Strong-Magnetic-Field States of the Pure Electron Plasma

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(Received 13 November 1986)

We study the zero-temperature electron plasma in a strong magnetic field in the Hartree-Fock approximation. The calculations are based on an expression for the density matrix which allows all Coulomb integrals to be performed explicitly and allows exchange to be treated exactly. We find that the ground state changes from a charge-density-wave state with **Q** parallel to the field, to a uniform-density state, then to a crystal state in the holes of the lowest Landau level, and finally to an electron-crystal state as the magnetic field is increased.

PACS numbers: 71.45.−d, 71.30.+h, 72.20.My

At sufficiently low electron densities the zero-temperature electron plasma (ZTEP) should undergo a transition to a Wigner-lattice state.[1] Following suggestions that a strong magnetic field would increase the density at which crystallization occurs,[2,3] Kaplan and Glasser[4] proposed an ordered state for the ZTEP in a strong field consisting of a two-dimensional hexagonal lattice of charged rods oriented parallel to the field and demonstrated that this state has lower energy then the uniform-density state formed by noninteracting electrons. In the Kaplan-Glasser (KG) state each of the charged rods behaves as a one-dimensional electron gas (1DEG) and Kleppman and Elliott[5] demonstrated that at very strong fields a further reduction of energy could be obtained by allowing the charge density to vary along the rods as well. As emphasized by later workers,[6,7] the state with a charge-density wave on the 1D rods evolves continuously into a Wigner crystal as the field is increased. In previous work the exchange between different charged rods has either been neglected or treated approximately, causing the reliability to become questionable in the region of field where the crystallization transition actually occurs. In this Letter we report the results of a calculation which treats exchange exactly. We find that the transition from uniform-density state to Wigner crystal state occurs in several steps and that the ZTEP has a richer phase diagram in the transition region than had been previously anticipated.

There have been many experimental attempts to observe magnetic-field-induced crystallization (MFIC) by studying magnetotransport properties in narrow-gap semiconductors,[8,9] and graphite.[10] Typical carrier densities in these materials correspond to values of the density parameter, r_s^*, which are ~ 1. [$r_s^* \equiv m^*(3/4\pi n a_0^3)/\varepsilon$ where m^*, n, and ε are the semiconductor's effective mass, carrier density, and dielectric constant.] At these densities kinetic-energy costs prevent crystallization at zero field and anomalies in magnetotransport properties have frequently been taken as evidence for MFIC. The situation is complicated by the possible importance of the inevitable ionized donors and controversy has arisen because of the qualitatively similar effect of magnetic freeze-out and MFIC on transport properties.[11] It is our hope that improved understanding of the expected properties of the pure electron plasma can contribute to the resolution of these controversies. It is worth remarking that a true pure electron plasma can be obtained through use of magnetic confinement.[12] However, at least at the densities achievable with current magnet technology ($r_s^* \gtrsim 500$) Wigner crystallization occurs even at zero-field strength[13] and MFIC cannot be studied.

Our calculation is based on the observation that the one-particle density matrix

$$\rho(k_z',k_z:X',X) \equiv \sum_\alpha n_\alpha \langle k_z' X' \mid \alpha \rangle \langle \alpha \mid k_z X \rangle \tag{1}$$

can be expressed without loss of generality in the form

$$\rho(k_z',k_z:X',X) \equiv \sum_{\mathbf{p}} \Delta(k_z:\mathbf{p}) \exp[\tfrac{1}{2} i p_x (X+X')] \delta_{X',X+l^2 p_y} \delta_{k_z',k_z+p_z}, \tag{2}$$

where we use the usual basis of Landau-gauge kinetic-energy eigenstates[14] and we consider the strong-field limit so that all electrons are in the lowest Landau level. In Eq. (2) k_z is the wave vector for motion along the field, X labels the states in the lowest Landau level for each value of k_z, and $l \equiv (\hbar c/eB)^{1/2}$. By use of Eq. (2), the matrix elements of the

effective single-particle Hamiltonian may be expressed in the form

$$\langle k_z'X'|H_{\rm HF}|k_zX\rangle=\delta_{k_z',k_z}\delta_{X',X}\frac{\hbar^2k_z^2}{2m^*}+\frac{e^2}{\varepsilon}\int\frac{dp_z}{\pi}\sum_{\mathbf{q}}\Delta(p_z:\mathbf{q})\delta_{X',X+l^2q_y}\delta_{k_z',k_z+q_z}\exp\left[\frac{iq_x}{2}(X+X')\right]\times\left[(1-\delta_{\mathbf{q},0})\frac{e^{-q_\perp^2l^2/2}}{q^2l^2}-X(q_\perp l,(k_z-p_z)l)\right],\quad(3)$$

where

$$X(u,v)=\int_0^\infty dt\,e^{-t^2/2}[J_0(ut)/(t^2+v^2)].\quad(4)$$

Similarly for the Fourier components of the charge density

$$\rho(\mathbf{q})\equiv\sum_\alpha\langle\alpha|e^{-i\mathbf{q}\cdot\mathbf{r}}|\alpha\rangle n_\alpha=\frac{\Omega}{(2\pi l^2)}\exp(-\tfrac{1}{4}q_\perp^2l^2)\int\frac{dk_z}{2\pi}\Delta(k_z:\mathbf{q}),\quad(5)$$

$\Delta(k_z:\mathbf{q})$ gives the contributions to $\rho(\mathbf{q})$, the Fourier transform of the charge density, from different k_z's. The first of the two terms inside the large parentheses in Eq. (3) gives the Hartree contribution from $\Delta(p_z:\mathbf{q})$ to the effective potential and the second is the exchange contribution whose nonlocality is reflected by its dependence on k_z and p_z.

For the Wigner-lattice state we seek solutions to the Hartree-Fock equations for which $\Delta(k_z:\mathbf{q})$ is nonzero only for $\mathbf{q}$ equal to a reciprocal-lattice vector. In that case the Hartree-Fock matrix elements for a given $\Delta(p_z:\mathbf{q})$ are of the same form as those coming from an external periodic potential of the same periodicity. Self-consistent solutions can be sought by starting with a potential which attracts the electrons to the lattice sites, evaluating $\Delta(p_z:\mathbf{q})$ from Eq. (2), diagonalizing the Hartree-Fock matrix, reevaluating $\Delta(p_z:\mathbf{q})$, and iterating. It is useful, however, to start with the consideration of solutions for which $\Delta(p_z:\mathbf{q})$ is nonzero only for $\mathbf{q}_\perp=(q_x,q_y)$ equal to a 2D reciprocal lattice vector and $q_z=0$. These solutions correspond to the 2D lattices of charged rods of Kaplan and Glasser[4] (KG) except that exchange between different rods is included *exactly* even when many rods overlap. For the KG states we see from Eq. (2) that k_z remains a good quantum number and we find self-consistent solutions for which only states with $|k_z|<k_F$ are occupied. The lowest-energy states have one electron for each occupied k_z at each 2D lattice site so that

$$n=\rho(\mathbf{q}=0)/\Omega=k_F\nu/2\pi^2l^2,\quad(6)$$

where $\nu=\Delta(k_z:\mathbf{q}=0)$ ($|k_z|<k_F$) is the fractional filling of each Landau level and equals the ratio of $2\pi l^2$ to the 2D unit-cell area.

We have found self-consistent solutions to the Hartree-Fock equations corresponding to KG states for a range of values of ν, n, and magnetic field.[15] The results for the energy per electron can be extremely accurately fitted to an expression motivated by considering the case of well-separated rods ($\nu\ll1$):

$$\varepsilon_{\rm KG}=2\gamma\{\delta^2/6+(1/\gamma^{1/2})[\varepsilon_1(\delta\sqrt{2})/\sqrt{2}+\delta\tilde{\varepsilon}(\nu,\delta)]\},\quad(7a)$$

where

$$\tilde{\varepsilon}(\nu,\delta)=(2\pi)^{-1}[-\ln\nu-1.6134+A\nu+B(\delta)e^{-1.8/\nu}]\ \text{for}\ \nu\le\tfrac{1}{2}.\quad(7b)$$

In Eq. (7b), the fitting parameters $A=2$ and $B=-3.2+0.04\delta$, $\delta=k_Fl$, energies are in units of the effective Rydberg (R^*), and $\gamma=\hbar\omega_c/2R^*=4.3\times10^{-6}(\varepsilon m/m^*)^2\times H(\text{tesla})$ is a dimensionless measure of the field strength. The first term inside the curly brackets in Eq. (7a) is the kinetic energy. The first term inside the square brackets in Eq. (7a) is the exchange energy for the 1DEG of a given charged rod and is closely related to the exchange energy of the uniform gas ($\nu=1$) state, $\varepsilon_1(\delta)$. [$\varepsilon_1(\delta)$ has been reduced to a single quadrature by Danz and Glasser.[16]] The first two terms in Eq. (7b) represent the Coulomb energy of the Kaplan-Glasser state for well-separated rods ($\nu\ll1$) which can be related[15] to the Madelung energy of a 2D one-component plasma on a triangular lattice.[17] The third and fourth terms in Eq. (7b) represent corrections to the Coulomb energy due to the finite diameter of the rods ($\sim l$) and exchange between separated rods. Finally, we can use particle-hole symmetry within each Landau level in the KG state to show that[15]

$$\tilde{\varepsilon}(\nu,\delta)=(2-\nu^{-1})\varepsilon_1(\delta)+(\nu^{-1}-1)\tilde{\varepsilon}(1-\nu,\delta),\quad(8)$$

where the ground state for $\nu\ge\frac{1}{2}$ is a KG state in the holes of the uniform-density state.

For a given density and field the energy must be minimized with respect to ν to find the lowest-energy KG

state. To avoid the necessity of finding self-consistent solutions to the Hartree-Fock equations at each possible value of ν we have used Eqs. (7) and (8) to minimize the energy. For $\nu < \frac{1}{2}$ decreasing ν separates the rods of electrons while for $\nu > \frac{1}{2}$ increasing ν increases the separation between the rods of holes in the otherwise uniform-density system. For $\nu < \frac{1}{2}$ decreasing ν increases the electron density in each charged rod which increases the magnitude of the 1DEG exchange energy of each rod and lowers the interaction energy of the system. For $\nu > \frac{1}{2}$ decreasing ν also tends to lower the interaction energy of the system except very near to $\nu = 1$ where the Madelung energy of well-separated hole rods dominates (see below). However, decreasing ν increases the kinetic energy ($\gamma\delta^2/3$) since states with higher values of k_z must be occupied when the Landau-level filling decreases [$\delta = 3\pi/(2r_s^{*3}\gamma^{3/2}\nu)$]. As γ increases each Landau level holds more electrons, the kinetic energy cost of separating rods decreases, and the lowest-energy KG state occurs at smaller values of ν.

In Fig. 1 we show the energy and Landau-level filling factor, ν, for the optimal KG state for $r_s^* = 2$ and a range of fields appropriate to narrow-gap semiconductors. The discontinuity in the optimal filling factor at $\nu = 1$ is due to the positive Madelung energy from widely separated hole rods for ν slightly below 1. The discontinuity near $\nu = \frac{1}{2}$ reflects a first-order phase transition between hole KG states and electron KG states as γ increases. For ν just below 1 the hole KG states are unstable with respect to a charge variation with wave vector $2k_F$ along each rod, and the ground state is a hole Wigner crystal [a $3-\mathbf{Q}$ charge-density-wave (CDW) state with one electron per unit cell]. An approximate stability requirement can be derived from the Hartree-Fock equations by averaging the exchange potential over k_z values to eliminate its nonlocality[18] and is used in Fig. 2 to produce a phase diagram of strong-field states of the ZTEP. For $r_s^{*2}\gamma \leq 2.231$ more than than one Landau level is occupied, even for a noninteracting system. This is the weak-field regime to which our calculations do not apply. In the strong-field regime kinetic energy is dominant at first, there is no charge variation perpendicular to the field ($\nu = 1$), and the system forms a CDW state with $\mathbf{Q}$ parallel to the field. As γ increases, k_F decreases, the wavelength of the CDW becomes longer, and the electrostatic energy cost of the CDW becomes too large so that the ground state has uniform density. Next, the Landau-level degeneracy increases sufficiently to allow a KG lattice of rods to be formed in the plane perpendicular to the field. For $\nu > \frac{1}{2}$ the lowest-energy KG states are rods of holes in the uniform state. Where these rods are unstable the ground state is a 3D Wigner lattice of holes. As γ increases further ν decreases below $\frac{1}{2}$ and electron KG states form. Finally, for sufficiently strong fields or sufficiently low densities the electron KG states become unstable and we obtain the expected electron Wigner crystal.

The accuracy of this phase diagram has been checked by finding numerically exact solutions to the full Hartree-Fock equations as a function of ν for selected values of r_s^* and γ. (Detailed results will be presented elsewhere.[15]) We can conclude from this work that MFIC in a pure electron plasma shows a richness of detail which has not been previously anticipated. The possibili-

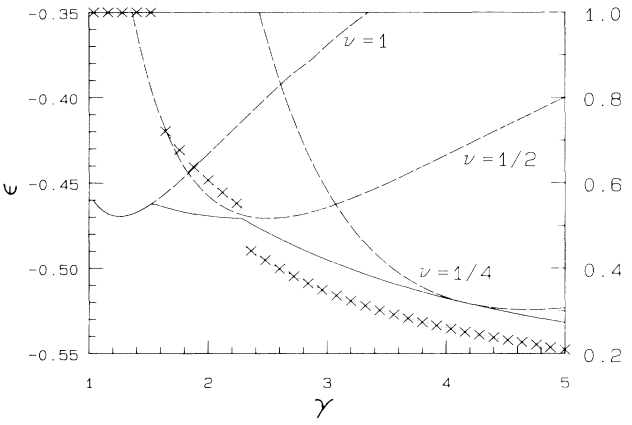

FIG. 1. KG state energies vs γ at $r_s^* = 2$. The crosses show the filling factor ν (scale on right), at which the KG state energy is minimized for each value of γ. The solid line is for the minimum-energy KG state while the dashed lines are for the $\nu = 1$, $\nu = \frac{1}{2}$, and $\nu = \frac{1}{4}$ states. Note that the $\nu = \frac{1}{2}$ state is not the minimum-energy state for any value of γ.

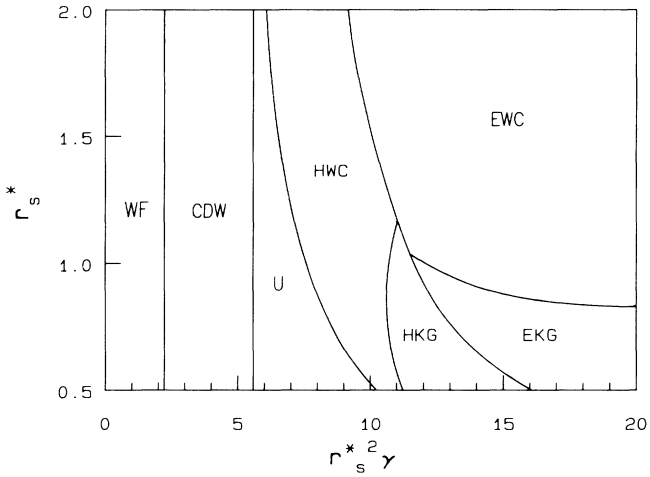

FIG. 2. Phase diagram for strong-field states of the ZTEP in a range of field and density appropriate to narrow-gap semiconductors. (WF, weak-field regime; CDW, charge-density wave with $\mathbf{Q} \| \mathbf{H}$; U, uniform-density state; HKG, hole Kaplan-Glasser state; HWC, hole Wigner crystal; EKG, electron Kaplan-Glasser state; EWC, electron Wigner crystal.)

ty that states in some regions of the phase diagram may be preempted by highly correlated uniform-density states related to those responsible for the fractional quantum Hall effect in 2D [19,20] only adds to the motivation for further studies of the strong-field ZTEP.

The authors acknowledge useful discussions with numerous colleagues. This work was performed in part under the McDonnell Douglas Corporation Independent Research and Development program.

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