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

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(Submitted 13 July 1978)
Zh. Eksp. Teor. Fiz. 76, 288–294 (January 1979)

The quantum problem of a two-dimensional electron crystal in a magnetic field is solved completely. The phase diagram of the system at $T = 0$ and at finite temperatures is constructed. It is found that the magnetic field reduces the amplitude of the zero-point vibrations of the lattice and thus increases the stability of the lattice. The maximal melting temperature of the lattice increases with increase of the magnetic field.

PACS numbers: 63.70. + h

1. INTRODUCTION

Recently, two-dimensional electron systems (inversion layers in semiconductor surfaces, size-quantized semiconducting films, electrons on the surface of liquid helium) have been intensively studied.[1] In these systems the motion of the electrons is quantized in one direction and free in the other two. It is especially interesting to elucidate the properties of two-dimensional electron systems in a perpendicular magnetic field. As is well known,[2] a strong magnetic field quantizes the transverse motion of the electrons, so that the energy spectrum of noninteracting electrons consists of discrete, infinitely degenerate Landau levels. The Coulomb electron-electron interaction lifts this degeneracy and, as shown below, leads in the limit of a strong magnetic field to the formation of a two-dimensional electron lattice (TEL), analogous to a Wigner lattice. We emphasize that, unlike a Wigner lattice, which is realized at low surface electron densities n_s, in a magnetic field a TEL arises for any initial electron density, as soon as the quantum Larmor radius $\lambda = (c\hbar/eB)^{1/2}$ of an electron in the magnetic field becomes appreciably smaller than the average electron-electron spacing r_0.

A TEL in a magnetic field has been considered in a number of recent papers. The vibrational frequencies of a TEL in a magnetic field were first determined by Chaplik[3] from the classical equations of motion. A quantum approach to the problem was developed by Fukuyama,[4] who found that the excitation energies of the system are proportional to the frequencies determined by Chaplik. As can be seen from what follows, to elucidate the form of the phase diagram of the system knowledge of the energy spectrum is not sufficient; it is also necessary to find the wavefunctions, which were not determined by Fukuyama.[4]

The phase diagram of a TEL in a magnetic field was first discussed in a paper by Lozovik and Yudson[5]; however, the authors confined themselves to the case of absolute zero temperature and did not take into account, even qualitatively, the low-frequency branch of the energy spectrum. In a paper by Chaplik[6] an attempt was made to construct the phase diagram of the system with allowance for the true form of the spectrum of the magnetized TEL. But since the mean square displacement of the lattice sites was calculated without taking the results of the solution of the quantum problem into account, a large part of the author's statements turn out to be erroneous.

Below we give a complete solution of the quantum problem of a TEL in a magnetic field. The phase diagram of the system is constructed for $T=0$ and for finite temperatures. It is found that the magnetic field reduces the amplitude of the zero-point vibrations of the lattice, and thus increases the stability of the TEL. The maximal melting temperature of the TEL increases with increase of the magnetic field.

Several cases must be distinguished. If the two-dimensional electron density in the system is such that a two-dimensional Wigner lattice exists in zero magnetic field,[7] it remains stable in any magnetic field and the melting temperature increases with increase of the field. But if the lattice does not exist in zero magnetic field, it can be realized when, at the least, the value of the magnetic field is greater than that at which all the electrons are in the lowest Landau level, and the average electron-electron spacing $r_0 \gg \lambda$. In the case $r_0 \lesssim \lambda$, to all appearances the lattice does not exist. Moreover, it seems highly likely that a TEL is formed by the electrons belonging to the last of the Landau levels occupied at $T=0$, in the case when the average spacing between them is appreciably greater than the corresponding Larmor radius.

2. THE QUANTUM PROBLEM OF A TEL IN A MAGNETIC FIELD

Suppose that we have a two-dimensional electron system with average spacing r_0 between the electrons. We take the perpendicular magnetic field to be so large that $\lambda \ll r_0$. It is natural to assume that in this case at $T=0$ the ground state of the system is a lattice. It will be shown below that the mean square displacement $\langle u^2\rangle$ of an electron from its lattice site is $\sim\lambda^2$, so that our assumption is justified.

Let R_i be the sites of a two-dimensional triangular lattice, and u_i the displacement of the electrons from the sites. Then, omitting the constant terms, we write the Hamiltonian of the system in the harmonic approximation[4]:

$$\hat{H}=\frac{1}{2\mu}\sum_{i,\alpha}\hat{\Pi}_{i\alpha}^2+\frac{1}{2}\sum_{i,j,\alpha,\beta}G_{ij}^{\alpha\beta}\hat{u}_{i\alpha}\hat{u}_{j\beta}. \quad (1)$$

Here the operator $\hat{\Pi}_{i\alpha}=\hat{P}_{i\alpha}+eA_\alpha(\mathbf{r}_i)/c$, where $\mathbf{A}$ is the vector potential of the external magnetic field $\mathbf{B}$, and the dynamical tensor $G_{ij}^{\alpha\beta}$ has the form

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$$G_{ij}^{\alpha\beta}=\begin{cases}-\left[\dfrac{\partial^2}{\partial r_\alpha\,\partial r_\beta}\dfrac{e^2}{r}\right]_{R_{ij}}, & i\neq j,\\ \sum\limits_{k\neq i}\left[\dfrac{\partial^2}{\partial r_\alpha\,\partial r_\beta}\dfrac{e^2}{r}\right]_{R_{ik}}, & i=j,\end{cases} \tag{2}$$

where $R_{ik}=|\mathbf{R}_i-\mathbf{R}_k|$. The operators $\hat{\Pi}_{i\alpha}$ and $\hat{u}_{j\beta}$ satisfy the commutation relations

$$[\hat{\Pi}_{i\alpha},\hat{\Pi}_{j\beta}]=-i\frac{\hbar^2}{\lambda^2}\delta_{ij}\varepsilon_{\alpha\beta},\quad [\hat{\Pi}_{i\alpha},\hat{u}_{j\beta}]=-i\hbar\delta_{ij}\delta_{\alpha\beta},\quad [\hat{u}_{i\alpha},\hat{u}_{j\beta}]=0, \tag{3}$$

where

$$\varepsilon_{\alpha\beta}=\begin{cases}1, & \alpha=x,\ \beta=y\\ -1, & \alpha=y,\ \beta=x\\ 0, & \alpha=\beta.\end{cases}$$

Unlike Fukuyama,[4] we introduce the following canonical transformation of the operators:

$$\hat{u}_{i\alpha}=\left(\frac{2}{N}\right)^{1/2}\sum_{k>0}\{\hat{x}_{\mathbf{k}}^{\alpha}\cos\mathbf{kR}_i+\hat{x}_{-\mathbf{k}}^{\alpha}\sin\mathbf{kR}_i\},$$
$$\hat{\Pi}_{i\alpha}=\left(\frac{2}{N}\right)^{1/2}\sum_{k>0}\{\hat{\Pi}_{\mathbf{k}}^{\alpha}\cos\mathbf{kR}_i+\hat{\Pi}_{-\mathbf{k}}^{\alpha}\sin\mathbf{kR}_i\}. \tag{4}$$

Here $k>0$ denotes the sum over half the states of the two-dimensional Brillouin zone of the reciprocal lattice. The operators $\hat{\Pi}_{\mathbf{k}}^{\alpha}$ and $\hat{x}_{\mathbf{k}}^{\alpha}$ are Hermitian and, as is easily verified, satisfy the same commutation rules (3), with the replacement $i\to\mathbf{k}$, $j\to\mathbf{k}'$.

The Hamiltonian (1) written in terms of the operators (4) is a sum of independent Hamiltonians:

$$\hat{H}=\sum_{\mathbf{k}}\hat{H}_{\mathbf{k}},\quad H_{\mathbf{k}}=\frac{1}{2u}\sum_{\alpha}(\Pi_{\mathbf{k}}^{\alpha})^2+\frac{1}{2}\sum_{\alpha,\beta}G^{\alpha\beta}(\mathbf{k})\hat{x}_{\mathbf{k}}^{\alpha}\hat{x}_{\mathbf{k}}^{\beta},$$
$$G^{\alpha\beta}(\mathbf{k})=\sum_j G_{ij}^{\alpha\beta}\exp[-i\mathbf{k}(\mathbf{R}_i-\mathbf{R}_j)]. \tag{5}$$

Our next problem will be to determine the energy eigenvalues and wave functions of a Hamiltonian of the type (5), and we shall not write out the index **k** explicitly.

The commutation relations (3) show that (5) is the Hamiltonian of a "particle" in a constant magnetic field and in a certain force field with tensor $G^{\alpha\beta}$. Since the operators $\hat{\Pi}_{\mathbf{k}}^{\alpha}$ and $\hat{x}_{\mathbf{k}}^{\alpha}$ are Hermitian, the commutation rules can be satisfied when we go over to the coordinate representation

$$\hat{x}_{\mathbf{k}}^{\alpha}=x^{\alpha},\quad \hat{\Pi}_{\mathbf{k}}^{\alpha}=-i\hbar\frac{\partial}{\partial x_\alpha}+\frac{e}{c}A_\alpha, \tag{6}$$

where curl $\mathbf{A}=\mathbf{B}$ (the specified external magnetic field).

Rotating the coordinate axes through the angle

$$\gamma_{\mathbf{k}}=\frac{G^{yy}(\mathbf{k})-G^{xx}(\mathbf{k})}{2G^{xy}(\mathbf{k})} \tag{7}$$

and putting

$$\mu\omega_1^2=G^{xx}\cos^2\gamma+G^{yy}\sin^2\gamma+2G^{xy}\sin\gamma\cos\gamma,$$
$$\mu\omega_2^2=G^{xx}\sin^2\gamma+G^{yy}\cos^2\gamma-2G^{xy}\sin\gamma\cos\gamma, \tag{8}$$

we bring the Hamiltonian to the form

$$\hat{H}=\frac{1}{2\mu}\left(\hat{\mathbf{P}}+\frac{e}{c}\mathbf{A}\right)^2+\frac{1}{2}\mu\omega_1^2x^2+\frac{1}{2}\mu\omega_2^2y^2. \tag{9}$$

In the case when a Wigner lattice exists in the absence of a magnetic field, the frequencies $\omega_1(\mathbf{k})$ and $\omega_2(\mathbf{k})$ obviously coincide with the frequencies of the longitudinal and transverse vibrations of a two-dimensional Wigner crystal, as determined in Refs. 3 and 7. But if there is no Wigner lattice in the absence of a magnetic field, we can still introduce the frequencies ω_1 and ω_2 by the formulas (5), (7), and (8). We assume that the potential energy of the system has a minimum for all values of the concentration; therefore, the corresponding quadratic form in the normal coordinates (4) should be positive-definite, so that only as a result of large zero-point vibrations might the lattice not exist.

The Hamiltonian (9) is a particular case of a Hamiltonian quadratic in the operators of the momenta and coordinates. The general method of diagonalization of this type of Hamiltonian is based on the following property. Since all the commutators of operators forming the Hamiltonian are c-numbers, it is easy to show that the result of the commutation of an arbitrary linear combination of momentum and coordinate operators with a quadratic Hamiltonian will again be a certain linear combination of these operators. This makes it possible, when solving the corresponding simple problem for the eigenvalues, to construct a system of lowering and raising operators for the given Hamiltonian.

Choosing henceforth the Landau gauge $\mathbf{A}=(0, Bx, 0)$, in our case we easily find that

$$[\hat{H},\hat{a}^+]=\hbar\omega_+\hat{a}^+,\quad [\hat{H},\hat{b}^+]=\hbar\omega_-\hat{b}^+, \tag{10}$$

where

$$\omega_\pm=\frac{1}{2}\{\omega_c^2+\omega_1^2+\omega_2^2\pm[(\omega_c^2+\omega_1^2+\omega_2^2)^2-4\omega_1^2\omega_2^2]^{1/2}\}^{1/2}$$

are the frequencies determined by Chaplik[3] (ω_c is the cyclotron frequency).

The operators $\hat{a}$ and $\hat{b}$ have the form

$$\hat{a}=(2\mu\hbar\omega_+)^{-1/2}\{\hat{p}_x\cos\alpha+\mu\omega_2\hat{y}\sin\alpha-i\mu\omega_+\hat{x}\cos\alpha+i(\omega_+/\omega_2)\hat{p}_y\sin\alpha\},$$
$$\hat{b}=(2\mu\hbar\omega_-)^{-1/2}\{-\hat{p}_x\sin\alpha+\mu\omega_2\hat{y}\cos\alpha+i\mu\omega_-\hat{x}\sin\alpha+i(\omega_-/\omega_2)\hat{p}_y\cos\alpha\}. \tag{11}$$

Here,

$$\mathrm{tg}\,2\alpha=-\frac{2\omega_c\omega_2}{\omega_c^2+\omega_1^2-\omega_2^2}.$$

It is easy to verify that the following commutation relations are fulfilled:

$$[\hat{a},\hat{a}^+]=1,\quad [\hat{b},\hat{b}^+]=1,\quad [\hat{a},\hat{b}]=0,\quad [\hat{a}^+,\hat{b}]=0, \tag{12}$$

and the Hamiltonian (9) can be represented in the form

$$\hat{H}=\hbar\omega_+(\hat{a}^+\hat{a}+1/2)+\hbar\omega_-(\hat{b}^+\hat{b}+1/2). \tag{13}$$

Obviously, therefore, the energy eigenvalues of the Hamiltonian (9) are

$$E(n_1,n_2)=(n_1+1/2)\hbar\omega_++(n_2+1/2)\hbar\omega_-, \tag{14}$$

and the wave functions are equal to

$$|n_1,n_2\rangle=(\hat{a}^+)^{n_1}(\hat{b}^+)^{n_2}|0\rangle. \tag{15}$$

Here $|0\rangle$ is the ground-state wave function, which is easily determined from the condition

$$\hat{a}|0\rangle=\hat{b}|0\rangle=0.$$

It has the following form:

$$|0\rangle=(2/\pi)^{1/2}(\alpha\beta)^{1/4}\exp\left(\alpha x^2+\beta y^2+i\gamma xy\right), \tag{16}$$

where

$$\alpha=-\frac{\mu\omega_1(\omega_++\omega_-)}{2\hbar(\omega_1+\omega_2)},\quad \beta=-\frac{\mu\omega_2(\omega_++\omega_-)}{2\hbar(\omega_1+\omega_2)},\quad \gamma=-\frac{\mu\omega_c\omega_2}{\hbar(\omega_1+\omega_2)}.$$

It can be seen clearly from (14)–(16) that, despite the equal-spacing character of the spectrum, the wave functions of the Hamiltonian (9) are not products of wave functions of harmonic oscillators with frequencies ω_+ and ω_-, as was assumed implicitly in Ref. 6.

We note also that if one of the frequencies $\omega_\pm$ vanishes (e.g., $\omega_-=0$ when ω_1 or $\omega_2=0$), this simply means that the corresponding raising operator and the Hamiltonian have common eigenfunctions. In this case the variables in the Schrödinger equation can usually be separated, and its solution is most simply found directly.

In discussing the phase diagram of the system we need to know the expectation value of the square of the position vector of the particle in the wave functions (15). Expressing r^2 in terms of the operators (11), it is easily found that

$$\langle n_1,n_2|r^2|n_2,n_1\rangle=\left(n_2+\frac{1}{2}\right)\frac{\hbar}{\mu}\frac{t-\omega_c^2}{\omega_-t}+\left(n_1+\frac{1}{2}\right)\frac{\hbar}{\mu}\frac{t+\omega_c^2}{\omega_+t}, \tag{17}$$

where

$$t=[(\omega_c^2+\omega_1^2+\omega_2^2)^2-4\omega_1^2\omega_2^2]^{1/2}.$$

3. THE PHASE DIAGRAM OF THE SYSTEM AT $T=0$

To construct the phase diagram one usually analyzes the Lindemann constant $\gamma=\langle u^2\rangle/r_0^2$, where u is the displacement of a particle from its equilibrium position; the angular brackets denote thermodynamic averaging. For γ less than a certain critical value γ_c a crystal lattice exists: for $\gamma>\gamma_c$ melting occurs. Thus, it is necessary to calculate $\langle\Sigma_\alpha(u_i^\alpha)^2\rangle$. Since the rotation transformation (7) leaves the quantity $\Sigma_\alpha(x_\mathbf{k}^\alpha)^2$ invariant, using (4) and (17) we find that

$$\left\langle\sum_\alpha(u_i^\alpha)^2\right\rangle=\frac{1}{N}\sum_\mathbf{k}\left\langle\sum_\alpha(x_\mathbf{k}^\alpha)^2\right\rangle$$

$$=\frac{\hbar}{N\mu}\sum_\mathbf{k}\left\{\left(\bar n_1(\mathbf{k})+\frac{1}{2}\right)\frac{t+\omega_c^2}{\omega_+t}+\left(\bar n_2(\mathbf{k})+\frac{1}{2}\right)\frac{t-\omega_c^2}{\omega_-t}\right\}, \tag{18}$$

where $\bar n_{1,2}(\mathbf{k})$ are the corresponding Bose occupation numbers.

The formula (18) generalizes the well known expression for the Lindemann parameter[8] to the case of nonzero magnetic fields. In the limit when $\omega_c\to0$, it takes the usual form.[8]

For $T=0$, from (18) we find an expression for the mean square amplitude of the zero-point vibrations of the TEL:

$$\left\langle\sum_\alpha(u_i^\alpha)^2\right\rangle\Big|_{T=0}=\frac{\hbar}{2\mu N}\sum_\mathbf{k}\frac{(\omega_1+\omega_2)^2}{\omega_1\omega_2}\frac{1}{[\omega_c^2+(\omega_1+\omega_2)^2]^{1/2}}. \tag{19}$$

We have made use of the identity $\omega_+\omega_-=\omega_1\omega_2$, and have put $\bar n_1=\bar n_2=0$. It can be seen from (19) that a magnetic field always reduces the amplitude of the zero-point

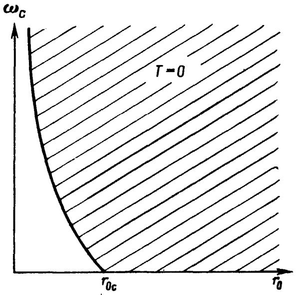

FIG. 1.

vibrations of the lattice. In the limit of a strong magnetic field $[\omega_c\gg\omega_0\sim(e^2/\mu r_0^3)^{1/2}$, where the frequency ω_0 plays the role of the Debye frequency], from (19) we find

$$\left\langle\sum_\alpha(u_i^\alpha)^2\right\rangle\approx\frac{\lambda^2}{N}\sum_\mathbf{k}\left\{1+\frac{1}{2}\left[\frac{\omega_1}{\omega_2}+\frac{\omega_2}{\omega_1}\right]\right\}. \tag{20}$$

In the isotropic model used by Chaplik,[6] we have $\omega_1(\mathbf{k})=sk$ for the transverse mode and $\omega_2(\mathbf{k})=(\alpha k)^{1/2}$ for the longitudinal mode. Here, $\alpha=4\pi e^2n_s/\mu\varepsilon\approx s^2k_0$, where $k_0=2(\pi n_s)^{1/2}$ is the Debye wave number, chosen in such a way that the correct number of degrees of freedom is obtained. Using these approximations we see that the integral (2) converges, and

$$\left\langle\sum_\alpha(u_i^\alpha)^2\right\rangle\approx2\lambda^2.$$

The phase diagram of the system at $T=0$ is depicted schematically in Fig. 1; the shaded region corresponds to the crystalline phase.

Thus, the amplitude of the zero-point vibrations is $\sim\lambda$ and decreases with increase of the magnetic field. Consequently, for any initial surface electron density there exists a magnetic field that crystallizes the electrons into a lattice. The assumption of the existence of a lattice in a strong magnetic field, which was postulated as the basis of our analysis, is thereby justified.

The erroneous conclusion reached in Ref. 6, concerning the cold melting of a TEL in a strong magnetic field, arose, as we see, because the author calculated the amplitude of the zero-point vibrations from the usual formulas for phonons ($\langle r^2\rangle=\hbar/\mu\omega_-$); from this he obtained (we reall that $\omega_-=\omega_1\omega_2/\omega_c$) the result that $\langle r^2\rangle\sim\omega_c$ and increases with increase of the field.

4. FINITE TEMPERATURES

We shall carry out the calculations for the most interesting case of a strong magnetic field ($\omega_c\gg\omega_0$) and not-too-high temperatures, when we may assume that the oscillators of the branch ω_+ are in the ground state. Then, from (18) we find

$$\left\langle\sum_\alpha(u_i^\alpha)^2\right\rangle=\left\langle\sum_\alpha(u_i^\alpha)^2\right\rangle\Big|_{T=0}+\frac{\hbar}{N\mu}\sum_\mathbf{k}\bar n_2(\mathbf{k})\frac{t-\omega_c^2}{\omega_-t}. \tag{21}$$

In a strong field, for the branch ω_- we have $\omega_-\approx\omega_1\omega_2/\omega_c$; therefore, for not-too-low temperatures, $\hbar\omega_-\lesssim T$, so that for the average number of quanta we obtain $\bar n_2(\mathbf{k})\approx T/\hbar\omega_-$. On the other hand, under the condition $\omega_c\gg\omega_0$ it is easy to find that

$$\frac{t-\omega_c^2}{\omega_-t}\approx\frac{1}{\omega_c}\left(\frac{\omega_1}{\omega_2}+\frac{\omega_2}{\omega_1}\right).$$

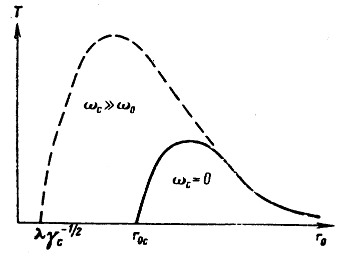

FIG. 2.

Thus, the mean square displacement in the lattice is equal to

$$\left\langle \sum_\alpha (u_i^\alpha)^2 \right\rangle = 2\lambda^2 + \frac{T}{\mu N}\sum_k \left(\frac{1}{\omega_1^2}+\frac{1}{\omega_2^2}\right). \quad (22)$$

It can be seen from this expression that the magnetic field has a strong effect on the zero-point vibrations of the system, while the thermal corrections for $T > \hbar\omega_-$ do not depend on the magnetic field.

As is well known,[7] in the two-dimensional case at $T \neq 0$ the mean square displacement in the lattice diverges logarithmically. This corresponds to the logarithmic divergence of the sum over **k** in (22). Thus, the theorem concerning the impossibility of a phase transition in an infinite two-dimensional system remains true in a magnetic field. This does not prevent, however, the existence at $T \neq 0$ of a polycrystalline two-dimensional lattice, as assumed by Chaplik.[6] In this case the expression (22) contains $\ln(k_0 L)$, where L is the characteristic size of the crystallites and k_0 is the Debye wave number.

Finally, we obtain

$$\left\langle \sum_\alpha (u_i^\alpha)^2 \right\rangle \simeq 2\lambda^2 + \frac{4}{3}\frac{T}{\mu\omega_0^2}\ln k_0 L. \quad (23)$$

Since $\omega_0^2 \sim e^2/\mu r_0^3$, in a given field a lattice exists at values of the concentration and temperature such that the inequality

$$2\lambda^2 + \frac{4}{3}T\frac{\ln(k_0 L)}{e^2}r_0^3 \lesssim \gamma_c r_0^2 \quad (24)$$

is fulfilled.

The form of the phase diagram at $T \neq 0$ is given qualitatively in Fig. 2. We note that $T_{max} \sim 1/\lambda$ increases with increase of the magnetic field.

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Translated by P. J. Shepherd