The Hartree-Fock state for the 2DEG at $\nu = \frac{1}{2}$ revisited: analytic solution, dynamics and correlation energy.

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Abstract

The CDW Hartree-Fock state at half filling and half electron per unit cell is examined. Firstly, an exact solution in terms of Bloch-like states is presented. Using this solution we discuss the dynamics near half filling and show the mass to diverge logarithmically as this filling is approached. We also show how a uniform density state may be constructed from a linear combination of two degenerate solutions. Finally we show the second order correction to the energy to be an order of magnitude larger than that for competing CDW solutions with one electron per unit cell.

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I. INTRODUCTION

For almost two decades the fractional quantum Hall effect has been one of the main focus of interest in condensed matter physics. Much progress has been made towards its understanding, and even general theories exist today aspiring to be fully coherent descriptions of the underlying physics. These theories do not rest on an actual solution of the basic quantum mechanical equations of motion, however, but are rather cast from ansatz wave functions exhibiting a large overlap with accurate numerical solutions of such equations for a few particles. A more basic theory, although highly desirable, is very difficult to attain because electron-electron interactions and correlations are at the core of the effect.

A first step in a perturbative approach was developed in the early years by Yoshioka and Lee, who constructed a mean field Hartree-Fock theory for the spin polarized case (HFT1). It received little attention, however, because it failed to provide the empirical selection rule that distinguishes even from odd denominator filling fractions, which characterizes the effect in an essential way. It was later shown by one of us, that if the mean field solution is constructed in a slightly different way, such distinction arises naturally, giving the same

gap structure at the various filling fractions as experiment, and producing the proper step like Hall conductivity dependence with magnetic field (HFT2). It predicts a gap at every odd denominator fraction, and a metallic state at all even denominators, within a band spectrum whose fine structure at or near the Fermi energy scales with the denominator in the fraction. Energies were too high, however, even compared to the state proposed by Yoshioka and Lee. One potential problem of Hartree-Fock spin polarized states in the lowest Landau level is that they necessarily have non uniform electron density at fractional filling, and, if space fluctuations are severe, possibly pin the many-body electronic state to the underlying impurities, an effect for which there appears to be no experimental evidence except perhaps at fillings below 1/7. However, it should be also stressed that a crystalline ordered state ("Hall Crystal") can be fully compatible with a quantized Hall conductivity thanks to its magnetic field dependent crystal parameters.

Simple charge density wave (CDW) mean field states are found assuming they form a periodic lattice of rectangular or triangular geometry. The size of the unit cell is an additional degree of freedom characterized by the quantity γ , the number of electrons per unit cell. The main difference between the mean field theories described above is that HFT1 assumes one electron per unit cell, that is, $\gamma = 1$, while HFT2 assumes $\gamma = 1/2$ or some other fraction of denominator 2^k , with k an integer. Keeping the geometry fixed and changing γ yields local minima at $\gamma = 1/2, 1$. Although neither show energies near the one corresponding to the true ground state, one may ask which one is a better perturbative precursor of the ground state. HFT1 gives a lower energy, but HFT2 provides the basic selection rule distinguishing even and odd denominators as required by experiment, and has less pronounced charge density fluctuations.

In this work we present an analytic solution for the $\nu=1/2,\,\gamma=1/2$ state. In particular, we address the question of sensitivity to perturbation theory in both theories. Within HFT1, Yoshioka and Lee obtained a correction to second order of about 0.002 in units of $\frac{e^2}{r_o}$, where r_o is the magnetic length. Here we show the same correction to be an order of magnitude larger for HFT2. This result confirms the suggestion made in a former work by one of us about that this latter state is more sensitive to correlations than HFT1. Our solution is constructed in terms of Bloch-like running waves which solve the Hartree Fock problem exactly and form a complete orthonormal set, save for a single point in the Brillouin zone. This remarkable property may be unique to filling 1/2 and $\gamma=1/2$, since then exactly one flux quanta traverses the unit cell of the underlying CDW. Having analytic solutions allows for a study of the dynamics at the Fermi surface. We find that the cyclotron effective mass diverges logarithmically as half filling is approached, in agreement with RPA estimates and with some experimental data.

In Section 2 the single particle solutions and their self-energies are given. Close expressions in terms of products of elliptic theta functions are presented, and the order parameter is explicitly given. We also show that degenerate Hartree-Fock solutions may be superposed to form a state of uniform charge density. In Sec. 3 a semiclassical analysis of the response to a small additional field is given, and the resulting cyclotron mass discussed. Section 4 is devoted to the evaluation of the second order correction to the energy. A short review and discussion of our results is given in the Summary. In the appendices we derive some symmetry properties of our solutions and show that filling the rotated central square of the Brillouin zone indeed yields the lowest self-consistent energy solution.

II. ANALYTIC SINGLE PARTICLE SOLUTIONS AND ORDER PARAMETERS

We consider N electrons constrained to move in a plane of area S under a perpendicular magnetic field \mathbf{B} . As shown by Wannier, to study this system one can construct an orthogonal set of single particle Bloch-like states from the zero angular momentum eigenfunction in the lowest Landau level

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{2\pi}r_o} \exp(-\frac{x^2}{4r_o^2}),\tag{1}$$

in the form [d,9,8],

$$\varphi_k(\mathbf{x}) = \frac{1}{N_k} \sum_{\ell} (-1)^{\ell_1 \ell_2} \exp(i \ \mathbf{k}.\ell) \ \mathbf{T}_{\ell} \ \phi(\mathbf{x}). \tag{2}$$

Eigenstates are labeled by a wave vector $\mathbf{k} = \mathbf{p}/\hbar$ where \mathbf{p} is the quasi-momentum, and the sum runs over all integers ℓ_1, ℓ_2 defining a planar square lattice L, with $\ell = a(\ell_1, \ell_2, 0), \ a = 2\pi r_o^2$ and $r_o = \sqrt{\frac{\hbar c}{|e|B}}$. The magnetic translation operator \mathbf{T}_ℓ acting on any function f introduces a phase:

$$\mathbf{T}_{\ell} f(\mathbf{x}) = \exp(\frac{\mathbf{i}\mathbf{e}}{\mathbf{h}\mathbf{c}}\mathbf{A}(\ell).\mathbf{x}) f(\mathbf{x} - \ell),$$
 (3)

where the vector potential is assumed in the axial gauge $\mathbf{A}(\mathbf{x}) = \frac{B}{2}(-x_2, x_1, 0)$ and the electron charge e is taken with its negative sign.

We want to study the case in which one flux quanta traverses each lattice cell. Then, there is one state per plaquette in the lowest Landau level and at filling one half the charge in each cell is just half the electron charge, and thus, $\gamma = 1/2$. The wave-function (2) and the normalizing factor $N_{\mathbf{k}}$ can then be expressed in terms of elliptic theta functions thanks to their simple properties under special shifts of the complex arguments in their quasi-periods. They are given, respectively, by

$$\varphi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{2\pi}r_{o}N_{k}} \exp(-\frac{x^{2}}{4r_{o}^{2}}) \left(\Theta_{3}(\frac{k_{1}^{*}a}{\pi} \mid -\frac{1}{\tau})\Theta_{3}(\frac{k_{2}^{*}a}{2\pi} \mid \tau) + \Theta_{2}(\frac{k_{1}^{*}a}{\pi} \mid -\frac{1}{\tau})\Theta_{4}(\frac{k_{2}^{*}a}{2\pi} \mid \tau) \right),$$

$$N_{k}^{2} = N_{\phi_{0}}(\Theta_{3}(\frac{k_{1}a}{\pi} \mid -\frac{1}{\tau})\Theta_{3}(\frac{k_{2}a}{2\pi} \mid \tau) + \Theta_{2}(\frac{k_{1}a}{\pi} \mid -\frac{1}{\tau})\Theta_{4}(\frac{k_{2}a}{2\pi} \mid \tau)),$$

where $\tau = \frac{i}{2}$. The components of the wave vectors appearing in these expressions are related through $\mathbf{k}^* = \mathbf{k} + (\mathbf{n} \times \mathbf{x} - i \mathbf{x})/2r_0^2$, where $\mathbf{n} = (0,0,1)$ is the unit vector normal to the plane. The orthonormal set is well defined except at the single point $\mathbf{k} = (\pi/a, \pi/a, 0)$, where the norm vanishes \mathbf{n} . In what follows we shall ignore this singular point.

As may be easily verified, the functions $\varphi_{\mathbf{k}}$ satisfy the eigenvalue equation

$$T_{\ell} \varphi_{\mathbf{k}}(\mathbf{x}) = \lambda_{\mathbf{k}}(\ell) \varphi_{\mathbf{k}}(\mathbf{x}),$$

$$\lambda_{\mathbf{k}}(\ell) = (-1)^{\ell_1 \ell_2} \exp(-i \ \mathbf{k}.\ell).$$
(4)

As was shown earlier they are exact solutions of the Hartree-Fock (HF) single particle Schrodinger equation associated to an arbitrary Slater determinant formed by selecting an

also arbitrary group as filled states. This occurs because the HF single particle Hamiltonian commutes with all translations leaving L invariant. Since the functions (2) are common eigenfunctions of the commuting magnetic translations leaving invariant the lattice L and the set of eigenvalues (4) uniquely determines them, the HF potential associated with the Slater determinant can not change those eigenvalues. Therefore $\varphi_{\mathbf{k}}$ should be an eigenfunction.

The explicit expression for the self-energy of the state $\varphi_{\mathbf{k}}$ has the form,

$$\epsilon(\mathbf{k}) = \frac{S}{2\pi r_o^2} \sum_{\mathbf{Q}} \Delta_{\mathbf{k}}(\mathbf{Q}) \ \Delta^*(\mathbf{Q}) \exp(-\frac{r_o^2 Q^2}{4}) \left(\frac{1 - \delta_{Q,0}}{r_o Q} \exp(-\frac{r_o^2 Q^2}{4}) - \sqrt{\frac{\pi}{2}} I_o(\frac{r_o^2 Q^2}{4})\right) \frac{e^2}{\varepsilon r_o},\tag{5}$$

where $\mathbf{Q} = 2\pi(n_1, n_2, 0)/a$ is the set of reciprocal lattice vectors and I_0 is the modified Bessel function. The momentum dependence of the self-energy is fully contained in the factor $\Delta_{\mathbf{k}}(\mathbf{Q}) = 2\pi r_o^2 \lambda_{\mathbf{k}}(\mathbf{x}^*)/S$, where $\mathbf{x}^* = r_o^2 \mathbf{n} \times \mathbf{Q}$. The order parameter is in turn given by

$$\Delta(\mathbf{Q}) = \frac{2\pi r_o^2}{S} \sum_{\mathbf{k} \in F} \lambda_{\mathbf{k}}(\ell)$$

$$= \frac{2\pi r_o^2}{S} (-1)^{n_1 n_2} \sum_{\mathbf{k} \in F} \exp(-i \ \mathbf{k}.\mathbf{x}^*),$$
(6)

where the sum is over all filled states in the Brillouin zone B, the set of which we call $F \subset B$. From general symmetry properties it is shown in Appendix B that an energy minimum is obtained among all possible Slater determinants by filling states inside the square bounded by the constant energy lines $\pm k_x \pm k_y = \pi/a$, which we take as the Fermi surface. The number of states in this square is just half the total, as required, since we are studying the half filling case. Note that the energy function is continuous across these lines so there is no gap in the single particle spectrum at the Fermi energy. Turning the sum into an integral one then gets,

$$\Delta(\mathbf{Q}) = (-1)^{n_1 n_2} a^2 \int_{p \in F} \frac{d\mathbf{k}}{(2\pi)^2} \exp(-i \ \mathbf{k}.\mathbf{x}^*)$$

$$= \left(\frac{\delta_{n_1, n_2}}{2} - \frac{2}{\pi^2} \lim_{\epsilon \to 0} \frac{\sin[(n_1 - n_2)\frac{\pi}{2}] \sin[(n_1 + n_2)\frac{\pi}{2}]}{n_1^2 - n_2^2 + \epsilon}\right).$$
(7)

Notice that these quantities vanish if n_1, n_2 have the same parity, save at the origin. Using the above expressions the total energy per electron may be easily computed, to obtain $\epsilon_{\frac{1}{2}} = -0.394 \frac{e^2}{\varepsilon r_o}$, a value somewhat above the result for $\gamma = 1$, $\epsilon_1 = -0.443 \frac{e^2}{\varepsilon r_o}$? The charge density may also be obtained from the above expressions since their Fourier

The charge density may also be obtained from the above expressions since their Fourier coefficients and (7) are related through $\Delta(\mathbf{Q}) = 2\pi r_o^2 e^{\frac{r_o^2 Q^2}{4}} \rho(\mathbf{Q})$, yielding a space fluctuation of a mere 17% about the average $n_0 = N/S$, while the $\gamma = 1$ state electron density varies between $0.1n_0$ and $1.85n_0$, representing a fluctuation of close to 90% about the average.

Finally in this section we would like to underline the curious point that using our Hartree-Fock solutions it is possible to construct a state of uniform charge density. To see this we consider the function $\Psi = (\Phi^{HF} + \tilde{\Phi}^{HF})/\sqrt{2}$, where as before Φ^{HF} is the Slater determinant formed with all states in F, while $\tilde{\Phi}^{HF}$ is the Slater determinant of all states in B - F, the complement of F in the Brillouin zone B. Both regions are separated by the Fermi surface, the square $\pm k_x a \pm k_y a = \pi$. Because all single-particle states are orthogonal to each other the crossed term in the charge density vanishes and one has $\rho(x) = (\rho^{HF}(x) + \tilde{\rho}^{HF}(x))/2 = \sum_{\mathbf{k} \in B} |\varphi_{\mathbf{k}}(\mathbf{x})|^2/2$, half the density of a completely filled Landau level, which equals $(4\pi r_o^2)^{-1}$ and is uniform throughout the sample.

We now show that the above linear combination has the minimal energy. To see this we first note that $\tilde{\Phi}^{HF}$ is obtained simply by shifting all momenta in Φ^{HF} by the vector $\delta=(1,-1)\pi/a$, since in the extended zone scheme this vector maps all states in F onto B-F. However, according to Eq. A.2 such shift may be done with the aid of a single magnetic translation $T_{\mathbf{R}}$, with $\mathbf{R}=r_o^2$ $\mathbf{n}\times\delta=(1,1)a/2$. Thus, both Slater determinants are related by a single translation in space. But, all the N states forming each of these Slater determinants are orthogonal with all the ones defining the other, and also the energy operator is a linear combination of products of merely four creation or annihilation operators. It therefore follows that the mean value of the energy operator in the state Ψ is just half what one obtains adding the mean values of Φ^{HF} and $\tilde{\Phi}^{HF}$, and thus the mean energy of the superposition state coincides with the HF energy.

III. DYNAMICS AND MASS

It has been suggested that the effective mass of the charged carriers may diverge at the Fermi surface, a property that remains controversial. Taking advantage of our analytic results we examine these questions. The semiclassical equations of motion may be solved for particles at the Fermi surface moving in the external field corresponding to half filling, $B_{\frac{1}{2}}$, with the result that if motion starts at $\mathbf{k} = \frac{\pi}{2\mathbf{a}}(1,1)$ then, after a time t, the particle quasi-momentum has reached the point $k_x = \frac{2}{a}\arctan[\exp(-t/T)]$, $ak_y = \pi - ak_x$, with a time constant of order $\tau = 2\hbar/\epsilon^*$, where $\epsilon^* = \frac{e^2}{\varepsilon r_o}$. It thus takes an infinite time to reach a corner of the square Fermi surface, and the trajectory in real space is a straight line covering just a fraction of the unit cell. One can thus claim that the Fermi particles behave as if there was no external field at all, in agreement with previous work.

In order to examine the effective mass that this solution provides we consider the period of a cyclotron orbit when the filling is slightly above or below 1/2. For definiteness we assume the later. For simplicity me keep the lowest order Fourier components in the dispersion relation only, and assume that the slight change in filling fraction does not perturb significantly the particle density. The self energy of state \mathbf{k} is then of the form $\epsilon = \epsilon_o - \epsilon_1(\cos(ak_x) + \cos(ak_y))$, with $\epsilon_o = -\frac{1}{2}\sqrt{\frac{\pi}{2}}\epsilon$ and $\epsilon_1 = 0.087 \ \epsilon^*$. We study the dynamics governed by the equations

$$\hbar \frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar c} \frac{\partial \epsilon}{\partial \mathbf{k}} \times \mathbf{B}.$$

For an orbit over the Fermi surface, no longer square in shape, this equation becomes, for the component k_y ,

$$\hbar \frac{dk_y}{dt} = -\frac{a\epsilon_1}{\delta^2} \sqrt{1 - (\eta + \cos(ak_y))^2},$$

from whose solution and the constant energy condition the itinerary of k_x may be extracted. Here $\delta^2 = \hbar c/eB = 2\pi r_o^2$, and $\eta = (\epsilon - \epsilon_o)/\epsilon_1$ measures the departure from the half filling square Fermi surface. Integrating this equation one obtains for the time it takes for a particle to go around the energy contour once,

$$T = \frac{4\hbar}{\pi\epsilon_1} \frac{K(\frac{\eta^2 - 4}{\eta^2})}{\eta},$$

where K(u) denotes the complete elliptic function of the first kind. A cyclotron effective mass may be obtained from this expression through the usual definition $m^* = eTB/(2\pi c)$. One obtains the result $m^* = 8\hbar^2 n_0 K(\frac{\eta^2-4}{\eta^2})/(\pi\epsilon_1\eta)$. Noting that $K(\frac{\eta^2-4}{\eta^2}) \sim -0.57\eta \log \eta$ as $\eta \to 0$ we get the final result,

$$m^* = -\frac{16.7 \ \hbar^2 n_0}{\epsilon^*} \log (\eta),$$

which diverges logarithmically as half filling is approached.

IV. ENERGY PER PARTICLE IN SECOND ORDER

We now turn our attention to the second order correction to the energy per particle for the $\nu=\frac{1}{2},\ \gamma=\frac{1}{2}$, state. A similar evaluation for $\gamma=1$ was done by Yoshioka and Lee, obtaining a correction of the order of 0.5% of the total result. However, as it was underlined in the increased degree of overlap of the single electron states associated to the $\gamma=\frac{1}{2}$ wave-functions could change the situation drastically. The study of this question is the main objective of the present paper.

For evaluating the second order correction the following formula will be employed

$$E^{(2)} = \sum_{i} \langle \Phi^{HF} \mid (H - H_F^{(HF)}) \mid \Phi_i \rangle \frac{1}{E^{(HF)} - E_i} \langle \Phi_i \mid (H - H_F^{(HF)}) \mid \Phi^{HF} \rangle$$

$$= \sum_{i} \frac{|\langle \Phi^{HF} \mid H \mid \Phi_i \rangle|^2}{E^{(HF)} - E_i}$$
(8)

where Φ^{HF} , $E^{(HF)}$ are the Slater determinant and total Hartree-Fock energy, respectively, and H is the projection of the exact Hamiltonian onto the first Landau level. The many particle excited states Φ_i are Slater determinants constructed with the Hartree-Fock basis states $\{\varphi_{\mathbf{k}}\}$, $\mathbf{k} \in B$. It follows that $\langle \Phi^{HF} \mid \Phi_i \rangle = 0$, a property that allowed to write the last equality in (8). In the second quantized representation the Hamiltonian H will have non-vanishing matrix elements linking the HF state and excited states of the form $|\Phi_i\rangle = a_\eta \, a_{\eta'} \, a_\xi^+ \, a_{\xi'}^+ \, |\Phi^{HF}\rangle$, where a_ξ^+ creates an electron of wavevector ξ , etc. The index i is a shorthand notation for pairs of filled $(\eta, \eta' \in F)$ and empty $(\xi, \xi' \in B - F)$ electron states. The total energies of the excited states are given by $E_i = E^{(HF)} + \epsilon(\xi) + \epsilon(\xi') - \epsilon(\eta) - \epsilon(\eta')$. Then, the second order correction can be rewritten in the form

$$E^{(2)} = \sum_{(\eta,\eta')} \sum_{(\xi,\xi')} \frac{|\langle \Phi^{HF} | H a_{\eta} a_{\eta'} a_{\xi}^{+} a_{\xi'}^{+} | \Phi^{HF} \rangle|^{2}}{\epsilon(\eta) + \epsilon(\eta') - \epsilon(\xi) - \epsilon(\xi')}, \tag{9}$$

where the total projected Hamiltonian has the form

$$H = \frac{e^2}{2} \int \int d\mathbf{x} d\mathbf{x}' \ \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|} \Psi(\mathbf{x}') \Psi(\mathbf{x})$$

$$= \frac{e^2}{2} \sum_{\alpha, \alpha'} \sum_{\beta, \beta'} M(\alpha, \alpha' | \beta, \beta') \ a_{\alpha}^+ a_{\alpha'}^+ a_{\beta} a_{\beta'},$$
(10)

with the matrix element of the coulomb interaction given by

$$M(\alpha, \alpha' \mid \beta, \beta') = \int \int d\mathbf{x} d\mathbf{x}' \ \varphi_{\alpha}^*(\mathbf{x}) \varphi_{\alpha'}^*(\mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|} \varphi_{\beta'}(\mathbf{x}') \varphi_{\beta}(\mathbf{x}). \tag{11}$$

By using the anti-commutation relations $[a_{\mathbf{q}}, a_{\mathbf{q}'}^+] = \delta_{\mathbf{q}, \mathbf{q}'}$, formula (11) can be expressed in terms of our basis as,

$$E^{(2)} = \sum_{(\eta,\eta')} \sum_{(\xi,\xi')} \frac{|e^2 \int \int d\mathbf{x} d\mathbf{x}' \, \Phi_{\eta,\eta'}^*(\mathbf{x},\mathbf{x}') \frac{1}{|\mathbf{x}-\mathbf{x}'|} \Phi_{\xi,\xi'}(\mathbf{x},\mathbf{x}') |^2}{\epsilon(\eta) + \epsilon(\eta') - \epsilon(\xi) - \epsilon(\xi')}, \tag{12}$$

where the two particle states Φ are defined as

$$\Phi_{\eta,\eta'}(\mathbf{x}, \mathbf{x}') = \frac{\varphi_{\eta}(\mathbf{x})\varphi_{\eta'}(\mathbf{x}') - \varphi_{\eta'}(\mathbf{x})\varphi_{\eta}(\mathbf{x}')}{\sqrt{2}}.$$
(13)

This quantity can be evaluated by use of the series (2), to obtain

$$M(\alpha', \alpha \mid \beta, \beta') = N_{\phi_0} \delta_P^{(K)}(\alpha + \alpha', \beta + \beta') I(\beta' - \alpha, \beta' - \alpha') *$$

$$\frac{\varphi_{\alpha}^*(-r_o^2 \mathbf{n} \times (\beta' - \alpha)) \varphi_{\alpha'}^*(r_o^2 \mathbf{n} \times (\beta' - \alpha))}{N_{\beta'} N_{\beta}},$$
(14)

where the Coulomb interaction is contained in the function I, given by

$$I(\beta' - \alpha, \beta' - \alpha') = \sum_{\mathbf{Q}} \frac{2\pi}{|\beta' - \alpha + \mathbf{Q}|} \times \exp\left(-\frac{r_o^2}{2}(\beta' - \alpha + \mathbf{Q})^2\right) \exp\left(i r_o^2 \mathbf{n} \times (\alpha' - \beta') \cdot \mathbf{Q}\right). \tag{15}$$

The inherent translation invariance of the problem is reflected in the delta function expressing the conservation of the quasimomentum of the four particle states defining the matrix element,

$$\delta_{\mathbf{P}}^{(K)}(\eta + \eta', \xi + \xi') = \sum_{\mathbf{Q}} \delta^{(K)}(\eta + \eta', \xi + \xi' + \mathbf{Q}). \tag{16}$$

Finally, by using the above expression for the matrix element, the second order correction to the energy per particle can be expressed as

$$\epsilon^{(2)} = \frac{E^{(2)}}{N} = \frac{1}{2(2\pi)^2} \int \int \int \frac{d\mathbf{q}}{(2\pi)^2} \frac{d\mathbf{q'}}{(2\pi)^2} \frac{d\mathbf{p}}{(2\pi)^2} \frac{M(\mathbf{q}, \mathbf{q'} \mid \mathbf{p})}{\epsilon(\mathbf{q}) + \epsilon(\mathbf{q'}) - \epsilon(\mathbf{p}) - \epsilon(\mathbf{q} + \mathbf{q'} - \mathbf{p})} \frac{e^2}{\epsilon r_o}, (17)$$

where the momentum variables have been rescaled to be dimensionless through the changes of variables $\mathbf{q} = a \, \eta$, $\mathbf{q}' = a \, \eta'$, $\mathbf{p} = a \, \xi$, and the usual equivalence in the high area limit $\sum_{\mathbf{q}} g(\mathbf{p}) \equiv S \int \frac{d\mathbf{q}}{(2\pi)^2} g(\mathbf{p})$ has been employed. The expression for the kernel in (13) becomes

$$M(\mathbf{q},\mathbf{q}'\mid\mathbf{p}) = \mid I(\mathbf{q}'-\mathbf{p},\mathbf{q}-\mathbf{p})\vartheta_{\mathbf{q}}(-\frac{\mathbf{n}\times(\mathbf{q}'-\mathbf{p})}{2\pi})\vartheta_{\mathbf{q}'}(\frac{\mathbf{n}\times(\mathbf{q}'-\mathbf{p})}{2\pi}) -$$

$$-I(\mathbf{p}-\mathbf{q},\mathbf{p}-\mathbf{q}')\vartheta_{\mathbf{q}}(-\frac{\mathbf{n}\times(\mathbf{p}-\mathbf{q})}{2\pi})\vartheta_{\mathbf{q}'}(\frac{\mathbf{n}\times(\mathbf{p}-\mathbf{q})}{2\pi})|^{2}\frac{1}{\vartheta_{\mathbf{q}}(0)\vartheta_{\mathbf{q}'}(0)\vartheta_{\mathbf{p}}(0)\vartheta_{\mathbf{q}+\mathbf{q}'-\mathbf{p}}(0)}$$
(18)

Relation (19) allows an estimate of $\epsilon^{(2)}$ by evaluating the three momentum integrals. The integration was performed partitioning the Brillouin zone into a lattice of $(2n+1)^2$ points, over which the integration variables take the values $\mathbf{q}(m_1, m_2) = \frac{\pi}{2n+1} (m_1 - m_2, m_1 + m_2)$, $-n \leq m_1, m_2 \leq n$, and similarly for $\mathbf{q}'(m_1, m_2)$, $\mathbf{p}(m_1, m_2)$. These partitions have the property that the points do not touch the boundary of F, and from which they are at least a distance equal to half the distance between the points of the partition. This property was implemented in order to avoid in a regular manner the singularity which appears when the momenta of the two states inside and outside F are all on the Fermi boundary. When at least one of the states is outside F the difference of energies in (53) is always non vanishing due to the form of the self energy surface. The results in units of $\frac{e^2}{\varepsilon r_o}$ for partitions involving up to 225 points are

- $n = \epsilon^{(2)} \left(\frac{e^2}{r_o}\right)$
- $1 -0.057\overline{2742}$
- 2 -0.02460706
- 3 -0.02515106
- 4 0.02762403
- 5 -0.02992157
- 6 -0.03175841
- 7 -0.0307658

Comparison with the $\gamma=1$ value $0.002e^2/\varepsilon r_o$ shows an increase in the correction for $\gamma=1/2$ of over an order of magnitude. Together with the significantly smaller space fluctuations of the charge density, we interpret this result as a larger sensitivity of the $\gamma=1/2$ state to the introduction of correlations, leading to a faster lowering of the energy and possibly melting of the charge density wave. Extension of this work to other filling fractions will be reported elsewhere.

V. SUMMARY

An analytic solution of the Hartree-Fock problem at filling $\nu = \frac{1}{2}$ and half a particle per unit cell $(\gamma = \frac{1}{2})$ has been discussed. The same state was formerly studied numerically. The solution is found to have a more uniform charge density in space than the $\gamma = 1$ state of Yoshioka and Lee, and the correction to the energy is an order of magnitude larger than that obtained with one electron per cell. Besides yielding no gap as required for filling 1/2,

our results suggest that the Hartree-Fock state with half of an electron per unit cell is a better perturbative precursor to the true ground state of the system, and calls for a more detailed investigation of its properties for the filling considered, as well as other fractions.

It should be stressed that after finishing this work Dr. N. Maeda have communicated us about two references: in which the same HF electronic state at $\nu=\frac{1}{2}$ was considered by him and other collaborators as possibly related with the composite fermions at this filling fraction. In the present work, from a technical point of view, we have intended to present and analytical solution to the mean field problem as a new result. Alternatively, on the physical side, our main purpose was to decide about wether the enhanced electron overlapping at $\gamma=\frac{1}{2}$ is able to also increase the correlation energy of the state at $\gamma=\frac{1}{2}$ over the one for $\gamma=1$.

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VII. APENDIX A

The following properties of the basis functions under translations and reflections are needed in the body of the text.

A. Translations

Let us argue that the effect of an arbitrary translation on the basis functions is, modulo a phase factor, equivalent to a shift in the momentum label $\overline{}$. Operating over a basis function twice with the translation operator involving a lattice vector ℓ and an arbitrary vector a one gets,

$$T_{\mathbf{a}} T_{\ell} \varphi_{\mathbf{p}}(\mathbf{x}) = \lambda_{\mathbf{p}}(\ell) T_{\mathbf{a}} \varphi_{\mathbf{p}}(\mathbf{x})$$

$$= \exp(-2 \frac{ie}{\hbar c} \mathbf{A}(\mathbf{a}) \cdot \ell) T_{\ell} T_{\mathbf{a}} \varphi_{\mathbf{p}}(\mathbf{x}),$$
(A.1)

where we have used Eq. (4) and the identity

$$T_{\mathbf{a}}T_{\ell} = \exp(2\frac{ie}{\hbar c}A(\mathbf{a}).\ell)T_{\ell}T_{\mathbf{a}}$$
.

Again using (4),

$$T_{\ell}T_{\mathbf{a}} \ \varphi_{\mathbf{p}}(\mathbf{x}) = \lambda_{\mathbf{p}+2\frac{ie}{\hbar c}\mathbf{A}(\mathbf{a})}(\ell)T_{\mathbf{a}} \ \varphi_{\mathbf{p}}(\mathbf{x}).$$

Then, taking into account that the set of eigenvalues defines uniquely the wavefunctions modulo a phase, it follows

$$T_{\mathbf{a}} \varphi_{\mathbf{p}}(\mathbf{x}) = F_{\mathbf{p}}(\mathbf{a}) \varphi_{\mathbf{p}+2\frac{ie}{\hbar c}\mathbf{A}(\mathbf{a})}(\mathbf{x}).$$
 (A.2)

That is, a magnetic translation is equivalent to a shift in the quasi-momentum. The factor F, being a phase, satisfies

$$F_{\mathbf{p}}(\mathbf{a})F_{\mathbf{p}}^{*}(\mathbf{a}) = 1.$$

We now consider a special translation in the vector $\mathbf{a} = r_o^2 \mathbf{n} \times \delta$, with $\delta = (-\frac{\pi}{a}, \frac{\pi}{a})$. Using Eq. A.2 one finds that it amounts to a shift in the momentum by the quantity $2\frac{e}{\hbar c}\mathbf{A}(\mathbf{a}) = \delta$. Then, the magnetic translation in a vector a transforms any momentum $\mathbf{p} \in F$ into a corresponding momentum $\mathbf{p}^{\delta} \in B - F$ through the relation

$$\mathbf{p}^{\delta} = \mathbf{p} + \delta \tag{A.3}$$

thus transforming all of F in all B - F.

B. Reflections

Consider the axis D in the plane determined by the vector

$$\mathbf{d} = (1, 1),\tag{A.4}$$

and define the operation R of a reflection on D within the plane by

$$\mathbf{x}^{R} = (x_2, x_1) = R \mathbf{x},$$

$$\mathbf{p}^{R} = R \mathbf{p},$$
(A.5)

and its self-inverse property

$$R = R^{-1}$$
.

After acting with the operator R over any function f the following property follows:

$$RT_{\ell} f(\mathbf{x}) = R \exp(\frac{ie}{\hbar c} \mathbf{A}(\ell).\mathbf{x}) f(\mathbf{x} - \ell)$$

$$= \exp(\frac{ie}{\hbar c} \mathbf{A}(\ell).R\mathbf{x}) f(R\mathbf{x} - \ell)$$

$$= \exp(\frac{ie}{\hbar c} \mathbf{A}(R\ell).\mathbf{x}) f(R(\mathbf{x} - R\ell))$$

$$= T_{R\ell} R f(\mathbf{x}),$$

from which one gets

$$R\varphi_{\mathbf{p}}(\mathbf{x}) = \frac{1}{N_{\mathbf{p}}} \sum_{\ell} (-1)^{\ell_1 \ell_2} \exp(i \ R\mathbf{p}.\ell) \ T_{\ell} \ \phi(\mathbf{x})$$
$$= \varphi_{R\mathbf{p}}(\mathbf{x}), \tag{A.6}$$

meaning that the action of a space reflection on the basis function is equivalent to a reflection of its quasi-momentum.

VIII. APENDIX B

That the lowest energy state for half filling is obtained by occupying all states within the square bounded by the lines $ak_x + ak_y = \pi$ may be shown as follows. First, let us inspect the commutation properties of the reflection R under the line containing the vector $\mathbf{d} = (1, 1)$, as well as the particular translation T_a which transforms the filled states F into the empty sates in B - F, with the Hartree-Fock single particle Hamiltonian. Both operations are defined in Appendix A. As the action of this hamiltonian is represented by a kernel with two arguments due to the projection on the first Landau level, it turns out to be useful to employ, when appropriate, the Dirac notation. Then the single particle HF equation can be expressed as

$$H_U^{(HF)} \mid \varphi_{\mathbf{p}} \rangle = \epsilon(\mathbf{p}) \mid \varphi_{\mathbf{p}} \rangle$$
 (B.1)

where the kernel associated to the Hartree-Fock Hamiltonian is

$$H_{U}^{(HF)}(\mathbf{x}, \mathbf{x}') = \hbar \omega_{o} \delta(\mathbf{x}, \mathbf{x}') + \int d\mathbf{y} d\mathbf{y}' \ P_{o}(\mathbf{x}, \mathbf{y}) \frac{e^{2}}{|\mathbf{y} - \mathbf{y}'|} \times$$

$$\{ (\sum_{\mathbf{q} \in U} \varphi_{\mathbf{q}}^{*}(\mathbf{y}') \varphi_{\mathbf{q}}(\mathbf{y}') - n_{o}) \ P_{o}(\mathbf{y}, \mathbf{x}') -$$

$$(\sum_{\mathbf{q} \in U} \varphi_{\mathbf{q}}^{*}(\mathbf{y}') \varphi_{\mathbf{q}}(\mathbf{y})) \ P_{o}(\mathbf{y}', \mathbf{x}') \}.$$
(B.2)

Here P_o is the projection operator in the first Landau level and the direct and exchange contributions are determined by the set U formed by the momenta associated to the selected filled states. At this point, let us assume that U = F. From the properties of the reflections it follows that

$$R \int H_F^{(HF)}(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') d\mathbf{x}' = \int H_F^{(HF)}(R\mathbf{x}, R\mathbf{x}') R f(\mathbf{x}') d\mathbf{x}'.$$
(B.3)

Noting the invariance property that follows from Eq. A.8,

$$P_o(R\mathbf{x}, R\mathbf{x}') = \sum_{\mathbf{q} \in B} \varphi_{\mathbf{q}}(R\mathbf{y}) \ \varphi_{\mathbf{q}}^*(R\mathbf{y}')$$
$$= \sum_{\mathbf{q} \in B} \varphi_{R\mathbf{q}}(\mathbf{y}) \ \varphi_{R\mathbf{q}}^*(\mathbf{y}')$$
$$= P_o(\mathbf{x}, \mathbf{x}')$$

the invariance of the Hamiltonian follows,

$$H_F^{(HF)}(R\mathbf{x}, R\mathbf{x}') = \hbar \omega_o \delta(\mathbf{x}, \mathbf{x}') + \int d\mathbf{y} d\mathbf{y}' \ P_o(R\mathbf{x}, R\mathbf{y}) \frac{e^2}{|R\mathbf{y} - R\mathbf{y}'|} \times$$

$$\{ (\sum_{\mathbf{q} \in F} \varphi_{\mathbf{q}}^*(R\mathbf{y}') \varphi_{\mathbf{q}}(R\mathbf{y}') - n_o) \ P_o(R\mathbf{y}, R\mathbf{x}') -$$

$$(\sum_{\mathbf{q} \in F} \varphi_{\mathbf{q}}^*(R\mathbf{y}') \varphi_{\mathbf{q}}(R\mathbf{y})) \ P_o(R\mathbf{y}', R\mathbf{x}') \}$$

$$= H_F^{(HF)}(\mathbf{x}, \mathbf{x}'),$$
(B.4)

where in the sums again use of A.8 has been made, as well as the fact that if $q \in F$ then its reflection about D is also in F. Using the above property in Eq. B.3 one gets

$$R \int H_F^{(HF)}(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') d\mathbf{x}' = \int H_F^{(HF)}(\mathbf{x}, \mathbf{x}') R f(\mathbf{x}') d\mathbf{x}'$$

From the arbitrariness of f then follows the commutativity of the reflection operator with $H^{(HF)}$,

$$[H_F^{(HF)}, R] = 0.$$

and consequently

$$RH_F^{(HF)} \mid \varphi_{\mathbf{p}} \rangle = \epsilon(\mathbf{p}) R \mid \varphi_{\mathbf{p}} \rangle$$
$$= H_F^{(HF)} R \mid \varphi_{\mathbf{p}} \rangle$$
$$= \epsilon(R \mathbf{p}) \mid \varphi_{R\mathbf{p}} \rangle,$$

leading to the symmetry of the spectrum with respect to reflection about the line D defined by $\mathbf{d} = (1, 1)$,

$$\epsilon(\mathbf{p}) = \epsilon(R\,\mathbf{p}). \tag{B.5}$$

Clearly, the same conclusion arises with respect to reflections on the line \overline{D} defined by $\overline{\mathbf{d}} = (-1, 1)$.

The next task is to consider symmetry properties under a translation in the special vector a defined in Appendix A . In this sense, it is worth noting that if $\mathbf{p} \in F$ then $\mathbf{p} + \delta \in B - F$ and moreover, R \mathbf{p} exactly gives $\mathbf{p} + \delta$ under a reflection about the line defined by the boundary of F and B - F. As we shall see, the relation between values of the self energies under such operations will allow us to show the property we are after.

We start out by considering the states in the sector B - F and exploit particle hole symmetry. Adding the hamiltonian obtained through such states to that given in B.4 one obtains the Hartree-Fock form appropriate for a filled Brillouin zone,

$$H_{B}^{(HF)}(\mathbf{x}, \mathbf{x}') = H_{F}^{(HF)}(\mathbf{x}, \mathbf{x}') + H_{B-F}^{(HF)}(\mathbf{x}, \mathbf{x}')$$

$$= \hbar \omega_{o} \delta(\mathbf{x}, \mathbf{x}') - \int d\mathbf{y} d\mathbf{y}' \ P_{o}(\mathbf{x}, \mathbf{y}) \frac{e^{2}}{|\mathbf{y} - \mathbf{y}'|}$$

$$= \sum_{\mathbf{q} \in B} \varphi_{\mathbf{q}}^{*}(\mathbf{y}') \varphi_{\mathbf{q}}(\mathbf{y}) \ P_{o}(\mathbf{y}', \mathbf{x}')$$

$$= \hbar \omega_{o} \delta(\mathbf{x}, \mathbf{x}') - \int d\mathbf{y} d\mathbf{y}' \ P_{o}(\mathbf{x}, \mathbf{y}) \frac{e^{2}}{|\mathbf{y} - \mathbf{y}'|}$$

$$= P_{o}(\mathbf{y}, \mathbf{y}') \ P_{o}(\mathbf{y}', \mathbf{x}').$$
(B.6)

It can be readily verified that the kernel $H_B^{(HF)}$ commutes with all the magnetic translations, that is,

$$[T_a, H_B^{(HF)}] = 0.$$
 (B.7)

Henceforth, since in particular it commutes with all the T_{ℓ} leaving invariant the lattice L, it follows that the $\varphi_{\mathbf{p}}$ are eigenfunctions of $H_B^{(HF)}$. Additionally, they all have exactly the same eigenvalue. This can be verified by considering a translation in any vector $a' = r_o^2 n \times \delta'$ commuting with it, which changes the momenta in an also arbitrary quantity δ' (Appendix A). One has $H_B^{(HF)} \mid \varphi_p \rangle = \epsilon_B(\mathbf{p}) \mid \varphi_{\mathbf{p}} \rangle$, that may also be written as $H_B^{(HF)} T_{r_o^2 \mathbf{n} \times \delta'} \mid \varphi_{\mathbf{p} - \delta'} \rangle = \epsilon_B(\mathbf{p}) T_{r_o^2 \mathbf{n} \times \delta'} \mid \varphi_{\mathbf{p} - \delta'} \rangle$. Multiplying this latter expression from the left by the inverse translation one gets $H_B^{(HF)} \mid \varphi_{\mathbf{p} - \delta'} \rangle = \epsilon_B(\mathbf{p}) \mid \varphi_{\mathbf{p} - \delta'} \rangle$, which also equals $\epsilon_B(\mathbf{p} - \delta') \mid \varphi_{\mathbf{p} - \delta'} \rangle$. Therefore, $\epsilon_B(\mathbf{p}) = \epsilon_B(\mathbf{p} - \delta') = \epsilon_B$, a constant. This property enforces the proportionality of $H_B^{(HF)}$ with the projection operator P_o . At this point it is worthwhile to recall that since we are considering functions on the first Landau level, the Dirac delta function appearing in the definition of the HF kernels is equivalent to the projection operator. Then,

$$H_B^{(HF)}(\mathbf{x}, \mathbf{x}') = \hbar \omega_o \delta(\mathbf{x}, \mathbf{x}') + \epsilon_L P_o(\mathbf{x}, \mathbf{x}')$$
(B.8)

Thus, all the basis functions are eigenfunctions of the Hartree-Fock hamiltonian associated with the filled Landau level $H_B^{(HF)} \mid \varphi_{\mathbf{p}} \rangle = \epsilon_B \mid \varphi_{\mathbf{p}} \rangle$, with the same eigenvalue $\epsilon_B = \hbar \omega_o + \epsilon_L$.

The next point to consider is the connection between the kernels $H_F^{(HF)}$ and $H_{B-F}^{(HF)}$. It follows from expressing the basis functions with momenta in B-F by means of translations of the basis states with momenta in F, and considering the transformation properties under the special translations $T_{r_o^2 \mathbf{n} \times \delta}$ of the projection operator and the Coulomb potential, as discussed in Appendix A. It follows

$$H_{B-F}^{(HF)}(\mathbf{x}, \mathbf{x}') = \hbar \omega_o \delta(\mathbf{x}, \mathbf{x}') + \int d\mathbf{y} d\mathbf{y}' \ P_o(\mathbf{x}, \mathbf{y}) \frac{e^2}{|\mathbf{y} - \mathbf{y}'|}$$

$$\left\{ \sum_{\mathbf{q} \in F} T_{r_o^2 \ \mathbf{n} \times \delta} \varphi_{\mathbf{q}}(\mathbf{y}') \ [T_{r_o^2 \ \mathbf{n} \times \delta} \ \varphi_{\mathbf{q}}(\mathbf{y}')]^* - n_o \right\} \ P_o(\mathbf{y}, \mathbf{x}') -$$

$$\sum_{\mathbf{q} \in F} T_{r_o^2 \ \mathbf{n} \times \delta} \varphi_{\mathbf{q}}(\mathbf{y}) \ [T_{r_o^2 \ \mathbf{n} \times \delta} \varphi_{\mathbf{q}}(\mathbf{y}')]^* \ P_o(\mathbf{y}', \mathbf{x}') \right\}$$

$$= \hbar \omega_o \delta(\mathbf{x}, \mathbf{x}') + \int d\mathbf{y} d\mathbf{y}' \ P_o(\mathbf{x}, \mathbf{y}) T_{r_o^2 \ \mathbf{n} \times \delta}^{(\mathbf{y})} \frac{e^2}{|\mathbf{y} - \mathbf{y}'|}$$

$$\left\{ \left(\sum_{\mathbf{q} \in F} \varphi_{\mathbf{q}}^*(\mathbf{y}') \varphi_{\mathbf{q}}(\mathbf{y}') - n_o \right) T_{-r_o^2 \ \mathbf{n} \times \delta}^{(\mathbf{y})} P_o(\mathbf{y}, \mathbf{x}') -$$

$$\sum_{\mathbf{q} \in F} \varphi_{\mathbf{q}}(\mathbf{y}) \varphi_{\mathbf{q}}^*(\mathbf{y}') \ T_{-r_o^2 \ \mathbf{n} \times \delta}^{(\mathbf{y}')} P_o(\mathbf{y}', \mathbf{x}') \right\},$$
(B.9)

which may be expressed in the more compact Dirac notation as,

$$H_{B-F}^{(HF)} = T_{r_o^2 \, \mathbf{n} \times \delta} \, H_F^{(HF)} T_{-r_o^2 \, \mathbf{n} \times \delta}.$$
 (B.10)

Physically, this relation means that the HF state associated to F is simply the space translation of the state associated to B-F. Therefore, within the first Landau level the following relation holds,

$$\epsilon_B = H_E^{(HF)} + T_{r^2 \, \mathbf{n} \times \delta} H_E^{(HF)} T_{-r^2 \, \mathbf{n} \times \delta},$$
(B.11)

which after acting over a basis function produces

$$\epsilon_B = \epsilon(\mathbf{p}) + \epsilon(\mathbf{p} - \delta),$$
 (B.12)

The sum of the energies at p and the shifted value is strictly constant. Using the symmetry of the spectrum under reflection it also follows that

$$\epsilon_B = \epsilon(\mathbf{p}) + \epsilon(R(\mathbf{p} - \delta)).$$
 (B.13)

Thus, the sum of the energies associated to the states which have momenta related by a reflection in the boundary of the regions F and B-F is also exactly constant. Finally by selecting $\mathbf{p} = \mathbf{p}_F$, with \mathbf{p}_F in the boundary between both regions, and noticing that in that case $\mathbf{p}_F = R(\mathbf{p}_F - \delta)$, it follows that, due to the continuity of the spectrum (absence of gaps) the energy at any point of the boundary of the filled states strictly equals $\epsilon(\mathbf{p}_F) = \epsilon_F/2$. Therefore, the criterium for a minimum given in reference is satisfied, and the Hartree-Fock solution with all states in F has a local minimum of the energy.

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