Phase diagram of a two-dimensional Wigner crystal in a magnetic field

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The regions of existence of the solid phase of a two-dimensional system of electrons in a magnetic field are ascertained for $T=0$ and for finite temperature values. It is shown that "magnetic" melting of the Wigner lattice is possible. The phase diagram of the system, based on the assumption that the solid phase has a polymicrocrystalline structure, is constructed.

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1. INTRODUCTION

The properties of two-dimensional electron systems—inversion layers in metal-dielectric-semiconductor (MDS) structures and electrons on a liquid-helium surface—are currently being intensively investigated. The most interesting of the questions that have arisen is that of the behavior of the system in the low-density limit (the mean distance r_0 between the particles is much greater than the effective Bohr radius a^*), when we should expect crystallization of the electrons (or holes).[1,2] Important arguments in favor of the reality of a two-dimensional Wigner crystal are the machine experiment of Hockney and Brown[3] and the computer calculations performed by Meissner, Namaizawa and Voss.[4] In Ref. 4, using the example of a metal-SiO_2-Si structure, the energy of the electrons in an inversion channel was calculated and it was shown that a triangular lattice is the most favorable. The square lattice has energy only 0.5% above that of the triangular lattice, but is dynamically unstable: the square of the vibrational frequency of the transverse branch becomes negative near the [10] direction. In the machine experiment of Ref. 3 a system of 10^4 particles moving in one plane and interacting by the Coulomb law was considered. The calculation was performed in the framework of classical machanics: the equations of motion were integrated numerically and then the thermodynamic functions of the system were calculated. It was found that at a sufficiently low temperature the particles are indeed arranged at the sites of a triangular lattice, the whole "sample" being divided into domains differing from each other in the orientation of the lattice axes. With increase of temperature the number of domains increases and their sizes decrease. At a certain temperature T_c (in the conditions of Ref. 3, $T_c=3.1$ K for a particle density of 10^{10} cm^{-2}, and the charge and mass of the particles correspond to those of a free electron), the specific heat of the system passes through a maximum. In the region $T>T_c$ the domains disappear and the arrangement of the particles becomes disordered (the liquid phase). Thus, a Wigner crystal should exist, albeit in polycrystalline form, at perfectly attainable values of the temperature and surface electron density.1) It is therefore of interest to elucidate the form of the phase diagram of such a system, and also its behavior in a magnetic field perpendicular to the plane of the lattice. The present article is devoted to this.

The phase diagram of two-dimensional electron crystal in a magnetic field was discussed in the paper by Lozovik and Yudson,[5] in which the authors confined themselves to the case of absolute-zero temperature and performed the calculation in the framework of the Einstein model of the vibrational spectrum. It turns out that allowance for the true form of the vibrational spectrum of the "magnetized" Wigner crystal in the region of small wave numbers substantially alters the result. In particular, in sufficiently strong fields "magnetic" melting of the electron lattice at a constant temperature, including at $T=0$, turns out to be possible. Increases in the temperature and magnetic-field intensity act in the same direction—the crystalline phase disappears, principally because of the contribution of the transverse branch of the vibrational spectrum to the displacements of the particles from their equilibrium positions. Physically this is easily explained if we note that the vibrational spectrum of the system is degenerate at the point $\mathbf{k}=0$. A magnetic field lifts this degeneracy and, as in the usual "pushing apart" of two close terms, the lower (transverse) branch decreases its frequencies, which favors melting.

2. A WIGNER CRYSTAL IN A MAGNETIC FIELD AT AT $T=0$

The solution of the vibrational problem for a two-dimensional Wigner crystal in a magnetic field perpendicular to the lattice plane (x, y) was obtained earlier.[2] The frequencies $\tilde{\omega}_\parallel$ and $\tilde{\omega}_\perp$ of the longitudinal (plasma) and transverse (shear) branches are expressed in terms of the same quantities in the absence of a magnetic field ($\omega_\parallel$ and $\omega_\perp$) by the formulas

$$\tilde{\omega}_{\parallel,\perp}^2={}^1/_2(\omega_\parallel^2+\omega_\perp^2+\Omega^2)\pm{}^1/_2[(\omega_\parallel^2+\omega_\perp^2+\Omega^2)^2-4\omega_\parallel^2\omega_\perp^2]^{1/2}, \qquad (1)$$

where $\Omega=eH/mc$ is the cyclotron frequency. In the region of small wave numbers ($kr_0\ll 1$) the following dependences2) are valid for the quantities $\omega_\parallel$ and $\omega_\perp$:

$$\omega_\parallel^2=\frac{4\pi e^2N_s k}{m(\varepsilon_1+\varepsilon_2\operatorname{cth}kD)},\qquad \omega_\perp^2=s_{ij}^2k_ik_j,\qquad i,j=x,y. \qquad (2)$$

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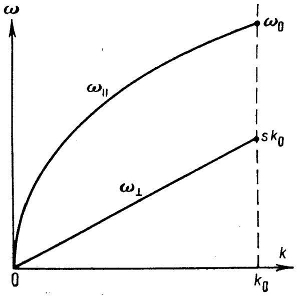

FIG. 1.

Here $N_s = r_0^{-2}$ is the density of the surface electrons, ε_1 and ε_2 are the dielectric constants of the semiconductor and dielectric, respectively, and D is the thickness of the dielectric (the distance to the metallic electrode, in the case of electrons on liquid helium). The transverse-sound velocity s is of the order of $(e^2/(\varepsilon_1+\varepsilon_2)mr_0)^{1/2}$. Numerical calculations of the dependences $\omega_{\parallel}(k)$ and $\omega_{\perp}(k)$ for the two characteristic directions Λ and Δ in the planar hexagonal Brillouin zone are given in Ref. 4.

Our aim is to ascertain those regions of values of the density, magnetic field and temperature for which the electron crystal is stable. We shall use the Lindemann melting criterion, i.e., we shall find the ratio $\langle u^2\rangle/r_0^2 \equiv \gamma$, where u is the displacement of a particle from the equilibrium position and the angular brackets denote thermodynamic averaging. When γ is smaller than a certain critical value γ_c the crystalline lattice is stable, the melting occurs for $\gamma > \gamma_c$. We have the following expression for the Lindemann parameter (cf., e.g., Ref. 6):

$$\gamma(T,H)=\frac{\hbar}{4\pi^2 m}\sum_{\lambda}\int\left[n(\tilde{\omega}_\lambda)+\frac{1}{2}\right]\frac{d\mathbf{k}}{\tilde{\omega}_\lambda(\mathbf{k})}, \qquad (3)$$

where the n are Bose occupation numbers and λ labels the branches of the vibrational spectrum, i.e., $\tilde{\omega}_\lambda = \tilde{\omega}_{\parallel}$, $\tilde{\omega}_{\perp}$.

We now consider the isotropic model, in which $\omega_{\perp} = sk$ and $\omega_{\parallel}$ is determined by the first of the formulas (2) for all k from zero to a limiting value k_0, which is chosen in such a way that the correct number of degrees of freedom is obtained: $k_0 \equiv 2(\pi N_s)^{1/2} = 2\pi^{1/2}/r_0$. Then, from (3) for $T=0$, $\Omega=0$, it is easy to obtain

$$\gamma(0,0)\equiv\gamma_0=\frac{1}{3\pi^{3/4}}\sqrt{\frac{a^*}{r_0}}+\frac{\hbar k_0}{4\pi ms}\sim\sqrt{\frac{a^*}{r_0}}, \quad \text{if} \quad D\gg r_0, \qquad (4a)$$

$$\gamma_0=\frac{1}{4\pi}\sqrt{\frac{a^*}{D}}, \quad \text{if} \quad D\ll r_0, \qquad (4b)$$

In the low-density limiting case considered here, the condition $r_0 \gg a^*$ should be fulfilled. If it is compatible with the condition (4a), for which we should have $D \gg a^*$, then $\gamma(0,0) \ll 1$ and decreases with decrease of the particle density. Thus, the lattice is stable for sufficiently large r_0 ($r_0 > r_c$, $r_c \sim a^*/\gamma_c^2$). However, for $r_0 > D$ screening of the electron-electron interaction by the electrostatic-image potential (the term with $\coth kD$ in formula (2)) becomes important. In this case γ_0 ceases to depend on the particle density (the case (4b)). The existence of the electron system in the liquid or crystalline phase is then determined entirely by the quantity D: the crystal is stable if $D > a^*/16\pi^2\gamma_c^2$. In all cases of practical interest this condition is amply fulfilled; therefore, we shall assume below that $D \gg r_0$. Then, in the isotropic model, $\omega_{\parallel} = (\alpha k)^{1/2}$, where $\alpha = 4\pi e^2 N_s/m(\varepsilon_1+\varepsilon_2) \sim s^2 k_0$: The vibrational spectrum of the model under consideration is depicted in Fig. 1.

Substituting $\omega_{\parallel}$ and $\omega_{\perp}$ into (1) and then integrating in formula (3), in which it is necessary to put $n=0$, we find $\gamma(0,H)$ in two limiting cases.

A weak magnetic field, $\Omega \ll \omega_0 \equiv (\alpha k_0)^{1/2}$, $\omega_0 \sim (e^2/mr_0^3)^{1/2}$:

$$\gamma(0,H)=\gamma_0+\frac{\hbar k_0\Omega^2}{4\pi ms\omega_0^2}\left[\ln\frac{2\omega_0^2}{\Omega(\omega_0+sk_0)}+\frac{1}{2}\right]. \qquad (5a)$$

A strong magnetic field, $\Omega \gg \omega_0$:

$$\gamma(0,H)=\frac{\hbar k_0\Omega}{2\pi ms\omega_0}\sim\gamma_0\frac{\Omega}{\omega_0}. \qquad (5b)$$

Here γ_0 is defined by formula (4a), so that $\hbar k_0/2\pi ms$ and γ_0 are quantities of the same order. The magnetic correction to $\gamma(0,H)$ from (5a) contains contributions from the longitudinal and transverse branch. These contributions are of the same order of magnitude and opposite in sign, but the resultant effect is such that $\gamma(0,H)$ grows with increase of H. As regards the case of (5b), here the principal role is played by the transverse branch, while the longitudinal branch gives a small contribution of the order of $\gamma_0\omega_0/\Omega$. Thus, increase of $\gamma(0,H)$ with magnetic field occurs for any value of ω_0, i.e., for any particle density.

When $H = H_c$ (the value such that $\gamma(0', H_c) = \gamma_c$), magnetic melting of the Wigner crystal should occur. The melting curve $\gamma(0,H) = \gamma_c$ is depicted schematically in the variables Ω, r_0 in Fig. 2; the shaded region corresponds to the crystalline phase. Near r_c the form of the curve is determined by formula (5a):

$$\Omega\propto\left(\frac{r_0-r_c}{\ln(r_0-r_c)}\right)^{1/2}.$$

The asymptotic form for $r_0 \gg r_c$ follows from (5b): $\Omega \propto r_0^{-1}$.

It is interesting that there exists a certain optimal value of the density (of order r_c^{-2}) for which the magnetic field that destroys the lattice is a maximum. At the point of the maximum $\Omega(r_m) \sim \omega_0$, which gives the estimate $\Omega_{\max} \sim me^4\gamma_c^3/\bar{\varepsilon}^2\hbar^3$, where $\bar{\varepsilon} \equiv \frac{1}{2}(\varepsilon_1+\varepsilon_2)$. For most solids the value of γ_c is close to 6×10^{-2} (see below), so that the limiting magnetic field is of the order of 10^5 Oe

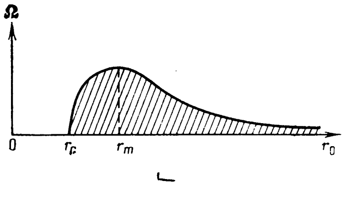

FIG. 2.

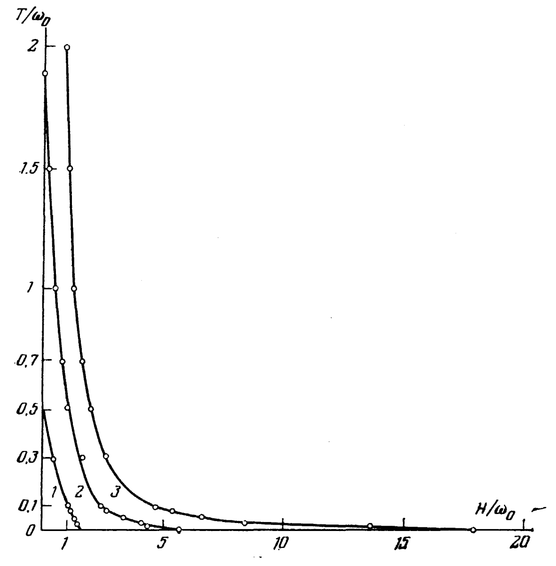

FIG. 3. Melting curves ($sk_0 = 0.5\omega_0$, $\bar{\varepsilon} = 1$, $m = m_e$): 1) for $N_s = 10^{12}$ cm^{-2}, 2) for $N_s = 10^{10}$ cm^{-2}, 3) for $N_s = 10^8$ cm^{-2}.

in the case of electrons on liquid helium and $10^2 - 10^3$ Oe for the inversion layers of semiconductors ($\bar{\varepsilon} \sim 10$, $m \sim (0.1 - 1)\, m_e$).

3. FINITE VALUES OF THE TEMPERATURE

For $T \neq 0$ the integral in (3) corresponding to the transverse branch diverges at the lower limit-logarithmically for $H = 0$ and like $\int dk/k^2$ for finite H. The point is that at small momenta $\tilde{\omega}_\perp(k)$ behaves like $\alpha^{1/2} s k^{3/2}/\Omega$. Thus, a two-dimensional electron lattice of arbitrarily large size cannot exist. We shall associate this circumstance with the fact, established in Ref. 3, that the sample breaks up into crystallites (in conditions of thermodynamic equilibrium!) whose sizes decrease as the temperature is raised. We shall assume that the lower limit $k_{\min}$ of the divergent integrals is determined by the mean size $L = 2\pi/k_{\min}$ of the monocrystalline domains that exist for the given T and H. In other words, the dependence of L and T and H is determined from the equation $\gamma(T, H, L) = \gamma_c$. In order to check this statement we shall make use of the results of the calculation in Ref. 3, in which the pair correlation function was calculated for nine different temperature values (in the absence of a magnetic field). The value of ω_0 corresponding to the density 10^{10} cm^{-2} is 2.4 $\times 10^{12}$ sec^{-1}, i.e., the Debye temperature $\Theta \approx 17$ K. Inasmuch as the melting temperature $T_c = 3.1$ K found in Ref. 3. is appreciably below Θ, we must make use of the low-temperature limit in formula (3):

$$\gamma(T,0) = \gamma_0 + \frac{T}{2\pi m s^2} \ln\left(\frac{LT}{2\pi\hbar s}\right) \quad (T \ll \Theta), \qquad (6)$$

$$L(T) = (2\pi\hbar s/T) \exp\{2\pi m s^2 (\gamma_c - \gamma_0)/T\}.$$

Below we give the values of the correlation length $N = L/r_0$, calculated from the equation $\gamma(T, 0) = \gamma_c$ with $\gamma(T, 0)$ from (6):

T, K:	0.16	0.65	1.9	2.81	3.3	3.61	4.46	6.29	8.91
$N = (7/T)e^{4/T}$:	$5\cdot10^{12}$	$4\cdot10^3$	31.7	10.4	7.1	5.9	3.9	2.1	1.2
$N_{\exp}$:	>100	>100	30	12	6	4	4	3	2

The corresponding values of $N_{\exp}$, borrowed from Ref. 3, are given in the last line. The adjustable parameters are the averaged transverse-sound velocity s and the difference $\gamma_c - \gamma_0$. The values of N given above were obtained for $s = 1.5\times10^6$ cm/sec and $\gamma_c - \gamma_0 = 4\times10^{-2}$. Knowing s we can find $\gamma_0 = 2\times10^{-2}$, whence $\gamma_c = 0.06$. The latter number is extremely close to the Lindemann parameter of other solids. For example, for Na we have $\gamma_c = \frac{1}{16}$ (cf. Ref. 6), and for solid He^4, by Abrikosov's estimate,[7], $\gamma_c = 5.65\times10^{-2}$. The quantity s is also in fair agreement with the caluulations of Ref. 4: $s(\Lambda) = 1.78\times10^6$ cm/sec, $s(\Delta) = 1.85\times10^6$ sm/sec. Thus, making allowance for the crudity of the isotropic model used here, the agreement between formulas (6) and the machine experiment might be considered satisfactory. It must be remembered, however, that the results of Hockney and Brown[3] were obtained in the framework of classical mechanics, while the formulas (6) pertain to the region $T \ll \Theta$, where quantum effects play an essential role.

We shall assume, further, that melting in the presence of a magnetic field occurs at those values of H, T and r_0 at which the crystallite size reaches the critical value L_c, i.e., $\gamma(T, H; L_c) = \gamma_c$. From the data of Ref. 3, $L_c \approx 9r_0$. We shall consider only the low-temperature limit $T \ll \hbar\omega_0$. Different relations between T and the magnetic energy $\hbar\Omega$ are possible. We write out the quantities $N = L/r_0$ in several characteristic regions (we put $\hbar = 1$):

$$N = \frac{2\sqrt{\pi}\,\omega_0 s k_0}{\Omega T}\left[\frac{\gamma_c}{\gamma(0,H)} - 1\right], \quad T \ll \omega_0 \ll \Omega, \quad 4\Omega T \ll \omega_0^2; \qquad (7a)$$

$$N = 2\pi\gamma_c \omega_0^2 m s^2/\Omega^2 T, \quad T \ll \omega_0 \ll \Omega, \quad 4\Omega T \gg \omega_0^2. \qquad (7b)$$

The case (7b) can be realized only if, besides the conditon $4\Omega T \gg \omega_0^2$, the condition $2\pi m s^2 \gg \Omega$ is also fulfilled. In principle this is possible, since $ms^2/\omega_0 \sim (r_0/a^*)^{1/2} \gg 1$. In the region $T \ll \Omega \ll \omega_0$,

$$N = 2\pi[\gamma_c - \gamma(0, H)]\, m s^2 \omega_0^2/\Omega^2 T. \qquad (8)$$

In the region $\Omega \ll T \ll \omega_0$,

$$N = 2\pi\gamma_c m s^2 \omega_0^2/\Omega^2 T. \qquad (9)$$

The melting curve in the (T, H) plane (for a given density) is determined by the relations (7)–(9) from the formula $Nr_0 = L_c$. The values of $\gamma(T, H)$ were calculated (in the isotropic model) at 250 points in the plane of the dimensionless variables $(T/\omega_0, H/\omega_0)$. The curves $\gamma(T, H; L_c) = \gamma_c$ are given in Fig. 3; the particle density $N_s = r_0^{-2}$ is the parameter of the curves. The region bounded by a curve and the coordinate axes corresponds to the polycrystalline phase.

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APPENDIX

We shall confine ourselves for simplicity to an idealized model in which the dielectric constants have the same value ε on both sides of the plane ($z=0$) of the electron lattice. In the long-wavelength limit of interest to us, the transverse vibrations can be described by the equations of motion of a continuous medium:

$$\ddot{\mathbf{u}}-s^2\Delta\mathbf{u}=e\mathbf{E}/\varepsilon m. \tag{A.1}$$

In the equation for the electric field $\ddot{\mathbf{E}}$ we take into account that the volume density of the current of electrons is equal to $e\dot{\mathbf{u}}N_s\delta(z)$[3]:

$$\Delta\mathbf{E}-\frac{\varepsilon}{c^2}\ddot{\mathbf{E}}=\frac{4\pi eN_s}{c^2}\delta(z)\ddot{\mathbf{u}}. \tag{A.2}$$

As will be clear from the result, the region of wave vectors in which the interaction manifest themselves through the transverse fields correspond to such small frequencies that we can take the static value for ε in (A.1) and (A.2).

The vectors $\mathbf{u}$ and $\mathbf{E}$ lie in the (x, y) plane. The solution, in the form of a plane wave, is

$$\mathbf{u}(\mathbf{r},\ t)=\mathbf{u}_0e^{i(\mathbf{kr}-\omega t)},\quad \mathbf{E}(\mathbf{r},\ t)=\mathbf{E}_0e^{i(\mathbf{kr}-\omega t)}e^{-\beta|z|}\ . \tag{A.3}$$

The singular factor in the expression for $\mathbf{E}(r, t)$ appears because of the need to compensate the term with the δ-function in (A.2).

We substitute (A.3) into (A.1) and (A.2) and separately equate the singular and regular terms. This gives first, a determination of the parameter β:

$$\beta^2=k^2-\omega^2\varepsilon/c^2,$$

and second, the dispersion equation:

$$(s^2k^2-\omega^2)\left(k^2-\frac{\varepsilon\omega^2}{c^2}\right)^{1/2}=\frac{2\pi N_se^2\omega^2}{\varepsilon mc^2}\equiv\alpha\frac{\omega^2}{c^2},\quad \alpha\sim s^2k_0. \tag{A.4}$$

Investigation of Eq. (A.4) leads to the following results: for $k \gg s^2k_0/c^2$ the dependence $\omega(k)$ remains as before: $\omega=sk$; for $k \ll s^2k_0/c^2$ we obtain $\omega(k)=sc\alpha^{-1/2}k^{3/2} \sim ck(k/k_0)^{1/2}$.

Thus, the retarded interaction is important only in the region of wave vectors $k/k_0 \lesssim s^2/c^2 \sim 0.3\times10^{-9} - 0.3\times10^{-7}$ in the range of values of N_s from 10^8 to 10^{12} cm^{-2}. In this case the speed of light appears explicitly in the dispersion law. The corresponding wavelengths (from 3×10^5 to 30 cm) are much greater than the linear dimensions ($L \sim 0.1-1$ cm) of real quasi-two-dimensional electron systems, both in the case of MDS structures and for electrons on liquid helium. Therefore, the spectrum of values of k always has a lower cutoff ($k \gtrsim 1/L$) far outside the limits of the region discussed here.

[1] The breakup of the sample into crystallites is, possibly, the process by which the fact that the crystalline phase is energetically favored is reconciled in the system with the impossibility of the existence of long-range order in the two-dimensional case for infinite sample sizes.

[2] These formulas were obtained in Ref. 2 under the assumption that the electron-electron interaction is instantaneous and corresponds to the Coulomb law. There is also the retarded interaction via the transverse fields that arise from the electron-lattice vibrations. The effect of these fields on the shear branch (the most important branch in the problem in the stability of the crystalline phase) is treated in the Appendix. It is found to be negligibly small.

[3] The corresponding three-dimensional problem is solved in Ref. 8.

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