Relativistic positrons dynamics in the electrostatic field of perfect periodic positively charged structures

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Abstract. In this paper, the channeling effect is considered, which consists in the ability of charged particles to penetrate relatively large distances into the interior of the crystal, in which particles move in the interplanar space and are affected by an electrostatic field created by ions of the crystal lattice. Interest in this effect arises due to the fact that channeling is accompanied by directed electromagnetic radiation. This was facilitated, on the one hand, by the versatility and complexity of the problem from a theoretical point of view and, on the other hand, by the practical possibility of using such radiation, the parameters of which can vary in a wide range by changing the parameters of the crystal structure in many fields of science and technology. In the work, the electrostatic field inside an arbitrary periodic structure is considered and a mathematical model is constructed that describes the main characteristics of the field in the ellipsoidal approximation: the scalar potential of the electric field and its intensity. The paper also provides all the necessary mathematical relationships.

1. Mathematical modeling of the electrostatic field

We will consider the electrostatic field within a crystalline structure consisting of the same ions that are located in the vertices of a parallelepiped unit cell. We will be interested in the electrostatic field in the interplanar space at large distances from the ions. Therefore, we will use the ellipsoidal approximation for a single ion, taking into consideration only three spatial parameters of an ion $a$, $b$, $c$ along the Cartesian axes $x$, $y$, $z$ and total charge of an ion $Q$.

Thus, we consider the field of a large number of charged ellipsoids constituting the periodic structure. First, we define a set of parameters that determine a rectangular three-dimensional grid. Let the quantity $n = \{n_x, n_y, n_z\}$ set the numbers of the nodal planes of the grid along one of the Cartesian axes. The set of the nodal points, at which the centers of ellipsoids are located, will be formed as the points of intersection of three mutually perpendicular nodal planes. Let $\vec{\rho}_i$ be $i$-th set of the Cartesian coordinates of $i$-th ellipsoid center, $i = 1, n_x n_y n_z$. Herewith, the quantity $T = \{T_x, T_y, T_z\}$ sets three linear periods of the three-dimensional grid. We reduce the constructed rectangular grid to the general
form by means of six values of displacement \( D = \{ D_{x+y}, D_{x+y}, D_{xy}, D_{z+y}, D_{zy}, D_{zx}, D_{zy} \} \), where \( D_{ijk} \) sets the amount of mutual displacement of the nodal planes of the rectangular grid, that are parallel to the coordinate plane \( O_{ij} \), along the axis \( O_{k} \).

We will calculate the electrostatic field potential of the solitary conductive charged ellipsoid \[1\] with the center at the point \( \rho_i \) for the observation point \( r_i \) within the ellipsoidal coordinates system, whose coordinate surfaces are confocal with the ellipsoid:

\[
\frac{x_i^2}{a^2} + \frac{y_i^2}{b^2} + \frac{z_i^2}{c^2} = 1,
\]

and we construct a new Cartesian system as a result of shift of the initial system, i.e. \( \tilde{r}_i = r_i - \rho_i \).

With condition \( a > b > c > 0 \), the ellipsoidal coordinates are given as roots \( u = \xi, \eta, \zeta \) of the cubic equation:

\[
\frac{x_i^2}{a^2 + u} + \frac{y_i^2}{b^2 + u} + \frac{z_i^2}{c^2 + u} = 1,
\]

and belong to the intervals \( \xi \geq -c^2, -c^2 \geq \eta \geq -b^2, -b^2 \geq \zeta \geq -a^2 \). We consider that the condition \( a > b > c > 0 \) does not restrict the generality, because fulfillment of the condition can be achieved by extra transformation of the coordinate systems \( \rho_i \).

Since the electrostatic field potential has the ellipsoidal symmetry, we will be further interested in the root \( \xi \) being the analogue of the radial coordinate in the ellipsoidal system.

We rewrite the equation (1) in the form:

\[
f(u) = u^3 + A_2u^2 + A_1u + A_0,
\]

where:

\[
A_2 = a^2 + b^2 + c^2 - r_i^2, \quad A_1 = a^2b^2 + a^2c^2 + b^2c^2 - x_i^2 \left(b^2 + c^2\right) - y_i^2 \left(a^2 + c^2\right) - z_i^2 \left(a^2 + b^2\right),
\]

\[
A_0 = a^2b^2c^2 - x_i^2b^2c^2 - y_i^2a^2c^2 - z_i^2a^2b^2.
\]

We will calculate the major root \( \xi \geq -c^2 \) of the equation (2) by means of Vieta's trigonometric formula for the cubic equation [2]. The expression for the root will have the form:

\[
\xi = -2\sqrt{S} \cos \left( \phi + \frac{2\pi}{3} \right) - \frac{A_2}{2},
\]

\[
\phi = \frac{1}{3} \arccos \left( \frac{R}{\sqrt{S^3}} \right),
\]

\[
S = \frac{A_2^2 - 3A_1}{9},
\]

\[
R = \frac{2A_1^2 - 9A_1A_2 + 27A_0}{54}.
\]
The electric potential of \( i \)-th ellipsoid is the elliptical integral of the first kind over \( \xi \) being the solution of the Laplace equation in the ellipsoidal coordinates:

\[
\Delta \varphi_i = \frac{4}{(\xi - \eta)(\xi - \zeta)(\eta - \zeta)} \left[ (\eta - \xi) R_y \frac{\partial}{\partial \xi} \left( R_y \frac{\partial \varphi_i}{\partial \xi} \right) + (\xi - \eta) R_y \frac{\partial}{\partial \eta} \left( R_y \frac{\partial \varphi_i}{\partial \eta} \right) + 
\right.
\]

\[
+ (\xi - \zeta) R_y \frac{\partial}{\partial \zeta} \left( R_y \frac{\partial \varphi_i}{\partial \zeta} \right) \right] = 0,
\]

\[
R_y = \sqrt{(u + a^2)(u + b^2)(u + c^2)}.
\]

Since the coordinate surface \( \xi = 0 \) coincides with the surface of the charged ellipsoid, all the surfaces \( \xi = \text{const} \) will be the level surfaces. Therefore, the Laplace equation reduces to the form:

\[
\frac{\partial}{\partial \xi} \left( \sqrt{\xi \xi + a^2}(\xi \xi + b^2)(\xi \xi + c^2) \frac{\partial \varphi_i}{\partial \xi} \right) = 0,
\]

where \( \xi_i \) is the ellipsoidal coordinate of an observation point in the system associated with an \( i \)-th ellipsoid. Therefore:

\[
\varphi_i = \frac{Q_i}{2} \int_{\xi_i}^{\infty} \frac{d\xi}{\sqrt{(\xi + a^2)(\xi + b^2)(\xi + c^2)}}.
\]

The integral (5) is the elliptical integral of the first kind [3]. Let us rewrite it in the canonical form by means of the substitution:

\[
\xi_i = \frac{a^2 - c^2}{\sin^2 \psi_i} - a^2,
\]

\[
\psi_i = \arcsin \left( \frac{a^2 - c^2}{\sqrt{a^2 + \xi_i}} \right),
\]

\[
d\xi = -2\left( a^2 - c^2 \right) \frac{\cos \psi_i}{\sin^3 \psi_i} d\psi_i,
\]

\[
(\xi_i + a^2)(\xi_i + b^2)(\xi_i + c^2) = (a^2 - c^2) \frac{\cos^2 \psi_i}{\sin^2 \psi_i} \left( 1 - \frac{a^2 - b^2}{a^2 - c^2} \sin^2 \psi_i \right).
\]

\[
\varphi_i = \frac{Q_i}{\sqrt{a^2 - c^2}} \int_{0}^{\psi_i} \frac{d\psi}{\sqrt{1 - k^2 \sin^2 \psi}}, \quad k^2 = \frac{a^2 - b^2}{a^2 - c^2} < 1.
\]

We will further calculate the integral (6) by means of Simpson's rule [4] with fourth order of the accuracy and with the calculation error which is inversely proportional to \( N_{\psi_i}^4 \) by nodal points \( \psi_{ia} = m \psi_i / N_{\psi_i} \):

\[
\int_{0}^{\psi_i} g(\psi_i) d\psi_i = \frac{\psi_i}{3N_{\psi_i}} \left[ \sum_{m=0, m \neq 1, 3, \ldots}^{N_{\psi_i} / 2} g(\psi_{im}) + 4g(\psi_{i(m+1)}) + g(\psi_{i(m+2)}) \right].
\]
and the calculation error of the approximation will have the form:

\[
E(g(\psi_1),\psi_2,N) = \frac{\psi_1^2}{2880N^2} \cdot \left. \frac{d^4}{d\psi_1^4} g(\psi_1) \right|_{\Theta=\cos[0.6\psi_1]} \cdot \frac{d\psi_1}{\sqrt{1-k^2\sin^2\psi_1}}.
\]

We will obtain the total electrostatic field potential of the ellipsoids system by means of the superposition principle:

\[
\varphi(\vec{r}) = \sum_i \varphi_i(\vec{r} - \vec{\rho}_i).
\]

2. **Mathematical modeling of the relativistic particles dynamics**

To assess the force of the electrostatic field, we define the expression for the potential gradient, which determines the electric field strength as \( E = -\nabla \varphi \). Let us present the necessary partial derivatives of function (7). Taking into account the integral (5) with (7), we write:

\[
\frac{\partial \varphi}{\partial r_j} = -\frac{Q}{2} \sum_i \frac{\partial \xi_i / \partial r_j}{\sqrt{(\xi + a^2)(\xi + b^2)(\xi + c^2)}},
\]

where \( \xi_i \) are the ellipsoidal coordinates in the systems associated with \( i \)-th ellipsoid, which were found earlier in the form (3), and quantity \( j = x, y, z \) denotes three constituents of the gradient.

We define the expression for the derivative \( \partial \xi_i / \partial r_j \) and obtain the following results:

\[
\frac{\partial \xi_i}{\partial r_j} = \sqrt{S} \left( 2 \sin \left[ \phi + \frac{2\pi}{3} \right] \frac{\partial \phi}{\partial r_j} - \frac{1}{S} \cos \left[ \phi + \frac{2\pi}{3} \right] \frac{\partial S}{\partial r_j} - \frac{1}{3} \frac{\partial A_j}{\partial r_j} \right),
\]

\[
\frac{\partial \phi}{\partial r_j} = \frac{1}{\sqrt{S^3 - R^2}} \left( R \frac{\partial S}{\partial r_j} - \frac{1}{3} \frac{\partial R}{\partial r_j} \right),
\]

\[
\frac{\partial S}{\partial r_j} = \frac{2}{9} A_j \frac{\partial A_j}{\partial r_j} - \frac{1}{3} \frac{\partial A_j}{\partial r_j},
\]

\[
\frac{\partial R}{\partial r_j} = \left( \frac{1}{9} A_j^2 - \frac{1}{6} \right) \frac{\partial A_j}{\partial r_j} + \frac{1}{6} \frac{\partial A_j}{\partial r_j} + \frac{1}{2} \frac{\partial A_j}{\partial r_j},
\]

where the quantity \( \partial A_j / \partial r_j \) can be written in the form of the matrix:

\[
\frac{\partial A_j}{\partial r_j} = -2 \begin{pmatrix}
\frac{x - \rho_x}{b^2 + c^2} & \frac{y - \rho_y}{a^2 + c^2} & \frac{z - \rho_z}{a^2 + b^2} \\
\frac{b^2 c^2 (x - \rho_x)}{a^2} & \frac{a^2 c^2 (y - \rho_y)}{b^2} & \frac{a^2 b^2 (z - \rho_z)}{c^2}
\end{pmatrix} \cdot
\]

herewith, everywhere the quantities \( S, R, \phi, \partial A_j / \partial r_j \) are indexed with \( i \), corresponding to the index of an ellipsoid.

The relativistic dynamics equation with the electrostatic force is the system of three second order ordinary differential equations. The Cauchy problem for the system will have the form:
\[
\frac{d\tilde{v}}{dt} = \tilde{f}(r, \tilde{v}), \quad \frac{d\tilde{r}}{dt} = \tilde{v}, \quad \tilde{v}(t_0) = \tilde{v}_0, \quad \tilde{r}(t_0) = \tilde{r}_0,
\]
\[f = \frac{e}{m} \left( \frac{\partial \varphi}{\partial x} \left( 1 - \frac{v_x^2}{C^2} \right) - \frac{1}{C^2} \left( v_y \frac{\partial \varphi}{\partial y} + v_z \frac{\partial \varphi}{\partial z} \right) \right) \sqrt{1 - \frac{v_x^2 + v_y^2 + v_z^2}{C^2}},
\]
\[f = \frac{e}{m} \left( \frac{\partial \varphi}{\partial y} \left( 1 - \frac{v_y^2}{C^2} \right) - \frac{1}{C^2} \left( v_x \frac{\partial \varphi}{\partial x} + v_z \frac{\partial \varphi}{\partial z} \right) \right) \sqrt{1 - \frac{v_x^2 + v_y^2 + v_z^2}{C^2}},
\]
\[f = \frac{e}{m} \left( \frac{\partial \varphi}{\partial z} \left( 1 - \frac{v_z^2}{C^2} \right) - \frac{1}{C^2} \left( v_x \frac{\partial \varphi}{\partial x} + v_y \frac{\partial \varphi}{\partial y} \right) \right) \sqrt{1 - \frac{v_x^2 + v_y^2 + v_z^2}{C^2}}.
\]

We will solve the Cauchy problem (8) by the fourth order Runge-Kutta method for the grid functions \(v_i^n = v_i(t_n), \ r_i^n = r_i(t_n), \ i = x, \ y, \ z, \ n = 0...N_t\). Let \(t_n = n\tau\) be the nodal points of one-dimensional time grid, \(\tau = T/N_t\) be the time step, \(T\) be the final moment of time and \(N_t + 1\) be the number of the nodal points. The difference scheme that approximates the solution of the Cauchy problem (8) will have the form:

\[
\begin{align*}
k_{1,i} &= f_i \left( r_i^n, r_i^n, v_i^n, v_i^n, v_i^n, v_i^n, k_{2,i} \right), \quad k_{1,i} = v_i^n, \\
k_{2,i} &= f_i \left( \left\{ r_i^n + \frac{\tau}{2} k_{1,i} \right\}, \left\{ v_i^n + \frac{\tau}{2} k_{1,i} \right\}, \right), \quad k_{2,i} = v_i^n + \frac{\tau}{2} k_{1,i}, \\
k_{3,i} &= f_i \left( \left\{ r_i^n + \frac{\tau}{2} k_{2,i} \right\}, \left\{ v_i^n + \frac{\tau}{2} k_{2,i} \right\}, \right), \quad k_{3,i} = v_i^n + \frac{\tau}{2} k_{2,i}, \\
k_{4,i} &= f_i \left( \left\{ r_i^n + \tau k_{3,i} \right\}, \left\{ v_i^n + \tau k_{3,i} \right\}, \right), \quad k_{4,i} = v_i^n + \tau k_{3,i}, \\
v_i^{n+1} &= v_i^n + \frac{\tau}{6} \left( k_{1,i} + 2k_{2,i} + 2k_{3,i} + k_{4,i} \right), \quad r_i^{n+1} = r_i^n + \frac{\tau}{6} \left( k_{1,i} + 2k_{2,i} + 2k_{3,i} + k_{4,i} \right).
\end{align*}
\]

### 3. Conclusion

As a result, a mathematical model of the electrostatic field of arbitrary three-dimensional periodic structure is obtained. The model approximates the field in the region of space which is the most important for the channelling problem, i.e. in the interplanar space at large distances from the ions of the structure under consideration. The model considers the ellipsoidal symmetry of the field of a single element of the structure and uses the principle of superposition to calculate the characteristics of the resulting field.

### References

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