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Density of states of a two-dimensional electron gas in a long-range random potential

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The thermodynamic density of states and the density of states as obtained from the activation energy of the conductivity are calculated taking into account both linear and nonlinear electron screening. In the linear screening regime the density of states in a strong magnetic field is negative, and it is determined by electron-electron interaction. Linear screening fails when the filling factor is close to an integer. In the nonlinear screening regime the density of states is positive. The crossover between these regimes is shown to be very sharp. The quantitative results are obtained by computer modeling. They are in a good agreement with recent magnetocapacitance measurements and previous measurements of the activation energy in the regime of the quantum Hall effect.

I. INTRODUCTION

A. Long-range potential and screening

The long-range potential and electron screening play a very important role both in GaAs/Ga$_{1-x}$Al$_x$As structures and in silicon metal-insulator-semiconductor structures (see the review[1]). In silicon structures the source of the long-range random potential is not known for sure, but in the modulation-doped GaAs/Ga$_{1-x}$Al$_x$As structures the long-range random potential is caused by fluctuations in the density of the remote ions. The energy scheme of a simple heterostructure is shown in Fig. 1. The layer with ionized donors is usually thin enough to consider it as a plane. This layer is separated from the two-dimensional electron liquid (2DEL) by an undoped spacer layer. Thus, the electrostatic model of a heterojunction with a wide spacer is a plane condenser with a 2DEL as one plate and with a thin layer of the randomly distributed donors as the other plate. The distance between the two plates is the spacer width s. The fluctuations in the density of charged donors create a random potential $F_b(\mathbf{r})$ in the plane of 2DEL. We assume here that the spatial distribution of the charged donors $C(\mathbf{r})$ is random, and that it is not correlated. Thus, $\langle C(\mathbf{r})\rangle = 0$ and

$$\langle C(\mathbf{r}_1)C(\mathbf{r}_2)\rangle = C\delta(\mathbf{r}_1-\mathbf{r}_2), \tag{1}$$

where $\langle\,\rangle$ represents averaging over different configurations of the donor density. It has been shown[2] that in order to take into account correlation in the charge distribution one should replace C with some effective reduced density.

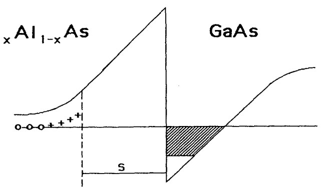

FIG. 1. Energy diagram of a GaAs heterostructure, where the region occupied by the 2DEL is shaded.

The random potential created by fluctuations in the donor density $F_b(\mathbf{r})$, called the bare potential, can be written in the form

$$F_b(\mathbf{r}) = \frac{e^2}{\kappa}\int\frac{C(\mathbf{r}')d^2r'}{\sqrt{|\mathbf{r}-\mathbf{r}'|^2+s^2}}. \tag{2}$$

Expressed as a Fourier integral this potential becomes

$$F_b(\mathbf{r}) = 2\pi\frac{e^2}{\kappa}\int\frac{d^2q}{q}C(\mathbf{q})e^{i\mathbf{qr}-qs}, \tag{3}$$

where

$$C(\mathbf{q}) = \int\frac{d^2r}{(2\pi)^2}C(\mathbf{r})e^{-i\mathbf{qr}}. \tag{4}$$

The Fourier transform of Eq. (1) will take the form

$$\langle C(\mathbf{q}_1)C(\mathbf{q}_2)\rangle = C(2\pi)^2\delta(\mathbf{q}_1+\mathbf{q}_2). \tag{5}$$

By using Eqs. (1) and (3) one can show that $\langle F_b\rangle = 0$ and that the dispersion of the bare potential is

$$\langle F_b^2(\mathbf{r})\rangle = 2\pi C\int_{q_{\min}}^{\infty}\frac{dq}{q}e^{-2qs}, \tag{6}$$

where $q_{\min}\approx 1/L$. In the limit of large size $L\to\infty$, this expression for the mean-square potential diverges according to

$$\sqrt{\langle F_b^2\rangle} = W\sqrt{\ln\frac{L}{2s}}, \tag{7}$$

where

$$W = \sqrt{2\pi}\frac{e^2}{\kappa}\sqrt{C}. \tag{8}$$

Here κ is the dielectric constant, s is the distance between the donor plate and the 2DEL plate. For a GaAs heterostructure, with a donor concentration of $C = 1.0\times 10^{11}$ cm^{-2}, one obtains $W = 9.2$ meV. Thus, the fluctuations in the bare potential of a macroscopic 2DEL are very large.

To understand this divergence one should consider the following argument. The average charge fluctuation within an $R \times R$ square is $\sqrt{CR^2}$. If $R < s$, then the potential created in the plane of the 2DEL by this charge fluctuation will be damped exponentially. Otherwise, if $R > s$, the charge fluctuation will generate a potential of order $e^2\sqrt{CR^2}/\kappa R = e^2\sqrt{C}/\kappa$. Thus, all harmonics with wavelengths greater than s give similar contributions to the dispersion of the potential. This results in a logarithmic divergence in the integral of Eq. (6) at small q.

The effect of electron screening is to remove the divergence in the dispersion of the potential. If one considers the case where the concentration of electrons is large relative to the changes in the concentration brought about by fluctuations in the bare potential, then the potential will be screened linearly. This linear screening can be accounted for by replacing q by $q + q_s$ in the denominator of the integrand in Eq. (3), giving

$$F(\mathbf{r}) = 2\pi \frac{e^2}{\kappa} \int C(\mathbf{q}) e^{i\mathbf{qr} - qs} \frac{d^2q}{(q + q_s)}, \tag{9}$$

where

$$q_s = 2\pi \frac{e^2}{\kappa} \frac{dn}{dE_f}. \tag{10}$$

In Eq. (10) n is the electron density and E_f is the chemical potential of the 2DEL.

These results are well known for the case of free electrons.[3] However, Eqs. (9) and (10) are valid in the general case of interacting electrons, both with and without a magnetic field[4] if the following conditions are satisfied:

The redistribution of the electron density is small, i.e., linear screening.

A smooth bare potential. The relevant values of q in the integral in Eq. (9) should be much smaller than q_s.

A simple derivation of this statement is given in Sec. II.

The derivation of the dispersion of this potential is similar to the derivation of the dispersion of the unscreened potential, and it gives

$$\langle F^2 \rangle = W^2 \frac{1}{4(q_s s)^2}. \tag{11}$$

This equation is valid, when $2|q_s|s \gg 1$, which is usually satisfied for structures with a large spacer width.

It is apparent that linear screening dramatically reduces the dispersion of the potential. For an ideal 2DEL, without a magnetic field, q_s does not depend on the electron density, and it is given by $q_s = 2/a$, where a is the Bohr radius.[3] For GaAs $a \approx 10$ nm, and, thus, for a spacer $s = 40$ nm the factor $2|q_s|s$ is about 16.

Linear screening is very effective in reducing fluctuations in the potential, but it is not valid when changes in the electron concentration, brought about by the fluctuations in the bare potential, are not small relative to the average concentration; in this case fluctuations in the long-range potential are of the order of W. Lowering the electron concentration will result in a metal-nonmetal transition, which is an example of a breakdown in linear screening. In a strong magnetic field linear screening breaks down each time the filling factor is close to an integer value (or a fractional value in a clean sample). The study of these two phenomena is the main topic of this paper.

B. Metal-nonmetal transition without a magnetic field

Without a magnetic field, the long-range potential of the impurities is the driving force of the metal-nonmetal transition.[5–7] On the metallic side of this transition, at high electron concentration, the mobility of the 2DEL, in structures with large spacer layers, is not controlled by the remote impurities. One reason for this is effective linear screening, but another reason is that the transport cross section in a long-range potential contains a small factor $1/(2q_f s)^2$ due to small-angle scattering (q_f is the Fermi wave vector; see Das Sarma and Stern[8]). Experimental data confirms this picture. The data show[6] that at high densities the mobility of the 2DEL is almost independent of the spacer width, but near the transition the dependence is very strong. This is important evidence that the transition is driven by the long-range potential.

At large s weak localization effects can be neglected,[5] and the transition can be described in terms of nonlinear screening and percolation. The advantages of these approaches is that they are exact in the limit of large spacer width s.

The concept of the nonlinear screening of a random potential has been developed by Shklovskii and Efros[9] during the early 1970s in connection with the theory of compensated semiconductors. Efros[4,10] has generalized this theory to two-dimensional systems with and without a magnetic field. Below are given the order of magnitude estimates, which follow from this theory. The main idea is that the entire 2DEL screens each harmonic of the impurity charge distribution independently. The average excess density of impurities in a square of area $R \times R$ is given by $\sqrt{CR^2}/R^2$. If the density of electrons is much greater than this excess density, $n \gg \sqrt{C}/R$, then the harmonics with wavelength R will be screened linearly. If $n \ll \sqrt{C}/R$, then the R wavelength harmonics are not screened effectively, and the 2DEL density becomes strongly inhomogeneous on a scale of order R. This failure in screening results from the fact that, in the process of screening an entire harmonic, the most the electron concentration can increase at a point is twice its average concentration. Thus, since the excess density of the short-wavelength harmonics is large, the 2DEL cannot balance them. This point can be stated very simply in terms of a nonlinear screening length $R_c = \sqrt{C}/n$. Harmonics in the impurity distribution with wavelengths $R \gg R_c$ are screened linearly, while those with wavelengths $R \ll R_c$ are screened very poorly.

For large electron density, $R_c \ll s$, and all significant harmonics in the bare potential are screened linearly. If the electron density is lowered, the nonlinear screening length becomes larger, and, eventually, for small enough electron density, R_c becomes of the same order as s. Then the density becomes strongly inhomogeneous on the scale of order s. At small densities, $R_c \gg s$, and fluctuations include all harmonics with wavelengths between s and R_c. To obtain quantitative results one should solve a system of nonlinear equations; these equations are given in Sec. II.

The metal-nonmetal transition occurs when percolation through the 2DEL disappears. The corresponding electron density is called the percolation threshold n_c, and it is of the same order of magnitude as the electron density in which the transition from linear to nonlinear screening occurs. Thus,

$$n_c = \beta \frac{\sqrt{C}}{s}, \tag{12}$$

where β is a numerical coefficient. An estimate by Efros[5] gives $\beta \approx 0.1$. A computer stimulation by Nixon and Davies[11] roughly confirms this number. Our result (see Sec. III C) is $\beta \approx 0.11$.

C. Linear and nonlinear screening in a magnetic field

Linear screening in a magnetic field is an interesting problem. At zero temperature the compressibility, in the free-electron approximation, is either zero or infinite, because the density of states is either zero or infinite.

A self-consistent screening theory has been proposed by Das Sarma and co-workers,[12–14] and separately by Murayama and Ando,[15] which takes into account broadening of the Landau levels due to disorder. We believe that this theory should be applicable if the resulting width of the Landau levels, due to disorder, is larger than the energy of the electron-electron interaction. Otherwise, the electron-electron interaction will provide the compressibility that is needed for screening; this is the case for structures with high mobility.

A new approach to linear screening has been proposed recently,[4] which emphasizes the electron-electron interaction. For a given level of disorder the smallest fractional gaps are smeared out, so that the energy density $H_N(\nu)$ of the 2DEL is a smooth function of the filling factor ν, within the intervals between the remaining singularities. Here $\nu = n/n_0$, N is the Landau level number, and $n_0 = eB/2\pi\hbar c$. It can be shown (see Sec. II) that within these intervals the Thomas-Fermi theory of linear screening is applicable, and that

$$q_s = 2\pi \frac{e^2}{\kappa} G(B), \tag{13}$$

where $G(B)$ is the thermodynamic density of states (TDS) of the 2DEL in a magnetic field B, which is related to the chemical potential E_f and the energy density H_N by the following equation:

$$G^{-1}(B) = dE_f/dn = d^2H_N/dn^2. \tag{14}$$

These equations allow one to determine the reciprocal screening wavelength q_s if one knows the energy density as a function of n.

In the case when only the lowest Landau level is occupied, one can use the approximation of Fano and Ortolani[16] for the energy density

$$H_0(\nu) = \sqrt{2\pi} \left(\frac{e^2}{\kappa}\right) n_0^{3/2} g(\nu), \tag{15}$$

where

$$g(\nu) = -0.6267\nu^2 - 0.7821x^{3/2} + 0.55x^2 - 0.463x^{5/2}, \tag{16}$$

and $x = \nu(1-\nu)$. This is a self-consistent approximation, which completely ignores fractional singularities. For this approximation both the TDS and the screening length are negative. This theory has been confirmed[17,18] by experimental data on the magnetocapacitance of GaAs structures, obtained in the ultraquantum limit by Smith, Wang, and Stiles.[19] The data show a very good quantitative agreement with the theory, without any fitting parameters. A negative TDS in Si structures has been reported, but no quantitative agreement with the theory has yet been achieved.[20] A possible reason for this is the mixing of different Landau levels.

An interesting experiment has been performed recently by Eisenstein, Pfeiffer, and West[21] on a double quantum-well GaAs structure. They measured the penetration of an external electric field through one quantum well into the other. The ratio of the penetrated field to the applied field is $1/(2q_sd+1)$, where q_s is given by Eq. (13), and d is the distance between the wells. Thus, by measuring the ratio of the penetrated field to the external field, they can find q_s. Their experimental results are shown by a dashed line in Fig. 9. Eisenstein, Pfeiffer, and West[21] have found a good agreement with the theory based on Eqs. (15) and (16) in the filling-factor range $0.2 \le \nu \le 0.7$. However, near integer filling factors the penetrated field increases dramatically. Below this increase is explained in terms of nonlinear screening.

In a strong magnetic field, the random potential generated by the impurities is screened by the highest occupied Landau level only; the lower levels are completely occupied and, thus, cannot respond to the random potential. Nonlinear screening theory, in this case, is very similar to nonlinear screening without a magnetic field, but the total electron density must be replaced by the density of electrons in the highest Landau level only.

There are many experimental manifestations of nonlinear screening in a magnetic field. It has been observed that the photoluminescence spectra of a 2DEL in a magnetic field[1,22,23] have a width that varies very strongly with the filling factor. If the filling factor is close to a half integer, this width is small, but if the filling factor is close to an integer, the width is large. Such a strong variation in the photoluminescence width can be explained in terms of screening. When the filling factor is close to a half integer, linear screening will be applicable, and fluctuations in the potential will be small. In the other case, when the filling factor is close to an integer, nonlinear screening will be applicable, and fluctuations in the potential will be large.

The transition from linear to nonlinear screening also manifests itself in the recombination of electrons and holes. For example, Dahl *et al.*[24] recently observed a sharp suppression of optical recombination near filling factor $\nu = 1$. This can be explained in terms of the above transition because, for $\nu = 1$, fluctuations in the smooth random potential will be large, and this will separate electrons and holes.

In the regime of the nonlinear screening a density of states can be obtained from the activation energy E_a of the resistivity ρ_{xx} in the regions of the plateaus of the integer quantum-Hall effect (IQHE).[25] One can define an activation density of states (ADS)as

$$G_a(E_a) = |dn/dE_a|. \qquad (17)$$

It has been observed, experimentally,[25] that this ADS is very large and relatively constant in the regions between Landau levels. This result has been interpreted in terms of a so-called "background" density of states. It is in contradiction to a one-electron theory of the density of states, because all one-electron theories give an exponential drop in the density of states between Landau levels. We explain here the background density of states in terms of nonlinear screening. It appears as a sharp broadening of the Landau level, when the filling factor is close to an integer.

II. EQUATIONS AND SCALING RELATIONS FOR LINEAR AND NONLINEAR SCREENING IN A MAGNETIC FIELD

To find the density of electrons in the highest Landau level $N(\mathbf{r}) = n + n'(\mathbf{r})$, where n is the average electron density in this level, and n' the local redistributed electron density, one should minimize the following expression for the energy of the system:

$$\Phi = \frac{e^2}{2\kappa}\int\int \frac{n'(\mathbf{r})n'(\mathbf{r}')d^2r\,d^2r'}{|\mathbf{r}-\mathbf{r}'|} + \int H_N(n+n')d^2r + \int n'(\mathbf{r})F_b(\mathbf{r})d^2r - E_f\int n'(\mathbf{r})d^2r \qquad (18)$$

with respect to $n'(\mathbf{r})$. The external potential $F_b(\mathbf{r})$ is given by Eq. (2). The first term in Eq. (18) describes the Coulomb interaction of the redistributed charge. The second term represents the difference in energy of a real electron liquid and a uniformly charged background. If it is neglected, the screening will be perfect.

For $|n'| \ll n$, one can expand the energy density $H_N[n + n'(\mathbf{r})]$ in terms of $n'(\mathbf{r})$ to obtain

$$H_N[n+n'(\mathbf{r})] = H_N(n) + \frac{dH_N(n)}{dn}n'(\mathbf{r}) + \frac{1}{2}\frac{d^2H_N(n)}{dn^2}n'^2(\mathbf{r}) + \cdots. \qquad (19)$$

By using the first three terms of this expansion and Eqs. (13) and (14), one can write Eq. (18) as

$$\Phi = \frac{e^2}{\kappa}\int \frac{n'(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^2r\,d^2r' + \int H_N(n)d^2r + \frac{2\pi e^2}{q_s\kappa}\int n'^2(\mathbf{r})d^2r + \int n'(\mathbf{r})F_b(\mathbf{r})d^2r. \qquad (20)$$

Minimizing this expression with respect to $n'(\mathbf{r})$ gives the equation

$$\frac{2\pi e^2 n'(\mathbf{r})}{\kappa q_s} + F_b + \frac{e^2}{\kappa}\int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^2r' = 0. \qquad (21)$$

It can be written in the form

$$F(\mathbf{r}) = -\frac{2\pi e^2 n'(\mathbf{r})}{\kappa q_s}, \qquad (22)$$

where

$$F(\mathbf{r}) = F_b + \frac{e^2}{\kappa}\int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^2r' \qquad (23)$$

is the resulting potential energy of the electrons. Equations (21)–(23) are just the equations of linear screening theory; they are valid at $|n'| \ll n$.

If $n \ll n_c$, then nonlinear screening applies. In this case, screening is very weak, and the random potential tears the 2DEL into pieces. The solution of this electrostatic problem can be found by minimizing total energy of the system

$$\Phi = \frac{e^2}{2\kappa}\int\int \frac{N(\mathbf{r})N(\mathbf{r}')d^2r\,d^2r'}{|\mathbf{r}-\mathbf{r}'|} + \int F_bN(\mathbf{r})d^2r + \int H(N(\mathbf{r}))d^2r - E_f\int N(\mathbf{r})d^2r \qquad (24)$$

with respect to $N(\mathbf{r})$. To do this one must impose the condition that the density of electrons in the highest Landau level cannot be negative. This is equivalent to letting $N(\mathbf{r}) = \xi^2(\mathbf{r})$ and minimizing

$$\Phi = \frac{e^2}{2\kappa}\int\int \frac{\xi^2(\mathbf{r})\xi^2(\mathbf{r}')d^2r\,d^2r'}{|\mathbf{r}-\mathbf{r}'|} + \int F_b\xi^2(\mathbf{r})d^2r + \int H_N(\xi^2(\mathbf{r}))d^2r - E_f\int \xi^2(\mathbf{r})d^2r \qquad (25)$$

within the class of real functions ξ. In the nonlinear screening regime the third term is small relative to the random potential (see below), so it can be neglected. As a result, one gets

$$\delta\Phi = 2\int d^2r\,\delta\xi\xi\left(\left[\frac{e^2}{\kappa}\int\frac{\xi^2(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^2r' + F_b - E_f\right]\right) = 0, \qquad (26)$$

which can be expressed as

$$\xi\left[\frac{e^2}{\kappa}\int \xi^2(\mathbf{r}')\frac{d^2r'}{|\mathbf{r}-\mathbf{r}'|} + F_b - E_f\right] = 0. \qquad (27)$$

This condition is satisfied if either the electron density is zero, or

$$F(\mathbf{r}) - E_f = 0, \qquad (28)$$

where Eq. (23) has been used. By considering the second variation of Eq. (25) one can show that the condition for this extremum to be a minimum is

$$F(\mathbf{r}) - E_f \geq 0, \tag{29}$$

which applies to the entire 2DEL. Thus, the minimization of the functional of Eq. (25) results in the following electrostatic problem. The plane of the 2DEL should be divided into metallic regions and dielectric regions. In the metallic regions the electron density must be nonzero, and the resulting potential must be equal to the chemical potential, while in the dielectric regions the electron density must be zero, and the resulting potential must be greater than the chemical potential.

Note that the metallic condition Eq. (28) is the result of neglecting the third term in Eq. (25). It means that we assume "perfect" screening in the metallic regions. Actually, screening in these regions is described in terms of linear screening theory, and an order of magnitude estimate of the fluctuations in the random potential is given by Eq. (11). To obtain an estimate for the random potential in the dielectric regions one can use Eq. (7), substituting R_c instead of L. Comparing these two expressions one finds that the random potential in the metallic regions is much smaller than in the dielectric regions if $q_s s \gg 1$. This is the main parameter of the theory.

One can obtain a scaling relation which connects the chemical potential E_f with s, n, and C. This can be done by writing Eqs. (1), (23), and (28) in the following dimensionless variables:

$$F(\mathbf{r}) = \vartheta(\mathbf{x})\frac{e^2\sqrt{C}}{\kappa}, \quad E_f = -\varepsilon\frac{e^2\sqrt{C}}{\kappa}, \tag{30}$$
$$N(\mathbf{r}) = \gamma(\mathbf{x})n, \quad C(\mathbf{r}) = \alpha(\mathbf{x})n, \quad \mathbf{r} = \mathbf{x}R_c, \quad R_c = \frac{\sqrt{C}}{n},$$

where n is the average electron density. Substituting these relations into Eq. (23), one obtains

$$\vartheta = \int \frac{\alpha(\mathbf{x}')d^2x'}{\sqrt{(\mathbf{x}-\mathbf{x}') + \left(\frac{sn}{\sqrt{C}}\right)^2}} + \int \frac{\gamma(\mathbf{x}')d^2x'}{|\mathbf{x}-\mathbf{x}'|}, \tag{31}$$

where $\alpha(\mathbf{x})$ is a dimensionless Gaussian random function with the correlator

$$\langle\alpha(\mathbf{x})\alpha(\mathbf{x}')\rangle = \delta(\mathbf{x}-\mathbf{x}'). \tag{32}$$

As a result, it is apparent that the dimensionless chemical potential ε depends on only one dimensionless parameter $\eta = sn/\sqrt{C}$, which we call the dimensionless density. Thus,

$$E_f = -\frac{e^2\sqrt{C}}{\kappa}\varepsilon(\eta), \tag{33}$$

where ε is an unknown function of η. Equation (33) is a general relationship between the chemical potential E_f, the spacer s, the average impurity density C, and the average electron density n, which was derived by neglecting the third term in Eq. (25).

An analytic solution of the above problem is difficult to obtain. The nonlinear screening problem has been solved analytically for only a few symmetrical bare potentials; there are exact solutions for a single antidot[26] and a one-dimensional strip.[27] There is no analytical solution for a periodic external potential,[28] and, obviously, there is no analytical solution for a random potential.

III. COMPUTER MODELING A 2DEL SUBJECTED TO A RANDOM POTENTIAL

A. Computer model

We have solved the above problem by performing a computer modeling. In our model both the plane of the electron liquid and the plane of the impurities are approximated by finite square lattices, each of size $L \times L$; note that modeling an extended 2DEL with a finite square 2DEL is justified if the size of the square is much larger than the nonlinear screening length $R_c = \sqrt{C}/n$. The random functions $\vartheta(\mathbf{x})$, $\alpha(\mathbf{x})$, and $\gamma(\mathbf{x})$ become discrete functions on these square lattices. Our program first generates the random function $\alpha(\mathbf{x})$ at all points in the impurity lattice, by using the correlator of Eq. (32), and then it sets the total impurity charge equal to zero; this is done to reduce the variation of our results for different arrays, and, as a result, it makes the 2DEL easier to model. From this charge distribution the dimensionless bare potential $\vartheta_b(\mathbf{x})$ is calculated on the lattice of the 2DEL. The program then finds the distribution of electronic charge for a given ε. This is done by going through each point in the lattice and determining if the potential there is less than, or greater than, ε. If it is less than ε, a small charge is added to the lattice point, while if it is greater than ε a small charge is subtracted from the lattice point, with the restriction that the electron concentration be non-negative. The change in the potential at all points in the lattice is then calculated. The program then proceeds to the next point and repeats this procedure. Note that each time the program adds, or subtracts, a charge to a point it also adds, or subtracts, the same amount of charge to a background density; this background density is uniform and equal to the negative of the average electron density. Thus, the total charge of the system is always zero. This process continues until all points that have a potential greater than ε have no electronic charge, and all points that have an electronic charge have a potential, within a given accuracy, equal to the chemical potential. The total electronic charge is then calculated, and averaged over many configurations of the impurity charge distribution $\alpha(\mathbf{x})$. We use periodic boundary conditions when calculating the potential. It means that the charge distributions of both the impurities and the electrons are periodic (of period L, where L is the side length of the finite 2DEL of our model). The potential at a particular lattice site is determined by considering only those charges of the periodic charge distribution that are within a square, of size $L \times L$, centered about the lattice site. This periodic condition is implemented in the program, when it calculates the potential at a lattice point. If the x (or y) component of the lateral distance between two lattice points Δx (or Δy) is greater than $L/2$, it is replaced by $L - \Delta x$ (or $L - \Delta y$).

Approximating the two-dimensional continuum by a lattice is justified if the lattice constant is smaller than s, because harmonics in the impurity charge distribution with wavelengths smaller than s are damped exponentially, see Eq. (3).

B. The dependence of the chemical potential on the concentration

Computations were performed on a Cray Y-MP8, at the San Diego Supercomputer Center. The time required to find the concentration depended greatly upon the chemical potential. As the magnitude of E_f decreased the computation time increased. For a dimensionless Fermi energy of $\varepsilon = 0.001$, the computation time, for an array of size 150 × 150, was about an hour.

Two typical plots of the potential $\vartheta(\mathbf{x})$ are shown in Fig. 2. Note that in the metallic regions $\vartheta = \varepsilon$ and that in the dielectric regions $\vartheta \geq \varepsilon$. These pictures look like a flooded mountain system, in which the water level corresponds to the chemical potential.

Figure 3 shows the dimensionless chemical potential $\varepsilon(\eta)$, as defined by Eq. (33), plotted against the reciprocal dimensionless electron density η^{-1}, for three values of s and for two different values of array size. Note that the chemical potential is negative in our model at all densities and that it decreases as the electron density is decreased, because, for low densities, screening becomes weak and fluctuations in potential become large. When $1/\eta < 25$, all points with a different s, and a different number of lattice sites, form a universal curve. This confirms the scaling relation as given by Eq. (33). At smaller η, deviations appear. These deviations are probably connected with the size effect, which occurs at small η.

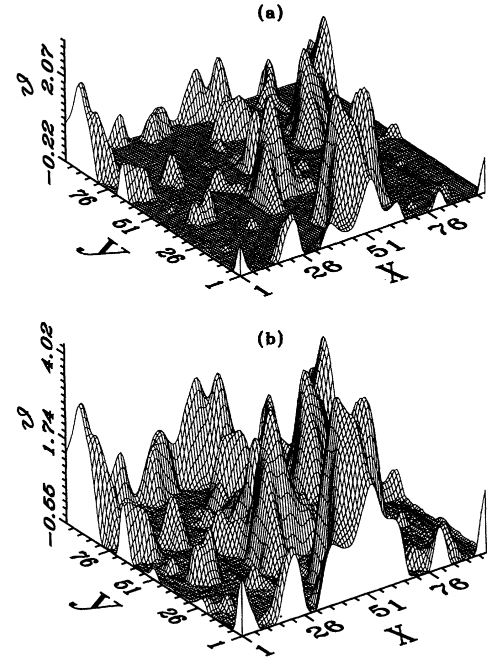

FIG. 2. Dimensionless potential $\vartheta(\mathbf{r})$ obtained from computer modeling at a spacer width of $s = 3$ (in units of the lattice constant), an array size of 100 × 100 sites, and at a dimensionless chemical potential of (a) $\varepsilon = 0.2$ and (b) $\varepsilon = 0.5$.

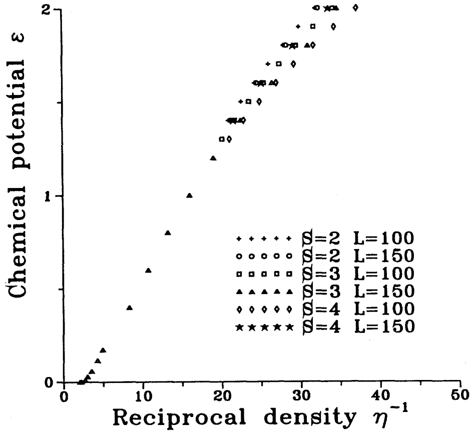

FIG. 3. Chemical potential ε vs reciprocal concentration η^{-1} as given by computer modeling at different s and L (in units of the lattice constant). Below $\eta^{-1} = 20$, the points for different s and L are indistinguishable, so only one point is given at these η^{-1}.

In the range of η shown in Fig. 3 the dimensionless function $\varepsilon(\eta)$ appears to be linear in η^{-1}. With good accuracy it obeys the equation

$$\varepsilon(\eta) = \frac{1}{14}\left(\frac{1}{\eta} - 2.4\right). \qquad (34)$$

An important point is that in the scale used in Fig. 3 this function becomes zero at $\eta^{-1} = 2.4$, and it looks like a phase transition.

To understand this behavior we introduce an effective charge density C_{eff}, which is located in the plane of the 2DEL and produces the same bare potential as the donor distribution $C(\mathbf{r})$ that is in a plane at a distance s from the 2DEL. The Fourier transforms of these two densities are related by

$$C_{\text{eff}}(\mathbf{q}) = C(\mathbf{q})e^{-qs}. \qquad (35)$$

Thus,

$$C_{\text{eff}}(\mathbf{r}) = \frac{1}{(2\pi)^2}\int d^2q\, C(\mathbf{q})e^{i\mathbf{qr}-qs}. \qquad (36)$$

Since $C_{\text{eff}}(\mathbf{r})$ is connected linearly with $C(\mathbf{r})$ it is also a random Gaussian function. It follows from Eqs. (1) and (36) that $\langle C_{\text{eff}}(\mathbf{r})\rangle = 0$ and

$$\langle C_{\text{eff}}^2\rangle = \frac{C}{8\pi s^2}. \qquad (37)$$

At large electron densities E_f tends to zero, because $C_{\text{eff}}(\mathbf{r})$ is neutralized by the electronic charge and by the homogeneous background charge, which has a sign opposite to the electrons. However, the electron density $N(\mathbf{r})$ has a definite sign (in our computer program it is taken to be positive), while $C_{\mathrm{eff}}(\mathbf{r})$ fluctuates around zero. Thus, the positive charge fluctuations of the remote impurities can only be screened by the homogeneous negative background density of the 2DEL. It follows then that the electron density required to completely screen the impurities will be greater than $\sqrt{\langle C_{\mathrm{eff}}^2\rangle}$. The condition of complete charge neutralization is

$$C_{\mathrm{eff}}(\mathbf{r}) + N(\mathbf{r}) - n = 0, \tag{38}$$

where n is the density of the uniform background, which is just the average electron density. Since $N(\mathbf{r}) \geq 0$, Eq. (38) is fulfilled, at all $\mathbf{r}$, only if n exceeds the maximum value of $C_{\mathrm{eff}}(\mathbf{r})$. The maximum value of the Gaussian random function $C_{\mathrm{eff}}(\mathbf{r})$ over an infinite plane is infinite. Thus, complete neutralization never occurs and the chemical potential will be nonzero for any finite electron density. We show, however, that at high electron densities the chemical potential is exponentially small. This is why the behavior shown in Fig. 3 looks as if there is a phase transition at a threshold density of $\eta_{\mathrm{th}} \approx 0.4$.

One can estimate this apparent threshold value by the following mean-field method. We assume that $C_{\mathrm{eff}}(\mathbf{r})$ is a harmonic function,

$$C_{\mathrm{eff}} = C_0 \cos\left(\frac{2\pi x}{s}\right) \cos\left(\frac{2\pi y}{s}\right). \tag{39}$$

Then we choose the amplitude C_0 in such a way that the square average as taken from Eq. (39) is the same as the square average for the random function of Eq. (37). One obtains

$$C_0^2/4 = C/8\pi s^2. \tag{40}$$

The wavelength of the harmonic function was taken to be s, because this harmonic gives the main contribution to the mean-square potential. It is not important, however, for the estimate given below. For the function of Eq. (39), complete charge neutralization is possible at a finite value of n. One can show that Eq. (38) is satisfied if $N(\mathbf{r}) = C_0 - C_{\mathrm{eff}}$ and $n = C_0$. Making use of Eq. (40) one finds that in dimensionless units this condition of the complete neutralization becomes

$$\eta_{\mathrm{th}} = \frac{n_{\mathrm{th}} s}{\sqrt{C}} = \frac{1}{\sqrt{2\pi}} \approx 0.4. \tag{41}$$

This is very close to the value of the apparent threshold.

By magnifying the region below the apparent threshold in Fig. 3, one can see an exponential tail in the plot of the chemical potential (see Fig. 4). This can be explained in terms of the Gaussian fluctuations of C_{eff}. For large n, there are a small number of regions where $C_{\mathrm{eff}} > n$. The fraction of the 2DEL occupied by these regions is proportional to $\exp(-4\pi\eta^2)$ [see Eq. (37)]. These negatively charged dielectric regions are surrounded by positively charged clouds, while the rest of the plane of the 2DEL is relatively neutral. Neglecting numerical coefficients, one can estimate the function $\varepsilon(\eta)$ (see the Appendix) and show

$$\varepsilon \approx \eta^{-3} e^{-4\pi\eta^2}. \tag{42}$$

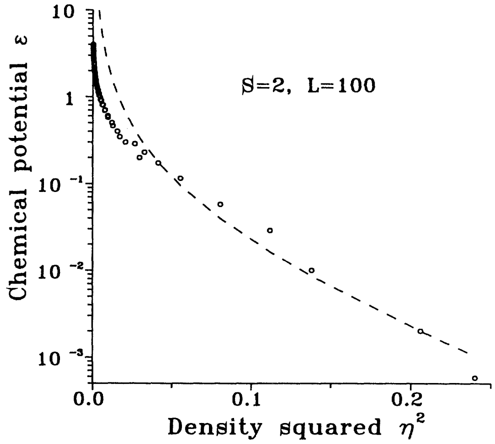

FIG. 4. Dimensionless chemical potential ε vs square of the dimensionless concentration η^2, in the region of high electron density. Those results obtained by computer modeling are shown by circles, while the dependence of Eq. (42) is shown by the dashed line.

A plot of Eq. (42) is shown, with a trial numerical coefficient, in Fig. 4, by a dashed line.

C. Activation energy and activation density of states

If there is percolation through metallic regions, the conductivity of a 2DEL, without a magnetic field, will be metallic. Otherwise, the conductivity of the system will be due to the activation of electrons from energies near the chemical potential to the percolation level, where the percolation level is the energy, for which an equipotential contour can be made that extends from one end of the 2DEL to the other. The activation energy E_a is defined as the difference in energy between this percolation level and the chemical potential.

The activation energy obeys the same scaling relation as the chemical potential, namely,

$$E_a = \frac{e^2\sqrt{C}}{\kappa}\varepsilon_a(\eta), \tag{43}$$

where ε_a is a function of $\eta = sn/\sqrt{C}$.

Our computer model has been extended to determine the function $\varepsilon_a(\eta)$. For a particular chemical potential ε, and dimensionless concentration η, our program finds the energy, which is less than the potential energies of half the lattice sites but greater than the potential energies of the other half. This energy is then averaged over many configurations of the impurity distribution to give the percolation level of the extended system, for the corresponding chemical potential. The program then subtracts the chemical potential from this percolation level to obtain the activation energy. This process is repeated for several different chemical potentials to obtain the activation energy as a function of the dimensionless con-

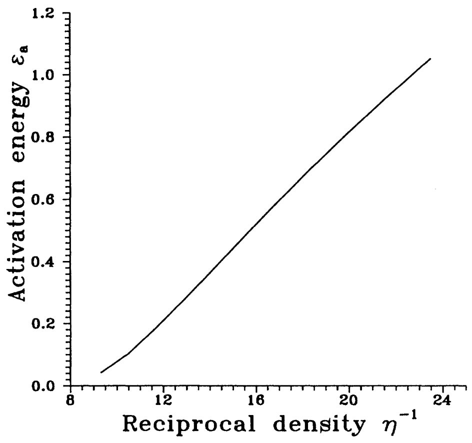

FIG. 5. Dimensionless activation energy ε_a vs dimensionless concentration η as obtained by computer modeling. These results were obtained for $s = 2, 3,$ and 4 (in units of the lattice constant), and for a 100 × 100 array size. Due to the scaling relation, Eq. (45), the points for different values s form a universal curve.

centration η.

A plot of the dimensionless activation energy ε_a versus the reciprocal dimensionless electron concentration η^{-1} is shown in Fig. 5. At $\eta^{-1} < \frac{1}{25}$ it obeys the equation

$$\varepsilon_a(\eta) = \frac{1}{14}\left(\frac{1}{\eta} - 8.8\right). \tag{44}$$

Comparing this result with Eq. (34) for the dimensionless chemical potential one can conclude that the dimensionless percolation energy is approximately −0.54 independently of η. Note that random bare potential is statistically symmetric with respect to zero energy. For such a potential the percolation energy is zero. Electron screening violates the symmetry of the potential in such a way that the percolation energy becomes negative.

The point where $\varepsilon_a = 0$ is the threshold of the metal-nonmetal transition without an applied magnetic field. At this point the dimensionless electron density is $\eta \approx 0.11$ [see Eq. (12)]. In the case of no applied magnetic field, one can use this plot to find the dependence of the activation energy on the electron density.

In the case of a strong magnetic field one can use Fig. 5 to find the activation energy in the regime of the plateaus of the quantum Hall effect as a function of the applied magnetic field or electron density. Note that in this case η is the dimensionless density of the highest occupied Landau level rather than the total density. If the total density n_t is fixed and η changes due to the magnetic field, one can find the magnetic field dependence of the activation energy. The value of B corresponding to a given value of η can be found from the equation

$$B = \frac{ch}{Ie}\left(n_t - \frac{\eta\sqrt{C}}{s}\right), \tag{45}$$

where I is the number of the highest completely occupied Landau level.

A plot of the activation energy versus the applied magnetic field at three different spacer widths, obtained by the above method, is shown in Fig. 6. By using Fig. 5 and the definition of the ADS [see Eq. (17)], one can determine the dimensionless activation density of states (DADS), contributed by the highest occupied Landau level of the 2DEL, as a function of the activation energy ε_a. The results are shown in Fig. 7. Note that so far it has been assumed that only the highest Landau level contributes to the ADS. This is not a good approximation, when E_a is midway between two Landau levels. In this case both the highest and the second highest occupied Landau levels should contribute equally to the ADS. In the future we are planning to model two-level screening. In this paper we approximate two-level screening in the following way. First each ε_a in Fig. 7 is multiplied by $e^2\sqrt{C}/\kappa$ giving E_a, while the corresponding DADS is multiplied by $e^2/(s\kappa)$ to give the ADS from the highest Landau level. The combined ADS is obtained by inverting the plot of the ADS vs E_a obtained above, and then shifting it in energy by an amount equal to $-\hbar\omega$, where $\hbar\omega$ is distance in energy between Landau levels. This inverted and shifted plot, which is just a plot of the ADS of the holes in the second highest Landau level vs E_a, can then be added to the original plot of the ADS vs E_a to give a new plot, which is a sum of the ADS of the holes in the second highest Landau level and the ADS of electrons in the highest Landau level. This plot of the total ADS will be symmetric with respect to the energy point midway between the highest and second highest Landau levels.

The ADS of a 2DEL in a strong magnetic field has been measured as a function of the activation energy by Weiss and co-workers.[25] Their results for a GaAs-Al$_x$Ga$_{1-x}$As sample with an electron density of $n = 1.8 \times 10^{11}$ cm are shown in Fig. 8(a). A plot of the ADS vs E_a, obtained from Fig. 7 by using the parameters $s = 30$ nm, $C = n = 1.8 \times 10^{11}$ cm^{-2}, and $\kappa = 12.56$, is shown in Fig. 8(b).

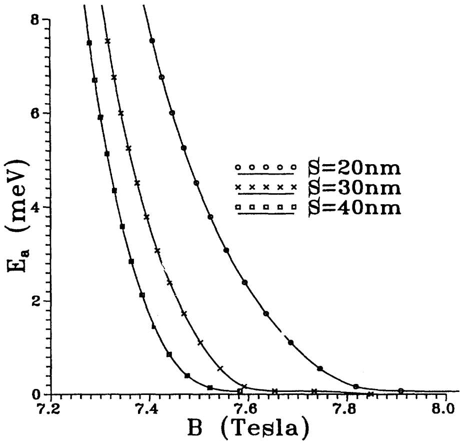

FIG. 6. Plot of the activation energy E_a vs the applied magnetic field B for an electron density of 3.5×10^{11} cm^{-2} and three spacers $s = 20$ nm (circles), $s = 30$ nm (crosses), and $s = 40$ nm (squares). The solid lines are just to guide the eye.

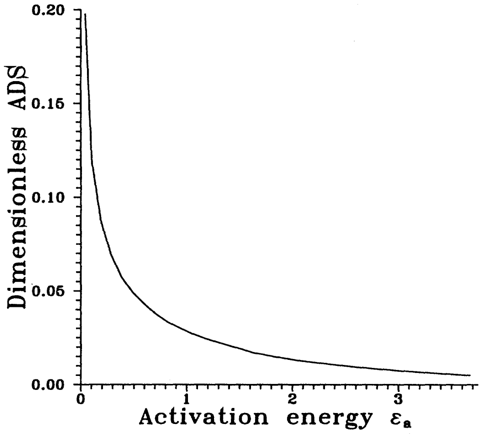

FIG. 7. Dimensionless ADS as a function of the dimensionless activation energy ε_a, obtained from Fig. 5.

One can see that our theory gives a quantitative explanation of the apparent density of states between the Landau levels.

Using Eqs. (17) and (44) we can write an analytical expression for the ADS in the middle between two Landau levels,

$$G_a\left(\frac{\hbar\omega}{2}\right) = \frac{\kappa}{7e^2 s}\left(\frac{\hbar\omega\kappa}{2e^2\sqrt{C}} + 0.63\right)^{-1}. \tag{46}$$

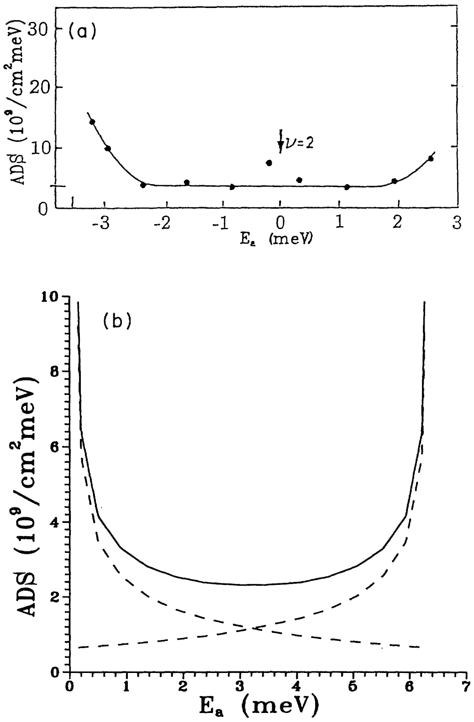

FIG. 8. Plot of the ADS vs the activation energy E_a. (a) Experimental data by Weiss, Klitzing, and Mosser (Ref. 25) at $n = 1.8\times10^{11}$ cm^{-2} for the filling factor close to $\nu = 2$. (b) The solid line is the theoretical plot as obtained from Fig. 7 at $s = 300$ Å, and $n = 1.8\times10^{11}$ cm^{-2} as described in Sec. III. The dashed lines are the ADS of the lower and higher Landau levels. Note $\hbar\omega$ was determined for $\nu = 2$.

D. The thermodynamic density of states

To fit the experimental data obtained by Eisenstein, Pfeiffer, and West[21] we consider both linear and nonlinear screening. Since the characteristic energies of these two regimes are very different, we can use an extrapolation formula

$$E_f = \frac{dH}{dN} - \frac{e^2\sqrt{C}}{\kappa}\varepsilon(\eta), \tag{47}$$

where the energy density H is given by Eqs. (15) and (16). In the region of linear screening $\varepsilon(\eta)$ is close to zero, and disorder does not play any important role, while in the nonlinear regime the first term is small as compared with the second. That is why we can obtain a good approximation without taking into account any interference of the linear and nonlinear screening.

By using Eqs. (13)–(16) and (47), we can find q_s and then use this q_s to find the penetration ratio $1/(2q_s d+1)$. We use the values $s = 70$ nm, $d = 30$ nm.

Figure 9 shows the experimental results of Eisenstein, Pfeiffer, and West[21] (dashed line) and our theoretical results (solid line). One can see that our extrapolation explains the sharp transition from a negative to a positive density of states, and that it gives a nice quantitative description for a wide range of ν. We cannot explain the absence of symmetry with respect to the point $\nu = \frac{1}{2}$ in the experimental plot. It looks like the approximation Eq. (15) is not good enough at $\nu > \frac{1}{2}$. Note that the structure in the experimental data near fractional ν cannot be described by our theory, since the corresponding singularities are not included in the energy density [see Eq. (15)].

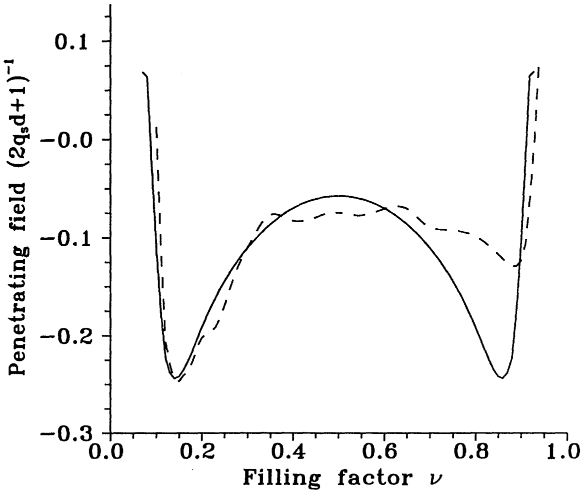

FIG. 9. Plot of the penetration field $(2q_s d + 1)^{-1}$ vs the filling factor ν, where the dashed line gives the results of Eisenstein, Pfeiffer, and West and the solid line gives the results of our computer stimulation.

IV. CONCLUSIONS

We have demonstrated the important role of the long-range random potential created by the remote impurities in the structures with two-dimensional electron liquid. Due to the logarithmic divergency this potential is very large, but it can be substantially suppressed by electron screening. In a strong magnetic field the 2DEL becomes incompressible at some filling factors, and this gives rise to a sharp increase of the random potential. The density of states between the Landau levels, as obtained from the activation energy of conductivity, becomes very large and almost energy independent. It has been interpreted before as a "background" density. But actually this background density strongly depends on the filling factor, and it is absent in the regime of the linear screening. Magnetocapacitance data are also very sensitive to the crossover from the linear to nonlinear screening regime, because electron density becomes strongly inhomogeneous. We have proposed here a system of nonlinear equations which describes the distribution of electron density and we have found out some important scaling relations for thermodynamic functions. This system is exact in the limit of a very smooth potential. Actually, this means that the spacer width is large. We have solved this system by computer modeling. The results are in a good agreement with experimental data.

ACKNOWLEDGMENTS

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APPENDIX

Here we derive Eq. (42) for the chemical potential at high electron densities. The distribution function for the effective impurity charge is

$$\omega(C_{\text{eff}}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\Delta^2}, \tag{A1}$$

where $\Delta^2 = C_{\text{eff}}^2/2\sigma^2$, and $\sigma^2 = \langle C_{\text{eff}}^2 \rangle = C/8\pi s^2$. (In the following derivation numerical coefficients in preexponential factors are ignored.) If $\eta = ns/\sqrt{C} \gg 1$, one can show that the fraction of the plane of the 2DEL, where $C_{\text{eff}}(\mathbf{r}) > n$, is

$$\omega_0 = \frac{\sqrt{C}}{ns} e^{-4\pi\eta^2}. \tag{A2}$$

Since this fraction is small, these regions will form small dielectric islands, which are surrounded by clouds of negative charge. In the same approximation, the average concentration of charge in these dielectric regions is

$$\delta C = \frac{\int_n^\infty (C_{\text{eff}} - n)\omega(C_{\text{eff}})dC_{\text{eff}}}{\int_n^\infty \omega(C_{\text{eff}})dC_{\text{eff}}} = \frac{C}{s^2 n}. \tag{A3}$$

Since the dielectric regions are far apart, and small, the energy density of the 2DEL is, approximately, the sum of the interaction energies of each dielectric region with its respective negative-charged cloud. The average charge within a dielectric region of size a is $e\delta C a^2$, while the net charge surrounding this dielectric region has the same magnitude but opposite sign. Thus, the interaction energy of the dielectric region with its cloud is $-e^2(\delta C a^2)^2/\kappa a$. To estimate the energy density of the 2DEL, this should be divided by the square of the average distance between dielectric regions l to give

$$H \approx -\frac{(e\delta C a^2)^2}{\kappa a l^2}. \tag{A4}$$

The value of l can be estimated from the condition $a^2/l^2 = \omega_0$. As a result,

$$H \approx -\frac{e^2}{\kappa} \frac{\sqrt{C}}{ns} \delta C^2 a e^{-4\pi\eta^2}. \tag{A5}$$

The parameter a can be estimated by the following argument. At $\eta \gg 1$, the dielectric regions are centered around the local maxima of the random function $C_{\text{eff}}(\mathbf{r})$. Near one of these local maxima, the spatial dependence of the effective impurity concentration has, approximately, the form

$$C_{\text{eff}}(\mathbf{r}) \approx C_{\max}\left(1 - \frac{r^2}{s^2}\right). \tag{A6}$$

At $r = a$, the effective impurity concentration $C_{\text{eff}}(a)$ must be equal to the average electron density n. Since $C_{\max} - n$ is of the same order as δC, this condition at $r = a$ takes the form

$$a^2 \approx s^2 \frac{C_{\max} - n}{C_{\max}} \approx s^2 \frac{\delta C}{n + \delta C}, \tag{A7}$$

which to first order in δC gives

$$a \approx \frac{\sqrt{C}}{n}. \tag{A8}$$

Putting this result into Eq. (A5), one obtains

$$H(n) \approx -\frac{e^2}{\kappa} \frac{C^3}{s^5 n^4} e^{-4\pi\eta^2}. \tag{A9}$$

When finding $E_f = dH(n)/dn$ at $\eta \gg 1$, one only has to differentiate the exponential term in Eq. (A9). Thus, one obtains Eq. (42).

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