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Scattering of ultrarelativistic electrons in ultrathin crystals

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ABSTRACT

Quantum theory is proposed of high energy electrons scattering in ultrathin crystals. This theory is based upon a special representation of the scattering amplitude in the form of an integral over the surface surrounding the crystal, and on the spectral method of determination of the wave function. The comparison is performed of quantum and classical differential scattering cross-sections in the transitional range of crystal thicknesses, from those at which the channeling phenomenon is not developed up to those at which it is established. It is shown that in this thickness range the quantum scattering cross-section, unlike the classical one, contains sharp peaks corresponding to some specific scattering angles, that is connected with the diffraction of the incident plane wave onto the periodically distributed crystal atomic strings. It is shown that the value of the scattering cross-section in the peaks varies periodically with the change of the target thickness. We note that this must lead to a new interference effect in radiation that is connected with the rearrangement of incident wave packet in transitional area of crystal thicknesses.

1. Introduction

At passing of fast charged particles through crystals the phenomenon of channeling is possible, at which the particles move inside the channels formed by crystal atomic strings or atomic planes, being periodically deviated to small angles from the channel direction [1,2]. In ultrathin crystals there is no room for channeling phenomenon to develop (see *Fig. 1*). However, there remains the possibility of appearance of several coherence and interference effects at interaction of particles with crystal atoms (at high energies the attention to this fact was paid in the works [3–5]). Such phenomena take place in several electromagnetic processes at high energies in crystals, such as scattering, radiation and electron–positron pairs creation (see [2,6] and references therein).

The present work is devoted to the development of classical and quantum theories of high energy charged particles scattering in transitional range of crystal thicknesses, from those thicknesses at which the channeling phenomenon is not developed up to those at which this regime of motion is established. Quantum theory is based upon the special representation of the scattering amplitude [7] in the form of an integral over the surface surrounding the region of influence of external crystal field onto the particle (in the considered problem this corresponds to the field of entire crystal), and upon the development of numeric methods of calculating of the wave function inside the crystal, that is realized by using the so-called spectral method of solving wave equations [8–10]. The classical theory is based upon the solution of the particle motion equation by numerical methods [11]. The main attention is paid to the comparative analysis of quantum and classical characteristics of the scattering process at different crystal thicknesses and particle energies.

The kinetic energies of particles in the considered calculation method may vary in a wide range, from several hundreds of keV up to hundreds of GeV. By varying energy inside this range, we can pass from the conditions at which the motion of particles is substantially quantum up to those at which it is quasi-classical and can be described with good precision by means of classical theory.

In the last years new possibilities have opened to carry out experimental research in this field, that is connected with the development of technologies of ultrathin crystals production for the accelerator experiments, and improving of the beam parameters [12,13]. Due to this, one can now speak about discovering quantum and classical effects in scattering discussed in the present paper.

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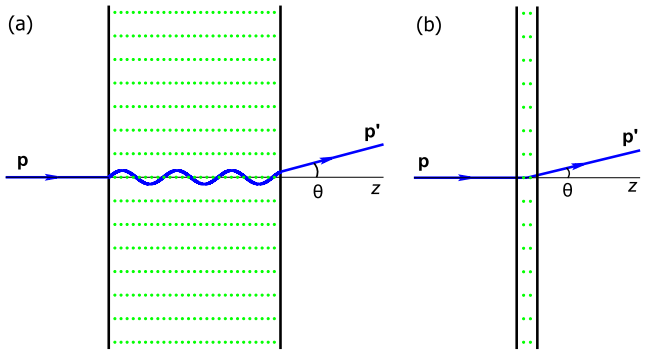

Fig. 1. Scattering in channeling regime (a) and in absence of channeling (b).

2. Quantum theory

Let us consider the scattering of relativistic electrons incident onto a thin crystal along one of its crystal axes. Differential scattering cross-section and scattering amplitude in this case are defined by the following formulas [2]:

$$\frac{d\sigma}{do} = |a(\vartheta)|^2, \tag{1}$$

$$a(\vartheta) = -\frac{1}{4\pi\hbar^2}\int_V d^3r\, e^{-\frac{i}{\hbar}\mathbf{p}'\mathbf{r}}\overline{u'}\gamma_0 U(\mathbf{r})\psi(\mathbf{r}), \tag{2}$$

where ϑ is the scattering angle, $\psi(\mathbf{r})$ – the wave function of the electron passing through crystal, $\overline{u'}$ and $\mathbf{p}'$ – bispinor and momentum of the scattered electron respectively, and $U(\mathbf{r})$ – the potential energy of interaction of the electron with crystal lattice field (we use the system of units in which the light velocity is equal to one, $c = 1$). Integration in (2) is performed inside the volume V where the particle is subject to the external field action.

At incidence of fast particles onto a crystal along one of its axes (we will name it z axis) the correlations between consequent collisions of the particle with lattice atoms are substantial. As a result of these correlations, the particle motion is mainly determined by the continuous potential of crystal atomic strings situated parallel to the z axis, so the lattice potential averaged along this axis is [1,2]:

$$U_c(\boldsymbol{\rho}) = \frac{1}{L}\int_0^L dz\, U(\mathbf{r}), \qquad 0 \le z \le L, \tag{3}$$

where L is the crystal thickness and $\boldsymbol{\rho}$ – the co-ordinates (x, y) in the plane orthogonal to the z axis (outside crystal $U_c(\boldsymbol{\rho}) = 0$).

By using the Dirac equation for the wave function of electron in the field $U(\mathbf{r})$:

$$(\varepsilon\gamma_0 + i\hbar\boldsymbol{\gamma}\nabla - m)\psi = \gamma_0 U(\mathbf{r})\psi, \tag{4}$$

we write the scattering amplitude (2) in the form

$$a(\vartheta) = -\frac{i}{4\pi\hbar}\int_V d^3r\, \mathrm{div}\left(\overline{u'}\boldsymbol{\gamma}\psi(\mathbf{r})e^{-\frac{i}{\hbar}\mathbf{p}'\mathbf{r}}\right). \tag{5}$$

The scattering amplitude in this case, with use of the Gauss theorem, can be presented in the form of integral over a closed surface surrounding the external field region [7]:

$$a(\vartheta) = -\frac{i}{4\pi\hbar}\oint d\mathbf{S}\,\overline{u'}\boldsymbol{\gamma}\psi(\mathbf{r})e^{-\frac{i}{\hbar}\mathbf{p}'\mathbf{r}}, \tag{6}$$

where $d\mathbf{S}$ is an element of the surface surrounding the crystal.

It is essential that the surface integral in (6) does not depend on the surface form, so as the only requirement imposed on this surface is that it surround the entire area of the external field action. In the considered problem it is convenient to choose as such a closed surface a cylinder whose bases coincide with the crystal sides. By neglecting the contribution of the cylinder lateral side parallel to the z axis in the surface integral (6), we come to the following expression for the scattering amplitude:

$$a(\vartheta) = -\frac{i}{4\pi\hbar}\int d^2\rho\, e^{-\frac{i}{\hbar}\mathbf{p}'\mathbf{r}}\overline{u'}\gamma_z\psi(\mathbf{r})\Big|_{z=0}^{z=L}. \tag{7}$$

For determining the wave function of electron in the field $U_c(\boldsymbol{\rho})$ we will use the squared Dirac equation [2]:

$$\left[\left(\varepsilon - U_c(\boldsymbol{\rho})\right)^2 - (i\hbar\nabla)^2 - m^2 + i\hbar\boldsymbol{\alpha}\nabla U_c(\boldsymbol{\rho})\right]\psi(\mathbf{r}) = 0, \tag{8}$$

where m and ε are particle mass and energy respectively, and $\boldsymbol{\alpha} = \gamma_0\boldsymbol{\gamma}$.

Before entering into the crystal, the electron wave function is represented as a plane wave characterized by momentum $\mathbf{p}$ and bispinor u_p. Then, by detaching from $\psi(\mathbf{r})$ the bispinor u_p and the plane wave factor (we define $\psi(\mathbf{r}) \equiv \varphi(\mathbf{r})u_p e^{\frac{i}{\hbar}\mathbf{p}\mathbf{r}}$), we come to the following equation for $\varphi(\mathbf{r})$:

$$i\hbar v\partial_z\varphi = \left[\frac{\hat{\mathbf{p}}^2}{2\varepsilon} + U_c(\boldsymbol{\rho}) - \frac{i\hbar}{2\varepsilon}\boldsymbol{\alpha}\nabla U_c(\boldsymbol{\rho}) - \frac{U_c^2(\boldsymbol{\rho})}{2\varepsilon}\right]\varphi(\mathbf{r}), \tag{9}$$

where $v = p/\varepsilon$ is the velocity of electron and $\hat{\mathbf{p}} = -i\hbar\nabla$ – operator of momentum.

Characteristic values for the scattering angles of high energy electrons in thin crystal are small compared to one. In this case, by resolving the Eq. (9), we can neglect spin effects in scattering (spin-field interaction), so far as the terms proportional to $U^2/2\varepsilon$ and $\hat{p}_z^2/2\varepsilon$. As a result, we come to the following equation for $\varphi(\mathbf{r})$:

$$i\hbar v\partial_z\varphi = \left[\frac{\hat{\mathbf{p}}_\perp^2}{2\varepsilon} + U_c(\boldsymbol{\rho})\right]\varphi, \tag{10}$$

where $\hat{\mathbf{p}}_\perp = -i\hbar\frac{\partial}{\partial\boldsymbol{\rho}}$.

The equation (10) is a Schrödinger-like equation, where the particle mass is replaced by the energy and instead of time we use z/v, so it can be solved with the help of numerical method developed in [8]. The process of determination of the wave function in the considered problem based upon this method consists in the following. Relying on the analogy of equation (10) with the Schrödinger equation, the evolution of the wave function with depth δz of particle's penetration into crystal is expressed, according to (10), in the following operator form:

$$\varphi(\boldsymbol{\rho}, z+\delta z) = \exp\left\{i\frac{\delta z}{\hbar v}\left[\frac{\hat{\mathbf{p}}_\perp^2}{2\varepsilon} + U_c(\boldsymbol{\rho})\right]\right\}\varphi(\boldsymbol{\rho}, z). \tag{11}$$

This expression is formally exact for any δz, but direct application of it leads to mathematical difficulties that are connected with the fact that the exponent index in (11) is composed of two non-commuting terms.

However, at small values of δz application of operator technique [14] lets one write (11) in approximated form in which the commutators of the order higher than $\left[\hat{A}, \hat{B}\right]$ are neglected, where $\hat{A} = (i/\hbar v)\cdot\left(\hat{\mathbf{p}}_\perp^2/2\varepsilon\right)$ and $\hat{B} = (i/\hbar v)\,U_c(\boldsymbol{\rho})$. So, with the precision up to the terms proportional to δz^3, such Zassenhaus product formula is true:

$$\exp\left(\delta z(\hat{A}+\hat{B})\right) \approx \exp\left(\delta z\frac{\hat{B}}{2}\right)\exp\left(\delta z\hat{A}\right)\exp\left(\delta z\frac{\hat{B}}{2}\right). \tag{12}$$