Enhancement of Wigner Crystallization in Multiple-Quantum-Well Structures

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We show that the density for Wigner crystallization to occur for the two-dimensional electron liquid in zero magnetic field can be increased in suitable multiple-quantum-well structures. Data from Monte Carlo calculations are used to determine the properties of each layer in isolation, and the layers interact through Coulomb forces. With this mechanism the maximum solidification density can be raised by as much as a factor of 3. At higher densities, charge-density-wave ground states can occur.

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The Wigner-crystal state of a pure electron system is expected to occur only at very low densities. This restriction comes from the competition between the kinetic and potential energies of the system. The kinetic-energy cost scales as the inverse square of the lattice constant, and this only becomes insignificant compared to the potential energy for very large values of the lattice constant, that is, for very low densities. Monte Carlo numerical simulations for the ground state of the electron system predict that at zero temperature the Wigner phase transition from liquid to solid occurs at $r_s \sim 110$ for a three-dimensional system [1] and $r_s \sim 37$ in two dimensions [2]. This has made observation of the quantum Wigner-crystallization phenomena very difficult, with a major obstacle being the tendency toward disorder-induced electron localization at densities much higher than those associated with crystallization. There is increasing experimental evidence that Wigner crystalization occurs in thin electron layers in very high magnetic fields [3]. In this case the quantized cyclotron orbit provides a localization scale for the electrons, which reduces the energy cost of localizing the electrons on lattice sites.

We propose here that the Wigner transition can be shifted to much higher electron densities in a multiple-quantum-well structure of parallel electron layers separated by potential barriers. Let us first consider two parallel layers of electrons each with the same layer density less than the Wigner-crystal transition density ($r_s \gtrsim 37$). In the ground state the electrons in both layers will be in the Wigner-crystal ground state. There has been recent interest in the effect of electron correlations between quantum wells on highly correlated many-body states within coupled electron layers [4], but here we are going to assume that the perpendicular separation between layers is sufficiently large that there is negligible hopping of electrons between the layers. Because of the Coulomb interaction between layers, the two Wigner lattices will be shifted relative to each other by half a lattice constant. Thus a lattice site in one layer will lie directly above the midpoint between two sites in the other layer. Now suppose the electron density in the layers is increased. Because of the additional potential gain arising from the interaction between layers [5], the electrons will not immediately liquify when density exceeds the transition density for a single layer ($r_s \simeq 37$), and for sufficiently small values of the perpendicular separation between the layers, this coupled crystal ground state can persist to densities significantly higher than $r_s = 37$.

If we continue to increase the density, the kinetic-energy cost of localizing the electrons on a length scale of the interparticle spacing will finally become too large for the potential-energy gain from the interlayer interaction to overcome. However, even then it can still be energetically favorable at densities higher than this point for there to exist a density modulation in the ground state with wave number $|\mathbf{q}| < 2k_F$. Such charge-density waves have been observed in many one-dimensional conductors (for a recent review see, for example, Ref. [6]), and in layered compounds, and there have even been suggestions that they may form the ground state of some simple bulk metals [7]. We believe this is a first suggestion that charge-density waves can be studied in multiple quantum wells. As a general requirement for the existence of a charge-density-wave ground state, we need to have a compensating polarizable background medium. In our system, each layer could act as the polarizing background medium for the other.

Our argument can be quantified by calculating the static response function for a system consisting of N evenly spaced, parallel layers of electrons, and by showing that it diverges for wave vectors equal to the reciprocal-lattice constant of the Wigner crystal, $\mathbf{q} \simeq \mathbf{G}$, or for a smaller wave vector ($|\mathbf{q}| < 2k_F$) in the case of a charge-density-wave transition.

Within linear-response theory the total potential acting on electrons in a particular layer l consists of the external potential $\Phi_l^{\rm ext}(\mathbf{q},\omega)$ plus the interaction induced by changes in electron density in other layers. The induced electron density in the lth layer $\delta n_l(\mathbf{q},\omega)$ is thus

$$\delta n_l(\mathbf{q},\omega) = \chi(\mathbf{q},\omega)\left[\Phi_l^{\rm ext}(\mathbf{q},\omega) - \sum_{l' \neq l} V_{ll'}(\mathbf{q})\delta n_{l'}(\mathbf{q},\omega)\right], \quad (1)$$

where $\chi(\mathbf{q},\omega)$ is the response function for a single isolated layer, and $V_{ll'}(\mathbf{q})$ is the interaction between electrons in the layers l and l'. We assume that there is negligible tunneling between layers, so that we can take the interaction between electrons in different layers to be the bare

Coulomb interaction for the intrinsic semiconductor with dielectric constant ϵ_0:

$$V_{ll'}(\mathbf{q}) = v_{\mathbf{q}} \int dz \int dz' e^{-q|z-z'|} |\zeta(z-la)|^2 |\zeta(z'-l'a)|^2 , \quad (2)$$

where $v_{\mathbf{q}} = 2\pi e^2/\mathbf{q}\epsilon_0$. The envelope wave function perpendicular to the layer, $\zeta(z-la)$, is assumed to be the same for all electrons, that is, only the lowest subband is occupied.

Equation (1) can be written in the form

$$\sum_{l'} \left[\left(\frac{1}{\chi(\mathbf{q},\omega)} - V_{ll}(\mathbf{q}) \right) \delta_{ll'} + V_{ll'}(\mathbf{q}) \right] \delta n_{l'}(\mathbf{q},\omega) = \Phi_l^{\text{ext}}(\mathbf{q},\omega) . \quad (3)$$

In this equation, the quantity in the square brackets is the inverse of the total response function matrix, $\chi_{ll'}^{\text{tot}}(\mathbf{q},\omega)$, for the multilayer system.

Equation (3) implies that a system which has a uniform density within each layer will be unstable to a phase transition into a state with a nonuniform density distribution if the determinant for $\omega = 0$ vanishes:

$$\det \left[\left(\frac{1}{\chi(\mathbf{q})} - V_{ll}(\mathbf{q}) \right) \delta_{ll'} + V_{ll'}(\mathbf{q}) \right] = 0 . \quad (4)$$

Here $\chi(\mathbf{q}) \equiv \chi(\mathbf{q},\omega=0)$. When this condition is satisfied, Eq. (3) has a nontrivial static solution in the absence of the external potential.

In the special case of two layers, when the matrix $\chi_{ll'}^{\text{tot}}(\mathbf{q})$ is diagonalized its elements are

$$\chi_{\pm}^{\text{tot}}(\mathbf{q}) = \frac{\chi(\mathbf{q})}{1 \pm V_{12}(\mathbf{q})\chi(\mathbf{q})} . \quad (5)$$

The plus label corresponds to the situation where density modulations parallel to the layers have the same phase in the two layers $[\delta n_1(\mathbf{q}) = \delta n_2(\mathbf{q})]$, and the minus to the case where they are π out of phase $[\delta n_1(\mathbf{q}) = -\delta n_2(\mathbf{q})]$.

We see that the denominator in Eq. (5) can vanish, causing the total response function $\chi_{\pm}^{\text{tot}}(\mathbf{q})$ to diverge, even when the response function for the single layer, $\chi(\mathbf{q})$, is finite. Since $V_{12}(\mathbf{q})$ and $\chi(\mathbf{q})$ are both nonnegative, it is $\chi_{-}^{\text{tot}}(\mathbf{q})$ which will diverge. If the density within each layer is close to the Wigner-crystal transition point, then $\chi(\mathbf{q})$ will be very large for values of $\mathbf{q}$ near the reciprocal-lattice vector $\mathbf{G}$ of the crystal. In this case even small values of the interlayer potential may be sufficient to cause $\chi_{-}^{\text{tot}}(\mathbf{q})$ to diverge. As we increase the density within both layers we will move away from the transition point and the peak in $\chi(\mathbf{q})$ will become less pronounced. In this case $V_{12}(\mathbf{q})$ will need to be larger for the denominator of Eq. (5) to vanish. This can be accomplished if the perpendicular spacing between the layers is decreased.

We now specify the response function for a single isolated layer. From the above argument it is vital that $\chi(\mathbf{q})$ should accurately reproduce the behavior of the electron liquid in the vicinity of the Wigner-crystal phase transition. We follow the procedure introduced in Ref. [8]. We determine the static response function for the single layer using the Monte Carlo numerical simulation data for the ground state of the pure two-dimensional electron liquid [2]. First $\chi(\mathbf{q},\omega)$ is written in the form [9]

$$\chi(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 + V(\mathbf{q})[1 - G(\mathbf{q})]\chi_0(\mathbf{q},\omega)} , \quad (6)$$

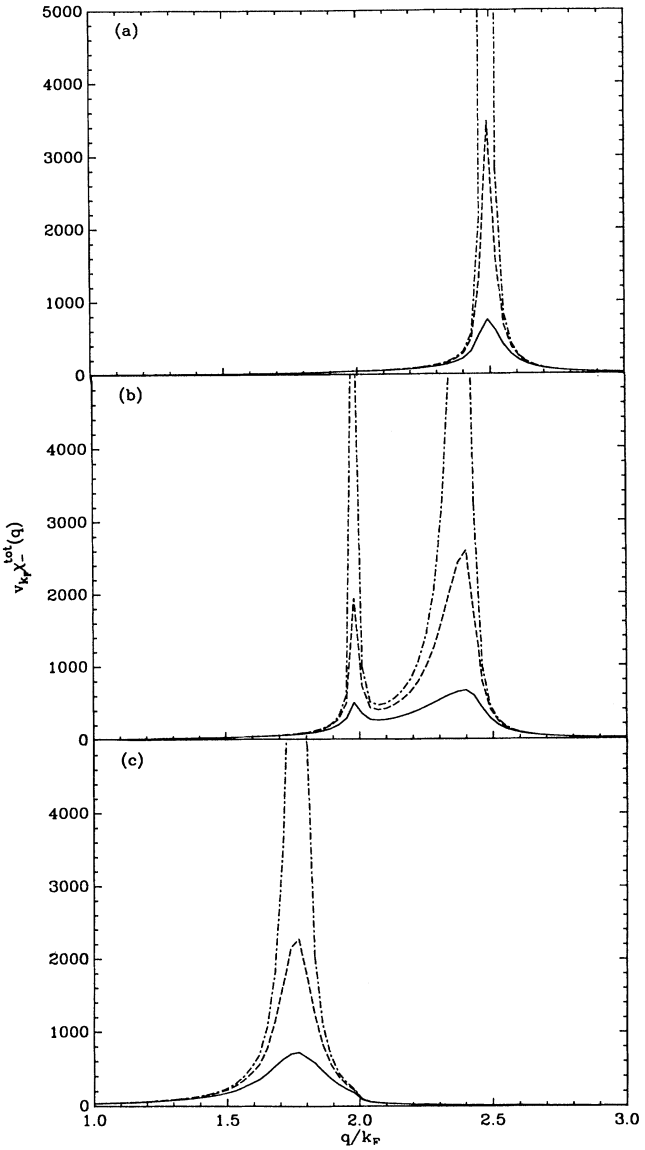

FIG. 1. Static response function $\chi_{-}^{\text{tot}}(\mathbf{q})$ for two layers. (a) Plots for density $r_s = 25$ and three different layer spacings, $a/a_B^* = 14.90$, 14.75, 14.71 (solid, dashed, and dot-dashed lines, respectively). Transition to the Wigner crystal occurs at critical layer spacing $a_c/a_B^* = 14.7$, with wave number $q_c = 2.5k_F$. (b) Similar to (a), but with $r_s = 20$ and $a/a_B^* = 9.65$, 9.57, and 9.55. Transition to the Wigner crystal at $a_c/a_B^* = 9.5$, with $q_c = 2.4k_F$. (c) Similar to (a), but with $r_s = 10$ and $a/a_B^* = 3.26$, 3.245, and 3.24. Transition to charge-density wave at $a_c/a_B^* = 3.2$, with $q_c = 1.8k_F$.

TABLE I. Wigner-crystal critical wave number q_c and critical layer spacing a_c. f_{10} denotes the Monte Carlo [2] occupation numbers for $r_s=10$, and f_0 the Fermi-Dirac occupation numbers. d is the layer thickness and N the number of layers.

	$\{N=2, f_{10}, d=a_B^*\}$		$\{N=2, f_0, d=a_B^*\}$		$\{N=2, f_{10}, d=2a_B^*\}$		$\{N=\infty, f_{10}, d=a_B^*\}$	
r_s	q_c/k_F	a_c/a_B^*	q_c/k_F	a_c/a_B^*	q_c/k_F	a_c/a_B^*	q_c/k_F	a_c/a_B^*
25	2.5	14.7	2.5	18.2	2.5	14.6	2.5	19.2
20	2.4	9.5	2.4	11.9	...	...	...	...

where $V(q)\equiv V_{ll}(\mathbf{q})$, and $\chi_0(\mathbf{q},\omega)$ is the Lindhard function for the two-dimensional system [10] with the single-particle occupation numbers $n(\mathbf{p})$ taken for the interacting electron liquid. The static local field factor $G(\mathbf{q})$ takes into account the static correlations between pairs of electrons due to their mutual exchange and interaction. Reference [2] gives the pair correlation function $g(\mathbf{r})$ for the ground state of the two-dimensional electron liquid for a range of densities down to the Wigner-crystallization point. $g(\mathbf{r})$ is related by a Fourier transformation to the static structure factor $S(\mathbf{q})$. This in turn is related to $\mathrm{Im}\chi(\mathbf{q},\omega)$ through the fluctuation-dissipation theorem. By assuming the form for $\chi(\mathbf{q},\omega)$ given by Eq. (6), we can thus use the $g(\mathbf{r})$ data in Ref. [2] to uniquely specify the local field factor $G(\mathbf{q})$.

Equation (5) can be rewritten with the help of Eq. (6) in the form

$$\chi_{\pm}^{\mathrm{tot}}(\mathbf{q})=\frac{\chi_0(\mathbf{q})}{1+\{V(\mathbf{q})[1-G(\mathbf{q})]\pm V_{12}(\mathbf{q})\}\chi_0(\mathbf{q})}. \quad (7)$$

We see that there is some cancellation between the effective potential within the layer, $V(q)[1-G(\mathbf{q})]$, and potential between layers, $V_{12}(\mathbf{q})$. It is this cancellation which can lead both to the enhancement of the Wigner crystallization and to the formation of a stable charge-density-wave state. While the charge-density wave is not very sensitive to the precise shape of $G(\mathbf{q})$, for the Wigner-crystal transition the local field $G(\mathbf{q})$ must have a maximum exceeding unity.

Using Eq. (7) we calculated $\chi_{-}^{\mathrm{tot}}(\mathbf{q})$ for two wells each of thickness $d=a_B^*$. For a GaAs/AlGaAs system the effective Bohr radius $a_B^*\simeq 98$ Å. At each density we varied the perpendicular spacing a between the layers to see how the interlayer interactions affected $\chi_{-}^{\mathrm{tot}}(\mathbf{q})$. For densities approaching the Wigner-crystal density for one layer ($r_s\simeq 37$) [2], the single-layer response function $\chi(\mathbf{q})$ diverges, causing the total response function $\chi_{-}^{\mathrm{tot}}(\mathbf{q})$ [Eq. (5)] to diverge for arbitrary layer spacing. If we consider a density higher than the critical density $r_s\simeq 37$, but smaller than $r_s\simeq 20$, then $\chi(\mathbf{q})$ is finite but with a large peak at $q_c/k_F\simeq 2.5$. This causes the total response function to diverge for a finite layer spacing a_c [Fig. 1(a)]. A Wigner transition is thus induced in this two-layer system for planar densities considerably larger than the critical density for one layer. The value of the critical wave number q_c for the Wigner-crystal transition should be insensitive to parameters of the system since it is given by the average spacing between electrons. On the other hand, the critical layer spacing a_c may weakly depend on details of the layer structure and also on the approximations used (see discussion below).

For densities approaching $r_s\simeq 20$ a second peak develops around $q_c/k_F\leq 2.0$ [Fig. 1(b)]. This wave number corresponds to a density modulation on a scale larger than the average interparticle distance, and we interpret it as a precursor for a two-dimensional charge-density wave in the plane of each layer. For $r_s=20$ the Wigner-crystal transition preempts any actual transition to a charge-density-wave ground state, but when the density increases there is a sharp crossover from the Wigner instability to the charge-density-wave phase transition.

At larger density $r_s=10$, only the peak corresponding to the charge-density wave survives. The critical wave number has now moved down to $q_c\simeq 1.8k_F$ [Fig. 1(c)]. By $r_s\simeq 5$ the charge-density-wave instability occurs for $a/a_B^*\simeq 2$. In this case appreciable tunneling between layers would be expected to occur [4], an effect which we have neglected in this calculation.

We turn now to a discussion of the influence on our results of the electron occupation numbers $n(\mathbf{p})$, the width of the layers d, and the number of the layers N. In Tables I and II we compare results for the Wigner crystal and the charge-density wave for the occupation numbers $n(\mathbf{p})$ taken from Ref. [2] for $r_s=10$, and for $n(\mathbf{p})$ set equal to the Fermi-Dirac step-function distribution (f_{10} and f_0, respectively). We also compare results for two values of the layer thickness ($d=a_B^*$ and $2a_B^*$), and for two layers and an infinite superlattice ($N=2$ and ∞).

(i) Occupation numbers.—Reference [2] gives results for the occupation numbers $n(\mathbf{p})$ for the interacting two-

TABLE II. Charge-density-wave critical wave number q_c and critical layer spacing a_c.

	$\{N=2, f_{10}, d=a_B^*\}$		$\{N=2, f_0, d=a_B^*\}$		$\{N=2, f_{10}, d=2a_B^*\}$		$\{N=\infty, f_{10}, d=a_B^*\}$	
r_s	q_c/k_F	a_c/a_B^*	q_c/k_F	a_c/a_B^*	q_c/k_F	a_c/a_B^*	q_c/k_F	a_c/a_B^*
20	...	...	...	...	2.0	9.6	2.0	13.5
10	1.8	3.2	2.0	4.7	1.7	3.4	1.5	5.1

dimensional electron liquid, but only for densities down to $r_s \simeq 10$. We found that the form of $n(\mathbf{p})$ is not critical to our results, and for the results in Fig. 1 we used $n(\mathbf{p})$ taken from Ref. [2] for $r_s = 10$. We obtain broadly similar results for the Fermi-Dirac distribution function (compare columns $\{N=2, f_{10}, d=a_B^*\}$ and $\{N=2, f_0, d=a_B^*\}$ in the tables). In this case, however, the singularity at $q=2k_F$ in $\chi_0(\mathbf{q})$ is stronger because of the larger discontinuity in $n(\mathbf{p})$ at $\mathbf{p} \simeq k_F$. This shifts the critical wave vector for the charge-density wave from $1.8k_F$ to $2.0k_F$.

(ii) Width of the layers.—In GaAs/AlGaAs systems the characteristic barrier height is 0.3 eV. This sets up a lower limit of around 100 Å on the spatial extent of the envelope function $\zeta(z)$. We found that the results were insensitive to the detailed shape of the potential well, and so for our results in Fig. 1 we confined $\zeta(z)$ by infinite potential walls at $z = \pm d/2$, with $d = a_B^*$. A larger value of d marginally favors the charge-density wave, pushing down the crossover to Wigner crystallization to slightly lower densities. In the tables we compare results for $\{N=2, f_{10}, d=2a_B^*\}$ with $\{N=2, f_{10}, d=a_B^*\}$.

(iii) Number of layers.—To check the sensitivity of the results to the number of electron layers, N, we consider the case of an infinite number of layers separated by a. In this case we can solve Eq. (1) by introducing a discrete Fourier transform in the direction perpendicular to the layer, obtaining for the static response function of the system

$$\chi^{\mathrm{tot}}(\mathbf{q},k) = \frac{\chi(\mathbf{q})}{1+[V(\mathbf{q},k)-V(\mathbf{q})]\chi(\mathbf{q})}, \tag{8}$$

where k is the quasimomentum perpendicular to the superlattice layers, and

$$V(\mathbf{q},k) = \sum_l e^{-ik(l-l')a} V_{ll'}(\mathbf{q}). \tag{9}$$

$\chi^{\mathrm{tot}}(\mathbf{q}, k=\pi/a)$ for the superlattice corresponds to $\chi^{\mathrm{tot}}_{-}(\mathbf{q})$ for two layers, in the sense that the modulated density distributions on adjacent layers are in both cases π out of phase. It is straightforward to show that $\chi^{\mathrm{tot}}(\mathbf{q},k)$ diverges most readily for $k=\pi/a$. The tables show that for two layers, $N=2$, the crossover to the Wigner crystal occurs at a slightly higher density than for the infinite superlattice ($N=\infty$).

We conclude that the behavior of the system is critically dependent only on the planar electron density and the spacing between the layers, and not on the form of the single-particle distribution function $n(\mathbf{p})$, the layer thickness, or the number of layers.

In summary, we have shown that in multiple electron layers, the Coulomb interaction between layers can cause the Wigner-crystal phase transition to occur at a factor of 3 higher planar density compared with the transition density for a single isolated layer. The transition density depends sensitively on the perpendicular spacing between the layers, but not on the number of layers. Combining this mechanism with other experimental tuning techniques may make the Wigner crystal in zero magnetic field more experimentally accessible than previously suspected. We have also shown that the same mechanism, when operating at higher planar densities, can produce charge-density-wave ground states.

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