

# Large-scale potential fluctuations in plane layers with impurities

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Large-scale fluctuations are investigated of a random potential produced by charged impurities that form a plane layer. These fluctuations are produced by remote donors in heterostructures with wide spacer layers, and influence the mobility of the two-dimensional electrons located in the channel. It is shown that if some of the donors in the layer are neutral, correlations are produced in the spatial distribution of the charged donors and decrease substantially the potential fluctuations. The correlations are investigated under various assumptions concerning the thermodynamic equilibrium in the system of electrons filling the donors. In a system that is in total equilibrium the problem reduces at low temperatures to calculation of the spatial distribution of the charge in the ground state. In thin layers the charge correlator is shown to be connected with the size of the mesoscopic fluctuations of the chemical potential of a finite system. Computer simulation yields independently the charge correlator and the magnitude of the chemical-potential fluctuations.

## 1. FORMULATION OF PROBLEM

The problem considered is encountered in the study of the density of states and of the mobility of a two-dimensional electron gas in heterostructures with thick spacer layers. Figure 1 shows the energy distribution of a modulation-doped GaAs–AlGaAs heterojunction. A two-dimensional electron gas (TEG) is located in a narrow layer near the junction. In a typical case, the wide-band solid solution is doped with donors (Si) at a density  $10^{18} \text{ cm}^{-3}$ . To increase the mobility of the two-dimensional electrons, an undoped solid-solution layer, called a spacer layer, is produced near the junction. The spacer layer can reach  $1000 \text{ \AA}$  and more. Heterostructures are sometimes produced with a  $\delta$ -function-like donor layer. In this case all the donors are practically in one plane at a distance  $d$  from the TEG. As a rule, the surface density  $n$  of the two-dimensional electrons is approximately equal to the density of the positively charged donors.

The locations of the charged donors are random, the surface charge density fluctuates, and as a result potential fluctuations are produced from which the two-dimensional electrons are scattered and which form the density of the electron states.

An important distinctive feature of the problem is that the two-dimensional electron gas is acted upon only by charged-donor density fluctuations having dimensions of the order of or larger than the spacer-layer thickness  $d$ . The potential of the small-scale fluctuations decreases exponentially with increase of the distance from the charged-donor layer. Assuming that  $d$  is much larger than the average distance between the charged donors, we shall investigate only large-scale fluctuations of the surface charge density. This is the main purpose of the present paper. It must also be kept in mind that a random potential can be produced not only by the charge-density fluctuations, but also because the charged donors are not in one plane. In the case of  $\delta$ -like layers this mechanism does not occur, but we shall show below that it plays an important role in the case of thick doped layers.

We assume for the donors a Poisson distribution in

space. If, however, some of the donors are charged and the rest are neutral, and if the electrons can go over from donor to donor, a correlation due to the interaction between the charges is produced in the distribution of the charged donors. For example, if the donors are located in a very thin layer and the fraction of the charged donors is small, the conditions are energywise favorable for the charge to form a structure reminiscent of a two-dimensional Wigner crystal. The fluctuations of the charge and the random potential produced by these fluctuations turn out to be much smaller than for a Poisson distribution of charged donors.<sup>1,2</sup>

The model considered below constitutes a parallel-plate capacitor, one electrode of which is the TEG and the other a layer of thickness  $h$  (Fig. 1) in which donors are randomly and uniformly distributed with a surface density  $N_d$ . The electron surface density in the TEG is equal to the density  $n$  of the charged donors ( $n \leq N_d$ ). The problem is to find the random potential produced by the charged donors, with account taken of their correlation. To calculate the correlation, some assumption must be made concerning the thermodynamic equilibrium in the system of electrons located on the donors. We are interested in the correlation at low (helium) temperatures, when the energy of the interaction

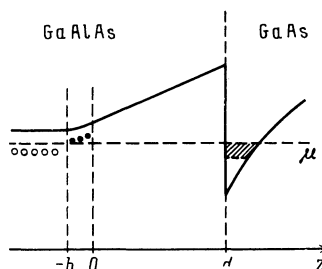


FIG. 1. Energy distribution in heterojunction. Solid line—energy of the bottom of the conduction band, which experiences a jump on the junction. The horizontal dashed line is the chemical-potential level. The electron states filling the TEG are shaded; closed circles—charged-donor levels; open circles—neutral-donor levels.

of the charges with one another is much larger than the thermal energy  $T$ . If it is assumed that at these temperatures the electrons can go over from donor to donor, for example through the TEG, the distribution of the electrons over the donors corresponds to the ground, i.e., lowest in energy, state of the system. The model for which this assumption is made will be dubbed the equilibrium model. It is the subject of Secs. 3–5. Section 3 contains a qualitative discussions of the charge fluctuations in this model, while Secs. 4 and 5 describe the procedure and the results of the computer simulation.

In the alternative nonequilibrium model (Sec. 2) the premise is that the electron distribution over the donors is “frozen” by the cooling at some temperature  $T_0$  and constitutes at lower temperatures a “snapshot” of the distribution existing at  $t = T_0$ . If this freezing is to be related to the onset of long-time photoconductivity, it must be assumed that  $T_0 \approx 100$  K. At this temperature the thermal energy exceeds the electron-interaction energy, so that the correlation in the disposition of the charges can be obtained analytically by methods valid for a weakly non-ideal plasma. The nonequilibrium model was first suggested and considered by one of us.<sup>1</sup> It is difficult at present to favor either model. It seems to us that an experimental confirmation of the nonequilibrium model would be observation of the dependence of the low-temperature mobility of the electrons on the cooling regime. The conductivity should in this case be sensitive to the rate of passage through the temperature region near  $T_0$ .

## 2. NONEQUILIBRIUM MODEL

It is assumed in this model that the charge correlation at low temperatures is the same as at  $T_0$ . We introduce the function  $c(\mathbf{r}) = n(\mathbf{r}) - n$ , which describes the fluctuation of the charged-donor density. We calculate the correlator

$$D(\mathbf{r}-\mathbf{r}') = \langle c(\mathbf{r})c(\mathbf{r}') \rangle \quad (1)$$

by the method of path integrals.<sup>3</sup> The probability of the fluctuation  $c(\mathbf{r})$  is proportional to  $\exp[-\Phi(c)]$ , where the functional  $\Phi(c)$  takes the form

$$\Phi(c) = \frac{1}{2n} \int c^2(\mathbf{r}) d^2r + \frac{1}{T_0} \int c(\mathbf{r})c(\mathbf{r}') G(\mathbf{r}-\mathbf{r}') d^2r d^2r'. \quad (2)$$

Here  $G(\mathbf{r}-\mathbf{r}')$  is the interaction energy of two electrons. It must be taken into account in its calculation that the TEG, which is located at a distance  $d$  from the donor layer, should be regarded as a metallic plane. Then

$$G(\mathbf{r}-\mathbf{r}') = \frac{e^2}{\kappa} \left\{ \frac{1}{|\mathbf{r}-\mathbf{r}'|} - \frac{1}{[(\mathbf{r}-\mathbf{r}')^2 + 4d^2]^{1/2}} \right\}. \quad (3)$$

The layer thickness  $h$  is assumed small compared with the dimension of the investigated fluctuations and the thickness of the spacer layer  $d$ . A Gaussian approximation in the first term of (2) is valid if the number of donors in the fluctuation is large. The correlator (1) can be written in the form of a path integral:

$$D(\mathbf{r}-\mathbf{r}') = \left\{ \int Dc c(\mathbf{r})c(\mathbf{r}') \exp[-\Phi(c)] \right\} \times \left\{ \int Dc \exp[-\Phi(c)] \right\}^{-1}. \quad (4)$$

As a result we find that the Fourier component

$$D(\mathbf{q}) = \int d^2r D(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}}$$

is equal to

$$D(q) = \frac{nq}{q + q_0 [1 - \exp(-2qd)]}, \quad (5)$$

where  $q_0 = 2\pi n e^2 / \kappa T_0$  is the reciprocal Debye radius. We are interested in the case  $q \ll q_0$ . For  $qd \gg 1$  we get  $D(q) = q\kappa T_0 / 2\pi e^2$ . Note that  $D(q) = n$  in the absence of correlation and the fluctuations are much stronger, since  $n \gg q\kappa T_0 / 2\pi e^2$ . For  $qd \ll 1$  we get

$$D(q) = \kappa T_0 / 4\pi e^2 d. \quad (6)$$

In this case the correlator has the same form as if there were no correlation, but the density  $n$  is replaced by the decreased effective density  $n_0 = \kappa T_0 / 4\pi e^2 d$ .

The random potential produced in the TEG plane by the density fluctuations of the charged phonons located at a distance  $d$  from the TEG is given by

$$F(\mathbf{r}, d) = \frac{e^2}{2\pi\kappa} \int \frac{c(\mathbf{q}) \exp(i\mathbf{q}\mathbf{r} - qd)}{q + q_s} d^2q, \quad (7)$$

where  $q_s$  is the TEG screening radius. In view of the linear relation between  $F$  and  $c$ , the potential is a Gaussian random function. With the aid of the correlator (5) we obtain

$$\langle F^2 \rangle = 3,77 \frac{e^4 n_0}{\kappa^2 (q_s d)^2}. \quad (8)$$

## 3. EQUILIBRIUM MODEL

In this model the spatial distribution of the charged donors corresponds to the ground state. As already mentioned, at very low charged-donor densities this distribution is reminiscent of a Wigner crystal. We, however, consider a more realistic case, when the average distances between the charged and neutral donors are comparable. We study in this section a donor layer of zero thickness ( $\delta$  layer). Layers of finite thickness are discussed in Sec. 5.

We show first that the considered problem of charge surface-density fluctuations is related to the mesoscopic problem of chemical-potential fluctuations in a finite square. We imagine, for this purpose, that the entire plane is broken up into  $R \times R$  squares. We assume that the distribution inside each square corresponds to the ground state, but under the condition that each square is electrically neutral. The neutrality is due in this case to the negative background that cancels the average charge of the donors. This is equivalent to taking the second electrode of the capacitor into account.<sup>4</sup> Equilibrium is thus reached inside each square, but flow of charge between squares is forbidden, so that the chemical potentials of the different squares differs from one another. Let  $R \ll d$ , so that a pure Coulomb electron interaction can be assumed. When total equilibrium is reached, charge flows between the squares, and the excess charge  $Q(R)$  of an  $R \times R$  square is of the order of  $\kappa \delta \mu(R) R / e$ , where  $\delta \mu(R)$  is the chemical-potential difference obtained under neutrality conditions. Let  $\langle \delta \mu^2 \rangle$  be the variance of the chemical potential in the  $R \times R$  square, obtained by averaging over all realizations of the random donor distribution in this square when the neutrality condition is met. It follows from the

preceding reasoning that the variance is connected with rms charge fluctuations  $\langle Q^2 \rangle$  in an  $R \times R$  square cut out of an infinite system, by the relation

$$\alpha \frac{e^2}{\kappa^2} \langle Q^2 \rangle = R^2 \langle \delta\mu^2 \rangle, \quad R \ll d, \quad (9)$$

where  $\alpha$  is a coefficient independent of  $R$ . To determine the  $Q(R)$  dependence it suffices therefore to study the fluctuations of the chemical potential in a finite system.

Under certain assumptions, which will be formulated below, the quantity  $\langle \delta\mu^2 \rangle$  can be calculated. We introduce a random function  $\mu(\mathbf{r})$  obtained by averaging the chemical potential of neutral squares over many squares in the vicinity of the point  $\mathbf{r}$ . The size of each square is assumed large compared with the average distance between charges. In essence,  $\mu(\mathbf{r})$  is the work function of a random two-dimensional system. The potential  $\varphi(\mathbf{r})$  that results from flow of charges between squares is connected with this work function by the relation

$$\mu(\mathbf{r}) + e\varphi(\mathbf{r}) = \mu, \quad (10)$$

where  $\mu$  is the equilibrium chemical potential of the infinite system. The simplest assumption is that the function  $\delta\mu(\mathbf{r}) = \mu(\mathbf{r}) - \mu$  is locally connected with the donor-density fluctuations:

$$\delta\mu(\mathbf{r}) = \frac{d\mu}{dN_d} [N_d(\mathbf{r}) - N_d]. \quad (11)$$

It follows from (10) and (11) that for Gaussian fluctuations we have

$$e^2 \langle \varphi(\mathbf{r}) \varphi(\mathbf{r}') \rangle = \left( \frac{d\mu}{dN_d} \right)^2 N_d \delta(\mathbf{r} - \mathbf{r}'). \quad (12)$$

The relation between the potential  $\varphi(\mathbf{r})$  and the excess charge  $ec(\mathbf{r})$  is given

$$\varphi(\mathbf{r}) = e \int c(\mathbf{r}') \left\{ \frac{1}{|\mathbf{r} - \mathbf{r}'|} - \frac{1}{[(\mathbf{r} - \mathbf{r}')^2 + 4d^2]^{1/2}} \right\} d^2r', \quad (13)$$

where the second term takes into account the presence of a metallic surface at a distance  $d$  from the donor layer. Using (1), (12), and (13) we get

$$D(q) = \frac{\kappa^2 q^2}{(2\pi)^2 e^4} \left( \frac{d\mu}{dN_d} \right)^2 \frac{N_d}{[1 - \exp(-2qd)]^2}. \quad (14)$$

It follows from (11) that the fluctuations of the chemical potential in a region of area  $S$  do not depend on the shape of the region and are described by the equation

$$\langle \delta\mu^2 \rangle = \left( \frac{d\mu}{dN_d} \right)^2 \frac{N_d}{S}. \quad (15)$$

This dependence of  $S$  is the usual one for systems with finite correlation radii. According to (9) and (14), the fluctuations of the charge  $Q(R)$  are independent of  $R$  if  $R \ll d$ , and amount to several elementary charges when  $n$  and  $N_d$  are comparable.

The dependence of  $\mu$  on  $n$  and  $N_d$  can be represented without loss of generality in the form

$$\mu = \frac{e^2 N_d^{1/2}}{\kappa} g \left( \frac{n}{N_d} \right), \quad (16)$$

where  $g$  is an unknown function. Equations (11), (12), (14), and (15) contain a derivative calculated under neutrality conditions, i.e., at a constant density  $n$  of the charged donors:

$$\frac{d\mu}{dN_d} = \frac{e^2}{N_d^{1/2} \kappa} \left( \frac{g}{2} - \frac{ng'}{N_d} \right). \quad (17)$$

Substituting  $q = 2\pi/R$  in (14), we obtain a universal connection between  $D(2\pi/R)$  and  $\langle \delta\mu^2 \rangle$ :

$$D \left( \frac{2\pi}{R} \right) = \frac{\kappa^2}{e^4} \langle \delta\mu^2 \rangle \left[ 1 - \exp \left( -\frac{4\pi d}{R} \right) \right]^{-2}. \quad (18)$$

The results (14)–(16) are based on Eq. (11) in which a local connection between  $\delta\mu(\mathbf{r})$  and  $N_d(\mathbf{r})$  is assumed. It must be noted, however, that a relation of type

$$D \left( \frac{2\pi}{R} \right) = \gamma(\nu) \frac{\kappa^2}{e^4} \langle \delta\mu^2 \rangle \quad (19)$$

follows from (9) for any  $D(q) \propto q$ . Here  $\gamma(\nu)$  is a numerical coefficient that depends on  $\nu$ , with  $\gamma(2) = 1$ . In Secs. 4 and 5 we describe a computer simulation that resulted in independent calculations of  $D(q)$  and  $\langle \delta\mu^2 \rangle$  as  $d \rightarrow \infty$ . Calculations performed for  $n/N_d = 5$  have confirmed the validity of (19). It has turned out here that  $\nu$  is closer to 1.7 than to 2 at the largest of the investigated values of  $R$  and the smallest  $q$ . It has also turned out that  $\gamma(\nu) \approx 1.1$ . We assume that the small deviation of  $\nu$  from the value  $\nu = 2$  predicted by the local theory is due to the long-range character of the Coulomb interaction and to the absence of screening of the large-scale fluctuations, i.e., to the same factors that lead to formation of a Coulomb gap in the density of states.<sup>5</sup>

#### 4. DESCRIPTION OF THE SIMULATION PROGRAM

In a three-dimensional array with dimensions  $R \times R \times h$  we generated random coordinates of a total of  $R^2$  donors, and varied their  $z$ -coordinates in the interval  $-h \leq z \leq 0$ . Each donor was assigned a charge 0 or 1 such that the fraction of the charged donors was equal to  $n/N_d$ . The second capacitor electrode, made up of the TEG, was taken into account by introducing an electric field perpendicular to the plane of the  $R \times R$  square and equal to  $2\pi\sigma$ . The total energy of the interaction of the charges with one another and with the external field was minimized with respect to all possible relocations of a given charge. This resulted in the so-called pseudo-ground states<sup>6</sup> from which it is possible to land in the ground state only by simultaneous rearrangement of several electrons. The program made it possible to run through several pseudoground states and choose from among them the states with lowest energy. A pure Coulomb energy of the interacting charges was assumed, i.e., the distance  $d$  to the metallic surface was assumed infinite. In addition, the presence of a negatively charged background that cancels the charge of the donors was assumed. We used quasiperiodic boundary conditions<sup>7</sup> consisting of the following: the initial  $R \times R$  square was surrounded by eight squares that were identical with it and had the same distribution of charged and neutral donors, so that the shortest distance between equivalent donors was equal to  $R$ . Only the interaction of charges on non-equivalent donors were taken into account. One of the interacting donors was always inside the initial square, and from the aggregate of donors equivalent to the

second we chose the nearest to the first, so that interaction could take place also through the boundary of the initial square.

After minimization, we calculated the chemical potential. To this end we chose a maximum-energy neutral donor and a minimum-energy charged donor. The chemical potential was defined as the arithmetic mean of these energies. We determined also the chemical potential averaged over the realizations and its variance. In addition, we calculated the distribution function  $f(z)$  of the charged donors in the coordinate  $z$  and the mean value  $\langle z \rangle$ . Both quantities were averaged over the realizations of the donor coordinates. To investigate the fluctuation potential produced by the charged donors, we calculated a function  $S(q, h)$  such that the rms potential [in units of  $(e^2 N_d^{1/2} / \chi)^2$ ] is given by

$$\langle F^2 \rangle = \sum_{m, n=-\infty}^{+\infty} D(q_{mn}, h) \frac{\exp(-2q_{mn}z)}{m^2 + n^2}, \quad (20)$$

where  $q_{mn} = 2\pi(m^2 + n^2)^{1/2}R$ . For  $h = 0$  the value of  $D(q, h)$  coincides with the charge correlator  $D(q)$  defined by relation (1). In the general case  $D(q, h)$  describes also potential fluctuations connected with the scatter of the  $z$  coordinates of the charged donors. The quantity  $D(q, h)$  was calculated using the equations

$$D(q_{mn}, h) = (16 - 12\delta_{m0} - 12\delta_{n0})^{-1} \sum_{j=1}^4 \langle C_{mn}^j \rangle, \quad (21)$$

$$C_{mn}^j = (4 - 2\delta_{m0} - 2\delta_{n0}) / R \sum_k \left\{ \exp \left[ \frac{2\pi z_k}{R} (m^2 + n^2)^{1/2} \right] \times \cos \left( \frac{2\pi x_k}{R} \right) \sin \left( \frac{2\pi y_k}{R} \right) \right\}. \quad (22)$$

The summation in (22) is over all the charged donors;  $x_k, y_k,$  and  $z_k$  are their coordinates. The three other coefficients  $C_{mn}^j$  differ by different possible replacements of the cosines by sines. The averaging in (21) is over the realizations of the donor coordinates.

It is easy to show for a charged-donor Poisson distribution

$$D(q, h) = n \frac{1 - \exp(-2qh)}{2qh}. \quad (23)$$

The simulation was with an EC 1055M computer having a speed of 0.5 MFLOPS. The maximum array used was  $R^2 = 1000$  and required about 2M of on-line memory. All the calculations described below required about 100 hours of processor time. The program was written in FORTRAN-77, with the exception of the two most frequently performed subprograms, viz., the random-number generator and the square-root extractor, which were written in Assembler language. When the standard square-root extraction function was used, this operation required more than half the program time. A "fast square root" subprogram was therefore developed, using a table of square roots for the choice of an initial approximation subsequently refined with the aid of one Newton iteration. At a result accurate to 6 decimal places and using a 32 K table, this subprogram was approximately twice as fast (and its variant using an argument-array was three times as fast) as the standard one.

## 5. SIMULATION RESULTS

### A. Simulation of $\delta$ -layer of donors

To simulate a  $\delta$  layer it suffices to put  $h = 0$ . We confine ourselves to the case  $n/N_d = 0.5$ . Figure 2 shows the dependence of the variance  $\langle (\delta\mu)^2 \rangle$  of the chemical potential on  $R^2$ . It can be seen that for the largest  $R$  the variance is  $\langle (\delta\mu)^2 \rangle \propto R^{-1.7}$  and differs from the  $\langle (\delta\mu)^2 \rangle \propto R^{-2}$  dependence given by Eq. (15).

Figure 3 shows a plot of the correlator  $D(q) - D(q, h)$  versus  $q$  for  $h = 0$ . It can be seen that for small  $q$  this  $D(q)$  dependence is given by  $D(q) \propto q^{1.7}$ . This fact follows from (19) at  $\langle (\delta\mu)^2 \rangle \propto R^{-1.7}$ . Figure 3 shows the values of  $D(q)$  obtained from Eq. (19) at  $\gamma(\nu) = 1.1$  from the data obtained for  $\langle (\delta\mu)^2 \rangle$  by simulation. It can be seen that (19) describes well the simulation result, with  $\gamma(1.7) = 1.1$  differing little from  $\gamma(2) = 1$ . For large  $q$ , such that  $qn^{-1/2} \gg 1$ , we have for the correlator  $D(q) = n$ , just as for uncorrelated charge distribution.

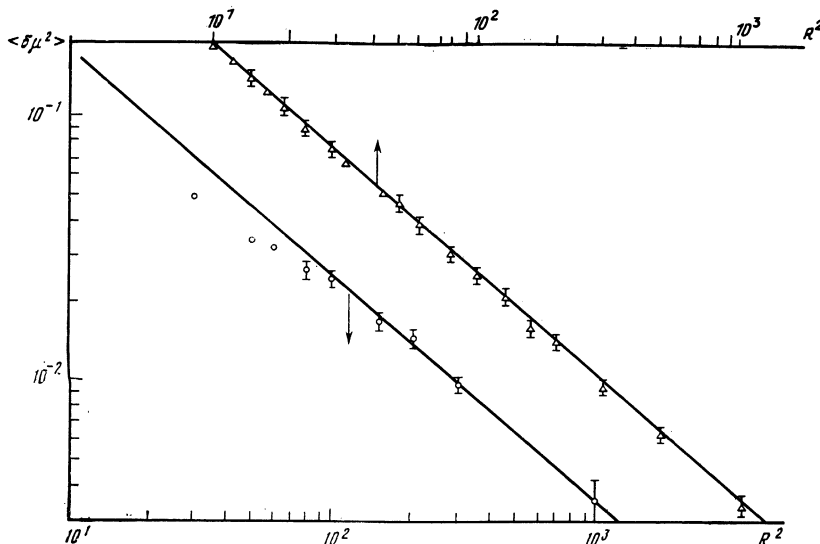


FIG. 2. Dependence of the chemical-potential fluctuations  $\langle (\delta\mu)^2 \rangle$  (in units of  $e^2 N_d / \chi^2$ ) on the number  $R^2$  of donors at  $n/N_d = 0.5$ :  $\circ$ — $h = 0$ ,  $\triangle$ — $h = N_d^{-1/2}$ . For convenience, these dependences are displaced from each other along the abscissa axis. The results for  $h = N_d^{-1/2}$  fit well a continuous line having a slope corresponding to  $\langle (\delta\mu)^2 \rangle \propto R^{-1.7}$ . This straight line is redrawn also in terms of the displaced coordinates.

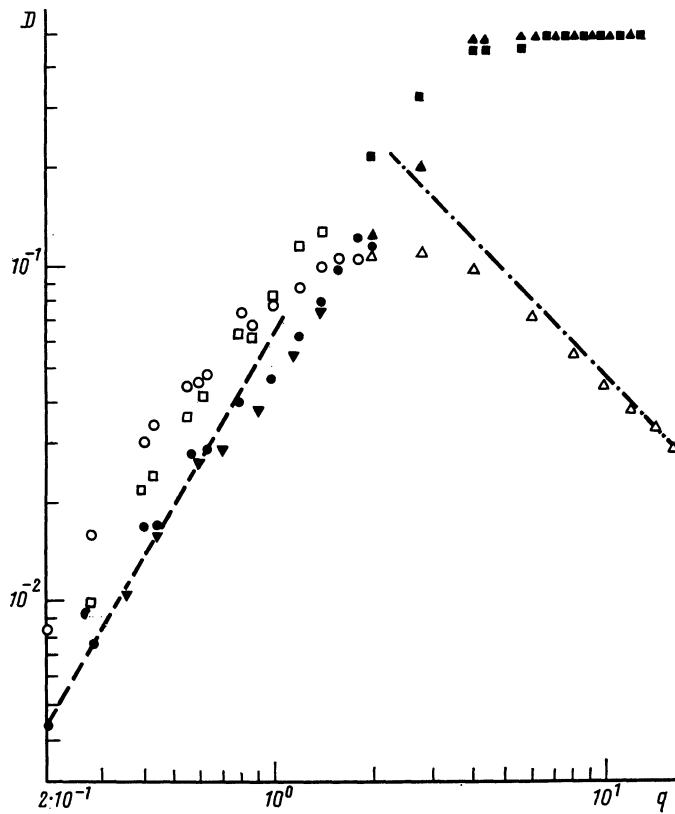


FIG. 3. Dependence of the correlator  $D(q, h)$  (in units of  $N_d$ ) on  $q$  (in units of  $N_d^{1/2}$ ) at  $\bullet$ — $h=0$ ,  $R^2=1000$ ;  $\blacktriangle$ — $h=0$ ,  $R^2=10$ ;  $\circ$ — $h=N_d^{-1/2}$ ,  $R^2=1000$ ;  $\triangle$ — $h=N_d^{-1/2}$ ,  $R^2=10$ ;  $\square$  and  $\blacksquare$  denote the density correlator of the charge projected on the plane  $z=0$  for  $h=N_d^{-1/2}$ ,  $R^2=1000$  and  $10$ , respectively. Dashed line— $D(q) \propto q^{1.7}$ , dash-dot line— $D=N_d/2\pi h$ ;  $\blacktriangledown$ —the  $D(q)$  correlator for  $h=0$ , calculated from (19) at  $\gamma(\nu)=1.1$  starting from the  $\langle(\delta\mu^2)\rangle$  data shown in Fig. 2.

### B. Simulation of volume distribution of donors

It is natural to define a  $\delta$  layer as a layer in which  $hN_d^{1/2} \ll 1$ . In this case the charge is uniformly distributed over the layer thickness and the quantities  $\langle(\delta\mu)^2\rangle$  and  $D(q)$  are independent of  $h$  (if  $R \gg h$  and  $qh \ll 1$ ). The layer for which  $hN_d^{1/2} \gg 1$ , will be called thick. The charged donors are located then in a thin layer of thickness on the order of  $N_d^{-1/2}$  near the  $z=0$  plane. The remainder of the layer contains practically no charged donors. In thick layers the fluctuating potential is produced not only by fluctuations of the surface charge density, but also by fluctuations of the  $z$  coordinates of the charged donors. The main purpose of simulating a thick layer is an assessment of the role of this fluctuation mechanism, and also of the influence of the layer thickness on the charge fluctuation.

Figure 4 shows the charged-donor distribution function  $f(z)$  representing the average volume density of the charged donors at a distance  $z$  from the layer boundary, referred to the donor volume density  $N_d/h$ . The value of  $h$  was varied, with  $n$  and  $N_d$  maintained constant and with  $n/N_d=0.5$ . It can be seen that a substantial inhomogeneity of the donor distribution sets in at  $hN_d^{1/2} > 0.2$ . Figure 5 shows a plot of  $D(q, h)$  in the region of small  $q$  for different values of  $h$  and constant  $n$  and  $N_d$ , with  $h/N_d=0.5$ . It can be seen that at

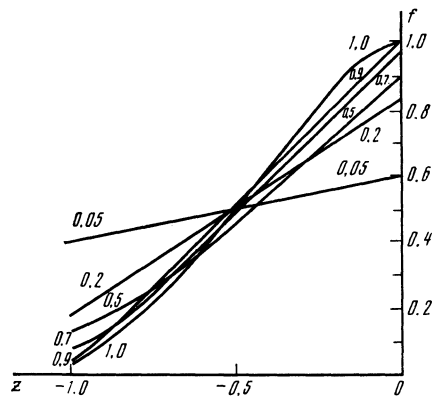


FIG. 4. Distribution function  $f(z)$  of charged donors for  $n/N_d=0.5$  and different values of  $h$  (marked on the curves).

$hN_d^{1/2} \leq 0.2$  the correlator  $D(q, h)$  is practically independent of  $h$ , so that from the standpoint of fluctuations the  $\delta$  layer should be defined to be the one with  $hN_d^{1/2} \leq 0.2$ . We have verified that a layer with  $hN_d^{1/2}=1$  can be regarded as thick, by showing that at  $h > N_d^{-1/2}$  an increase of  $h$  without changing the donor volume density  $N_d/h$  and the surface charge density  $n$  does not lead to a change of  $D(q, h)$ .

In Fig. 3, the data for a thick layer  $hN_d^{1/2}=1$  are compared with the data for a  $\delta$  layer ( $h=0$ ) in a wide range of  $q$ . It can be seen that at the very smallest values of  $q$  the correlator  $D(q, h)$  is approximately twice as large as for a  $\delta$  layer. To determine the cause of this difference we modified the simulation program: after minimizing the energy in the  $h=N_d^{-1/2}$  layer we assumed all the donors to have  $z=0$ . This was followed by calculation of the correlator  $D(q, h)$ , which in this case coincided with the charge density correlator projected on the  $z=0$  plane. This calculation excluded completely the fluctuations of the distance from the charged donors to the plane  $z=0$ , leaving the surface charge-density fluctuations unchanged. The correlator  $D(q)$  obtained as a result of this procedure is shown in Fig. 3. It can be seen that

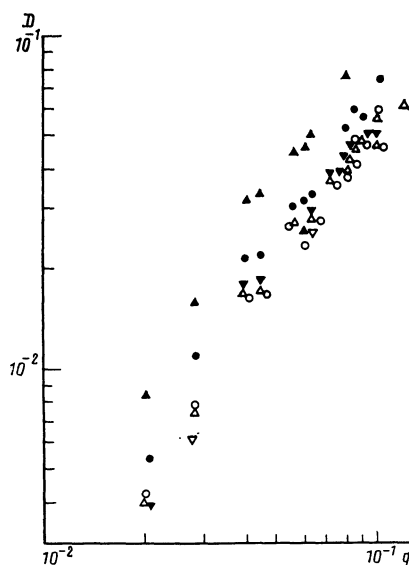


FIG. 5. The correlator  $D(q, h)$  (in units of  $N_d$ ) versus  $q$  (in units of  $N_d^{1/2}$ ) for  $n/N_d=0.5$ ;  $R^2=1000$ :  $\triangle$ — $h=0$ ,  $\circ$ — $h=0.05 N_d^{-1/2}$ ,  $\blacktriangledown$  ( $\nabla$ )— $h=0.2 N_d^{-1/2}$ ,  $\circ$ — $h=0.5 N_d^{-1/2}$ ,  $\blacktriangle$ — $h=N_d^{-1/2}$ .

for the smallest  $q$  it coincides with the correlator for the  $\delta$  layer. It follows hence that the aforementioned difference between the correlators for thick and  $\delta$  layers at small  $q$  is due just to fluctuations of the distance to the charge. A theoretical estimate of the contribution of these fluctuations leads to an expression of the same order of magnitude as (14). It is difficult, however, to estimate the numerical coefficient for this mechanism.

We examine now the asymptote of  $D(q, h)$  for  $qh \gg 1$ . In this case the main contribution to the correlator is made by a layer with thickness of order  $1/q$  near the  $z = 0$  plane. As seen from Fig. 4, for  $h = N_d^{-1/2}$  we have in this layer  $f(z) = 1$ , i.e., all the donors are charged. The correlator  $D(q, h)$  should consequently be the same as for the uncorrelated distribution of charged donors with surface density  $n = N_d$ . According to (23) we have

$$D(q, h) = \frac{2qh}{N_d}. \quad (24)$$

As seen from Fig. 3, Eq. (24) agrees splendidly with the simulation results for  $qh > 6$ . This serves as a reliable verification of the program.

The chemical-potential fluctuation  $\langle (\delta\mu)^2 \rangle$  as a function of  $R^2$  is shown for a thick layer ( $hN_d^{1/2} = 1$ ) in Fig. 2. Note that at large  $R$  the chemical-potential fluctuations are the same for thick and  $\delta$  layers.

As already mentioned,  $D(q, h)$  and  $\langle (\delta\mu)^2 \rangle$  were calculated not for the ground states but for pseudoground states. To verify whether this circumstance is important, we used the following procedure: for a given realization of the donor coordinates we carried out a set of ten minimizations with different initial arrangements of the electrons. This resulted in ten, generally speaking, different pseudoground states. From among these we chose the pseudoground state having the lowest energy, and used just this state for averaging  $D(q, h)$  and  $\langle (\delta\mu)^2 \rangle$  over the realizations of the donor coordinates. We have verified that the results obtained in this manner did not differ systematically from the values obtained by averaging over random pseudoground states.

Let us list the main results of using the equilibrium model.

1. When the donors making up a plane layer are only partly charged, a correlation appears in the spatial distribution of the charge and decreases substantially the fluctuations of the potential.

2. In the case of  $\delta$  layers the Fourier components of the potential fluctuations can be related to mesoscopic fluctuations of the chemical potential in a finite neutral system.

3. In a two-dimensional disordered system of localized electrons, at zero temperature, the chemical-potential fluctuations  $\langle (\delta\mu)^2 \rangle$  at the investigated system dimensions  $R$  are not proportional to  $R^{-2}$ . This may be due to the long-range character of the Coulomb interaction.

4. At a donor-layer thickness  $h > N_d^{-1/2}$  the potential fluctuations increase substantially with increase of  $h$ , so that at the lowest values of  $q$  investigated by us we have

$$D(q, h) \Big|_{h=N_d^{-1/2}} \approx 2D(q, 0).$$

It follows hence that within the framework of the equilibrium model the layers should ensure a substantially higher electron mobility in the channel than thick donor layers.

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