SCATTERING OF CHARGED PARTICLES IN A THIN SINGLE CRYSTAL

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Submitted July 11, 1967

Zh. Eksp. Teor. Fiz. 54, 822–825 (March, 1968)

It is shown that scattering of fast charged particles in a thin single crystal is accompanied by a spatial regrouping of the particle flux. The corrections that must be introduced in the cross section for the scattering of a fast electron in the crystal as a result of this spatial regrouping are determined.

1. The scattering of charged particles in a thin single crystal was considered in the Born approximation of perturbation theory by Ter-Mikaelyan[1], who pointed out the existence of interference effects with respect to the transmitted wavelength. In connection with experiments on the interaction of particles in thin single-crystal films[2-4], it is of interest to consider more accurately the scattering of charged particles in single crystals.

The wave function of the charged particle in the summary external potential of the crystal atoms

$$U(\mathbf{r})=\sum_a \int d\mathbf{q} U_0(\mathbf{q}) \exp(i\mathbf{q}(\mathbf{r}-\mathbf{R}_a)) \tag{1}$$

should satisfy the equation

$$(\Delta + p_0^2)\Psi(\mathbf{r}) = 2E_0 U(\mathbf{r})\Psi(\mathbf{r}), \tag{2}$$

which is valid for relativistic particles at $E_0 = (p_0^2 + m^2)^{1/2} \gg U$ (for nonrelativistic particles $E_0 = m$ and (2) coincides with the Schrödinger equation).

It is convenient to seek the solution of (2) in the form

$$\Psi(\mathbf{r}) = \text{const}\cdot\exp\{i\mathbf{p}_0\mathbf{r} + S_1 + iS_2\}.$$

The real functions of the coordinates S_1 and S_2 satisfy the equations

$$\begin{aligned}(\nabla S_1)^2 - 2\mathbf{p}_0\nabla S_2 + \Delta S_1 - (\nabla S_2)^2 &= 2E_0 U,\\ 2\mathbf{p}_0\nabla S_1 + \Delta S_2 + 2\nabla S_1\nabla S_2 &= 0.\end{aligned} \tag{3}$$

Assume that the direction of the initial motion of the particle makes an angle θ_0 with the crystallographic axis; the particle acquires in the crystal, as a result of the multiple scattering, an angle spread $\langle\theta^2\rangle_L$, which depends on the thickness of the crystal.

Let us consider the case of a thin crystal, when

$$\theta_0^2 \gg \langle\theta^2\rangle_L, \tag{4}$$

i.e., the multiple-scattering angle in the crystal is small compared with the entrance angle. In this case it is possible to neglect the term ∇S_2 in (3) compared with $p_{0\perp}$.

We now assume that the inequality

$$\Delta S_1 \gg (\nabla S_1)^2 \tag{5}$$

is satisfied, so that the term $(\nabla S_1)^2$ in (3) can be neglected. The solution (3) when conditions (4) and (5) are satisfied takes the form

$$S_1(\mathbf{r}) + iS_2(\mathbf{r}) = -2E_0\int \frac{d\mathbf{l}U_0(\mathbf{l})e^{i\mathbf{l}\mathbf{r}}}{l^2 + 2\mathbf{p}_0\mathbf{l} - i\delta}\sum_a e^{-i\mathbf{l}\mathbf{R}_a}. \tag{6}$$

Substitution of (6) in (5) causes (5) to be replaced by the equivalent condition

$$S_1(\mathbf{r}) \ll 1, \tag{7}$$

so that the wave function of the particle in the external field (1) becomes

$$\Psi(\mathbf{r}) = \text{const}\cdot\exp(i\mathbf{p}_0\mathbf{r} + iS_2)(1 + S_1), \tag{8}$$

where S_1 and S_2 are defined in (6). The limits of applicability of (8) are determined by the inequalities (4) and (7).

We note that by omitting S_1 and neglecting the quantity l^2 in the denominator of (6), it is possible to obtain from (8) the well known approximate solution of the Schrödinger equation for the motion of a fast particle ($E_0 \gg U$) in an external field:

$$\Psi(\mathbf{r}) = \exp\left\{ip_0 x - \frac{i}{v_0}\int_{-\infty}^{x} dx' U(x', y, z)\right\}, \tag{9}$$

$v_0 = p_0/E_0$ is the particle velocity. For a sufficiently thin crystal, the foregoing analysis is valid also for zero entrance angles.

2. The obtained solution makes it possible to show that the motion of charged particles in a crystal is accompanied by spatial regrouping of the particles. In fact, the probability-density distribution in space is given by

$$W(\mathbf{r}) = \text{const}\cdot\left\{1 - 2\,\text{Re}\,2E_0\int \frac{d\mathbf{l}U_0(\mathbf{l})e^{i\mathbf{l}\mathbf{r}}}{l^2 + 2\mathbf{p}_0\mathbf{l} - i\delta}\sum_a e^{-i\mathbf{l}\mathbf{R}_a - i\mathbf{l}\mathbf{u}_a}\right\} \tag{10}$$

($\mathbf{R}_a$ - equilibrium coordinate of the atom, $\mathbf{u}_a$ - thermal displacement). Let the transit time of the particle in the crystal be slow compared with the period of the lattice vibration. In this case the vibrations affect only the change in the positions of the atoms prior to the interaction with the particle. Averaging over the vibrations yields the expression

$$W(\mathbf{r}) = \text{const}\cdot\left\{1 - 2\,\text{Re}\,2E_0\int \frac{d\mathbf{l}U_0(\mathbf{l})e^{i\mathbf{l}\mathbf{r}}}{l^2 + 2\mathbf{p}_0\mathbf{l} - i\delta}e^{-l^2\overline{u^2}}\cdot\right.$$

$$\left.\left[\left(\frac{2\pi}{a}\right)^2\delta^{(2)}(\mathbf{l}_\perp)\sum_{n_\parallel}e^{il_\parallel n_\parallel a} + \left(\frac{2\pi}{a}\right)^2\sum_{n_\perp\neq 0}\delta^{(2)}\left(\mathbf{l}_\perp - \frac{2\pi}{a}\mathbf{n}_\perp\right)\sum_{n_\parallel}e^{il_\parallel n_\parallel a}\right]\right\}, \tag{11}$$

where we are considering a cubic crystal, a is the

lattice constant, $\bar{u}^2$ is the mean square of the thermal displacement of the atom, and the normal to the surface coincides with the axis of the crystal. The crystal is regarded as infinitely large in the transverse directions, and therefore the dependence on r_y and r_z in the probability distribution (11) is periodic, and we can consider only the case when r_y and r_z vary from $-a/2$ to $+a/2$. For the particular case of normal incidence of the particle (along the x axis) this distribution takes the form

$$W_0(\mathbf{r}) = \text{const}\cdot\left\{1-\frac{\alpha x^2}{v_0\bar{u}^2 pa}\left[\exp\left(-\frac{r_\perp^2}{2\bar{u}^2}\right)\right.\right.$$
$$\left.\left.-\frac{\bar{u}^2\varkappa^2}{2}\exp\left(\frac{\bar{u}^2\varkappa^2}{2}\right)\left(2K_0(r_\perp\varkappa)+\mathrm{Ei}\left(-\frac{r_\perp^2}{2\bar{u}^2}\right)\right)\right]\right\}, \quad \alpha = zZe^2. \tag{12}$$

The validity of this formula is limited to the thicknesses $L^2 \ll p\bar{u}^2 a v_0/\alpha$. Thus, the distribution of the probability density in the transverse plane (y, z) changes with the sign of the charge. The probability distribution ceases to be constant and varies significantly with the distance to the lattice site. For positively charged particles, the probability density in the interstices is larger than near the sites. Therefore the positive particles shift effectively towards the region of smaller electron densities. Negatively charged particles, to the contrary, have a large probability of passing near the lattice sites. Here, naturally, the particle flux through the entire cross section of the crystal remains constant.

3. In the case of oblique incidence at small angles of inclination, the picture remains the same, but the result can be obtained in close form for inclination angles $1 \gg \theta_0 \gg a/L$ (L - crystal thickness). In this case, by averaging at a specified θ_0 over the azimuthal angle and averaging near θ_0, it is possible to obtain from the small spread of the angles, on the order of a/L, for $x \sim L \gg a/\theta_0$,

$$W(\mathbf{r}_\perp, \theta_0) = \text{const}\cdot\left\{1-\frac{2\alpha}{v_0\theta_0^2 pa}\left[-\left(\frac{2\pi}{a\varkappa}\right)^2\right.\right.$$
$$\left.\left.+\exp\left(\frac{\bar{u}^2\varkappa^2}{2}\right)\left(2K_0(r_\perp\varkappa)+\mathrm{Ei}\left(-r_\perp^2/2\bar{u}^2\right)\right)\right]\right\}. \tag{13}$$

We emphasize that formula (13) is valid for a relatively thick crystalline plate, the thickness of which satisfies the inequality

$$\frac{a}{\theta_0} \ll L \ll \frac{\theta_0^2}{E_s^2} E^2 L_{\text{rad}}$$

(E_S = 21 MeV, L_{rad} - radiation length). Comparison of (12) and (13) shows that the spatial regrouping of the particles upon scattering in the crystal depends significantly on the angle θ_0 between the direction of the incidence and the crystallographic axis. At small entrance angles θ_0, the effect depends quadratically on the path x covered by the particle, and at relatively large entrance angles θ_0, the dependence on the path x disappears, starting with lengths $L \gtrsim a/\theta_0$. We note that the obtained formulas agree qualitatively with the experimental data on scattering of charged particles in a crystal[2,3], but the limited region of applicability of the obtained formulas, particularly condition (7), does not permit a quantitative comparison with the available experimental data.

4. Let us see how the ordering action of the crystal lattice will affect the process of scattering in the crystal. Let us calculate the mean square of the scattering angle in a thin crystal. In this case the usual Born analysis leads to interference effects[1]. The cause of these effects is that at high energies the longitudinal part of the momentum transferred to the Coulomb field of the nucleus becomes small. If this quantity becomes smaller than the vector of the reciprocal lattice of the crystal, then the screened Coulomb fields of the different atoms act coherently, and the resultant amplitude of the process increases. The effective number of the coherently-acting atoms depends on the angle of entrance of the particle relative to the crystallographic axes, leading to the occurrence of interference phenomena[1]. However, the influence of the crystal lattice on the scattering process will become manifest also in the fact that the number of particles with different impact parameters changes. When considering positively charged particles in a crystal, the particles will move predominantly in the region $r_\perp \sim a/2$, i.e., with large impact parameters, and consequently will be scattered less intensely, causing a decrease in the mean square of the scattering angle. Using the well known formula for the scattering amplitude

$$f(\mathbf{p}_2 - \mathbf{p}_1) = \text{const}\cdot\int e^{-i\mathbf{p}_2\mathbf{r}} U(\mathbf{r})\Psi_{\mathbf{p}_1}(\mathbf{r})\,d\mathbf{r}, \tag{14}$$

and choosing the wave function in the form (8), we substitute the amplitude obtained from (14) into the formula for the mean square of the scattering angle

$$\langle\theta^2\rangle = \int \theta^2 \frac{d\sigma}{d\Omega}\,d\Omega.$$

It is easy to obtain

$$\langle\theta^2\rangle = \langle\theta^2\rangle_{\text{T-M}}\{1+\Phi(\theta_0, L)\}, \tag{15}$$

where $\langle\theta^2\rangle_{\text{T-M}}$ is the mean square of the scattering angle, obtained in the paper by Ter-Mikaelyan[1]

$$\Phi(\theta_0, L) = \begin{cases} -\alpha\dfrac{L^2}{v_0\bar{u}^2 pa}, & \theta_0 \ll \dfrac{a}{L} \\ -\alpha\dfrac{2}{v_0\theta_0^2 pa}\ln\dfrac{2\gamma}{\bar{u}^2\varkappa^2}, & \theta_0 \gg \dfrac{a}{L} \end{cases} \tag{16}$$

It should be noted that the criterion for the applicability of the obtained formulas for $\Phi(\theta_0, L)$ are connected with the condition $|S_1(\mathbf{r})| \ll 1$, by the condition for the applicability of relation (8) for the wave function of the particle. In the case of small entrance angles $\theta_0 \ll a/L$, this condition imposes a limitation on the thickness of the crystal $L^2 \ll \bar{u}^2 a v_0/\alpha$, and in the latter case, $\theta_0 \gg a/L$, the expression for $\Phi(\theta_0, L)$ is applicable provided $\alpha/\theta_0^2 pa \ll 1$.

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Translated by J. G. Adashko
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