CHANNELING OF RELATIVISTIC ELECTRONS AND POSITRONS

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The quanta-mechanical problem of relativistic electron (positron) movement through the electro-static crystal field for the case of small angle between initial particle momentum and the atomic plane is considered for the case of electron energy larger than several MeV. The analytical expressions for the wave functions for electrons and positrons in the model potentials, which are similar to the state of the "one-dimensional relativistic atom", are presented.

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1. INTRODUCTION

Directional effects of positively charged heavy particles, which are penetrating through the single crystal targets, can be investigated in the frame of the classical theory of Lindhard [1], where the applicability of classical theory is justified. Such a way the finite motion of positively charged heavy particles along the crystal atomic plane (or atomic string) can be described. This directional effect, which is a result of correlated small angular scattering on the multitude of crystal atoms, which belongs to the plane (or string) named "channeling". Plane channeling can be described with good exactness using crystal potential averaged over the atomic plane.

Investigation of the directional effects of electrons (positrons), which are penetrating through the single crystal targets, requires different theoretical descriptions for different particle energies. It is well-known that for electrons with kinetic energy in the range from tens eV up to a few hundreds keV the angular distribution of scattered electrons in the thin mono-crystal targets demonstrate diffraction pattern [2]. For electrons in such energy range a classical approach fails, and the directional effects can be described in the terms of a few beam dynamical diffraction theory. For particle energies from hundreds keV up to the several Mev the wave packet is composed of a large number of partial waves and thus requires a many-beam description. If electrons with energies less than several MeV move along the atomic plane, they can not create the bound states with separate crystal plane. Only if electron energy is larger than several MeV, it can create the bound state with separate crystal plane, which can be considered as *"one dimensional atom"*. Such result for electrons in quantum-mechanical description contrasts with result for heavy particles in classical description, where finite motion is possible for arbitrary small kinetic energies. For electron with energies are larger than several MeV, the wave packet localized well enough, particularly in the transverse plane. With increasing the electron energy the number of partial plane waves increasing drastically, and therefore we need to search another type of basis functions, which are not similar to the plane waves, and which are suitable for presentation of electron bound state by superposition of small number of waves. The convenient basis can be created from solutions of Dirac equation with model continued plane potentials, which have simple analytical form and small difference from the real crystal potential. The task of the present work is to search such solutions. It should be noted that such quantum description becomes inconvenient in the case, when electron creates a large number of bound states with small difference between adjacent energy levels, which are realized at electron energies order of GeV and larger. In this case it's more convenient to apply the quasi-classical and classical descriptions [3].

2. PLANAR CHANNELING

We are interested in the investigation of the relativistic electron motion in the crystal potential in the case, when initial electron momentum $\vec{p}$ creates small angle respectively one of the main crystal planes (for example plane YZ in the Cartesian coordinate system XYZ). We assume that the projection of the electron momentum $\vec{p}$ on the X-axes satisfies the inequality $p_x^2/(2m\gamma) < V'$, where V' is the value of the potential energy of the interaction between relativistic particle and the atomic plane ($V' = |\pm eU_p(x)|$, where $U_p(x)$ is the plane potential). In our task the action of the real plane potential can be replaced by action of the averaged potential over the square of the crystal plane. The plane potential $U_p(x)$ creates the

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potential prison for negative charged particle. The potential of the couple of planes creates the potential prison for positive charged particle. So the electron (positron) motion is characterized by its localization near the potential deep minimum and may be considered as analogy with *"relativistic one-dimensional atom"*, that is moving along the crystal plane in the direction $\vec{n} = \vec{e}_y \sin(\theta) + \vec{e}_z \cos(\theta)$. So we will search solution of the Dirac equation

$$i\hbar \frac{\partial}{\partial t}\psi = \hat{H} \tag{1}$$

with Hamiltonian

$$\hat{H} = c\hat{\vec{\alpha}}\hat{\vec{p}} + \hat{\beta}mc^2 \pm eU_p(x),$$

where one-dimensional potential $U_p(x)$ is the potential of the separated crystal plane (or channel) averaged over the square in the YZ plane. One easily verifies the commutation relations and the corresponding constants of motion

$$\left[\hat{H}, i\hbar\frac{\partial}{\partial t}\right] = 0, \quad \textit{with eigenvalue } E \tag{2}$$

$$\left[\hat{H}, \hat{p}_y\right] = 0, \quad \textit{with eigenvalue } p_y \tag{3}$$

$$\left[\hat{H}, \hat{p}_z\right] = 0, \quad \textit{with eigenvalue } p_z \tag{4}$$

$$\left[\hat{H}, \hat{p}_x\right] \neq 0. \tag{5}$$

Using integrals of motion E, p_y, p_z one can look for solution of Dirac equation in the following form

$$\psi(\vec{r}, t) = \psi(x) e^{i(p_y y + p_z z - Et)/\hbar}. \tag{6}$$

So as the second order differential equations may be solved only for some simple potentials, and taking into account that coordinates of localization centers for particles with different sign do not coincide, we will use different model functions $V(x) = \pm eU_p(x)$ for description the potential energies of electron and positron in the plane potential. Therefore solutions for electron and positron will be considered separately, and Dirac equation in the considered case has the form:

$$\left[\hat{\alpha}_1\nabla_x - \frac{iV}{\hbar c}\right]\psi(x) = \tag{7}$$
$$= \frac{i}{\hbar c}\left[E - mc^2\hat{\beta} - p_2 c\hat{\alpha}_2 - p_3 c\hat{\alpha}_3\right]\psi(x).$$

Let us designate the momentum component, which is parallel to the atomic plane by $\hbar\vec{k}$ and angle between $\vec{k}$ and axis $\vec{z}$ by θ. Then $p_2 = \hbar k \sin\theta$ and $p_3 = \hbar k \cos\theta$. If we multiply equation (7) from the right side by $\hat{\alpha}_1$ and take into account that $\hat{\alpha}_1\hat{\alpha}_2 \equiv i\hat{S}_3$ and $\hat{\alpha}_1\hat{\alpha}_3 \equiv -i\hat{S}_2$, we can represent Dirac equation (7) in the following form:

$$\left[\nabla_x - k(\sin\theta\hat{S}_3 - \cos\theta\hat{S}_2)\right]\psi(x) = \tag{8}$$
$$= \frac{i}{\hbar c}\left[(E + V(x))\,\hat{\alpha}_1 - mc^2\hat{\alpha}_1\hat{\beta}\right]\psi(x).$$

Expression $\sin\theta\hat{S}_3 - \cos\theta\hat{S}_2$ is equal the x projection of the vector product of the spin operator $\hat{\vec{S}}$ on the direction $\vec{n} = \vec{k}/k$ i.e. $[\hat{\vec{S}}, \vec{n}]_x$. The eigenvalues of operator $\sin\theta\hat{S}_3 - \cos\theta\hat{S}_2$ are:

$$\lambda_1 = +1, \quad \lambda_2 = -1, \quad \lambda_3 = +1, \quad \lambda_4 = -1, \tag{9}$$

and corresponding eigenvectors are:

$$\bar{u}_1 = \begin{pmatrix} 1 \\ -i\xi \\ 0 \\ 0 \end{pmatrix}, \qquad \bar{u}_2 = \begin{pmatrix} -i\xi \\ 1 \\ 0 \\ 0 \end{pmatrix},$$

$$\bar{u}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -i\xi \end{pmatrix}, \qquad \bar{u}_4 = \begin{pmatrix} 0 \\ 0 \\ -i\xi \\ 1 \end{pmatrix}, \tag{10}$$

where
$\xi(\theta) = (\cos(\theta/2) - \sin(\theta/2))/(\cos(\theta/2) + \sin(\theta/2))$.

Eigenvectors (10) satisfies the following condition:

$$\bar{u}_i\bar{u}_j^+ = \bar{u}_i^+\bar{u}_j = (1 + \xi^2)\delta_{ij}. \tag{11}$$

It's easy to show, that:

$$\begin{aligned} &\hat{\alpha}_1\bar{u}_1 = \bar{u}_4, && \hat{\alpha}_1\bar{u}_2 = \bar{u}_3, \\ &\hat{\alpha}_1\bar{u}_3 = \bar{u}_2, && \hat{\alpha}_4\bar{u}_1 = \bar{u}_1; \\ &\hat{\alpha}_1\hat{\beta}\bar{u}_1 = \bar{u}_4, && \hat{\alpha}_1\hat{\beta}\bar{u}_2 = \bar{u}_3, \\ &\hat{\alpha}_1\hat{\beta}\bar{u}_3 = -\bar{u}_2, && \hat{\alpha}_1\hat{\beta}\bar{u}_4 = -\bar{u}_1. \end{aligned} \tag{12}$$

If we search solution of the Dirac equation (8) in the form

$$\psi(x) = \sum_{j=1}^{4} \bar{u}_j f_j(x), \tag{13}$$

where $f_j(x)$ are arbitrary functions, and use the conditions (11) and (12), we obtain the following system of equations:

$$\begin{aligned} \nabla_x f_1(x) - k f_1(x) &= \frac{i}{\hbar c}\left[E + mc^2 + V(x)\right] f_4(x), \\ \nabla_x f_2(x) + k f_2(x) &= \frac{i}{\hbar c}\left[E + mc^2 + V(x)\right] f_3(x), \\ \nabla_x f_3(x) - k f_3(x) &= \frac{i}{\hbar c}\left[E - mc^2 + V(x)\right] f_2(x), \\ \nabla_x f_4(x) + k f_4(x) &= \frac{i}{\hbar c}\left[E - mc^2 + V(x)\right] f_1(x). \end{aligned} \tag{14}$$

The system of four equations (14) is shared into two pairs of independent and identical systems of equations. Using the first equation we can write:

$$f_4(x) = -\frac{i\hbar c\,(\nabla_x - k)}{E + mc^2 + V(x)} f_1(x). \tag{15}$$

Substituting this expression into the fourth equation of the system (14) we obtain the second order differential equation:

$$\left[\frac{\hbar^2 c^2}{2E}\nabla_{xx}^2 + \frac{E^2 - \hbar^2 k^2 c^2 - m^2 c^4}{2E} + V(x) + \right. \tag{16}$$
$$\left. + \frac{V^2(x)}{2E} - \frac{\hbar^2 c^2}{2E}\frac{V'(x)_x\,(\nabla_x - k)}{E + mc^2 + V(x)}\right] f_1(x) = 0.$$

The last two terms in (16) are small, and in the first approximation we can neglect them. Then for obtaining basis functions we can use model potential $V(x)$, which has sufficient analytical form and small difference from the real potential. In the first approximation function $f_1(x)$ does not differ from $f_2(x)$, because equation for $f_2(x)$ differs from (16) only by the sign near the k in the small term. General solution of the Dirac equation for electrons can be represented in the form:

$$\psi_{(-e)}(x) = A\left(\bar{u}_1 - i\hbar c\frac{\nabla_x - k}{E + mc^2 + V(x)}\bar{u}_4\right) f_1(x) + B\left(\bar{u}_2 - i\hbar c\frac{\nabla_x + k}{E + mc^2 + V(x)}\bar{u}_3\right) f_2(x), \quad (17)$$

and for positrons in the form:

$$\psi_{(+e)}(x) = C\left(\bar{u}_3 - i\hbar c\frac{\nabla_x - k}{E - mc^2 + V(x)}\bar{u}_2\right) f_3(x) + D\left(\bar{u}_4 - i\hbar c\frac{\nabla_x + k}{E - mc^2 + V(x)}\bar{u}_1\right) f_4(x), \quad (18)$$

where arbitrary constants A, B, C and D become definite after using the boundary conditions.

2.1. ELECTRON WAVE FUNCTIONS

2.1.1. Model potential

The averaged crystal plane potential can be represented (in units $m_e c^2$) in the form of the sum of potentials of the separate planes $U_p(x)$:

$$U(x) = \sum_{n=-\infty}^{+\infty} U_p(x + d\cdot n), \quad (19)$$

$$\begin{aligned} U_p(x) &= 2Z\alpha\frac{\nu d}{v_c}\sum_{i=1}^{3} a_i U_i(x), \qquad where: \\ U_i(x) &= \frac{\pi}{\beta_i}\exp(-\beta_i x)\exp(u^2\beta_i^2)\times \\ &\times \left\{\frac{1}{2}\exp(2\beta_i x) erfc(\frac{x}{2u} + u\beta_i) + 1 - \right. \\ &- \left.\frac{1}{2} erfc(\frac{x}{2u} - u\beta_i)\right\}, \end{aligned} \quad (20)$$

Z is the atomic number, $\alpha = 1/137$, ν is the number of atoms in elementary cell, v_c is the volume of the elementary cell, d is the distance between planes, u^2 is the root mean atomic thermal displacement. Here we used the Moliere-type of atomic potential, where constants a_i and β_i defined as:

$$\begin{aligned} a_i &= \{0.1;\ 0.55;\ 0.35\} \quad (21)\\ b_i &= \{6.0;\ 1.2;\ 0.3\} \\ \beta_i &= \left(Z^{1/3}/121\right) b_i. \end{aligned}$$

At a distance $|x| \geq d$ from the plane the potential $U_i(x)$ has the following form $U_i(x) \approx \frac{\pi}{\beta_i}\exp(-\beta_i|x|)$. We get the sum of potentials of all planes (19) by adding to $U_i(x)$ the sum of asymptotical plane potentials from (20), which is a geometrical progression

$$\frac{\pi}{\beta_i}\sum_{n=1}^{\infty}\{\exp[-\beta_i(dn - x)] + \exp[-\beta_i(dn + x)]\} = \frac{2\pi}{\beta_i}\frac{\exp(-\beta_i d)}{1 - \exp(-\beta_i d)} ch(\beta_i x). \quad (22)$$

In order to investigate equation (16) let's suppose that potential energy of interaction between relativistic electron with plane potential can be presented by model function $V(x) = V_0/\operatorname{ch}^2(x/x_0) + C$, where constants V_0, x_0 and C can be obtained by fitting the model potential to the corresponding exact crystal plane potential [4]. For the case of relativistic electron motion with Lorentz factor $\gamma \sim 10$ near (100)-plane of the Si crystal the orders of these constants are: $|V_0| \sim 10^{-4}mc^2$ and $x_0 \sim 1.3\times 10^2\hbar/mc$ (look at (20)).

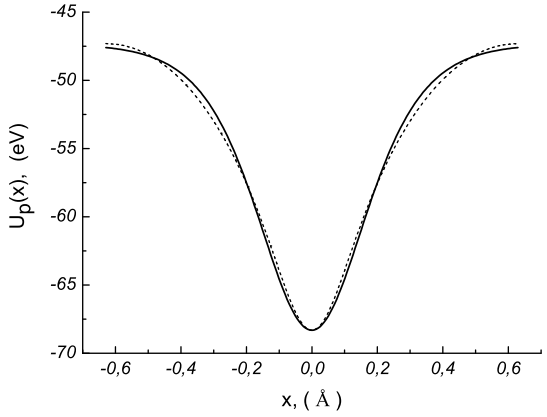

Fig.1. *Potential energy of electron interacting with continuum potential of (110) plane of diamond crystal. Solid line represents the model potential $V(x) = V_0/ch^2(x/x_0) + C$, where: $C = -47.3085\,eV$, $V_0 = -21.0048\,eV$, $x_0 = 0.2215\,Å$. Dashed line represents potential calculated using formulas 19 and 20*

2.1.2. Solution of the Schrödinger wave equation with potential $V(x) = V_0/\operatorname{ch}^2(x/x_0) + C$

Representing $2E = 2mc^2\gamma$, we can see, that equation (16) is a Schrödinger wave equation for the particle with mass $M = m\gamma$. The last two terms in the rectangular brackets of (16) are small corrections to the potential energy $V(x)$. Total expression of the potential energy for our case looks like $V(x)(1 + O(x))$, where $O(x) \sim 10^{-3}$. Let's neglect small terms in Schrödinger wave equation (16), replace $V(x)$ by model potential $V(x) = V_0/\operatorname{ch}^2(x/x_0) + C$ and

$$\left[-\frac{\hbar^2}{2M}\nabla_{xx}^2 + \frac{V_0}{\operatorname{ch}^2(x/x_0)}\right] f_1(x) = E_\perp f_1(x), \quad (23)$$

where $E_\perp = (E^2 - \hbar^2 k^2 c^2 - m^2 c^4 - 2EC)/2E$. As it was first shown in [5] and [6], the Schrödinger equation with such potential (23) can be solved analytically. We will go on to the new variable $y = ch^2(x/x_0)$, and then we obtain equation:

$$y(1-y)f''_{1yy} + \left(\frac{1}{2} - y\right) f'_{1y} - \left(\frac{u}{y} - \kappa^2\right) f_1 = 0, \quad (24)$$

where

$$\begin{aligned} -\kappa^2 &= [E^2 - m^2c^4 - \hbar^2 k^2 c^2] x_0^2/(4\hbar^2 c^2); \\ u &= \frac{1}{2}\left(\frac{V_0}{mc^2}\right)\left(\frac{2\pi x_0}{\lambda_c}\right)^2 \gamma; \end{aligned} \quad (25)$$

Then with the help of substitutions $f = y^\nu \cdot w(y)$, where while ν-is some arbitrary constant, we'll obtain the equation

$$y(1-y)w''_{yy} + \left[(2\nu + \frac{1}{2}) - (2\nu+1)y\right] w'_y + \\ + \left[(\nu^2 - \frac{\nu}{2} - u)y^{-1} - (\nu^2 - \kappa^2)\right] w = 0, \quad (26)$$

which turns to hyper geometric equation of Gauss if a coefficient equates to zero with y^{-1}. Setting this coefficient to be zero, we get the necessary value of ν

$$\nu = \left(1 \pm \sqrt{1 + 16u}\right)/4. \quad (27)$$

For reducing the hyper geometric equation to the standard form, let's introduce some new constants

$$a = \nu - \kappa, \qquad b = \nu + \kappa, \qquad c = 2\nu + \frac{1}{2}, \quad (28)$$

where κ was defined in (25) ($\kappa > 0$). We are interested in solution of the equation (26) in the area of changing the argument $0 \le |x| < \infty$, which corresponds to the sphere of changing the function $1 \le |y| < \infty$. The standard sphere of changing the argument of hyper geometrical function is a half line $-\infty < z \le 0$. So going on to the variable quantity $z = 1 - y$ we'll satisfy this requirement and obtain the following equation:

$$z(1-z)w''_{zz} + [c^* - (a+b+1)z] \cdot w'_z - abw = 0, \quad (29)$$

where $c^* = a + b + 1 - c \equiv 1/2$. Solution of the hypergeometric Gauss equation (29) may be presented by series

$$w(z) = z^\delta \sum_{k=0}^{\infty} C_k z^k,$$

where coefficients C_k satisfy the following request:

$$C_{k+1} = C_k \frac{(a+k+\delta)(b+k+\delta)}{(c^*+k+\delta)(1+k+\delta)},$$

and δ will be determined from the equation

$$\delta(\delta + c^* - 1) = 0.$$

So as c^* is not integer number and therefore the hypergeometric Gauss equation (29) has two linear independent solutions:

$$\begin{aligned} &w_1(z) = F(a,b,c^*;z) = \\ &= 1 + \frac{ab}{c^*}z + \frac{a(a+1)b(b+1)}{c^*(c^*+1)}\frac{z^2}{2!} + \\ &+ \frac{a(a+1)(a+2)b(b+1)(b+2)}{c^*(c^*+1)(c^*+2)}\frac{z^3}{3!} + ..., \end{aligned} \quad (30)$$

and

$$\begin{aligned} &w_2(z) = \\ &= z^{1-c^*}\left(1 + \frac{(a-c^*+1)(b-c^*+1)}{2-c^*}z + ...\right) = \\ &= z^{1-c^*}F(a-c^*+1, b-c^*+1, 2-c^*; z). \end{aligned} \quad (31)$$

So the general solution of hyper geometric equation (29) has the following form:

$$w(z) = A \cdot F(a,b,\frac{1}{2};z) + B \cdot z^{1/2} F(a+\frac{1}{2}, b+\frac{1}{2}, \frac{3}{2}; z), \quad (32)$$

where we denote the hyper geometric Gauss functions by $F(a,b,c;z)$ and the arbitrary constants by A and B. While $A = 1$ and $B = 0$ we'll obtain the standard even solution of the equation (24)

$$f_1^{(+)}(x) = ch^{2\nu}(x/x_0) F(a,b,\frac{1}{2}; -sh^2(x/x_0)). \quad (33)$$

While $A = 0$ and $B = i$ - we'll obtain the odd solution of (24)

$$\begin{aligned} &f_1^{(-)}(x) = ch^{2\nu}(x/x_0) sh(x/x_0) \cdot \\ &F(a+\frac{1}{2}, b+\frac{1}{2}, \frac{3}{2}; -sh^2(x/x_0)). \end{aligned} \quad (34)$$

Wave functions $f_1^+(x)$ and $f_1^-(x)$ should be normalized therefore it is necessary to satisfy the condition $\lim_{|x|\to\infty} f_1^\pm(x/x_0) = 0$. For investigation of solutions of (33) and (34) with large values of the argument let's use asymptotic equations:

$$\begin{aligned} ch(x/x_0) &\approx 2^{-1}\exp(|x/x_0|), \\ sh(x/x_0) &\approx \pm 2^{-1}\exp(|x/x_0|), \\ -sh^2(x/x_0) &\approx -2^{-2}\exp(2|x/x_0|), \end{aligned} \quad (35)$$

and let's use the identity

$$\begin{aligned} &F(a,b,c;z) = \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}(-z)^a \cdot \\ &\cdot F(a, 1-c+a, 1-b+a; \frac{1}{z}) + \\ &+ \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)}(-z)^{-b} \cdot \\ &\cdot F(b, 1-c+b, 1-a+b; \frac{1}{z}). \end{aligned} \quad (36)$$

While argument z is increasing infinitely, the hyper geometric functions in the right part of the equation

(36) run to the unity. Thus while the values of the argument are big, the asymptotic equations take place:

$$f_1^{(+)}(x) \approx 2^{-2\nu} \exp\left(2\nu \left|\frac{x}{x_0}\right|\right) \Gamma\left(\frac{1}{2}\right) \times \left[\frac{\Gamma(b-a)}{\Gamma(b)\Gamma(\frac{1}{2}-a)} 2^{2a} \exp\left(-2a\left|\frac{x}{x_0}\right|\right) + \frac{\Gamma(a-b)}{\Gamma(a)\cdot\Gamma(\frac{1}{2}-b)} 2^{2b} \exp\left(-2b\left|\frac{x}{x_0}\right|\right)\right], \tag{37}$$

and

$$f_1^{(-)}(x) \approx \pm 2^{-(2\nu+1)} \exp\left((2\nu+1)\left|\frac{x}{x_0}\right|\right) \Gamma\left(\frac{3}{2}\right) \times \left[\frac{\Gamma(b-a)}{\Gamma(b+\frac{1}{2})\Gamma(1-a)} 2^{2a+1} \exp\left(-(2a+1)\left|\frac{x}{x_0}\right|\right) + \frac{\Gamma(a-b)}{\Gamma(a+\frac{1}{2})\cdot\Gamma(1-b)} 2^{2b+1} \exp\left(-(2b+1)\left|\frac{x}{x_0}\right|\right)\right].$$

In the last expression sign " + " corresponds to $x > 0$, and " − " corresponds to $x < 0$. The first and the second items in brackets of the expressions (37) and (38) behave themselves as $\exp(\kappa|x|)$ and $\exp(-\kappa|x|)$. Since for the bound states conditions κ is real and is larger than zero therefore in order to obtain normalized solution it is necessary to go to zero the coefficients near $\exp(\kappa|x|)$. This is possible when functions $\Gamma(\zeta)^{-1}$ turn to zero. As a result we obtain arguments ζ are equal integer numbers $-n$, $(n = 0; 1; 2; ...)$. This condition is necessary, but not enough. It should be added by one more. In all cases of physical application of Gauss hyper geometric functions the condition $c - a > 0$ or $c - b > 0$ should be satisfied, therefore in expression (27) before the square root we choose the sign " − ", and it guarantees the values to be $\nu < 0$. Let's demand, that $b = -n$ for the even function $\psi_+(x)$ and $b + 1/2 = -n$, for the odd $\psi_-(x)$ function. Then to determine the energy levels of the bound states we'll obtain the conditions:

$$\kappa = -\nu - n \tag{38}$$

for the even function, and

$$\kappa = -\nu - n - 1/2 \tag{39}$$

for the odd function. Then taking into account (16) and our definition (25), we see that the energy of the crosswise motion $E_\perp$ respectively the crystal plane we can present in the form $E_\perp = \hbar^2 c^2 {k_\perp}^2/2E$. so finally we obtain

$$E_\perp^{(n)} = -\frac{\hbar^2 c^2}{2E}\left(\frac{2\nu+n}{x_0}\right)^2, \tag{40}$$

where even n corresponds to the even function, and the odd n corresponds the odd function. Such dependence is shown on Fig.2. Analogous result was obtained in [7] and [8].

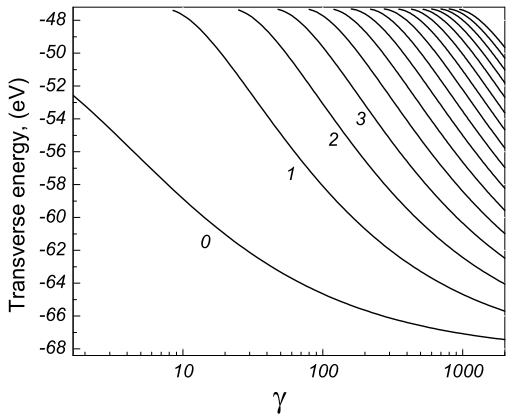

Fig.2. *Transverse electron energy as a function of $\gamma = E/mc^2$ in the plane* (110) *of the diamond crystal for quantum numbers $n = 0, ..., 15$*

While the condition that was discussed above is fulfilled, then the hyper geometric rows in the expressions (37) and (38) are broken on the term with number n and thus they are degenerated into Jacobi polynomials. Therefore the physical solutions of the equation (23) have the following forms:

$$f_1^{(+)}(n,x) = N_n ch^{2\nu}(x/x_0) \times G_n(2\nu + n/2, 1/2; -sh^2(x/x_0)), \tag{41}$$
$$f_1^{(-)}(n,x) = N_n ch^{2\nu}(x/x_0) sh(x/x_0) \times G_n(2\nu + (n-1)/2, 3/2; -sh^2(x/x_0)),$$

where

$$G_n(p,q;z) \equiv 1 + \sum_{k=1}^{n} (-1)^k \begin{pmatrix} n \\ k \end{pmatrix} \times \frac{(p)(p+1)...(p+k-1)}{q(q+1)...(q+k-1)} z^k, \tag{42}$$

and $\begin{pmatrix} n \\ k \end{pmatrix}$ are binomial coefficients.

2.1.3. Normalization

Functions $f_1^{(+)}(n,x)$ and $f_1^{(-)}(m,x)$ for $m \neq n$ are orthogonal, because they are eigenfunctions of Hermitian operator. Besides they must be normalized, i.e. must satisfy the condition $\left\langle f_m^{(\pm)}(x) \mid f_n^{(\pm)}(x) \right\rangle = \delta_{mn}$. Let us designate in (42) c_k - the coefficient with z^k. Then we can write down the condition of normalizing of wave functions $f_\pm(x)$ in the following form:

$$\left\langle f_m^{(\pm)}(x) \mid f_n^{(\pm)}(x) \right\rangle = N_n^2 \sum_{k=0}^{n}\sum_{j=0}^{n} c_k c_j x_0 \times \int_{-\infty}^{+\infty} ch^{4\nu}(x/x_0) sh^{2(k+j)}(x/x_0) dx = 1. \tag{43}$$

Integral in (43) can be transformed to the new variable $t = th(x/x_0)$ and can be represented in the form

of:

$$x_0 \int_0^1 (1-t^2)^p t^q dt = x_0 B(p,q)\,,$$
$$B(p,q) = \Gamma(p)\Gamma(q)/\Gamma(p-q)\,, \qquad (44)$$

where designations $p = k + j + 1/2$ and $q = -(\nu + 2 + k + j)$ are used. Whence we find out that for normalizing of functions which are presented by expression (43) it is necessary to multiply them by the normalizing factor:

$$N_n = \left[x_0 \sum_{k=0}^{n} \sum_{j=0}^{n} c_k c_j B(p,q) \right]^{-1/2}. \qquad (45)$$

Samples of bound state electron wave functions are shown on Fig.3 and in [4].

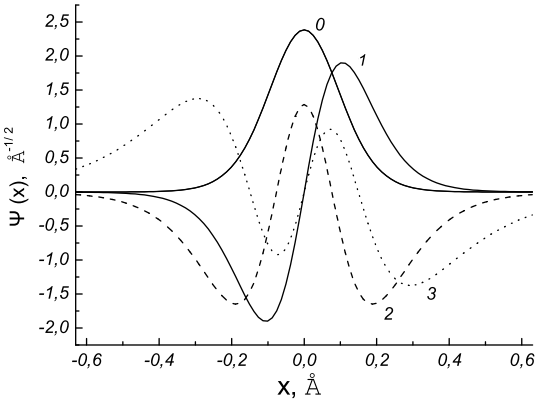

Fig.3. *Bound state wave functions ($n = 0; 1; 2; 3$) for electrons with Lorentz factor $\gamma = 500$, which moving along the plane (110) of the diamond crystal*

2.2. POSITRON WAVE FUNCTIONS

2.2.1. Solution of the Schrödinger wave equation for channeled positrons

Potential energy of positron interaction with planar continuous crystal potential near the center of isolated plane channel has its minimum, and in this region it can be approximated by parabolic function $V(x) = Kx^2/2 + C$, (Fig.4), [9]. We can see that such simple model potential is a good enough approximation for the planar channel potential. In this case from the main equation (16) we obtain one-dimensional equation for function $f_3(x)$, which is well-known equation of harmonic oscillator:

$$\left[-\frac{\hbar^2}{2M} \nabla_{xx}^2 + \frac{Kx^2}{2} \right] f_3(x) = E_\perp f_3(x), \qquad (46)$$

where designation $E_\perp = ((E + C)^2 - \hbar^2 k^2 c^2 - m^2 c^4)/2E$ is used. Introducing new variable $z = \alpha x$ and chose α to be $\alpha = (KM/\hbar^2)^{1/4}$, we obtain equation:

$$\left(\nabla_z^2 + \mu - z^2\right) f(z) = 0, \qquad (47)$$

where $\mu = 2E_\perp/\hbar\omega_c$ and $\omega_c = (K/M)^{1/2}$ is a classical oscillator frequency. Such representation is convenient because it operates by dimensionless values.

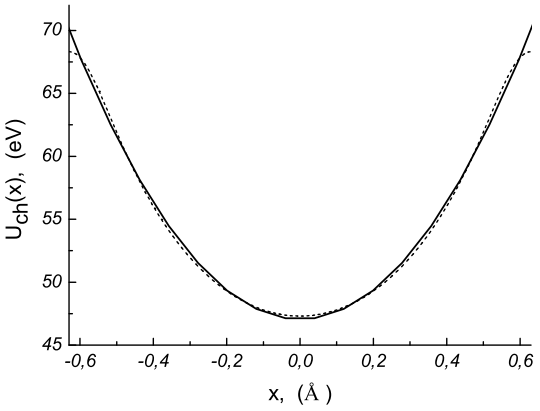

Fig.4. *Potential energy of positron interacting with continuum potential of (110) plane of diamond crystal. Solid line represents the model potential $V(x) = C + (x/x_0)^2$, where: $C = 47.04 \pm 0.04\,eV$, $x_0 = 570.2215\,Å$. Dashed line represents potential calculated using formulas 19 and 20*

Asymptotic solution of the equation (47) for $z \to \infty$ must satisfy the equation $(\nabla_z^2 - z^2) f(z) = 0$. General solution of this equation is $C_1 e^{-z^2/2} + C_2 e^{z^2/2}$. Normalized solution must satisfy the asymptotic condition $\lim_{z\to\infty} f(z) = 0$ i.e. we must put $C_2 = 0$. So we must look for the solution of (47) in the form $f(z) = e^{-z^2/2} H(z)$. Then we obtain equation for function $H(z)$

$$H''(z) - 2zH'(z) + (\mu - 1)H(z) = 0, \qquad (48)$$

that is the Hermite's equation. Let us look for the solution of (48) in the form of series $H(z) = z^s \sum_{k=0}^{\infty} a_k z^k$. Substituting such series into equation (48) one can obtain the requirements

$$(s+k+2)(s+k+1)a_{k+2} - (2s+2k+1-\mu)a_k = 0. \qquad (49)$$

From the first equation for index $k = 0$ $s(s-1)a_0 = 0$. If $a_0 \neq 0$, then $s = 0$ or $s = 1$. The second equation $(s+1)sa_1 = 0$ also satisfies by $s = 0$. Then it may be $a_0 \neq 0$ or $a_0 = 0$. But if $s = 1$ then must be $a_1 = 0$. General solution of (48) looks like

$$H(z) = e^{-z^2/2} \times$$
$$\left\{ a_0 \left[1 + \sum_{p=1}^{\infty} (-1)^p \frac{(\mu-1)...(\mu-4p+3)}{(2p)!} z^{2p} \right] + \right.$$
$$\left. a_1 z \left[1 + \sum_{p=1}^{\infty} (-1)^p \frac{(\mu-3)...(\mu-4p+1)}{(2p+1)!} z^{2p} \right] \right\}, \qquad (50)$$

where a_0 and a_1 are arbitrary constants. The first term is a sum of even powers of z and the second term is a sum of odd powers of z. In order to obtain the normalized solutions we must choose $\mu = 4p + 1$ and

$a_1 = 0$, or $\mu = 4p + 3$ and $a_0 = 0$. Under this requirement our series degenerate into the finite sums. In the first case we obtain the even solution and in the second case the odd one. Let us introduce new principle integer number $n = 2p$ if n even and $n = 2p + 1$ if n odd. Then we can join both solutions into the general expression. Each principle quantum number n corresponds to the positron transverse energy $E_\perp^{(n)}$

$$E_\perp^{(n)} = C + \hbar\omega_c \gamma^{-1/2}(n + 1/2). \qquad (51)$$

Such dependence is shown on the Fig.5.

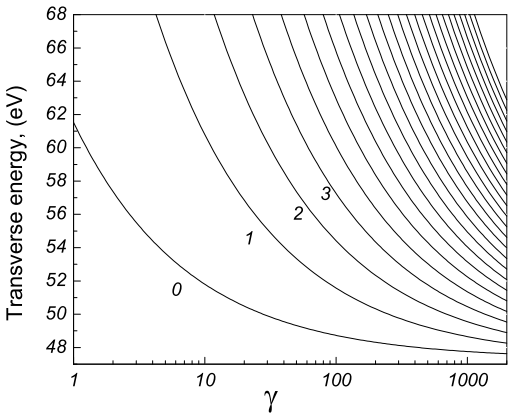

Fig.5. *Transverse positron energy as a function of $\gamma = E/mc^2$ in the plane (110) of the diamond crystal for quantum numbers $n = 0, ..., 25$*

Corresponding wave functions are represented by formula:

$$f_n^{(\pm)}(x) = N_n e^{-\alpha^2 x^2/2} H_n(\alpha x), \qquad (52)$$

where $H_n(\alpha x)$ are the Hermite's polynomials, N_n are normalization factors.

2.2.2. Normalization

Functions $f_1^{(+)}(n, x)$ and $f_1^{(-)}(m, x)$ for $m \neq n$ are orthogonal, because they are eigenfunctions of Hermitian operator. Besides they must be normalized, i.e. must satisfy the condition $\left\langle f_m^{(\pm)}(\alpha x) \mid f_n^{(\pm)}(\alpha x) \right\rangle = \delta_{mn}$. Such property of wave functions (52) can be proved by using Hermitian producing function[1]. We can write:

$$\int_{-\infty}^{\infty} e^{-t^2+2tx} e^{-s^2+2sx} e^{-x^2} dx = \sum_{n,m=0}^{\infty} \frac{t^n s^m}{n!m!} \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx. \qquad (54)$$

After integration on the left we obtain the following result:

$$\pi^{1/2} e^{2ts} = \sum_{n=0}^{\infty} \frac{(2ts)^n}{n!}. \qquad (55)$$

[1]Hermitian producing function is:

$$e^{-t^2+2tx} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n. \qquad (53)$$

Equating the coefficients near the equal powers of t and s in the right part of (57) and in the expression (55), we obtain:

$$\int_{-\infty}^{\infty} H_n(\alpha x) H_m(\alpha x) e^{-\alpha^2 x^2} dx = \begin{cases} \pi^{1/2} 2^n n!/\alpha, & n = m, \\ 0, & n \neq m. \end{cases} \qquad (56)$$

So the orthogonality of the wave function is proved, and the normalization factors N_n are:

$$N_n = \left(\frac{\alpha}{2^n n! \sqrt{\pi}} \right)^{1/2}. \qquad (57)$$

Samples of bound state electron wave functions with principle quantum numbers $n = 0, 1, 2, 3, 4$ are shown on Fig.6.

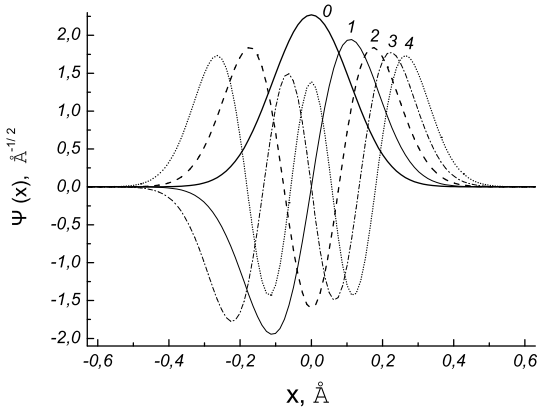

Fig.6. *Bound state wave functions ($n = 0; 1; 2; 3, 4$) for positrons with $\gamma = 500$, which are moving along the plane (110) of the diamond crystal*

2.2.3. Population probabilities

The distribution in the transverse energy varies significantly when the particle progresses through a crystal due to transitions between the transverse states. Here we shall not consider this problem. Now we shall consider only the initial distribution in the positron transverse energy at the crystal entrance. We propose that the particle enters the crystal at the definite angle θ_0 respectively to the plane. The probability $P_n(q)$ of capture to the state $|n\rangle$, where $q = E\theta_0/\hbar c$, can be expressed in the terms of the plane wave expansion in the transverse wave functions:

$$P_n(q) = |A_n(q)|^2, \quad A_n(q) = \int_{-\infty}^{\infty} f_n^{(\pm)}(\alpha x) e^{iqx} dx. \qquad (58)$$

Using the integral representation of the Hermitian functions:

$$H_n(x) = C \int_{-\infty}^{+0} e^{-t^2+2xt} t^{-(n+1)} dt$$

and changing the order of the priority of integration, we obtain:

$$A_n(q) = N_n(-i)^{-n}(2\pi)^{1/2}\alpha^{-1}e^{-(q/\alpha)^2/2}H_n(q/\alpha)\,. \tag{59}$$

3. OUTLOOK

The wave functions, which was obtained above for the model plane potentials, can be combined with orthogonalized plane waves and used as basis functions for representation the wave functions of relativistic particles in the crystal potential. Using these basis functions, we can modify the method of numerical calculations, which was developed by [10] for calculation the wave functions of the crystal electrons, and apply them for obtaining wave functions of the relativistic electrons and positrons in the close to reality crystal potential.

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КАНАЛИРОВАНИЕ РЕЛЯТИВИСТСКИХ ЭЛЕКТРОНОВ И ПОЗИТРОНОВ

В.Л. Мороховский

Рассмотрена квантово-механическая задача движения релятивистского электрона (позитрона) в электрическом поле кристалла в случае, когда начальный импульс электрона направлен под малым углом к атомной плоскости кристалла, для энергий электронов больших нескольких МэВ. Приведены аналитические выражения для волновых функций релятивистского электрона (позитрона) в модельном усредненном потенциале непрерывной плоскости, которые описывают связанные состояния релятивистского электрона с атомной плоскостью, подобные состояниям "одномерного релятивистского атома".

КАНАЛЮВАННЯ РЕЛЯТИВІСТСЬКИХ ЕЛЕКТРОНІВ ТА ПОЗИТРОНІВ

В.Л. Мороховський

Розглянуто квантово-механічна проблема руху релятивістського електрона (позитрона) в електричному полі кристалу у випадку, коли початковий імпульс електрона направлений під малим кутом відносно атомної площини кристалу, для енергій електронів більших кількох МеВ. Приведено аналітичні вирази для хвильових функцій релятивістського електрона (позитрона) в модельному усередненому потенціалі суцільної площини, які описують зв'язані стани релятивістського електрона з атомною площиною, які подібні станам "одновимірного релятивістського атома".