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Large-scale fluctuation potential and state density in doped and strongly compensated semiconductors

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A method is proposed for a self-consistent calculation of the large-scale fluctuation potential in doped and strongly compensated semiconductors with shallow impurities at $T=0$. It is shown that the fluctuation potential can range from zero to the energy difference Δ between the donor and acceptor levels. The position of the Fermi level and the mean value of the potential \bar{V} are determined. The potential probability density function $\mathcal{P}(V)$ is calculated in the energy interval $0 \leq V \leq \Delta$ for a degree of compensation $0.95 \leq K \leq 1$. The large-scale potential causes all the neutral donors to be on the Fermi level at the energy $E=0$, and causes the empty donor states to spread into a band with energies from zero to Δ . The electronic states below the Fermi level arise in the case $a_B^3 \bar{N}_d \ll 1$ only as a result of the Coulomb potential of the nearest empty donor, and in the case $a_B^3 \bar{N}_d \gg 1$ they are due to quantization of the electron in small-radius fluctuations. The tails of the state densities of the valence and empty bands differ in character. The valence band has a deep state-density tail on account of the large-scale potential (when $\bar{N}_d > \bar{N}_a$), while the conduction-band tail is due only to the small-radius fluctuations, in which the quantization is significant.

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INTRODUCTION

An inhomogeneous random distribution of the impurities in doped semiconductors violates the local electroneutrality and accordingly leads to the appearance of an inhomogeneous large-scale potential. It is known from experiment that when the degree of compensation is increased, the activation energy for the conductivity increases.¹⁻⁵ The influence of a fluctuation potential on the electron spectrum was considered in Refs. 6-13. Shklovskii and Efros¹⁰⁻¹² calculated the fluctuation potential in the following manner. They considered fluctuations of arbitrary radius R under the assumption that the impurities are uniformly distributed inside the fluctuation. Since fluctuations of sufficiently small radius cannot be screened by electrons, a "bare" charge appears in the region of the fluctuations, and is equal to $q\Delta N\Omega$, where $\Delta N = N_d - N_a - (\bar{N}_d - \bar{N}_a)$, where N_d and N_a are the concentrations of the donors and acceptors in the fluctuation, \bar{N}_d and \bar{N}_a are the average concentrations of the impurities in the crystal, and Ω is the

volume of the fluctuation. The potential in the region of the fluctuation is in this case approximately equal to $(q^2/\epsilon)\Delta NR^2$.

Assuming a Gaussian distribution for the fluctuations, the mean squared potential is calculated to be

$$\gamma = (q^2/\epsilon) (\bar{N}_d R)^{1/2},$$

from which it follows that without allowance for the screening γ diverges when R is increased.

The characteristic radius at which screening comes into play is estimated in Refs. 10 and 11 from the following considerations: since the mean squared deviation of the concentration decreases when the radius is increased, $\Delta N^2 = \bar{N}_d/R^3$, it follows that at $n > (\Delta N^2)^{1/2}$ ($n = \bar{N}_d - \bar{N}_a$ is the average concentration of the electrons in the free or impurity donor band) the electrons easily screen such fluctuations, and the latter make no contribution to the potential. Thus, the characteristic radius R_c is determined from the relation

$(\Delta N^2)^{1/2} = \bar{N}_d - \bar{N}_a$, and then

$$\gamma \approx \frac{q^2}{\epsilon} \frac{\bar{N}_d^{1/2}}{(1-K)^{1/2}}, \quad R_c^{-1} \approx \bar{N}_d^{1/2} (1-K)^{3/2}.$$

However, these estimates do not determine the fluctuation potential at $K = \bar{N}_d / \bar{N}_a \rightarrow 1$, for in this case γ again diverges. In Ref. 12 was considered the case of a fully compensated semiconductor, and it was shown that the growth of the fluctuation potential as $K \rightarrow 1$ is stopped by screening by electrons and holes from the free and valence bands, respectively. Thus, γ reaches its upper limit $\sim E_g/2$ at $K=1$ (E_g is the width of the forbidden band).

In addition, Shklovskii and Éfros¹¹ considered the influence of a small-scale potential on the position of the Fermi level in a strongly compensated semiconductor. The point is that the donor state can be substantially lowered because of a random approach of two donors to within a short distance, and the lowering of the Fermi level on account of the small-scale potential can become comparable with γ , but the maximum lowering must not exceed $4E_B$, where E_B is the donor ionization energy.

To analyze the large-scale potential in "pure form," the present paper deals with a doped semiconductor with shallow donors, when $E_B \ll \gamma$. The difficulty in the calculation of the large-scale potential lies in the nonlinearity of the screening of the fluctuations at low temperature. We take into account the screening nonlinearity at zero temperature, determine the position of the Fermi level, the probability density of the potential, and accordingly the state density of the local centers in the free and valence bands for a compensation degree K in the range $0.95 < K \leq 1$.

2. THE POISSON EQUATION AND THE CONCEPT OF SCREENED AND UNSCREENED FLUCTUATIONS

We consider a doped and compensated semiconductor. We assume that the doping is weak, that the impurity bands do not overlap the free and valence bands, and that the temperature is low enough so that the electrons and holes are mainly on impurity levels. In this case the fluctuation potential is determined by a Poisson equation of the form

$$\nabla^2 V(r) = \frac{4\pi q^2}{\epsilon} \left[N_d(r) - N_a(r) - \frac{N_d(r)}{1 + \exp(V(r)/kT)} + \frac{N_a(r)}{1 + \exp[(\Delta - V(r))/kT]} \right], \quad (1)$$

where $N_d(r)$ and $N_a(r)$ are the concentrations of the donors and acceptors at each point of the crystal, while the third and fourth terms in the right-hand side of (1) determine respectively the concentrations of the electrons on the donors and of the holes of the acceptors; $\Delta = E_d - E_a$, where E_d and E_a are the positions of the donor and acceptor levels, respectively. The origin of the potential $V(r)$ was chosen such that at $V(r)=0$ the donor level passes through the Fermi level.

We ascertain first of all the possible limits of the potential $V(r)$, meaning the limits of the spectrum for the donor states. Obviously, the maximum potential occurs in the region of large albeit low-probability fluctua-

tions, in which $N_d - N_a > 0$, (large fluctuations—large radius and large $N_d - N_a$), while the maximum potential occurs in large fluctuations with $N_d - N_a < 0$. In the central region of sufficiently large fluctuations the screening should give rise to electroneutrality. We call these fluctuations screened, and the value of the potential at the electroneutrality points can be easily determined from the condition $\rho = 0$, where ρ is determined by the right-hand side of (1),

$$V = \frac{\Delta}{2} + \frac{1}{2} kT \ln \frac{N_d}{N_a} - kT \operatorname{arcsinh} \frac{N_d - N_a}{2(N_d N_a)^{1/2}} e^{\Delta/2kT}. \quad (2)$$

Accordingly, unscreened fluctuations are called those for which there is no electroneutrality at the center.

It follows from (2) that at the electroneutrality point, as $T \rightarrow 0$, we have

$$V=0 \text{ if } N_d - N_a > 0, \quad V=\Delta \text{ if } N_d - N_a < 0, \quad (3)$$

from which it is seen that the potential in the system varies in the interval $0 \leq V(r) \leq \Delta$ and accordingly the donor impurities spread out into a band with energies from 0 to Δ relative to the Fermi level. The acceptors spread into a band with energies from $-\Delta$ to 0. At the points where $V=0$, the donor level passes through the Fermi level; the charge density $\rho=0$; the concentration of the neutral donors is $n_d(r) = N_d(r) - N_a(r)$; the concentration of the neutral acceptors is $p_a(r) = 0$. At the points where $V=\Delta$ the acceptor level passes through the Fermi level; the charge density $\rho=0$; the concentration of the neutral donors is $n_d(r) = 0$; the concentration of the neutral acceptors is $p_a(r) = N_a(r) - N_d(r)$.

At the points where $0 < V(r) < \Delta$, as follows from (1), $n_d(r) = 0$ and $p_a(r) = 0$, and the charge density is

$$\rho(r) = q[N_d(r) - N_a(r)].$$

Thus, at zero temperature the Poisson equation takes the form

$$\nabla^2 V(r) = \frac{4\pi q^2}{\epsilon} [N_d(r) - N_a(r)] [1 - \theta(-V) - \theta(V - \Delta)], \quad (4)$$

where

$$\theta(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z < 0 \end{cases}.$$

It is seen from (4) that the nonlinearity of the screening of the potential at zero temperature acquires a jump-like character. At potential values $0 < V < \Delta$ there are no electrons or holes, and the screening length is infinite. At $V=0$ and $V=\Delta$, on the other hand, the screening length vanishes jumpwise.

It should be noted that the Poisson equation (4) is actually valid also in the case of strong doping (neglecting the degeneracy energy), when the donor and acceptor impurity bands merge respectively with the free and valence bands, in which case $\Delta = E_g$ in Eq. (4).

The qualitative band picture in a semiconductor with an inhomogeneous impurity distribution is the following. Whereas, for example, in the case of a homogeneous semiconductor the Fermi level passed through a donor level and the state density of the donor and acceptor centers constituted two δ functions [$N_d(E) = \bar{N}_d \delta(E)$ and $N_a(E) = \bar{N}_a \delta(E + \Delta)$], now the donor

and acceptor centers become smeared out into bands of width Δ and with state densities $N_d(E) = N_d \mathcal{P}(E)$ and $N_a(E) = \bar{N}_a \mathcal{P}(E + \Delta)$, where $\mathcal{P}(E)$ is the probability density of the potential and must be calculated.

In addition, the semiconductor vacuum level also bends in accordance with the fluctuation potential. Since the contact phenomena, and in particular the work function, are determined by the position of the mean value of the vacuum level of the semiconductor relative to the Fermi level, it can be stated that the bottom of the conduction band and the Fermi level, and accordingly the position of the neutral donor, drop lower relative to the vacuum level by an amount equal to the average value of the potential \bar{V} . This means that in a doped and compensated n -type semiconductor the electron affinity and the work function increase by \bar{V} , and accordingly in a p -type semiconductor these quantities decrease by \bar{V} .

3. MEAN VALUE OF THE POTENTIAL

The mean value of the potential, by definition, is

$$\bar{V} = \int V \mathcal{P}(V) dV.$$

We assume that the impurity fluctuations have a Gaussian distribution, just as in an ideal gas, and the concentration of the impurities inside the fluctuation is homogeneous, so that the distribution function takes the form

$$f(x) = \pi^{-1/2} \exp[-(x-x_0)^2], \quad (5)$$

where

$$x = x_0 \frac{N_d - N_a}{\bar{N}_d - \bar{N}_a}, \quad x_0 = \left[\frac{2\pi R^3}{3(\bar{N}_d + \bar{N}_a)} \right]^{1/2} (\bar{N}_d - \bar{N}_a).$$

The fluctuation potential will be calculated as follows. We choose all the fluctuations of radius R , in which the difference of the donor and acceptor concentrations is equal to a certain value $N_d - N_a$. The potential within the fluctuation, as follows from the Poisson equation (4), is in the case of spherical symmetry

$$V(r) = a_1 + a_2 r^2 + a_3 r^{-1} \quad \text{for } R_1 \leq r \leq R, \quad (6)$$

$$\left. \begin{aligned} V &= 0 & \text{if } N_d - N_a > 0 \\ V &= \Delta & \text{if } N_d - N_a < 0 \end{aligned} \right\} \quad \text{for } 0 \leq r \leq R_1,$$

where

$$a_2 = \frac{2\pi q^2}{3\epsilon} (N_d - N_a),$$

R_1 is the radius of the sphere at the center of the fluctuation inside which an electroneutrality region can occur.

To determine the parameters a_1 , a_3 , and R_1 it is necessary to join the solution (6) together with the potential outside the fluctuation. We average the potential outside the fluctuation over all possible configurations that surround the fluctuation with given value of $N_d - N_a$. The potential at a certain point located at a distance R from the considered fluctuation is represented in the form

$$V(r) = E + \varphi(r),$$

where E is a random quantity that is distributed in accordance with the probability density function $\mathcal{P}(E)$, of the potential and $\varphi(r)$ is a certain regular function that characterizes the correlation properties of the poten-

tial and is determined by the fact that the fluctuation in question, with a certain charge Q , is located at a distance r from this point. Then the average potential at this point is equal to

$$\bar{V}(r) = \bar{V} + \varphi(r)$$

and $\varphi(r)$ is determined by the averaged Poisson equation

$$\begin{aligned} \nabla^2 \varphi(r) = \frac{4\pi q^2}{\epsilon} \iint \left[N_d - N_a - \frac{N_d(r)}{1 + \exp[(E + \varphi(r))/kT]} \right. \\ \left. + \frac{N_a(r)}{1 + \exp[(\Delta - E - \varphi(r))/kT]} \right] \\ \times f(N_d(r')) f(N_a(r')) DN_d(r') DN_a(r') \mathcal{P}(E) dE. \quad (7) \end{aligned}$$

Here $f(N_d(r'))$ and $f(N_a(r'))$ are the probabilities of the appearance of the configurations $N_d(r')$ and $N_a(r')$. Recognizing that there is no correlation in the distribution of the impurities in (7) and that the potential at the given point is independent of the impurity concentration at the same point (the latter is due to the non-local connection between the potential and the free-charge density), we obtain for zero temperature

$$\nabla^2 \varphi(r) = \frac{4\pi q^2}{\epsilon} \left[\bar{N}_d - \bar{N}_a - \bar{N}_d \int_0^{\Delta} \mathcal{P}(E) dE + \bar{N}_a \int_{-\Delta}^0 \mathcal{P}(E) dE \right]. \quad (8)$$

We have obtained a rather obvious equation that characterizes the screening of an external field in a semiconductor with distributed density of the donor and acceptor states. Thus, the screening of the potential that is produced by the considered fluctuation is taken into account exactly inside the fluctuation (screening occurs only if the potential reaches values $V=0$ and $V=\Delta$), while outside the fluctuation it is taken into account in terms of the averaged Poisson equation (8), which determines a certain effective screening radius.

We proceed now to calculate the concrete form of the potential inside and outside the fluctuations. For fluctuations with $N_d - N_a > 0$, the solution for $V(r)$ in the approximation where the potential density is constant near zero energy, neglecting the hole density, takes the form

$$\bar{V}(r) = \bar{V} + \frac{a}{r} \exp(-r/r_0), \quad r_0^{-1} = \left[\frac{4\pi q^2}{\epsilon} \bar{N}_d \mathcal{P}(E \approx 0) \right]^{1/2}. \quad (9)$$

Joining together the solutions (9) and (6) and changing over to the dimensionless variables x , x_0 , and $\zeta = r/R$, we obtain the potential inside the fluctuation for $N_d - N_a > 0$:

$$V(\zeta) = \bar{V} \left[1 + \frac{1}{3} \frac{x}{x_1} \left(-\frac{3r_d + R(1 + 2\zeta_1^2)}{r_d + R} + \zeta^2 + \frac{2\zeta_1^3}{\zeta} \right) \right], \quad (10)$$

$$\zeta_1 \leq \zeta \leq 1;$$

$$V(\zeta) = 0, \quad 0 \leq \zeta \leq \zeta_1,$$

where

$$x_1 = \frac{\bar{V}}{\gamma_c x_0^{1/2}}, \quad \gamma_c = \frac{q^2}{\epsilon} \left[18\pi \frac{(1+K)^2}{1-K} \bar{N}_d \right]^{1/2},$$

and ζ_1 is determined from the equation

$$\frac{2}{3} \frac{R}{r_d + R} \zeta_1^3 - \zeta_1^2 + \frac{3r_d + R}{3(r_d + R)} - \frac{x_1}{x} = 0. \quad (11)$$

for fluctuations with $N_d - N_a < 0$ ($x < 0$), neglecting the hole density in the right-hand side of (8), the solution

for the potential inside the fluctuation is

$$V(\zeta) = \bar{V} - \gamma_c x_0^{1/2} x \left[1 - \frac{1}{3} \zeta^2 - \frac{2}{3} \left(1 + \frac{\Delta - \bar{V}}{\gamma_c x_0^{1/2} x} \right)^{1/2} \frac{1}{\zeta} \right],$$

for

$$1 \geq \zeta \geq \zeta_2 = [1 + (\Delta - \bar{V}) / \gamma_c x_0^{1/2} x]^{1/2};$$

$$V(\zeta) = \Delta \text{ for } 0 \leq \zeta \leq \zeta_2. \quad (12)$$

We now calculate the average concentration of neutral donors at the Fermi level. As follows from (10) and (11), the neutral donor concentration in the fluctuation, referred to the volume of the fluctuation, is

$$n_d(x) = \frac{\bar{N}_d - \bar{N}_a}{x_0} \zeta_1^3(x) x. \quad (13)$$

The average concentration of the neutral donors is obtained by averaging (13) over the distribution function (5)

$$\bar{n}_d = \frac{\bar{N}_d - \bar{N}_a}{\pi^{1/2} x_0} \int_{x_1}^{\infty} \frac{(x-x_1)^{1/2}}{x^{3/2}} \exp[-(x-x_0)^2] dx. \quad (14)$$

This expression is written in the approximation $r_d \gg R$, and below we obtain the limits of applicability in this approximation and, where important, we indicate the results of allowance for the screening of the potential outside the fluctuation (the screening inside the fluctuation is taken into account exactly, as before).

We obtain analogously an expression for the average concentration of the neutral acceptors,

$$p_a = \frac{\bar{N}_d - \bar{N}_a}{\pi^{1/2} x_0} \int_{x_2}^{\infty} \frac{(x-x_2)^{1/2}}{x^{3/2}} \exp[-(x+x_0)^2] dx, \quad (15)$$

where $x_2 = x_1(\Delta - \bar{V})/\bar{V}$. Substituting (14) and (15) in the electroneutrality condition

$$\bar{N}_d - \bar{N}_a - \bar{n}_d + \bar{p}_a = 0, \quad (16)$$

we obtain

$$\int_{x_1}^{\infty} \frac{(x-x_1)^{1/2}}{x^{3/2}} \exp[-(x-x_0)^2] dx - \int_{x_2}^{\infty} \frac{(x-x_2)^{1/2}}{x^{3/2}} \exp[-(x+x_0)^2] dx = \pi^{1/2} x_0. \quad (17)$$

Equation (17) determines \bar{V} as a function of x_0 —the radius of the fluctuations ($x_0 \sim R^{3/2}$). It follows from (17) that in the case of complete compensation ($K=1$, $x_0=0$) we have $x_1=x_2$, whence we obtain

$$\bar{V} = \Delta/2 \text{ at } K=1. \quad (18)$$

At a degree of compensation $K < 1$, when $\gamma_c \ll \Delta$, the parameter $x_2 \gg 1$ and the second integral in (17) can be neglected. This means that at $\gamma_c \ll \Delta$ the number of neutral acceptors is negligibly small compared with the neutral donors. In this case it follows from (17) that at $x_0 \ll 1$ we have

$$\bar{V} \approx (q^2/\epsilon) [6\pi(\bar{N}_d + \bar{N}_a)R]^{1/2} = \gamma_c x_0^{1/2}. \quad (19)$$

At $x_0 > 1$ we get from (17)

$$\bar{V} = \frac{1}{3\pi^{1/2}} \gamma_c x_0^{1/2} [\exp(-x_0^2) - \pi^{1/2} x_0 (1 - \Phi(x_0))], \quad (20)$$

where $\Phi(x)$ is the error-function integral. It follows from (20) that with increasing fluctuation radius, in the region $x_0 > 1$, the mean value \bar{V} tends rapidly (exponentially) to zero.

A computer solution of (17) shows that \bar{V} has at

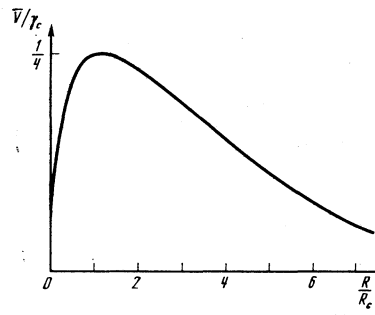


FIG. 1. Mean value of the potential as a function of the fluctuation radius.

$x_0 = x_{0c}$ and $x_1 = x_{1c}$ ($x_{0c} = 0.027$, $x_{1c} = 0.84$), a maximum equal to

$$\bar{V} = \gamma_c x_{1c} x_{0c}^{1/2}. \quad (21)$$

A more accurate expression for \bar{V} , with allowance for the finite value of the screening radius r_d is

$$\bar{V} = 1.5 \frac{q^2}{\epsilon} \frac{\bar{N}_d^{1/2}}{(1-K)^{1/2}} \frac{3r_d + R_c}{3(r_d + R_c)}. \quad (22)$$

The dependence of \bar{V} on the fluctuation radius is shown in Fig. 1. As seen from Fig. 1, \bar{V} has a maximum. We make use of the method of optimal fluctuations, proposed by Lifshitz.⁹ We assume that the decisive role is played by fluctuations with a radius corresponding to $x_0 = x_{0c}$. From the equation $x_0 = x_{0c}$ we determined the radius and the optimal fluctuations R_c :

$$R_c = \left(\frac{x_{0c}}{1-K} \right)^{2/3} \frac{1}{\bar{N}_d^{1/2}}. \quad (23)$$

Comparing \bar{V} and R_c with the values of γ and R_c obtained by Shklovskii and Efros,¹¹ we see that \bar{V} practically coincides with γ , and R_c in our case differs by a factor $x_{0c}^{2/3} = 0.09$.

However, there is a limitation on the radius of the fluctuations. We have a right to use a Gaussian distribution and the Poisson equation (1) only under the condition that the selected volume contains a large number of both donors and acceptors. Since $\bar{N}_d \gg \bar{N}_a$, this limitation follows from the requirement that the number of acceptors in a fluctuation of radius of R_c be > 1 (strictly speaking, $\gg 1$). It follows from this condition that

$$1 - K < 2x_{0c}. \quad (24)$$

From the inequality (24) we find that only at $K > K_1 \approx 0.95$ does the mean value \bar{V} satisfy Eq. (22). In addition, (22) is valid only at $K < K_2$, where K_2 is determined from the equation $\gamma_c \approx \Delta$:

$$K_2 = 1 - 72\pi \bar{N}_d (q^2/\epsilon \Delta)^2. \quad (25)$$

At $K > K_2$ the value of \bar{V} is close to $\Delta/2$ (Fig. 2).

It should be noted that the method of optimal fluctuations is valid, strictly speaking, only for an exponentially sharp maximum. As seen from Fig. 1, the maximum is not sharp and the applicability of this method is not obvious in this case. Therefore to assess the accuracy of the applicability of the method, the value of \bar{V} was calculated in the next order of approximation, namely: the fluctuation of radius R is broken up into two concentric regions of equal volume, in each of which

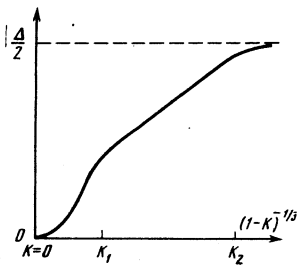


FIG. 2. Mean value of the potential as a function of the degree of compensation.

the concentration is assumed already to be arbitrary. A numerical solution of the obtained equations yields $\bar{V} = 0.252\gamma_c$; we note that Eq. (17) yields $\bar{V} = 0.251\gamma_c$, from which we see that allowance for the inhomogeneity inside the fluctuation changes the value of \bar{V} only in the third significant figure.

Thus, it can be stated that the approximation wherein the impurity distribution is uniform inside the fluctuation yields sufficiently good accuracy when \bar{V} is calculated.

4. PROBABILITY DENSITY OF POTENTIAL

In this section we calculate the probability density $\mathcal{P}(E)$ of the potential for energies $0 \leq E \leq \Delta$. We introduce the potential density for a fluctuation with radius R and concentration $N_d - N_a$:

$$P(E, R, N_d - N_a) = \frac{1}{\Omega} \int \delta(E - V(\mathbf{r})) d\mathbf{r}. \quad (26)$$

In dimensionless variables x , x_0 , and ζ Eq. (26) takes the form

$$P(E, x_0, x) = 3 \frac{\zeta^2}{|dV/d\zeta|} \Big|_{V(x, x_0, \zeta) = E}, \quad (27)$$

where $V(\zeta)$ is taken from Eqs. (10)–(12). By averaging (27) over the distribution function $f(x)$ we obtain the probability density $\mathcal{P}(E, x_0)$ of the potential for fluctuations of the radius x_0 :

$$\mathcal{P}(E, x_0) = \frac{1}{\pi^{1/2}} \int P(E, x_0, x) \exp[-(x-x_0)^2] dx. \quad (28)$$

The limits of integration with respect to x in (28) are determined from the equation $E = V(x, x_0, \zeta)$ under the condition that ζ can vary from 0 to 1. From the equation $V(x, x_0, \zeta) = E$, where $V(\zeta)$ takes the form (12) (without the third term in the square bracket), we obtain for ζ :

$$\zeta^2 = 3 \left[1 + \frac{E - \bar{V}}{\gamma_c x_0^{1/2} x} \right]. \quad (29)$$

It also follows from (12) that

$$dV/d\zeta = \frac{2}{3} \gamma_c x_0^{1/2} x \zeta. \quad (30)$$

Substituting (29) and (30) in (28) with allowance for (27), we get

$$\mathcal{P}(E, x_0) = \frac{3^{3/2}}{2\pi^{1/2} \gamma_c x_0^{1/2}} \int_{-x_0}^{-x_0} \frac{(x+x_0)^{1/2}}{|x|x^{1/2}} \exp[-(x-x_0)^2] dx, \quad (31)$$

where $x_3 = (E - \bar{V})/\gamma_c x_0^{1/2}$. For energies $E \gg \bar{V}$ in (31), the integrand has a sharp maximum and the integral is evaluated by the saddle-point method

$$\mathcal{P}(E, x_0) = \frac{3^{3/2} \exp[-(x_3+x_0)^2]}{2^{1/2} \gamma_c x_0^{1/2} x_3^{1/2} (x_3+x_0)^{1/2}}. \quad (32)$$

It follows from (32) that at $E \gg \bar{V}$ the radius of the optimal fluctuations corresponds to the minimum of the expression $x_3 + x_0$. Minimizing the latter with respect to x_0 we obtain

$$x_0 = \left(\frac{1}{3} \frac{E - \bar{V}}{\gamma_c} \right)^{2/3}$$

and for $\mathcal{P}(E)$ we get

$$\mathcal{P}(E) = \frac{3^{3/2}}{2} \frac{\bar{V}^{3/4}}{(E - \bar{V})^{1/4}} \exp \left[-\frac{2}{3^{1/2}} \left(\frac{E - \bar{V}}{\bar{V}} \right)^{3/2} \right] \quad (33)$$

The argument of the exponential for the tail of the probability density of the potential in (33) practically coincides with the analogous quantity obtained in Ref. 11. It is interesting that \bar{V} characterizes both the mean value of the potential and its variance [(see (33)].

For energies near \bar{V} we can confine ourselves in (31) to a fluctuation scale with $R = R_c(x_0 = x_{0c})$, and we obtain for $\mathcal{P}(E)$

$$\mathcal{P}(E) \approx \frac{0.6}{\bar{V}} \exp \left[-\left(\frac{E - \bar{V}}{\bar{V}} \right)^2 \right]. \quad (34)$$

It is seen from (34) that the maximum of $\mathcal{P}(E)$ is at the level $E = \bar{V}$ (Fig. 3).

For energies $E \gg \bar{V}$, the value $\mathcal{P}(E)$ was calculated accurate to the pre-exponential factor, owing to the presence in (32) of an exponentially sharp maximum with respect to R .

With decreasing E , the accuracy with which $\mathcal{P}(E)$ is calculated decreases, and at $E \ll \bar{V}$ we can no longer confine ourselves to only one fluctuation scale. On the other hand, the smaller E the larger the role assumed by the small scale of the fluctuations and, on the other hand, the small-radius fluctuations are themselves in a random potential produced by the surroundings. Here, however, we have a mitigating circumstance. In the limit of small fluctuation radii, the probability of finding the potential V produced by the environment in the region of the fluctuation is by definition equal to $\mathcal{P}(V)$, so that we can obtain an equation for $\mathcal{P}(V)$.

The potential in the region of the fluctuation with

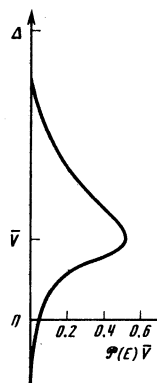


FIG. 3. Probability density of the potential at $0.95 < K < K_2$, where K_2 is determined from (25).

random boundary condition takes the form

$$V(\xi) = V - \gamma_c x_0^{1/2} x \left[1 - \frac{1}{3} \xi^2 - \frac{2}{3} \frac{\xi_1^3}{\xi} \right], \quad (35)$$

where V is a random function having a distribution function $\mathcal{P}(V)$, and

$$\xi_1 = (1 - V/\gamma_c x_0^{1/2} x)^{1/2}. \quad (36)$$

Just as in Sec. 3, we calculate the average concentration of the neutral donors. The reduced concentration of the neutral donors in fluctuations with boundary potential V with concentration x is equal to

$$n_d(V, x) = \frac{\bar{N}_d - \bar{N}_a}{x_0} \xi_1^3(V, x) x. \quad (37)$$

Averaging (37) over the distribution functions $\mathcal{P}(V)$ and over $f(x)$ we obtain the average concentration of the neutral donors and substituting it in the electroneutrality equation, we obtain an integral equation for $\mathcal{P}(V)$:

$$\int_0^\infty \mathcal{P}(V) dV \int_{V/\gamma_c x_0^{1/2}}^\infty x \left(1 - \frac{V}{\gamma_c x_0^{1/2} x} \right)^{3/2} \exp[-(x-x_0)^2] dx = \pi^{1/2} x_0. \quad (38)$$

It follows from (38) that $\mathcal{P}(V \approx 0) \sim x_0^{2/3}/\gamma_c$, and in the limit as $x_0 \rightarrow 0$ we have near $V=0$,

$$\mathcal{P}(V) = 16V^2/\gamma_c^3.$$

It should be noted, however, that we are not justified in decreasing the fluctuation radius to zero, since, on the one hand, for radii less than the mean distance between particles the Gaussian distribution (5) is no longer valid, and furthermore the Poisson equation (4) is likewise not valid because the charges are discrete; on the other hand, at small scales the quantization assumes an important role. Nonetheless, we shall deduce from (38) that the decisive role in the behavior of $\mathcal{P}(V)$ near zero is played by small fluctuation scales and it is necessary to ascertain here which scale is more substantial.

Without allowance for quantization, it was found that the fluctuation potential can vary only in the range from zero to Δ . The quantization should cause the potential in the fluctuation to become negative, so as to make possible at least one state with energy $E \leq 0$. We write down once more the potential in a fluctuation with a random boundary condition

$$V(r) = V - 2\pi \frac{q^2}{\epsilon} (N_d - N_a) \left[R^2 - \frac{1}{3} r^2 \right]. \quad (39)$$

Expression (39) is the potential energy for the electron in the region of the fluctuation, and takes the form of a spatial oscillator. For a spatial oscillator, $V(r) = (1/2)m\omega^2 r^2$ the energy levels are¹⁴

$$E_n = \hbar\omega(n + 1/2), \quad n=0, 1, 2, \dots \quad (40)$$

with wave functions

$$\psi_n \sim r^n \exp(-\alpha^2 r^2/2),$$

where $\alpha = (m\omega/\hbar)^{1/2}$, and with a degeneracy multiplicity $(n+1) \cdot (n+2)$. For the potential (39), with allowance for (40), the position of the energy levels takes the form

$$E_n(V, \Delta N, R) = V - 2\pi \frac{q^2}{\epsilon} \left[R^2 \Delta N - \frac{1}{2} (a_B \Delta N)^{1/3} \left(\frac{2}{3} n + 1 \right) \right], \quad (41)$$

where V is a random large-scale potential with vari-

ation intervals $0 \leq V \leq \Delta$, and with a distribution function $\mathcal{P}(V)$; $a_B = \hbar^2 \epsilon / q^2 m$ is the Bohr radius; $\Delta N = N_d - N_a$.

The average state density $\langle N(E) \rangle$ at the energy level E is determined by the number of fluctuations in which any one of the energy levels from (41) coincides with E :

$$\langle N(E) \rangle = \left(\frac{4\pi}{3} R^3 \right)^{-1} \frac{1}{x^{1/2}} \left(\frac{R^3}{N_d} \right)^{1/2} \sum_{n=0}^m (n+1)(n+2) \int_0^\Delta \mathcal{P}(V) dV \times \int_{-\infty}^\infty \exp\left(-\frac{R^3}{N_d} \Delta N^2\right) d\Delta N \delta(E - E_n(V, \Delta N, R)). \quad (42)$$

The summation over a finite number of excited levels in (42) is connected with the charge limitation that can be expressed in the form

$$Z < Q,$$

where Z is the number of electrons on m excited levels ($Z = 1/3 m^3 + 2m^2 + 11/3 m + 2$), and Q is the charge of the fluctuation ($Q = 4/3 \pi R^3 \Delta N$). For small radii an important role in (42) is played by the behavior of $\mathcal{P}(V)$ near $V=0$, so that we can confine ourselves to the approximation of constant probability density of the potential near $V=0$, after which we get

$$\langle N(E) \rangle = \left(\frac{4\pi}{3} R^3 \right)^{-1} \left(\frac{R^3}{\pi N_d} \right)^{1/2} \mathcal{P}(V \approx 0) \sum_{n=0}^m (n+1)(n+2) \times \int_{\Delta N_n(E)}^\infty \exp\left(-\frac{R^3}{N_d} \Delta N^2\right) d\Delta N, \quad (43)$$

where $\Delta N_n(E)$ is determined from the equation

$$E_n(V=0, \Delta N_n(E), R) = E$$

and $\Delta N_n(E)$ is equal to

$$\Delta N_n(E) = \frac{a_B}{4R^3} \left(\frac{2}{3} n + 1 \right)^2 - \frac{\epsilon E}{\pi q^2 R^2}. \quad (44)$$

Changing over to the variable $x = (R^3/\bar{N}_d)^{1/2} \Delta N$, we get

$$\langle N(E) \rangle = \frac{1}{2} \left(\frac{4\pi}{3} R^3 \right)^{-1} \mathcal{P}(V \approx 0) \sum_{n=0}^m (n+1)(n+2) [1 - \Phi(x_n(E))], \quad (45)$$

where $x_n(E) = (R^3/\bar{N}_d)^{1/2} \Delta N_n(E)$. Expressing the radius R of the fluctuation in terms of $x_n(E=0)$ ($x_n(E=0) = a_B (4R^5/2\bar{N}_d^{1/2})^{-1} (2/3 n + 1)^2$), we arrive at the following expression for $\langle N(E) \rangle$:

$$\langle N(E) \rangle = \frac{\bar{N}_d \mathcal{P}(V \approx 0)}{2^{1/2} (a_B^3 \bar{N}_d)^{1/2}} \sum_{n=0}^m \frac{(n+1)(n+2)}{(2/3 n + 1)^{1/2}} x_n^{1/2}(0) \times \left[1 - \Phi \left(x_n(0) - \frac{E}{E_1} \frac{x_n^{1/2}(0)}{(2/3 n + 1)^{1/2}} \right) \right]; \quad (46)$$

Here $E_1 = 2^{-2/5} \pi (q^2/\epsilon) \bar{N}_d^{1/3} (a_B \bar{N}_d^{1/3})^{1/5}$.

The physical meaning of the parameter $x_n(E=0)$ consists in the following: in a fluctuation with concentration $x = x_n(0)$ and radius R , the number of levels having energy $E \leq 0$ is equal to $n+1$. With this as a starting point we can transform the charge limitation $Z < Q$ to the simple expression

$$\frac{1/3 m^3 + 2m^2 + 11/3 m + 2}{(2/3 m + 1)^2} < \frac{a_B}{R}. \quad (47)$$

Minimizing (46) with respect to $x_n(0)$, we obtain the optimal radius that makes the maximal contribution to the state density at the energy level E . The maximum of (46) turns out to be at

$$x_n(0) = 0.6 \left(1 - 0.68 \frac{|E|}{E_1} \frac{1}{(2/3n+1)^{3/2}} \right) \quad \text{at } |E| \ll E_1, \quad (48)$$

$$x_n(0) = 1.61^{5/2} (2/3n+1)^{3/2} E_1^{3/2} / |E|^3 \quad \text{at } |E| \gg E_1,$$

and the optimal radius R_1 is

$$R_1 = \frac{0.7}{\bar{N}_d^{1/2}} (a_B \bar{N}_d^{1/2})^{3/2} \left(\frac{2}{3} n + 1 \right)^{3/2} \quad \text{at } |E| \ll E_1, \quad (49)$$

$$R_1 = \frac{1}{2\bar{N}_d^{1/2}} (a_B \bar{N}_d^{1/2})^{3/2} \frac{E^2}{E_1^2} \quad \text{at } |E| \gg E_1.$$

It is seen from (49) that the optimal radius R_1 turns out to be larger than the average distance between the impurity charges only at $a_B^3 \bar{N}_d > 1$, and only in this case is the foregoing analysis correct. From (47) with account taken of (49) it follows that at practically any realistic doping the inequality (47) is satisfied only at $m = 0$, so that it can be stated that the main contribution to the state density is made by the ground state in each fluctuation, and we can retain in (46) only the term with $n = 0$, after which we get for $\langle N(E) \rangle$

$$\langle N(E) \rangle = 0.28 \bar{N}_d \frac{\mathcal{P}(V \approx 0)}{(a_B \bar{N}_d^{1/2})^{3/2}} \begin{cases} 1 - 1.8|E|/E_1 & \text{at } |E| \ll E_1 \\ 1.8(E/E_1)^6 & \text{at } |E| \gg E_1. \end{cases} \quad (50)$$

The total number of states below the Fermi level $N_e \leq 0$ is determined by integrating $\langle N(E) \rangle$ over all the energies below $E = 0$:

$$N_{E \leq 0} = 0.14 \bar{N}_d \frac{\mathcal{P}(V \approx 0) E_1}{(a_B \bar{N}_d^{1/2})^{3/2}}. \quad (51)$$

Substituting (51) in the electroneutrality equation $N_{E \leq 0} = (1 - K) \bar{N}_d$, we obtain

$$\mathcal{P}(V \approx 0) = 7 \frac{(1 - K)}{E_1} (a_B \bar{N}_d^{1/2})^{3/2}, \quad (52)$$

and the state density at the Fermi level, as follows from (51) and (52), is

$$\langle N(E \approx 0) \rangle = 2 \frac{\bar{N}_d (1 - K)}{E_1}. \quad (53)$$

In the case of weak doping ($a_B^3 \bar{N}_d < 1$) there exists an impurity band in which the radius of electron localization on the impurity center is smaller than the average distance between the impurities. In this case the donor level becomes smeared out below the Fermi level as a result of the Coulomb potential of the nearest empty donor, and the characteristic smearing energy is $\approx 4E_B$.

The state density at the Fermi level can in this case be estimated at

$$\langle N(E=0) \rangle \approx \bar{N}_d (1 - K) / 4E_B. \quad (54)$$

Now, knowing $\langle N(E \approx 0) \rangle$, we can compare the effective screening radius (9) with a characteristic fluctuation radius R_c from (23):

$$\frac{r_d}{R_c} = \begin{cases} 3.4 (a_B \bar{N}_d^{1/2})^{1/2} (1 - K)^{1/2} & \text{at } a_B^3 \bar{N}_d \gg 1 \\ 6.3 (a_B \bar{N}_d^{1/2})^{-1/2} (1 - K)^{1/2} & \text{at } a_B^3 \bar{N}_d \ll 1 \end{cases} \quad (55)$$

It follows from (55) that at practically all realistic degrees of doping and compensation we have $r_d \approx R_c$, after which we get from V for (22)

$$V = \frac{q^2}{\epsilon} \frac{\bar{N}_d^{1/2}}{(1 - K)^{1/2}}. \quad (56)$$

If $\overline{V(r)}$ from (9) or $V(z)$ from (10) and (12) are expres-

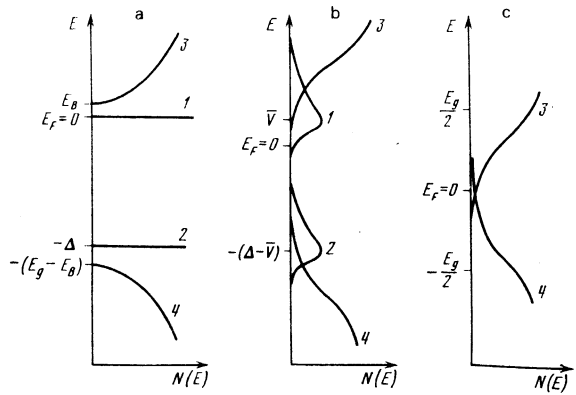


FIG. 4. State density in doped and compensated semiconductor: curve 1—for donor centers, 2—acceptors, 3—conduction band, 4—valence band; a) straight-band approximation, $a_B^3 \bar{N}_d \ll 1$, b) $0.95 < K < K_2$, $a_B^3 \bar{N}_d \ll 1$, c) $K = 1$, $a_B^3 \bar{N}_d \gg 1$.

sed in terms of the potential at the center of the fluctuation, and if the product $[\overline{V(r)} - \bar{V}][V(r=0) - \bar{V}]$ is averaged over $\mathcal{P}(V)$ then, by definition, we obtain the correlation function $K_V(r)$, which takes the form

$$K_V(r) \approx \begin{cases} (R_c/2r) \exp(1-r/R_c) [\bar{V}^2 - V^2] & \text{at } r \gg R_c \\ [1 - 1/2(r/R_c)^2] [\bar{V}^2 - V^2] & \text{at } r \leq R_c \end{cases}, \quad (57)$$

from which we see that a characteristic fluctuation radius R_c from (23) is in fact the correlation radius, and correlation exists in the potential, despite the total absence of correlation and the distribution of impurities:

$$\langle \Delta N(r+r_1) \Delta N(r_1) \rangle = (\bar{N}_d + \bar{N}_a) \delta(r).$$

Knowing the probability density of the potential, we can calculate in the quasiclassical approximation the state densities of the free and valence bands. For example, for the case $a_B^3 \bar{N}_d \gg 1$ the state density in the conduction band is

$$N_c(E) = \frac{m_c^{3/2}}{2^{1/2} \pi^2 \hbar^3} \int_{-E}^E (E - V)^{1/2} \mathcal{P}(V) dV,$$

and taking (52) into account we have for $E \geq 0$

$$N_c(E) \approx 3 \frac{\bar{N}_d (1 - K)}{E_1 (a_B \bar{N}_d^{1/2})^{3/2}} \left(1 + \frac{E}{E_1} \right)^{3/2}. \quad (58)$$

It follows from (58) that the quasiclassical state density is practically joined together with $\langle N(E) \rangle$ from (53).

The state density in the valence band is determined by the relation

$$N_v(E) = \frac{m_v^{3/2}}{2^{1/2} \pi^2 \hbar^3} \int_{\Delta - E}^{\Delta} (V - \Delta - E)^{1/2} \mathcal{P}(V) dV. \quad (59)$$

Substituting in (59) the value of $\mathcal{P}(V)$ from (33), we obtain a deep tail of the state density of the valence band:

$$N_v(E) = \left(\frac{\bar{N}_d}{a_B^3 (1 - K)} \right)^{1/2} \frac{|E|^{3/2}}{(\Delta - \bar{V} + E)^{1/2} \bar{V}^{1/2}} \exp \left[-\frac{2}{3} \left(\frac{\Delta - \bar{V} + E}{\bar{V}} \right)^{3/2} \right]. \quad (60)$$

The distribution of the state density in a compensated semiconductor is shown in Fig. 4.

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Nonequilibrium fluctuations in semiconductors in quantizing magnetic fields

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The effect of a quantizing magnetic field on nonequilibrium fluctuations in an electron gas is investigated. Besides solving the fluctuation problem, the linear response of the system to an external action is obtained, and this yields relations similar to the fluctuation-dissipation theorem. The cases of parallel electric and magnetic fields and of scattering of electrons by acoustic and optical phonons are considered. The author has shown previously that in a strong electric field such a system deviates greatly from equilibrium because two competing mechanisms act on the electrons: "runaway" of the electrons into the region of higher energies, and spontaneous optical-phonon emission that hinders the runaway. It is found that in strong electric field the fluctuations in the system are large, whereas the dependence of the current on the electric field is only slightly nonlinear. All this indicates, at least, that the study of the fluctuations is a very sensitive method of investigating nonequilibrium systems.

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1. INTRODUCTION

Electronic fluctuations in a nonequilibrium stationary state, which are produced in a semiconductor by a constant electric field, were investigated in a number of studies.¹⁻⁶ Most of them dealt with systems whose kinetic behavior is described by the ordinary Boltzmann equation. In Ref. 6, however, the fluctuations were considered under conditions of quantization of the motion of electrons in the electric field,⁷ when the ordinary kinetic equation cannot be used, and it was shown that the fluctuations can be anomalously large in that case. It is of interest to investigate other quantum systems in which one can expect new regularities of the nonequilibrium state.

The present paper deals with spatially-homogeneous current fluctuations in an electron-phonon system situated in parallel electric and quantizing magnetic fields. High-frequency fluctuations in crossed fields were investigated earlier in Ref. 8, and the method developed there will be used here.

The parallel orientation of the fields is of interest because in the case when the electric field is strong the electron energy distribution deviates greatly from

equilibrium,⁹ and this disequilibrium is not described by an effective electron temperature, as is the case in crossed electric and magnetic fields.¹⁰

In Ref. 9, under conditions of strong quantization ($\hbar\omega_c > \bar{\epsilon}$, where ω_c is the cyclotron frequency and $\bar{\epsilon}$ is the average electron energy), the author considered the kinetics of electrons interacting with acoustic and optical phonons. The latter prevent the penetration of electrons into the region of high energy, which takes place in a quantizing magnetic field if the electron scattering is quasielastic. It is precisely in such a system that we investigate in the present paper the longitudinal fluctuations of the current.

In Sec. 2 is discussed the fluctuation problem. Various approaches to the solution of this problem are cited and the possible situations in the theory of nonequilibrium fluctuations are analyzed. These situations are investigated in Secs. 3 and 4 for the cases of an electron gas in weak and strong disequilibrium under Landau quantization conditions. Besides solving the problem of the fluctuations, we obtain the linear response of the system to the external action, and this makes it possible to obtain relations similar to the