	0.0147
Ψ_{--}	4.5651	0.0150	4.7757	0.0149

3. CONCLUSIONS

The quantum mechanical problem of the charged particle interaction with the uniform potential of two neighboring atomic strings in crystal is considered.

The procedure for computing the energy levels of the particle transversal motion using the spectral method is designed. This procedure is used to study the quantum chaos manifestations in the considered system.

The inter-level distances distribution is well described by the Wigner distribution, however only if the variance of mean inter-level distance is small enough on the considered energy range.

ACKNOWLEDGEMENTS

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СТАТИСТИЧЕСКИЕ СВОЙСТВА УРОВНЕЙ ЭНЕРГИИ В КВАНТОВОЙ ТЕОРИИ АКСИАЛЬНОГО КАНАЛИРОВАНИЯ

Н. Ф. Шульга, В. В. Сыщенко, А. Ю. Исупов

При каналировании быстрых заряженных частиц в кристалле может иметь место квантование энергии поперечного движения частицы в непрерывных потенциалах атомных цепочек. В предлагаемой работе найдены уровни энергии электронов, движущихся в режиме аксиального каналирования в системе параллельных атомных цепочек (на примере цепочек [110] кристалла кремния). Показано, что распределение межуровневых расстояний в квазиклассической области, где плотность уровней велика, согласуется с предсказаниями теории квантового хаоса.

СТАТИСТИЧНІ ВЛАСТИВОСТІ РІВНІВ ЕНЕРГІЇ В КВАНТОВІЙ ТЕОРІЇ АКСИАЛЬНОГО КАНАЛЮВАННЯ

М. Ф. Шульга, В. В. Сищенко, О. Ю. Исупов

При каналюванні швидких заряджених частинок у кристалі може бути наявним квантування енергії поперечного руху в неперервних потенціалах атомних ланцюжків. У запропонованій роботі знайдені рівні енергії електронів, які рухаються у режимі аксиального каналювання у системі паралельних атомних ланцюжків (на прикладі ланцюжків [110] кристала кремнія). Показано, що розподіл міжрівневих відстанів у квазикласичній області, де щільність рівнів є великою, узгоджується з передбаченнями теорії квантового хаосу.