

Droplet state in an interacting two-dimensional electron system

Junren Shi

Department of Physics, Oklahoma State University, Stillwater, Oklahoma 74078

Song He

Hexaa Laboratory, Warren, New Jersey 07059

X. C. Xie

Department of Physics, Oklahoma State University, Stillwater, Oklahoma 74078

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It is well known that the dielectric constant of two-dimensional (2D) electron systems goes negative at low electron densities. A consequence of the negative dielectric constant could be the formation of the droplet state. The droplet state is a two-phase coexistence region of high density liquid and low density "gas." In this paper, we carry out energetic calculations to study the stability of the droplet ground state. The possible relevance of the droplet state to recently observed 2D metal-insulator transition is also discussed. [S0163-1829(99)50944-2]

The recent discovery of two-dimensional (2D) metal-insulator transition (MIT) by Kravchenko *et al.*¹ has challenged the scaling theory of localization^{2,3} in which a 2D MIT is forbidden. A noticeable character of the electron system in these experiments is that r_s , the parameter that measures the strength of the Coulomb interaction, is fairly large. We suspect that the electron system may be unstable against phase separation at these large values of r_s . We demonstrated in our previous paper⁴ that this assumption alone is sufficient to provide a theoretical description that is consistent with all the known experiments. For a two-dimensional (2D) electron system, there is believed to be two phases: a high density Fermi gas phase and a low density insulating Wigner crystal phase. The dielectric constant of the liquid phase becomes negative when $r_s \approx 2$,⁵ which indicates that the liquid phase is unstable. At lower densities, the Wigner crystal phase appears around $r_s \approx 37$ in the absence of disorder.⁶ This critical value of r_s appears to be reduced to around $r_s \approx 10$ with disorders.⁷ In the intermediate values of r_s , we believe that there is a *liquid* phase which we think is responsible for the observed MIT.

In this paper, we propose that a droplet state of the electron system resulted from the phase separation of the electrons into this new liquid phase and a low density "gas" phase. Here we call the low density phase "gas" purely for the reason that its density is low. In fact, in the presence of impurities, the "gas" phase is disordered Wigner crystal. To investigate our proposal, we have studied the energetics of such a droplet state. We find that both electron-electron interaction and potential fluctuations are crucial for the formation of the droplet state.

An obvious condition for the droplet state is that the electron gas is unstable. To investigate what possibilities the instability leads to, we study a simple but physically motivated model. Let us consider electrons in the disc of radius b with a positive background. Imagine that the electron system is shrunk to a new radius $a < b$ while the positive background remains intact. Clearly the charging energy due to the separation of the electrons from the positive background in-

creases the energy of the system. However, there can also be energy gained (decreasing total energy): since for a uniform electron gas the ground state energy E_g is at its minimum when $r_s \approx 2$,⁵ for $r_s > 2$ the system gains energy by shrinking the area occupied by electrons. Furthermore, in the presence of disorder, electrons tend to occupy the valleys of the disorder landscape. Thus, a slowly varying disorder potential is in favor for the formation of the droplet state. We calculate the energy changes when the electron disc is shrunk from b to a to determine whether a spontaneous shrinking can take place.

For electron-electron or electron and positive background interaction, we use screened Coulomb potential. For Si metal-oxide-semiconductor field effect transistors (MOSFET's), the image charge in the metal substrate induces the screening and the interaction in the momentum space can be written as⁸

$$V(k) = \frac{1}{\epsilon} \frac{2\pi e^2}{k} \frac{1 - e^{-2kD}}{1 - Ke^{-2kD}},$$

where D is the thickness of the Si₂O insulating layer and $\epsilon = \frac{1}{2}(\epsilon_1 + \epsilon_2)$, $K = (\epsilon_1 - \epsilon_2)/(\epsilon_1 + \epsilon_2)$, with ϵ_1 and ϵ_2 being the dielectric constants of Si and Si₂O, respectively. For other systems, such as GaAs/Al_xGa_{1-x}As, the screened interaction can be well represented by the following form:

$$V(r) = \frac{e^2}{\epsilon r} e^{-\lambda r},$$

and the corresponding moment space representation is

$$V(k) = \frac{2\pi e^2}{\epsilon} \frac{1}{\sqrt{k^2 + \lambda^2}}.$$

Both forms of the interactions define an interaction range ξ . For Si MOSFET's, $\xi = (\epsilon/\epsilon_2)D$, and for the screened Coulomb potential, $\xi = 1/2\lambda$. Outside the range the interaction is strongly screened.

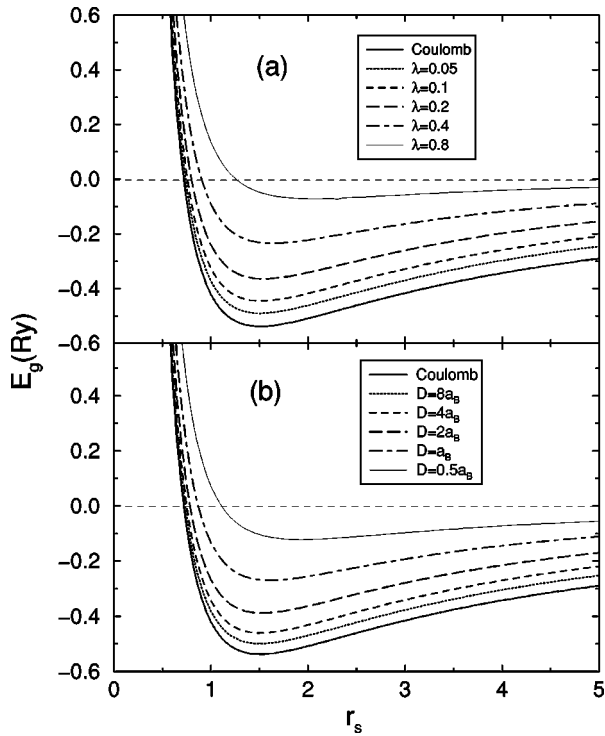


FIG. 1. The ground state energy of electron system for different screening strengths. (a) For screened Coulomb interaction. (b) For Si MOSFET's.

To calculate the ground state energy of the electron gas with the screened Coulomb interaction, we use the variational correlated-basis-function (CBF) method.⁹ This method has been applied to the bare Coulomb interaction and is proved to provide rather accurate results for the ground state energy of 2D electron systems.⁹ The accuracy of the ground state energy is found to within 10% compared with the best available quantum Monte Carlo results⁶ for densities down to $r_s = 20$. In the CBF approach, there is a variational variable α for which the ground state energy E_g has to be minimized:

$$E_g(r_s, \alpha) = \frac{A(\alpha)}{r_s^2} - U_c\left(\frac{\sqrt{\alpha}}{r_s}\right) \quad (\text{Ry}),$$

$$A(\alpha) = A_0^B(\alpha) + A_{01}^F(\alpha) + A_{02}^F(\alpha) + A_{03}^F(\alpha) + \dots,$$

$$A_0^B(\alpha) = \alpha^2 \left[\sum_{n=0}^{\infty} \frac{\alpha^n}{(n+2)^2} + \frac{\pi^2}{6} - \frac{5}{4} \right],$$

$$A_{01}^F(\alpha) = 1,$$

$$A_{02}^F(\alpha) = -\frac{16}{\pi} \int_0^1 [2 \arccos(y) - y(1-y^2)^{1/2}] \times y^3 e^{-2y^2/\alpha} dy,$$

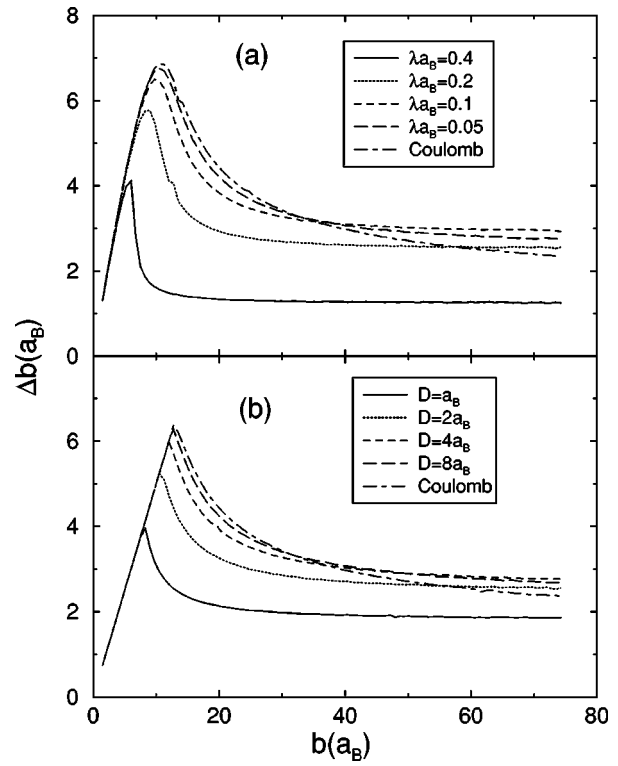


FIG. 2. The shrinking distance $\Delta b = b - a$ versus disc radius b for different screening strength. (a) For screened Coulomb potential. (b) For Si MOSFETs. The initial density parameter $r_s = 15a_B$.

$$A_{03}^F(\alpha) = -\frac{2}{\pi} \int_0^1 dy_1 \int_0^1 dy_2 \int_0^1 dy_3 \int_0^\pi d\theta y_{12}^2 \times \{1 - \exp[-y_{12}^2/2\alpha]\} \exp[-(y_1^2 + y_2^2 + 2y_3^2)/2\alpha] I_0[\alpha^{-1}(y_1^2 y_3^2 + y_2^2 y_3^2 + 2y_1 y_2 y_3^2 \cos \theta)^{1/2}],$$

where $1 \text{ Ry} = e^2/2\epsilon a_B$, $a_B = \epsilon \hbar^2/m^* e^2$, and $y_{12} = y_1 - y_2$. $U_c(\sqrt{\alpha}/r_s)$ is the cohesive energy which depends on the special form of the interaction,

$$U_c\left(\frac{\sqrt{\alpha}}{r_s}\right) = \frac{1}{2} \int \exp\left[-\left(\frac{k}{2\sqrt{\alpha}}\right)^2\right] V(k) \frac{d^2k}{(2\pi)^2}.$$

Figure 1 shows the calculated results for the ground state energy. The screening effect raises the ground state energy because the electron correlation is suppressed.

The shrinking of the electron disc will cause the redistribution of the charge, which will raise extra electrostatic energy because the positive background is fixed. The charge distribution can be written as

$$\rho(k) = 2N \left(\frac{J_1(ka)}{ka} - \frac{J_1(kb)}{kb} \right),$$

where N is the total number of the electrons in the disc. The charging energy is

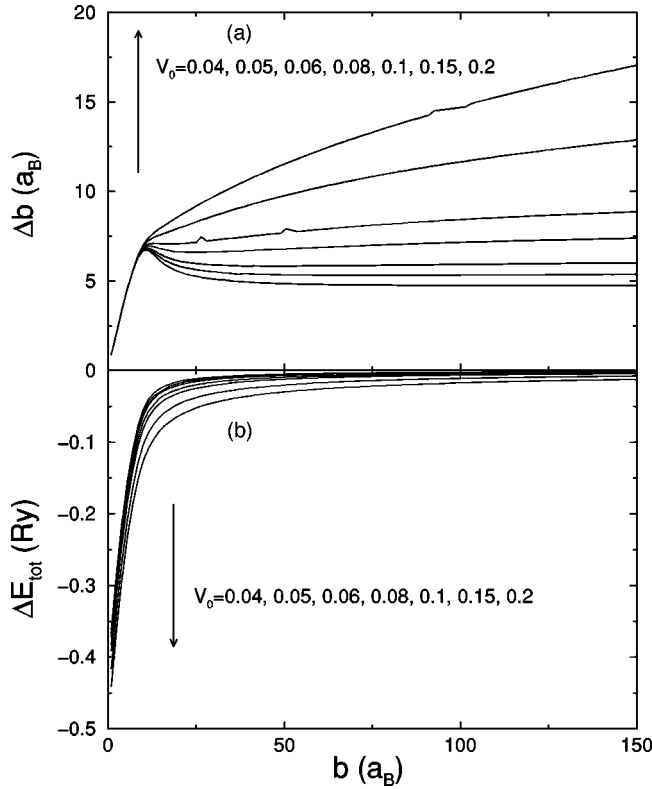


FIG. 3. (a) The shrinking distance $\Delta b = b - a$ versus radius b for Si MOSFET's with $D = 10a_B$. Top curves are for larger disorder potential V_0 's. (b) ΔE_{tot} versus radius b . Lower curves are for larger disorder potential V_0 's. The initial electron density parameter $r_s = 15a_B$.

$$E_c = \frac{1}{2N} \int \frac{d^2k}{(2\pi)^2} V(k) |\rho(k)|^2$$

$$= \frac{1}{\pi a_B^2 r_s^2} \int_0^\infty \frac{dx}{x} V\left(\frac{x}{b}\right) \left(\frac{J_1(\gamma x)}{\gamma} - J_1(x) \right)^2,$$

where $\gamma = a/b$ is the ratio of the radii after and before shrinking the electron disc. The charging energy shows distinct forms for different interaction ranges. When the interaction range ξ is much larger than the radius of the disk, $\xi \gg b$, the electron-electron interaction can be roughly considered as the bare Coulomb interaction. In this case, the electrostatic charging energy is

$$E_c \approx \frac{4b}{r_{s0}^2} \left(0.290545 - \frac{1}{\pi} \ln|1 - \gamma| \right) (1 - \gamma)^2 + \dots \text{ (Ry)}.$$

In the other limit $b \gg \xi$, the interaction is well screened and the electrostatic energy has the form

$$E_c = 4\xi \left| \frac{1}{r_s^2} - \frac{1}{r_s'^2} \right| \text{ Ry},$$

where r_s and r_s' are the inverse density parameters before and after the shrinking. The total energy difference can be written as

$$\Delta E_{tot} = E_c(\gamma) + \Delta E_g.$$

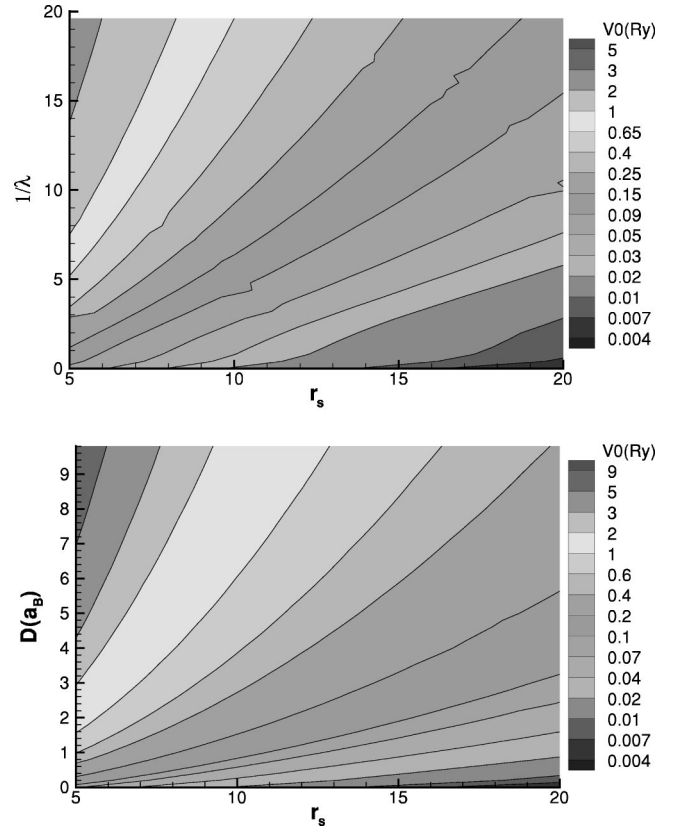


FIG. 4. The phase diagram in the $r_s - \xi$ plot. r_s is the initial density parameter of the electron disc. D or $1/\lambda$ represents the interacting range ξ of the electron-electron interaction. Each value of V_0 corresponds to a curve in the figure. On the right side of the curve, the electron disc will have a macroscopic shrinking.

For a small initial radius $b \ll \xi$, the energy gain ΔE_g dominates over the energy loss E_c , thus, there is always finite shrinking.

However, the above conclusion is not true in general as demonstrated in Fig. 2. Figure 2 shows the shrinking distance $\Delta b = b - a$ versus initial radius b . Δb approaches a constant for large b . However, the shrinking shown here cannot be considered as a macroscopic shrinking because the typical Δb is only about $2a_B$, which is far smaller than the average distance between the electrons, which is $r_s = 15a_B$ for this calculation. Similar behavior has also been observed for other values of r_s .

Thus, the intrinsic instability is not sufficient to overcome the charging energy cost in order to form the electron droplet state. The system is in a marginally stable situation. However, in real systems, there are always disorders. The low frequency component of a disorder potential forms the potential landscape, and electrons tend to occupy the low potential valleys. We assume that around each local minimum, the disorder potential is isotropic and slowly varying. We expand the disorder potential around the local minimum up to the quadratic term. Therefore, we adopt the following simple model for disorder potential:

$$W(r) = V_0 \frac{r^2}{b^2},$$

where V_0 is the potential depth from center to edge of the disc. The energy gain by shrinking to a radius a can be evaluated as

$$\Delta E_w = \Delta \frac{1}{N} \int W(r) \rho(r) dS = \frac{V_0}{2} (\gamma^2 - 1).$$

The total energy difference in the limit $b \gg \xi$ can be written as

$$\Delta E_{tot} = - \left(\frac{V_0}{2} - \frac{4\xi}{r_{s0}^2} \right) (1 - \gamma^2) + \Delta E_g.$$

The effect of the electrostatic energy will be suppressed by the potential fluctuation. A large value of V_0 is favorable for the disc to shrink.

Figure 3(a) plots the $\Delta b = b - a$ as a function of the initial radius b for Si MOSFET's with $D = 10a_B$ and $r_s = 15a_B$. There exists a critical V_0^c (~ 0.08) above which $\Delta b \propto b$. Thus, for large b there is a macroscopic shrinking for $V_0 > V_0^c$. A similar result has also been obtained for the screened Coulomb interaction with $1/\lambda$ places the role of D . In Fig. 3(b) we plot the energy change as a function of the initial radius b . It is clear that larger value of V_0 gives rise to larger energy gain. We have carried out the calculations for many values of r_s and the resulting phase diagrams are plotted in Fig. 4.

Figure 4 shows the phase diagram in the $r_s - \xi$ plot for the case of $b \gg \xi$. Each value of V_0 corresponds to a curve in the figure. The curves for larger V_0 are above those for smaller V_0 . On the right side of the curve for a given V_0 , the electron disc will have a macroscopic shrinking, thus, an electron droplet phase is stable. To form the electron droplet state, the screening of the electron-electron interaction and the potential fluctuation are both crucial. The smaller the interaction

range between the electrons and the lower the electron density, the easier it is to form the droplet phase.

Before summarizing, we would like to make several comments. (i) In this paper, we only consider one electron disc, corresponding to one drop in the droplet state. In real systems, electrons tend to occupy valleys of potential fluctuations to give rise to many such drops. The size of each drop is determined by local potential depth. (ii) We only consider zero temperature effect in this paper such that the "gas" phase is empty. At a finite temperature, the "gas" phase is occupied by lower density electrons. Thus, a finite temperature enhances the possibility for the droplet state since the density difference between the liquid and the "gas" is smaller and the charging energy is less costly. However, in order to form the droplet state, the temperature has to be below the cohesive energy (the energy cost to remove an electron from the liquid phase to the "gas" phase⁴). (iii) We believe that the recently observed 2D metal-insulator transition might be the percolation transition of the liquid phase in the droplet state.⁴ The percolation here is semiquantum in nature, different from the conventional classic percolation.¹⁰ (iv) In order to have a percolation, the "gas" phase needs to have a much smaller local conductivity than the liquid phase. This requires that a typical length scale of the "gas" region is larger than the localization length of the "gas" phase. The "gas" phase is low in electron density which gives rise to a short localization length. Thus, one may not need a large shrinking of electron drops to realize a percolation transition. We suspect that in experimental samples, a typical drop size is of the order of μm .

In summary, we have demonstrated that it is possible to have a droplet phase for 2D electron systems at low densities. Both electron-electron interaction and disorder potential fluctuations are important for the formation of the droplet phase.

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