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Exact solution of Dirac equation for axially channeled relativistic electrons

K. B. Korotchenko([1])([*]) and Yu. P. Kunashenko([1])([2])

([1]) *Department of Theoretical and Experimental Physics, Tomsk Polytechnic University Lenin Ave. 30, 634050 Tomsk, Russia*
([2]) *Department of Theoretical Physics, Tomsk State Pedagogical University Kiivskaya Str. 60, 634046 Tomsk, Russia*

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Summary. — The exact analytical solution of the Dirac equation for axial channeled electrons, with taking into account the spin direction of the channeled electron is found. It is shown that the longitudinal polarization manifests itself as the splitting of every energy level into two sublevels.

PACS 75.25.-j – Spin arrangements in magnetically ordered materials (including neutron and spin-polarized electron studies, synchrotron-source X-ray scattering, etc.).
PACS 61.85.+p – Channeling phenomena (blocking, energy loss, etc.).
PACS 03.65.-w – Quantum mechanics.

1. – Introduction

When relativistic charged particle enters a crystal at small angle with respect to crystal plane or axis, its interaction with separated crystal atoms can be described by continuous (averaged) potential of the crystal plane or axis [1]. In such situation the relativistic charged particle can be trapped into the channeling state [1-3]. The motion of channeled particle typically can be divided into transverse (perpendicular to the crystal plane or axis) and longitudinal motions (parallel to the crystal plane or axis). Channeled particle has the transverse discrete energy levels. If the particle is a high energy one, its motion should be described by the Dirac equation. Usually the Dirac equation is transformed to approximate Schrödinger-like equation. But within this approximation the information about particle spin is lost. In order to clarify spin problems one should solve the Dirac equation. The spin problem for planar channeled electrons and positrons

([*]) E-mail: korotchenko@tpu.ru

was considered in [4,5], where it was shown that in planar case spin effects in interaction of relativistic charged particles are negligibly small.

In the present report we study the spin effects in the interaction of relativistic channeled electrons with a crystal in axial case. Several theoretical works were dedicated to the solution of the Dirac equation for relativistic channeled electrons (see, *e.g.*, refs. [3,6,7] and references therein), but it seems that the problem has not been investigated in details yet. Here, we obtain the exact solution of the Dirac equation for relativistic electrons with orbital momentum and spin. We consider axial channeling of relativistic electrons, and use an axial model of continuous potential $V(r) = \text{const}/r$, where r is the distance from the electron to the crystal axis. The solution is found with the help of variables separation in cylindrical coordinates.

In order to estimate the role of electron spin, we define the bound energy levels of channeled electron and transition energies between these levels.

2. – Dirac equation for axial channeling

Within the framework of quantum theory the motion of relativistic electron is described by the Dirac equation

$$(\gamma^\mu P_\mu - mc)\Psi = 0, \tag{1}$$

where γ^μ is the Dirac matrix, $P_\mu = \mathrm{i}\hbar\partial_\mu - (e/c)A_\mu$ is the operator of generalized momentum, $A_\mu = (\varphi_o, \vec{A})$ is the 4-vector potential with the scalar potential φ_o and the vector potential $\vec{A}$ of the electromagnetic field, e is the electron charge and m is the electron rest mass.

Due to axial cylindric symmetry of averaged axial potential it is convenient to use cylindrical coordinates. We assume that the crystal axis is directed along the OZ coordinate axis.

When relativistic electron moves in the axial channeling regime, the longitudinal (parallel to the crystal axis) momentum of electron is a constant as well as the total energy. It is mean that electron motion along the crystal axis is free; therefore we can consider its wave function $\Psi(r, \varphi, z, t)$ as a product of transverse wave (which describes electron motion in a plane perpendicular to the crystal axis) and free plane wave propagates along the crystal axis (OZ axis)

$$\Psi(r, \varphi, z, t) = \begin{pmatrix} \chi_1(r, \varphi) \\ \chi_2(r, \varphi) \end{pmatrix} \exp\left[\frac{\mathrm{i}}{\hbar}(pz - Et)\right]. \tag{2}$$

Here $\chi_1(r, \varphi)$ and $\chi_2(r, \varphi)$ are two-component spinors of the transverse wave function. After substitution of wave function (2) into the Dirac equation (1) we derive

$$\begin{aligned} &(E - mc^2 - V(r))\chi_1(r, \varphi) - cp\sigma_3\chi_2(r, \varphi) + \mathrm{i}c\hbar\hat{D}_\perp\chi_2(r, \varphi) = 0, \\ &(E + mc^2 - V(r))\chi_2(r, \varphi) - cp\sigma_3\chi_1(r, \varphi) + \mathrm{i}c\hbar\hat{D}_\perp\chi_1(r, \varphi) = 0. \end{aligned} \tag{3}$$

Here $V(r) = e\varphi_o(r)$ is the potential energy of the electron in the electrostatic field of the axis and also we have used the operator as in [6], $\hat{D}_\perp = \sigma_{1z}\hat{\partial}_r + (1/r)\sigma_{2z}\hat{\partial}_\varphi$.

3. – Solution of spin equation for axial channeling

In order to find the solution of the Dirac equation with a fixed spin, we use spin covariant operator as obtained in [8]. This spin operator commutes with the Dirac equation and therefore has common eigenfunctions. In the absence of magnetic field, the component of the spin perpendicular to the electric field will be the integral of motion. In our case it is a Z-component of the spin $\hat{S}_z = \rho_3\sigma_{3z} - (\mathrm{i}\hbar/mc)\rho_1\partial_z$ [8]. Now the equation describing the electron spin can be written as follows:

$$\hat{S}\Psi(r,\varphi,z,t) = \rho_3\sigma_{3z}\Psi(r,\varphi,z,t) - \frac{\mathrm{i}\hbar}{mc}\rho_1\partial_z\Psi(r,\varphi,z,t) = \lambda_3\Psi(r,\varphi,z,t), \tag{4}$$

where λ_3 are the eigenvalues of the spin operator $\hat{S}_z$, and σ_{1z}, σ_{2z}, σ_{3z} are the Pauli matrixes in cylindrical coordinates, and

$$\rho_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \rho_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5}$$

After substitution of the channeled electron wave function (2) into eq. (4) we find

$$\begin{aligned} p\chi_2(r,\varphi) &= mc[\lambda_3\chi_1(r,\varphi) - \sigma_{3z}\chi_1(r,\varphi)], \\ p\chi_1(r,\varphi) &= mc[\lambda_3\chi_2(r,\varphi) + \sigma_{3z}\chi_2(r,\varphi)]. \end{aligned} \tag{6}$$

Therefore, in order to study the spin problem for the axially channeled electron we have to find a common solution of the system of eqs. (3) and (6). Following [6], we choose the spinor $\chi_1(r,\varphi)$ in the form

$$\chi_1(r,\varphi) = \begin{pmatrix} u_0(r)e^{\mathrm{i}\nu\varphi} \\ u_1(r)e^{\mathrm{i}(\nu+1)\varphi} \end{pmatrix}, \tag{7}$$

here ν is the orbital quantum number. Using (5) it is easily to find from the first equation of system (6) that

$$\chi_2(r,\varphi) = \frac{mc}{p}\begin{pmatrix} (\lambda_3-1)u_0(r)e^{\mathrm{i}\nu\varphi} \\ (\lambda_3+1)u_1(r)e^{\mathrm{i}(\nu+1)\varphi} \end{pmatrix}. \tag{8}$$

Substituting $\chi_2(r,\varphi)$ of the form (8) into the second equation of system (6) and some algebra we find the relation between electron momentum p and eigenvalues λ_3 of the spin operator

$$\lambda_3 = \xi\sqrt{1+\left(\frac{p}{mc}\right)^2} = \xi\gamma, \qquad \xi^2 = 1. \tag{9}$$

Here γ is the relativistic factor of the channeled electron. The value $\xi = +1$ corresponds to the spin vector direction as the longitudinal momentum of the channeled

electron, while $\xi = -1$ corresponds to the spin vector in the opposite direction. As follows from eq. (9) the $\chi_2(r,\varphi)$ has the form

$$\chi_2(r,\varphi) = \begin{pmatrix} \kappa u_0(r) e^{\mathrm{i}\nu\varphi} \\ (1/\kappa) u_1(r) e^{\mathrm{i}(\nu+1)\varphi} \end{pmatrix}, \qquad \kappa = \sqrt{\frac{\lambda_3 - 1}{\lambda_3 + 1}}. \tag{10}$$

4. – Solution of Dirac equation with fixed spin for axial channeling

After substitution of the spinors $\chi_1(r,\varphi)$ and $\chi_2(r,\varphi)$ in the forms (8), (10) into (3) we obtain that now the Dirac equation depends only on one variable r for the arbitrary potential function $V(r)$:

$$\begin{cases} (E - mc^2 - V(r) - cp\kappa)u_0(r) + \mathrm{i}c\hbar\left[u_1(r)(1+\nu)/r + \partial_r u_1(r)\right]/\kappa = 0, \\ (E + mc^2 - V(r) + cp\kappa)u_1(r) + \mathrm{i}c\hbar\kappa\left[-u_0(r)\nu/r + \partial_r u_0(r)\right] = 0, \\ (E + mc^2 - V(r) - cp/\kappa)u_0(r) + \mathrm{i}c\hbar\left[u_1(r)(1+\nu)/r + \partial_r u_1(r)\right]/\kappa = 0, \\ (E - mc^2 - V(r) + cp/\kappa)u_1(r) + \mathrm{i}c\hbar\kappa\left[-u_0(r)\nu/r + \partial_r u_0(r)\right] = 0. \end{cases} \tag{11}$$

A similar result was obtained in [7]. The structure system of eq. (11) is similar to the structure system of the equation for electron motion in a spherically symmetric field [9,10].

For further calculation we use the continuous potential of the separated crystal axis in the form

$$V(r) = -\frac{Ze^2}{r}, \tag{12}$$

here r is the distance from the axis, Z is the atomic number of crystal atoms. Approximation (12) for the crystal axis potential was used for example in [3,6]. This approximation is valid when the average distance from the electron to the crystal axis is greater than the root mean-square displacement of the crystal atoms from equilibrium positions.

Following the well-known method [10], we find the common solution of first and second pairs of eq. (11):

$$\begin{aligned} u_0(r) = -\frac{\mathrm{i}}{\kappa\mu} e^{-\frac{r}{\alpha}} r^{s-1} \Bigg[\left(\frac{\pi+s}{q+s} + C \right) U\left(\pi+s, 2s, \frac{2r}{\alpha}\right) \\ - \frac{2r}{\alpha}\frac{\pi+s}{q+s} U\left(1+\pi+s, 1+2s, \frac{2r}{\alpha}\right) \Bigg], \end{aligned} \tag{13}$$

$$\begin{aligned} u_1(r) = e^{-\frac{r}{\alpha}} r^{s-1} \Bigg[\left(C - \frac{\pi+s}{q+\nu} \right) U\left(\pi+s, 2s, \frac{2r}{\alpha}\right) \\ - \frac{2r}{\alpha}\frac{\pi+s}{q+\nu} U\left(1+\pi+s, 1+2s, \frac{2r}{\alpha}\right) \Bigg]. \end{aligned}$$

Here C is the normalization constant, $U(a,c,r)$ is the confluent hypergeometric function, and

$$q=\frac{\beta}{2}\left(\mu+\frac{1}{\mu}\right)+\frac{1}{2}\,,\qquad \pi=\frac{\beta}{2}\left(\mu-\frac{1}{\mu}\right)-\frac{1}{2} \tag{14}$$

$$s=\frac{1}{2}+\sqrt{\left(\frac{1}{2}+\nu\right)^2-\beta^2},\qquad \beta=\frac{Ze^2}{c\hbar}\,.$$

In order to write the solution of the first and second pairs of eqs. (11) by the same formulas, we introduced different notations for the first and second pairs of eq. (11). For the first pair we introduced

$$\alpha=\frac{c\hbar}{\sqrt{-(E-mc^2-cp\kappa)(E+mc^2+cp\kappa)}}\,,\qquad \mu=\sqrt{1-\frac{E-mc^2-cp\kappa}{E+mc^2+cp\kappa}} \tag{15}$$

and for the second pair

$$\alpha=\frac{c\hbar}{\sqrt{-(E+mc^2-cp\kappa)(E-mc^2+cp\kappa)}},\qquad \mu=\sqrt{1-\frac{E+mc^2-cp/\kappa}{E-mc^2+cp/\kappa}}. \tag{16}$$

The solution, which satisfied the condition at infinity, is obtained only for negative integer (or zero) values $\pi+s=-n$ in a first confluent hypergeometric function, when this function reduces to a polynomial one. Otherwise it diverges at infinity. This condition results in formulae for electron energy levels with fixed spin orientation (left for the first pair, right for the second pair):

$$E_{n\kappa 1}=E_{nD}\left(1+\frac{p\kappa}{mc}\right),\qquad E_{n\kappa 2}=-E_{nD}\left(1-\frac{p}{mc\kappa}\right),\quad D=(+,-). \tag{17}$$

Here,

$$E_{n+}=mc^2/\sqrt{1+(\beta/n_s)^2},\qquad E_{n-}=mc^2/\sqrt{1-(\beta/n_s)^2}, \tag{18}$$

where $n_s=n+s-1/2$. It should be mentioned that formula (18) for energy E_{n+} is similar to the well-known formula for the electron energy in a Coulomb field [9] and formulae (18) for energies E_{n+} and E_{n-} differ from each other only in the 4th order by β:

$$E_{n+}=E_{n-}=mc^2(1-(\beta/n_s)^2/2)+O(\beta^4). \tag{19}$$

As noticed in [9], further terms of the expansion have no meaning, since radiative corrections are more than these terms.

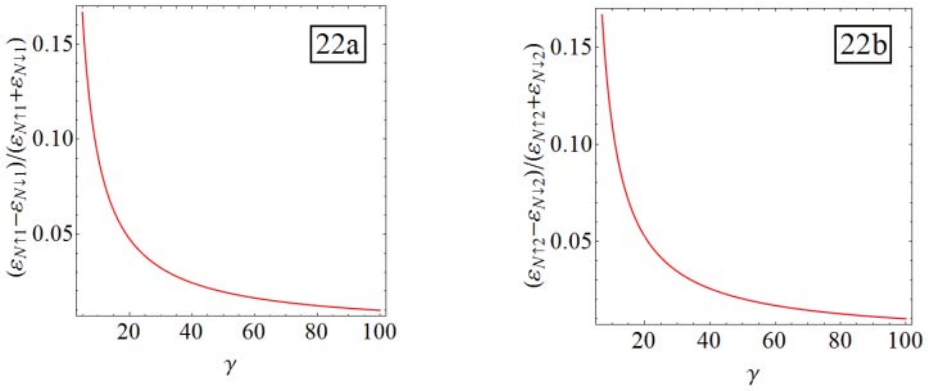

Fig. 1. – Relative difference of transverse energies of the axially channeled electron with the spin directed in the direction of longitudinal electron momentum and with the spin directed in the opposite direction as a function of the relativistic factor of electron γ for Si ($Z = 14$).

5. – Numerical results

Using notations (14)–(16) formulas (17) for an axially channeled electron with fixed spin direction can be rewritten as (left for the first pair of eq. (11), right for the second pair)

$$E_{N\xi 1} = (mc^2 + E_N)(1 - \xi + \gamma), \qquad E_{N\xi 2} = (mc^2 - E_N)(1 + \xi - \gamma), \tag{20}$$

here $E_N\,(\beta \ll 1)$ is the energy of the electron, obtained from the two-dimensional Schrödinger equation with potential (12) [11]:

$$E_N = -\frac{mc^2\beta^2}{2(N - 1/2)^2}\,. \tag{21}$$

Here we follow ref. [10] where $N = 1 + \nu + n$ is denoted as a principal quantum number.

It should be mentioned that expressions (20) for electron energies describe the total relativistic energy of the channeled electron. From a practical point of view it is more convenient to consider transverse energy $\varepsilon_{N\xi 1}\,(\varepsilon_{N\xi 2})$. The transverse energy is obtained by subtraction of the energy of the longitudinal motion $mc^2\gamma$ from the total energy (20), then the result is shifted on the constant $\pm mc^2$:

$$\varepsilon_{N\xi 1} = E_N(1 - \xi + \gamma), \tag{22a}$$

$$\varepsilon_{N\xi 2} = -E_N(1 + \xi - \gamma). \tag{22b}$$

Figure 1 shows the relative difference of the transverse energies $\varepsilon_{N\xi 1}$ (and $\varepsilon_{N\xi 2}$) of the axially channeled electron with the spin directed in the direction of longitudinal electron momentum and with the spin directed in the opposite direction as a function of the relativistic factor of electron γ for Si ($Z = 14$). The result does not depend on the principal quantum number$N$. The calculation was done using both eqs. (22a), (22b); the results are very close.

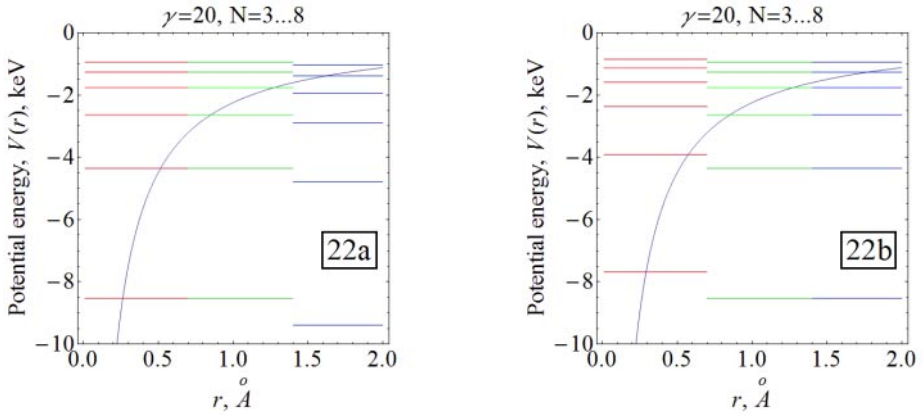

Fig. 2. – Left: the energies of axially channeled electron: $\varepsilon_{N\uparrow 1}$ —left lines, $\varepsilon_{N\downarrow 1}$—right lines, $\varepsilon_{N0} = \varepsilon_N\gamma$—central lines. Right (as on the left, but for the second set of energies): $\varepsilon_{N\uparrow 2}$, $\varepsilon_{N\downarrow 2}$ and $\varepsilon_{N0} = \varepsilon_N\gamma$.

In fig. 2 we show the energies of axially channeled electron with and without taking into account electron spin direction. In both the pictures there are three lines: left lines correspond to electron energies with spin directed in the direction of electron momentum $\varepsilon_{N\uparrow I}\,(I = 1, 2)$, right lines correspond to electron energies with opposite spin direction $\varepsilon_{N\downarrow I}\,(I = 1, 2)$, central lines are the energies of unpolarized electrons calculated by the formulas obtained in [6], $\varepsilon_{N0} = E_N\gamma$.

6. – Conclusion

We have derived the exact analytical solution of the Dirac equation for an axially channeled electron for the model continuous potential $V(r) = \text{const}/r$, with taking into account spin effects. From this solution it follows that the longitudinal polarization manifests itself in the splitting of every energy level into two sublevels that corresponds to two possible spin projections onto the channeled electron longitudinal momentum. In principle, one could observe the splitting of spectral lines in the channeling radiation spectrum (emitted at fixed angle) from axially channeled electrons; the problem lies mainly in the experimental equipment enabling to separate these lines.

A similar result was obtained in [9]. The advantage of this work is that we have obtained the exact analytical solution of the Dirac equation.

There are two different solutions, which give different formulas for electron energies. Both formulas result in approximately the same value of the electron energy splitting due to the spin interaction. Unfortunately, it is not clear which solution should be chosen. The reason of the existence of two formulas for electron energy is connected with the dependence of energy on the electron longitudinal momentum p. In the limit $p = 0$ both formulas are identical.

In the future we plan to calculate the radiation spectrum from axially channeled polarized electrons and to use a more real approximation for crystal axial potential.

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REFERENCES

[1] Lindhard J., *Vidensk. Kgl. Dan. Selsk. Mat.-Fys. Medd*, **34** (1965) 1.
[2] Gemmel D. S., *Rev. Mod. Phys*, **46** (1974) 129.
[3] Bazylev V. A. and Zhevago N. K., *Radiation of Fast Particles in Matter and External Fields* (Nauka, Moscow) 1987 (in Russian).
[4] Babaev A. A., *Proc. SPIE*, **6634** (2007) 66340A.
[5] Babaev A. A., *Poverkhn. Rentgenov., Sinkhrotron. Neitron. Issled.*, **50** (2007) 95.
[6] Olsen H. A. and Kunaschenko Yu., *Phys. Rev. A*, **56** (1997) 527.
[7] Augustin J., Schäfer A. and Greiner W., *Phys. Rev. A*, **51** (1995) 1367.
[8] Sokolov A. A. and Ternov I. M., *The Relativistic Electron* (Nauka, Moscow) 1974 (in Russian).
[9] Beresterskii V. B., Lifshits E. M. and Pitaevskii L. P., *Quantum Electrodynamics Pergamon* (Oxford) 1980.
[10] Flüge S., *Practical Quantum Mechanics II* (Springer-Verlag, Berlin) 1974.
[11] Galickij V. M., Karnakov B. M. and Kogan V. I., *Zadachi po kvantovoj mehanike* (Nauka, Moscow) 1981 (in Russian).