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Electric fields in a weakly doped compensated semiconductor

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We obtain the distribution function $F(E)$ of the electric field produced by charged donors and acceptors on neutral impurity centers in a weakly doped compensated semiconductor at absolute zero temperature. For the case of a low degree of compensation of the main impurity ($K \ll 1$), when the charged impurities are situated in the crystal in the form of individual pairs comprising an ionized donor and an ionized acceptor, we obtain an analytic expression for $F(E)$. At higher degrees of compensation (up to $K = 0.95$) the function $F(E)$ is obtained with the aid of computer experiments. The method of Efros *et al.* [J. Phys. C: Solid St. Comm. 22, 623 (1977)] is used to realize in the computer the ground state of the model of a weakly doped compensated semiconductor. It is found that up to the highest investigated K the most probable electric field at the neutral impurity, a field corresponding to the maximum $F(E)$, is much less than the value that would be obtained if the charged impurities were disposed relative to each other and relative to the neutral impurities in a completely uncorrelated manner, so that $F(E)$ would correspond to a Holtzmark distribution. This result points to a strong correlation between the charges in the considered disordered system.

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I. INTRODUCTION

In weakly doped compensated semiconductors at low temperatures, when all the carriers are frozen out (we consider for the sake of argument an n -type semiconductor with a donor density N_D and an acceptor density $N_A < N_D$), the uncompensated electrons are situated on the donors, so that a unit volume contains $N_D - N_A$ neutral donors, N_A positively charged donors, and N_A negatively charged acceptors. The static electric fields produced by the ionized donors and acceptors cause a Stark shift and a splitting of the levels of those impurity centers that had remained neutral and contribute to the impurity optical absorption. Since the electric fields at the different impurity centers are different, this effect leads to a broadening of the spectral lines of the impurity optical absorption and of the photoconductivity; this line broadening mechanism is decisive in many cases (the analogous effect of Stark

broadening of spectral lines in a gas plasma is well known).

The usual approach¹⁻⁸ in the calculation of the Stark broadening of the spectral lines in weakly doped compensated semiconductors reduces to the following. It is assumed that the charged donor and acceptor distributions are perfectly random (uncorrelated) relative to the radiation-absorbing neutral donors. In this case the field distribution that determines the shape of the spectral lines is well known: it is described by the Holtzmark formula,^{9,15} in which the concentration of the charged particles must be taken to be equal to $2N_A$. This approach is valid when the crystal temperature is much higher than the characteristic scatter of the levels in the impurity band. At not too large a compensation this scatter is of the order of the Coulomb energy of the interaction of the charges over the average distance between the impurities, i. e., $\sim e^2 N_D^{1/3} / \kappa$, where κ is the

dielectric constant of the crystal. Usually, however, in the measurements of optical and photoelectric spectra of shallow impurities, the opposite inequality holds, i. e., $kT \ll e^2 N_D^{1/3} / \kappa$. Under these conditions the state of the remaining uncompensated electrons, with concentration $N_D - N_A$, is close to the ground state and is determined by the minimum of the Coulomb energy, so that the relative disposition of the neutral and charged impurities is strongly correlated. The role of this correlation in the problem of Stark broadening of lines was pointed out earlier in Refs. 10 and 11. In Ref. 11 they observed an appreciable line broadening in the photoconductivity spectra of *n*-GaAs and *n*-CdTe with shallow donors when the sample temperatures were raised from 4 to 10 K. The authors have attributed this effect to a transition from a correlated to an uncorrelated disposition of the electrons on the donors.

We examine first the nature of the correlation between the charged and neutral impurities in the limiting cases of weak and very strong compensation, using the known ideas concerning the structure of the ground state of the electrons on the donors in these two limiting cases.¹² In the case of weak compensation of the main impurities $K = N_A / N_D \ll 1$ and at $T = 0$ the only donors ionized are those which are nearest neighbors of acceptors. As a rule, near each (negatively charged) acceptor there is one positively charged donor. Only near a small fraction of the acceptor (~2.6%) we have either no donor or two charged donors per acceptor. If we neglect these relatively rare charge configurations, then we assume that all the charged donors are grouped into dipoles with displacements on the order of the average distance between the donors. The greater part of the neutral donors, the field at which is the value of interest for the calculation of the Stark broadening of the lines, is located at distances on the order of $N_A^{-1/3} \gg N_D^{-1/3}$ from these dipoles. A typical value of the electrostatic field acting on a neutral impurity is in this case $E_d = eN_A / \kappa N_D^{1/3}$. At the same time, at high temperatures when the ionized donors are "torn away" from the acceptors and have positions uncorrelated with the latter, the characteristic value of the Holtmark field is $E_H \approx eN_A^2 / \kappa$. The ratio of the characteristic fields at low and high temperatures is of the order of $E_d / E_H \approx K^{1/3}$. At $K \ll 1$ this ratio is small. Thus, the correlation between the charged donors and the acceptors, which manifests itself in the dipole formation, leads at $K \ll 1$ and $T = 0$ to a strong decrease of the characteristic value of the electric field, compared with the value that would be obtained if the locations of the positive and negative charges in the semiconductors were disordered.

Attention was called in Ref. 10 to the fact that in a very strong compensated semiconductor ($1 - K \ll 1$) the correlation can lead to an opposite effect. At very strong compensation, the carriers that have remained uncompensated are concentrated on the impurity pairs, i. e., on donors that have close to them, at a distance $R \ll N_D^{-1/3}$, another charged donor.¹² The concentration of the electrons on the donors is in addition modulated by the large-scale potential produced by the statistical fluctuations of the concentrations of the charged donors

and acceptors. If we do not consider a large-scale potential then, for a given value of K , the electrons are situated only on pairs having $R \leq R_p = (3/2\pi)^{1/3} (1 - K)^{1/3} N^{-1/3}$. For these pairs, the electric field produced by a charged donor on a neutral one

$$E \geq E_p = [3(1 - K)/2\pi]^{-1/3} eN_D^{1/3} / \kappa \approx E_H (1 - K)^{-1/3},$$

i. e., is larger than in the case of a disordered distribution of the charged impurities relative to the neutrals. Thus, in the limit of a very strong compensation, the correlation should increase rather than decrease the characteristic fields in which the neutral donors are located.

The question of the structure of the ground state of the electrons on the donors at an arbitrary degree of compensation can not be solved analytically. A direct numerical method for numerically solving this problem was recently developed.¹³

We shall describe briefly the calculation scheme. A random-number generator produces in a cube of length $L = (N/ND)^{1/3}$ the coordinates of N donors and KN acceptors. This is followed by distributing $(1 - K)N$ electrons randomly over the donors and calculation of the Coulomb energies on all the donors. A succession of electron permutations that lead to a lowering of the energy of the system then yields the ground state of the system at a given realization of the donor and acceptor coordinates. In other words, it is found which of the N donors are occupied and which are empty, i. e., ionized.

The idea of the present paper is to use the so-obtained ground state of a compensated semiconductor to calculate directly with a computer, by summing the fields from all the charged centers, the electric fields at all the neutral donors for each given realization of the donor and acceptor coordinates, and then find the distribution function of the electric fields at the neutral donors by averaging over the various realizations. The results of these calculations are the subject of Sec. 3.

In the limiting case of small compensation $K \ll 1$, when the charged donors and acceptors form dipoles that are randomly disposed in the crystal, the distribution function of the electric field at the neutral donors can be calculated analytically. The calculation of this function is dealt with in Sec. 2.

2. DISTRIBUTION FUNCTION OF ELECTRIC FIELD IN A WEAKLY COMPENSATED SEMICONDUCTOR

In the case of weak compensation the energy of interaction of each dipole with other dipoles is of the order of $(e^2 N_D^{1/3} / \kappa) K$. As a rule this energy can not lead to rotation of the dipole or to an increase of its separation distance, since such a process ionizes not the donor closest to the acceptor but, say, the next farther away. This would require energies on the order of $e^2 N_D^{1/3} / \kappa$, i. e., much higher than the energy of interaction of the given dipole with the others. Thus, despite the interaction between the dipoles, practically each of them is oriented in the direction from the acceptor to the nearest donor. This means that the di-

poles are randomly oriented, and the distribution function with respect to their separation distance r is

$$f(r) = 4\pi r^2 N_D \exp(-4/3\pi N_D r^3). \quad (1)$$

Since the acceptor impurities are randomly distributed in the crystal, the dipole centers are distributed in the same manner.

Let $W(E)dE$ be the probability that the vector of the electric field at the neutral donor lands in the element dE , and $F(E)dE = 4\pi E^2 W(E)dE$ is the probability that the absolute value of this field lies in the interval from E to dE .

We calculate the distribution function $F_d(E)$ of the field produced in a crystal by the randomly disposed and randomly oriented dipoles with concentration N_A and with a distribution function (1) with respect to the separations. We use well known Markov method (see, e.g., Ref. 14) of finding the distribution functions of quantities that constitute the sums of the contributions from randomly distributed sources. As a result we get

$$W_d(E) = \int \frac{d^3t}{(2\pi)^3} e^{-i\mathbf{t}\cdot\mathbf{E}} \exp\left\{-N_A \int d^3R \frac{1}{4\pi} \int dr \sin\vartheta d\vartheta d\varphi f(r) [1 - e^{i\mathbf{t}\cdot\mathbf{E}(\mathbf{R},\vartheta)}]\right\}. \quad (2)$$

Here \mathbf{R} is the radius vector of the center of the dipole,

$$\mathbf{E}(\mathbf{R}, \mathbf{d}) = \frac{3(\mathbf{n}\mathbf{d})\mathbf{n} - \mathbf{d}}{\kappa R^3}$$

is the field produced by the dipole at the origin, $\mathbf{d} = e\mathbf{r}$ is the dipole moment of a pair made up of an ionized donor and an ionized acceptor, $\mathbf{n} = \mathbf{R}/R$, and ϑ and φ are the angles that determine the dipole orientation.

We change to the dimensionless variables

$$\mathbf{u} = E\mathbf{d}t, \quad E_d = \frac{eN_A}{\kappa N_D^{1/3}}, \quad \mathbf{x} = N_A^{1/3}\mathbf{R}, \quad \mathbf{y} = N_D^{1/3}\mathbf{r},$$

and choose in the integrand of the exponential a coordinate frame in which the polar axis is directed along \mathbf{u} . We denote by θ the angle between \mathbf{R} and \mathbf{u} , $\xi = \cos\theta$, and $\eta = \cos\vartheta$. Then the expression in the second exponential in (2) takes the form

$$-(2\pi)^2 N_A N_D \int_{-1}^{+1} d\xi \int_{-1}^{+1} d\eta \int_0^\infty dy y^2 \exp\left(-\frac{4\pi}{3} y^3\right) \int_0^\infty dx x^2 \times \left[1 - \exp\left\{i\left(3\xi^2 - 1\right)\eta \frac{xy}{x^3}\right\} J_0\left(3\xi\left[(1-\xi^2)(1-\eta^2)\right]^{1/2} \frac{xy}{x^3}\right)\right],$$

where J_0 is a Bessel function of zero order.

After straightforward but cumbersome calculations we obtain

$$F_d(E) = 4\pi E^2 W_d(E) = \frac{4}{\pi E_{md}} \frac{(E/E_{md})^2}{[1 + (E/E_{md})^2]^2}, \quad (3)$$

where

$$E_{md} = \beta E_d = \beta K e N_D^{1/3} / \kappa \quad (3a)$$

is the field corresponding to the maximum of the distribution function $F_d(E)$, and

$$\beta = 6^{-1/3} \pi^{1/3} \Gamma\left(\frac{4}{3}\right) \left[1 + \frac{1}{2\sqrt{3}} \ln(2 + \sqrt{3})\right] = 2.515.$$

The distribution of the field in the system of disordered and randomly oriented dipoles with fixed spacing length d/e was obtained by Holtmark.¹⁵ It takes the same functional form as (3), but the characteristic field

in it is

$$E_{dH} = \frac{\pi^2}{3} \left[1 + \frac{1}{2\sqrt{3}} \ln(2 + \sqrt{3})\right] \frac{N_A d}{\kappa} = 4.54 \frac{N_A d}{\kappa}. \quad (4)$$

It is seen that the characteristic field in (3), which equals E_{md} , coincides with E_{dH} if we assume in the latter that the effective separation distance of the dipole is

$$\frac{d_{eff}}{e} = \left(\frac{3}{4\pi}\right)^{1/3} \Gamma\left(\frac{4}{3}\right) N_D^{-1/3} = 0.55 N_D^{-1/3},$$

i.e., the average distance from the acceptor to the nearest donor.¹⁴

3. RESULTS OF COMPUTER EXPERIMENTS

As already indicated in the Introduction, the procedure used to find the distribution function of the electric field at the neutral donors, in a wide range of degrees of compensation K , was to find the ground state of a compensated semiconductor, a method developed by Efros *et al.*¹³ The calculations were performed for the values $K = 0.1, 0.3, 0.7, 0.9$, and 0.95 . For each K the total number of donors was assumed to be $N = 100, 200, 400, 800$, and 1600 . The number of realization of the donor and acceptor coordinates, over which the averaging was carried out, depended on N and decreased from 400 to 15 when N increased from 100 to 1600, inasmuch as calculations with larger N required longer computer time. Figure 1 shows the distribution functions $F(E)$ for an aggregate of donors $N = 1600$ and various degrees of compensation. Each curve is a smoothed histogram with more than 40 intervals on the abscissa axis. The deviation of the smoothed curve from the calculated points of the histogram does not exceed 10% at $K \leq 0.9$ and 15% at $K = 0.95$.

The simplest characteristic of the $F(E)$ curves is the most probable field E_m corresponding to the maximum of this function. To ascertain the extent to which the results obtained at the donor numbers N employed in the work enable us to assess $F(E)$ for an infinite system, Fig. 2 shows the values of E_m^N corresponding to various N . It is natural to assume that the size effect, (i.e., the dependence of the results on N) is due to the fact that in the regions near the faces of the cube the

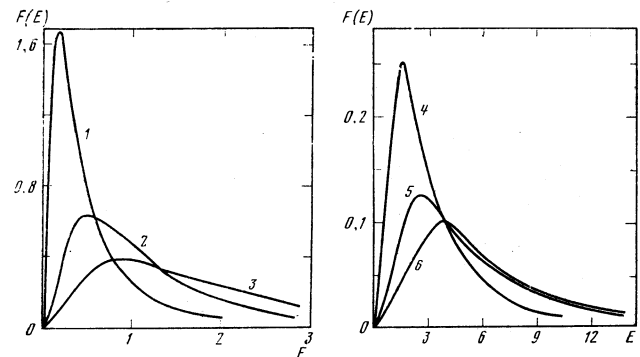


FIG. 1. Distribution function of electric field at neutral donors at various degrees of compensation K . The field E is plotted in units of $eN_D^{1/3}/\kappa$ and $F(E)$ in units of $[eN_D^{1/3}/\kappa]^{-1}$. The values of K are: 1—0.1, 2—0.3; 3—0.5; 4—0.7; 5—0.9; 6—0.95.

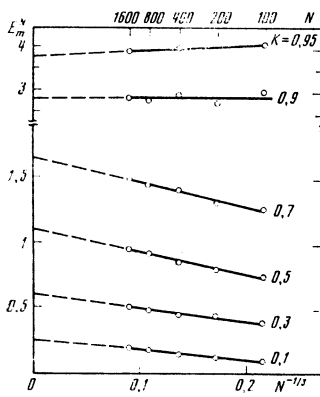


FIG. 2. Dependence of the most probable electric field E_m^N on the total number of donors N in a computer experiment for different degrees of compensation K . The field E_m^N is measured on the ordinate axis in units of $eN_D^{2/3}/\kappa$.

neutral donors have a smaller number of charged neighbors than the donors deep inside the cube, and the characteristic field at them is weaker. The fraction of these "near-surface" neutral donors should be proportional to $N^{-1/3}$, therefore the abscissa scale is in fact $N^{-1/3}$. It is seen that the dependence of E_m^N on $N^{-1/3}$ is really linear with good approximation. It is also seen that the relative magnitude of the size effect is most appreciable at small degrees of compensation K . The reason is that at $K \ll 1$ the thickness of the "near-surface" layer, which determines the size effect, is equal to the average distance between the acceptor-donor dipoles $N_A^{-1/3} = K^{-1/3}N_D^{-1/3}$ and increases with decreasing K .

At intermediate degrees of compensation, the thickness of the "near-surface" layer is of the order $N_D^{1/3}$ and the size effect remains of the same sign but has a smaller relative value. At the strong compensation limit, as seen from Fig. 2, the size effect is small and is apparently of opposite sign. The possible cause will be discussed below.

The values of E_m obtained by extrapolation to $N \rightarrow \infty$ in Fig. 2 are shown in Fig. 3 as functions of K (curve 1). The same figure shows a plot of $E_{mH}(K)$ corresponding to the Holtmark distribution for randomly distributed charges with concentration $2N_A = 2KN_D$. In this case^{9,14,15}

$$F(E) = F_H(E) = \frac{2}{\pi E} \int_0^\infty dx x \sin x \exp \left[- \left(\frac{E_H}{E} x \right)^2 \right] \quad (5)$$

and

$$E_{mH} = 1.6 E_H, \quad (5a)$$

where

$$E_H(K) = 2.60(2K)^{1/2} eN_D^{1/3} / \kappa.$$

Figure 3 shows at $K < 0.5$ a plot of $E_m(K)$ obtained from Eq. (3a) for the limiting case $K \ll 1$.

It is seen from Fig. 3 that at all $K \leq 0.9$ the most probable electric field E_m is considerably less than the value E_{mH} that would be obtained if the impurity distribution were uncorrelated relative to the neutral ones. The correlation effect is very strong. For example, at $K = 0.5$ we have a ratio $K_{mH}/E_m \approx 4$.

At $K \ll 1$ the result of the computer experiment agrees with the result of the theory developed in Sec. 2. It is important to note that the $E_m(K)$ dependence obtained in the computer experiment is very close to the $E_{mH}(K)$ dependence [Eq. (3a)] for the field produced by acceptor-donor dipoles, even at $K = 0.5$. This indicates that at so appreciable a compensation the correlation that takes place in the considered system of charges manifests itself primarily in the formation of acceptor-donor dipoles. It is possible that the cause of this effect is the fact that even at $K = 0.5$ the average distance from the acceptor to the nearest donor, $0.55N_D^{-1/3}$, is somewhat less than the average distance $K^{-1/3}N_D^{-1/3}$ between the dipoles.

At $K > 0.9$, the field E_m increases rapidly when K approaches unity, in qualitative agreement with the conclusion¹⁰ based on the donor-pair representation. However, even at $K = 0.95$ the field E_m is still weaker than the field F_{mH} corresponding a random distribution of the charges. This result seems somewhat unexpected, and will be discussed separately in Sec. 4.

We have dealt so far with the position of the maximum of the field distribution function $F(E)$. We now discuss the form of this function. To this end, the obtained field distribution functions for different values of K are plotted in such a way that the positions of their maxima on the abscissa axis coincide, i. e., the functions $E_m^N F^N(E)$ are plotted against E/E_m^N at $N = 1600$. For comparison the figure shows also the theoretical curves corresponding to the distribution (3) for the field of the randomly disposed acceptor-donor dipoles and to the Holtmark distribution (5) for randomly disposed charges.

It is seen in Fig. 4 that for all $K \leq 0.9$ the electric-field distribution functions are very similar in shape and are close to the theoretical function (3) obtained for randomly disposed acceptor-donor dipoles. All these curves have a much larger asymmetry with respect to the maximum and a larger effective width compared with the Holtmark distribution (5).

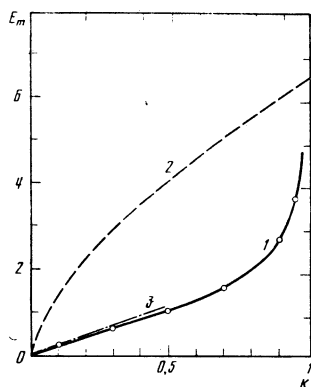


FIG. 3. Dependence of the most probable electric field on the degree of compensation K . The field E is plotted in units of $eN_D^{2/3}/\kappa$. Curve 1—result of computer experiment; curve 2 corresponds to the Holtmark distribution for randomly disposed charges [Eq. (5a)]; line 3 corresponds to Eq. (3a) derived for the limiting case $K \ll 1$.

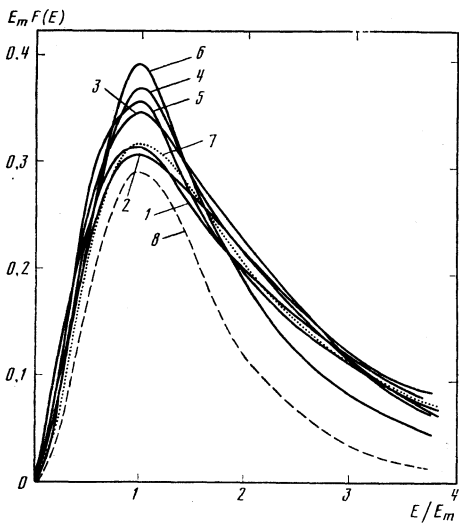


FIG. 4. Comparison of the field distribution functions obtained as a result of computer experiments (solid curves) with the theoretical distribution functions. The abscissas represent the field in units of E_m . For the calculated plots we used $F(E)$ and E_m for a total number of donors $N = 1600$. The calculated curves correspond to the degrees of compensation K : 1—0.1; 2—0.3; 3—0.5; 4—0.7; 5—0.9; 6—0.95. Curve 7—distribution described by Eq. (3), curve 8—Holtsmark distribution (5), which is normalized for clarity to $1/2$, in contrast to the other curves, which are normalized to unity.

4. DISCUSSION OF THE STRONG COMPENSATION CASE

In the theory of strong compensated semiconductors¹² it is shown that the principal part in the lowering of the Fermi level as $K \rightarrow 1$ should be played by two characteristic spatial scales of the random potential. The first corresponds to the length (β is a numerical coefficient)

$$R_s = \beta N_D^{-1/3} / (1-K)^{1/3}, \quad (6)$$

representing the radius of the nonlinear screening of the charge-density fluctuations of the ionized donors and acceptors. The second scale is connected with the formation of compact donor pairs. If we neglect a potential with wave vectors smaller than $N_D^{-1/3}$ then, as stated in the Introduction, in the case of strong compensation an ionized donor is located near each neutral donor, at a distance $R \leq R_p \ll N_D^{-1/3}$, and lowers the level of the latter. Since the interaction of the neutral donor with the remaining charged impurities is disregarded in this approximation, we shall call this approximation "paired."

In the paired approximation the Fermi level measured upward from the unperturbed donor level is equal to $\mu_p = -e^2 / \kappa R_p$. In order of magnitude, an equal lowering of the Fermi level is made by potential of scale R . It turns out as a result that as $K \rightarrow 1$ the Fermi level $\mu \approx 2.2 \mu_p$.¹³ According to Ref. 12, potentials with scales intermediate between R_p and R_s have an amplitude smaller than $|\mu_p|$, and have a relatively small effect on the position of the Fermi level. Unfortunately, the theory¹² does not make it possible to calculate $F(E)$ as $K \rightarrow 1$, with account taken of potentials of all scales. In the paired approximation, the calculation of the distribution function of the electric field at the neutral donors entails no difficulty. It yields

$$F(E) = \begin{cases} 0, & E < E_p = e / \kappa R_p^2 \\ 3/2 E_p^{3/2} / E^{3/2}, & E > E_p \end{cases}, \quad (7)$$

with the most probable field E_m coinciding with the minimal field E_p .

At $K = 0.95$ the field $E_p = 12$ (the fields are expressed here and below in units of $e N_D^{2/3} / \kappa$). At the same time, as seen from Fig. 3, at $K = 0.95$ we have the field $E_m \approx 4$. This means that the potential whose scale of variation is $\geq N_D^{-1/2}$ plays a significant role in the distribution of the neutral donors in the crystal, and greatly weakens the electric fields at the neutral donors. It is natural to assume that the mechanism of the action of this potential consists in the fact that it modulates the depths of the levels produced in the donor pairs. The electrons flow over from the points where their energy is increased into the potential-relief wells. By the same token, the pairs with $R > R_p$, in each of which the charged donor produces at its neutral partner a field smaller than E_p , turn out to be filled in the wells. This should shift the distribution function $F(E)$ towards weaker fields.

To study the role of the different scales of the potential in the decrease of the characteristic field at the filled donors, the following computer experiment was performed. In the entire computer program, both for the calculation of the ground state of the crystal and for the calculation of the electric fields at the impurities, the Coulomb potentials were multiplied by $\exp(-r/r_0)$. At $r_0 \ll N_D^{-1/3}$ the introduction of this factor, naturally, suppressed the potentials with scales larger than $N_D^{-1/3}$, and in the case of strong compensation it made it possible to describe the ground state in the paired approximation. In this case only the donor pairs with $R < R_p$ should be filled and the Fermi level should be lower than the isolated donor level E_0 by an amount equal to the energy of the interaction of the electron with the ionized donor located at a distance R_p , i. e.,

$$\mu = -\frac{e^2}{\kappa R_p} \exp\left(-\frac{R_p}{r_0}\right), \quad R_p = \left[\frac{3}{2\pi} (1-K)\right]^{1/3} N_D^{-1/3}. \quad (8)$$

The most probable (and at the same time minimal) field at the neutral donors should equal in this model

$$E_m = \frac{e}{\kappa R_p} \left(\frac{1}{r_0} + \frac{1}{R_p}\right) \exp\left(-\frac{R_p}{r_0}\right). \quad (9)$$

In Fig. 5, formulas (8) and (9) are compared with the results of the computer experiment for $K = 0.95$ and $N = 800$ (such a comparison was first carried out for the Fermi level μ at $N = 100$ in Ref. 13). It is seen that with decreasing r_0 the calculated points approach the theoretical curves, thus attesting to the applicability of the paired model at small r_0 and confirms the correctness of the problem. With the aid of Fig. 5 we can estimate the characteristic spatial scales l_μ and l_E of the potential harmonics responsible for the deviations of μ and E_m from the values (7) and (8) corresponding to the paired model. We shall assume that l_μ is approximately equal to the value of r_0 at which the difference between the calculated value and (8) is half the difference at $r_0^{-1} = 0$. We assume a similar definition also for l_E . We then obtain $l_\mu = 2N_D^{-1/3}$ and $l_E = 0.5N_D^{-1/3}$.

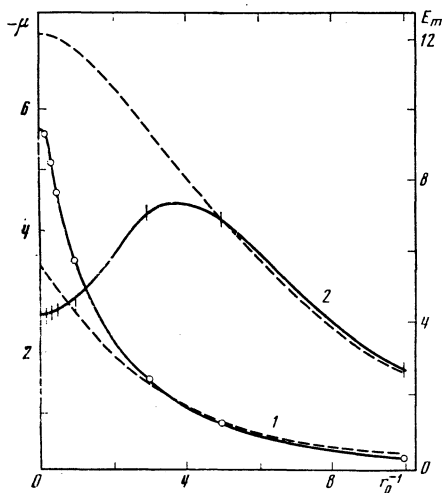


FIG. 5. Dependence of the Fermi level μ (curves 1, left-hand scale) and of the most probable field E_m (curve 2, right-hand scale) on the reciprocal "screening radius" r_0^{-1} of the model potential at $K=0.5$. The Fermi level is plotted in units of $eN_D^{1/3}/\kappa$, the field in units of $eN_D^{2/3}/\kappa$, and r_0^{-1} in units of $N_D^{1/3}$. Solid curves—computer experiment at $N=800$. The dashed curves correspond to formulas (8) and (9).

The obtained value $l_\mu = 2N_D^{-1/3}$ agrees qualitatively with the statement that as $K \rightarrow 1$ the difference between μ and μ_p is connected with a potential having a characteristic scale much larger than $N_D^{-1/3}$, i. e., with the general premises¹² concerning the role of potentials with different scales. It is therefore natural to assume that l_μ should be close to R_c . Then the coefficient β in (6) should be ≈ 0.3 , which is not unlikely.

On the other hand, the obtained value $l_E = 0.5N_D^{-1/3} \ll l_\mu$ is somewhat unexpected. This result means that the principal role in the decrease of E_m , compared with the paired model, is played by modulation of the densities of the pairs by a potential with a characteristic scale $\leq N_D^{-1/3}$, and not with a scale much larger than $N_D^{-1/3}$, as might have been assumed prior to the performance of the described computer experiments. More accurately speaking this means that an appreciable fraction of the electrons is located not on well isolated pairs, but on small clusters consisting of three or four donors, which ensure with the aid of the large-scale potential a lowering of the electron to below the Fermi level. The point is that in such clusters the fields produced by the different donors can cancel each other, whereas the potentials add up. The simplest example is that of three donors lying on a single straight line so that the two outer (charged) donors are equidistant from the central neutral one. In such an impurity "triad," the field at the neutral donor is zero, but the potential can be appreciable. As a rule, of course, the distances from the neutral to the charged donors are different. Therefore when r_0 decreases and becomes less than $N_D^{-1/3}$, the fields of the different donors

cease to cancel each other, and the decisive action is that of the field of the nearest charged donor, and this leads to an increase of the characteristic field. Further decrease of r_0 leads to a decrease of the characteristic field [in accordance with (9)] because of the exponential decrease ("screening") of the potential of the nearest donor. This explains the nonmonotonic character of the $E_m(1/r_0)$ curve obtained in the computer experiment.

Within the framework of the same concepts it is possible also to explain the anomalous sign and the relatively small value of the size effect at $K=0.95$ (Fig. 2). In the case of strong compensation a decrease of the dimension of the system leads to an effective suppression of the large-scale potential. This decreases the modulation of the pair density in space and the associate weakening of the field E_m . As a result, when N decreases the field E_m^N increases. The size effect for E_m however, turns out to be very weak compared with the size effect for μ , since, as we have seen above, the principal role in the weakening of the field is played by the relatively small scales of variation of the random potential, and the size of the system has little effect on these scales.

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