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Influence of Landau-level mixing on the charge-density-wave state of a two-dimensional electron gas in a strong magnetic field

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The influence of Landau-level mixing on the charge-density-wave (CDW) state of the two-dimensional electron gas in a strong magnetic field has been investigated. We find that it is necessary to calculate the mixing self-consistently. The results show that little change in the ground-state energy results even when the interaction energy becomes stronger than the Landau-level separation but that there is a substantial change of the charge-density variation, especially for electron CDW states.

I. INTRODUCTION

Recently Yoshioka and Lee[1] have presented accurate calculations of the ground-state energy of the charge-density-wave (CDW) state of a two-dimensional electron gas in a strong magnetic field. This state, which was first studied by Fukuyama *et al.*[2] and by Yoshioka and Fukuyama,[3] had been proposed[4] as a possible explanation for the fractional quantum Hall effect,[5,6] but the calculations of Yoshioka and Lee[1] showed that the ground-state energy did not have the requisite cusps as a function of a Landau-level filling factor. Moreover, it has recently been established by Laughlin[7] that an "incompressible-quantum-fluid" state, which he invented, has lower energy than the CDW state, at least at some filling factors ($\nu = N/N_L$ where N_L is the number of states in a Landau level). This state is now thought to be the basis of the fractional quantum Hall effect. Nevertheless, the CDW state is still of interest since the energy difference between this state and Laughlin's state (or hierarchies thereof[8,9]) helps to determine the set of filling factors at which the fractional effect occurs.

In this paper we describe an investigation of the influence of Landau-level mixing on the CDW state. In most calculations it has been assumed that this mixing can be ignored, although it has been discussed in Appendix B of Ref. 1 and briefly by Yoshioka and Fukuyama.[10] In Sec. II we briefly describe the calculation and in Sec. III we discuss the consequence of including Landau-level mixing without allowing the charge density to relax. Finally in Sec. IV we allow the charge density to be determined self-consistently. We find that while the charge density changes substantially especially for electron (rather than hole) CDW states, there is only a small reduction in the ground-state energy. This is expected since, even without Landau-level mixing, the interaction energy is near the minimum value defined in the classical Madelung energy, and any gain in interaction energy is at the expense of a cost of kinetic energy. Our findings are summarized in Sec. V.

II. HARTREE-FOCK APPROXIMATION FOR THE CHARGE-DENSITY-WAVE STATE IN A STRONG MAGNETIC FIELD

For a two-dimensional electron gas in a magnetic field, if a Landau gauge is chosen, the eigenstates of the kinetic energy operator may be written as

$$\phi_{n,X}(\vec{r}) \equiv \langle \vec{r} \,|\, n,X \rangle = \frac{1}{(L_y)^{1/2}} \exp\left[\frac{iXy}{a_L^2}\right] \phi_n(x-X) \, , \qquad n = 0,1,2,\ldots \, , \tag{1}$$

where $\phi_n(x)$ is a one-dimensional harmonic-oscillator eigenstate with oscillator frequency $\omega_c = eH/mc$, $a_L = (\hbar c/eH)^{1/2}$ is the Larmor radius, and, for a finite system, the allowed values of the quantum number X are separated by $2\pi a_L^2/L_y$. Many of the unusual properties of this system in a strong field are due to the fact that the eigenvalue associated with the state $|n,X\rangle$, $\epsilon_{n,X} \equiv \epsilon_n = \hbar\omega_c(n+\frac{1}{2})$, is independent of X. (The manifold of states associated with a quantum number n is referred to as a Landau level.) In this paper we restrict ourselves to the Hartree-Fock approximation and, for clarity, use the language of single-particle wave functions (i.e., first, rather than second, quantization). Thus the Fourier components of the electron density are given by

$$\rho(\vec{q}) = \sum_{\alpha} n_\alpha \langle \alpha \,|\, \exp(i\vec{q}\cdot\vec{r}) \,|\, \alpha \rangle \, , \tag{2}$$

where the normalized single-particle eigenstates ($|\alpha\rangle$) solve the self-consistent equations

$$\sum_{n,X} \left[\hbar\omega_c(n+\tfrac{1}{2})\delta_{X',X}\delta_{n',n} + \sum_{\alpha'} n_{\alpha'} \left(\langle n',X';\alpha' \,|\, V_c \,|\, n,X;\alpha' \rangle - \langle n',X';\alpha' \,|\, V_c \,|\, \alpha';n,X \rangle \right) \right] \langle n,X \,|\, \alpha \rangle = \epsilon_\alpha \langle n',X' \,|\, \alpha \rangle \, , \tag{3}$$

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where $V_c(\vec{r},\vec{r}\,')=e^2/|\vec{r}-\vec{r}\,'|$ is the Coulomb interaction. The ground state is determined by choosing $n_\alpha=1$ for the N lowest eigenvalues and 0 otherwise, where N is the number of electrons in the system. The ground-state energy is conveniently expressed as

$$E=\tfrac{1}{2}\hbar\omega_c\left[N+\sum_\alpha n_\alpha\sum_n n\sum_X|\langle n,X|\alpha\rangle|^2\right]+\tfrac{1}{2}\sum_\alpha n_\alpha\epsilon_\alpha\ . \tag{4}$$

We want to find solutions for which $\rho(\vec{q})$ is nonzero only for $\vec{q}=\vec{G}$ where $\vec{G}$ is a reciprocal-lattice vector of a two-dimensional lattice. $\rho(\vec{q})$ may be expressed as

$$\rho(\vec{q})=\sum_{n,n'}\sum_{X',X}\rho_{nn'}(X,X')\langle n',X'|\exp(-i\vec{q}\cdot\vec{r})|n,X\rangle\ , \tag{5}$$

where the density matrix is given by

$$\rho_{nn'}(X,X')=\sum_\alpha n_\alpha\langle n,X|\alpha\rangle\langle\alpha|n',X'\rangle\ . \tag{6}$$

The matrix element

$$\langle n',X'|\exp(i\vec{q}\cdot\vec{r})|n,X\rangle=\delta_{X',X+a_L^2q_y}\exp[\tfrac{1}{2}iq_x(X+X')]F_{n',n}(\vec{q})\ , \tag{7a}$$

where

$$F_{n',n}(\vec{q})\equiv\frac{n!}{(n')!}\left[\frac{(-q_y+iq_x)a_L}{\sqrt{2}}\right]^{n'-n}\times\exp\left[\frac{-q^2a_L^2}{4}\right]L_n^{n'-n}\left[\frac{q^2a_L^2}{2}\right] \tag{7b}$$

for $n'\geq n$. [$L_n^\alpha(x)$ is the generalized Laguerre polynomial. For $n'<n$, $F_{n',n}(\vec{q})$ can be determined using the identity $F_{n,n'}(\vec{q})=F^*_{n',n}(-\vec{q})$.] It follows that the density matrix must take the form

$$\rho_{m_1m_2}(X_1,X_2)=\sum_j\Delta_{m_2m_1}(\vec{G}_j)\exp[\tfrac{1}{2}iG_{jx}(X_1+X_2)]\times\delta_{X_2,X_1-a_L^2G_{jy}} \tag{8}$$

and that

$$\rho(\vec{G})=\sum_{n',n}\Delta_{n',n}(\vec{G})F_{n',n}(-\vec{G})\ . \tag{9}$$

The sum in Eq. (8) is over the reciprocal-lattice vectors for the two-dimensional crystal structure.

Both the Hartree and Fock terms in Eq. (3) can be expressed in terms of $[\Delta_{n',n}(\vec{G})]$. For the Hartree term, we express the result in the form

$$\sum_\alpha\langle n_1,X';\alpha|V_c|n_2X;\alpha\rangle n_\alpha=\frac{e^2}{a_L}\sum_j\exp[\tfrac{1}{2}iG_{jx}(X+X')]\times\delta(X'-X-a_L^2G_{jy})\mathcal{H}(n_1,n_2;\vec{G})\ , \tag{10a}$$

where

$$\mathcal{H}(n_1,n_2;\vec{G})=\sum_{m_1,m_2}H(n_1,m_1;n_2,m_2;\vec{G})\Delta_{m_2,m_1}(\vec{G}) \tag{10b}$$

and

$$H(n_1,m_1;n_2,m_2;\vec{G})=\frac{1}{Ga_L}F_{n_1,n_2}(\vec{G})F_{m_2,m_1}(-\vec{G}) \tag{10c}$$

for $G\neq0$ and 0 otherwise.

The exchange term has an analogous form:

$$\sum_\alpha\langle n_1,X';\alpha|V_c|\alpha;n_2,X\rangle n_\alpha=\sum_j\exp[\tfrac{1}{2}iG_{jx}(X+X')]\times\delta(X'-X-a_L^2G_{jy})\mathcal{X}(n_1,n_2;\vec{G})\ , \tag{11a}$$

where

$$\mathcal{X}(n_1,n_2;\vec{G})=\sum_{m_1,m_2}X(n_1,m_1;n_2,m_2;\vec{G})\Delta_{m_2,m_1}(\vec{G}) \tag{11b}$$

and

$$X(n_1,m_1;n_2,m_2;\vec{G})=\int_0^\infty dq\,a_L\int_0^{2\pi}d\theta(2\pi)^{-1}\exp[ia_L^2(G_yq_x-q_yG_x)]F_{n_1,m_1}(\vec{q})F_{m_2,n_2}(-\vec{q})\ . \tag{11c}$$

The integral over θ in Eq. (11c) gives Bessel functions of integral order and, if the explicit form is used for the Laguerre polynomials, the integration over q may be performed to yield

$$X(n_1,m_1;n_2,m_2;\vec{G})=\exp(il\theta_G)[\mathrm{sgn}(l)]^l(i)^{s_1-i_1-s_2+i_2}M(s_1,i_1;s_2,i_2;|l|;G)\ , \tag{12a}$$

where $s_j=\max\{n_j,m_j\}$ and $i_j=\min\{n_j,m_j\}$ $(j=1,2)$, $l=n_1-m_1-n_2+m_2$,

$$M(n_1,m_1;n_2,m_2;l;G)=\left[\frac{\pi m_1!m_2!}{2n_1!n_2!}\right]^{1/2}G^l\exp\left[\frac{-G^2}{2}\right](\sqrt{2})^{m_1+m_2-n_1-n_2-2l}\times\sum_{k_1=0}^{m_1}\sum_{k_2=0}^{m_2}2^{-k_1-k_2}C_{k_1,m_1}^{n_1-m_1}C_{k_2,m_2}^{n_2-m_2}\frac{(t+l-1)!!}{l!}\,{}_1F_1(\tfrac{1}{2}(1+l-t);l+1;\tfrac{1}{2}G^2)\ , \tag{12b}$$

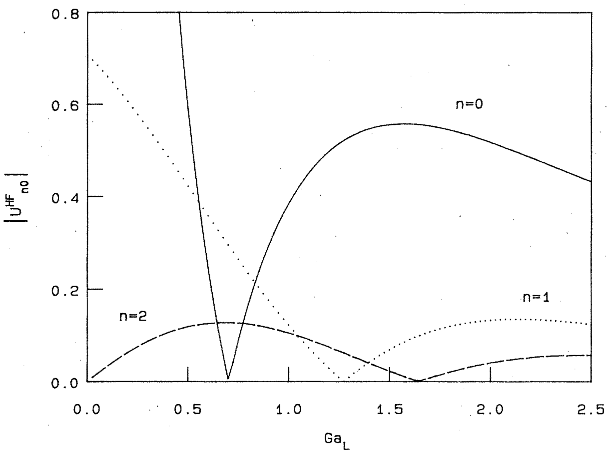

FIG. 1. $|U^{\mathrm{HF}}_{n0}(G)|$ versus Ga_L for $n=0$, 1, and 2. The effective coupling to higher Landau levels is strongest for $n=1$ at most G values.

and

$$t=n_1+n_2-m_1-m_2+2(k_1+k_2)\ .$$

[In Eq. (12b) $C^{\alpha}_{k,m}$ is the coefficient of x^k in $L^{\alpha}_m(x)$.]

In the calculations which we discuss below we consider the case in which only the lowest Landau level is partially occupied. Thus, as we shall see, $\Delta_{m'm}$ is near zero unless m' and m are both zero. Many of our results can be understood in terms of the $m_1=m_2=0$ term in Eqs. (10b) and (11b). This makes it useful to define the quantity

$$U^{\mathrm{HF}}_{n'n}(\vec{\mathrm{G}})=H(n',0;n,0;\vec{\mathrm{G}})-X(n',0,n,0;\vec{\mathrm{G}})\ , \qquad (13)$$

which is plotted in Fig. 1 versus $|\vec{\mathrm{G}}|$ for $n=0$ and $n'=0$, 1, 2. [$U^{\mathrm{HF}}_{n'n}(\vec{\mathrm{G}})$ equals $U_{nn'}(\vec{\mathrm{G}})$ as defined by Eq. (B1) of Ref. 1. Note, however, that there are misprints in that paper.] The small magnitudes for the $n'\neq n$ terms shown in Fig. 1 are in accord with the expectation that the Landau-level mixing will be weak.

In Eqs. (10a) and (11a) the factors $\mathscr{H}(n_1,n_2;\vec{\mathrm{G}})$ and $X(n_1,n_2;\vec{\mathrm{G}})$ are independent of X and X'. As a result the eigenvalue equations which we are required to solve at any stage in the iteration procedure are of the same form as those for an external potential of the same periodicity as that asumed for the CDW state. These equations can be solved for any assumed crystal structure of the CDW state in the manner discussed in Ref. 12. Our calculations were performed in the following steps.

(i) For $\hbar\omega_c\rightarrow\infty$ find the eigenstates for the case of noninteracting electrons in an external potential which produces a charge density of the desired form. As far as is known, for each crystal structure the lowest-energy CDW state has one electron per unit cell for $\nu<\frac{1}{2}$ and one hole (one electron less than a single full Landau level) for $\nu>\frac{1}{2}$. [By $\hbar\omega_c\rightarrow\infty$ here we mean, simply, that the mixing of the eigenstates into $n\neq0$ Landau levels is assumed to be negligible and the sum over n in Eq. (3) is truncated at $n=0$, i.e., there is no Landau-level mixing.] From these eigenstates $\Delta_{0,0}(\vec{\mathrm{G}})$ is calculated using

$$\Delta_{0,0}(\vec{\mathrm{G}})=L_x^{-1}\int dX_1\rho_{00}(X_1,X_1-a_L^2G_y)\times\exp\left[-\frac{i}{2}G_x(X_1-\tfrac{1}{2}a_L^2G_y)\right]. \qquad (14)$$

Note that $\Delta_{0,0}(\vec{\mathrm{G}}=\vec{0})=\nu$.

(ii) Self-consistently solve the Hartree-Fock equations without allowing Landau-level mixing. At each stage $\Delta_{0,0}(\vec{\mathrm{G}})$ is "mixed" with its value on the previous iteration. That is

$$[\Delta^{(j+1)}_{0,0}(\vec{\mathrm{G}})]_{\mathrm{in}}=\alpha[\Delta^{(j)}_{0,0}(\vec{\mathrm{G}})]_{\mathrm{in}}+(1-\alpha)[\Delta^{(j)}_{0,0}(\vec{\mathrm{G}})]_{\mathrm{out}}\ , \qquad (15)$$

where (j) is an iteration index, $[\Delta_{0,0}{}^{(1)}(\vec{\mathrm{G}})]_{\mathrm{in}}=\Delta^{(0)}_{0,0}(\vec{\mathrm{G}})$, $[\Delta^{(i)}_{0,0}(\vec{\mathrm{G}})]_{\mathrm{in}}$ is used to evaluate Eqs. (10b) and (11b) and (truncated to $m_1=m_2=0$) $[\Delta^{(j)}_{0,0}(\vec{\mathrm{G}})]_{\mathrm{out}}$ is obtained from the resulting eigenstates from Eq. (14) [the eigenstates from step (i) are used for $j=0$], and α is a numerical factor. We found that $\alpha\sim0.7$ gave reasonably rapid convergence. The sums over j in Eqs. (10a) and (10b) were truncated to include all $\vec{\mathrm{G}}$ vectors with $|\vec{\mathrm{G}}|<G_{\max}$, and $G_{\max}$ was chosen to be sufficiently large to have the sum rule[13]

$$\sum_j|\Delta_{0,0}(\vec{\mathrm{G}}_j)|^2=\nu \qquad (16)$$

satisfied to four figures ($G_{\max}\sim8a_L^{-1}$ for $\frac{1}{3}\leq\nu\leq\frac{2}{3}$).

(iii) Starting from the self-consistent solution without Landau-level mixing, continue iterating with Landau-level mixing allowed until a new self-consistent solution is reached. In this case the eigenvalue equations for the single-particle wave functions were determined by truncating after the $n_{\max}$ lowest Landau levels. The criteria used to determine $n_{\max}$ are discussed in the next section. The ground-state wave function and the ground-state energy in units of e^2/a_L, depend on the ratio of e^2/a_L to $\hbar\omega_c$ and calculations were performed for several values of this parameter for square- and triangular-lattice CDW states and for $\nu=\frac{1}{3}$, $\frac{1}{2}$, and $\frac{2}{3}$.

III. UNRELAXED LANDAU-LEVEL MIXING

Assume that a self-consistent solution of the Hartree-Fock equations has been found for the limit $\hbar\omega_c\rightarrow\infty$. For finite $\hbar\omega_c$ we must allow Landau-level mixing. For small values of $(e^2/a_L)/\hbar\omega_c$ the new single-particle wave functions and energies can be determined by leading-order (degenerate state) perturbation theory. Using Eqs. (10), (11), and (13) it follows that

$$|\alpha\rangle'=|\alpha\rangle-\frac{1}{\hbar\omega_c}\sum_{n,X'}{}'n^{-1}\langle n,X'|\delta H|\alpha\rangle|X'\rangle\ , \qquad (17a)$$

$$\epsilon_{\alpha'}=\epsilon_\alpha-\frac{1}{\hbar\omega_c}\sum_{n,X'}{}'n^{-1}|\langle n,X'|\delta H|\alpha\rangle|^2\ , \qquad (17b)$$

where

$$\langle n,X' \,|\, \delta H \,|\, \alpha \rangle = \frac{e^2}{a_L} \sum_{j,X} \exp[\tfrac{1}{2} i G_{jx}(X+X')] \delta_{X'-X-a_L^2 G_{jy}} U_{n0}^{\mathrm{HF}}(\vec{G}_j) \Delta_{0,0}(\vec{G}_j) \langle 0,X \,|\, \alpha \rangle \ . \tag{17c}$$

Using, in addition, Eqs. (6) and (8), gives

$$\begin{aligned} \delta E_{\mathrm{sp}} &\equiv \sum_{\alpha} (\epsilon_\alpha' - \epsilon_\alpha) n_\alpha \\ &= \frac{-(e^2/a_L)^2}{\hbar\omega_c} N_L \sum_{\vec{G}_1,\vec{G}_2}{}' \Delta_{0,0}(\vec{G}_1) \Delta_{0,0}(\vec{G}_2) \Delta_{0,0}(-\vec{G}_1 - \vec{G}_2) \exp[\tfrac{1}{2} i a_L^2 (G_{2x} G_{1y} - G_{1x} G_{2y})] \\ &\qquad \times \sum_{n}{}' n^{-1} U_{n,0}^{\mathrm{HF}}(\vec{G}_1) U_{0,n}^{\mathrm{HF}}(\vec{G}_2) \ . \end{aligned} \tag{18}$$

This is the quantity listed as ΔE in Eq. (B7) of Ref. 1. The primes on the sums over n in Eqs. (17) and (18) indicate that $n=0$ is excluded while the prime on the sums over $\vec{G}_1$ and $\vec{G}_2$ in Eq. (18) indicates that terms with $\vec{G}_1=\vec{0}$ or $\vec{G}_2=\vec{0}$ may be excluded since

$$|\, U_{n,0}(\vec{G}=\vec{0}) \,| = |\, U_{0,n}(\vec{G}=\vec{0}) \,| = 0$$

if $n \neq 0$.

The change in the total energy, for unrelaxed Landau-level mixing, is given to leading order in $(e^2/a_L)/\hbar\omega_c$ by

$$\begin{aligned} \delta E &= \tfrac{1}{2} \sum_{\alpha} n_\alpha \left[\epsilon_\alpha' - \epsilon_\alpha + \hbar\omega_c \sum_{n,X}{}' n \,|\, \langle n,X \,|\, \alpha \rangle' \,|^2 \right] \\ &= \tfrac{1}{2} \sum_{\alpha} n_\alpha \left[\epsilon_\alpha' - \epsilon_\alpha + \frac{1}{\hbar\omega_c} \sum_{n,X}{}' n^{-1} \,|\, \langle n,X \,|\, \delta H \,|\, \alpha \rangle \,|^2 \right] \\ &\equiv 0 \ . \end{aligned} \tag{19}$$

The first form on the right-hand side of Eq. (19) follows directly from Eq. (4) upon noting that $\langle n,X \,|\, \alpha \rangle = 0$ for $n \neq 0$, and the second form follows from using Eq. (17a) in the first term. Comparing the second form with Eq. (17b) makes it clear that this quantity vanishes. This result, which is surprising at first sight, provides a check on our computer code for calculating Landau-level mixing and we have verified that the energy change calculated for unrelaxed Landau-level mixing vanishes to leading order in $(e^2/a_L)/\hbar\omega_c$. There is an exact cancellation to this order between a gain in interaction energy and a cost in kinetic energy. δE_{sp} is negative because it double counts the change in the interaction energy. It is important to realize that when the Landau-level mixing is relaxed to self-consistency, as discussed in the next section, changes in the energy do occur to leading order in $(e^2/a_L)/\hbar\omega_c$, but these are not directly related to δE_{sp}. [Note from Eqs. (10b) and (11b) that if $\Delta_{n,0} \sim (e^2/a_L)/\hbar\omega_c$, this produces changes in the Hartree-Fock matrix elements within the lowest Landau level which are $\sim (e^2/a_L)^2/\hbar\omega_c$ and these must be determined self-consistently.] However, to the extent that it provides a measure of the degree of Landau-level mixing present before we relax to self-consistency, δE_{sp} does give some notation of the forces at play and helps us to understand the various numerical results we report in the next section.

Results for δE_{sp} are summarized in Table I. The sum in Eq. (18) is dominated by those terms with $\vec{G}_2 = -\vec{G}_1$ which all have the same sign. This contribution to the sum is

$$\delta \tilde{E}_{\mathrm{sp}} = \frac{-(e^2/a_L)^2 \,|\, N_L \nu}{\hbar\omega_c} \sum_{\vec{G}}{}' \,|\, \Delta_{0,0}(\vec{G}) \,|^2 \,|\, U_{\mathrm{eff}}(G) \,|^2 \ , \tag{20a}$$

where $U_{\mathrm{eff}}(G)$ gives a measure of the contribution to Landau-level coupling of charge variations with wave vector G and is defined by

$$|\, U_{\mathrm{eff}}(G) \,|^2 \equiv \sum_{n=1}^{\infty} \frac{|\, U_{n,0}^{\mathrm{HF}}(\vec{G}) \,|^2}{n} \ . \tag{20b}$$

This quantity is plotted in Fig. 2. Using Eq. (16) in Eq. (20a) gives

$$\delta E_{\mathrm{sp}} \simeq \delta \tilde{E}_{\mathrm{sp}} \simeq -\frac{(e^2/a_L)^2 N_L \nu^2 (1-\nu)}{\hbar\omega_c} \langle \,|\, U_{\mathrm{eff}}(G) \,|^2 \rangle \ , \tag{21}$$

where $\langle \,|\, U_{\mathrm{eff}}(G) \,|^2 \rangle$ is an average of $|\, U_{\mathrm{eff}}(G) \,|^2$ over the

TABLE I. Change in the average single-particle energy in leading order of perturbation theory. The $\nu=\frac{1}{3}$ CDW states have the periodicity of an electron Wigner lattice while the $\nu=\frac{2}{3}$ states have the periodicity of a hole Wigner lattice. For $\nu=\frac{1}{2}$ calculations were done for both electron and hole CDW states. δE_{sp} is in units of $10^{-3} N_L (e^2/a_L)^2/\hbar\omega_c$.

Lattice	Filling factor	Type of state	$-\delta E_{\mathrm{sp}}$
Square	$\frac{1}{3}$	Electron	0.861
Hexagonal	$\frac{1}{3}$	Electron	0.840
Square	$\frac{1}{2}$	Electron	1.845
Hexagonal	$\frac{1}{2}$	Electron	2.180
Square	$\frac{1}{2}$	Hole	1.848
Hexagonal	$\frac{1}{2}$	Hole	2.180
Square	$\frac{2}{3}$	Hole	1.184
Hexagonal	$\frac{2}{3}$	Hole	1.116

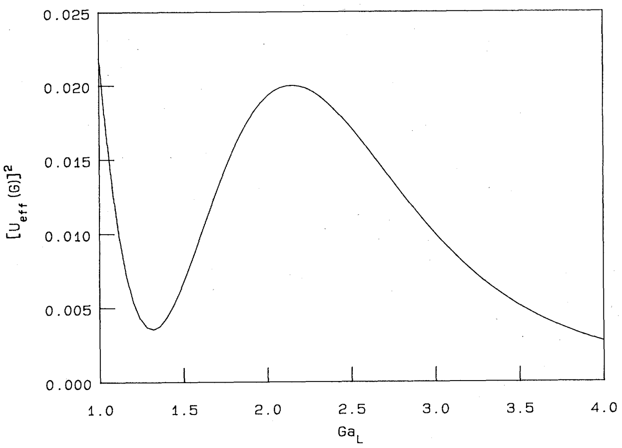

FIG. 2. $[U_{\text{eff}}(G)]^2$ versus Ga_L.

reciprocal-lattice vectors which dominate this sum rule, which for the case considered here are those in the first two shells. $Ga_L=1.447$ and 1.555, respectively, for the first shell of reciprocal-lattice vectors in square and hexagonal lattices from both the electron CDW state at $\nu=\frac{1}{3}$ and the hole CDW state at $\nu=\frac{2}{3}$. For both the electron and hole states at $\nu=\frac{1}{2}$, the same numbers are 1.772 and 1.904. Comparing with Fig. 2 it is clear that $\langle\, |U_{\text{eff}}(G)|^2\rangle$ should be larger at $\nu=\frac{1}{2}$. This, combined with the explicit filling factor dependence in Eq. (21), suggests that δE_{sp} should be largest near the middle of the Landau level. The numbers reported in Eq. (21) bear this out. We shall see in the next section that $\delta\widetilde{E}_{\text{sp}}$ is, in this aspect, a reliable indicator of the dependence of the change in ground-state energy on the filling factor. Equation (21) also suggests that δE_{sp} should be larger for the hole CDW states at $\nu>\frac{1}{2}$ than for the electron CDW states at $\nu<\frac{1}{2}$.[14] This impression turns out to be entirely misleading.

Another useful piece of information comes from the calculation of $\delta\widetilde{E}_{\text{sp}}$. We find that the entries in Table I have converged to within $\sim 1\%$ when the sum over Landau levels is truncated at the fifth level and to within better than a part in 10^4 when it is truncated at the tenth Landau level. We have used this fact to justify performing the calculations reported on in the next section in a Hilbert space truncated, for the most part, to the five lowest Landau levels. These calculations also show that δE_{sp} is relatively insensitive to the crystal structure. This insensitivity was verified for the ground-state energy calculations discussed in the next section and, although we performed calculations for several crystal structures, the results are reported only for the hexagonal case. In the absence of Landau-level mixing this structure gives the lowest energy except very near to $\nu=\frac{1}{2}$ where the ground-state energy is extremely insensitive to crystal structure and the square lattice seems to be narrowly preferred.[15]

IV. SELF-CONSISTENT CDW STATES

Our results for the energy are summarized in Table II, where results are reported for a series of values of $(e^2/a_L)/\hbar\omega_c$ and for electron CDW states at $\nu=\frac{1}{3}$ and $\frac{1}{2}$ and hole CDW states at $\nu=\frac{1}{2}$ and $\frac{2}{3}$. [The two $\nu=\frac{1}{2}$ CDW states become degenerate as $(e^2/a_L)/\hbar\omega_c$ approaches zero.] The most striking feature is that the energy change is much larger for the electron states. It is easy to understand why this must be so. The minimum of the interaction energy occurs for electron wave functions localized, as closely as possible, about the lattice sites. The ratio of the electron density at a lattice site to the average electron density is a measure of the degree to which this localization occurs for the electron CDW state. The maximum possible electron density at any position, when Landau-level mixing is not allowed, is $(2\pi a_L^2)^{-1}$ which is the uniform density of a filled Landau level. To the accuracy of our calculations[15] this density is achieved in the CDW states and so the ratio mentioned above is $1/\nu$, which becomes large for small ν. For small ν the interaction energy of the electron CDW state is very near to the classical limit but as ν approaches $\frac{1}{2}$ the maximum densi-

TABLE II. Energy per electron in units of e^2/a_L for hexagonal-lattice CDW states for several values of e^2/a_L. As usual, the zero of energy has been chosen to be the noninteracting (kinetic plus Zeeman) energy of the lowest Landau level. Results for the interaction energy and total energy are given for several values of $(e^2/a_L)/\hbar\omega_c$. The minimum possible interaction energy occurs for a lattice of point electrons. This Madelung energy is, in the above units -0.4516 at $\nu=\frac{1}{3}$, -0.5531 at $\nu=\frac{1}{2}$, and -0.6387 at $\nu=\frac{2}{3}$. The energy of Laughlin's state at $\nu=\frac{1}{3}$ is $\simeq -0.410$.

		$(e^2/a_L)/\hbar\omega_c$						
State	Energy type	0.0	0.5	1.0	2.0	3.0	5.0	10.0
$\nu=\frac{1}{3}$	Interaction	-0.3885	-0.3956	-0.4006	-0.4070	-0.4108	-0.4149	-0.4196
Electron CDW	Total	-0.3885	-0.3916	-0.3939	-0.3973	-0.3999	-0.4032	-0.4076
$\nu=\frac{1}{2}$	Interaction	-0.4435	-0.4580	-0.4681	-0.4805	-0.4875	-0.4950	-0.5022
Electron CDW	Total	-0.4435	-0.4497	-0.4545	-0.4617	-0.4666	-0.4731	-0.4811
$\nu=\frac{1}{2}$	Interaction	-0.4435	-0.4440	-0.4445	-0.4452	-0.4457	-0.4463	-0.4470
Hole CDW	Total	-0.4435	-0.4438	-0.4440	-0.4445	-0.4449	-0.4450	-0.4460
$\nu=\frac{2}{3}$	Interaction	-0.5076	-0.5080	-0.5084	-0.5090	-0.5095	-0.5100	-0.5107
Hole CDW	Total	-0.5076	-0.5078	-0.5080	-0.5084	-0.5087	-0.5091	-0.5098

TABLE III. Electron and hole densities at the lattice sites of electron and hole CDW states. For the electron CDW states we list $n(\vec{R})2\pi a_L^2$ and for the hole CDW states we list $1-n(\vec{R})2\pi a_L^2$.

	$(e^2/a_L)/\hbar\omega_c$						
State	0.0	0.5	1.0	2.0	3.0	5.0	10.0
$\nu=\frac{1}{3}$ Electron CDW	1.000	1.145	1.262	1.424	1.532	1.658	1.812
$\nu=\frac{1}{2}$ Electron CDW	1.000	1.210	1.376	1.610	1.765	1.946	2.167
$\nu=\frac{1}{2}$ Hole CDW	1.000	1.000	1.000	1.000	0.999	0.999	0.999
$\nu=\frac{2}{3}$ Hole CDW	1.000	1.000	1.000	1.000	0.999	0.999	0.999

ty restriction becomes more severe and the difference between these energies grows rapidly. When Landau-level mixing is allowed it is possible to increase the electron density at a lattice site at the cost of increasing the kinetic energy. For the hole CDW states the situation is very different. The maximum hole density is also $(2\pi a_L^2)^{-1}$ compared to an average density of $(1-\nu)(2\pi a_L^2)^{-1}$. But this corresponds to a physical electron density of zero and this, obviously, cannot be decreased further. We believe this is the reason that the energy of the hole CDW state decreases only slightly when Landau-level mixing is allowed.

In Table III we list values for $n(\vec{R})(2\pi a_L^2)$, for $\vec{R}$ at a lattice site of the electron CDW states, and $1-n(\vec{R})(2\pi a_L^2)$ for $\vec{R}$ at the lattice site of the hole CDW states. As expected, the electron density at the electron-lattice sites increases quite rapidly as $(e^2/a_L)/\hbar\omega_c$ increases. This corresponds to a narrowing of the electron density distribution around the lattice sites and is responsible for the increase in the magnitude of the interaction energy noted in Table II. On the other hand, for the hole-lattice sites the hole density changes little. The small increase in the magnitude of the interaction energy in this case comes from a slight change in the shape of the charge distribution around a lattice site.

In concluding this section we note that all of the results listed in Tables II and III are based on calculations for which the Hilbert space was restricted to the five lowest Landau levels. For the electron CDW state at $\nu=\frac{1}{2}$ we also performed several calculations which allowed mixing within the ten lowest Landau levels. The changes in the ground-state energy were ~ 0.00002 and ~ 0.0001 at $(e^2/a_L)/\hbar\omega_c$ equal to 1 and 5, respectively. The corresponding changes in the electron density at the lattice sites were $\sim 0.003(2\pi a_L^2)^{-1}$ and $\sim 0.01(2\pi a_L^2)^{-1}$.

V. SUMMARY AND CONCLUSIONS

We have solved the Hartree-Fock equations for the electron and hole CDW states of a two-dimensional electron gas in a strong magnetic field. We find that, for the electron CDW states, there is a substantial increase in the degree to which the charge density is localized around lattice sites when mixing between different Landau levels is allowed. For the hole CDW states, the hole charge density already has its maximum value (zero electron density) at the lattice sites for the one-Landau-level CDW state and the increase in binding energy resulting from Landau-level mixing is therefore much smaller. For $(e^2/a_L)/\hbar\omega \rightarrow 0$ the electron CDW states are lowest in energy for $\nu<\frac{1}{2}$ and the hole CDW states are lower in energy for $\nu>\frac{1}{2}$. As $(e^2/a_L)/\hbar\omega_c$ increases the crossover point must move to larger values of ν for the reasons given above. For example, at $\nu=\frac{2}{3}$, calculations not discussed in detail here show that the electron CDW state has lower energy for $e^2/a_L \gtrsim 3\hbar\omega_c$. Since the increase in binding energy of the electron CDW state, when Landau-level mixing is allowed, is associated with its nonuniform density distribution it is likely that the increase for Laughlin's uniform state[7] is much smaller. However, for the ratio of (e^2/a_L) to $\hbar\omega_c$ appropriate to the GaAs-$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ heterostructures[16] (~ 0.7 at $H=10$ T and ~ 0.5 at $H=20$ T) it is clear that the energy difference between the two states is not greatly altered. In the case of an inversion layer at Si-SiO$_2$ interfaces, however, $(e^2/a_L)/\hbar\omega_c \sim 4$ at $H=10$ T and ~ 3 at $H=20$ T (Ref. 16), it seems that Landau-level mixing may contribute to making the appearance of a fractional Hall effect less likely.

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[11] Essentially the difference is that for the second argument of the confluent hypergeometric function in Eq. (12b) they have $l+\frac{1}{2}$ rather than $l+1$.

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[13] This sum rule was proved in Appendix A of Ref. 1 for a hexagonal-lattice charge-density-wave state but is actually valid for any single Slater-determinant state in the lowest Landau level.

[14] Electron and hole CDW states in the lowest Landau level differ only by the replacements $\Delta_{0,0}(\vec{G}=\vec{0})\rightarrow 1-\Delta_{0,0}(\vec{G}=\vec{0})$ and $\Delta_{0,0}(\vec{G}\neq\vec{0})\rightarrow -\Delta_{0,0}(\vec{G}\neq\vec{0})$. Thus $|\delta\tilde{E}_{\rm sp}|$ for a hole CDW state at $\nu>\frac{1}{2}$ is ν/ν' times greater than the same quantity for the electron CDW state at $\nu'=1-\nu$. For $\nu=\frac{2}{3}$ and $\nu'=\frac{1}{3}$ this ratio is 2. The ratio for the $\delta E_{\rm sp}$ values in Table I is less than this because of the contribution of $\vec{G}_1+\vec{G}_2\neq 0$ terms in Eq. (18).

[15] A. H. MacDonald (unpublished).

[16] The effective interaction between electrons in the inversion layer is altered by the medium. In the crudest approximation—see, for example, A. H. MacDonald and G. C. Aers [Phys. Rev. B **29**, 5976 (1984)]—the interaction may be replaced by a Coulomb interaction reduced by a dielectric constant which is the average of the bulk values on the two sides of the interface. In addition $\hbar\omega_c$ should be calculated using the effective mass for motion in the plane of the interface. The estimates for the ratio of interaction and cyclotron energies have taken these corrections into account. For the Si case we used the effective mass appropriate to the (100) surface.