Wigner transition temperature of a two-dimensional electron gas in a strong magnetic field

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Within the Hartree-Fock approximation the transition temperature T_c of a two-dimensional electron gas of density n in a strong magnetic field B is studied in the nondegenerate limit $n/B \to 0$. By means of an asymptotically correct calculation it is shown that the ansatz of a strongly anharmonic, unidirectional charge-density wave (CDW) for the condensed state leads, apart from weak logarithmic corrections, to the limiting form $T_c \sim n^{1/2}$. The ansatz of an essentially harmonic, though triangular symmetric CDW leads to much smaller limiting values $T_c \sim nB^{-1/2}$. This demonstrates the importance of the anharmonicity of the CDW or, equivalently, of the sharp localization of electronic wave functions in the nondegenerate limit.

I. INTRODUCTION

Wigner crystallization of a two-dimensional electron gas in a strong magnetic field has been discussed by several authors.[1-3] A Hartree-Fock (HF) calculation[3] in the magnetic quantum limit yields for the temperature T_2, at which the free energy of the homogeneous state becomes unstable against the formation of charge-density waves (CDW)

$$k_B T_2 = 0.557 \nu(1-\nu) e^2/\epsilon l \quad . \tag{1.1}$$

Here $l = (\hbar c/eB)^{1/2}$ is the Larmor radius of an electron in a magnetic field of strength B, ϵ is a static dielectric constant, and $\nu = 2\pi l^2 n_0$ is the fraction of occupied states in the lowest Landau level, with n_0 the mean electron density. In a recent paper[4] (hereafter referred to as I) it was pointed out, that the limiting behavior $T_2 \sim n_0 B^{-1/2}$ for small n_0 and large B is unreasonable.

The correct transition temperature T_c is expected to become small in the limit of small n_0 values as $T_c \sim n_0^{1/2}$, but to saturate for $B \to \infty$. Therefore, one expects in the limit of small ν values

$$T_c/T_2 \sim \nu^{-1/2} \quad . \tag{1.2}$$

A weak enhancement of the critical temperature is already obtained, if, instead of a single harmonic CDW, a superposition of three CDW's with a density pattern of triangular symmetry is considered.[3] It was shown in I, that for small ν values the T_c enhancement increases rapidly, if one allows for the evolution of higher harmonics of the triangular CDW. It was argued, that in the limit of small ν values all harmonics become important to produce a first-order phase transition at a temperature T_c, which satisfies Eq. (1.2). But the actual calculation of I could not be extended properly to this limit, since it was based on a Taylor expansion of the free energy with respect to the order parameters (OP) characterizing the harmonics. This restricted the validity of the calculations to relatively small values of the OP and, furthermore, only a relatively small number of OP could be taken into account.

In the present paper we want to avoid these restrictions. We want to calculate, in the limit $\nu \to 0$, the free energy and the transition temperature, taking all harmonics into account properly. This becomes possible, if we restrict our consideration to a unidirectional CDW with a particle density $n(\vec{r})$ of the form

$$2\pi l^2 n(\vec{r}) = \nu + \nu \sum_{m=1}^{\infty} 2\psi_m \cos(mQx) \exp(-\tfrac{1}{4} m^2 l^2 Q^2) \quad , \tag{1.3}$$

where $\vec{r} = (x,y)$. With the ansatz

$$\psi_n = \psi \exp(-\alpha |n|), \quad \text{for } n = \pm 1, \pm 2, \ldots , \tag{1.4}$$

where ψ and α are non-negative real numbers, we will obtain in the limit of small ν the minimum of the free energy for $\psi = 1$ and $\alpha \sim \nu$, and a diverging ratio of T_c/T_2.

II. FREE ENERGY OF THE UNIDIRECTIONAL CDW

We consider a two-dimensional system of electrons in the magnetic quantum limit.[3,4] The electrons interact via the Coulomb potential $v(\vec{r}) = e^2/r\epsilon$. A homogeneous background of positive charge makes the system electrically neutral. We calculate the free energy within the HF approximation. For the matrix elements of the effective single-particle Hamiltonian

in the Landau representation we make the ansatz[4]

$$h_{jk}=\delta_{jk}\left[E^{(0)}+k_BT\sum_{n\neq 0}x_n\exp(-il^2Qnj)\right] , \quad (2.1)$$

where $E^{(0)}$ is the HF energy of the homogeneous state at the same temperature T, x_n is a dimensionless OP, and Q is a wave number, which must be determined variationally. This ansatz leads to the electron density of Eq. (1.3) with the self-consistency equations[4]

$$x_n=-\gamma_n\psi_n/\tau , \quad (2.2)$$

with $\tau=(1-\nu)T/T_2$, $k_BT_2=\nu(1-\nu)u_0e^2/\epsilon l$, and with

$$\gamma_n=u(\tfrac{1}{4}n^2l^2Q^2)/u_0 , \quad (2.3)$$

where u_0 is the maximum value of the function

$$u(x)=(\tfrac{1}{2}\pi)^{1/2}e^{-x}I_0(x)-\tfrac{1}{2}x^{-1/2}e^{-2x} . \quad (2.4)$$

Since the chemical potential μ_0 in the homogeneous HF state ($x_n\equiv 0$) is related to the density by

$$\exp[(E^{(0)}-\mu_0)/k_BT]=(1-\nu)/\nu , \quad (2.5)$$

the difference of the free energies of the CDW and of the homogeneous state is, apart from an unimportant common prefactor, given by the sum ϕ of

$$\phi_1=\eta-(2\pi\nu)^{-1}\int_{-\pi}^{\pi}dt\,\ln\{1-\nu+\nu\exp[\eta-x(t)]\} \quad (2.6)$$

and

$$\phi_2=\sum_{n=1}^{\infty}\gamma_n|\psi_n|^2/\tau , \quad (2.7)$$

where $\eta=(\mu-\mu_0)/k_BT$ and

$$x(t)=\sum_{n\neq 0}x_n\exp(-int) . \quad (2.8)$$

The chemical potential μ in the CDW state is determined by

$$\int_{-\pi}^{\pi}dt\,\{\nu+(1-\nu)\exp[x(t)-\eta]\}^{-1}=2\pi . \quad (2.9)$$

Converting sums over Landau quantum numbers into t integrals, we assumed $LQ\gg 1$, where L is the linear dimension of our system.

III. ASYMPTOTIC CALCULATION FOR SMALL ν

In the limit of small ν values Eq. (2.9) reduces to

$$\eta=-\ln I_1+\nu(I_2/I_1^2-1) , \quad (3.1)$$

where

$$I_m=(2\pi)^{-1}\int_{-\pi}^{\pi}dt\exp[-mx(t)] . \quad (3.2)$$

With Eq. (3.1), we obtain from Eq. (2.6) in this limit

$$\phi_1=-\ln I_1+\tfrac{1}{2}\nu(I_2/I_1^2-1) . \quad (3.3)$$

It is important for the following to note that with the ansatz of Eq. (1.4) the integrals I_m become singular in the limit $\alpha=0$. To demonstrate this, we note that Eq. (2.4) implies the asymptotic behavior

$$u(x)\sim\begin{cases}-\tfrac{1}{2}x^{-1/2}, & \text{for } 0<x\ll 1\\ +\tfrac{1}{2}x^{-1/2}, & \text{for } x\gg 1 .\end{cases} \quad (3.4)$$

Then

$$\gamma_n=\gamma/|n|+\Gamma_n , \quad (3.5)$$

where $\gamma=1/u_0lQ$ and $u_0\Gamma_n\sim\frac{1}{2}(lQ|n|)^{-3}$ for $|n|lQ\gg 1$. This yields with Eqs. (1.4), (2.2), and (2.8)

$$x(t)=(\gamma\psi/\tau)\ln(1+e^{-2\alpha}-2e^{-\alpha}\cos t)+X(t) , \quad (3.6)$$

where

$$X(t)=-2\frac{\psi}{\tau}\sum_{n=1}^{\infty}\Gamma_ne^{-\alpha n}\cos nt \quad (3.7)$$

is finite and well behaved, even for small values of t and of α. The first term on the right-hand side of Eq. (3.6) becomes singular in this limit:

$$x-X\sim(\gamma\psi/\tau)\ln(\alpha^2+t^2) . \quad (3.8)$$

If we put $\gamma\psi/\tau=y$, we obtain for $2my\geq 1$ and for small values of α

$$I_m\approx\alpha^{1-2my}Z(my)\exp[-mX(0)] , \quad (3.9)$$

where

$$Z(y)=\int_0^{\infty}dt(1+t^2)^{-y}=\tfrac{1}{2}\sqrt{\pi}\,\Gamma(y-\tfrac{1}{2})/\Gamma(y) . \quad (3.10)$$

In this limit the leading contributions to ϕ_1 of Eq. (3.3) come from

$$\ln I_1\approx X(0)-(2y-1)\ln\alpha+\ln Z(y) \quad (3.11)$$

and

$$I_2/I_1^2\approx q(y)/\alpha , \quad (3.12)$$

where

$$q(y)=Z(2y)/Z^2(y) . \quad (3.13)$$

Asymptotic evaluation of ϕ_2, Eq. (2.7), for small α yields

$$\phi_2=-\psi y\ln(1-e^{-2\alpha})+\phi_0 , \quad (3.14)$$

where the last term

$$\phi_0 = \frac{\psi^2}{\tau} \sum_{n=1}^{\infty} \Gamma_n e^{-2\alpha n} \tag{3.15}$$

remains finite in the limit $\alpha \to 0$, whereas the first becomes large as $\psi y \ln(1/2\alpha)$. For small α we have

$$\phi_0 \approx -\tfrac{1}{2}\psi X(0) \approx \psi y \sum_{n=1}^{\infty} \frac{\Gamma_n}{\gamma} \tag{3.16}$$

independent of α. We do not neglect this term, since it becomes large for small values of lQ, which become important for small values of ν. If, in the limit of small ν, we neglect the second term on the right-hand side of Eq. (3.3), we obtain for the free energy

$$\phi \sim -c \ln(1/\alpha) \tag{3.17}$$

with

$$c = [1-(1-\psi)^2]\gamma/\tau - 1 \ . \tag{3.18}$$

For $\gamma > \tau$ the coefficient c becomes maximum for $\psi = 1$, and the lowering of the free energy due to the formation of the CDW becomes infinite for $\alpha = 0$. Since $\tau/\gamma = 0.557 lQT/T_2$, this leads us to expect in the limit of vanishing ν a phase transition at an arbitrarily large value of T/T_2 to a CDW with a very small value of lQ. For small but finite values of ν, the second term on the right-hand side of Eq. (3.3) becomes dominant for small α. The α-dependent part of ϕ,

$$\phi_\alpha = c \ln\alpha + \tfrac{1}{2}\nu q/\alpha \ , \tag{3.19}$$

assumes for

$$\alpha = \tfrac{1}{2}\nu q/c \tag{3.20}$$

its minimum value

$$\phi_{\alpha,\min} = -c[\ln(2c/\nu q) - 1] \ . \tag{3.21}$$

Minimizing this with respect to ψ, we obtain for $\nu \to 0$ the optimum value $\psi = 1$, for which c assumes its maximum value $c = \gamma/\tau - 1 = y - 1$. Inserting the optimum values of α and ψ, we obtain with the ansatz of Eq. (1.4) the minimum value of the free energy for given values of ν, τ an $\gamma = (u_0 lQ)^{-1}$ as

$$\phi_{\min} = -(y-1)\{\ln[2(y-1)/\nu q(y)] - 1\} - y\ln 2 - \ln Z(y) - \phi_0 \ , \tag{3.22}$$

where ϕ_0 is given by Eq. (3.16) with $\psi = 1$ and $y = \gamma/\tau$. For given values of ν and of γ the critical temperature is determined by $\phi_{\min} = 0$. This determines a critical value $\tau_c(\nu, \gamma)$. In a final step we have to maximize τ_c for given ν as a function of γ. This yields, for the given value of ν, the transition temperature τ_c and the optimum value of γ, i.e., the period of the CDW. Since we expect the optimum values of γ to become very large for very small values of ν, we calculate ϕ_0 asymptotically correct in this limit.

IV. OPTIMUM Q VALUE

In order to evaluate ϕ_0 from Eq. (3.16) ($\psi = 1$), we note that Γ_n depends on n in the form $u_0\Gamma_n = G(nlQ)$, as follows from Eqs. (2.3) and (3.5). Then, choosing $N = \lambda/lQ$, we see that the sum

$$u_0 lQ \sum_{n=N}^{\infty} \Gamma_n \approx \int_{\lambda}^{\infty} dx G(x) \tag{4.1}$$

approaches in the limit of small lQ values a constant value independent of lQ. For $0 < \lambda << 1$ we obtain from Eq. (3.4)

$$u_0 lQ \sum_{n=1}^{N} \left(\gamma_n - \frac{\gamma}{n}\right) \approx -2\ln N \ . \tag{4.2}$$

Equations (3.16), (4.1), and (4.2) yield the asymptotic expression

$$\phi_0 \approx -y \ln\lambda'\gamma^2 \ , \tag{4.3}$$

with $\gamma = (u_0 lQ)^{-1}$ and some constant λ', which in principle can be calculated numerically. Retaining for small values of ν and $1/\gamma$ only the most relevant terms, we obtain from Eq. (3.22) the condition

$$\phi_{\min} \approx -(y-1)\ln[2(y-1)/\nu q(y)] + y\ln\lambda\gamma^2 = 0 \ , \tag{4.4}$$

where λ is some constant. This determines $y = y(\gamma)$ and, thereby, $\tau = \gamma/y(\gamma)$. The condition that $\tau(\gamma)$ should become maximum can, by virtue of Eq. (4.4), be written in the form

$$y[1 + (y-1)q'(y)/q(y)] = \ln[2(y-1)/q(y)] - \ln\nu \ . \tag{4.5}$$

The function $q(y)$, defined by Eqs. (3.10) and (3.13), increases with increasing values of $y \geq 1$ monotonically from the value $q(1) = 1/\pi$ and has the asymptotic form $q(y) \sim (2y/\pi)^{1/2}$ for $y >> 1$. As a consequence, Eq. (4.5) has two solutions, if ν is sufficiently small. There is one solution for y, which approaches unity in the limit $\nu \to 0$ ($y - 1 \sim \nu$). This solution must be ruled out, since it is not consistent with our asymptotic calculation of $\phi_{\min}$, Eq. (4.4). The y values of the second solution become large for small values of ν. For $y >> 1$ we may approximate Eq. (4.5) by

$$\tfrac{3}{2}y = \tfrac{1}{2}\ln(2y/\pi) - \ln\nu \ , \tag{4.6}$$

which has the asymptotic solution $y = \frac{2}{3}\ln(1/\nu)$. Inserting this into Eq. (4.4) we obtain asymptotically in

the limit of small ν

$$\gamma = (\lambda\nu)^{-1/2}[(4\pi/3)\ln(1/\nu)]^{1/4} \sim \nu^{-1/2}\ln^{1/4}(1/\nu) \tag{4.7}$$

and

$$\tau_c = \gamma/y \sim \nu^{-1/2}\ln^{-3/4}(1/\nu) \quad . \tag{4.8}$$

V. CONCLUSIONS

In the limit $\nu \to 0$ the two-dimensional electron system becomes nondegenerate and we expect a phase transition to a classical Wigner crystal with a lattice spacing $b \sim n_0^{-1/2}$ at a transition temperature $T_c \sim n_0^{1/2}$, where b and T_c both are independent of the magnetic field. For the magnetic field-dependent, dimensionless units of the previous sections, this means $\gamma \sim b/l \sim \nu^{-1/2}$ and $\tau_c \sim T_c/T_2 \sim \nu^{-1/2}$. This type of asymptotic behavior was obtained in I by means of an extrapolation of a calculation, which considered several types of harmonics of a triangular CDW. But the actual calculation, which took into account only a relatively small number of harmonics, yielded finite limiting values for both γ and τ_c. The present calculation, where we made the ansatz of a unidirectional but strongly anharmonic CDW, yields on the other hand with Eqs. (4.7) and (4.8) essentially the expected asymptotic result, with only weak logarithmic corrections. Since for $\nu \to 0$ the OP ψ_n of Eq. (1.4) approach unity, the CDW assumes a Gaussian form in this limit [cf. Eq. (1.3)]. The width of a single Gaussian approaches the Larmor radius l and the spacing between neighboring Gaussians becomes $b \sim n_0^{-1/2}$, apart from logarithmic corrections. This result leads us to attribute the essential lowering of the free energy in the CDW state to the spatial separation of sharply localized (in one direction) electronic wave functions and not simply to a more or less harmonic modulation of the electronic density. It is then very likely, that a triangular symmetric arrangement of totally localized (in both directions) wave functions would be even more favorable than our unidirectional CDW, so that eventually Eqs. (4.7) and (4.8) would be obtained without the logarithmic factors. Certainly, our asymptotic calculation can yield only a lower bound to the correct HF transition temperature T_c. But a similar calculation with the more reasonable ansatz of a strongly anharmonic triangular CDW would be much more complicated since it requires the diagonalization of a very large Hamiltonian matrix.

Kuramoto[1] has shown that in the classical regime of small ν values a unidirectional CDW yields a cohesive energy (for zero temperature) which is only slightly weaker than that obtained for a triangular CDW. He obtained as the optimum unidirectional CDW Eq. (1.3) with $\psi_n = (\pi n \nu)^{-1}\sin(\pi n \nu)$. If we replace the ansatz (1.4) in view of this result by $\psi_n = (\psi/n\alpha)\sin(n\alpha)$, we obtain again the same asymptotic results of Eqs. (4.7) and (4.8). Only the analytical evaluation of the sums, e.g., Eq. (3.16), becomes somewhat more complicated. Kuramoto's results are consistent with our expectation that the asymptotic results of Eqs. (4.7) and (4.8) agree apart from the weak logarithmic factors with the correct HF results for a triangular CDW.

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