Fluctuation Levels of an Electron in a System of Disordered Short-range Dislocations

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We have investigated the fluctuation region of the electron energy spectrum in a system of disordered short-range dislocations. In the case of an attraction potential, the asymptotic form of the density of the lowlying levels obeys a power law. For a repulsion potential, the density of state near the true end of the point of the spectrum has the same form as in a two-dimensional system of disordered impurities. We have also investigated the structure of the spectrum near the mean potential, irrespective of the sign of the interaction between the electron and the dislocation.

1. INTRODUCTION

THE determination of the structure of the electronic energy spectrum of disordered systems is one of the principal problems of physics of the condensed state of matter. In the simplest model, this spectrum was determined from the solution of the Schrödinger equation for a particle moving in a random potential field (see, for example,[1,2]). In most papers, the origin of the random field is either not specified concretely at all, or else is connected with the presence of disordered "point" defects (impurities, vacancies, etc.). In pure crystals, however, a random potential can be generated by a system of disordered dislocations. A distinguishing feature of these dislocations is the fact that they have length, which affects substantially the structure of the electronic energy spectrum[3]. Just like point defects, disordered dislocations can lead to the appearance of new allowed values of the energy and to an essential change in the density and in the character of the quantum states in the initial spectra. In particular, a new section of the spectrum may arise near a level corresponding to a two-dimensional bound state of an electron on an individual dislocation[4]. The corresponding quantum states are localized on two or several dislocations, the distances between which can greatly exceed the mean values. In the present paper we investigate the fluctuation region of the spectrum, corresponding to states localized on macroscopic clusters of dislocations.

Considering the simplest model, we shall assume that the dislocations are linear and pass through the entire crystal. The parameters determining the positions of the individual dislocations are assumed to be independent and uniformly distributed random quantities (an ideal gas of extended defects). Therefore the only characteristic of such an ensemble is the average distance l_0 between dislocations that are parallel to an arbitrary direction. We consider dislocations with randomly distributed directions. The average distance between them, determined in the usual manner, is $l_0(2\pi)^{-1/2}$. The potential of the individual dislocations does not depend on the coordinate along its axis and is equal to $-\beta u(\mathbf{R}_\perp)$ ($\hbar^2/2m = 1$), where $\mathbf{R}_\perp$ is a two-dimensional radius vector in a plane perpendicular to the dislocation axis, and $u(\mathbf{R}_\perp)$ is a delta-like function with smearing radius a and normalization $\int u d\mathbf{R}_\perp = 1$. The dimensionless parameter β determines the intensity of the dislocation potential. Positive β correspond to attraction of an electron by a dislocation, and negative ones to repulsion. Such a model describes, in particular, charged dislocations in semiconductors. In this case a coincides in order of magnitude with the screening radius of the charge connected with the dislocation. For a reasonable dislocation density, present estimates of a[3] indicate a ratio $l_0/a \gg 1$. In some case (for example, in metals), a decisive role is played by the interaction between the electrons and the long-range deformation potential. The structure of the energy spectrum is then quite distinct, and its study calls for a separate analysis.

In the description of the fluctuation region of the spectrum, it is natural to introduce the local dimensionless concentration ρ_n of the dislocations parallel to the direction n ($n^2 = 1$):

$$\rho_n(\mathbf{X}_n) = \frac{l_0^2 dN_n(\mathbf{X}_n)}{d^2\mathbf{X}_n}.$$

Here $\mathbf{X}_n$ is the two-dimensional radius vector in a plane perpendicular to n, the area element $d^2\mathbf{X}_n$ is intersected by a large number $dN_n(\mathbf{X}_n)$ of dislocations, but its dimensions are small compared with the fluctuation radius. Since the quantity $\rho_n(\mathbf{X}_n)$ is equal to the number of parallel dislocations intersecting an area l_0^2 perpendicular to them, a homogeneous dislocation distribution corresponds to a concentration $\rho_0 = 1$.

In the limiting case $|\beta| \ll 1$ (for concreteness we consider an attraction potential), the field of the individual dislocation contains a two-dimensional ground state of electrons with energy $|E_\perp| \sim a^{-2}\exp(-\beta^{-1})$, exponentially close to the edge of the initial continuous spectrum $E_k = k^2$. It follows therefore that the accumulation of a large number (relative to the parameter $1/\beta$) of dislocations is necessary for the formation of sufficiently deep levels. In the case of point defects, the theory of such fluctuation levels was constructed by I. Lifshitz[5]. The procedure proposed in[5] can also be used for the following investigation of dislocation fluctuation levels.

2. CALCULATION OF DENSITY OF STATES

1. We introduce the dimensionless radius $\mathbf{r} = \mathbf{R}l_0^{-1}|\beta|^{1/2}$, the two-dimensional radius vector $\mathbf{x}_n = \mathbf{X}_n l_0^{-1}|\beta|^{1/2}$, the two-dimensional concentration

$c_{\mathbf{n}}(\mathbf{x_n}) \equiv \rho_{\mathbf{n}}(\mathbf{X_n})$[1], and the energy $\epsilon = -E l_0^2 \beta^{-1}$ (in the spectral regions of interest to us, $\epsilon > 0$ irrespective of the sign of β). Then the density of states is equal to

$$\nu(E) = l_0^{-2} \nu(\varepsilon) / |\beta|,$$

and $\nu(\epsilon)$ is the ratio of two continual integrals[5]

$$\nu(\varepsilon) = \left(\int e^{S\{c\}} Dc \right)^{-1} \int e^{S\{c\}} \delta[\varepsilon - \varepsilon_0\{c\}] Dc. \tag{1}$$

The symbol c in (1) denotes a set of two-dimensional concentrations $c_{\mathbf{n}}(\mathbf{x_n})$ for all the possible directions of $\mathbf{n}$, and the dimensionless energy $\epsilon_0\{c\}$ corresponds to the ground state of the electron on the fluctuation. The functional $S\{c\}$ represents the change of the entropy of the system as a result of the deviation of the concentration $c_{\mathbf{n}}(\mathbf{x_n})$ from the mean value c_0:

$$S\{c\} = \frac{1}{2|\beta|} \int d\mathbf{n} \int d^2\mathbf{x}_{\mathbf{n}} [\sigma(c_{\mathbf{n}}) - \sigma(c_0) - (c_{\mathbf{n}} - c_0)\sigma'(c_0)], \tag{2}$$

and the quantity $l_0^{-2}\sigma(c)$ is the entropy density of the system of parallel dislocations with homogeneous concentration c.

The presence of the large parameter $|\beta|^{-1}$ in the argument of the exponential allows us to use the saddle-point method in the calculation of the density of states. Since there are no physical considerations that lead to anisotropy of the extremal fluctuations, we can assume that the two-dimensional extremal concentrations $\tilde{c}_{\mathbf{n}}(\mathbf{x_n})$ do not depend on the direction of $\mathbf{n}$: $\tilde{c}_{\mathbf{n}}(\mathbf{x}) \equiv \tilde{c}(\mathbf{x})$. Under this assumption we obtain a system of equations for the sought extremal $\tilde{c}(\mathbf{x})$ and for the corresponding wave function of the ground state $\varphi_0(\mathbf{r})$:

$$\sigma'(c) - \sigma'(c_0) = -\operatorname{sign}\beta \int dz\, \varphi_0^2(\mathbf{x}, z). \tag{3a}$$

$$\operatorname{sign}\beta \Delta\varphi_0 + \left(\frac{1}{2} \int d\mathbf{n} \tilde{c}[\mathbf{r} - \mathbf{n}(\mathbf{rn})] - \varepsilon \right) \varphi_0 = 0 \tag{3b}$$

with boundary conditions

$$\varphi_0|_\infty = (\tilde{c} - c_0)|_\infty = 0.$$

Unlike the case of pointlike impurities, the right-hand side of (3a) contains a quantity proportional to the probability of finding the electron at a given point of $\mathbf{x}$-space, and the additional integration with respect to the third coordinate is connected precisely with the fact that the dislocation has length. The expression

$$\tilde{c}_3(\mathbf{r}) = \frac{1}{2} \int d\mathbf{n}\, \tilde{c}[\mathbf{r} - \mathbf{n}(\mathbf{rn})] \tag{4}$$

has a simple physical meaning: if we represent the dislocation as an aggregate of point defects located along its axis, then $\tilde{c}_3(\mathbf{r})$ is the three-dimensional concentration of these defects on the extremal fluctuation.

The principal term $\nu_0(\epsilon)$ in the expression for the density of states is connected with the solution of the system (3) by the relation

$$\ln \nu_0(\varepsilon) = \frac{\pi}{|\beta|} \int d^2\mathbf{x} [\sigma(\tilde{c}) - \sigma(c_0) - (\tilde{c} - c_0)\sigma'(c_0)]. \tag{5}$$

2. We investigate first the behavior of the density of states in the vicinity of the mean potential $\epsilon = 2\pi$. This region of the spectrum is defined by the inequality

$$0 < \xi = (\varepsilon - 2\pi) \operatorname{sign}\beta \ll 1.$$

We shall consider henceforth isotropic two-dimensional fluctuations of $\tilde{c}(x)$, which are connected, by virtue of (4), with the three-dimensional concentration $\tilde{c}_3(r)$ by the relations

$$\tilde{c}_3(r) = \frac{2\pi}{r} \int_0^r \frac{x\tilde{c}(x)\,dx}{\sqrt{r^2 - x^2}}, \tag{6}$$

$$\tilde{c}(x) = \frac{1}{\pi^2} \int_0^x \frac{c_3(r) + rc_3'(r)}{\sqrt{x^2 - r^2}}. \tag{7}$$

In the investigated region of the spectrum, the presence of the small parameter ξ allows us to assume that the extremal concentration $\tilde{c}(x) \equiv c_0 + \delta(x)$ differs little from the average concentration, so that $|\delta(x)| \ll c_0$. In this case the left-hand side of Eq. (3a) is simply $\sigma''(1)\delta(x)$. Substituting the obtained expression for $\delta(x)$ in (3b) and carrying out a scale transformation

$$r = r'\xi^{-1/2}, \quad x = x'\xi^{-1/2}, \quad z = z'\xi^{-1/2},$$

$$\varphi_0^2(x, z) = \frac{\xi^{3/2}|\sigma''(1)|}{2\pi} \varphi^2(x', z'),$$

we arrive at an equation without parameters

$$\Delta'\varphi - \varphi + \frac{\varphi}{r'} \int_0^{r'} dx'' \int_{-\infty}^{\infty} dz'' \frac{x''\varphi^2(x'', z'')}{\sqrt{r'^2 - x''^2}} = 0.$$

Therefore the fluctuation of the concentration

$$\delta(x) = \operatorname{sign}\beta \frac{\xi}{2\pi} \Phi(x') \equiv \operatorname{sign}\beta \frac{\xi}{2\pi} \int_{-\infty}^{\infty} dz' \varphi^2(x', z')$$

turns out to be of the order of $\xi \ll 1$, which justifies the assumptions made. For the principal term in the density of states we obtain in accordance with (5)

$$\ln \nu_0(\varepsilon) = \frac{2\pi^2}{|\beta|} |\sigma''(1)| \int \delta^2(x)\, x\, dx = -\frac{\xi|\sigma''(1)|}{2|\beta|} \Phi_2, \tag{8}$$

where the numerical constant Φ_2 is determined from the formula

$$\Phi_n = \int_0^{\infty} \Phi^n(t)\, t\, dt.$$

As seen from (8), in the immediate vicinity of the average potential $\xi \ll 1$, the quantity $|\ln \nu_0(\epsilon)|$ is not too large. In this connection, it is of interest to obtain the preexponential factor in the expression for $\nu(\epsilon)$. The calculations are carried out in accordance with the well-known scheme[5] and lead to the following result for the density of states:

$$\nu(\varepsilon) \sim \left| \frac{\sigma''(1)}{\beta\xi} \right|^{1/2} \exp\left[-\frac{\Phi_2}{2} \left| \frac{\sigma''(1)}{\beta} \right| \xi \right]. \tag{9}$$

The entire analysis in this subsection was carried out in terms of the arbitrary function $\sigma(c)$. However, the succeeding calculations can be carried through to conclusion only if account is taken of the concrete dependence of the entropy on the concentration. For concreteness, we shall consider henceforth the simplest model of an ideal gas of dislocations, corresponding to

$$\sigma(c) = -c \ln(c/e). \tag{10}$$

3. With increasing deviation from the mean potential, the dislocation concentration in the region of the fluctuation differs considerably from the mean concentration. The method described above cannot be used in this case and it would be necessary, strictly speaking, to

[1] By virtue of the definition of the quantity $\rho_{\mathbf{n}}(\mathbf{X_n})$, a uniform distribution of the dislocations in a plane corresponds to a concentration $c_0 = 1$. In some of the succeeding problems, however, we retain the symbol c_0, since it leads to more symmetrical expressions.

solve the system (3) exactly, a complicated mathematical problem. However, since the density of states is not very sensitive to the details of the form of the fluctuation, we shall employ a direct variational method.

When choosing the appropriate class of trial functions, we note the following. For all two-dimensional concentrations c(x) such that $(c - c_0)$ sign $\beta > 0$ and[2)]

$$\left| \int [c(x) - c_0] x\, dx \right| < \infty,$$

relation (6) leads to the asymptotic form

$$c_3(r) \simeq 2\pi c_0 + \frac{2\pi}{r^2} \int_0^\infty [c(x) - c_0] x\, dx. \tag{11}$$

The result (11) is obvious, since the aggregate of finite-radius dislocation tubes emerging from the center of the fluctuation transfers to the point r a potential proportional to the solid angle at which the nucleus of the fluctuation is seen from the point of observation.

It is therefore natural to consider a class of trial functions of the form

$$c_3(r) = \begin{cases} 2\pi c_1, & r < r_0, \\ 2\pi c_0 + 2\pi (c_1 - c_0) r_0^2 / r^2, & r > r_0. \end{cases} \tag{12}$$

Here the variational parameters are the radius r_0 and the concentration c_1 at the nucleus of the fluctuation.

Substituting (12) in the Schrödinger equation (3b) we obtain an equation for the spectrum. This equation leads to a definite connection between the ground-state energy ϵ and the parameters r_0 and c_1. For all the values of ϵ of interest to us, this connection is given by

$$r_0 \sqrt{(2\pi c_1 - \varepsilon) \operatorname{sign} \beta} = q(c_1, \varepsilon), \tag{13}$$

where the slowly-varying function $q(c_1, \epsilon) \sim 1$ is positive everywhere and does not exceed π.

After determining from (7) the concentration $\tilde{c}(x)$ corresponding to the assumed approximation $c_3(r)$ (12) and substituting into the expression for the density of states (5), we get

$$\ln \nu_0(\varepsilon) = -\frac{2\pi^2}{\beta} \frac{q^2(c_1, \varepsilon)}{(2\pi c_1 - \varepsilon)} \left[c_1 \ln \frac{c_1}{e} + 1 + 2I(c_1) \right], \tag{14}$$

where

$$I(c_1) = \int_0^{\pi/2} dt \frac{\cos t}{\sin^3 t} \{ [1 + (c_1 - 1) f(t)] \ln [1 + (c_1 - 1) f(t)] - (c_1 - 1) f(t) \}, \tag{15}$$

and $f(t) = (2t - \sin 2t)/\pi$.

It is convenient to analyze (14) separately for attraction or repulsion of an electron by a dislocation.

We consider first the attraction ($\beta > 0$). It is physically understandable that in this case, in the far region of the spectrum $\epsilon \gg 1$, the concentration c_1 is much larger than the average concentration $c_0 = 1$, so that $c_1 \gg 1$ in (15) and therefore

$$I(c_1) \approx \tfrac{1}{2} c_1 \ln (c_1 / e),$$

and

$$\ln \nu_0(\varepsilon) \approx -\frac{2\pi}{\beta} \frac{c_1 \ln (c_1/e)}{c_1 - \varepsilon/2\pi} q^2(c_1, \varepsilon). \tag{16}$$

After minimizing (16) with respect to the parameter c_1 and neglecting the derivative $\partial q / \partial c_1$, we obtain

$$\nu_0(\varepsilon) \sim (\varepsilon / 2\pi)^{-2\pi q^2/\beta}, \tag{17}$$

$$c_1 \approx \frac{\varepsilon}{2\pi} \ln \frac{\varepsilon}{2\pi}, \quad r_0 \approx q \left(\varepsilon \ln \frac{\varepsilon}{2\pi} \right)^{-1/2}. \tag{18}$$

In the case of a repulsion potential ($\beta < 0$) there exists a true end point of the spectrum $\epsilon = 0$. The states near this point ($\epsilon \ll 1$) are realized on fluctuations of large radius $r_0 \gg 1$ and small dislocation concentration $c_1 \ll 1$, and in this case $q(c_1, \epsilon)$ tends to π. To determine the density of states, it suffices therefore to put $q = \pi$ and $c_1 = 0$ in (14), after which we get

$$\ln \nu_0(\varepsilon) \approx -\frac{2\pi^4}{\varepsilon |\beta|} [1 + 2I(0)]. \tag{19}$$

The concentration c_1 at the nucleus of the extremal fluctuation is determined, just as before, by minimizing expression (14) and is equal to

$$c_1 \approx \exp \left\{ -\frac{2\pi}{\varepsilon} [1 + I(0)] \right\}, \tag{20}$$

while the radius of the nucleus of the fluctuation, as follows from (13) and (20), is

$$r_0 \simeq \pi \varepsilon^{-1/2}. \tag{21}$$

In the vicinity of the mean potential we have $|\epsilon - 2\pi| \ll 1$ and $|c_1 - c_0| \ll 1$, and by using the procedure described above we obtain for the density of states

$$\ln \nu_0(\varepsilon) = -Q(\varepsilon - 2\pi)/\beta, \quad Q \sim 1, \tag{22}$$

which differs only by a numerical factor ~ 1 from expression (8).

3. DISCUSSION OF RESULTS

Since the physical situation depends significantly on whether the electron is attracted or repelled by the dislocation, the results must be analyzed separately for $\beta > 0$ and $\beta < 0$.

1. Attraction ($\beta > 0$). As already noted, in this case there are two characteristic values of the energy, the mean potential $|E_c| \sim \beta l_0^{-2}$ and the energy of the two-dimensional bound state on an individual dislocation $|E_\perp| \sim a^{-2} \exp(-\beta^{-1})$ (see Fig. 1). Depending on the relation between the dislocation concentration $(a/l_0)^2 \ll 1$ and the coupling constant β, the "transverse" energy $E_\perp$ can be either larger or smaller than the mean potential E_c.

a) We consider first the case $|E_c| \gg |E_\perp|$ (Fig. 1a). The smallest parameter of the problem is in this case β, so that the inequality

$$\beta \exp(\beta^{-1}) \gg (l_0/a)^2 \gg 1 \tag{23}$$

is satisfied. The density of states for deep levels $|E| \gg |E_c|$ is then determined by formula (17). We see that the length of the dislocations leads to a slower

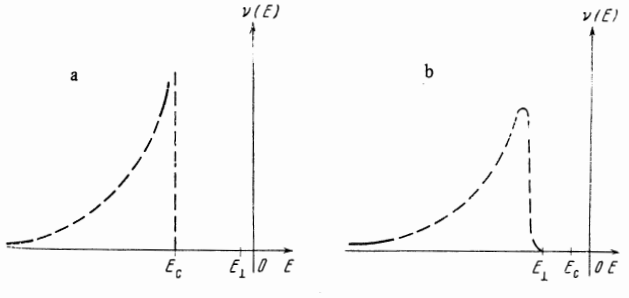

FIG. 1

[2)]The condition that follows is connected with the conservation of the total number of dislocations in the system.

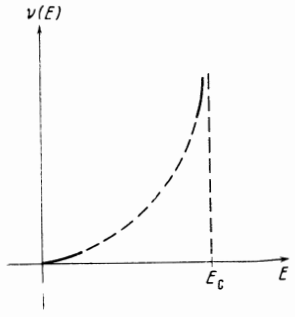

FIG. 2

(power-law) decrease of the density of states on the tail of the spectrum, as distinguished from the exponential decrease characteristic of point defects[6]. The characteristic dimension of the extremal fluctuation is $R_0 \sim l_0\beta^{-1}|E/E_c|^{-1/2}$, and the average distance between dislocations is $l \sim l_0 c_1^{-1/2} = l_0|E/E_c|^{-1/2}$, so that the excess number of dislocations on the fluctuation is $N \sim (R_0/l)^2 \sim \beta^{-1}$. The wave function of the electron is localized over a distance on the order of R_0.

The region of applicability of formula (17) is bounded from below by the condition $|E| \ll |E_c|(l_0/a)^2$, since the distance l for deeper levels becomes of the order of the interatomic distance, and a description of such a formation in dislocation terms becomes meaningless.

In the vicinity of the mean potential, to the left of the point E_c($|(E - E_c)/E_c| \ll 1$), the density of states is given by formula (9). The inaccuracy δE in the determination of the position of the dislocation level, which is connected with the macroscopic description, is of the order of $|\delta E| \sim \beta|E - E_c| \ll |E - E_c|$. The requirement that the density of states be exponentially small does not make it possible to assume the energy in formula (9) to be too close to E_c:

$$\left|\frac{E-E_c}{E_c}\right| \gg \beta|\ln\beta|.$$

The excess number of dislocations on the fluctuation in this region of the spectrum is $N \sim \beta^{-1}$.

b) With decreasing concentration, the point E_c on Fig. 1 approaches $E_\perp$. Levels close to E_c can be realized on clusters with a small number $N \sim 1$ of dislocations already when $\beta\exp(\beta^{-1}) \gtrsim (l_0/a)^2$, and the approach developed above does not hold in the region $E \to E_c$. At the same time, at these and lower concentrations, $(l_0/a)^2 \gg \beta\exp(\beta^{-1})$ (see Fig. 1b), formula (17) for the tail of the density of states remains valid as before, but the condition for its applicability takes the form

$$\left(\frac{l_0}{a}\right)^2 \gg \left|\frac{E}{E_c}\right| \gg \frac{(l_0/a)^2}{\beta\exp(\beta^{-1})}. \qquad (24)$$

In the case of strong attraction ($\beta \sim 1$), the deep levels $|E| \ll |E_\perp|$, just as for $\beta \ll 1$, are due to fluctuations, but each of them corresponds to many almost equally-probable fluctuations. Therefore the use of the saddle-point method to calculate the functional integral (1) is not justified and the result (17) is incorrect (the latter is also confirmed by the fact that when $\beta \sim 1$ the inequality (24) "collapses"). At the same time, a spectrum region adjacent on the left to $E_\perp$[4] is distinctly formed (dashed curve on Fig. 1b).

2. Repulsion ($\beta < 0$). In this case the only characteristic energy is the mean potential $E_c \sim |\beta|l_0^{-2}$ (see Fig. 2). In the vicinity of the mean potential, to the left of E_c, the density of states is determined by formula (9), the applicability of which is limited by the conditions $1 \gg |(E - E_c)/E_c| \gg \beta\ln|\beta|$. Near the true end point of the spectrum ($E = 0$), expression (19) holds true for the density of states. The levels $E \ll E_c$ correspond to fluctuations with a large radius $R_0 \sim l_0\beta^{-1/2}|E/E_c|^{-1/2}$ and with exponentially small dislocation concentration (20) (rarefaction of the "dislocation cloud"). The wave function of the electron is localized on the nucleus of the fluctuation.

For strong repulsion ($|\beta| \sim 1$) the mean potential ceases to be a singled-out point of the spectrum. States close to E_c can be realized on different microscopic fluctuations, and the density of states is not described by formula (9). Yet the result (19) remains valid in the vicinity of the true end point of the spectrum $E \to 0$, as before. The reason for this is that the large parameter of the theory is in fact not β^{-1} but the deviation of the number of dislocations on the fluctuation from the mean value. For a repulsion potential near the true boundary, this deviation $\Delta N \sim \beta^{-1}E_c/E$ is large even when $\beta \sim 1$.

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