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DISLOCATION BANDS IN ELECTRON ENERGY SPECTRUM

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The influence of randomly distributed dislocations on the electron energy spectrum of a crystal is investigated. Two models of interaction between an electron and a dislocation are studied: one with a deformation potential and one with a short-range delta-like potential. It is shown that the presence of a large number of dislocations in the crystal leads to the appearance of new ranges of allowed electron energy—dislocation bands—in the electron spectrum. The width of the dislocation band in the case of a deformation potential is of the order of $\Lambda bc^{1/2}$, where Λ is the deformation interaction constant, b the absolute value of the Burgers vector, and c the dislocation concentration. The maximal density of states in this case is proportional to $c^{3/4}$. Dislocations with a short-range attraction potential produce a band of width $|E_\perp| \exp(-k_\perp^2/c)$ ($E_\perp$ is the energy of a two-dimensional electron bound state on a single dislocation and $k_\perp$ is the corresponding wave number) with a maximal state density which is proportional to $\exp(k_\perp^2/c)$.

1. INTRODUCTION

EXTENDED crystal-lattice defects, and above all dislocations, can exert a noticeable and unique influence on the electronic energy spectrum of a crystal. In real samples, the dislocations are, as a rule, located at random. The influence of the dislocations on the electronic properties of crystals is therefore part of the problem of the energy spectrum of a disordered system.

If the dislocation has an attraction potential, then two-dimensional bound states of the electron can arise in its vicinity. In such states the particle executes a finite motion in a plane perpendicular to the dislocation line, and infinite motion along the dislocation. The essential difference between the spectrum generated by the dislocation and the spectrum due to "point" defects such as impurities, vacancies, etc., is due precisely to the motion of the electrons along the dislocations. This infinite motion is the main cause of the appearance of an entire energy band instead of a single level. We shall call this the dislocation band. The concept of dislocation bands was first introduced by Bonch-Bruevich and Glasko[1,2], who investigated certain essential characteristics of the spectrum in this band.

Another cause of the dislocation band is the concentration broadening of the two-dimensional bound states. In the case of point defects, this is the only mechanism for producing the impurity band. A sufficiently complete study of the structure of a dislocation band with allowance for concentration broadening is possible only in the case of low dislocation concentration. A corresponding detailed analysis for point defects was carried out by I. Lifshitz[3]. In the present paper, using his ideas and procedure, we attempt to describe the main features of the singularities of the dislocation band.

It should be noted first that the dislocation band arises only in the case when an individual isolated dislocation in an infinite crystal leads to the appearance of a two-dimensional bound (local) state. We therefore consider the quantum-mechanical problem of electron motion in a field of an individual dislocation. Naturally, in the study of such complicated objects as dislocations, we are forced to limit ourselves to consideration of rather crude models. Namely, we assume that the electron dispersion is isotropic and quadratic, and that the dislocations are straight and pass through the entire crystal.

If the dislocation axis is chosen to be the z axis, then the potential energy of the interaction of the electron with the dislocation depends only on the two variables x and y, i.e., $U = U(x, y)$. The concrete form of this function is determined by the type of dislocation, i.e., by its Burgers vector **b**, and also by whether the crystal is a metal, semiconductor, or dielectric. These questions are discussed in greater detail, for example, in[1,2] or in Friedel's book[4].

In many cases it can be assumed that the dislocation potential is due to the lattice deformation, i.e., it has the form $U = \Lambda_{ik}u_{ik}$, where Λ_{ik} are the components of the deformation-potential tensor. The strain tensor u_{ik}, in polar coordinates r and φ on the xy plane, which is perpendicular to the dislocation axis, has the well-known form[4]

$$u_{ik}(r,\varphi) = \frac{b}{r} f_{ik}(\varphi), \tag{1}$$

where $f_{ik}(\varphi)$ is a dimensionless tensor that depends on the character of the anisotropy of the crystal, and on the type and orientation of the dislocation relative to the crystallographic axes. In order of magnitude, the components of this tensor are equal to unity. It is important that

$$\int_0^{2\pi} f_{ik}(\varphi)\,d\varphi = 0, \quad i, k = 1.2\ 3.$$

As seen from (1), the deformation potential is long-range. There are, however, cases, for example in certain types of semiconductors[1], when the principal role in the creation of the dislocation potential is played either by the little-investigated distortions near the core of this dislocation, or by the screened charge of the carriers captured by the dislocation. In these cases, the potential is short-range, and to simplify the calculation we assume the following model:

$$U = -\beta\delta(\mathbf{r}), \tag{2}$$

where $\delta(\mathbf{r})$ is a two-dimensional δ function, $\beta = U_0 b^2$, U_0 is the characteristic depth of the potential well, and b the characteristic dimension of the well, which is equal in order of magnitude to the length of the Burgers vector (for more details see[5]). We shall henceforth consider only these two models, which are in a certain sense polar, although the final results are applicable to a much broader class of models.

It is well known (see, for example,[6]) that in a two-dimensional potential well there is always a bound state. This statement is valid for model (2) if $\beta > 0$. As to model (1), this statement is not valid a priori, owing to the alternating sign of the functions $f_{ik}(\varphi)$, i.e., owing to the presence of both a "well" and a "hill" on the potential relief. A simple quantum-mechanical calculation shows that the bound state in a potential relief of the type (1) appears only in the case when the dimensionless parameter $\lambda = 2\pi m\hbar^{-2}\int |U|\,dxdy$ (the integral is taken over the region in which $U < 0$) exceeds a certain critical value $\lambda_{cr} \sim 1$. For a deformation potential, the corresponding integral formally diverges. Actually, however, it is necessary to recognize that the presence of other dislocations causes this integral to be cut off at distances on the order of the average distance between dislocations. If we take this remark into consideration, then it turns out that $\lambda \gg 1$ practically always, i.e., there is a large number of levels in this well. When we consider the concentration broadening, we shall have in mind one such level. In other words, we assume that the broadening of the individual levels is much smaller than the distance between them.

Let us discuss the localization radius of the bound state. In the case of a short-range potential, the localization radius, i.e., the dimension of the region within which the wave function differs noticeably from zero, is of the order of[6]

$$r_\perp = 1 / k_\perp = b(e^{1/\lambda} - 1)^{1/2}. \tag{3}$$

At small λ, the localization radius can be very large. However, it is difficult to indicate the physical reasons why the parameter λ can differ noticeably from unity. In the case of a long-range potential, the localization radius coincides in order of magnitude with the dimensions of the well.

In describing the system of dislocations, we assume that the positions of the individual dislocations are not correlated with one another. Therefore the only parameter of the distribution of such a system of straight lines is their concentration. By dislocation concentration c is meant their total length per unit volume of the crystal. The dimensionality of c is thus cm^{-2}. For a system of parallel dislocations, the concentration coincides with the number of dislocation lines crossing a unit area perpendicular to their direction. For dislocations with randomly distributed directions, their number contained in a solid-angle element $d\Omega$ crossing the corresponding unit area is $c\,d\Omega/2\pi$.

Physical considerations similar to those advanced in[3] show that the presence of many dislocations with long-range interaction potential leads to a classical concentration broadening of the levels. This broadening is in essence the result of the random variation of the point from which the energy is reckoned at the location of the given dislocation, owing to the influence of the "tails" of the potential relief of the remaining dislocations. A fundamentally new situation arises in the case of a short-range potential (the quantum case). The foregoing calculations show that the presence of even two crossing dislocations leads to the appearance of a three-dimensional bound state in which the particle is localized in the region where the dislocations come close together. This state is due to the tunneling of the electron from one dislocation to the other. The position of the discrete level corresponding to this state is determined mainly by the overlap of the wave functions localized near the individual dislocations. In turn, this overlap depends on the distance between dislocations, on the angle between them, on the influence of the remaining dislocations, etc. The aggregate of the discrete levels obtained in this manner forms the quantum section of the dislocation band. If we take this section into consideration, then the net result will consist of a broadening of the "unperturbed" dislocation band, which we shall henceforth call the quantum concentration broadening. It must be emphasized once more, however, that this broadening is due not to the smearing of the initial levels, but to the appearance of a fundamentally new section of the spectrum, adjacent to the initial spectrum. Of course, the three-dimensional states, and accordingly, the new section of the spectrum, can arise also in the case of a long-range potential, but in this case they do not play any role, since they are completely "suppressed" by the classical concentration broadening. Roughly speaking, the quantum concentration broadening predominates in the case when the localization radius of the wave function exceeds the radius of action of the potential, and the classical broadening predominates in the opposite limiting case. The corresponding more accurate estimates are analogous to those obtained by I. Lifshitz for point defects.

In view of all the foregoing, we present a theory of classical broadening for a deformation potential and a theory of quantum broadening for a δ-like dislocation potential.

2. CLASSICAL CONCENTRATION BROADENING

The task of the theory is to find the spectral density $\nu(E)$. It is clear that in the case of classical concentration broadening, the dislocation distribution with respect to the directions is immaterial. We can therefore assume for the sake of clarity that all the dislocations are parallel to the z axis. But then it is necessary to find first the "two-dimensional" density of states $\nu_\perp(E - p_z^2/2m)$, and the integrate the result with respect to p_z. The method of finding the two-dimensional density of states is somewhat different from that proposed in[3] for the case of point defects. The difference lies in the use of a bilateral Fourier transformation in lieu of a unilateral Laplace transformation. This difference is due to the alternating sign of the deformation potential of the interaction. We therefore permit ourselves to present the calculation in a relatively detailed form.

Let $E_\perp$ be the two-dimensional level generated by one dislocation. The random shift of this level is given by

$$\varepsilon \equiv E - \frac{p_z^2}{2m} - E_\perp = \sum_{\alpha=1}^{N} U(\mathbf{r}_\alpha), \tag{4}$$

where $U(\mathbf{r}_\alpha)$ is the potential of the α-th dislocation at the location of the given dislocation, and N is the total number of dislocations in the sample. The random quantities are the two-dimensional radius vectors $\mathbf{r}_\alpha$ of the individual dislocations. Obviously, the distribution density $p(\epsilon)$ of the random quantity ϵ is the sought two-dimensional density of states, normalized to a single dislocation. It should not be stated beforehand that the sum of mutually independent random quantities of the form (4) has a normal distribution, since these quantities are not suitably normalized. To find $p(\epsilon)$ we proceed as follows. We introduce the characteristic function

$$F(z) = \overline{e^{i\varepsilon z}} = \int_{-\infty}^{\infty} p(\varepsilon) e^{i\varepsilon z}\, d\varepsilon. \tag{5}$$

A bar denotes here statistical averaging. The characteristic function is obtained directly, after which $p(\epsilon)$ is sought with the aid of the inverse Fourier transformation. We present the corresponding derivations:

$$\begin{aligned} F(z) &= \overline{\exp(i\varepsilon z)} = \overline{\exp\Big[iz \Big(\sum_\alpha U(\mathbf{r}_\alpha) \Big) \Big]} \\ &= \overline{\prod_\alpha \exp(izU(\mathbf{r}_\alpha))} = \overline{[\exp(izU(\mathbf{r}))]^N} \\ &= \Big[\int_{-\infty}^{\infty} p(U) \exp(izU)\, dU \Big]^N = \Big[\frac{1}{S} \iint \exp(izU(r,\varphi))\, r\, dr\, d\varphi \Big]^N \\ &= \Big\{ \frac{1}{S} \iint [1 - 1 + \exp(izU(r,\varphi))]\, r\, dr\, d\varphi \Big\}^N \\ &= \Big\{ 1 - \frac{1}{S} \iint [1 - \exp(izU(r,\varphi))]\, r\, dr\, d\varphi \Big\}^N. \end{aligned} \tag{6}$$

In the chain (6), S denotes the area of the sample cross section and p(U) is the density of the distribution of the potential of one dislocation. At large values of N we have $F(z) = \exp[-c\varphi(z)]$, where

$$\begin{aligned} \varphi(z) &= \int_0^\infty \int_0^{2\pi} [1 - \exp(izU(r,\varphi))]\, r\, dr\, d\varphi \\ &= \int_0^\infty \int_0^{2\pi} \Big[1 - \exp\Big(iz \frac{b}{r} \Lambda_{ik} f_{ik}(\varphi) \Big) \Big]\, r\, dr\, d\varphi. \end{aligned} \tag{7}$$

From (7) we see that at small values of r the integral converges rapidly, and at large r it diverges logarithmically (we recall that $\int_0^{2\pi} f_{ik}(\varphi) d\varphi = 0$). This divergence seems natural to us. A similar logarithmic divergence arises also in the calculation of the elastic energy of a dislocation in a crystal. Owing to the logarithmic character of the divergence, the exact distances at which the integral in (7) should be cut off (of course, these must be large compared with interatomic distances), do not matter greatly. We shall assume that the cutoff radius coincides in order of magnitude with the transverse dimensions L. Then we obtain for $\varphi(z)$ the formula

$$\varphi(z) = \Lambda^2 b^2 z^2 \ln(L/\Lambda b z), \tag{8}$$

where Λ is of the same order of magnitude as the arbitrary tensor component Λ_{ik}.

We can now calculate also

$$p(\varepsilon) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\Big(-cb^2\Lambda^2 z^2 \ln \frac{L}{\Lambda b z} - i\varepsilon z \Big)\, dz. \tag{9}$$

With logarithmic accuracy, the result of the integration is

$$p(\varepsilon) = [2\pi c b^2 \Lambda^2 \ln(Lc^{1/2})]^{-1/2} \exp\Big[-\frac{\varepsilon^2}{2cb^2\Lambda^2 \ln(Lc^{1/2})} \Big], \tag{10}$$

i.e., the two-dimensional density of states is described by a Gaussian curve with average fluctuation $\Lambda bc^{1/2}$ (the logarithm does not play a significant role, since it is of the order of 10–20 at ordinary dislocation concentrations $c = 10^6$–10^{10} cm^{-2} and at dimensions $L \sim 1$ cm).

The true three-dimensional density of states, normalized to the unit volume, is determined from the formula

$$\nu(E) = \frac{NL_\parallel}{2\pi\hbar V} \int_{-\infty}^{\infty} p\Big(E - E_\perp - \frac{p_z^2}{2m} \Big)\, dp_z, \tag{11}$$

where V is the volume of the crystal and $L_\parallel$ is the longitudinal dimension of the sample. Since $NL_\parallel$ is the total length of the dislocation lines, we get $NL_\parallel/V = c$. When (10) is substituted in (11), the integral can be calculated in terms of parabolic-cylinder functions with index $-1/2$. We present here only the corresponding asymptotic forms, when the absolute value of the distance from the two-dimensional level $|E - E_\perp|$ is much larger than the average fluctuation $\Lambda bc^{1/2}$.

When $E > E_\perp$ we have

$$\nu(E) \approx cm^{1/2}/2^{1/2}\pi\hbar(E - E_\perp)^{1/2}. \tag{12a}$$

The asymptotic form on the low-energy side, $E < E_\perp$, is

$$\nu(E) \approx \frac{cm^{1/2}}{2\pi\hbar(E_\perp - E)^{1/2}} \exp\Big[-\frac{(E_\perp - E)^2}{2cb^2\Lambda^2 \ln(Lc^{1/2})} \Big]. \tag{12b}$$

A plot of $\nu(E)$ is shown schematically in Fig. 1. Without allowance for the mutual influence of the dislocations, the density of states will be proportional to $c(E - E_\perp)^{-1/2}$, i.e., it would have a square-root singularity at the point $E = E_\perp$. The classical broadening leads to a strong smearing of this singularity. It is replaced by a maximum whose magnitude is of the order of $\nu_{\max} \sim c^{3/4}(m/b\Lambda\hbar^2)^{1/2}$. It is shifted relative to $E_\perp$ towards higher energies by an amount on the order of $\Lambda bc^{1/2}$, whereas the bound-state energy itself is of the order of Λ. In addition, an exponential "tail" appears on the low-energy side, having the same characteristic average-fluctuation parameter $\Lambda bc^{1/2}$. If we assume for estimating purposes a Burgers vector $b \sim 10^{-8}$ and a dislocation concentration $c \sim 10^8$ cm^{-2}, then the smearing of the spectral density will be of the order of $10^{-4}\,\Lambda$, i.e., the smearing is small, as expected, to the extent that the concentration is small. If we compare the smearing $\Lambda bc^{1/2}$ with the deformation potential $\Lambda b/r$, then it becomes clear that the main contribution to the broadening is made by dislocations located at distances $r_* \sim c^{-1/2}$ from each other, i.e., at medium distances.

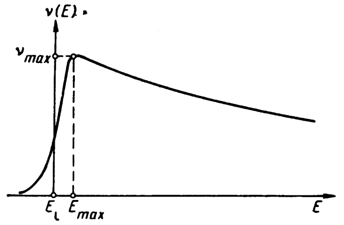

FIG. 1

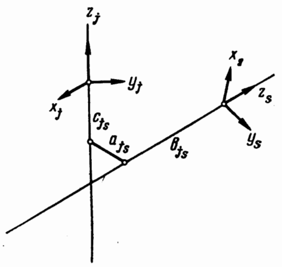

FIG. 2

3. QUANTUM CONCENTRATION BROADENING

We now proceed to study the density of states in the dislocation band for a short-range potential. We first introduce certain geometrical characteristics that are needed for the description of the mutual placement of the straight-line dislocations. To this end, we examine Fig. 2, which shows the mutual locations of the j-th and s-th dislocations. If we assign to each dislocation its own reference frame, then to make the s-th and j-th systems congruent it is necessary to perform a definite set of rotations and translations, the number and form of which is evident from an examination of Fig. 2. In this figure, the symbol a_{js} denotes the shortest distance between the crossing straight lines. We denote by θ_{js} the angle between these lines. It is physically quite understandable, and it will be furthermore seen from the formulas, that the spectral density is determined essentially only by the quantities a_{js} and θ_{js} ($j, s = 1, 2, \ldots, N$), and depends very little on the translations b_{js} and c_{js}. Therefore to simplify the formulas we shall exclude these translations entirely from consideration. In other words, we shall perform the calculations assuming $b_{js} = c_{js} = 0$.

The Schrödinger equation for an electron moving in the field produced by a system of N randomly distributed dislocations is

$$-\frac{\hbar^2}{2m}\Delta\psi + \sum_{j=1}^{N} U_j\psi = E\psi. \tag{13}$$

If the coordinate system is chosen with the z axis along the j-th dislocation, the action of the potential U_j on the wave function is written, in accordance with (2), in the form

$$U_j\psi(x, y, z) = -\beta\psi(0, 0, z)\,\delta(x)\,\delta(y). \tag{14}$$

We recall that we assume $\beta > 0$. This corresponds to attraction of the electron to the dislocation. An extremely localized potential of the type (14) leads, as is well known, to the appearance of a logarithmic divergence in many of the integrals that arise in this problem. The divergence will therefore be eliminated where necessary by smearing out the δ function by introducing a suitable cutoff parameter.

We rewrite Eq. (13) in a coordinate system connected with an arbitrary but fixed j-th dislocation:

$$-\frac{\hbar^2}{2m}\Delta\psi - \beta\sum_{s=1}^{N}\psi(z_s)\,\delta(x_s)\,\delta(y_s) = E\psi. \tag{15}$$

In Eq. (15), x_s, y_s, and z_s are coordinates in a system connected with the s-th dislocation, and $\psi(z_s)$ is taken to mean the wave function at the points belonging to the s-th dislocation.

A study of the spectrum of the operator (15) is best carried out by a method which is a generalization of the method of degenerate (local) perturbations[3]. To this end we change over in (15) to the Fourier representation

$$\frac{\hbar^2k^2}{2m}\psi(\mathbf{k}) - \beta\sum_{s}\exp(ik_{y_s}a_{sj})\,\psi(k_{z_s}) = E\psi(\mathbf{k}), \tag{16}$$

$$\psi(k_{z_s}) = \int_{-\infty}^{\infty}\psi(z_s)\exp(ik_{z_s}z_s)\,dz_s. \tag{17}$$

In writing down (16) we took into account the fact that rotation around the dislocation axis is physically immaterial, and therefore the direction of the common normal to the s-th and j-th dislocations can be chosen, for example, to be the y axis common to the s-th and j-th coordinate systems. The vector $\mathbf{k}_s$ is connected with $\mathbf{k}_j$ by the linear transformation

$$\begin{cases} k_{x_s} = k_{x_j}\cos\theta_{js} - k_{z_j}\sin\theta_{js}, & \\ k_{y_s} = k_{y_j}, & 0 \leqslant \theta_{js} \leqslant \pi/2, \\ k_{r_s} = k_{x_j}\sin\theta_{js} + k_{z_j}\cos\theta_{js}. & \end{cases} \tag{18}$$

Thus, the object of our investigation is the equation

$$\psi(\mathbf{k}) - \frac{\beta\sum\limits_{s}\exp(ik_{y_s}a_{js})\,\psi(k_{z_s})}{(\hbar^2k^2/2m) - E} = 0. \tag{19}$$

It is seen from (19) that the problem consists of finding N unknown "one-dimensional" functions $\psi(k_{zs}) \equiv \psi_s(k)$, whereas in the analogous problem with impurities we dealt with the determination of N numbers. In the problem with random impurities, these N numbers are the solution of a system of linear algebraic equations.

Proceeding analogously in our case, we obtain a system of integral equations for the determination of $\psi_j(k)$ ($j = 1, 2, \ldots, N$). To this end we take the scalar products of both sides of (19) with $\psi^*(k_z^j)$. Then the first term takes the form

$$\int\psi(\mathbf{k})\,\psi^*(k_{z_j})\,d\mathbf{k} = \int\psi(\mathbf{k})\left[\int_{-\infty}^{\infty}\psi^*(z_j)\exp(-ik_{z_j}z_j)\,dz_j\right]d\mathbf{k}$$
$$= \int_{-\infty}^{\infty}\psi^*(z_j)\left[\int\psi(\mathbf{k})\exp(-ik_{z_j}z_j)\,d\mathbf{k}\right]dz_j$$
$$= \int_{-\infty}^{\infty}\psi^*(z_j)\,\psi(z_j)\,dz_j = \int_{-\infty}^{\infty}\psi(k_{z_j})\,\psi^*(k_{z_j})\,dk_{z_j},$$

and the last equation of this chain expresses the invariance of the scalar product on going from one representation to the other. We thus have the equations

$$\int_{-\infty}^{\infty}\left\{\psi(k_{z_j}) - \frac{2m\beta}{\hbar^2}\iint\frac{\sum\limits_{s}\exp(ik_{y_j}a_{js})\,\psi(k_{z_s})\,dk_{x_j}dk_{y_j}}{k^2 - 2mE/\hbar^2}\right\}\psi^*(k_{z_j})\,dk_{z_j} = 0. \tag{20}$$

Equating the expressions in the curly brackets to zero, we obtain the system of equations

$$\psi_j(\varkappa) - \frac{2m\beta}{\hbar^2}\sum_{s=1}^{N}\iint\frac{\exp(ika_{js})\,\psi_s(q\sin\theta_{js} + \varkappa\cos\theta_{js})}{q^2 + k^2 + \varkappa^2 - 2mE/\hbar^2}\,dq\,dk = 0,$$
$$j = 1, 2, \ldots, N. \tag{21}$$

The integration with respect to k is elementary. In addition, at $s = j$, when $\theta_{js} = 0$ and $a_{js} = 0$, we can also integrate with respect to q, but the corresponding interval diverges. As already indicated above, this divergence is connected with the limiting localization of the potential. In this case, the divergence is eliminated by cutting off the integral at large momenta $k_0 \sim 1/b$. (We recall that $\beta \sim U_0 b^2$, where b is the Burgers vector.) After performing the indicated integrations and introducing the dimensionless parameter $\lambda = 2\pi m\beta\hbar^{-2}$, the system (21) can be written in the following form, which can be conveniently investigated:

$$\psi_j(\varkappa) - \frac{\lambda}{f(\varkappa)} \cdot$$

$$\times \sum_{s\neq j} \int_{-\infty}^{\infty} \frac{\exp[-a_{js}(q^2 - 2\varkappa q\cos\theta_{js} + \varkappa^2 - 2mE\hbar^{-2}\sin^2\theta_{js})^{1/2}/\sin\theta_{js}]}{(q^2 - 2\varkappa q\cos\theta_{js} + \varkappa^2 - 2mE\hbar^{-2}\sin^2\theta_{js})^{1/2}}$$

$$\times \psi_s(q)\,dq = 0, \tag{22}$$

$$f(\varkappa) = 1 - \lambda\ln\left(1 + \frac{k_0^2}{\varkappa^2 - 2mE/\hbar^2}\right). \tag{22'}$$

The energy eigenvalues are determined from the condition that the system (22) have a nontrivial solution. Its study must be started with a consideration of the particular cases N = 1 and N = 2.

1) N = 1. If there is only one dislocation, then the system (22) reduces to the single equation

$$\psi(\varkappa)\left[1 - \lambda\ln\left(1 + \frac{k_0^2}{\varkappa^2 - 2mE/\hbar^2}\right)\right] = 0. \tag{23}$$

The general solution of (23) is

$$\psi(\varkappa) = C_1\delta\left(\varkappa - \frac{1}{\hbar}\sqrt{2m(E - E_\perp)}\right) + C_2\delta\left(\varkappa + \frac{1}{\hbar}\sqrt{2m(E - E_\perp)}\right), \tag{24}$$

where C_1 and C_2 are arbitrary constants and the "transverse" energy is given by

$$E_\perp = -\hbar^2 k_0^2 / 2m(e^{1/\lambda} - 1). \tag{25}$$

It is assumed in (24) that $E > E_\perp$, for with $E < E_\perp$ there is no nontrivial solution of (23). Equation (24) is a formal expression of the already discussed result, namely that the electron is captured by a two-dimensional potential well (the energy of the bound state is $E_\perp$) and moves freely along the dislocation—along its potential "corridor" in the direction of the z axis.

We introduce the transverse momentum defined by the relation

$$k_\perp^2 = -2mE_\perp / \hbar^2 = k_0^2 / (e^{1/\lambda} - 1). \tag{26}$$

If we substitute (24) in (19), then we can calculate the wave function $\psi(\mathbf{k})$. It turns out here that in the coordinate representation the wave function decreases like $\exp(-k_\perp r)$ at large distances r from the dislocation axis. By the same token we confirm formally that the dislocation radius of a two-dimensional wave function is given by (3). It is seen from (26) that $k_\perp$, and consequently also the localization radius, are exceedingly sensitive to changes of the parameter λ. It is clear, however, that in practice, we always have $k_\perp \lesssim k_0$. So long as λ is sufficiently small, we have $k_\perp \sim k_0\exp(-1/2\lambda) \ll k_0$.

An important role in the subsequent analysis is played by the behavior of the function (22′). This function has a root κ_* only in the case when $E > E_\perp$. The asymptotic form of $f(\kappa)$ at small κ and $\epsilon = E_\perp - E$ is

$$f(\varkappa) \approx \frac{\lambda}{k_\perp^2}\left(\varkappa^2 + \frac{2m\varepsilon}{\hbar^2}\right). \tag{27}$$

2) N = 2. In this case the system (22) consists of two equations. We write out only one of them, since the other is obtained simply by replacing the indices $1 \rightleftarrows 2$. In addition, to simplify the notation we put $a_{12} = a$ and $\theta_{12} = \theta$:

$$\psi_1(\varkappa) - \frac{\lambda}{f(\varkappa)}\int_{-\infty}^{\infty} \frac{\exp[-a(q^2 - 2\varkappa q\cos\theta + \varkappa^2 - 2mE\hbar^{-2}\sin^2\theta)^{1/2}/\sin\theta]}{(q^2 - 2\varkappa q\cos\theta + \varkappa^2 - 2mE\hbar^{-2}\sin^2\theta)^{1/2}}$$

$$\times \psi_2(q)\,dq = 0. \tag{28}$$

We shall investigate the system (28) under the assumption that $ak_\perp \gg 1$. This means that the dislocations are separated by a distance much larger than the localization radius of the "single-particle" wave function. The object of the analysis will be the region of the discrete spectrum. The corresponding wave function of the k-representation should not have any poles on the real k axis. Yet it is seen from (28) that when $E > E_\perp$ the function $\psi_1(\kappa)$ (meaning, in accordance with (19), also $\psi(\mathbf{k})$) has a pole at the point $\kappa = \kappa_*$, which is a root of the function $f(\kappa)$. When making this statement, we took into consideration the fact that there are no physical reasons why the integral in (28) should vanish at the same point. Consequently, the sought energy levels lie in the region $E < E_\perp$. It is physically obvious that at $ak_\perp \gg 1$ the three-dimensional discrete level (or levels) should be separated only slightly from the edge of the continuous spectrum, i.e., $\epsilon \ll |E_\perp|$. But in this case the wave function decreases very slowly along the dislocation axis. For the k-representation this means that the functions ψ_1 and ψ_2 are noticeably different from zero only at small values of the arguments; more accurately speaking, as will be subsequently verified, at q, $\kappa \ll \kappa_\perp\sin\theta$. The last argument is confirmed also by the fact that the "unperturbed" functions ψ_1 and ψ_2 are exact δ functions, and the perturbation is assumed weak.

Taking all the foregoing into account, we can expand the argument of the exponential in (28) in powers of small q and κ, put in the denominator q = κ = 0, replace E by $E_\perp$ in the integrand, and confine ourselves to the asymptotic form (27) of the function $f(\kappa)$. We then obtain

$$\psi_1(\varkappa) - \frac{k_\perp e^{-ak_\perp}}{\sin\theta(\varkappa^2 + 2m\varepsilon/\hbar^2)} \tag{29}$$

$$\times \int_{-\infty}^{\infty} \exp\left(-\frac{ak_\perp}{2}\frac{q^2 - 2\varkappa q\cos\theta + \varkappa^2}{k_\perp^2\sin^2\theta}\right)\psi_2(q)\,dq = 0.$$

It is seen from (29) that the integrand is a product of two competing functions: one is maximal at the point $q = \kappa\cos\theta$ and decreases rapidly at distances on the order of $k_\perp\sin\theta\,(ak_\perp)^{-1/2}$, while the other, $\psi_2(q)$, is maximal at zero, and the characteristic distance over which it decreases is determined by the smaller of the two quantities $k_\perp\sin\theta\,(ak_\perp)^{-1/2}$ and $(m\epsilon)^{1/2}/\hbar$. We shall show later that in practice we have for all the values of the parameters of the problem

$$\sqrt{m\varepsilon}/\hbar \ll \sqrt{k_\perp/a}\,\sin\theta. \tag{30}$$

Therefore the function $\psi_2(q)$ is "sharper" than the exponential in (29). We can therefore put q = 0 in the argument of the exponential. Then (29) changes into the degenerate integral equation

$$\psi_1(\varkappa) = \frac{k_\perp\exp(-ak_\perp - a\varkappa^2/2k_\perp\sin^2\theta)}{(\varkappa^2 + 2m\varepsilon/\hbar^2)\sin\theta}\int_{-\infty}^{\infty}\psi_2(q)\,dq. \tag{31}$$

From this, in particular, follows the statement made concerning the distances over which the function $\psi_1(\kappa)$ decreases.

The system of integral equations corresponding to (31) now reduces to a system of two linear equations with two unknown numbers (the integrals of ψ_1 and ψ_2).

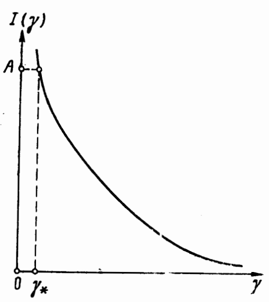

FIG. 3

Equating its determinant to zero, we obtain an equation for the determination of the spectrum:

$$\frac{k_\perp e^{-ak_\perp}}{\sin\theta}\int_{-\infty}\frac{\exp(-a\varkappa^2/2k_\perp\sin^2\theta)\,d\varkappa}{\varkappa^2+2m\varepsilon/\hbar^2}=\pm 1. \tag{32}$$

Since $\epsilon > 0$ ($E < E_\perp$), Eq. (32) can have a solution only if the plus sign is chosen in the right-hand side. This choice of the sign corresponds to a symmetrical wave function ($\psi_1(q) \equiv \psi_2(q)$). To find ϵ from (32), we change over to integration with respect to the dimensionless variable $t = (ak_\perp/2)^{1/2}\kappa/k_\perp \sin\theta$, and introduce the dimensionless parameter

$$\gamma=\left(\frac{\varepsilon a k_\perp}{2|E_\perp|}\right)^{1/2}\frac{1}{\sin\theta}. \tag{33}$$

Equation (32) can then be rewritten in the form

$$I(\gamma)\equiv\int_{-\infty}^{\infty}\frac{e^{-t^2}\,dt}{t^2+\gamma^2}=A \quad \equiv\left(\frac{2}{ak_\perp}\right)^{1/2}\sin^2\theta e^{ak_\perp}. \tag{34}$$

The integral in the left-hand side of (34) is expressed in terms of the probability integral. We, however, are interested only in the asymptotic forms of $I(\gamma)$ at small and large values of the argument: $I(\gamma) \approx \pi/\gamma$ at $\gamma \ll 1$ and $I(\gamma) \approx \pi^{1/2}/\gamma^2$ at $\gamma \gg 1$.

Figure 3 shows a graphic solution of Eq. (34). It is obvious from Fig. 3 that there is only one solution. This means that in a system of two crossing dislocations there is only one three-dimensional bound state of the electron. The origin of this state can be clearly explained in the following manner. The electron is captured in the dislocation potential corridor, along which it moves freely. In the place where one dislocation is closest to another, there is a definite (albeit quite small) probability of tunneling from one dislocation to the other. By the same token, the electron becomes localized in the region where the dislocations come close together.

The energy of such a bound state is somewhat smaller than $E_\perp$, and for a more accurate determination of this energy we reason as follows. Let the sought energy $\epsilon \equiv E_\perp - E$ be such that the corresponding root of Eq. (34) is $\gamma_* \ll 1$. For the solution of this equation we then use the asymptotic form of $I(\gamma)$ at small γ, and obtain the answer in the form

$$\varepsilon/|E_\perp|=\pi^2 e^{-2ak_\perp}/\sin^2\theta. \tag{35}$$

It is seen from (35) and (33) that in this case

$$\gamma_*=\pi(ak_\perp/2)^{1/2}e^{-ak_\perp}/\sin^2\theta. \tag{36}$$

Since we have assumed that $ak_\perp \gg 1$, it is obvious that the inequality $\gamma_* \ll 1$ is satisfied practically for all angles, with the exception of a small vicinity near zero angle. This region is determined by the inequality $\theta \lesssim e^{-1/2 ak_\perp}(ak_\perp)^{1/4}$ and is exponentially small when $ak_\perp \gg 1$, so that from the practical point of view it can be disregarded, since the dislocations cannot be strictly parallel.

By the same token, we obtain the position of the discrete level in explicit form, and, in addition, we verify the inequality (30). Since the gap ϵ between the energy of the discrete level and the edge of the continuous spectrum is exponentially small, the radius of the localization of the corresponding finite motion along the dislocation, the order of magnitude of which is $\hbar(m\epsilon)^{-1/2}$ (see (31)), is exponentially large $\sim(\exp[ak_\perp])$. This means that in this state, too, the electron moves along the dislocation almost freely. This leads precisely to the statement made at the beginning of this section to the effect that allowance for the translations along the dislocation axes cannot greatly influence the spectrum of the dislocation band in the considered case of a short-range potential.

It is seen from (35) that the main influence on the position of the discrete level is exerted by the distance between the dislocations whereas the influence of the angle between them is appreciably smaller. At a fixed distance a, the smallest gap is obtained for mutually-perpendicular dislocations. With decreasing angle θ, this splitting increases, and formula (35) remains valid all the way to exponentially small angles. At such angles, when the condition for the validity of Eq. (34) is already violated, a qualitatively correct answer for ϵ (accurate to within the pre-exponential factor) can nevertheless be obtained from (34) by using the asymptotic form of $I(\gamma)$ at large values of γ. The same results can also be derived from formula (35) by putting $\gamma_* \sim 1$, i.e., $\theta \sim \exp(-\frac{1}{2}ak_\perp)$. By any of these methods we obtain

$$\varepsilon/|E_\perp|\approx(2\pi/ak_\perp)^{1/2}e^{-ak_\perp}. \tag{37}$$

Consequently, at very small angles θ, the splitting ceases to depend on θ and increases substantially in comparison with (35). This is apparently connected with the large effective overlap of the "single-particle" wave functions in the case of almost parallel dislocations. Incidentally, the case of strictly parallel dislocations can be investigated quite simply. To this end, it is convenient to start directly from (21)

$$\psi_1(k_z)f(k_z)-\lambda\psi_2(k_z)\int_{-\infty}\frac{\exp[-a(k_x^2+k_z^2-2mE\hbar^{-2})^{1/2}]\,dk_x}{(k_x^2+k_z^2-2mE\hbar^{-2})^{1/2}}=0.$$

The problem now becomes two-dimensional, the motion of the electron along the z axis is free, and we are dealing with determination of the shift of the transverse energy, i.e., the quantity ϵ in the relation $E = \hbar^2k_z^2/2m + E_\perp + \epsilon$. The calculation of this shift at $ak_\perp \gg 1$ is carried out in the same manner as before, and the result is

$$\varepsilon=\pm(2\pi/ak_\perp)^{1/2}e^{-ak_\perp}. \tag{38}$$

Unlike the case of nonparallel dislocations, the two-dimensional state is split here into two (the ± sign), but both these states pertain already to the continuous spectrum, whereas in the case of crossing dislocations only one state of the discrete level was split off. As seen from (37) and (38), at very small angles the energy of the discrete level comes close to the lower limit of the continuous spectrum, and a transition from finite to infinite motion of the electron along the dislocation takes place.

Let us proceed to study a system of N dislocations. We assume that the dimensionless parameter $k_\perp c^{-1/2}$ is much larger than unity. Usually, the dislocation concentration is $c \sim 10^6-10^{10}$ cm^{-2}, and $k_\perp$ is a quantity of the order of 10^8-10^6 cm^{-1}, so that the indicated parameter is always large in real situations. Therefore the distances between the dislocations a_{js} should be regarded as large. Using this circumstance, and also assuming that the angles θ_{js} between the dislocations are not exponentially small, we can reduce the system of integral equations (22) to a system of degenerate integral equations, i.e., in essence to a system of linear algebraic equations. The method of such a reduction was given above for the case of two dislocations. The characteristic equation of the system obtained in this manner is of the form

$$\begin{vmatrix} -\sqrt{\dfrac{\varepsilon}{|E_\perp|}} & \dfrac{\pi e^{-a_{12}k_\perp}}{\sin\theta_{12}} & \dfrac{\pi e^{-a_{13}k_\perp}}{\sin\theta_{13}} & \cdots \\ \dfrac{\pi e^{-a_{12}k_\perp}}{\sin\theta_{12}} & -\sqrt{\dfrac{\varepsilon}{|E_\perp|}} & \dfrac{\pi e^{-a_{23}k_\perp}}{\sin\theta_{23}} & \cdots \\ \dfrac{\pi e^{-a_{13}k_\perp}}{\sin\theta_{13}} & \dfrac{\pi e^{-a_{23}k_\perp}}{\sin\theta_{23}} & -\sqrt{\dfrac{\varepsilon}{|E_\perp|}} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix} = 0. \tag{39}$$

If we introduce the unknown x in accordance with the relation $x = -(\epsilon/|E_\perp|)^{1/2}$ and perform the calculation with logarithmic accuracy (i.e., we disregard $\sin\theta_{js}$ in the denominators of the matrix elements), then it is easy to establish the formal analogy between Eq. (39) and the characteristic equation given in the paper of I. Lifshitz[3] for the case of pointlike impurities. The only but quite important difference between these equations is that in our case it is necessary to take into consideration only the negative roots x of Eq. (39).

To explain better the situation arising here, let us consider a concrete example of three mutually perpendicular dislocations with $\theta_{12} = \theta_{13} = \theta_{23} = \pi/2$. Without loss of generality we can assume that the distance a_{12} is smaller than the other two distances. Then Eq. (39) takes the form

$$x^3 - \pi^2 e^{-2a_{12}k_\perp} x + 2\pi^3 e^{-(a_{12}+a_{13}+a_{23})k_\perp} = 0. \tag{40}$$

Equation (40) has one negative root corresponding to a state collectivized between the two closest-lying dislocations, and two positive roots, which should simply be discarded. We recall that in the case of three impurities[3] the situation is entirely different, namely, one of the positive roots and the negative root correspond to pairing of the states near centers 1 and 2, while the third root corresponds to a state localized near the center 3. This difference between the situations is due to the absence of a three-dimensional bound state near the individual isolated dislocation. The bound state is due to the presence of a pair of dislocations.

The formal equivalence of the characteristic equation (39) and of the corresponding equation of[3] makes it possible to extend to our situation the main conclusions obtained in[3]. We make use of the fact that the main contribution to the density of states is made by states localized near pairs of nearest dislocations. Naturally, in our case we are dealing with discrete-spectrum levels for which $E < E_\perp$.

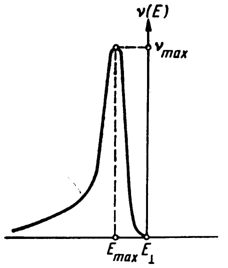

FIG. 4

If we take into account only the influence of the nearest neighbors on the formation of the spectrum, then the density of states (normalized to one dislocation), as shown in[3], can be calculated in accordance with the formula

$$\nu(\varepsilon) = ce^{-cS(\varepsilon)}\left|\frac{dS(\varepsilon)}{d\varepsilon}\right|, \quad \varepsilon = E_\perp - E, \tag{41}$$

where $S(\epsilon)$ is the cross-sectional area of a cylinder surrounding the given dislocation and such that if the nearest dislocation crosses this cylinder, then the energy of the corresponding bound state $\epsilon(a, \theta)$, calculated from formula (35), is larger than the given energy ϵ.

Let us calculate the density of states with logarithmic accuracy, i.e., we disregard the influence of the angle θ. Then $S(\epsilon) = (4k_\perp^2)^{-1} \cdot \ln^2(\epsilon/|E_\perp|)$ and

$$\nu(\varepsilon) = \frac{c}{2k_\perp^2}\frac{1}{\varepsilon}\left|\ln\frac{\varepsilon}{|E_\perp|}\right| \quad \exp\left(-\frac{c}{4k_\perp^2}\ln^2\frac{\varepsilon}{|E_\perp|}\right). \tag{42}$$

A plot of the state density (42) is shown in Fig. 4.

The maximum value of the density of states is obtained at the point $E_{\max}$, which is located very close ($\sim\exp[-2k_\perp^2/c]$) to the edge of the continuous spectrum. In the vicinity of the maximum, the width of which is of the order of $|E_\perp|\exp(-k_\perp^2/c)$, the density of states $\nu_{\max}$ is quite large (proportional to $\exp[-k_\perp^2/c]$). A comparison of the data of Fig. 4 with formula (35) shows that the main contribution to the quantum part of the density of states is made by dislocations located at distances $c^{-1/2}(k_\perp c^{-1/2})$ greatly exceeding the mean values. Yet, as we have seen earlier, the classical concentration broadening is due mainly to dislocations that are separated from one another by average distances of the order of $c^{-1/2}$.

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