ISSN 1027-4510, Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques, 2023, Vol. 17, No. 3, pp. 707–711. © Pleiades Publishing, Ltd., 2023.
Russian Text © The Author(s), 2023, published in Poverkhnost', 2023, No. 6, pp. 88–93.

On the Effect of Quantum Tunneling on the Energy Spectrum of the Transverse Motion of Channeled Positrons in a Silicon Crystal

V. V. Syshchenko[a, *], A. I. Tarnovsky[a], V. I. Dronik[a], and A. Yu. Isupov[b]

[a] *Belgorod State University, Belgorod, 308015 Russia*

[b] *Laboratory of High Energy Physics, Joint Institute for Nuclear Research, Dubna, 141980 Russia*

**e-mail: syshch@yandex.ru*

Received September 22, 2022; revised November 24, 2022; accepted November 24, 2022

Abstract—The movement of charged particles in a crystal can be both regular and chaotic. At the quantum level, chaos manifests itself in the statistical properties of the set of energy levels. Systems, in which regions of regular motion are separated in the phase space by a region of dynamic chaos, are of particular interest. The statistics of the energy levels of such systems substantially depends on the possibility of tunneling between phase-space domains that are dynamically isolated from each other. Consideration of this effect leads to the Podolskiy–Narimanov distribution function. In this study, we estimate the matrix elements of such tunneling transitions in the problem of the transverse motion of positrons with energies of 20 and 40 GeV, which are transmitted in the axial channeling mode in the [100] direction of a silicon crystal. The Podolskiy–Narimanov distribution parameter is found on the basis of this estimate, and it is shown that the former actually describes the statistics of the distances between neighboring energy levels of the transverse motion.

Keywords: regular dynamics, chaotic dynamics, quantum chaos, channeling, semiclassical approximation, level spacing statistics, Berry–Robnik distribution, dynamical tunneling, chaos-assisted tunneling, Podolskiy–Narimanov distribution

DOI: 10.1134/S1027451023030321

INTRODUCTION

The statistical properties of the set of energy levels of a quantum system that is chaotic in the classical limit differ sharply from those for an integrable system with regular dynamics [1–4]. These differences are due to the fact that the energy levels of an integrable system do not interact with each other, while there is interaction between the energy levels of a nonintegrable (chaotic in the classical limit) system, which leads to their mutual repulsion. As a consequence, distances s between adjacent energy levels of the system in the latter case are described by Wigner's distribution function

$$P_W(s) = (\pi s/2)\exp(-\pi s^2/4), \tag{1}$$

where the average interlevel distance in an array is assumed to be normalized to one, while the distribution function in the case of an integrable system has an exponential form that is typical for a Poisson flow of events and expressed as follows:

$$P_P(s) = \exp(-s). \tag{2}$$

The manifestations of dynamic chaos in electron tunneling [5, 6] were studied in [7–11] for the case of channeling near the [110] direction of a silicon crystal. In this case, pairs of neighboring atomic chains create a double-well potential, above the saddle point of which the motion of electrons turns out to be almost completely chaotic. It was found that the statistical properties of the levels in this region are well described by Wigner's distribution (1).

There is a more complicated case when the classical dynamics of a particle turns out to be regular for some initial conditions and chaotic for others for a given energy value, while the regions of regular motion are separated in the phase space by a region of dynamic chaos (for example, such a situation is substantiated when an electron moves near the [100] direction of a silicon crystal [12, 13]). It was assumed in [14] that regular and chaotic domains generate two sequences of levels independent of each other (with the relative level densities ρ_1 and ρ_2, $\rho_1 + \rho_2 = 1$), which leads to the Berry–Robnik distribution expressed as follows:

$$P_{BR}(s) = \exp(-\rho_1 s) \times \left\{\rho_1^2 \operatorname{erfc}\left(\frac{\sqrt{\pi}}{2}\rho_2 s\right) + \left(2\rho_1\rho_2 + \frac{\pi}{2}\rho_2^3 s\right)\exp\left(-\frac{\pi}{4}\rho_2^2 s^2\right)\right\}, \tag{3}$$

where

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \exp(-t^2)dt = 1 - \operatorname{erf}(x). \tag{4}$$

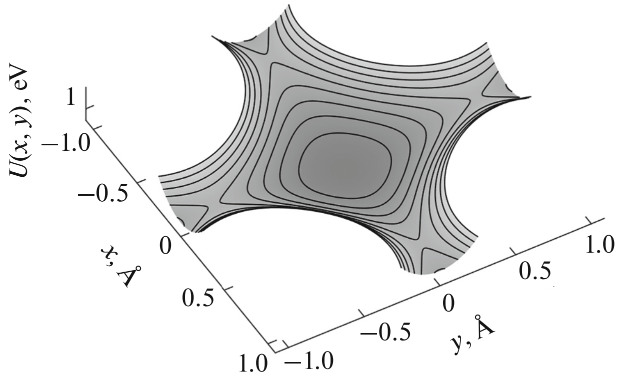

Fig. 1. Potential energy (7) of a positron moving near the [100] direction of a silicon crystal.

However, tunneling between phase-space domains that are dynamically isolated from each other will lead to the interaction of energy levels generated by states localized in such domains. In this case, tunneling between two regular domains can occur in two ways, for example, as described in [15, 16]. Direct tunneling is an unlikely first-order process described by a dimensionless amplitude (the same as s) with a characteristic value of $V_{RR} \ll 1$. Along with this, a second-order process called chaos-assisted tunneling (CAT) is possible, in which the particle first tunnels only beyond the limits of its own regular domain, and this process is described by the V_{RC} constant. A particle picked up by a chaotic flow can find itself near the boundary of another regular domain, in which it tunnels inwards with the amplitude V_{RC}. Thus, this is a second-order process, the resulting amplitude of which is $V_{RC}^2 \sim V_{RR} \ll 1$ [17].

A theory that takes into account the effects of tunneling transitions on the statistics of the levels was proposed in [17]; this leads to the Podolskiy–Narimanov distribution

$$P_{PN}(s) = \exp(-\rho_1 s)\left\{\rho_1^2 \operatorname{erfc}\left(\frac{\sqrt{\pi}}{2}\rho_2 s\right) F\left(\frac{s}{V_{RC}^2}\right) + \left(2\rho_1\rho_2 F\left(\frac{s}{V_{RC}}\right) + \pi s \rho_2^3\right)\exp\left(-\frac{\pi}{4}\rho_2^2 s^2\right)\right\}, \quad (5)$$

where

$$F(x) = 1 - \left(1 - \sqrt{\pi/2}x\right)\Big/\left(\exp(x) - x\right). \quad (6)$$

The technique for estimating the matrix elements of such transitions (from the values of which the V_{RC} parameter is extracted) was described in [18]. In this study, we analyze the statistics of the interlevel distances of the energy of the transverse motion of high-energy positrons (20 and 40 GeV) for the case of channeling in the [100] direction of a silicon crystal. It has been established that the Podolskiy–Narimanov function (5) well describes the distribution of the interlevel distances, and the parameter in this distribution corresponds to the found average value of the matrix elements of tunneling transitions.

CALCULATION TECHNIQUES

The motion of a relativistic particle at a small angle to the crystallographic axis densely packed with atoms in a crystal can be described as two-dimensional motion in a transverse (with respect to this axis) plane under the influence of continuous potentials averaged along atomic chains that are perpendicular to this plane with conservation of the longitudinal component $p_\parallel$ of the particle momentum. In the (100) plane of a silicon crystal, such chains form a square lattice with a period of $a \approx 1.92$ Å. For a positron, the continuous potential of the chain is repulsive, and a small potential well appears near the center of the square, at the vertices of which there are four chains in the positions closest to each other (Fig. 1). In this well, the finite motion of a positron is possible in the transverse plane, which is called axial channeling [5, 6]. Taking into account the contributions of these four chains, the potential energy of the positron is described by the following sum:

$$\begin{aligned} U(x, y) = {} & U_1(x - a/2, y - a/2) \\ & + U_1(x - a/2, y + a/2) \\ & + U_1(x + a/2, y - a/2) \\ & + U_1(x + a/2, y + a/2) - 7.96 \text{ eV}, \end{aligned} \quad (7)$$

where a constant is added to make the potential equal to zero at the center of the cell. The continuous potential of an individual atomic chain is approximated by the folowing formula [5]:

$$U_1(x, y) = U_0 \ln\left(1 + \frac{\beta R^2}{x^2 + y^2 + \alpha R^2}\right), \quad (8)$$

where $U_0 = 66.6$ eV, $\alpha = 0.48$, $\beta = 1.5$, and $R = 0.194$ Å (the Thomas–Fermi radius) for the [100] chain of a silicon crystal. The quantum description of axial channeling is given by the two-dimensional Schrödinger equation, in which the $E_\parallel/c^2$ parameter plays the role of the mass of the particle, and $E_\parallel = (m^2c^4 + p_\parallel^2 c^2)^{1/2}$ is the energy of longitudinal motion [5].

In this study, the channeling of positrons with energies $E_\parallel$ of 20 and 40 GeV is considered. The eigenvalues (energy levels of channeled positrons) and eigenfunctions of the Hamiltonian were numerically found using the so-called spectral method [19], the details of which as regards the channeling problem are described in [7–10].

The technique for estimating the relative contribution of regular dynamics regions ρ_1 to the average semiclassical density of energy levels is described in [12, 13]. A region with

$$1.2 \le E_\perp \le 1.43 \text{ eV}, \quad (9)$$

was selected for analysis, in which the ρ_1 value is approximately constant (Fig. 2), as required for the applicability of distributions (3) and (5). This value is approximately 0.313 for positrons with $E_\parallel = 20$ GeV, and about 0.285 for positrons with an energy of $E_\parallel = 40$ GeV. The weighted average value in this region is

$$\rho_1 = 0.294^{+0.021}_{-0.013}. \quad (10)$$

The uncertainty of the estimate is due to the complexity of taking into account the contribution of small domains of regular dynamics in the phase space of a channeled particle.

Since potential (7) has square symmetry, all available states of transverse motion can be classified according to irreducible representations of the D_4 group (or the isomorphic C_{4v} group, see for example, in [20]) as a function of the symmetry type of the wave function. This group has four one-dimensional irreducible representations, denoted as A_1, A_2, B_1, and B_2, which correspond to nondegenerate energy levels, and one two-dimensional representation E corresponding to doubly degenerate levels. We will analyze further only nondegenerate levels. We emphasize that the interlevel distances should be singled out for the states of each of the four types of symmetry independently [3], normalized to a unit average interlevel distance, and only then the data should be combined for statistical analysis.

We also emphasize that the quantum-chaos theory describes fluctuations in the distribution of levels that change relatively smoothly with a change in the average density of states [2]. To isolate these fluctuations, the initial sequence of energy levels is subjected to the unfolding procedure [2, 4], which results in a new sequence of levels that automatically has a unit-average interlevel distance. It is for such sequences that distributions (1)–(3) and (5) are formulated. However, the average density of states is practically unchanged within small interval (9), which makes it possible to omit the deployment procedure. Instead, we only normalize each of the initial sequences of levels by the average value of the interlevel distance D in it (see Table 1).

The technique used for estimating the amplitudes of tunneling transitions V_{ij} is described in [18]. The found amplitudes also need to be normalized to the average interlevel distance. However, given that tunneling transitions occur between the superpositions of states with a certain type of symmetry (A_1, A_2, B_1, and B_2), as shown in [18], the weighted average from all four D_k values for given $E_\parallel$ should be used for normalization. This value is $D = 0.0099$ for $E_\parallel = 20$ GeV and $D = 0.0050$ for $E_\parallel = 40$ GeV. In accordance with the above,

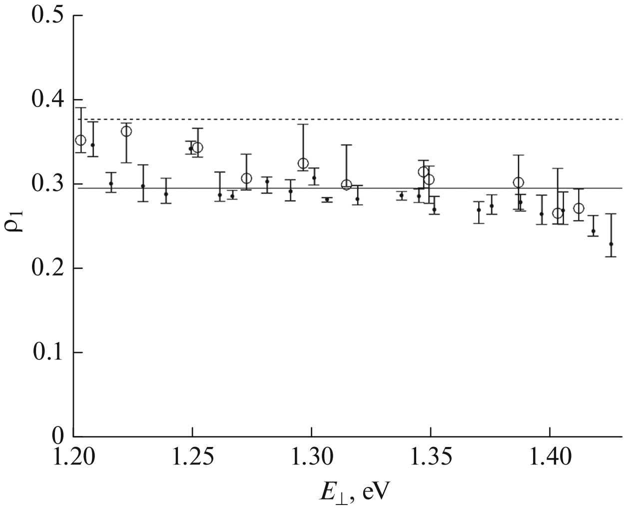

Fig. 2. Relative contribution of regular dynamics domains to the semiclassical density of levels in interval (9) for positrons with energies $E_\parallel$ of 20 (circles) and 40 GeV (dots). The solid horizontal line marks the weighted average value (10) of this quantity, and the dashed line marks value (13), which satisfies the maximum likelihood criterion.

the V_{RC} parameter in the Podolskiy–Narimanov distribution (5) should be set equal to the square root of the average of the absolute value of the found amplitudes, normalized to the unit interlevel distance, as follows:

$$V_{RC} = \sqrt{\langle |V_{ij}|/D \rangle}. \quad (11)$$

For the set of arrays of energy levels of transverse motion in interval (9), this value was

$$V_{RC} = 0.1548. \quad (12)$$

Table 1. Number of states belonging to different types of symmetry and the average distance between energy levels in interval (9)

Symmetry type	N_k	D_k, eV
$E_\parallel = 20$ GeV		
A_1	24	0.009312
A_2	23	0.010102
B_1	22	0.010483
B_2	24	0.0099168
$E_\parallel = 40$ GeV		
A_1	47	0.0048609
A_2	46	0.0050508
B_1	44	0.0052105
B_2	48	0.0048027

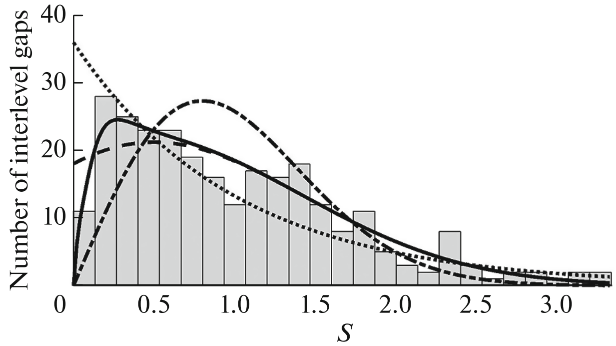

Fig. 3. Distribution of interlevel distances in interval (9) for positrons with energies $E_{||}$ of 20 and 40 GeV (histogram) and theoretical curves corresponding to the Wigner (1) (dash-and-dotted line; $\chi^2 = 242.1434$ and $p = 0$), Poisson (2) (dashed line; $\chi^2 = 47.4105$ and $p = 0.00298$), Berry–Robnik (3) (dashed line; $\chi^2 = 30.171$ and $p = 0.17915$), and Podolskiy–Narimanov (5) (solid line; $\chi^2 = 24.0133$ and $p = 0.46083$) distributions.

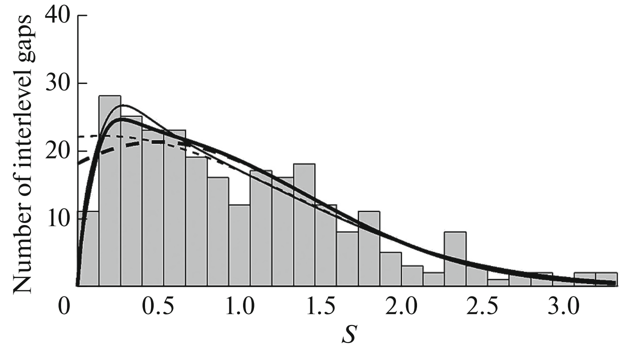

Fig. 4. Berry–Robnik and Podolskiy–Narimanov distributions with parameters (10) and (12), as in Fig. 3 (bold lines), and with parameters (13) and (14) found by the maximum likelihood criterion (thin lines).

RESULTS AND DISCUSSION

The distribution of interlevel distances in energy interval (9) of the transverse motion for positrons with energies $E_{||}$ of 20 and 40 GeV, which are normalized to the unit average in the manner described above, is given as a histogram in Fig. 3. Curves corresponding to predictions (1)–(3) and (5) are superimposed on the histogram, and the value of the relative contribution of regular dynamics domains to the semiclassical local average density (10) of levels is substituted into the Berry–Robnik distribution (3). Into the Podolsky–Narimanov distribution (5), the value of parameter V_{RC} (12) is substituted in addition to this parameter value. For these four distributions, the values of quantity χ^2 and the corresponding p values for 24 degrees of freedom are also determined. One can see that the distribution of interlevel distances agrees well with the prediction of Podolskiy–Narimanov theory [17].

It was also interesting to construct distributions (3) and (5) with free parameters selected according to the maximum likelihood criterion. The corresponding graphs are shown in Fig. 4 by thin lines. For the Berry–Robnik distribution, the result of fitting is as follows:

$$(\rho_1)_{BR}^{fit} = 0.376. \tag{13}$$

In this case, the χ^2 value and the corresponding p values for 23 degrees of freedom (which takes into account the presence of one fitting parameter) are as follows:

$$\chi^2 = 26.1299, \quad p = 0.2948.$$

The fitting results for the Podolskiy–Narimanov distribution are as follows:

$$(\rho_1)_{PN}^{fit} = 0.389, \quad (V_{RC})_{PN}^{fit} = 0.188. \tag{14}$$

The χ^2 value and the corresponding p values for 22 degrees of freedom (taking into account the presence of two fitting parameters) are as follows:

$$\chi^2 = 19.2549, \quad p = 0.6295.$$

The similaratity of the curves corresponding to the actual values of the system parameters and the curves found by the maximum likelihood criterion also indicates good agreement between the distribution of interlevel distances in the considered system and the predictions of quantum-chaos theory.

CONCLUSIONS

The channeling of positrons with energies of 20 and 40 GeV near the [100] direction of a silicon crystal is studied. Numerical methods are used to find all energy levels of the transverse motion of positrons and the wave functions corresponding to them in interval (9) near the upper edge of the potential well. The earlier developed methods [12, 13, 18] are used to find the relative contribution of regions of regular motion to the semiclassical average density of energy levels and the probability of tunneling transitions between such regions. According to the prediction published in [17], the presence of such transitions leads to the mutual repulsion of neighboring energy levels, which modifies the distribution of interlevel distances.

The statistical analysis of the array of interlevel distances, which is performed in this study, shows that the Podolskiy–Narimanov distribution [17] describes the characteristic features of this array much better than the Berry–Robnik distribution [14] as it does not take into account chaos-assisted tunneling. Good agreement of the actual distribution with the predictions of the theory [17] is also evidenced by the closeness of the values of the distribution parameters extracted from analysis of the dynamics of the system under consideration and the values selected by the maximum likelihood criterion.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

REFERENCES

1. M. V. Berry, Proc. R. Soc. A **413**, 183 (1987). https://doi.org/10.1098/rspa.1987.0109
2. O. Bohigas and M.-J. Giannoni, Lect. Notes Phys. **209**, 1 (1984). https://doi.org/10.1007/3-540-13392-5_1
3. H.-J. Stöckmann, *Quantum Chaos* (Cambridge Univ. Press, Cambridge, 2000; Fizmatlit, Moscow, 2004).
4. L. E. Reichl, *The Transition to Chaos: Conservative Classical Systems and Quantum Manifestations*, 2nd ed. (Springer, New York, 2004; RKhD, Moscow, 2008).
5. A. I. Akhiezer and N. F. Shul'ga, *Electrodynamics of High Energies in Matter* (Nauka, Moscow, 1993) [in Russian].
6. A. I. Akhiezer, N. F. Shul'ga, V. I. Truten', A. A. Grinenko, and V. V. Syshchenko, Phys.—Usp. **38**, 1119 (1995). https://doi.org/10.1070/PU1995v038n10ABEH000114
7. Shul'ga, N.F., V. V. Syshchenko, and V. S. Neryabova, J. Surf. Invest.: X-ray, Synchrotron Neutron Tech. **7**, 279 (2013). https://doi.org/10.1134/S1027451013020183
8. N. F. Shul'ga, V. V. Syshchenko, A. I. Tarnovskii, A. Yu. Isupov, J. Surf. Invest.: X-ray, Synchrotron Neutron Tech. **9**, 721 (2015). https://doi.org/10.1134/S1027451015040199
9. N. F. Shul'ga, V. V. Syshchenko, A. I. Tarnovsky, and A. Yu. Isupov, Nucl. Instrum. Methods Phys. Res., Sect. B **370**, 1 (2016). https://doi.org/10.1016/j.nimb.2015.12.040
10. N. F. Shul'ga, V. V. Syshchenko, A. I. Tarnovsky, and A. Yu. Isupov, J. Phys.: Conf. Ser. **732**, 012028 (2016). https://doi.org/10.1088/1742-6596/732/1/012028
11. V. V. Syshchenko and A. I. Tarnovsky, J. Surf. Invest.: X-ray, Synchrotron Neutron Tech. **15**, 728 (2021). https://doi.org/10.1134/S1027451021040200
12. V. V. Syshchenko, A. I. Tarnovsky, A. Yu. Isupov, and I. I. Solovyev, J. Surf. Invest.: X-ray, Synchrotron Neutron Tech. **14**, 306 (2020). https://doi.org/10.1134/S1027451020020354
13. N. F. Shul'ga, V. V. Syshchenko, A. I. Tarnovsky, V. I. Dronik, A. Yu. Isupov, J. Instrum. **14**, C12022 (2019). https://doi.org/10.1088/1748-0221/14/12/C12022
14. M. V. Berry and M. Robnik, J. Phys. A **17**, 2413 (1984). https://doi.org/10.1088/0305-4470/17/12/013
15. H. Tureci, H. Schwefel, A. D. Stone, and E. E. Narimanov, Opt. Express **10**, 752 (2002). https://doi.org/10.1364/OE.10.000752
16. Y. Bolotin, A. Tur, and V. Yanovsky, *Chaos: Concepts, Control and Constructive Use* (Springer, Cham, 2017). https://doi.org/10.1007/978-3-319-42496-5
17. V. A. Podolskiy and E. E. Narimanov, Phys. Lett. A **362**, 412 (2007). https://doi.org/10.1016/j.physleta.2006.10.065
18. V. V. Syshchenko, A. I. Tarnovskii, V. I. Dronik, A. Yu. Isupov, J. Surf. Invest.: X-ray, Synchrotron Neutron Tech. **15**, S73 (2021). https://doi.org/10.1134/S1027451022020203
19. M. D. Feit, J. A. Fleck, Jr., and A. Steiger, J. Comput. Phys. **47**, 412 (1982). https://doi.org/10.1016/0021-9991(82)90091-2
20. L. D. Landau and E. M. Lifshits, *Theoretical Physics*, Vol. 3: *Quantum Mechanics. Nonrelativistic Theory* (Fizmatlit, Moscow, 2016) [in Russian].

Translated by O. Kadkin