Correlation and exchange of three-dimensional and quasi-two-dimensional electron gases in a strong magnetic field

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Generalizations of different trial wave functions for two-dimensional (2D) electrons to 3D and quasi-2D situations are discussed. The question of optimizing the Coulomb and kinetic energies with respect to the occupied fraction of available angular momentum states is studied. A "transition" where the planar filling factor becomes less than 1 is found. The possibility of observing the fractional quantized Hall effect in 3D systems is investigated.

I. INTRODUCTION

Recently there has been much interest in the quantum physics of electrons in strong magnetic fields, stimulated partly by the possible observation of a Wigner solid or charge-density wave[1–5] (CDW) in three-dimensional (3D) systems and partly by the observation of the integral and the fractional quantized Hall effects (FQHE) in two-dimensional (2D) systems.[6,7] In 2D, the planar filling factor, ν_{2D}, defined as the fraction of available angular momentum states that are filled, can be changed by varying the external magnetic field. For ν_{2D} very small, the system is expected to form a CDW. At intermediate ν_{2D} the system is much more complicated, however. Chui *et al.*[8] have investigated a series of correlated Gaussian wave functions with different amounts of correlations. They came to the conclusion that, because of the exchange, there are large positional fluctuations in the system. The lowest energy state that they found corresponds to a classical solid at a finite temperature. Laughlin[9] proposed a fluidlike wave function that seems to agree well with results from small sample diagonalizations. It is generally agreed now that the nature of the ground state is quite different at integer and at fractional filling factors.[8–10] For both filling factors, there is no long-range positional order in the xy direction. The present paper examines possible generalizations of these wave functions to 3D and quasi-2D systems. We shall study a system with no impurities and shall use the angular momentum gauge in what follows.

In 3D and quasi-2D systems, the single-particle wave functions are characterized by both the z momentum as well as the quantum numbers such as the angular momentum and Landau-level index that characterized 2D systems. We mean by a quasi-2D system here one that consists of a stack of planes with interplanar spacing d; the hopping integral t in the z direction is usually quite small. When the z momentum is small, the kinetic energy in the z direction can be approximated by the continuum form but with a large effective mass.

One of the simplest class of wave functions for 3D and quasi-2D systems consists of symmetrized products of 2D wave functions φ previously studied and plane waves along the z direction, viz.,

$$\psi=\sum_P(-1)^P\prod_j\varphi(r_{P(1,j)},r_{P(2,j)},\ldots)\exp i\sum_m(k_jz_{P(m,j)}) \quad (1)$$

where one sums over all possible permutations P. We have written the wave function in a general form so as to encompass a class of possibilities as φ is changed. A simple choice is $\varphi=\varphi_F$, a determinant of the angular momentum orbitals. The electrons are labelled by two subscripts: m, for the angular momentum and k, the z momentum. Two electrons must have different m if they have the same z momentum k_j. Assume that, on the average, a total K and M of z- and angular-momentum states, respectively, are occupied. Then $KM=N\nu$ where N is the total number of states and $\nu=N_e/N$ is the ratio of the total number of electrons to the total number of states. It is only the product KM that is fixed. The maximum m is given by $M_{\max}=A/(2\pi l^2)$ where A is the planar area. For a quasi-2D system one can fill the k states up to a maximum of $K_{\max}=\pi/d$. For a 3D system so that the z motion is continuous, the maximum z momentum is determined by the requirement that only one Landau level is filled. Otherwise one needs to fill up the next Landau level. This implies $(\hbar K_{\max})^2/2m=\hbar\omega_c$. To make a connection with one's understanding of 2D systems, one can define a planar filling factor $\nu_{2D}=M/M_{\max}$ as the fraction of angular momentum states that are filled. In the absence of the electron-electron (e-e) interaction, the lowest energy state corresponds to $\nu_{2D}=1$. As the external magnetic field is varied, only the Fermi wave vector along the z direction, k_F, is changed. Because there is no gap in exciting an electron to a different z momentum, the fractional quantized Hall effect (FQHE) will not be seen in 3D systems of this nature. In the presence of the e-e interaction, this picture may change. If the Coulomb repulsion is strong, the electrons will try to stay apart in the xy direction as well as in the z direction. If one had picked $M=M_{\max}$, then there is no way one can adjust the xy motion to lower the potential energy in the xy direction, hence we expect $M<M_{\max}$ and the physics may be similar to the 2D situation at some filling factor. If the kinetic energy is strong, then $K=\nu K_{\max}$, $M=M_{\max}$ and the noninteracting picture

will be a good starting point from which detailed calculations can be carried out. We shall show in this paper that the recently studied experimental systems[11,1] exhibit parameters near the region such that a "transition" where M becomes less than $M_{\max}$ is expected to occur (Figs. 1 and 3).

This "transition" can also be appreciated from a different perspective. At low densities and strong magnetic fields, CDW's are expected to develop.[1-5] The CDW in the 3D systems is expected to exhibit long-range positional order. On the other hand, if the planar filling factor is 1 there cannot be long-range positional order in the xy plane. For any transition to a state with long-range order in the transverse direction to take place, the planar filling factor has to be less than 1. Thus as the strength of the e-e interaction is increased, we expect a tendency towards the formation of a CDW and the planar filling will become less than 1. However, that the planar filling factor is less than 1 does not imply the existence of long-range translational order, as is evidenced by the investigations in the 2D FQHE. Thus in principle there can be two "transitions" whereby the planar filling factor becomes less than 1; then long-range order in the xy direction is developed. In addition, a CDW (Peierls) or SDW instability may also develop along the z direction but not necessarily at the same time.

To understand the nature of the ground states under different regimes, we have investigated wave functions of increasing complexity. Our results suggest that, in order to achieve a state such that the $\nu_{2D}<1$ with no long-range order in the xy plane, it is necessary that a CDW be formed and a corresponding gap developed along the z direction. Otherwise the charge fluctuation along the z direction reduces the Coulomb energy that might be gained with a smaller ν_{2D}. The energies of representative cases will be discussed and compared with each other at the end.

II. NO CDW ALONG THE z DIRECTION

We first examine a class of wave functions with no CDW along the z direction. In general, because of the anisotropic nature of the system, a CDW is expected to occur along the z direction at zero temperature. The present calculation is not superfluous, however. First, it examines wave functions that are still not too complex so that they will be good model systems by which we can gain understanding of the driving force behind different phenomena that might be manifested. It may also be a good starting point from which the ordering in the z direction can be incorporated. Secondly, it may approximate the real situation when the gap along the z direction is not big. Thirdly, the CDW may disappear at a finite temperature and our calculation may shed some light for that case.

A. $\nu_{2D}=1$

We first look at the case for which the planar filling factor is 1. Assuming that the z part of the wave function is free-electron-like, the wave function assumes the form in Eq. (1). The structure factor of this state is equal to[12]

$$S(q,p)=1-\exp(-q^2/2)f(p)+(2\pi)^2\delta(\mathbf{q})\delta(p)\alpha \tag{2}$$

where, for quasi-2D systems such as heterojunctions which consist of discrete planes

$$f(p)=\alpha d\sum_z \exp(ipz)\sin^2(k_F z)/(k_F z)^2 , \tag{3a}$$

where one sums over all the planes labelled by z. α is the number of electrons per unit length along the z direction. For 3D systems so that z becomes continuous

$$f(p)=[1-|p|/(2k_F)]\Theta(|p|<k_F). \tag{3b}$$

Here Θ is the step function that is 1 only when the condition imposed by its argument is satisfied. Otherwise it is zero. $S(q,p)$ does not exhibit any "Bragg peaks" as a function of q. Hence for $\nu_{2D}=1$ the system is a fluid. Long-range order in the xy plane can only develop after the planar filling factor becomes smaller than 1. The dependence on q is exact. The pair-correlation function, defined as the Fourier transform of S by

$$g(r)=\int\int \rho^{-1}(S-1)dp\, d^2q/(2\pi)^3,$$

is given by $g_F(r)=1+h_2(r)h_1(z)$ where

$$h_1(z)=[\sin(k_F z)/(k_F z)]^2.$$

$h_2(r)=-\exp(-r^2/2)$ is defined in terms of the 2D pair-correlation function by $1+h_2(r)=g_2(r)$. The in-plane correlation at $z=0$ is thus the same as that for the 2D fully filled case. When Fourier transformed back into real space, the function f becomes h_1. It keeps the electrons apart and represents the effect of the exchange hole in the z direction.

The magnetoplasmons of this state, including both the ladder and the bubble contribution and the possibility of interplane hopping, has been recently discussed by the author[13] and will not be repeated here.

B. $\nu_{2D}<1$

When the planar filling factor is less than 1, one possible way to extend the trial wave functions discussed in the FQHE to the present case is to use Eq. (1) except that φ is now replaced by a wave function that can be, in increasing amount of positional fluctuation, the uncorrelated Wigner solid φ_W,[14] the magnetophonon wave function,[8] the correlated Wigner solid discussed by Chui, Hakim, and Ma[8] φ_{CHM}, or the fluid wave function by Laughlin[9] φ_L. This class of wave functions is the simplest choice if a CDW has not developed along the z direction. Whereas the Laughlin wave function can be defined only at specific filling factors, such is not the case for the other wave functions.

In contrast to the FQHE, because of the possibility of exciting to a state with a different z momentum, the excitations in the present case for the above wave functions may not possess a gap. There are two limits corresponding to very little transverse order ($\varphi=\varphi_L$) and a lot of transverse order ($\varphi=\varphi_W$) that are simple enough that the results are analytically tractable. The results of these limits suggest that the former is not energetically favorable, whereas for the latter the excitations are gapless. Hence

the FQHE will not be seen unless long-range order, either intrinsic (due to a CDW along the z axis) or extrinsic (such as is imposed by the quasi-2D layer structure when all the planes are occupied) is developed along the z direction. We now examine these two limits in detail.

For $\varphi=\varphi_L$, any permutation P_0 that does not permute the electron between planes (no change in j) should be excluded in the form in Eq. (1). This is due to the following. The Laughlin wave function is fully antisymmetric, i.e.,

$$\varphi_L[r_{P_0}(1,j),r_{P_0}(2,j),\dots]=(-1)^{P_0}\varphi_L(r_{1,j},r_{2,j},\dots)\ .$$

Any permutation P_0 that does not change the z coordinate only changes the sign of the different contributions to the wave function and does not generate new terms in the sum. Hence they should be excluded.

The pair-correlation function of this function can be expressed in terms of the one-particle density matrix of φ_L. More precisely, the pair-correlation function is given by

$$\sum_P(-1)^P\int_{l,a\neq m,b;n,c}\prod_j\varphi(r_{P(1,j)},r_{P(2,j)},\dots)\varphi^*(r_{1,j},r_{2,j},\dots)\exp\left[i\sum_m(k_{P^{-1}j}-k_j)z_{m,j}\right]$$

where one integrates over all variables except the two labelled by m,b and n,c. The direct term corresponds to $P=1$ and provides for the contribution

$$\int_{l,a\neq m,b;n,c}\prod_j|\varphi(r_{1,j},r_{2,j},\dots)|^2.$$

When the two electrons labelled by m,b and n,c are on the same plane ($b=c$) this is equal to $V\rho g_2(r_{mn})$ where $g_2(r)$ is the 2D pair-correlation function. When the two electrons are on different planes ($b\neq c$), it is simply equal to ρ. We next focus on the exchange contribution with $P\neq1$. It is straightforward to see that the only contributions come from two-particle exchanges. The z integration requires all except two of the j's to be the same. As we argue at the beginning of this section, we need only sum over those permutations P such that $c\neq b$. We get the contribution

$$-\sum_{k,k'}\int\varphi(r_{m,b},\dots,r,\dots)\varphi(r_{n,c},\dots,r',\dots)\varphi^*(r_{n,c},\dots,r,\dots)\varphi^*(r_{m,b},\dots,r',\dots)\exp[i(k-k')(z_{m,b}-z_{n,c})]$$

where the variables r,r' are being integrated. The integral

$$\int\varphi(r_{m,b},r,\dots)\varphi^*(r_{n,c},r,\dots)=\frac{\nu_{2D}}{2\pi}\exp\{-|\mathbf{r}_{m,b}-\mathbf{r}_{n,c}|^2/4+[(x_{m,b}-iy_{m,b})(x_{n,c}+iy_{n,c})-(x_{m,b}+iy_{m,b})(x_{n,c}-iy_{n,c})]/4\}$$

is the Green's function. Collecting the different contributions, we obtain the result

$$g(r_{m,b},r_{n,c})=\rho[(Nk-1)+g_2(r_{m,b;n,c})]/Nk-\rho h_1(z_{m,b}-z_{n,c})\exp(-|\mathbf{r}_{m,c}-\mathbf{r}_{n,c}|^2/2). \tag{4}$$

The term $[-1+g_2(r)]/N$ is infinitesimally small in the thermodynamic limit and can be ignored. Hence $g(r)$ is given by the same form as the fully filled case except that the Fermi wave vector k_F is larger. Thus for this type of wave function, the exchange-correlation hole does not exhibit a larger transverse dimension. Even though electrons with the same k are kept apart, electrons with different k's are quite close to each other in the xy direction. The Coulomb energy is not enhanced and will be larger than that for which the planar filling factor is 1. This calculation suggests that no FQHE can be observed in 3D systems if no CDW is developed along the z direction.

We next consider the other limit with $\varphi=\varphi_W$. This may be a better approximation at low densities. The electrons occupied a symmetrized product wave function consisting of uncorrelated Gaussian orbitals $\exp(-|\mathbf{r}-\mathbf{R}_j|^2/4)$ located on a triangular lattice in the transverse direction at positions labelled by $\mathbf{R}_j$. We can write the structure factor S as a sum of a direct and an exchange contribution, viz.,

$$S=1+S_d+S_e.$$

For a quasi-2D system, the z motion is discrete; the direct contribution is given by

$$S_d=\sum_{i,j}\sum_{z_{1,2}}\int d\mathbf{r}_1d\mathbf{r}_2\frac{1}{N_z^2(2\pi)^2}\exp(-|\mathbf{r}_1-\mathbf{R}_i|^2/2-|\mathbf{r}_2-\mathbf{R}_j|^2/2-i\mathbf{q}\cdot\mathbf{r}_{12}+ipz_{12})/N$$

$$=\sum_{n,m}\exp(-G_m^2)\delta(p=K_n)\delta(\mathbf{q}=\mathbf{G}_m)N-\exp(-q^2)\sum_n\delta(p=K_n)$$

where $K_n=2\pi n/d$. G is the reciprocal-lattice vector in the transverse direction. The exchange contribution is given by

$$S_e=\sum_{i,j}\sum_{z_{1,2}}\int d\mathbf{r}_1\mathbf{d}_2\frac{1}{N_z^2(2\pi)^2}\exp[i\mathbf{z}\times\mathbf{R}_{ij}\cdot\mathbf{r}_{ij}/2-|\mathbf{r}_1-\mathbf{R}_i|^2/4$$

$$-|\mathbf{r}_2-\mathbf{R}_j|^2/4-|\mathbf{r}_2-\mathbf{R}_i|^2/4-|\mathbf{r}_1-\mathbf{R}_j|^2/4-i\mathbf{q}\cdot\mathbf{r}_{12}+i(p-k)z_{12}]/N$$

where $k=k_1-k_2$. The calculation of this overlap is identical to that in the 2D situation. For filling factors less than

one-third, the sites R_i are far enough apart so that the overlap contribution to S from terms with $R_i \neq R_j$ is quite small. After the r,z integrations are performed, the exchange contribution is given by

$$S_e = -\sum_{\mathbf{R}} \exp(-|q|^2 - Z^* q - |R_{ij}|^2/2) f(p)$$

where $f(p)$ is defined in Eq. (3). $Z = X + iY$, $q = q_x + iq_y$. Collecting the different contributions to S, we thus get

$$S(q,p) = 1 - \sum_{\mathbf{R}} \exp(-|q|^2 - Z^* q - |R_{ij}|^2/2) f(p) + \sum_{n,m} \exp(-G_m^2)\delta(p = K_n)\delta(\mathbf{q} = \mathbf{G}_m) N - \exp(-q^2) \sum_n \delta(p = K_n), \tag{5}$$

$Z = X + iY$, $q = q_x + iq_y$. The pair-correlation function in real space is dominated by the contribution from electrons in the same cylinder and is equal to

$$1 - \sum_R \exp - (|\mathbf{R}_{ij}|^2|/2) h_1(z) \exp - (r^2/4).$$

We now have a factor $\exp-(r^2/4)$ instead of the factor $\exp-(r^2/2)$ that appears in the pair distribution function $g_F(r)$ for the $\nu_{2D}=1$ case discussed in Sec. II A. This crucial difference comes from a correlation in the mean xy position of electrons with different momenta in the present case. As a consequence of this term, the exchange-correlation hole exhibits a larger transverse dimension than that for the fully filled case. Hence this state can be more favorable than the case $\nu_{2D}=1$ when the Coulomb energy is strong.

There are two different kinds of excitations for this case, one associated with exciting electrons to a higher kinetic energy along the z axis, the other with a phonon motion of the lattice along the z direction. Both excitations are gapless; hence no FQHE can be observed for this case as well.

The energy of this state relative to that at fully filled is discussed in the last section. We found that some of the recently studied heterojunctions possess parameters close to the region such that the present state is more favorable than the case with $\nu_{2D}=1$.

For all the ground states discussed so far, the single-electron excitation energy does not exhibit a dispersion in the transverse direction. Because of this, a Peierls (CDW) instability in the z direction will most likely result at low temperatures. We next turn our attention to this possibility.

III. A CDW EXISTS ALONG THE z DIRECTION

When a CDW (or SDW) is developed along the z direction, we expect the FQHE to be observable. A trivial example of this occurs when all the planes of a heterojunction are filled. In that case it is easy to write down an alternative wave function

$$\psi' = \sum_P (-1)^P \prod_j \varphi(r_{P(1,j)}, r_{P(2,j)}, \ldots) \prod_m s(Z_j - z_{P(m,j)}) \tag{6}$$

where in place of plane waves along the z direction, we can use Wannier orbitals s since a Slater determinant of completely filled band of plane-wave states is the same as the Slater determinant of Wannier orbitals. The crucial feature is that there will be a gap in the electronic excitation spectrum in the z direction so that the FQHE can be observed for this case.

When not all the planes are filled a reasonable generalization that corresponds to a CDW along the z direction consists of assuming that the electrons occupy Wannier orbitals $s(z\text{-}Z)$ with the plane positions z on which the electrons are located regularly spaced. Functions of this type may be important when the interplane hopping is small. Depending upon the choice of φ, there may or may not be long-range order in the xy plane. This type of wave function can possess exchange-correlation holes with much wider transverse dimensions.

In both the 3D and quasi-2D limits, a simple but approximate formula for the pair distribution function can be obtained by interpolation between the limits $r=0$, arbitrary z and $z=0$, arbitrary r as $g(r) = 1 + h_2(r) h_1(z)$ where $h_2(r)$ is the corresponding 2D distribution function for the wave function φ and h_1 is the 1D pair distribution function for two electrons in the same state for their xy motion. This formula also reduces to Eq. (2) when the planar filling factor is equal to 1. The total energy consists of the kinetic energy due to the one-dimensional motion of the electrons and the Coulomb energy,

$$-\nu_{2D} \int d\mathbf{q} \sum_{z=nd} \exp(-q|z|) h_2(\mathbf{q}) h_1(z)/2\pi q,$$

of the 2D wave function φ.

It is interesting to ask what the best choice of φ will be. From physical considerations, we expect that at low densities $\varphi = \varphi_{HF}$. This corresponds to a 3D CDW such as is discussed by Kuramoto.[15] At high densities the system may exhibit large positional fluctuations in the xy direction. $\varphi = \varphi_L, \varphi_{\mathrm{CHM}}$ may be more appropriate. The excitations may exhibit a gap and the FQHE may be observable in this case. k_F can now be varied. As is discussed in the Introduction, only the product of the linear density and the planar density is a constant. The energy of this case, as well as that in the previous sections, will be discussed in detail in the next section. We found that this state is energetically more favorable than the case with $\nu_{2D}=1$ when the Coulomb energy is large.

A mean-field calculation of the effect of interplane coupling on the CDW order in the transverse direction has been discussed by Chui[12] and will not be repeated here.

IV. ENERGIES

We look at the energies of some representative cases in this section. The calculation of the energy of the quasi-2D case, the case with Laughlin-type correlations for the continuum 3D limit [$\varphi=\varphi_L$ in Eq. (1)], and the cases with the CDW developed along the z direction are new. For the sake of completeness, we have also recalculated some other phases that have been discussed previously so that these results can be compared with each other. The difference between the quasi-2D limit that consists of discrete planes and the continuum 3D limit lies in the fact that in the quasi-2D limit the interplane spacing d as well as the interplane hopping matrix element can be varied. Hence the available "phase space" is much richer. The potential energy E has been computed numerically from the structure factor $S(q)$ discussed in the previous sections with the formula

$$E=\int d\mathbf{q}[S(q)-1]v(q).$$

Here $v(q)$ is the Fourier transform of the Coulomb interaction. Our results are summarized in Figs. 1–3 which we now discuss in detail.

We first look at the quasi-2D limit and investigate, as the strength of the Coulomb interaction is increased with respect to the kinetic energy, when ν_{2D} starts becoming less than 1. We calculate the energy of a wave function of type ψ as in Eq. (1) first with $\varphi=\varphi_F$ when all available angular momentum states are occupied, then with $\varphi=\varphi_W$ for the uncorrelated solid corresponding to partially occupied angular momentum states. For the latter case, we calculate lattices with different spacings to determine the optimum value. The results are summarized by a "phase diagram" in Fig. 1 as a function of the interplane spacing d and ratio of kinetic energy of the z motion to the electrostatic energy $c=(\hbar^2/m^*l^2)/(e^2/\varepsilon l)$. The squares represent regions where the "partially filled" solid has the same energy as the "fully filled" fluid. Regions with $K=k_{\max}$ lie in the lower right and regions with $M=m_{\max}$ lie in the upper left of this diagram. We have assumed that the kinetic energy associated with the motion in the z direction can be described by an effective mass approximation. We have also compared the energy of ψ ($\varphi=\varphi_F$) with the "partially filled correlated" fluid ψ' ($\varphi=\varphi_L$) with a CDW developed along the z axis. For this calculation, we have assumed that the spatial ex-

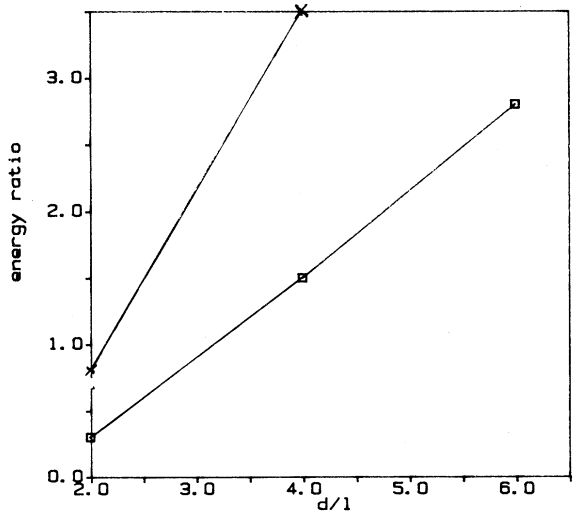

FIG. 1. A phase diagram as a function of the interplane spacing d and ratio of kinetic energy of the z motion to the electrostatic energy $c=(\hbar^2/m^*l^2)/(e^2/\varepsilon l)$. The squares represent regions where the "partially filled" solid has the same energy as the "fully filled" fluid; the squares, the energy of ψ ($\varphi=\varphi_F$) equals that of the "partially filled" fluid ψ' ($\varphi=\varphi_L$) with a CDW developed along the z axis. The lines are drawn through the points to guide the eye. Regions with $K=k_{\max}$ lie in the lower right and regions with $M=m_{\max}$ lie in the upper left of this diagram.

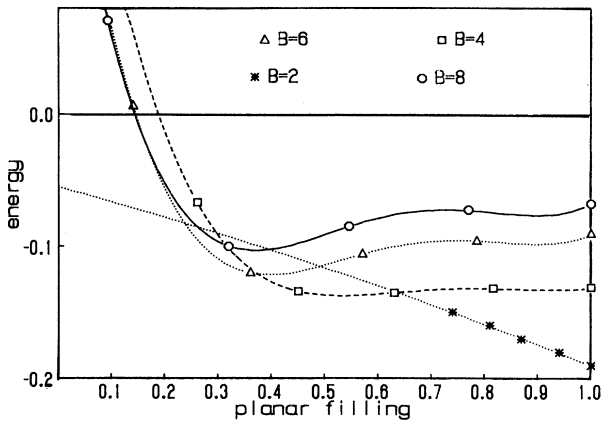

FIG. 2. The energy for a square lattice as a function of the planar filling $\nu_{2D}=2\pi l^2/\rho$ for magnetic field strengths $B=8$ (squares), 6 (triangles), 4 (diamonds), 2 (crosses) kG. The lines are drawn through the points to guide the eye. For each magnetic field, the planar filling stops at $\nu_{\min}$.

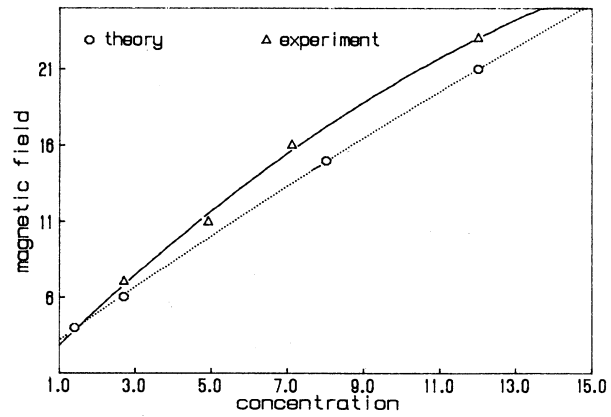

FIG. 3. A phase diagram for the depinning transition as a function of the electron concentration with parameters appropriate for $Hg_{1-x}Cd_xTe$. The magnetic field is expressed in units of kG. The concentration is in units of $10^{14}\,cm^{-3}$. Also shown are the experimental boundaries of Goldman *et al.*

tent of the function s is small enough compared with the spacing between the layers that they can be approximated by a δ function. The transition region is shown by the crosses in the figure. These two results together provide for an estimate as to when the angular momentum states become partially filled. On the upper left corner, we have a fully filled fluid that resembles the noninteracting state. On the lower right-hand corner, we have the partially filled states which can be a fluid or a solid as far as the transverse dimension is concerned. The two lines provide for an estimate of the uncertainty that can come in because of our lack of a definitive understanding of the correlation at this point. We considered it premature to compare the energy of the partially filled "uncorrelated" solid and the partially filled "correlated" fluid with a CDW along the z direction. A fair comparison would require a detailed study and the incorporation of correlations in the partially filled solid as well.

For the GaAs heterojunction studied by Stormer *et al.*,[11] the bandwidth w due to interplane hopping is of the order of $0.03\hbar\omega_c$, the interplane spacing d is 226 Å and the planar electron density is 4.5×10^{11} cm^{-2}. For this density, the cyclotron radius l at $\frac{1}{3}$ filled will be 35 Å. Hence $d/l=6.5$ and the ratio of the kinetic energy of the z motion to the electrostatic energy $c\simeq2.8$. Hence from Fig. 1 one is close to the transition regions between the limits of $K=k_{\max}$ and $M=m_{\max}$. We thus expect this sample at higher magnetic field, or samples made with larger interplane spacing but at the same magnetic field, to exhibit either SDW or CDW instabilities and insulating behavior in the z direction. In our calculation, we have used a very simplified form for s. A better estimate of s will include the effect of the depletion region and will provide for accurate estimates of the transition regions.

Near the "transition" to a nonunity planar filling factor, the magnitude of the direct energy is usually $\frac{1}{3}$ to $\frac{1}{4}$ the total energy. The changes of this direct energy as the "transition" takes place are significant. For example, at $c=1.6$, $d=4$, $\frac{1}{3}$ filling, the minimum in energy occurs at a planar filling factor of approximately 0.5. As the planar filling factor is changed from 0.67 to 0.5, the total energy changes by 0.02, whereas the direct energy changes by 0.03. This direct energy has not been properly treated in previous calculations even for the continuum case.

We next look at the continuum 3D limit. There has been much experimental work recently on investigating the possibility of the formation of a CDW in the semiconductor $Hg_{0.76}Cd_{0.24}Te$.[1] Now the Larmor radius $l=811B^{-1/2}$Å where B is expressed in units of kG. The maximum Fermi wave vector $k_{\max}$ is determined by the requirement that the Fermi energy is less than the magnetic energy. We obtain $k_{\max}=\sqrt{2}/l$. For a given density ρ, this determines a minimum planar filling factor $\nu_{\min}=2.82\rho(l/1000)^3$. For a CDW, the system forms a lattice and is no longer circularly symmetric. We generalize the definition of the planar filling factor as $2\pi l^2/\rho$. Using these parameters, we have calculated the energy for both a square and a hexagonal lattice as a function of the planar filling for different magnetic field strengths. The results for the two lattices are quite close. Since we shall be comparing some of our results to a 3D tetragonal lattice we show in Fig. 2 the energies for the square lattice for an electron concentration $\rho=1.4\times10^{14}$ cm^{-3} as a function of the planar filling factor ν_{2D}. For $B=2$ kG the energy is lowest at $\nu_{2D}=1$. For $B>4$ kG, the transition has taken place and $\nu_{2D}<1$. An analysis of the different contributions to the total energy indicates that for small filling factor, the exchange energy E_e dominates. As the filling factor is increased towards the transition, both the kinetic energy and the direct energy E_d become important with E_d about half as big as the kinetic energy. We have carried out calculations for different electron concentrations c. The resulting phase diagram is shown in Fig. 3.

Shayegan *et al.*[1] recently observed that in heavily doped $Hg_{0.76}Cd_{0.24}Te$ the resistivities ρ_{zz}, ρ_{xx}, ρ_{xy} develop temperature dependences at different magnetic field strengths; which they call B_l, B_t, B_H, respectively. As a function of the concentration of the charge carriers, B_t is quite close to the calculated value of the field strengths for the depinning transition discussed here (Fig. 3). It is possible that B_t is associated with the depinning transition since at that point a change in the density of states for particle-hole excitation is expected to take place. This will have a stronger effect on ρ_{xx} than ρ_{xy}. At these field strengths, the extent of the wave functions are still big enough so that magnetic freezeout is not important. However, detailed studies of impurity effects need to be made before conclusive statements can be reached. The transition at a still higher magnetic field B_H is then presumably a localization transition, which may be connected with the CDW state but modified by the presence of the impurities. This affects both ρ_{xx} and ρ_{xy}.

V. SUMMARY

To summarize, in this paper we discuss generalizations of different trial wave functions for 2D electrons to 3D and quasi-2D situations. The question of optimizing the Coulomb and kinetic energies with respect to the occupied fraction of available angular momentum states is studied. A "transition" where the planar filling factor becomes less than 1 is found. Some recently studied experimental systems[11,1] exhibit parameters near the region where this "transition" is expected to occur (Figs. 1 and 3). Study of different trial wave functions suggests that the FQHE will not be seen unless long-range order, either intrinsic (due to a CDW along the z axis) or extrinsic (such as is imposed by the quasi-2D layer structure when all the planes are filled) is developed along the z direction.

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