THEORY OF THE SHADOW EFFECT

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The theory of the shadow effect is considered from the standpoint of multiple-scattering theory. Thermal vibrations of atoms are taken into account by introducing an effective temperature-dependent potential. The problem of classical scattering by an effective potential is solved. A formula is derived for the spot width which is in qualitative agreement with the experimental data. The results are compared with the data of Lindhard and with qualitative considerations based on the uncertainty principle.

THE basic theory of the shadow effect developed by Lindhard[1] in the purely classical approximation is well known. The Born approximation is used in such problems with great reservations[2]. Discussion of the effect from the kinetic point of view[3] gives the complete picture, but the estimates of the widths of the spots and lines and their temperature dependence do not agree with experiment. The recent work of Vedrinskiĭ and Sharko[4], which was based on the theory of double scattering, apparently does not yet permit specific results to be obtained which relate to the shadow effect.

1. We will discuss the problem of scattering of protons with energy ~ 1 MeV in a crystal lattice from the point of view of multiple-scattering theory. Let the proton-lattice system be described by the Hamiltonian

$$H+\sum_l V_l,$$

where V_l is the potential for interaction of the proton with the l-th lattice site. Then the solution of the scattering problem is given by the equations (see, for example, Goldberger and Watson[5])

$$\psi_N^{(+)}=\chi+\sum_l \frac{1}{E-H+i\eta}T_l\psi_l,$$

$$\psi_l=\chi+\sum_{l'\neq l}\frac{1}{E-H+i\eta}T_{l'}\psi_{l'}, \qquad (1)$$

where χ is the incident wave and the operators T_l are determined by the equations

$$T_l=V_l+V_l\frac{1}{E-H+i\eta}T_l. \qquad (2)$$

The solution of the problem in explicit form without additional assumptions is difficult. The principal assumption which will be used here is that we can neglect back-scattering in propagation of the particle to the point of observation. The possibility of neglecting back-scattering is due to the high energy of the particle and is confirmed by the calculation made by us previously[2]. We showed in that work that the scattering amplitude is large in a narrow range of angles near $\vartheta = 0$.

Let us consider, in particular, scattering by a single straight string of atoms. From Eq. (1) it follows that

$$\psi_l\approx\chi+\sum_{l'=1}^{l-1}\frac{1}{E-H+i\eta}T_{l'}\psi_{l'},$$

which gives

$$\psi_N^{(+)}=\left(1+\frac{1}{E-H+i\eta}T_N\right)\left(1+\frac{1}{E-H+i\eta}T_{N-1}\right)\dots \dots\left(1+\frac{1}{E-H+i\eta}T_1\right)\chi. \qquad (3)$$

Equation (3) gives the solution of the problem in quadratures if the operators T_l are known. With a more complicated location of the atoms the contribution to scattering into a given solid angle will be given by several strings of atoms, each of which can be taken into account sequentially.

The operators T_l are determined from Eq. (2) with the known potential V_l. We will assume that all atoms are identical, and then

$$V_l = V(\mathbf{r}-\mathbf{l}-\mathbf{u}_l),$$

where $\mathbf{l}$ is the radius vector of the site of the l-th atom and the quantity $\mathbf{u}_l$ is the deviation of a nucleus from its equilibrium position at the center of the site. If we consider the motion of the nucleus as quasiclassical, its coordinates cannot change greatly during the time of interaction with the proton. The final result must be averaged over the various configurations of the nuclei, for which it is necessary to know the probability distribution for the various configurations. The quantum-mechanical averaging is carried out directly in calculations of the matrix elements of the scattering matrix.

2. We will consider those cases in which the Born approximation is valid for scattering by a single atom, and the potential describing the interaction of the proton with the atom we will take as a screened Coulomb potential:

$$V(r)=\frac{Ze^2}{r}\exp\left(-\frac{r}{r_0}\right)$$

We have

$$T_l\approx V(\mathbf{r}-\mathbf{l}-\mathbf{u}_l)$$

The operators inside the parentheses in Eq. (3) are the operators for scattering by individual atoms, including both elastic and inelastic channels. We will limit ourselves to discussion of elastic processes. This means that we are excluding from consideration all processes which lead to a change in the vibrational state of the lattice in each of the scattering events.

Let us complete the transformation of the potential, which permits separation of the terms leading to elastic processes from the remaining terms. We will expand the deviation $\mathbf{u}_l$ in normal coordinates:

$$\mathbf{u}_l = \frac{1}{N^{1/2}} \sum_{\mathbf{q}}' Q_{\mathbf{q}} e^{i\mathbf{q}\mathbf{l}}.$$

Substituting this expression into the Fourier expansion of the potential, we have

$$V(\mathbf{r}-\mathbf{l}-\mathbf{u}_l) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{l})} V_{\mathbf{k}} \prod_{\mathbf{q}} \exp\left\{-\frac{i\mathbf{k}}{N^{1/2}} Q_{\mathbf{q}} e^{i\mathbf{q}\mathbf{l}}\right\}.$$

Utilizing the fact that $Q_{-\mathbf{q}} = Q_{\mathbf{q}}^*$ and expanding the exponentials which occur under the product sign, we obtain

$$V(\mathbf{r}-\mathbf{l}-\mathbf{u}_l) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{l})} V_{\mathbf{k}} \prod_{\mathbf{q}>0} \left\{1 - i\frac{\mathbf{k}}{N^{1/2}}\left(Q_{\mathbf{q}} e^{i\mathbf{q}\mathbf{l}} + Q_{-\mathbf{q}} e^{-i\mathbf{q}\mathbf{l}}\right) - \frac{|\mathbf{k}Q_{-\mathbf{q}}|^2}{N} - \frac{1}{2N}\left[(\mathbf{k}Q_{\mathbf{q}})^2 e^{2i\mathbf{q}\mathbf{l}} + (\mathbf{k}Q_{-\mathbf{q}})^2 e^{-2i\mathbf{q}\mathbf{l}}\right] + \ldots\right\}.$$

Here the notation $\mathbf{q} > 0$ means that the product is taken of all possible terms for which the vector $\mathbf{q}$ takes on all values in the half space.

We have, then,

$$V(\mathbf{r}-\mathbf{l}-\mathbf{u}_l) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{l})} V_{\mathbf{k}} \left[\prod_{\mathbf{q}}\left(1 - \frac{|\mathbf{k}Q_{\mathbf{q}}|^2}{N}\right)\right]^{1/2} \times \prod_{\mathbf{q}>0}\left[1 - \frac{i}{N^{1/2}} \frac{\mathbf{k}(Q_{\mathbf{q}} e^{i\mathbf{q}\mathbf{l}} + Q_{-\mathbf{q}} e^{-i\mathbf{q}\mathbf{l}})}{1 - |\mathbf{k}Q_{\mathbf{q}}|^2/N} + \ldots\right].$$

Using the relation

$$\prod_{\mathbf{q}}\left(1 - \frac{|\mathbf{k}Q_{\mathbf{q}}|^2}{N}\right) = \exp\left(-\sum_{\mathbf{q}} |\mathbf{k}Q_{\mathbf{q}}|^2\right),$$

we obtain

$$V(\mathbf{r}-\mathbf{l}-\mathbf{u}_l) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{l})} V_{\mathbf{k}} \exp\left(-\frac{1}{2}\sum_{\mathbf{q}} |\mathbf{k}Q_{\mathbf{q}}|^2\right) \times \prod_{\mathbf{q}>0}\left[1 - \frac{i}{N^{1/2}} \frac{\mathbf{k}(Q_{\mathbf{q}} e^{i\mathbf{q}\mathbf{l}} + Q_{-\mathbf{q}} e^{-i\mathbf{q}\mathbf{l}})}{1 - |\mathbf{k}Q_{\mathbf{q}}|^2/N} + \ldots\right].$$

The contribution to inelastic processes originates from terms containing $e^{\pm i\mathbf{q}\cdot\mathbf{l}}$ to any nonzero power. Rejecting these terms, we find that the part of the potential responsible for elastic processes has the form

$$V_{\text{el}}(\mathbf{r}-\mathbf{l}-\mathbf{u}_l) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{l})} V_{\mathbf{k}} \exp\left(-\frac{1}{2}\sum_{\mathbf{q}} |\mathbf{k}Q_{\mathbf{q}}|^2\right).$$

In the Born approximation the potential enters linearly into the matrix elements. Carrying out the integration over generalized coordinates, we obtain a potential dependent only on the proton coordinates and the number of the site:

$$V_{eff}(\mathbf{r}-\mathbf{l}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{l})} V_{\mathbf{k}} e^{-k^2 W}, \qquad (4)$$

where k^2W is the exponent of the Debye-Waller factor:

$$W = \frac{1}{2MN}\sum_{\mathbf{q}} \frac{n_{\mathbf{q}} + 1/2}{\omega_{\mathbf{q}}}.$$

Averaging this expression over the statistical ensemble then gives

$$W = \frac{3\hbar^2}{8M\Theta}\left[1 + 4\left(\frac{T}{\Theta}\right)^2 \int_0^{\Theta/T} \frac{x\,dx}{e^x - 1}\right].$$

The exact expression for V_{eff} has the form[2]

$$V_{eff} = \frac{Ze^2}{2r}\exp\left(\frac{W}{r_0^2}\right)\left\{\exp\left(-\frac{r}{r_0}\right)\left[1 - \Phi\left(\frac{W^{1/2}}{r_0} - \frac{r}{2W^{1/2}}\right)\right] - \exp\left(\frac{r}{r_0}\right)\left[1 - \Phi\left(\frac{W^{1/2}}{r_0} + \frac{r}{2W^{1/2}}\right)\right]\right\}.$$

For $W^{1/2} \gg r_0$ we have approximately

$$V_{eff} = \frac{Ze^2 r_0^2}{2\pi^{1/2} W^{3/2}} \exp\left(-\frac{r^2}{4W}\right).$$

The assumptions which have been made lead to the assertion that if we are interested in elastic scattering, then in calculation of the T operator from Eq. (2) the potential V_l can be replaced by $V_{\text{eff}}(\mathbf{r}-\mathbf{l})$ and subsequently it is not necessary to take into account the motion of the lattice. This statement follows from quantum theory and it gives us the right, in making a calculation in the classical approximation, to consider the problem of scattering of a proton by a string of atoms as the problem of scattering by a string of effective potentials. Below we carry out the calculation in the classical approximation.

3. Let us consider the problem of scattering in the classical approximation in a potential averaged along the string of atoms, following Lindhard[1]. If we spread the potential V_{eff} introduced above by Eq. (4) along the string of atoms, we obtain

$$V(\rho) = \frac{2Ze^2}{a}\int_0^\infty \frac{e^{-x^2} J_0(\rho x/2W^{1/2})}{x^2 + w} x\,dx, \quad w \equiv \frac{W}{r_0^2}, \qquad (5)$$

where ρ is the deviation from the string, a is the lattice parameter, and J_0 is a Bessel function of zero order. For $\rho < W^{1/2}$ the potential reduces to the form

$$V(\rho) = \frac{Ze^2 a_0}{wa}\left[1 - \left(\frac{\rho^2}{4W}\right) b_1 + \frac{1}{2}\left(\frac{\rho^2}{4W}\right)^2 b_2\right],$$

where

$$a_0 = -we^w \operatorname{Ei}(-w),$$
$$b_1 = -[we^w \operatorname{Ei}(-w) + 1]/e^w \operatorname{Ei}(-w),$$
$$b_2 = -\frac{-(w)^2 e^w \operatorname{Ei}(-w) - w + 1}{2e^w \operatorname{Ei}(-w)};$$

Ei is the exponential integral. The asymptotes of the coefficients a_0, b_1, and b_2 are as follows: for $w \to \infty$

$$a_0 \approx 1, \quad b_1 \approx 1, \quad b_2 \approx 1,$$

and for $w \to 0$

$$a_0 \approx w \ln\frac{1}{w}, \quad b_1 \approx 1/\ln\frac{1}{w}, \quad b_2 \approx \left(2\ln\frac{1}{w}\right)^{-1}.$$

We have considered a spherically isotropic proton beam with its center at the string of atoms, which was then scattered by the smeared effective potential (4). Scattering at small angles was investigated. For $\rho < W^{1/2}$ the result is expressed in terms of the elliptic integrals K(k), F(φ, k). It was possible to evaluate the shadow width:

$$\Delta\vartheta \approx (Ze^2\xi/aE)^{1/2}; \qquad (6)$$

here E is the proton energy and

$$\xi = 2\frac{[we^w \operatorname{Ei}(-w) + 1]^2}{-we^w \operatorname{Ei}(-w) - w + 1}.$$

the asymptotes of ξ have the form

$$\xi \approx r_0^2/W \quad \text{for } W/r_0^2 \to \infty;$$
$$\xi \approx 2 \quad \text{for } W/r_0^2 \to 0.$$

The shadow width obtained (6) is in good agreement with experiment[6]. Equation (6) gives the experimentally observed decrease in shadow width with increasing temperature. This dependence is determined mainly by the ratio $w \equiv W/r_0^2$. It is weaker for $w \ll 1$ than for $w \gg 1$. This provides the possibility of evaluating the screening radius r_0, which apparently has a value in a crystal which is smaller than the value given for a free atom by the Fermi-Thomas method.

The evaluation carried out shows that the dependence of the shadow width on the thickness of the crystalline sample is very weak. Investigation of the dependence of shadow depth on temperature gave qualitative agreement with experiment—a decrease in depth with increasing temperature. However, the numerical value of the depth turned out to be significantly greater than given by experiment. Apparently the filling of the shadow is accomplished also by protons scattered by other strings of atoms, and these are not taken into account in the present problem.

4. Previously[2] it was shown that use of the Born approximation for calculation of the temperature dependence of the shadow width leads to the following result:

$$\Delta\vartheta \sim 1/kW^{1/2}. \qquad (7)$$

Application of the Born approximation to the shadow effect is justified for the following reasons:

1) The Born approximation is always valid if the perturbation is small. For the case of a particle moving in a lattice with a large impact parameter, $\rho > r_0$, where r_0 is the screening radius, this condition is satisfied, since the greater part of the nuclear charge is screened.

2) If $\rho < r_0$, we can assume that the particle motion occurs in the pure Coulomb field of the nucleus, and in this case the classical and quantum descriptions lead to an identical result[7].

It is of interest to compare the result (7) with the result of Sec. 3 and with qualitative reasoning. We have for the value of the scattering angle in an individual scattering event $\Delta\vartheta = \Delta p_y/p$, where Δp_y is the change in the transverse component of the proton momentum. In scattering of protons by a string of atoms with allowance for the thermal vibrations of the latter, the region of localization of a particle of any energy cannot be less than a certain quantity equal to the amplitude of the thermal displacements of the nuclei, i.e.,

$$\Delta y \geqslant W^{1/2},$$

where $W^{1/2}$ is the rms displacement of the lattice nucleus. According to the uncertainty principle $\Delta p_y \geq \hbar/W^{1/2}$. If this is taken into account, the smallest value of proton scattering angle, with thermal vibrations of the lattice nuclei taken into account, is found to be given by Eq. (7). The classical formula (6) leads to the same function (7), but only for the condition that the amplitude of the vibrations of the nuclei is larger than the screening radius. However, the experimental results[6] apparently indicate that this condition is satisfied. Thus, Eq. (7) is confirmed from three different points of view. A more careful analysis of the problem on the basis of more accurate quantum theory (3) will be undertaken later.

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