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Screening by fixed charges in compensated semiconductors*

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Donor and acceptor ions in compensated semiconductors at low temperatures are not completely randomly distributed—positive and negative charges tend to be closer to each other than allowed by chance. This gives rise to a kind of screening effect, which is usually taken into account in calculations by replacing the ion Coulomb potential by a Debye-type screened potential. We show that this replacement is wrong in principle; it leads to a statistical fluctuation of potential which is too small by a factor of 2 and, at least in the case of small screening lengths, to a distribution of the total ion potential whose shape is substantially different from that obtained in a more fundamental calculation.

A number of experimental properties of compensated semiconductors depend upon the statistics of the spatial fluctuations of the total electrostatic potential from all of the ionized donors and acceptors contained inside the sample crystal. These fluctuations affect mobility and freeze-out of carriers at low temperatures as well as optical linewidths in, for example, luminescence, impurity absorption and spin-flip Raman scattering.

This paper is concerned with screening at low temperatures in semiconductors of high purity. By low temperatures, we mean temperatures T such that kT is much smaller than the energy difference between the ground state and first excited state of a bound carrier. By high purity we mean that typical separations of nearest-neighbor impurity centers are much greater than the effective Bohr radius of bound carriers. Under conditions of low temperature and high purity, it is a very good approximation to assume that the donor and acceptor ions present can be treated as a static arrangement of point charges; our discussion will be based on this assumption.[1]

The Coulomb potential U of an impurity ion of charge q_i (for definiteness we will consider $q_i = \pm|e|$) has the familiar form

$$U(\vec{r}-\vec{r}_i) = q_i/\epsilon_0|\vec{r}-\vec{r}_i| , \tag{1}$$

where $\vec{r}_i$ locates the center of the impurity ion (taken to be a point charge) and ϵ_0 is the static dielectric constant of the host lattice. (We will always be concerned with values of $|\vec{r}-\vec{r}_i|$ much larger than the lattice spacing.)

Because of certain theoretical difficulties associated with the slowness of decay of $U(r)$ with r, it is customary in doing calculations to replace (1) by the more tractable potential

$$U_s(\vec{r}-\vec{r}_i) = \frac{q_i \exp(-|\vec{r}-\vec{r}_i|/r_s)}{\epsilon_0|\vec{r}-\vec{r}_i|} , \tag{2}$$

where r_s is some "screening length" and is independent of $\vec{r}$.

Although the replacement of U by U_s may be justifiable in some cases, it is not correct in principle when the concentration of free carriers is negligible (the carriers having been localized on donor or acceptor impurities). Nevertheless, this replacement is made quite routinely in studies of compensated semiconductors with very low free-carrier concentration.[2-6]

We shall show that U_s can be understood only as an average potential—not as an actual physical potential at the point $\vec{r}$. A consequence of this in, for example, ionized-impurity-scattering calculations, is that it is not correct in principle to calculate the scattering from potentials of the form (2) (which amounts to averaging the potential first and then computing the scattering). One should instead average the scattering from the various charge configurations which give rise to the average potential. Whether there are any physical situations for which these two procedures are equivalent does not seem to have been investigated.

In problems of carrier freeze-out in compensated semiconductors the statistical distribution of the total potential, U_T, given by

$$U_T = \sum_i U(\vec{r}-\vec{r}_i) , \tag{3}$$

where the sum is over all impurity ions, is of direct interest. Correlations in impurity positions can affect this distribution, but, as we shall show here, such correlations cannot in general be properly accounted for by replacing the U's in the right-hand side of (3) by their average values.

An elementary argument shows why (2) cannot represent the real variation of potential around any impurity ion in the absence of mobile charges. The extra charge density ρ which must surround the impurity at $\vec{r}_i$ to produce the screened potential U_s in (2) can be found from Poisson's equation,

$$\epsilon_0\nabla_r^2[U_s(\vec{r}-\vec{r}_i)-U(\vec{r}-\vec{r}_i)]=-4\pi\rho(\vec{r}-\vec{r}_i)$$
$$=\frac{q_i}{r_s^2}\,\frac{\exp(-|\vec{r}-\vec{r}_i|/r_s)}{|\vec{r}-\vec{r}_i|}\,. \tag{4}$$

It is easy to verify that

$$\int\rho(\vec{r}-\vec{r}_i)\,d^3r=-q_i\,. \tag{5}$$

Clearly it is impossible to construct a charge distribution at all resembling $\rho(\vec{r}-\vec{r}_i)$ in (4) by some arrangement of charged impurity ions, each one with charge $\pm|e|$, around the ith impurity atom, even if we remove (as we will) all constraints of discreteness of allowed impurity positions arising from the lattice structure in locating the various screening impurities.

In order to understand the meaning of U_s in (2) let us evaluate at point $\vec{r}$ the "average" potential of all the impurity ions in the crystal, given that a positive charge is located at $\vec{r}_1$. What we are after is the result of a hypothetical experiment in which we measure the potential at a displacement $\vec{r}-\vec{r}_1$ from each positive ion in the crystal and take the average. As we change this displacement the average will change and we will obtain a function describing the dependence of this average as a function of displacement, $\overline{U}(\vec{r}-\vec{r}_1)$. We assume that $\overline{U}$ can be calculated by fixing $\vec{r}$ and $\vec{r}_1$ and averaging over an ensemble of ion configurations specified by the ionic positions $\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{2N}$, with the probability density of any configuration given by $p(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_{2N})$. We shall further assume that (i) the impurity system is sufficiently dilute and correlations are of sufficiently long range that we can treat the crystal as a continuum, (ii) there are equal numbers N of positive and negative impurity ions, and (iii) N and V are so large that it is always permissible to take the limit $N\to\infty$ holding N/V constant.

We require that $p(\vec{r}_1\cdots\vec{r}_{2N})$ be normalized to 1 and that the system be spatially homogeneous so that

$$\int^{(j)}p(\vec{r}_1\cdots\vec{r}_{2N})=p(\vec{r}_j)=1/V\,, \tag{6}$$

where $\int^{(j)}$ means the multiple integral over all ion coordinates except $\vec{r}_j$.

From the statistical theory[7] we know that the probability of finding a value U_T of the total potential at point $\vec{r}$ is given by

$$D(U_T,\vec{r},\vec{r}_1)=\int_{-\infty}^{\infty}dk\,e^{ikU_T}f(k,\vec{r},\vec{r}_1)\,, \tag{7}$$

where

$$f(k,\vec{r},\vec{r}_1)=\frac{1}{2\pi p(r_1)}\int^{(1)}\exp\Big[-ik\sum U(\vec{r}-\vec{r}_i)\Big]p(\vec{r}_1\cdots\vec{r}_{2N})\,d^3r_2\cdots d^3r_{2N}\,. \tag{8}$$

The mean value of U_T at r is given by

$$\overline{U}(\vec{r},\vec{r}_1)=\int_{-\infty}^{\infty}U_T D(U_T,\vec{r},\vec{r}_1)\,dU_T\,. \tag{9}$$

Inserting (7) into (9) and integrating by parts yields

$$\overline{U}(\vec{r},\vec{r}_1)=-\frac{1}{i}\int_{-\infty}^{\infty}dU_T\int_{-\infty}^{\infty}dk\,e^{ikU_T}\frac{\partial f(k,\vec{r},\vec{r}_1)}{\partial k}\,.$$

Interchanging orders of integration and using

$$\int_{-\infty}^{\infty}dU_T\,e^{ikU_T}=2\pi\delta(k)\,,$$

we obtain in the infinite-volume limit

$$\overline{U}(\vec{r},\vec{r}_1)=-\frac{2\pi}{i}\frac{\partial f(0,\vec{r},\vec{r}_1)}{\partial k}$$
$$=U_+(\vec{r}-\vec{r}_1)+NV\Big[\int U_+(\vec{r}-\vec{r}_a)p_{++}(\vec{r}_1,\vec{r}_a)\,d^3r_a+\int U_-(\vec{r}-\vec{r}_a)p_{+-}(\vec{r}_1,\vec{r}_a)\,d^3r_a\Big]\,, \tag{10}$$

where

$$U_\pm(\vec{r}-\vec{r}_a)=\pm|e|/\epsilon_0|\vec{r}-\vec{r}_a|\,,$$

$$p_{++}(\vec{r}_a,\vec{r}_b)\equiv\int^{(a,b)}p(\vec{r}_1\cdots\vec{r}_{2N})\,,$$

both $\vec{r}_a$ and $\vec{r}_b$ being coordinates of positive charges, and

$$p_{+-}(\vec{r}_a,\vec{r}_b)\equiv\int^{(a,b)}p(\vec{r}_1\cdots\vec{r}_{2N})\,,$$

$\vec{r}_a$ and $\vec{r}_b$ being coordinates of charges of opposite sign. [The superscript (a,b) on the integrals means that the integral is over all ion coordinates except $\vec{r}_a$ and $\vec{r}_b$.] In (10) we have, of course, made allowance for the possibility that a positive charge may have a different pair-correlation function for other positive charges than it has for negative charges. We shall assume here, however, in order to simplify future discussion that

$$p_{--}(\vec{r}_a, \vec{r}_b) = p_{++}(\vec{r}_a, \vec{r}_b).$$

What we learn from (10) is that the quantity

$$|e|\, VN[p_{++}(\vec{r}_1, \vec{r}_a) - p_{+-}(\vec{r}_1, \vec{r}_a)] \tag{11}$$

acts as the effective charge distribution producing the average screening potential $\overline{U}(\vec{r}, \vec{r}_1) - U_+(\vec{r} - \vec{r}_1)$ associated with the positively charged ion at $\vec{r}_1$. No assumption as to the specific form of $p(\vec{r}_1 \cdots \vec{r}_N)$ has yet been made. This shows that pair correlations alone determine the *average* potential at $\vec{r}$. [However, to obtain the *distribution* of potential at $\vec{r}$ we must know the detailed form of $p(\vec{r}_1 \cdots \vec{r}_N)$.]

From the foregoing we conclude that the replacement of U by U_s requires an implicit assumption about pair correlations of charges. In fact, this assumption amounts to

$$VN[p_{++}(\vec{r}_1, \vec{r}_2) - p_{+-}(\vec{r}_1, \vec{r}_2)] = -\frac{1}{4\pi r_s^2} \frac{\exp(-|\vec{r}_1 - \vec{r}_2|/r_s)}{|\vec{r}_1 - \vec{r}_2|}, \tag{12a}$$

in view of (4). For the screening of a negative charge at point $\vec{r}_1$ (12a) changes to

$$-VN[p_{--}(\vec{r}_1, \vec{r}_2) - p_{+-}(\vec{r}_1, \vec{r}_2)] = \frac{1}{4\pi r_s^2} \frac{\exp(-|\vec{r}_1 - \vec{r}_2|/r_s)}{|\vec{r}_1 - \vec{r}_2|}. \tag{12b}$$

Let us turn now to a related but slightly different problem, the problem of calculating the mean square fluctuation of total potential at some arbitrarily chosen point in the crystal. This quantity is important in, for example, the theory of freeze-out.[4]

To obtain an exact answer we should resort again to the statistical theory, using equations similar to (7) and (8), except that now we no longer require that an ion be fixed at $\vec{r}_1$. We consider instead all possible configurations of ions surrounding an arbitrarily chosen fixed field point, where we place the origin of coordinates. Denoting the distribution of the total potential at the origin by $D(U_T)$ and its first and second moments by $\langle U_T \rangle$ and $\langle U_T^2 \rangle$ we obtain from the statistical theory the analogs of (7)–(9):

$$D(U_T) = \int_{-\infty}^{\infty} dk\, e^{ikU_T} f(k), \tag{13a}$$

$$f(k) = \frac{1}{2\pi} \int \cdots \int e^{-ik\sum U(r_i)} p(\vec{r}_1 \cdots \vec{r}_{2N})\, d^3r_1 \cdots d^3r_{2N}. \tag{13b}$$

The fact that the crystal is homogeneous with an equal number of positive and negative ions present implies that $\langle U_T \rangle = 0$. By a development similar to that leading to (10) it is straightforward to show that

$$\langle U_T^2 \rangle = \int_{-\infty}^{\infty} U_T^2 D(U_T)\, dU_T = -2\pi \frac{\partial^2 f(0)}{\partial k^2}$$
$$= \int \cdots \int \left(\sum_{i=1}^{2N} U(r_i) \right)^2 p(\vec{r}_1 \cdots \vec{r}_{2N})\, d^3r_1 \cdots d^3r_{2N}. \tag{14}$$

Because the potential U is a function of a single ion coordinate, evaluation of (14) requires knowledge of the pair correlation functions only. All three of these functions appear upon integrating (14), corresponding to the three types of products (e.g., U_+U_+, U_+U_-, and U_-U_-) in $[\sum_{i=1}^{2N} U(r_i)]^2$. We obtain

$$\langle U_T^2 \rangle = \left(\frac{e}{\epsilon_0} \right)^2 \int d^3r_a \left(\frac{2N}{r_a^2} p(r_a) + \int d^3r_b \frac{N^2}{r_a r_b} [p_{++}(\vec{r}_a, \vec{r}_b) + p_{--}(\vec{r}_a, \vec{r}_b) - 2p_{+-}(\vec{r}_a, \vec{r}_b)] \right).$$

Taking $p_{--} = p_{++}$ and $p(r_a) = 1/V$ we have

$$\langle U_T^2 \rangle = \left(\frac{e}{\epsilon_0} \right)^2 \frac{2N}{V} \int d^3r_a \left(\frac{1}{r_a^2} + \int d^3r_b \frac{NV}{r_a r_b} [p_{++}(\vec{r}_a, \vec{r}_b) - p_{+-}(\vec{r}_a, \vec{r}_b)] \right). \tag{15}$$

Specializing to Debye-type screening, we substitute (12) into (15), arriving at

$$\langle U_T^2 \rangle = \left(\frac{e}{\epsilon_0} \right)^2 \frac{2N}{V} \int d^3r_a\, d^3r_b \left(\frac{1}{V} \frac{1}{r_a^2} - \frac{1}{4\pi r_s^2} \frac{\exp(-|\vec{r}_a - \vec{r}_b|/r_s)}{r_a r_b |\vec{r}_a - \vec{r}_b|} \right). \tag{16}$$

The multiple integral in (16) can be performed analytically. [It is convenient to introduce new variables of integration by $\vec{R} = \frac{1}{2}(\vec{r}_a + \vec{r}_b)$, $\vec{r}_{ab} = \vec{r}_a - \vec{r}_b$ and integrate first over d^3R. The resulting divergence of the integral of the first term in the large parentheses in (16) is exactly cancelled by that of the second.] Our result is

$$\langle U_T^2 \rangle = 4\pi r_s \frac{2N}{V} \left(\frac{e}{\epsilon_0} \right)^2. \tag{17}$$

A different result, given in (18), has been obtained or quoted in the literature[3,5,6] by replacing the true potential (1) by the average potential (2) for the ions and then further assuming that the ions are randomly distributed. In this case the statistical theory gives for the mean square fluctuation of the total screened potential at an arbitrary point

$$\langle U_{sT}^2\rangle = -\frac{\partial^2}{\partial k^2}\exp\left(\frac{2N}{V}J(0)\right),$$

where

$$J(k)=\int\left[\cos\left(\frac{e}{\epsilon_0}k\frac{\exp(-r/r_s)}{r}\right)-1\right]d^3r.$$

Since $\partial J(0)/\partial k=0$ and $J(0)=0$, we have

$$\langle U_{sT}^2\rangle = -\frac{2N}{V}\frac{\partial^2 J(0)}{\partial k^2}=\frac{2N}{V}4\pi\left(\frac{e}{\epsilon_0}\right)^2\int_0^\infty e^{-2r/r_s}dr$$
$$=2\pi r_s\frac{2N}{V}\left(\frac{e}{\epsilon_0}\right)^2 \qquad (18)$$

which is the standard result[3,5,6] and is smaller by a factor of 2 than (17).

In the foregoing derivation of $\langle U_{sT}^2\rangle$ we have explicitly assumed that our system of charges consists of $2N$ randomly scattered ions, N positive and N negative, with screened potentials given by (2). From this model, which we shall call the SPM (screened-potential model), we can calculate not only $\langle U_{sT}^2\rangle$ but a complete distribution function for U_{sT}. We have just established that this distribution function is, crudely speaking, too narrow when compared to distributions arising from charges which have Debye-type pair correlations, as given by (12). Still, we may wonder if the distribution of potential from the SPM has a shape at least qualitatively similar to those which one would compute from models of charge distributions obeying (12).

In an attempt to answer this question, we shall construct a specific charge distribution satisfying (12), consisting, for simplicity, of randomly placed pairs of positive and negative charge, and compare the resulting distribution of potential to that calculated from the SPM. (We shall use subscripts RPM to denote quantities calculated in our random-pair model.) Thus we hope to be able to judge how reliable the SPM may be in general for calculating quantities dependent on the shape of the distribution of potential (or, by extension, on the shape of the distribution of potential gradients, etc.).

Labeling the positions of the N positive ions by $\vec{r}_1\cdots\vec{r}_N$, and those of the negative ions by $\vec{r}_{N+1}\cdots\vec{r}_{2N}$, we assume that $p(\vec{r}_1\cdots\vec{r}_{2N})$ is a product of pair functions g of the form

$$p(\vec{r}_1\cdots\vec{r}_{2N})$$
$$=\frac{1}{V^N}\frac{1}{N!}\sum_{P-}g(\vec{r}_1-\vec{r}_{N+1})g(\vec{r}_2-\vec{r}_{N+2})\cdots g(\vec{r}_N-\vec{r}_{2N}), \qquad (19)$$

where $\sum_{P-}$ means the sum on all permutations of the indices of the negative charges and

$$\int g(r)\,d^3r=1. \qquad (20)$$

One can verify that p is normalized and that

$$p_{+-}(\vec{r}_a,\vec{r}_b)=\frac{g(\vec{r}_a-\vec{r}_b)}{NV}+\frac{1}{V^2}, \qquad (21a)$$

$$p_{++}(\vec{r}_a,\vec{r}_b)=p_{--}(\vec{r}_a,\vec{r}_b)=\frac{1}{V^2}. \qquad (21b)$$

The statistical distribution of the total potential U_T at the origin is given by (13a), but $f(k)$ now has the special form

$$f(k)=\frac{1}{2\pi V^N}\prod_{j=1}^{N}\int d^3r_j\int d^3r_{N+j}\exp\left[-ik\frac{|e|}{\epsilon_0}\left(\frac{1}{r_j}-\frac{1}{r_{N+j}}\right)\right]g(\vec{r}_j-\vec{r}_{N+j})$$
$$=\frac{1}{2\pi}\left[\int d^3s_j\,g(s_j)\left(1+\frac{1}{V}\int d^3R_j\left\{\exp\left[-ik\frac{|e|}{\epsilon_0}\left(\frac{1}{r_j}-\frac{1}{r_{N+j}}\right)\right]-1\right\}\right)\right]^N$$
$$=\frac{1}{2\pi}\exp\left(-\frac{N}{V}\int d^3s\,g(\vec{s})J(\vec{s},k)\right), \qquad (22)$$

where we have introduced relative coordinates $\vec{s}_i=\vec{r}_i-\vec{r}_{N+i}$ and $\vec{R}_i=\frac{1}{2}(\vec{r}_i+\vec{r}_{N+i})$, taken the usual limit $N\to\infty$ ($V\to\infty$, N/V constant), and defined

$$J(\vec{s},k)=\int\left\{1-\exp\left[-ik\frac{|e|}{\epsilon_0}\left(\frac{1}{r_i}-\frac{1}{r_{N+i}}\right)\right]\right\}d^3R_i. \qquad (23)$$

So far we have made no approximations.

Specializing now to

$$g(\vec{s})=\frac{1}{4\pi r_s^2}\frac{e^{-s/r_s}}{s}, \qquad (24)$$

we notice that only pairs of charges whose separation is less than or of the order of r_s contribute to the integral in the exponent in Eq. (22). For r_s sufficiently small compared to $(N/V)^{-1/3}$ this means that for the overwhelming majority of configurations $s_i \ll R_i$, so that we can make the dipole approximation in (23),

$$\frac{1}{r_i}-\frac{1}{r_{N+i}}=\frac{1}{|\vec{R}_i+\vec{s}_i/2|}-\frac{1}{|\vec{R}_i-\vec{s}_i/2|}$$
$$\cong -\frac{\vec{s}_i\cdot\vec{R}_i}{R_i^3}\,, \tag{25}$$

where now $\vec{R}_i$ is the position of the dipole i, which has moment $|e|\vec{s}_i$. In this approximation, then, $f(k)$ in (22) is the Fourier transform of the distribution of potential (at a randomly chosen point) due to randomly placed point dipoles of random orientation whose distribution of dipole-moment magnitudes is proportional to $g(s)$.

Evaluating $J(\vec{s}, k)$ from (23) and (25), inserting into (22) for $f(k)$ and then applying (13a), we obtain

$$D_{\mathrm{RPM}}(u_T)=\frac{1}{\pi}\int_0^\infty \cos k u_T\, e^{-\beta k^{3/2}}\,dk\,, \tag{26}$$

where $\beta=\frac{4}{15}(2\pi)^{3/2}$ and $U_T=(\overline{\mu}_{\mathrm{eff}}/\epsilon_0)(N/V)^{2/3}u_T$. Here u_T is the potential in dimensionless form; $\overline{\mu}_{\mathrm{eff}}$ is an effective mean dipole moment defined by

$$\overline{\mu}_{\mathrm{eff}}=|e|\left[\int_0^\infty g(s)s^{3/2}\,d^3s\right]^{2/3}=(\tfrac{15}{8}\sqrt{\pi})^{2/3}|e|r_s$$
$$\cong 2.227\,|e|r_s\,. \tag{27}$$

It is easy to show that $D_{\mathrm{RPM}}(u_T)$ in (26) is just the distribution of potential from point dipoles of random position and orientation with fixed dipole moment $\overline{\mu}_{\mathrm{eff}}$ and of concentration N/V.[8]

The dipole model will most accurately reproduce $D_{\mathrm{RPM}}(u_T)$ when $p(\vec{r}_1\cdots\vec{r}_{2N})$ is of form (19) with g given by (24), when r_s is small compared to $(V/N)^{1/3}$, a typical interdipole spacing. For configurations of charges such that the charge closest to the origin is much farther away than r_s the approximation (25) will be accurate. Such configurations become overwhelmingly probable as $(N/V)^{1/3}r_s$ becomes very small. Charges in those few configurations for which the nearest charge (e.g., the charge nearest to the origin) is approximately of distance r_s or less from the origin will produce potentials with magnitudes of order $|e|/\epsilon_0 r_s$ or greater. Thus the high-potential tail of $D_{\mathrm{RPM}}(u_T)$ will not be properly given by the dipole model. [As an example, for $r_s=0.01(V/N)^{1/3}$ we expect that $D_{\mathrm{RPM}}(u_T)$ as calculated from (26) should become inaccurate for $u_T\gtrsim 100$.]

We have no physical reason for expecting r_s to be small in compensated semiconductors; we have discussed the case of small r_s because $D_{\mathrm{RPM}}(u_T)$ can be calculated in a simple way when r_s is small and, for comparison, the distribution of total screened potential $D_{\mathrm{SPM}}(u_{sT})$ can also be easily calculated in this limit.

For $r_s\ll (N/V)^{-1/3}$, $D_{\mathrm{SPM}}(U_{sT})$ can be accurately approximated (for U_{sT} not too small) by supposing that the only charge contributing to U_{sT}, the total screened potential at the origin, is the charge nearest to the origin, which we have called the "nearest charge." The reason for this is that if, in a given charge configuration, r_n is the nearest distance, i.e., the distance of the nearest charge from the origin, then other charges give important contributions to U_{sT} only if they lie within a distance r_n+Ar_s from the origin, where A is a constant greater than, say, 3.

The probability that no charges lie in the spherical shell with inner radius r_n and outer radius r_n+Ar_s can be calculated from the general formula for the probability that within a large volume V containing $2N$ particles the small volume ΔV is empty (ΔV is fixed and we assume $N\to\infty$, N/V fixed):

$$\lim_{N\to\infty}\left(1-\frac{\Delta V}{V}\right)^{2N}=e^{-(2N/V)\Delta V}\,. \tag{28}$$

From (28) we conclude that the probability that one or more ions lie between r_n and r_n+Ar_s is

$$\begin{aligned}&1-e^{-(2N/V)h(r_n)}\cong(2N/V)h(r_n)\,,\\&h(r_n)=4\tfrac{\pi}{3}[(r_n+Ar_s)^3-r_n^3]\,.\end{aligned} \tag{29}$$

Clearly, as r_s approaches zero this probability vanishes linearly with r_s, and the nearest charge gives the main contribution to U_{sT} for the overwhelming majority of configurations.

For a given value of r_s we can estimate the region of U_{sT} in which $D_{\mathrm{SPM}}(U_{sT})$ is accurately approximated by the distribution of potential from the nearest charge. For example if we take $r_s=0.01(N/V)^{-1/3}$ and require

$$(2N/V)h(r_n)\leqslant 0.05\,,$$

with $A=5$, we obtain $r_n\lesssim 0.174(N/V)^{-1/3}$ and

$$|u_{sT}|\equiv\left[\frac{e}{\epsilon_0}\left(\frac{N}{V}\right)^{1/3}\right]^{-1}|U_{sT}|\geqslant\frac{e^{-r_n/r_s}}{r_n}\left(\frac{V}{N}\right)^{1/3}$$
$$\cong 1.6\times 10^{-7}\,.$$

To compute the distribution of potential from the nearest charge we observe that the probability that a positive (or negative) charge has the nearest distance, r_n, is, in view of (28),

$$p(r_n)\,dr_n=4\pi\left(\frac{N}{V}\right)r_n^2\exp\left[-\frac{2N}{V}\left(\frac{4\pi r_n^3}{3}\right)\right]dr_n\,,$$

from which we deduce

$$D_{\mathrm{SPM}}(u_{sT})\cong 4\pi\left(\frac{N}{V}\right)r_n^2(u_{sT})\exp\left(\frac{-8\pi}{3}\frac{N}{V}r_n^3(u_{sT})\right)$$
$$\times\left(\frac{du_{sT}}{dr_n}\right)^{-1}, \tag{30a}$$

where

$$u_{sT} = \pm \frac{\exp(-r_n/r_s)}{r_n}\left(\frac{V}{N}\right)^{1/3} . \qquad (30b)$$

We have calculated D_{SPM} from (30a) by numerically inverting (30b) to obtain r_n as a function of u_{sT}. The resulting distribution is plotted in Fig. 1, where $D_{\mathrm{RPM}}(u_T)$ is also displayed for comparison. To ensure that the approximations used in calculating these distributions are valid in the range plotted, we have chosen a small value of r_s $[r_s = 0.01(N/V)^{-1/3}]$. The steep increase of D_{SPM} near the origin is a general characteristic of distributions of short-range potentials (or other field quantities of short range). The marked difference between D_{SPM} and D_{RPM} evident in Fig. 1 suggests that the SPM should be used with great caution.

In closing, we wish to point out that linewidth studies can give information about the degree of randomness of donor and acceptor ions in compensated semiconductors. Analysis of linewidths of certain magneto-optical transitions of neutral donors in compensated GaAs samples has led to the suggestion that donor and acceptor ions may be weakly paired in these samples.[9] In strong magnetic fields certain donor absorption lines in GaAs are broadened by the quadratic Stark effect (linewidths are proportional to the distribution of a weighted sum of squares of components of the total electric field), while other lines have widths proportional to the width of the distribution of the gradient of the electric field along the magnetic-field direction. The assumption of a completely random distribution of ions gives calculated quadratic-Stark-effect–induced widths which are too large relative to the calculated field-gradient-induced widths, when compared to the experimental observations.

We have reinvestigated this question of relative widths using the independent-pair model introduced here. Indeed, we find that decreasing r_s decreases the quadratic-Stark-effect widths relative to the field-gradient widths, as conjectured in Ref. 9. However, our results are valid only for $r_s \ll (N/V)^{-1/3}$, whereas we expect that $r_s > (N/V)^{-1/3}$ in semiconductors, so that no quantitative conclusions can be drawn. It should also be pointed out that we have no strong reason to expect that an independent-pair model accurately represents the distribution of ions in compensated semiconductors; furthermore, it is not at all certain that the Debye-type pair correlation given in (12) accurately approximates pair correlations in real semiconductors.

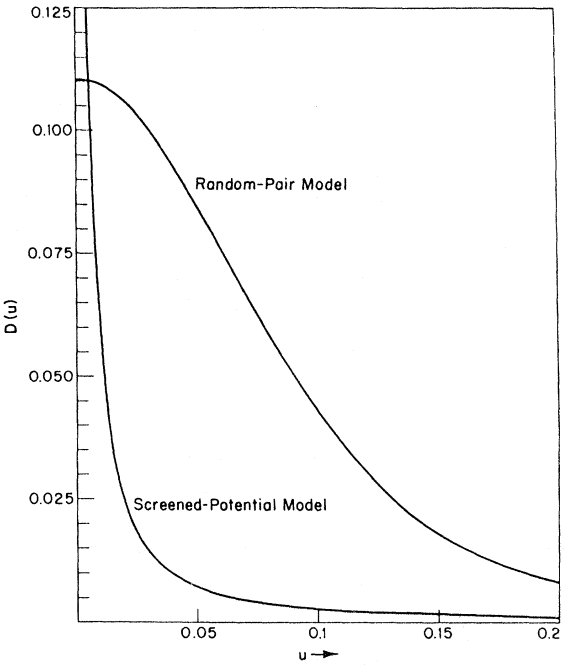

FIG. 1. Comparison of probability distributions of potential, $D(u)$, for the random-pair model (RPM) and screened-potential model (SPM) for $r_s = 0.01(N/V)^{-1/3}$. The potential u is plotted in units of $(|e|/\epsilon_0)\,(N/V)^{1/3}$.

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[1] An electron bound to a donor ion (or, in p-type material, a hole bound to an acceptor ion) is here assumed to completely neutralize its ion, forming an uncharged center. This approximation can be valid only if the electron (or hole) is not smeared over more than one ion. As one increases temperature and/or impurity concentration, the carriers, which are initially bound, tend to become delocalized. In that case, one can no longer classify centers as either neutral or charged and the discussion given here does not apply.

[2] L. V. Keldysh and G. P. Proshko, Fiz. Tver. Tela 5, 3378 (1963) [Sov. Phys.—Solid State 5, 2481 (1964)].

[3] T. N. Morgan, Phys. Rev. 139, A343 (1965). We refer here to the last part of the discussion in Sec. IV.

[4] M. I. Dyakonov, A. L. Efros, and D. L. Mitchell, Phys. Rev. 180, 813 (1969).

[5] G. F. Neumark, Phys. Rev. B 5, 408 (1972).

[6] F. Stern, Phys. Rev. B 9, 4597 (1974).

[7] For a useful review of the statistical theory see A. M. Stoneham, Rev. Mod. Phys. 41, 82 (1969).

[8] A cautionary note should be added at this point. The dipole model can also be used to approximate the distribution of electric fields and field gradients from the paired-charge model discussed above. However, the proper effective dipole moment to be employed is not $\bar{\mu}_{\mathrm{eff}}$ in (27), but should be recalculated for each field quantity whose distribution is to be found.

[9] D. M. Larsen, Phys. Rev. B 8, 535 (1973).