

Phase diagram of the two-dimensional electron liquid

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The phase diagram of a two-dimensional electron liquid immersed in a uniform background of charge is analyzed. We present a qualitative argument based on energy considerations alone which yields the shape of the liquid-solid boundary. To determine absolute values of the density and temperature we utilize a microscopic theory based on the self-consistent harmonic approximation to the phonon spectrum of a solid. This theory is a one-phase instability theory of the long-wavelength transverse mode in the solid phase alone. It yields values of $r_s \approx 5$ in the quantum regime and $\Gamma_0 = 3$ in the classical case.

I. INTRODUCTION

Recent experimental work^{1,2} has focused attention on the two-dimensional electron liquid. Electrons on the surface of liquid helium¹ are a particularly ideal system. A finite concentration of them ($10^5 < n < 10^{10} \text{ cm}^{-2}$) are held onto the free surface by the combination of an external field and an image potential which traps the electrons in their lowest quantum state for motion perpendicular to the surface. Motion parallel to the surface is essentially unrestricted so that the arrangement is very accurately characterized by a two-dimensional electron gas immersed in a uniform positive background of charge.³

At the interface of a metal-oxide-semiconductor sandwich excess electrons accumulate in their lowest quantum state and a similar situation arises.² The model system, in this case, is somewhat more complicated in that the law of force becomes dipolar at distances characteristic of the oxide layer thickness, which is usually of the order of tens of angstroms, and anisotropic band structure effects are not unimportant. However, it too, for some rather limited region of parameter space, may be thought of as a two-dimensional electron liquid immersed in a uniform neutralizing background of charge.

From a theoretical point of view one of the features of these experimentally accessible systems which makes them intriguing is the wide range of densities (\approx six orders of magnitude) which can be produced by essentially turning a knob. This large variation in density (and temperature) leads to a correspondingly large variation (\approx four orders of magnitude) in the ratio of mean potential to mean kinetic energy of the electrons. Such large variations would suggest that a possible crystallization, into a two-dimensional Coulomb solid⁴ (TDCS) might occur. In three dimensions there has been a great deal of work and discussion of the transition from a gas (liquid) to a so-called Wigner

solid.⁵⁻⁷ In this paper we consider the phase diagram of such a TDCS and conclude that the liquid-solid transition is a definite experimental possibility.

II. SIMPLEST ESTIMATE

Physically we expect any liquid to crystallize when the potential energy dominates the kinetic energy. We can get a qualitative picture of the shape and nature of the phase diagram by calculating both these quantities (potential $\langle V \rangle$ and kinetic energies $\langle K \rangle$) in the gas phase and setting their ratio equal to some constant Γ_0 (greater than 1), i.e.,

$$\langle V \rangle / \langle K \rangle \equiv \Gamma_0. \quad (1)$$

For the case under consideration here, a two-dimensional electron gas with a density per unit area $n \equiv (\pi r_0^2)^{-1}$ in the presence of a uniform positive background, the mean potential energy is approximated by

$$V = e^2 / r_0 = e^2 \pi^{1/2} n^{1/2}. \quad (2)$$

On the other hand, the mean kinetic energy per particle (for fermions of mass m) is given by an integral over the Fermi function, i.e.,

$$\langle K \rangle = \frac{2}{n} \int \frac{d^2 p}{(2\pi)^2} \frac{\epsilon_p}{e^{\beta(\epsilon_p - \mu)} + 1}. \quad (3)$$

In Eq. (3) μ is the chemical potential, β the inverse temperature ($\kappa T = \beta^{-1}$), and $\epsilon_p = p^2 / 2m$ the kinetic energy. The number density n is defined in the usual way in terms of the chemical potential,

$$n = 2 \int \frac{d^2 p}{(2\pi)^2} \frac{1}{e^{\beta(\epsilon_p - \mu)} + 1}. \quad (4)$$

In the high-temperature classical regime where $\langle K \rangle = \kappa T$, the melting curve [given by (1)] is simply

$$n = (\kappa T \Gamma_0 / \pi^{1/2} e^2)^2. \quad (5)$$

At zero temperature the $\langle K \rangle = \pi n / 2m$ and the melting density n_c at $T=0$ is simply

$$n_c = \frac{4m^2 e^4}{\pi \Gamma_0^2} = \frac{4}{\pi a_0^2} \frac{1}{\Gamma_0^2}, \quad (6)$$

where $a_0 = (me^2)^{-1}$ is the three-dimensional Bohr radius. If, as is the custom in three dimensions, the mean interparticle spacing is measured in units of a_0 and is called r_s , then Eq. (6) tells us that $r_s = (\pi/4)^{1/2} \Gamma_0$ at melting.⁸

At arbitrary temperatures and densities the integrals in Eqs. (3) and (4) may be evaluated analytically. Substituting the results of these integrations into Eq. (1), one arrives at the parametric equations (parametric in the chemical potential $z \equiv e^{-\beta\mu}$) for the phase boundary, i.e.,

$$n = F_1^4(z) / F_3^2(z) \quad (7)$$

and

$$T = F_3^3(z) / F_3^2(z). \quad (8)$$

We have picked units in Eqs. (7) and (8) such that the density n in Eq. (7) is measured in units of n_c [see Eq. (6)] while the temperature T is to be measured in units of T_c , where

$$\kappa T_c = 2e^4 m / \Gamma_0^2. \quad (9)$$

The functions F_1 and F_3 are given by

$$F_1(z) = \frac{1}{2} \ln(1+1/z)$$

$$F_3(z) = \frac{1}{2} \left\{ \frac{1}{2} \left[\ln \left(1 + \frac{1}{z} \right) \right]^2 + f \left(\frac{1}{1+z} \right) \right\}, \quad (10)$$

where $f(x)$ is the so-called di-logarithm or Spence function⁹:

$$f(x) = - \int_1^x \frac{\ln|1-y|}{y} dy. \quad (11)$$

It has been tabulated in Ref. 9. Equations (7) and (8) are plotted in Fig. 1. The curve is labeled at each point by the value of z , i.e., the degree of degeneracy. To get an idea of the real temperature and densities involved we note that $n_c = 1.2 \times 10^{14} \text{ cm}^{-2}$, $T_c = 10^3 \text{ }^\circ\text{K}$ for a $\Gamma_0 = 20$.¹⁰

III. MEAN-FIELD THEORY

While Fig. 1 no doubt gives a good qualitative picture of the shape of the phase diagram it suffers from the fact that the absolute magnitudes of the temperature and density scale depend quadratically on the parameter Γ_0 .

In 1968 Kugler^{6,7} suggested that the so-called self-consistent harmonic approximation (SCHA)¹¹ to the phonon spectrum of a solid might be applied to the stability of a Wigner lattice in three dimensions at 0 K. In Ref. 7 (hereafter to be called I) these

concepts were developed. The idea as presented there focuses on an instability of the transverse sound mode in the solid. Such a theory has been shown to be analogous to and in some cases (three-dimensional simple phonon spectrum) identical with Lindemans empirical melting law¹² without an empirical parameter.

For a set of particles with position vectors \vec{r}_i which are the sum of an equilibrium position \vec{R}_i and a deviation $\delta\vec{r}_i$, Lindemans law states that when the root-mean-square deviation reaches some fraction δ of the lattice spacing $b[\langle \delta r_i^2 \rangle / b^2 = \delta^2]$, the solid will melt. In two-dimensions, at any finite temperature the mean square displacement at a fixed site, averaged over the phonon spectrum, diverges logarithmically. Thus we cannot use Lindemans criterion to simply determine a melting curve. In fact, the divergence of the fluctuations has been used as an argument to conclude that true long-range order never really exists in two dimensions except perhaps at zero temperature.¹³⁻¹⁵ Several workers, notably Mermin,¹⁴ have pointed out that other correlation functions, for example ones involving the angular correlation between two parallel vectors, remain finite in two as well as three dimensions, implying that some types of long-range order may in fact exist in two dimensions.

In the theory, as presented in I, we will most naturally be concerned with the correlation function

$$\frac{1}{2} \langle [\vec{q} \cdot (\delta\vec{r}_i - \delta\vec{r}_j)]^2 \rangle \equiv D(\vec{q}, \vec{R}_{i,j}). \quad (12)$$

This correlation function is finite for any finite R_{ij} and only diverges (in two dimensions) logarithmically at finite temperature as $R_{ij} \rightarrow \infty$. Such a divergence is in fact equivalent to the logarithmic divergence present in Lindemans law. Within the framework of the SCHA, it is quite easy to show that this divergence is sufficient to force the Debye-Waller factor, i.e., the intensity in the Bragg peak, to be identically zero at any finite temperature. In this restricted sense no long-range order exists. However, within the framework of this same theory, we also find that such a weak logarithmic divergence of D does *not* necessarily destroy the existence of an infinitely-long-wavelength transverse mode at any finite temperature. The physical reason for this is simply related to the fact that the transverse restoring force (even for infinitely long wavelengths) is strongly dependent on the relative displacements of near neighbors; i.e., the important i, j differences in Eq. (12) are not those which go to infinity. Since solids have transverse modes and liquids do not, it is the existence of a long-wavelength transverse mode which we use to define the existence of a solid.

Since melting is a first-order transition between liquid and solid phases a true theory of melting should of necessity consider both phases. The Lindeman approach to melting, like the current approach, is a one-phase theory. It only treats the solid and says nothing about the liquid. Such theories evolve from an intuitive sense of what must be occurring. Physically we know that liquids do not support transverse modes so that it is reasonable to assume that an instability of the transverse modes signals the onset of melting. The transverse-model instability may be considered a superheating transition.

In the SCHA¹¹ the normal-mode frequencies ($\omega_{\vec{k}\lambda}$) of a group of particles of mass m interacting via a two-particle potential $V(\vec{r}_{ij})$ are

$$\omega_{\vec{k}\lambda}^2 = \frac{1}{m} \sum_{i < j} \epsilon_{\lambda\alpha}^*(\vec{k}) \epsilon_{\lambda\beta}(\vec{k}) (1 - e^{i\vec{k}\cdot\vec{r}_{ij}}) \times \langle \nabla_{i\alpha} \nabla_{j\beta} V(\vec{r}_{ij}) \rangle. \quad (13)$$

The position \vec{r}_{ij} is the sum of the equilibrium position \vec{R}_i and a displacement which is to be averaged over the phonon distribution at temperature T . This type of mean-field theory quite accurately describes the low-temperature phonon spectra of a variety of anharmonic solids.¹¹

The average over the oscillators is easily carried out and, in terms of the Fourier coefficients $v_{\vec{q}}$ of the potential, Eq. (13) may be written as

$$\omega_{\vec{k}\lambda}^2 = \frac{1}{m} \sum_{\vec{q}, R \neq 0} [\epsilon_{\lambda\alpha}^*(\vec{k}) \cdot \vec{q}] [\epsilon_{\lambda\beta}(\vec{k}) \cdot \vec{q}] e^{i\vec{q}\cdot\vec{R}} \times (e^{i\vec{k}\cdot\vec{R}} - 1) v_{\vec{q}} e^{-D(i\vec{q}, \vec{R})}. \quad (14)$$

The effects of self-consistency are contained in

$$D(\vec{q}, \vec{R}) = \frac{1}{2Nm} \sum_{\vec{k}', \lambda'} [\epsilon_{\lambda'}^*(\vec{k}') \cdot \vec{q}]^2 (1 - \cos \vec{k}' \cdot \vec{R}) \omega_{\vec{k}'\lambda'}^{-2} \times \coth(\beta \omega_{\vec{k}'\lambda'}/2). \quad (15)$$

In I it was shown for a variety of simple models in three dimensions that, at a fixed density, a maximum temperature T_m exists above which no self-consistent solution of Eq. (14) for the transverse mode exists. The simple picture which emerged was that as the temperature increases the fluctuations increase and the shear restoring forces decrease leading to a subsequent decrease in the transverse sound velocity and a further increase in the fluctuations. At some temperature the potential runs away from the sound velocity and a first-order transition occurs. In this section we will attempt to apply this kind of reasoning to the two-dimensional Coulomb solid.

In order to evaluate $D(\vec{q}, \vec{R})$ we must know some-

thing about the properties of the phonon spectrum of the two-dimensional Coulomb solid. In the Appendix we give the results of a simple harmonic calculation (no fluctuation effects) for a triangular Coulomb lattice (lattice constant b). (The triangular lattice, owing to its close-packed nature, is expected to be the configuration of lowest potential energy.¹⁶) Recent calculations¹⁷ of this spectrum for a square lattice give a phonon spectrum with somewhat more structure but roughly similar to the results shown in Figs. 5-7. The essential features of the phonon spectrum are the existence of a more or less isotropic linear transverse mode ($\omega = ck$) and a longitudinal plasmon mode.¹⁸

In evaluating $D(\vec{q}, \vec{R})$ we parametrize the spectrum by assuming a linear transverse mode having a velocity c which is to be determined self-consistently and a longitudinal plasmon mode of the form

$$\omega_l^2 = (2\pi ne^2/m)k$$

independent of fluctuations and or self-consistency requirements. This is an approximation which we expect to be reasonably accurate. In I it was shown that the longitudinal mode is less effected by fluctuations than the transverse mode, and that an instability of the type discussed here for the transverse mode is not expected to be present for the longitudinal mode. Physically we expect this to be true since the longitudinal mode (plasmon) exists in both the liquid and solid phases. In addition we will see that the presence of longitudinal

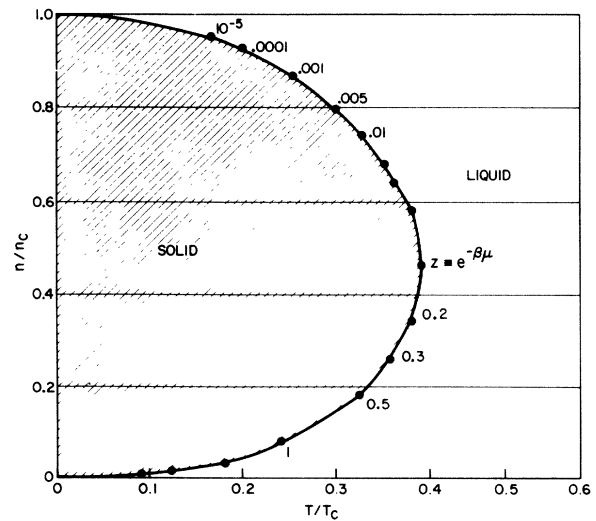


FIG. 1. Parametrized phase diagram of the two-dimensional Coulombic system. [$n_c = (4/\pi a_0^2)(1/\Gamma_0^2)$, $T_c = (2e^4 m/\Gamma_0^2)$].

fluctuations only effects the transition by about 20% in its entirety.

Using the above assumed form for the phonon spectrum the angular integrals in Eq. (14) are readily done and we are left with an expression of the form

$$D(\vec{q}, \vec{R}) = \frac{q^2 k_D}{8nm\pi c} \int_0^1 x dx \{ \coth(ck_D x/2\kappa T)/x [1 - J_0(k_D R x) - \cos(2\theta') J_2(k_D R x)] + (ck_D/\gamma x^{1/2}) \coth(\gamma x^{1/2}/2T) \times [1 - J_0(k_D R x) + \cos(2\theta') J_2(k_D R x)] \}, \quad (16)$$

where J_ν is the Bessel function and the wave vector $|\vec{k}_D| = (4\pi n)^{1/2}$ sets the scale for the circular Brillouin zone used in these calculations, i.e.,

$$\int_{|\mathbf{k}| < k_D} \frac{d^2 k}{(2\pi)^2} \equiv \frac{k_D^2}{(4\pi)} = n = (\pi r_0^2)^{-1} = (\frac{1}{2} \sqrt{3} b^2)^{-1}. \quad (17)$$

The angle θ' is the angle between \vec{q} and \vec{R} ; and the quantity $\gamma = (2\pi n e^2 / m k_D)^{1/2}$ is the plasmon frequency at the zone boundary. Equation (16) cannot be integrated further without numerical work. In order to make progress it is worth looking at some of the properties of D and of the self-consistent equations in two limiting cases.

A. Classical regime ($kT \gg \gamma$)

In this regime the occupation-number factors $\coth(\hbar\omega/2\kappa T)$ are replaced by $2\kappa T/\hbar\omega$. The behavior of the integrals at large and small $k_D R$ can be extracted. Our conclusions are that the angular-dependent pieces are unimportant. The angular-independent part, arising from the transverse mode, goes like $T \ln(k_D R)$ at large R and like $T(k_D R)^2$ at small R . A reasonably good approximation for all R is given by

$$\int_0^1 \frac{2T}{ck_D} \frac{dx}{x} [1 - J_0(k_D R x)] \cong \frac{T}{ck_D} \ln[1 + (k_D R)^2/4]. \quad (18)$$

The longitudinal-mode contribution to D in Eq. (16) starts out like $(k_D R)^2$ and rapidly approaches a constant. It is well approximated by

$$\frac{2Tk_D c}{\gamma^2} \int_0^1 dx [1 - J_0(k_D R x)] \cong \frac{T}{ck_D} \left[\left(\frac{2\sqrt{3}}{\pi} \right)^{1/2} \left(\frac{c^2}{v_0^2} \right) \frac{(k_D R)^2/12}{1 + (k_D R)^2/12} \right], \quad (19)$$

where $v_0^2 = e^2/m\hbar$.

The net effect of these approximations is that

$$D(\vec{q}, \vec{R}) \cong q^2 l^2. \quad (20)$$

In Eq. (20),

$$l^2 = \delta^2 \gamma_0^2 \left[\ln \left[1 + \frac{1}{4} (k_D R)^2 \right] + \left(\frac{2\sqrt{3}}{\pi} \right)^{1/2} \left(\frac{c^2}{v_0^2} \right) \frac{(k_D R)^2}{1 + (k_D R)^2/12} \right] \quad (21)$$

and

$$\delta^2 = \kappa T / 8mc^2. \quad (22)$$

Substituting (20) into (14) and integrating over \vec{q} we obtain, for the transverse mode,

$$\omega_{kt}^2 = \frac{e^2}{2m} \sum_{\vec{R} \neq 0} (e^{i\vec{k} \cdot \vec{R}} - 1) \frac{1}{R^3} \times \int_0^\infty dx x^2 e^{-x^2(l^2/R^2)} [J_0(x) + \cos(2\theta') J_2(x)], \quad (23)$$

where l^2 is given by (21) and $J_\nu(x)$ is the Bessel function. By use of the equation

$$\int_0^\infty dx e^{-a^2 x^2} J_{2\nu}(x) = \frac{\sqrt{\pi}}{2a} e^{-(\pi a^2)^{-1}} I_\nu \left(\frac{1}{8a^2} \right),$$

where $I_\nu(x) = e^{-\nu\pi i/2} J_\nu(ix)$ and a is a real positive number, we can rewrite Eq. (23) as

$$\omega_{kt}^2 = \frac{e^2}{2m} \sum_{\vec{R} \neq 0} (e^{i\vec{k} \cdot \vec{R}} - 1) \frac{1}{R^3} [\Phi_1(z) + \cos(2\theta)\Phi_2(z)], \quad (24)$$

where $z = R^2/8l^2$ and

$$\Phi_1 = 4\sqrt{2\pi} z^{3/2} e^{-z} [(1-2z)I_0 + 2zI_1], \quad (25)$$

$$\Phi_2 = 4\sqrt{2\pi} z^{3/2} e^{-z} [zI_0 + (1-2z)I_1 + zI_2]. \quad (26)$$

The quantity θ is the angle between \vec{k} and \vec{R} . (Note that in the absence of fluctuations, i.e., $l=0$, $z=\infty$, $\Phi_1 = -1$, and $\Phi_2 = 3$.)

Equation (24) is valid for any \vec{k} . We could in principle use it to discuss the behavior of the entire anisotropic spectrum. However, we have already assumed in calculating D that the phonon spectrum even in the presence of fluctuations is roughly isotropic. In order to be consistent we will work with the average of both sides or Eq. (22), over the direction of \vec{k} , i.e.,

$$\langle \omega_{\mathbf{k}t}^2 \rangle \equiv \frac{1}{(2\pi)} \int_0^{2\pi} d\theta \omega_{\mathbf{k}t}^2 = \frac{-e^2}{2m} \sum_{\mathbf{R} \neq 0} \frac{1}{R^3} \times \{ \Phi_1(z)[1 - J_0(kR)] + \Phi_2(z)J_2(kR) \}. \quad (27)$$

Expanding the Bessel Functions appearing in Eq. (27) and setting $\langle \omega_{\mathbf{k}t}^2 \rangle = c^2 k^2$ at long wavelengths we arrive at the final self-consistent equation for c^2 :

$$c^2 = c_0^2 - \Delta c^2. \quad (28)$$

The velocity c_0^2 is the average transverse velocity in the absence of fluctuation effects. It has a value (see Figs. 5-7) equal to $0.269v_0^2 \equiv 0.269(e^2/m\bar{b})$. The quantity

$$\Delta c^2 = \frac{v_0^2}{16} \sum \frac{b}{R} [\Phi_2 + 2\Phi_1 - 1]. \quad (29)$$

To obtain the melting temperature in this classical regime, we have numerically solved Eqs. (28) and (29) by a simple iteration procedure. Since Δc^2 is a function of both γ and c^2 we fixed γ , and performed the sum in Eq. (29) over a triangular lattice for several values of c^2 until we found (by trial and error) that value of c^2 which satisfied Eq. (28) self-consistently. The results obtained are shown in Fig. 2. The velocity c^2 is plotted as a function of temperature.

The point labeled $T_m/8mv_0^2 = 0.085$ is the highest temperature for which a self-consistent solution of the equations exist. At higher temperatures the lack of a solution (in this picture) implies that we are in the liquid regime. For varying densities the equation of state is simply given by

$$\frac{T}{8mv_0^2} \equiv \frac{Tb}{8e^2} = 0.085. \quad (30)$$

Using the relation between b and Γ_0 given in Eq. (5) we find a $\Gamma_0 = 2.8$.

In three dimensions this same (SCHA) instability theory yields a Γ_0 of 20, almost an order of magnitude larger than the value found here and about an order of magnitude smaller than the numerical results in three dimensions.¹⁵ The smaller Γ_0 in two dimensions implies a greater stability for the solid. Without getting into a discussion of the correctness of the absolute magnitude of Γ_0 we can safely conclude that this trend, from three to two dimensions, is real and that the behavior of the velocity (see Fig. 2) is indicative of this effect. As the temperature increases in two dimensions we see (Fig. 2) that the transverse sound velocity increases for a while. This increased rigidity due to fluctuations is at first sight unusual and in fact is not characteristic of three dimensions, where the velocity decreases monotonically with temperature. An examination

of the effective potential $v(\vec{r})$ in the two cases is consistent with this picture.

For three dimension,

$$\begin{aligned} \bar{v}_3(r) &= \frac{1}{(2\pi)^3} \int d^3q e^{i\vec{q}\cdot\vec{r}} \frac{4\pi e^2}{q^2} e^{-q^2 r^2} \\ &= \frac{2e^2}{\pi r} \int_0^\infty dx \frac{\sin x}{x} e^{-x^2 r^2/r^2} \\ &= \frac{e^2}{r} \operatorname{erf}\left(\frac{r}{2l}\right) \equiv \frac{e^2}{r} f_3(r/l), \end{aligned}$$

where $\operatorname{erf}(x) = 2/\sqrt{\pi} \int_0^x dt e^{-t^2}$. For two dimensions,

$$\begin{aligned} \bar{v}_2(r) &= \frac{1}{(2\pi)^2} \int d^2q e^{i\vec{q}\cdot\vec{r}} \frac{2\pi e^2}{q} e^{-q^2 r^2} \\ &= \frac{e^2}{r} \int_0^\infty dx J_0(x) e^{-x^2 r^2/r^2} \\ &= \frac{e^2}{r} f_2(r/l), \end{aligned}$$

where

$$f_2(x) = 2^{-1} \sqrt{\pi} x e^{-x^2/8} I_0(x^2/8).$$

The quantities $f_2(z)$ and $f_3(z)$ are shown in Fig. 3. Note that $f_3(z) < 1$ for all z , which implies that the fluctuations reduce the mutual potential. On the other hand, $f_2(z) > 1$ for $z > 1.42$, and $f_2(z)$ has a maximum $f_2(z) = 1.18$ at $z = 2.6$. This means that in two dimensions the fluctuations (if they are small enough, i.e., $b/l > 1.42$) actually strengthen

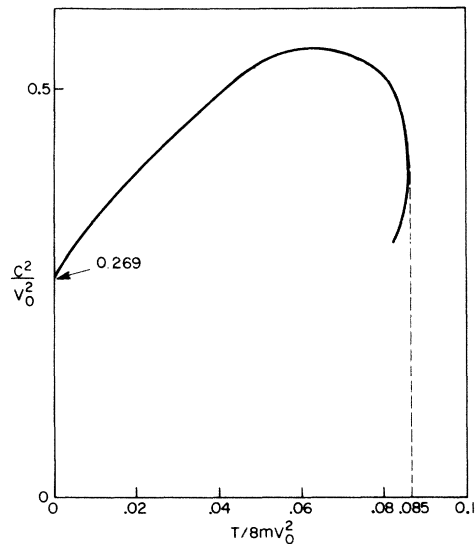


FIG. 2. Transverse sound velocity as a function of temperature. ($v_0^2 = e^2/m\bar{b}$).

the mutual interactions between every pair of electrons. This increased potential in turn leads to an increased restoring force (see Fig. 4). As the fluctuations increase further the nearest-neighbor forces finally do become weakened (see Fig. 2), giving rise to a softening of the mode frequency. Note that the velocity of the transverse mode is larger at the melting than that of the harmonic phonons, even though a rapid softening is occurring in the vicinity of melting.

B. Quantum regime

At zero temperature it is possible to determine the melting density r_s without any numerical work.

Since the occupation-number factors ($\coth \hbar \omega / 2kT$) in Eq. (16) are equal to 1 we are not plagued by the logarithmic divergences present at higher temperatures. This implies that it is quite a good approximation to neglect the R dependence of $D(\vec{q}, R)$, i.e.,

$$D(\vec{q}, \vec{R}) = \frac{q^2 k_D}{8nm\pi c} \left(1 + \frac{2}{3} \frac{ck_D}{\gamma} \right). \quad (31)$$

Since $D(\vec{q}, \vec{R})$ is roughly independent of \vec{R} the sum over \vec{R} [in Eq. (23)] yields

$$\tilde{v}_{\vec{k}t}^2 = \frac{N}{m} \sum_{\nu \neq 0} [\vec{K}_\nu \cdot \vec{\epsilon}_t(\vec{k})]^2 (\tilde{v}_{\vec{k}+\vec{K}_\nu} - \tilde{v}_{\vec{K}_\nu}), \quad (32)$$

where

$$\tilde{v}_{\vec{q}} = v_q e^{-D(q)} \equiv (2\pi e^2/q) e^{-D(q)}. \quad (33)$$

Near melting (as we shall see) D is in fact larger than 1 for $q = |K_1| = 2\pi/b$ (the smallest reciprocal-lattice vector) so that the sum in Eq. (31) is very accurately approximated by the sum over the six

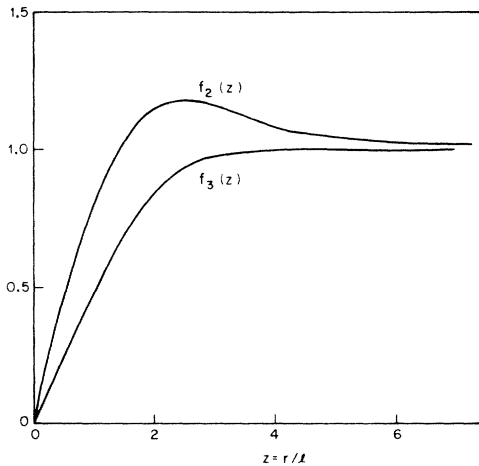


FIG. 3. Plot of the functions which describe the effect of fluctuations on the effective potential.

nearest-neighbor reciprocal-lattice vectors $K_1 = (\pi/b)[\pm \hat{x} \pm \sqrt{3} \hat{y}]$, $K_1 = \pm (2\pi/b)\hat{x}$.

Expanding the difference in potentials appearing in Eq. (32) about $k=0$ and averaging over the direction of k as discussed in Eq. (27) we arrive at a self-consistent equation for the sound velocity c ,

$$c^2 = 0.226(1/r_s) e^{-R} (-1 - 4R + 4R^2), \quad (34)$$

with

$$R \equiv D(K_1) = \frac{2.72}{r_s c} + \frac{1.81}{r_s^{1/2}}. \quad (35)$$

In Eq. (35) we have used atomic units ($e^2 = \hbar = m = 1$); in these units $r_s = r_0$, $b = 1.9r_s$, and $k_D = 2/r_s$.

The maximum value of r_s for which there is a self-consistent solution of Eq. (35) is easily found to be $r_s = 4.5$.¹⁹ As in the classical case the number found here for two dimensions implies a more stable solid. What is more this number is roughly consistent with the simple estimate (see Fig. 1):

$$\langle V \rangle / \langle K \rangle = \Gamma_0 \approx 3.$$

IV. CONCLUSIONS

Estimating transition temperatures for real many-body systems is often a difficult and tricky task. However, it seems to be clear from this work that the solidification line of the two-dimensional Coulomb solid may be experimentally within

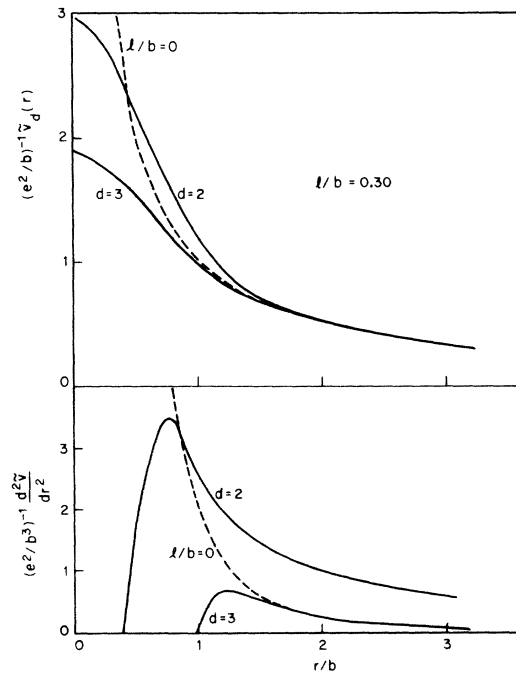


FIG. 4. Effective potential and restoring force in the presence of fluctuations in two and three dimensions.

reach. While peculiar behavior of the dc resistivity² of the metal-oxide-semiconductor devices has been observed in the neighborhood of $r_s=3$, the experimental situation is sufficiently cloudy that we do not wish to claim this is evidence for the existence of the transition and/or the theoretical predictions. For electrons on the surface of He Γ_0 's of 10 are easily within reach and a Γ_0 's of a few hundred are not out of the question. Since this system is so clean and so unambiguously a real physical idealization of a two-dimensional electron gas it offers exciting possibilities for future experimental and theoretical investigations.

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APPENDIX: PHONON SPECTRUM OF A TRIANGULAR LATTICE IN THE HARMONIC APPROXIMATION

We consider a triangular lattice with lattice spacing b . The frequency $\omega_{\mathbf{k}\lambda}$ of a phonon with wave vector \mathbf{k} and polarization λ is given by

$$\omega_{\mathbf{k}\lambda}^2 = \frac{1}{m} \sum_{i \neq j; \alpha, \beta} \tilde{\epsilon}_{\lambda\alpha}^*(\mathbf{k}) \tilde{\epsilon}_{\lambda\beta}(\mathbf{k}) (1 - e^{i\mathbf{k} \cdot \mathbf{R}_{ij}}) \frac{\partial^2 v(\mathbf{R}_{ij})}{\partial R_{i\alpha} \partial R_{j\beta}} \quad (\text{A1})$$

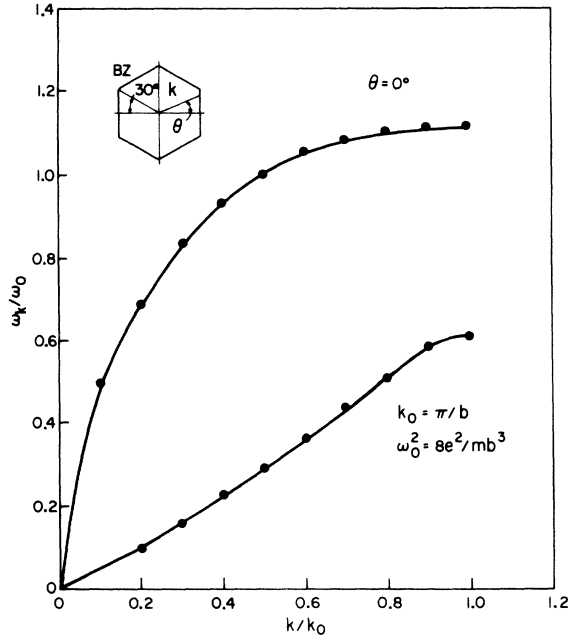


FIG. 5. Phonon spectrum in the two-dimensional Coulomb lattice where the momentum vector \mathbf{k} makes an angle $\theta=0^\circ$ with respect to the Brillouin zone shown in the inset.

Here m is the electron mass and $v(R) = e^2/R$. α and β refer to the components of vectors and $\tilde{\epsilon}_\lambda(\mathbf{k})$ is the polarization vector of the mode. By use of

$$\frac{\partial^2 v(\mathbf{R}_{ij})}{\partial R_{i\alpha} \partial R_{j\beta}} = e^2 \left(3 \frac{(\mathbf{R}_{ij})_\alpha (\mathbf{R}_{ij})_\beta}{R_{ij}^5} - \frac{\delta_{\alpha\beta}}{R_{ij}^3} \right),$$

(A1) can be written as

$$\omega_{\mathbf{k}\lambda}^2 = \frac{e^2}{m} \sum_{\mathbf{R} \neq 0} \left(3 \frac{(\mathbf{R} \cdot \tilde{\epsilon}_\lambda(\mathbf{k}))^2}{R^5} - \frac{1}{R^3} \right) (1 - \cos \mathbf{k} \cdot \mathbf{R}). \quad (\text{A2})$$

It is easy to perform the summations over lattice sites $[\mathbf{R} = (r, \sqrt{3}s)b$ and $\mathbf{R} = (r + \frac{1}{2}, \sqrt{3}s + \frac{1}{2}\sqrt{3})b]$ in (A2). The quantities r and s are integers and x, y in $\mathbf{R} = (x, y)$ are components of the vector R in a Cartesian coordinate system. The Brillouin zone for such a triangular lattice is the hexagon shown in the insert in Fig. 5. The lattice spacing in the reciprocal lattice is $K_0 = 2\pi/b$. The results of numerical summations of Eq. (A2) for three different directions of k are shown in Figs. 5–7. Both modes are roughly isotropic, particularly at long wavelengths. The velocity $c = \omega_{\mathbf{k}\lambda}/k$ of the transverse mode is very nearly ($\approx 5\%$) constant and equal to $0.5(e^2/mb)^{1/2}$.

Although (A2) is convenient for numerical calculations it is not a convenient form for discussing several interesting analytical properties of the spectrum. To facilitate such a discussion we rewrite the right-hand side of (A1) in terms of the Fourier transform of $v(R)$, $v_{\mathbf{k}} = 2\pi e^2/k$, i.e.,

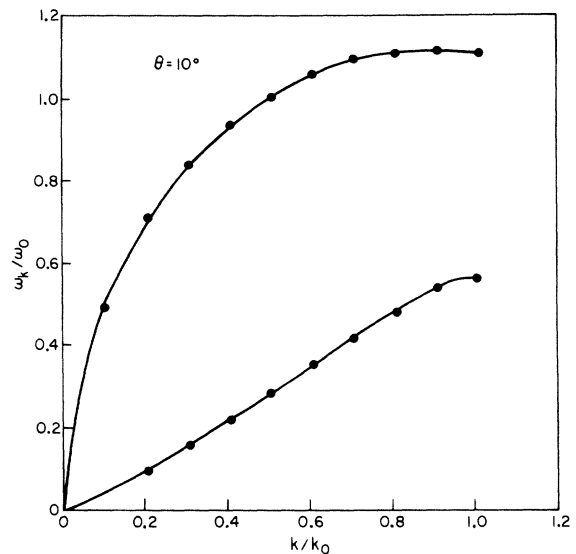


FIG. 6. Phonon spectrum in the two-dimensional Coulomb lattice with $\theta=10^\circ$.

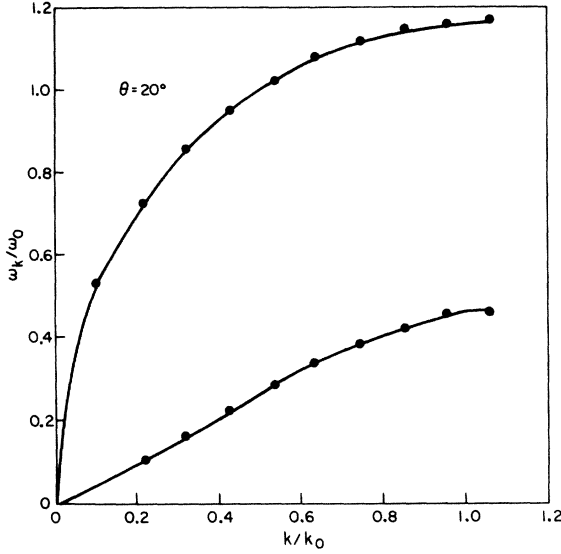


FIG. 7. Phonon spectrum in the two-dimensional Coulomb lattice with $\theta = 20^\circ$.

$$\begin{aligned} \omega_{\vec{k}\lambda}^2 &= \frac{n}{m} v_{\vec{k}} [\vec{k} \cdot \vec{\epsilon}(\vec{k})]^2 \\ &+ \frac{n}{m} \sum_{\nu \neq 0} \{ v_{\vec{k} + \vec{K}_\nu} [(\vec{k} + \vec{K}_\nu) \cdot \vec{\epsilon}_\lambda(\vec{k})]^2 \\ &- v_{\vec{K}_\nu} [\vec{K}_\nu \cdot \vec{\epsilon}_\lambda(k)]^2 \}, \end{aligned} \quad (\text{A3})$$

where n and \vec{K}_ν are the number of lattice sites in a unit area and the reciprocal-lattice vector, respectively. For long wavelengths, i.e., $k/K_0 \ll 1$, the frequency of the longitudinal phonon is given by the first term of (A3):

$$m\omega_{\vec{k}\lambda}^2 \stackrel{k \rightarrow 0}{\approx} 2\pi n e^2 k. \quad (\text{A4})$$

This result is independent of the lattice structure.

Unlike three dimensions this longitudinal mode approaches zero as $k \rightarrow 0$. This feature of the spectrum arises from the fact that the attractive force between two parallel strips, which are oppositely charged and have a fixed charge density per unit area, is proportional to the inverse of the distance between the strips. This is in contrast to the three-dimensional system, where two oppositely

charged plates have a constant attractive force independent of the distance between the plates. In the latter case we have the familiar result:

$$m\omega_{\vec{k}\lambda}^2 \stackrel{k \rightarrow 0}{\approx} 4\pi n e^2. \quad (\text{A5})$$

The frequency of the transverse phonon, on the other hand, is linear in k in this region and dependent weakly on the lattice structure. It is possible to write an explicit formula for the transverse anisotropic velocity, i.e.,

$$\begin{aligned} m\omega_{\vec{k}t}^2 &= n \sum_{\nu \neq 0} [\vec{K}_\nu \cdot \vec{\epsilon}_t(\vec{k})]^2 (v_{\vec{k} + \vec{K}_\nu} - v_{\vec{K}_\nu}) \\ &\stackrel{k \rightarrow 0}{\approx} n\pi e^2 \sum_{\nu \neq 0} \frac{[\vec{K}_\nu \cdot \vec{\epsilon}_t(k)]^2}{K_\nu^3} \left[3(\vec{k} \cdot \vec{K}_\nu)^2 \frac{1}{K_\nu^2} - k^2 \right] \\ &\approx mc^2 k^2. \end{aligned} \quad (\text{A6})$$

We would like to make one additional point regarding the validity of the well-known sum rule for $\omega_{\vec{k}\lambda}$:

$$\sum_{\lambda} \omega_{\vec{k}\lambda}^2 = 4\pi n e^2 / m. \quad (\text{A7})$$

This relation holds only for three-dimensional Coulombic systems. In the present case where a two-dimensional array of electrons interacts via three-dimensional Coulomb forces no such simple sum rule exists. If on the other hand, we had a group of electrons interacting via really two-dimensional Coulomb forces such that $\Delta v(r) = 0$ or, equivalently, $v(k) = 2\pi e^2 / r_0 k^2$, analogous sum rule, i.e.,

$$\sum_{\lambda} \omega_{\vec{k}\lambda}^2 = 2\pi n e^2 / m r_0. \quad (\text{A8})$$

The apparent divergence of the sum over \vec{K}_ν in (A6) comes from the fact that we have added and subtracted the term with $\vec{K}_\nu = 0$ to the summation in (A1) in order to obtain (A2). This is not really legitimate if $v(R)$ is rigorously taken as e^2/R , since its second derivative is highly singular at $R = 0$. To avoid this unphysical complexity we can assume $v(k) = (2\pi e^2/k) e^{-\lambda k^2}$ everywhere in the calculations and then let $\lambda \rightarrow 0$ at the end. This type of procedure leads to the correct physical results.

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- ¹⁹If we neglect fluctuations from plasmons, we obtain $r_s = 5.9$.