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Analytic mean-field charge-density-wave solution at $\nu=1/3$: Composite-fermion-like subbands and correlation effects

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An analytic solution of the Hartree-Fock problem for a 2DEG at filling 1/3 and half an electron per unit cell is presented. The Coulomb interaction dynamically breaks the first Landau level in three narrow subbands, one of which is fully occupied and the others empty, as in the composite fermion model. Strong correlations are expected owing to large charge density overlap between neighboring plaquettes. Numerical evaluations show an enhancement of the cohesive correlation energy, bringing the energy per particle to the proximity of that obtained in competing variational models. Correlations are long range, requiring over 98 particles in numerical computations to approach convergence.

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I. INTRODUCTION

It is well accepted today that the fractional quantum Hall effect in the lowest Landau level results from the formation of a strongly correlated spin polarized electron liquid that crystallizes below filling 1/7.[1–3] It is intriguing, however, that mean field charge density wave solutions (CDW) exist at all fillings, which yield in a natural way the odd-denominator rule that characterizes the effect.[4,5] In spite of such remarkable property, detailed investigation of this class of mean field states was stopped largely due to their higher energy compared to the state proposed by Laughlin.[2] Also, the correlation energy for another class of mean field solutions, the Wigner Solid (WS), was computed by Yoshioka and Lee (YL) yielding a correction to the energy of less than 2%.[6] The two sets of solutions differ in that while in a WS state there is one whole electron per plaquette, in a CDW state each plaquette contains a fraction of an even denominator of an electron charge, such as $e/2$. While in the former case the charge density is formed by nearly Gaussian peaks around lattice points with little overlap of electrons from neighboring cells, in the latter the charge density forms continuous ridges between cells, opening the way for an appreciable increase of the cohesive correlation energy.[7] This idea was first explored in the simplest case of 1/2 filling.[8] The results confirmed the effect yielding a second order correlation correction an order of magnitude larger than for the best WS state. The same line of thinking was also recently considered by Mikhailov.[9]

In this work we report results for the correlation energy of the CDW at 1/3 filling and one half electron per unit cell. The work rests on an analytic solution of the mean field problem constructed using symmetry considerations. We show that the electron-electron interaction breaks the single particle degeneracy of the lowest Landau level (LLL), splitting it into three remarkably flat bands. All bands contain the same number of states so that only one is filled while the other two are empty, separated by a large gap from the filled one. While the CDW unit cell traps 3/2 flux quanta of the original field, it is only pierced by one flux quanta of the reduced field $B^{*}=B_{1/3}-B_{1/2}$, where $B_{1/3}$ and $B_{1/2}$ are the fields at 1/3 and 1/2 filling factor, respectively. The narrowness of the occupied band and this latter fact suggest that the magnetic Wannier states are approximate solutions of the problem and behave as nearly free quasiparticles filling the LLL of the effective field B^{*}, much as the composite fermion model predicts.[3,10]

For better comparison with earlier results we study the correlation energy using the YL method, that is, we evaluate the second order perturbation correction to the Hartree-Fock (HF) solution. Two computational procedures are used, one employing a Monte Carlo approach for evaluation of the space integrals over a large sample, and the other by computing in momentum space using a discrete set defined by periodic boundary conditions applied to a comparatively small sample. As in the half-filling case, both methods yield for filling 1/3 an energy correction about ten times larger than that for the WS state,[6] adding support to the conjecture that at all fillings the high electron overlap of the CDW enhances significantly the cohesive energy corrections.[7,9] This reopens the case for the CDW state as a serious candidate for precursor to the true ground state in a perturbative approach in the thermodynamic limit.

One further outcome is that having included up to 98 particles in our numerical calculation convergence is yet not reached, suggesting that an even larger number of particles is needed to fully capture correlation effects through numerical computation, way above current permissible sizes used in first principles numerical diagonalization, which treat at most 27 particles.[11] Since, as we show, the CDW charge distribution exhibits large intercell overlap through rather steep hexagonal ridges, it is likely that the slowness in reaching the thermodynamic limit is due to the presence of long range cooperative ring exchange effects which, to be effective, require a matching large sample.[12] It is of interest to underline in addition that the states discussed in this work can be also considered as possible realizations of the so-called “Hall Crystal” states, introduced in Ref. 13 to argue the possible compatibility of the occurrence of the QHE and the presence of a crystal structure.

In Sec. II the single particle Hartree-Fock Hamiltonian is diagonalized analytically. In Sec. III the second order correction to the mean field solution is evaluated. Finally, in Sec. IV we present our conclusions. Details of the calculation are given in the Appendices. In particular, in Appendix B a formula is derived expressing the single particle Hartree-Fock Hamiltonian in terms of the magnetic translations associated with a lattice of arbitrary periodicity that, to our knowledge, is absent in the literature.

II. BLOCH REDUCTION OF THE HF PROBLEM AT $\nu=\frac{1}{3}$

A. One particle Hamiltonian and magnetic translations

Let us consider a 2DEG in a strong perpendicular magnetic field. We are interested in an analytic treatment of the Hartree-Fock problem at filling $1/3$. The Hartree-Fock Hamiltonian of this problem can be written in the compact form

$$H_{\mathrm{HF}} = \sum_{Q} v(\mathbf{Q})\exp\left(-\frac{r_o^2\mathbf{Q}^2}{4}\right)T_{r_o^2\mathbf{n}\times\mathbf{Q}}, \tag{1}$$

where the coefficients $v(\mathbf{Q})$ are given by

$$v(\mathbf{Q}) = 2\pi r_o^2\rho(\mathbf{Q})\exp\left(\frac{r_o^2\mathbf{Q}^2}{4}\right)\left(\frac{1-\delta_{\mathbf{Q},0}}{r_o|\mathbf{Q}|}\exp\left(-\frac{r_o^2\mathbf{Q}^2}{4}\right) - \sqrt{\frac{\pi}{2}}I_o\left(\frac{r_o^2\mathbf{Q}^2}{4}\right)\right)\frac{e^2}{\varepsilon_o r_o}, \tag{2}$$

and ε_o is the background dielectric constant. The magnetic translation operators T are defined in Appendix A, while form (1) is derived in Appendix B. The particle density in real space $\rho(\mathbf{x})$ is assumed to be periodic under displacements covering the triangular lattice defined by the vectors

$$\mathbf{R} = r_1\mathbf{a}_1 + r_2\mathbf{a}_2,\ r_1,r_2 = 0, \pm 1, \pm 2, \ldots; \tag{3}$$

$$\mathbf{a}_1 = \sqrt{\frac{6\pi}{\sqrt{3}}}(1,0)r_o,$$

$$\mathbf{a}_2 = \sqrt{\frac{6\pi}{\sqrt{3}}}\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)r_o.$$

The Fourier components of the density are defined as

$$\rho(\mathbf{Q}) = \frac{1}{A_{\mathrm{cell}}}\int \mathbf{dx}\rho(\mathbf{x})\exp(i\mathbf{Q}\,.\,\mathbf{x}), \tag{4}$$

where A_{cell} is the unit cell area

$$A_{\mathrm{cell}} = \mathbf{n}\,.\,\mathbf{a}_1\times\mathbf{a}_2 = 3\pi r_o^2. \tag{5}$$

Here $\mathbf{n}$ is a unit vector normal to the electron gas plane. Through this cell traverse a flux $\frac{3}{2}$ in units of the magnetic flux quantum $\phi_o = hc/e$. Associated with the above real space lattice is the reciprocal lattice

$$\mathbf{Q} = Q_1\mathbf{s}_1 + Q_2\mathbf{s}_2, \tag{6}$$

$$Q_1, Q_2 = 0, \pm 1, \pm 2, \ldots\ ,$$

$$\mathbf{s}_1 = -\frac{2}{3r_o^2}\mathbf{n}\times\mathbf{a}_2,$$

$$\mathbf{s}_2 = \frac{2}{3r_o^2}\mathbf{n}\times\mathbf{a}_1,$$

$$\mathbf{s}_i\,.\,\mathbf{a}_j = 2\pi\delta_{ij}.$$

The triangular lattice was here chosen owing to the fact that it has the lowest energy in two dimensions. Our treatment can be extended to lattices with other symmetries.[5,6,14]

B. Block diagonalization of the HF Hamiltonian

We next show that it is possible to find a basis in which the matrix representation of (1) has a diagonal form composed of simple three-dimensional blocks. In addition, the functions have such a structure that they automatically furnish the translation symmetry of the total density over the lattice (3). For this purpose we consider the basis functions $\varphi_{\mathbf{p}}(\mathbf{x})$ defined in Appendix A, constructed over the lattice with primitive vectors

$$\mathbf{b}_1 = \mathbf{a}_1, \quad \mathbf{b}_2 = \tfrac{2}{3}\mathbf{a}_2. \tag{7}$$

The magnetic translations then have the form

$$T_{r_o^2\mathbf{n}\times\mathbf{Q}} = T_{-(2/3)Q_2\mathbf{b}_1+Q_1\mathbf{b}_2}. \tag{8}$$

Since the flux piercing the unit cell of the lattice (3) is not an integral number of flux quanta, the set of translation operators obtained by varying the integers Q_1 and Q_2 in (8) do not commute and it is not possible to find common eigenfunctions to all of them. The basis we shall construct decomposes in a set of three dimensional subspaces, closing each of them under the action of translations for all values of $\mathbf{Q}$.

A first step in finding the basis is to define a set of eigenfunctions of a translation in the vector $\mathbf{a}_2$, which is a period of the density. For a given value of the momentum $\mathbf{p}$ such orbitals may be written as

$$\chi_{\mathbf{p}}^{\sigma}(\mathbf{x}) = \frac{1}{\sqrt{2}}\left(\varphi_{\mathbf{p}}(\mathbf{x}) + \frac{\sigma}{\exp(-i\mathbf{a}_2\,.\,\mathbf{p})}T_{\mathbf{a}_2}\varphi_{\mathbf{p}}(\mathbf{x})\right), \sigma = \pm 1. \tag{9}$$

Using the formulas in Appendix A it can be readily proven that these functions satisfy the eigenvalue relation

$$T_{\mathbf{a}_2}\chi_{\mathbf{p}}^{\sigma}(x) = \sigma\exp(-i\mathbf{a}_2\,.\,\mathbf{p})\chi_{\mathbf{p}}^{\sigma}(\mathbf{x}). \tag{10}$$

The two values of σ appearing in these equations will play an important role in what follows. They will allow us to impose the periodicity of the density under the shifts in $\mathbf{a}_1$ and $\mathbf{a}_2$, in spite of the impossibility of obtaining a basis of eigenvectors of all the magnetic translations in the lattice. It should be stressed that the range of values of $\mathbf{p}$ defining independent functions in the new basis have been reduced in half, the two values of σ compensating for this reduction. The restriction comes from the singular property of the basis $\{\varphi_{\mathbf{p}}\}$, that a magnetic translation is fully equivalent to a shifting of the momenta argument as implied by the relation

$$T_{\mathbf{R}}\varphi_{\mathbf{p}}(\mathbf{x}) = \mathcal{F}_{\mathbf{p}}(\mathbf{R})\varphi_{\mathbf{p}+(2e/\hbar c)\mathbf{A}(\mathbf{R})}(\mathbf{x}), \tag{11}$$

where $\mathcal{F}_{\mathbf{p}}(\mathbf{R})$ is a pure phase factor. See Appendix A and Ref. 16 for the justification of this relation. It directly implies that the shift done in $\mathbf{a}_2$ in constructing the new basis precisely changes the momentum $\mathbf{p}$ of the particle in $-\mathbf{s}_1/2$. Therefore, what has been basically done is to form linear combinations of the original functions associated with different values of the momentum. In the new basis the magnetic translation in $\mathbf{a}_1$ has the simple effect

$$T_{\mathbf{a}_1}\chi_{\mathbf{p}}^{\sigma}(\mathbf{x}) = \exp(-i\mathbf{a}_1 . \mathbf{p})\chi_{\mathbf{p}}^{-\sigma}(\mathbf{x}), \tag{12}$$

that is, it merely changes the sign of σ and multiplies it by a phase factor.

As the next step let us employ the fact that, although the functions are not eigenvectors of translations in $\mathbf{a}_1$, they are eigenfunctions of the double sized translations in $2\mathbf{a}_1$. This is because its effect, when considered as two consecutive shifts in $\mathbf{a}_1$, have the simple result of making two consecutive changes of sign of σ that reproduce the original function. Therefore, if for $\mathbf{p}$ and σ fixed we construct the triplet of states formed by the function $\chi_{\mathbf{p}}^{\sigma}(\mathbf{x})$ and the other two obtained by a pair of successive translations in the vector $-2\mathbf{a}_1/3$, the operation of performing a translation in an arbitrary multiple of these vectors leaves the triplets invariant.

A specific linear combination within each triplet which is also an eigenfunction of the translation in $-2\mathbf{a}_1/3$ can be obtained by constructing the new basis

$$\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \sum_{s=-1,0,1} c_r^s(\mathbf{p})T_{-(2/3)s\mathbf{b}_1}\chi_{\mathbf{p}}^{\sigma}(\mathbf{x}),\ r=-1,0,1. \tag{13}$$

After solving the linear equations for the constants c_r^s obtained by imposing the condition that these functions be solutions of the eigenvalue problem

$$T_{-(2/3)\mathbf{b}_1}\chi_{\mathbf{p}}^{(r,\sigma)}(x) = \lambda\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x})$$

one finds

$$\lambda^{(r)}(\mathbf{p}) = \exp\left(\frac{2}{3}i\mathbf{p} . \mathbf{a}_1 + \frac{2\pi r}{3}\right), \tag{14}$$

$$c_s^r(\mathbf{p}) = \frac{1}{\sqrt{3}}\exp\left(-\frac{2}{3}i\mathbf{p} . \mathbf{a}_1 s - \frac{2\pi irs}{3}\right),$$

$$r,s=-1,0,1.$$

Substituting in (13) yields

$$\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \frac{1}{\sqrt{3}}\sum_{s=-1,0,1}\exp\left(-\frac{2}{3}i\mathbf{p} . \mathbf{a}_1 s - \frac{2\pi irs}{3}\right)T_{-(2/3)s\mathbf{b}_1}\chi_{\mathbf{p}}^{\sigma}(\mathbf{x}), \tag{15}$$

$$r=-1,0,1,$$

$$\sigma=\pm 1,$$

$$\mathbf{p} \equiv \mathbf{p} + n\frac{\mathbf{s}_1}{2} + m\frac{\mathbf{s}_2}{2},\ n,m=0,\pm 1,\pm 2,\ldots\ . \tag{16}$$

The last relation expresses that, modulo a phase factor, the states of the new basis are equivalent upon a shift of their momenta $\mathbf{p}$ in any linear combination with integer coefficients of half the unit cell vectors of the reciprocal lattice corresponding to the periodicity of the density. The periodicity of the states under the shifts in $\mathbf{s}_1/2$ was discussed above, and the one related with $\mathbf{s}_2/2$ similarly follows from relation (A8) in Appendix A, expressing the equivalence of a magnetic translation with a shift in momentum. The functions just defined have an alternative and more compact form given by

$$\chi_{\mathbf{p}}^{(r,\sigma)}(x) = \frac{1}{\sqrt{6}N_{\mathbf{p}}^{(3,2)}}\sum_{\mathbf{m}}\exp\left(i\mathbf{P}^{(\mathbf{p},r,\sigma)} . \mathbf{m} + \frac{5\pi i}{6}m_1m_2\right)T_{\mathbf{m}}\phi(\mathbf{x}), \tag{17}$$

$$N_{\mathbf{k}}^{(3,2)} = \sqrt{N_{\phi_0}}\sqrt{\sum_{\ell}(-1)^{\ell_1\ell_2}\exp\left(i\mathbf{k} . \ell - \frac{\ell^2}{4r_0^2}\right)}, \tag{18}$$

$$\ell = \ell_1(3\mathbf{c}_1) + \ell_2(2\mathbf{c}_2), \tag{19}$$

where the effective momenta and the new elementary lattice of vectors $\mathbf{m}$ over which the sum is performed are given by

$$\mathbf{P}^{(\mathbf{p},r,\sigma)} = \mathbf{p} - r\mathbf{s}_1 + \frac{\sigma-1}{2}\frac{3}{2}\mathbf{s}_2, \tag{20}$$

$$\mathbf{m} = m_1\mathbf{c}_1 + m_2\mathbf{c}_2,$$

$$\mathbf{c}_1 = \frac{\mathbf{a}_1}{3},$$

$$\mathbf{c}_2 = \frac{\mathbf{a}_2}{3}.$$

The double sum (17) can be evaluated to obtain an explicit formula in terms of the elliptic theta functions as follows:

$$\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \frac{\exp\left(-\frac{\mathbf{x}^2}{4r_0^2}\right)}{\sqrt{6}\sqrt{2\pi r_0^2}N_{\mathbf{p}}^{(3,2)}} \times \sum_{\beta=0,\ldots,5}\sum_{\alpha=0,1} \exp\left(27\pi i\tau_1\alpha^2 + \pi i\tau_1\beta^2 + a_2\beta + 2\pi i\alpha\left(\frac{3a_2}{\pi i} - \frac{3a_1}{2\pi i} - \frac{15\alpha}{2} + \left(\frac{9\tau_1}{2} - \frac{5}{4}\right)\beta\right)\right)$$
$$\times\Theta_3\left(\frac{6a_2}{\pi i} - \frac{3a_1}{\pi i} - (15-54\tau_1)\alpha + 2\left(\frac{9\tau_1}{2} - \frac{5}{4}\right)\beta\middle|108\tau_1\right) \times \Theta_3\left(\frac{a_1}{2\pi i} + \frac{5\alpha}{2} + \left(\frac{\tau_1}{2} + \frac{5}{12}\right)\beta\right)\Big|\tau_1), \tag{21}$$

where

$$a_1 = i\mathbf{P}^{(\mathbf{p},r,\sigma)}\,.\,\mathbf{c}_1 + \frac{1}{2r_o^2}(\mathbf{c}_1 - i\mathbf{n}\times\mathbf{c}_1)\,.\,\mathbf{x},$$

$$a_2 = i\mathbf{P}^{(\mathbf{p},r,\sigma)}\,.\,\mathbf{c}_2 + \frac{1}{2r_o^2}(\mathbf{c}_2 - i\mathbf{n}\times\mathbf{c}_2)\,.\,\mathbf{x},$$

$$\tau_1 = \frac{i}{6\sqrt{3}}.$$

Let us inspect now the action of a magnetic translation by $\frac{2}{3}\mathbf{a}_2$ on the new functions. If such a transformation leaves the triplets invariant, then the matrix reduction of the Hartree-Fock Hamiltonian will follow. One has

$$T_{(2/3)\mathbf{a}_2}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \frac{1}{\sqrt{3}}\sum_{s=-1,0,1}\exp\left(-\frac{2}{3}i\mathbf{p}\,.\,\mathbf{a}_1 s - \frac{2\pi irs}{3}\right)$$
$$\times T_{(2/3)\mathbf{a}_2}T_{-(2/3)s\mathbf{b}_1}\chi_{\mathbf{p}}^{\sigma}(\mathbf{x}). \tag{22}$$

But after using (A4) in Appendix A for changing the order of the two operators within the sum, it follows that

$$T_{(2/3)a_2}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \lambda_{\mathbf{p}}\left(\frac{2}{3}\mathbf{a}_2\right)\chi_{\mathbf{p}}^{([r-1],\sigma)}(\mathbf{x}), \tag{23}$$

where the square bracket defines the number among the set $\{-1,0,1\}$ that is equivalent, modulo 3, to the integer in the argument.

For fixed $\mathbf{p}$ and σ the matrix elements of the Hamiltonian (1) in the new basis can readily be found to have the form

$$h_{\mathbf{p},\sigma}^{(r',r)} = \sum_{Q} v(\mathbf{Q})\exp\left(-\frac{\mathbf{Q}^2r_o^2}{4}\right)$$
$$\times\exp\left(i\mathbf{p}\,.\,\mathbf{n}\times\mathbf{Q}r_o^2 + \frac{2\pi i}{3}Q_2\right.$$
$$\left.\times(r+Q_1)\right)\delta_{r',[r-Q_1]}. \tag{24}$$

The problem has thus been reduced to the self-consistent diagonalization of a three dimensional matrix for each value of momenta $\mathbf{p}$ and parameter σ. The basis can be checked to have the following set of transformations properties:

$$T_{2\mathbf{c}_1}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \exp\left(-2i\mathbf{p}\cdot\mathbf{c}_1 - \frac{2\pi ri}{3}\right)\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}), \tag{25}$$

$$T_{2\mathbf{c}_2}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \exp(-2i\mathbf{p}\cdot\mathbf{c}_2)\chi_{\mathbf{p}}^{([r-1],\sigma)}(\mathbf{x}),$$

$$T_{3\mathbf{c}_1}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \exp(-3i\mathbf{p}\cdot\mathbf{c}_1)\chi_{\mathbf{p}}^{(r,-\sigma)}(\mathbf{x}),$$

$$T_{3\mathbf{c}_2}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \sigma\exp(-3i\mathbf{p}\cdot\mathbf{c}_2)\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}),$$

$$I\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \chi_{-\mathbf{p}}^{(-r,\sigma)}(\mathbf{x}),$$

where the parity transformation I is defined as usual by $I\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \chi_{\mathbf{p}}^{(r,\sigma)}(-\mathbf{x})$. As shown in Appendix A, from these symmetry properties it follows that the density associated with any Slater determinant constructed by selecting one orbital within each triplet has exact periodicity under shifts in all vectors $\mathbf{R}$.

In order to find the solution of the mean field problem by an iterative technique it is sufficient to make an ansatz for the density in the first step, and then diagonalize numerically the matrices for a sufficiently high partition of the reduced Brillouin cell momenta $\mathbf{p}$ defined by (16). By selecting the normalized lowest energy state within each three-dimensional quantum mechanical problem, the Fourier components of the density corresponding to the new step should be constructed. Following its definition, it can be done by means of the following expression:

$$\rho(\mathbf{Q}) = \frac{1}{A_{\text{cell}}}\sum_{p,\sigma=\pm1}\int\mathbf{dx}\left|\sum_{r} g_r^0(\mathbf{p})\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x})\right|^2\exp(i\mathbf{Q}\cdot\mathbf{x})$$
$$= \frac{\exp\left(-\frac{\mathbf{Q}^2r_o^2}{4}\right)}{A}\sum_{\mathbf{p}}\sum_{\sigma=\pm1}\exp\left(i\mathbf{p}\cdot\mathbf{n}\times\mathbf{Q}r_o^2\right.$$
$$\left.+\frac{2\pi i}{3}Q_2Q_1\right)\sum_{r,r'=-1,01} g_{r'}^0(\mathbf{p})^*g_r^0(\mathbf{p})$$
$$\times\exp\left(-\frac{2\pi ir}{3}Q_2\right)\delta_{r',[r+Q_1]}. \tag{26}$$

This formula can be obtained by evaluating the Gaussian integrals appearing after substituting the expansions defining the functions $\chi_{\mathbf{p}}^{(r,\sigma)}$. The coefficients g_r^0, g_r^1, and g_r^2, define the components of the eigenvectors of the single particle HF Hamiltonian in the basis of states χ. They fix the wave functions of the filled band and the empty bands as

$$\Phi_{\mathbf{p}}^{(b,\sigma)}(\mathbf{x}) = \sum_{r=-1,0,1} g_r^b(\mathbf{p})\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}), \tag{27}$$

$b=0,1,2$. Here $b=0$ labels the filled band in each triplet, and $b=1,2$ label the two empty bands.

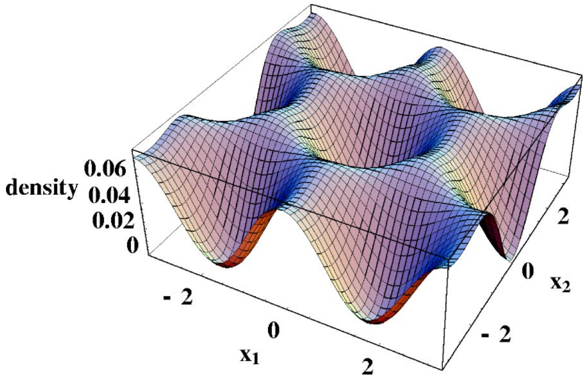

FIG. 1. Particle density associated with the CDW state at filling 1/3.

The fact that the first Landau level is split in just three bands is a manifestation of the fact that the Hartree-Fock equations map into a generalized form of Harpers equation.[5] As is well known, the Landau level is split into p bands, where p is the numerator in the rational fraction that expresses the number of flux quanta traversing the unit cell.[10] Since in our case this integer equals 3, then the spectrum contains exactly three bands.

C. Functions that vanish at the origin

In order to proceed within an analytical context let us consider the observation from former numerical studies, that the particle density for the state considered essentially vanishes at all lattice points.[5] Then, let us assume that the density rigorously vanishes at this set of points. If this is the case, the wave function of any of the filled states should then also vanish at those points. This requirement follows from the fact that the Hartree-Fock particle density is a sum over the individual densities of all occupied orbitals,

$$\sum_{\mathbf{p},\sigma=\pm 1}\left|\sum_{r} g_r^0(\mathbf{p})\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x})\right|^2=\rho(\mathbf{x}). \tag{28}$$

We can then use this property to fix the coefficients of the wave functions within each triplet.

After imposing the vanishing conditions at the origin, the coefficients defining the functions (27) are fully determined and take the form

$$g_0^0(\mathbf{p})=\frac{1}{\mathcal{N}_{\mathbf{p}}^*},$$

$$g_{-1}^0(\mathbf{p})=-\frac{1}{\mathcal{N}_{\mathbf{p}}^*}\,\frac{\chi_{\mathbf{p}}^{(0,+)}(0)\chi_{\mathbf{p}}^{(+1,-1)}(0)-\chi_{\mathbf{p}}^{(0,-1)}(0)\chi_{\mathbf{p}}^{(-1,-1)}(0)}{\chi_{\mathbf{p}}^{(-1,+1)}(0)\chi_{\mathbf{p}}^{(+,-1)}(0)-\chi_{\mathbf{p}}^{(+1,+1)}(0)\chi_{\mathbf{p}}^{(-1,-1)}(0)}, \tag{29}$$

$$g_{+1}^0(\mathbf{p})=-\frac{1}{\mathcal{N}_{\mathbf{p}}^*}\,\frac{\chi_{\mathbf{p}}^{(0,-1)}(0)\chi_{\mathbf{p}}^{(-1,+1)}(0)-\chi_{\mathbf{p}}^{(0,+1)}(0)\chi_{\mathbf{p}}^{(+1,+1)}(0)}{\chi_{\mathbf{p}}^{(-1,+1)}(0)\chi_{\mathbf{p}}^{(+1,-1)}(0)-\chi_{\mathbf{p}}^{(+1,+1)}(0)\chi_{\mathbf{p}}^{(-1,-1)}(0)},$$

$$1=|g_0^0(\mathbf{p})|^2+|g_{-1}^0(\mathbf{p})|^2+|g_1^0(\mathbf{p})|^2.$$

Note that the coefficients g are all independent of σ. This completes the definition of our functions. The proof that the above discussed vanishing condition gives the exact solution and not simply a very approximate one, will be considered elsewhere.

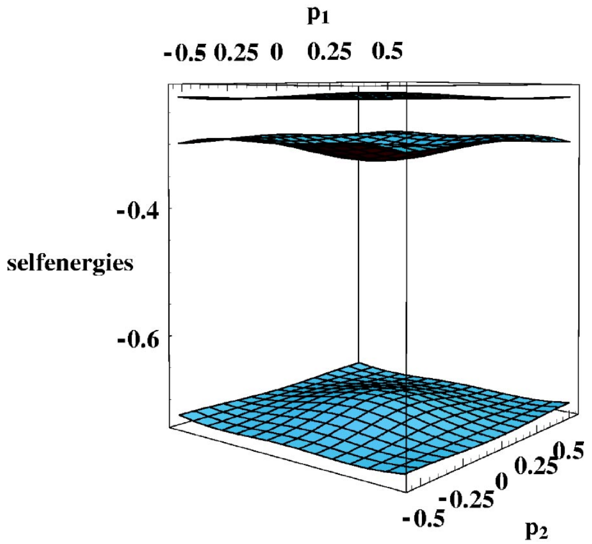

FIG. 2. Single particle band structure for the CDW state at filling 1/3.

The particle density may now be computed replacing these functions in Eq. (28). The real space particle density thus obtained is shown in Fig. 1.

A main property to be noticed in this figure is the formation of sharp hexagonal channels surrounding the low density regions at the center of which the vanishing density occurs. These structures mark the difference with the Wigner solid whose unit cell encloses three flux quanta. The charge density in this latter instance is made up essentially of well localized Gaussians centered at each lattice point. In our case there is strong overlap, suggesting that cooperative ring exchange involving many unit cells is a large contribution to the correlation energy.

Furthermore, the insertion of the calculated density in the eigenvalue equation associated with the matrix representation of the Hamiltonian in each triplet, Eqs. (2) and (24), allows for the evaluation of the one particle spectrum of the system. As it was expected, three energy bands appear, each associated with a value of the index b and covering the full range of $\mathbf{p}$ within each triplet. We also note that states associated with $\sigma=\pm 1$ turn out to be degenerate. The bands dispersion relations are illustrated in Fig. 2.

Note the narrowness of the bands as compared with the gaps separating them. This fact leads to the idea that in this mean field approximation the Coulomb interaction, although breaking the degeneracy of the first Landau level, reorganizes the states in three equally populated separate sets that again are approximately degenerate, as if they were Landau levels of a renormalized problem. Since at 1/3 filling one band is full and the other two are empty, one expects the electrons to behave dynamically similarly to filling one, except for a different effective mass, as the composite fermion model suggests.[8,10] The magnetic Wannier states are expected to be approximate solutions, playing the role of the angular momentum states in the noninteracting problem at filling one.

These properties seem to corroborate the possibility of tracing a link between weakly interacting composite fermions and the Bloch or Wannier orbitals in the mean field solutions considered earlier by one of us.[4,5] To complete this section we note that the mean field energy per particle obtained from the above formalism for the solution we have constructed confirms the value reported in an earlier numerical computation,[5]

$$\epsilon = -0.362\frac{e^2}{\varepsilon_o r_o}. \tag{30}$$

III. CORRELATION ENERGY IN SECOND ORDER

In order to obtain the energy correction to second order of perturbation theory we proceed similarly as in Ref. 8, starting with the expression[6]

$$\begin{aligned} E^{(2)} &= \sum_i \langle \Psi^{\mathrm{HF}} | (H - H_{\mathrm{HF}}) | \Psi_i \rangle \frac{1}{E^{\mathrm{HF}} - E_i} \langle \Psi_i | (H - H_{\mathrm{HF}}) | \Psi^{\mathrm{HF}} \rangle \\ &= \sum_i \frac{|\langle \Psi^{\mathrm{HF}} | H | \Psi_i \rangle|^2}{E^{\mathrm{HF}} - E_i}. \end{aligned} \tag{31}$$

Here Ψ^{HF}, E^{HF} are the mean field Slater determinant and total Hartree-Fock energy associated with the ground state, respectively, and H is the projection of the exact many particle Hamiltonian onto the first Landau level. The many particle excited states Ψ_i are Slater determinants constructed with the basis (27), mixing states in the filled band with states in the empty bands. It follows that $\langle \Psi^{\mathrm{HF}} | \Psi_i \rangle = 0$, a property that allowed to write the last equality in (31). In the second quantized representation the Hamiltonian H will have nonvanishing matrix elements linking the HF state and excited states of the form $|\Phi_i\rangle = a_\eta a_{\eta'} a^+_\xi a^+_{\xi'} |\Phi^{\mathrm{HF}}\rangle$ only, where a^+_ξ creates an electron of quantum numbers ξ, etc. The index i is a shorthand notation for the set of two pairs of filled $(\eta, \eta' \in F)$ and empty $(\xi, \xi' \in T - F)$ electron states, where T and F are the set of all states in the Landau level and just the filled ones, respectively. The indices $\eta = (0, \mathbf{p}, \sigma)$ and $\xi = (b, \mathbf{p}, \sigma)$ for $b = 1, 2$ denote the quantum numbers of filled and empty states, respectively. The total energy of an excited state is $E_i = E^{(\mathrm{HF})} + \epsilon(\xi) + \epsilon(\xi') - \epsilon(\eta) - \epsilon(\eta')$. Then, the second order correction can be rewritten in the form[8]

$$E^{(2)} = \sum_{(\eta,\eta')} \sum_{(\xi,\xi')} \frac{|\langle \Phi^{\mathrm{HF}} | H a_\eta a_{\eta'} a^+_\xi a^+_{\xi'} | \Phi^{\mathrm{HF}} \rangle|^2}{\epsilon(\eta) + \epsilon(\eta') - \epsilon(\xi) - \epsilon(\xi')}, \tag{32}$$

where the total projected Hamiltonian is

$$\begin{aligned} H &= \frac{e^2}{2\varepsilon_o} \int\int d\mathbf{x} d\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|} \Psi(\mathbf{x}') \Psi(\mathbf{x}) \\ &= \frac{e^2}{2\varepsilon_o} \sum_{\alpha,\alpha'} \sum_{\beta,\beta'} M(\alpha, \alpha' | \beta', \beta) a^+_\alpha a^+_{\alpha'} a_{\beta'} a_\beta. \end{aligned} \tag{33}$$

The matrix elements of the Coulomb interaction are given by

$$\begin{aligned} & M(\alpha, \alpha' | \beta', \beta) \\ &= \int\int d\mathbf{x} d\mathbf{x}' \Phi^*_\alpha(\mathbf{x}) \Phi^*_{\alpha'}(\mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|} \Phi_{\beta'}(\mathbf{x}') \Phi_\beta(\mathbf{x}), \end{aligned} \tag{34}$$

where we have used the shorthand notation $\Phi_\alpha = \Phi^{(b,\sigma)}_{\mathbf{p}}$. By using the anticommutation relations $[a_\alpha, a^+_{\alpha'}] = \delta_{\alpha,\alpha'}$, formula (31) can be expressed as

$$\begin{aligned} E^{(2)} &= \frac{e^4}{\varepsilon_o^2} \sum_{(\eta,\eta')} \sum_{(\xi,\xi')} \\ &\quad \times \frac{\left| \int\int d\mathbf{x} d\mathbf{x}' \Phi^*_{\eta,\eta'}(\mathbf{x}, \mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|} \Phi_{\xi,\xi'}(\mathbf{x}, \mathbf{x}') \right|^2}{\epsilon(\eta) + \epsilon(\eta') - \epsilon(\xi) - \epsilon(\xi')}, \end{aligned} \tag{35}$$

where the two particle states $\Phi_{\eta,\eta'}$ are defined by

$$\Phi_{\eta,\eta'}(\mathbf{x}, \mathbf{x}') = \frac{\Phi_\eta(\mathbf{x}) \Phi_{\eta'}(\mathbf{x}') - \Phi_{\eta'}(\mathbf{x}) \Phi_\eta(\mathbf{x}')}{\sqrt{2}}. \tag{36}$$

The pairs (η, η') and (ξ, ξ') are considered as unordered.

A. Correlation energy: First evaluation

As pointed out above the single particle bands are remarkably flat. We can use this property to simplify the calculation of the energy correction. First, we approximate the filled band energies appearing in the denominator of (35) by their mean value,

$$\epsilon(\eta) = \epsilon_0. \tag{37}$$

In addition, and slightly more crudely, we substitute the energies in the excited bands by a common energy equal to half the sum of the mean energies of the two bands,

$$\epsilon(\xi) = \frac{\epsilon_1 + \epsilon_2}{2}. \tag{38}$$

This last approximation is taken in view of the small relative gap separating these two bands.

With this simplifying substitution (35) can be expressed in the simpler form

$$\begin{aligned} E^{(2)} &= \frac{e^4}{2(2\epsilon_0 - \epsilon_1 - \epsilon_2)\varepsilon_o^2} \int\int d\mathbf{x}' d\mathbf{x} \\ &\quad \times \int\int d\mathbf{y} d\mathbf{y}' \\ &\quad \times \frac{1}{|\mathbf{x} - \mathbf{x}'|} \frac{1}{|\mathbf{y} - \mathbf{y}'|} (\pi_f(\mathbf{x}', \mathbf{y}') \pi_f(\mathbf{x}, \mathbf{y}) \\ &\quad - \pi_f(\mathbf{x}', \mathbf{y}) \pi_f(\mathbf{x}, \mathbf{y}')) \pi_e(\mathbf{y}, \mathbf{x}) \pi_e(\mathbf{y}', \mathbf{x}'), \end{aligned} \tag{39}$$

where π_f is the projection operator on the subspace of states of the filled band, and π_e the projector associated with the subspace of states formed by the union of the empty bands. The projectors have the following expression in terms of the corresponding densities

$$\begin{aligned}\pi_f(\mathbf{x},\mathbf{x}') &= \sum_{\mathbf{p},\sigma} \Phi_{\mathbf{p}}^{(0,\sigma)}(\mathbf{x})(\Phi_{\mathbf{p}}^{(0,\sigma)}(\mathbf{x}\,\prime\,))^* \\ &= P(\mathbf{x},\mathbf{x}')2\pi r_o^2 \sum_Q \rho_f(\mathbf{Q}) \\ &\quad\times \exp\left(i\mathbf{Q}\cdot\left(\frac{\mathbf{x}+\mathbf{x}'}{2}+\frac{1}{2}i\mathbf{n}\times(\mathbf{x}-\mathbf{x}')\right)\right),\end{aligned} \tag{40}$$

$$\begin{aligned}\pi_e(\mathbf{x},\mathbf{x}') &= \sum_{\mathbf{p},b,\sigma} \Phi_{\mathbf{p}}^{(b,\sigma)}(\mathbf{x})(\Phi_{\mathbf{p}}^{(b,\sigma)}(\mathbf{x}'))^* \\ &= P(\mathbf{x},\mathbf{x}')2\pi r_o^2 \sum_Q \rho_e(\mathbf{Q}) \\ &\quad\times \exp\left(i\mathbf{Q}\cdot\left(\frac{\mathbf{x}+\mathbf{x}'}{2}+\frac{1}{2}i\mathbf{n}\times(\mathbf{x}-\mathbf{x}')\right)\right),\end{aligned}$$

$$\rho_e(\mathbf{Q}) = \frac{1}{2\pi r_o^2}\delta_{\mathbf{Q},0} - \rho_f(\mathbf{Q}),$$

where $\delta_{\mathbf{Q},\mathbf{0}}$ is the ordinary Kronecker delta and $P(\mathbf{x},\mathbf{x}')$ is the projection operator onto the first Landau level, defined in Appendix A. These expressions can be obtained from formula (B10) in Appendix B. After evaluating a few spatial integrals, the correlation energy per particle $\epsilon^{(2)}=E^{(2)}/N$ becomes

$$\begin{aligned}\epsilon^{(2)} = {} & \frac{e^4}{2(2\epsilon_{0-}\epsilon_{1-}\epsilon_2)\varepsilon_o^2}\frac{4\pi\sqrt{\pi}r_o(\pi r_o^2)^2}{\nu}\sum_{\mathbf{Q}_1}\sum_{\mathbf{Q}_2}\sum_{Q_3}\rho_f(\mathbf{Q}_1)\rho_f(\mathbf{Q}_2)\rho_e(\mathbf{Q}_3)\rho_e(-\mathbf{Q}_1-\mathbf{Q}_2-\mathbf{Q}_3)\exp\left(\frac{(\mathbf{Q}_1+\mathbf{Q}_2)^2r_o^2}{4}\right)\int \mathbf{dz}\frac{1}{\sqrt{\mathbf{z}^2}} \\ & \times\exp\left(-\frac{\mathbf{z}^2}{4r_o^2}\right)\exp\left(-(\mathbf{Q}_1+\mathbf{Q}_3)\cdot\frac{\mathbf{n}\times\mathbf{z}}{2}-i(\mathbf{Q}_2+\mathbf{Q}_3)\cdot\frac{\mathbf{z}}{2}\right)I_0\left(\frac{1}{8}\left(\frac{\mathbf{z}}{r_o}-\mathbf{n}\times(\mathbf{Q}_1+\mathbf{Q}_3)r_o-i(\mathbf{Q}_2+\mathbf{Q}_3)r_o\right)^2\right) \\ & \times\left(\exp\frac{1}{8}\left(\frac{\mathbf{z}}{r_o}-\mathbf{n}\times(\mathbf{Q}_1+\mathbf{Q}_3)r_o-i(\mathbf{Q}_2+\mathbf{Q}_3)r_o\right)^2-\exp\left(-\frac{1}{8}\left(\frac{\mathbf{z}}{r_o}-\mathbf{n}\times(\mathbf{Q}_1+\mathbf{Q}_3)r_o-i(\mathbf{Q}_2+\mathbf{Q}_3)r_o\right)^2\right)\right),\end{aligned} \tag{41}$$

where I_0 is a modified Bessel function. In evaluating the sums we found sufficient for convergence to keep the 36 Fourier components associated with the shortest values of **Q**. Of these, terms in the longest **Q** are slightly altered to assure that the sum rule[5]

$$\sum_Q |\rho_f(\mathbf{Q})|^2 \exp\left(\frac{\mathbf{Q}^2r_o^2}{2}\right) = \frac{\nu}{(2\pi r_o^2)^2} \tag{42}$$

is satisfied. This condition is used to cancel various fictitious divergences in the formula defining the correlation energy.[6] We then obtain

$$\begin{aligned}\epsilon^{(2)} = {} & \frac{(e^2/\varepsilon_o r_0)^2}{4\nu\sqrt{\pi}(2\epsilon_{0-}\epsilon_{1-}\epsilon_2)}\sum_{\mathbf{Q}_1}\sum_{\mathbf{Q}_2}\sum_{\mathbf{Q}_3}\Delta_f(\mathbf{Q}_1)\Delta_f(\mathbf{Q}_2)\Delta_e(\mathbf{Q}_3)\Delta_e(\mathbf{Q}_1+\mathbf{Q}_2+\mathbf{Q}_3) \\ & \times\exp\left(-i\frac{r_o}{2}(\mathbf{Q}_2+\mathbf{Q}_3)\cdot\mathbf{n}\times(\mathbf{Q}_1+\mathbf{Q}_3)r_o+\frac{(\mathbf{Q}_2+\mathbf{Q}_3)^2r_o^2}{2}\right) \\ & \times\int \mathbf{du}\exp\left(-\frac{(\mathbf{u}-\mathbf{i}(\mathbf{Q}_2+\mathbf{Q}_3)r_o)^2}{4}-ir_o(\mathbf{Q}_2+\mathbf{Q}_3)\cdot\frac{(\mathbf{u}-\mathbf{i}(\mathbf{Q}_2+\mathbf{Q}_3)r_o)}{2}\right) \\ & \times I_0\left(\frac{1}{8}(\mathbf{u}-i(\mathbf{Q}_2+\mathbf{Q}_3)r_o)^2\right)\sinh\left(\frac{1}{8}(\mathbf{u}-i(\mathbf{Q}_2+\mathbf{Q}_3)r_o)^2\right)\times\left(\frac{1}{\sqrt{(\mathbf{u}+\mathbf{n}\times(\mathbf{Q}_1+\mathbf{Q}_3)r_o)^2}}-\frac{\delta_{\mathbf{Q}_2+\mathbf{Q}_3,0}}{\sqrt{\mathbf{u}^2}}\right),\end{aligned} \tag{43}$$

where the order parameters of the filled and empty bands have been defined as usual,

$$\Delta_f(\mathbf{Q}) = 2\pi r_o^2 \rho_f(\mathbf{Q}) \exp\left(\frac{(\mathbf{Q})^2 r_o^2}{4}\right),$$

$$\Delta_e(\mathbf{Q}) = 2\pi r_o^2 \rho_e(\mathbf{Q}) \exp\left(\frac{(\mathbf{Q})^2 r_o^2}{4}\right),$$

respectively. The integrals in Eq. (43) were evaluated using the Monte Carlo integration method with a variable number N_{mc} of sample points. The region of integration was taken as a square of size 50 r_o, centered at the origin. Results were obtained for sixteen values of N_{mc} evenly spaced in the interval $\{10000,\ 160000\}$. From these data we obtained (all energy values below given in units of $e^2/\varepsilon_o r_o$)

$$\epsilon_{\mathrm{corr}} = -0.0364 \mp 0.0048, \tag{44}$$

where the first figure is the average over the 16 values, and the one following, the mean square deviation. As a check, the case $N_{\mathrm{mc}} = 320000$ was also computed, yielding $\epsilon_{\mathrm{corr}} = -0.0371$, which falls within 2% of the average (44).

It is possible to perform an independent evaluation of the correlation energy that avoids approximations (37) and (38) and uses as parameter the number N of particles in the sample. This is done next.

B. Correlation energy: Second method

Using the formulas derived in Appendix C it is possible to recast Eq. (35) to give it the form

$$\epsilon^{(2)} = \frac{3\left(\dfrac{e^2}{\epsilon_o r_0}\right)^2}{(N_{\phi_0})^3} \sum_{(p_\beta,\sigma_\beta)} \sum_{(p_{\beta'},\sigma_{\beta'})} \sum_{(b,p_\alpha,\sigma_\alpha)} \sum_{(b',p_{\alpha'},\sigma_{\alpha'})} \frac{1}{\epsilon^{(0,p_\beta,\sigma_\beta)} + \epsilon^{(0,p_{\beta'},\sigma_{\beta'})} - \epsilon^{(b,p_\alpha,\sigma_\alpha)} - \epsilon^{(b',p_{\alpha'},\sigma_{\alpha'})}} \times \Bigg| \sum_{r_\alpha,r_{\alpha'},r_\beta,r_{\beta'}} \delta^{(K)}(\mathbf{P}_{\beta',r_{\beta'}} + \mathbf{P}_{\beta,r_\beta}$$
$$- \mathbf{P}_{a,r_\alpha} - \mathbf{P}_{\alpha',r_{\alpha'}}, 0) \times \mathcal{F}^*(\mathbf{p}_\alpha, r_\alpha, \sigma_\alpha) g_{r_\alpha}^{*b}(\mathbf{p}_\alpha) \mathcal{F}^*(\mathbf{p}_{\alpha'}, r_{\alpha'}, \sigma_{\alpha'}) g_{r_{\alpha'}}^{*b'}(\mathbf{p}_{\alpha'}) \mathcal{F}(\mathbf{p}_{\beta'}, r_{\beta'}, \sigma_{\beta'}) g_{r_{\beta'}}^0(\mathbf{p}_{\beta'})$$
$$\times \mathcal{F}(\mathbf{p}_\beta, r_\beta, \sigma_\beta) g_{r_\beta}^0(\mathbf{p}_\beta) \mathcal{F}^*_{\mathbf{P}_{a,r_\alpha}}(\mathbf{n} \times (\mathbf{P}_{\beta,r_\beta} - \mathbf{P}_{a,r_\alpha}) r_0^2) \times \mathcal{F}^*_{\mathbf{P}_{\alpha',r_{\alpha'}}}(\mathbf{n} \times (\mathbf{P}_{\beta',r_{\beta'}} - \mathbf{P}_{\alpha',r_{\alpha'}}) r_0^2) \times V(\alpha,\alpha',\beta,\beta') \Bigg|^2, \tag{45}$$

where the function V is defined by

$$V(\alpha,\alpha',\beta,\beta') = \sum_{\mathbf{Q}^*} \frac{2\pi}{r_0 |\mathbf{P}_{\beta',r_{\beta'}} - \mathbf{P}_{\alpha',r_{\alpha'}} + \mathbf{Q}^*|} \times \exp(-r_0^2(\mathbf{P}_{\beta',r_{\beta'}} - \mathbf{P}_{\alpha',r_{\alpha'}} + \mathbf{Q}^*)^2) \times \exp[-i r_0^2 \mathbf{n} \times \mathbf{Q}^* \cdot (\mathbf{P}_{\alpha,r_\alpha} + \mathbf{P}_{\beta,r_\beta} - \mathbf{P}_{\beta',r_{\beta'}} - \mathbf{P}_{\alpha',r_{\alpha'}})].$$

The form of the pure phase factors $\mathcal{F}^*$ and $\mathcal{F}^*_{\mathbf{p}}$, the momenta $\mathbf{P}_{\alpha,r}$ and the special reciprocal lattice vectors $\mathbf{Q}^*$ are all specified in Appendix C. As before, the functions $g_r^b(\mathbf{p})$ are the coefficients determining the single particle HF excitations. We remark that once the coefficients for the filled band are known the other set of coefficients for the empty bands can be evaluated analytically as the two eigenvectors of the (3×3) matrix representation of the single particle HF Hamiltonian, orthogonal to the vector $g_r^0(\mathbf{p})$.

In order to evaluate numerically expression (45) we restrict the Hilbert space of the single particle HF problem by defining a cell of sides $2N_1\mathbf{a}_1$, $2N_2\mathbf{a}_2$ with N_1, N_2 integers, and impose periodic boundary conditions over its borders. Using the symmetry properties (25) we have

$$T_{N_1 6\mathbf{c}_1} \chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \exp(-i6\mathbf{p}\,.\,\mathbf{c}_1 N_1) \chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}),$$

$$T_{N_2 6\mathbf{c}_2} \chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) = \exp(-i6\mathbf{p}\,.\,\mathbf{c}_2 N_2) \chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}).$$

These constraints can be translated into the relations

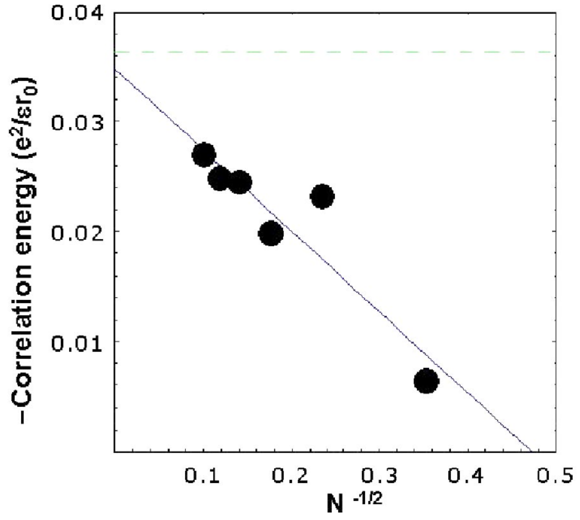

FIG. 3. The negative of the correlation energy correction as a function of sample size. N is the number of particles in the sample. The plotted values were obtained from Eq. (45). The dashed line indicates the result of Eq. (44).

$$-6\mathbf{p}\,.\,\mathbf{c}_1 = 2\pi\frac{n_1}{N_1},$$

$$-6\mathbf{p}\,.\,\mathbf{c}_2 = 2\pi\frac{n_2}{N_2}.$$

They restrict the values of the quasimomentum $\mathbf{p}$ to a discrete set, as expressed in compact form by the condition

$$\mathbf{p} = -\frac{n_1}{N_1}\frac{\mathbf{t}_1}{2} - \frac{n_2}{N_2}\frac{\mathbf{t}_2}{3}, \tag{46}$$

$$0 \leqslant n_1 < N_1,\ 0 \leqslant n_2 < N_2,$$

where $\mathbf{t}_1$ and $\mathbf{t}_2$ are defined in Appendix A. The cell chosen traps $6N_1N_2$ flux quanta and contains $2N_1N_2$ particles. In order to keep the computing time within practical limits, the values of m_1 and m_2 in the expression defining the summation argument

$$\mathbf{Q}^* = m_1\frac{3}{2}\mathbf{t}_1 + m_2\frac{2}{3}\mathbf{t}_2 \tag{47}$$

were restricted to the regions $-4 \leqslant m_1 \leqslant 4$ and $-4 \leqslant m_2 \leqslant 4$, ranges found sufficient to assure numerical convergence. The energy correction was calculated for samples with $N_1 = N_2 = N_s$, yielding an aspect ratio close to one. The upper bound for N_s, set by computing limitations, was $N_s = 7$. The number of particles associated with this value is $N = 2N_s^2 = 98$. Results are shown in Fig. 3 as filled circles. The straight line is a linear fit in the variable $N^{-1/2}$ whose intercept in the limit of large N yields the value

$$\varepsilon_{\text{corr}} = -0.0347 \mp 0.0027, \tag{48}$$

consistent with that given in (44) and obtained with the previous method, shown as an horizontal dashed line in the figure. Notice that the linear fit in terms of the variable $N^{-1/2}$ is suggested by the fact that making the sample finite produces a boundary energy which in two dimensions varies as the square root of the number of particles.

As Fig. 3 suggests, convergence to the thermodynamic limit requires the inclusion of a large number of particles, even beyond our largest value of 98. This outcome points to the relevance of long distance correlations in reaching the correct value of the energy through numerical computations, possibly dominated by cooperative ring exchange effects.[12]

Adding the value (48) to the Hartree-Fock result (30) one obtains the energy per particle $\epsilon = -0.397$. Published values taking one electron per cell and including correlations are $\epsilon_{\text{YL}} = -0.3901$ using perturbation theory,[6] and $\epsilon_{\text{LG}} = -0.3948$ using a variational approach.[17] We notice that our result is slightly lower than either value, suggesting that the CDW state is a serious candidate for the correct Hartree-Fock precursor to the true ground state of the system.

IV. SUMMARY

An analytic solution of the Hartree-Fock problem for a 2DEG at filling 1/3 and half electron per unit cell is found by employing symmetry considerations and a special complete set of common eigenfunctions of the magnetic translations. A triplet of bands arises that turn out surprisingly flat as functions of the two- dimensional quasimomentum. The Coulomb interaction breaks the first Landau level in three narrow subbands resembling effective Landau levels of composite fermions, one of which is fully occupied and the other two, empty. The energy per particle reproduces an earlier numerical result for this quantity.[5] We find that the charge density forms hexagonal rings throughout the lattice, suggesting strong long range correlations owing to cooperative ring exchange. An evaluation of the correlation energy using second order perturbation theory yields a correction an order of magnitude larger than that for the localized single-particle features of the usual Wigner Crystal state.[6] Our results also indicate that the thermodynamic limit may not be reached even when 98 particles are included, thus suggesting the relevance of long range correlation effects in the generation of the enhanced cohesive correlations. Further, numerical results we have obtained at fillings 1/5, 1/7, and 1/9 show that the CDW charge distribution also has hexagonal ridges that become sharper as the filling decreases. One can then speculate that these states have a large correlation energy, making them good candidates for the ground state at such low electron densities. Further results for these latter fillings will be reported elsewhere.

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APPENDIX A

1. Eigenfunctions of magnetic translations

Consider a 2DEG constrained to move in a plane of area A under a perpendicular magnetic field $\mathbf{B}$. A useful basis set of single particle Bloch-type states in the lowest Landau level can be defined in terms of linear combinations of the normalized zero angular momentum eigenfunction

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{2\pi}r_o}\exp\left(-\frac{\mathbf{x}^2}{4r_o^2}\right) \tag{A1}$$

in the compact form,[7,15,16,18]

$$\varphi_k(\mathbf{x}) = \frac{1}{N_{\mathbf{k}}}\sum_{\ell}(-1)^{\ell_1\ell_2}\exp(i\mathbf{k}\,.\,\ell)T_{\ell}\phi(\mathbf{x}), \tag{A2}$$

$$N_{\mathbf{k}} = \sqrt{N_{\phi_0}}\sqrt{\sum_{\ell}(-1)^{\ell_1\ell_2}\exp\left(i\mathbf{k}\,.\,\ell - \frac{\ell^2}{4r_0^2}\right)}.$$

Due to its role in the above definition the function ϕ is called the "seed" function. The sum runs over all integers ℓ_1, ℓ_2 defining a planar lattice L, through $\ell = \ell_1\mathbf{b}_1 + \ell_2\mathbf{b}_2$, where the unit cell intercepts one flux quantum, so that $\mathbf{n}.\mathbf{b}_1\times\mathbf{b}_2=2\pi r_o^2$. The magnetic translation operators $T_{\mathbf{R}}$ acting on any function f are defined by

$$T_{\mathbf{R}}\, f(\mathbf{x}) = \exp\left(\frac{2ie}{\hbar c}\mathbf{A}(\mathbf{R})\,.\,\mathbf{x}\right) f(\mathbf{x}-\mathbf{R}), \tag{A3}$$

where the vector potential is assumed in the axial gauge $\mathbf{A}(\mathbf{x})=B(-x_2,x_1,0)/2$ and the electron charge e is taken with its negative sign. This basis was employed before to obtain exact mean field solutions of the related problem at filling 1/2.[8] For arbitrary vectors $\mathbf{R}_1$ and $\mathbf{R}_2$ the translation operators satisfy the commutation relation

$$T_{\mathbf{R}_1}T_{\mathbf{R}_2} = \exp\left(\frac{ie}{\hbar c}\mathbf{A}(\mathbf{R}_1)\,.\,\mathbf{R}_2\right)T_{\mathbf{R}_2}T_{\mathbf{R}_1}. \tag{A4}$$

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

$$T_{\ell}\varphi_{\mathbf{k}}(\mathbf{x}) = \lambda_{\mathbf{k}}(\ell)\varphi_{\mathbf{k}}(\mathbf{x}), \tag{A5}$$

$$\lambda_{\mathbf{k}}(\ell) = (-1)^{\ell_1\ell_2}\exp(-i\mathbf{k}\,.\,\ell). \tag{A6}$$

Arranged in an arbitrary Slater determinant these functions are exact solutions of the Hartree-Fock problem.[18,19] This strong property happens because the HF single particle Hamiltonian commutes with all translations leaving L invariant.[18] The functions (A2) are common eigenfunctions of the commuting magnetic translations. Moreover, the set of eigenvalues (A6) uniquely determines them. Therefore, the HF Hamiltonian associated with the Slater determinant cannot change those eigenvalues and the $\varphi_{\mathbf{k}}$ should be eigenfunctions.

Finally, let us show that the effect of an arbitrary translation on the basis functions is equivalent to a shift in the momentum label, modulo a phase factor.[16] Operating twice with the translation operator involving an arbitrary vector $\mathbf{a}$ and a vector in the lattice ℓ and using Eqs. (A4) and (A5) one readily gets,

$$T_{\mathbf{a}}T_{\ell}\varphi_{\mathbf{p}}(\mathbf{x}) = \lambda_{\mathbf{p}}(\ell)T_{\mathbf{a}}\varphi_{\mathbf{p}}(\mathbf{x}) = \exp\left(2\frac{ie}{\hbar c}\mathbf{A}(\mathbf{a})\,.\,\ell\right)T_{\ell}T_{\mathbf{a}}\varphi_{\mathbf{p}}(\mathbf{x}). \tag{A7}$$

Again using (A5) we have

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

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

$$T_{\mathbf{a}}\varphi_{\mathbf{p}}(\mathbf{x}) = \mathcal{F}_{\mathbf{p}}(\mathbf{a})\varphi_{\mathbf{p}+2(e/\hbar c)\mathbf{A}(\mathbf{a})}(\mathbf{x}), \tag{A8}$$

from which also follows,

$$\mathcal{F}_{\mathbf{p}}(\mathbf{a}) = \frac{\varphi_{\mathbf{p}}(0)}{\varphi_{\mathbf{p}+2(e/\hbar c)\mathbf{A}(\mathbf{a})}(\mathbf{a})}. \tag{A9}$$

That is, a magnetic translation is equivalent to a shift in the quasimomentum.

2. A $\varphi_{\mathbf{p}}$-transform

Any function f in the first Landau level, and its inverse, can be represented as

$$\begin{aligned} f(\mathbf{x}) &= \sum_{\mathbf{p}\in\tilde{B}} c(\mathbf{p})\varphi_{\mathbf{p}}(\mathbf{x}) \\ &= \int_{\mathbf{p}\in\tilde{B}}\frac{d\mathbf{p}}{(2\pi)^2}\tilde{c}(\mathbf{p})\overline{\varphi_{\mathbf{p}}}(\mathbf{x}),\tilde{c}(\mathbf{p}) \\ &= \int d\mathbf{x}\overline{\varphi}^{*}_{\mathbf{p}}(\mathbf{x})f(\mathbf{x}), \end{aligned}$$

where $\overline{\varphi_{\mathbf{p}}}(\mathbf{x})=\sqrt{S}\varphi_{\mathbf{p}}(\mathbf{x})$, $\tilde{c}(\mathbf{p})=\sqrt{S}c(\mathbf{p})$, with $S=2\pi r_0^2N_{\phi_0}$, with N_{ϕ_0} the number of flux quanta in the system area, $\tilde{B}$ is the Brillouin zone defined by the unit cell vectors

$$\mathbf{t}_1 = -\frac{1}{r_0^2}\mathbf{n}\times\mathbf{b}_2,$$

$$\mathbf{t}_2 = \frac{1}{r_0^2}\mathbf{n}\times\mathbf{b}_1.$$

The orthogonality and completeness relations in the first Landau level of the modified functions take the forms

$$\int_A d\mathbf{x}\overline{\varphi}^{*}_{\mathbf{p}}(\mathbf{x})\overline{\varphi}_{\mathbf{p}'}(\mathbf{x}) = (2\pi)^2\delta(\mathbf{p}-\mathbf{p}'),$$

$$P(\mathbf{x},\mathbf{x}') = \sum_{\mathbf{p}\in\tilde{B}}\varphi_{\mathbf{p}}(\mathbf{x})\varphi^{*}_{\mathbf{p}}(\mathbf{x}') = \int_{p\in\tilde{B}}\frac{dp}{(2\pi)^2}\overline{\varphi_{\mathbf{p}}}(\mathbf{x})\overline{\varphi}^{*}_{\mathbf{p}}(\mathbf{x}'). \tag{A10}$$

3. The orbitals $\chi_{\mathbf{p}}^{(r,\sigma)}$ as special cases of the basis functions $\varphi_{\mathbf{p}}(\mathbf{x})$

Let us now verify that the functions $\chi_{\mathbf{p}}^{(r,\sigma)}$ constructed to diagonalize in blocks the HF Hamiltonian in Sec. II are simply constant phase factors multiplied by a particular kind of basis functions $\varphi_{\mathbf{p}}$. These differ from the orbitals considered in Sec. II and defined by the unit cell vectors (7) in that their basis vectors are given by

$$\mathbf{b}_1 = \tfrac{2}{3}\mathbf{a}_1, \mathbf{b}_2 = \mathbf{a}_2. \tag{A11}$$

To start out it will be useful to consider the $\varphi_{\mathbf{p}}$-transform of a translated "seed" function $\phi(x)$. For this purpose we notice that it is possible to fix the second argument of the projector operator to be equal to the translation vector $\mathbf{a}$. It follows that the projector operator in the first Landau level can be rewritten as

$$P(\mathbf{x},\mathbf{a}) = \frac{1}{2\pi r_0^2}\exp\left(-\frac{(\mathbf{x}-\mathbf{a})^2}{4r_0^2}\right)\exp\left(\frac{ie}{\hbar c}\mathbf{A}(\mathbf{a})\,.\,\mathbf{x}\right)$$
$$= \frac{1}{\sqrt{2\pi r_0^2}}T_a\phi(\mathbf{x}) = \int_{p\in\tilde{B}}\frac{dp}{(2\pi)^2}\overline{\varphi}_{\mathbf{p}}(\mathbf{x})\overrightarrow{\varphi}^{*}_{\mathbf{p}}(\mathbf{a}), \tag{A12}$$

where the last equality is merely the definition of the projector operator in coordinate space. Therefore, these relations determine the following $\varphi_{\mathbf{p}}$-transform of the translated "seed" function

$$T_a\phi(\mathbf{x}) = \int_{\mathbf{p}\in\tilde{B}}\frac{d\mathbf{p}}{(2\pi)^2}\left(\sqrt{2\pi r_0^2}\,\overrightarrow{\varphi}^{*}_{\mathbf{p}}(\mathbf{a})\right)\overline{\varphi}_{\mathbf{p}}(\mathbf{x}). \tag{A13}$$

Next we will consider the definition

$$\chi_{\mathbf{p}}^{(r,\sigma)}(x) = \frac{1}{\sqrt{6}N_{\mathbf{p}}^{(3,2)}}\sum_{\mathbf{m}}\exp\left(i\mathbf{P}^{(\mathbf{p},r,\sigma)}\,.\,\mathbf{m} + \frac{5\pi i}{6}m_1m_2\right)T_{\mathbf{m}}\phi(\mathbf{x}), \tag{A14}$$

and represent the vectors **m** in terms of alternative vectors ℓ and the indices α and β defined through the expressions

$$\mathbf{m} = \ell + \delta,$$

$$\ell = \ell_1 2\mathbf{c}_1 + \ell_2 3\mathbf{c}_2,$$

$$\delta = u\mathbf{c}_1 + v\mathbf{c}_2.$$

The symbols α, β, ℓ_1, and ℓ_2 are specified by the relations

$$u = \langle m_1\rangle = \begin{cases} 0 \text{ if } m_1 = 0 \text{ Modulo}(2) \\ 1 \text{ if } m_1 = 1 \text{ Modulo}(2), \end{cases}$$

$$v = [m_1] = \begin{cases} -1 \text{ if } m_2 = -1 \text{ Modulo}(3) \\ \ \ 0 \text{ if } m_2 = 0 \text{ Modulo}(3) \\ \ \ 1 \text{ if } m_2 = 1 \text{ Modulo}(3), \end{cases}$$

$$\ell_1 = \frac{m_1 - \langle m_1\rangle}{2},$$

$$\ell_2 = \frac{m_2 - [m_2]}{3}.$$

The use of these alternative definitions allows to write (A14) in the form

$$\chi_{\mathbf{p}}^{(r,\sigma)}(x) = \frac{1}{\sqrt{6}N_{\mathbf{p}}^{(3,2)}}\sum_{\ell}(-1)^{\ell_1\ell_2}\exp(i\mathbf{P}^{(\mathbf{p},r,\sigma)}\cdot\ell)T_\ell$$
$$\times\left\{\sum_{u=0,1}\sum_{v=-1,0,1}\exp\left(\frac{5\pi i}{6}uv + i\mathbf{P}^{(\mathbf{p},r,\sigma)}\right.\right.$$
$$\left.\left.\times(u\mathbf{c}_1+v\mathbf{c}_2)\right)T_{u\mathbf{c}_1+v\mathbf{c}_2}\phi(\mathbf{x})\right\}. \tag{A15}$$

Now, it can be noticed that the above expression differs from the definition (A2) only in that the "seed" function is changed by a superposition of itself translated to the points $u\mathbf{c}_1+v\mathbf{c}_2$. However, it was shown in Ref. 16 that the basis functions are completely independent of an arbitrary change in the "seed" for any other function in the first Landau level.

An alternative proof of this curious property is possible. To see it let us represent the "seed" functions in (A15) by their $\varphi_{\mathbf{p}}$-transform (A13), yielding

$$\chi_{\mathbf{p}}^{(r,\sigma)}(x) = \frac{1}{\sqrt{6}N_{\mathbf{p}}^{(3,2)}}\sum_{\alpha=0,1}\sum_{\beta=-1,0,1}\exp\left(\frac{5\pi i}{6}uv + i\mathbf{P}^{(\mathbf{p},r,\sigma)}\right.$$
$$\left.\times(u\mathbf{c}_1+v\mathbf{c}_2)\right)\int\frac{d\mathbf{q}}{(2\pi)^2}\sqrt{2\pi r_0^2}\,\overrightarrow{\varphi}^{*}_{\mathbf{q}}$$
$$\times(u\mathbf{c}_1+v\mathbf{c}_2)\overline{\varphi}_{\mathbf{q}}(\mathbf{x})\sum_{\ell}\exp(i(\mathbf{P}^{(\mathbf{p},r,\sigma)}-\mathbf{q})\cdot\ell),$$

after employing the character of eigenfunctions of the operators T_ℓ that the functions $\overline{\varphi}_{\mathbf{q}}$ have. But now the following identity can be employed:

$$\sum_{\ell\in\mathbf{A}}\exp(i(\mathbf{q}-\mathbf{q}')\cdot\ell) = \frac{(2\pi)^2}{2\pi r_0^2}\delta(\mathbf{q},\mathbf{q}'),$$

where the δ function is nonvanishing for equal arguments modulo a vector of the reciprocal lattice $Q=\frac{3}{2}Q_1\mathbf{t}_1+\frac{2}{3}Q_2\mathbf{t}_2$. This relation allows to show the desired connection between the basis functions $\chi_{\mathbf{p}}^{(r,\sigma)}$ and $\overline{\varphi}_{\mathbf{p}}(\mathbf{x})$,

$$\chi_{\mathbf{p}}^{(r,\sigma)}(x) = \mathcal{F}(\mathbf{p},r,\sigma)\overline{\varphi}_{\mathbf{P}^{(\mathbf{p},r,\sigma)}}(\mathbf{x}),$$

where the phase factor is given by

$$\mathcal{F}(\mathbf{p},r,\sigma) = \frac{1}{\sqrt{6}\sqrt{2\pi r_0^2}N_{\mathbf{p}}^{(3,2)}}\sum_{u=0,1}\sum_{v=-1,0,1}\exp\left(\frac{5\pi i}{6}uv\right.$$
$$\left.+ i\mathbf{P}^{(\mathbf{p},r,\sigma)}\cdot(u\mathbf{c}_1+v\mathbf{c}_2)\right)\overrightarrow{\varphi}^{*}_{\mathbf{P}^{(\mathbf{p},r,\sigma)}}(u\mathbf{c}_1+v\mathbf{c}_2).$$

4. Periodicity of the Slater determinants of triplet orbitals

Here we show that the single particle density associated with a Slater determinant formed with a set of functions, each one corresponding to an arbitrary linear combinations of the triplet of orbitals characterized by the indices $(\mathbf{p},\sigma)$, is periodic over the lattice **R**. To consider this question, let us use the basic property that the density of a many electron Slater determinant constructed with orthogonal orbitals is the sum of the individual densities of each orbital. Writing the selected linear combinations as

$$\Psi_{\mathbf{p}}^{(\sigma)}(\mathbf{x}) = \sum_r C_{\mathbf{p}}^{(r,\sigma)}\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}), \tag{A16}$$

where the coefficients $C_{\mathbf{p}}^{(r,\sigma)}$ are arbitrary, and considering the symmetry properties (25), it follows that

$$
\begin{aligned}
\rho(\mathbf{x}) &= \sum_{\mathbf{p}} \sum_{\sigma=\pm 1} |\Psi_{\mathbf{p}}^{(\sigma)}(\mathbf{x})|^2 \\
&= \sum_{\mathbf{p}} \sum_{\sigma=\pm 1} |\Psi_{\mathbf{p}}^{(-\sigma)}(\mathbf{x})|^2 = \sum_{\mathbf{p}} \sum_{\sigma=\pm 1} \sum_{r} \sum_{r'} C_{\mathbf{p}}^{(r',\sigma)*} C_{\mathbf{p}}^{(r,\sigma)} \\
&\quad \times (\exp(i\mathbf{p}\cdot\mathbf{a}_1) T_{a_1} \chi_{\mathbf{p}}^{(r',\sigma)}(\mathbf{x}))^* \exp(i\mathbf{p}\cdot\mathbf{a}_1) T_{a_1} \chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}) \\
&= \sum_{\mathbf{p}} \sum_{\sigma=\pm 1} \sum_{r} \sum_{r'} C_{\mathbf{p}}^{(r',\sigma)*} C_{\mathbf{p}}^{(r,\sigma)} \left(\exp\left(\frac{ie}{\hbar c} \mathbf{A}(\mathbf{a}_1)\cdot\mathbf{x} \right) \chi_{\mathbf{p}}^{(r',\sigma)} \right. \\
&\quad \left. \times (\mathbf{x}-\mathbf{a}_1) \right)^* \exp\left(\frac{ie}{\hbar c} \mathbf{A}(\mathbf{a}_1)\cdot\mathbf{x} \right) \chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x}-\mathbf{a}_1) \\
&= \sum_{\mathbf{p}} \sum_{\sigma=\pm 1} |\Psi_{\mathbf{p}}^{(\sigma)}(\mathbf{x}-\mathbf{a}_1)|^2 = \rho(\mathbf{x}-\mathbf{a}_1).
\end{aligned}
$$

One can show in a similar way that $\rho(\mathbf{x})=\rho(\mathbf{x}-\mathbf{a}_2)$.

APPENDIX B

Here we shall derive the general formula expressing the single particle Hartree-Fock Hamiltonian as a sum of magnetic translation operations. The arguments of these operators are spatial vectors determined by the reciprocal lattice associated with the Fourier components of the density. It is worth remarking here that the lattice considered in this Appendix is not restricted in any way. Therefore, the representation of the single particle HF Hamiltonian is valid for a general though periodic mean field problem.

Consider the action of the kernels of the direct and exchange interactions defining the HF Hamiltonian over any of the elements φ_p of the complete basis functions as follows:

$$
\begin{aligned}
\tilde{\varphi}^{(d)}(\mathbf{x}) &= H_{\mathrm{HF}}^{(d)} \varphi_{\mathbf{p}}(\mathbf{y}') \\
&= \frac{e^2}{\varepsilon_o} \int d\mathbf{y} d\mathbf{y}' P(\mathbf{x},\mathbf{y}') \frac{\rho(\mathbf{y}) - n_0/e^2}{|\mathbf{y}-\mathbf{y}'|} \varphi_{\mathbf{p}}(\mathbf{y}'),
\end{aligned} \tag{B1}
$$

$$
\begin{aligned}
\tilde{\varphi}^{(e)}(\mathbf{x}) &= H_{\mathrm{HF}}^{(e)} \varphi_{\mathbf{p}}(\mathbf{y}') \\
&= -\frac{e^2}{\varepsilon_o} \int d\mathbf{y} d\mathbf{y}' P(\mathbf{x},\mathbf{y}') \frac{\rho(\mathbf{y},\mathbf{y}')}{|\mathbf{y}-\mathbf{y}'|} \varphi_{\mathbf{p}}(\mathbf{y}'),
\end{aligned} \tag{B2}
$$

where n_0 is the jellium background charge density making the overall system neutral. The representation we shall derive is valid for both direct and exchange kernels and will be discussed below for each case separately.

1. Direct Coulomb interaction

The potential term representing the direct Coulomb interaction can be written in its Fourier transform representation as follows:

$$
\begin{aligned}
v^{(d)}(\mathbf{x}) &= \frac{e^2}{\varepsilon_o} \int d\mathbf{x}' \frac{\rho(\mathbf{x}') - n_0/e^2}{|\mathbf{x}-\mathbf{x}'|} \\
&= \frac{e^2}{\varepsilon_o} \sum_{\mathbf{Q}\neq 0} \rho(\mathbf{Q}) \int d\mathbf{x}' \frac{\exp(i\mathbf{Q}\cdot\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|} \\
&= \sum_{\mathbf{Q}} \frac{2\pi e^2}{\varepsilon_o} \frac{\rho(\mathbf{Q})(1-\delta_{\mathbf{Q},0})}{|\mathbf{Q}|} \exp(i\mathbf{Q}\cdot\mathbf{x}) \\
&= \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp(i\mathbf{Q}\cdot\mathbf{x}).
\end{aligned} \tag{B3}
$$

Then, using the representation of the kernel for the projection operator in the first Landau level

$$
P(\mathbf{x},\mathbf{x}') = \frac{1}{2\pi r_0^2} \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^2}{4r_0^2} \right) \exp\left(\frac{ie}{\hbar c} \mathbf{A}(\mathbf{x}')\cdot\mathbf{x} \right)
$$

we obtain,

$$
\tilde{\varphi}_p^{(d)}(\mathbf{x}) = \int d\mathbf{y}' P(\mathbf{x},\mathbf{y}') \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp(i\mathbf{Q}\cdot\mathbf{y}') \varphi_{\mathbf{p}}(\mathbf{y}'). \tag{B4}
$$

Recalling definition (A2) we get for each translation term

$$
\begin{aligned}
L_\ell^{(d)}(\mathbf{x}) &= \int d\mathbf{y}' P(\mathbf{x},\mathbf{y}') \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp(i\mathbf{Q}\cdot\mathbf{y}') T_\ell \phi(\mathbf{y}') \\
&= \frac{1}{\sqrt{2\pi} r_0} \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp\left(-\frac{1}{4} r_0^2 \mathbf{Q}^2 \right) \exp\left(i \frac{\mathbf{Q}\cdot\ell}{2} \right) \\
&\quad \times \exp\left(-\frac{1}{4r_0^2} (\mathbf{x} - (\ell - \mathbf{r}_0^2 \mathbf{Q}\times\mathbf{n}))^2 \right. \\
&\quad \left. - \frac{i}{2r_0^2} \mathbf{x}\cdot(\ell + \mathbf{r}_0^2 \mathbf{n}\times\mathbf{Q}) \right) \\
&= \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp\left(-\frac{1}{4} r_0^2 \mathbf{Q}^2 \right) \\
&\quad \times \exp\left(i \frac{\mathbf{Q}\cdot\mathbf{l}}{2} \right) T_{\ell + \mathbf{r}_0^2 \mathbf{n}\times\mathbf{Q}} \phi(\mathbf{x}).
\end{aligned} \tag{B5}
$$

This last relation can be further simplified by employing relation (A7) and the similar property

$$
T_{\mathbf{R}_1} T_{\mathbf{R}_2} = \exp\left(\frac{ie}{\hbar c} \mathbf{A}(\mathbf{R}_1)\cdot\mathbf{R}_2 \right) T_{\mathbf{R}_1+\mathbf{R}_2},
$$

leading to the formula

$$
\begin{aligned}
&\int d\mathbf{y}' P(\mathbf{x},\mathbf{y}') \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp(i\mathbf{Q}\cdot\mathbf{y}') T_\ell \phi(\mathbf{x}) \\
&\quad = \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q}) \exp\left(-\frac{1}{4} r_0^2 \mathbf{Q}^2 \right) T_{\mathbf{r}_0^2 \mathbf{n}\times\mathbf{Q}} T_\ell \phi(\mathbf{x}).
\end{aligned}
$$

After adding corresponding the integrals over all translations ℓ one obtains

$$H_{\mathrm{HF}}^{(d)}\varphi_{\mathbf{p}}(\mathbf{x}) = \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}\varphi_{\mathbf{p}}(\mathbf{x}).$$

Since the equality is valid for any element of the complete basis $\varphi_{\mathbf{p}}(\mathbf{x})$ it then follows,

$$H_{\mathrm{HF}}^{(d)} = \sum_{\mathbf{Q}} v^{(d)}(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}. \qquad \text{(B6)}$$

2. Exchange interaction

The derivation of the analogous representation for the exchange interaction kernel is more involved and needs for some special properties of the one particle density matrix. Then, let us initially consider these properties.

a. One particle density matrix transformations

The definition of the one-particle density matrix in terms of the Slater determinant $\Phi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4,\ldots,\mathbf{x}_N)$ can be transformed by performing a simultaneous magnetic translation operation in a vector $\mathbf{R}$ of the periodic lattice over all the particle coordinates. Since this is assumed to be a symmetry transformation of the system, this map should leave the many particle state invariant. Thus by assumption

$$\begin{aligned}
\rho(\mathbf{x}_1,\mathbf{x}_2) &= \int\cdots\int d\mathbf{x}_3 d\mathbf{x}_3\cdots d\mathbf{x}_N|\Phi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4,\cdots,\mathbf{x}_N)|^2\\
&= \int\cdots\int d\mathbf{x}_3 d\mathbf{x}_3\cdots d\mathbf{x}_N\left|\prod_{i=3}^{N} T_R(\mathbf{x}_i)\Phi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4,\cdots,\mathbf{x}_N)\right|^2\\
&= \sum_s \Psi_s(\mathbf{x}_1)\Psi_s^*(\mathbf{x}_2)\\
&= \sum_s T_R(\mathbf{x}_1)\Psi_s(\mathbf{x}_1)(T_R(\mathbf{x}_2)\Psi_s(\mathbf{x}_2))^*\\
&= \sum_s \exp\left(\frac{ie}{\hbar c}\mathbf{A}(\mathbf{R})\cdot(\mathbf{x}_1-\mathbf{x}_2)\right)\exp(\Psi_s(\mathbf{x}_1-R)\ (\Psi_s(\mathbf{x}_2-R))^*\rho(\mathbf{x}_1,\mathbf{x}_2)\\
&= \exp\left(\frac{ie}{\hbar c}\mathbf{A}(\mathbf{R})\cdot(\mathbf{x}_1-\mathbf{x}_2)\right)\rho(\mathbf{x}_1-R,\mathbf{x}_2-R),
\end{aligned} \qquad \text{(B7)}$$

an expression that furnishes the transformation law of the one particle density matrix under spatial shifts in the vectors of the periodic lattice.

b. The density determines the density matrix

Below we will show that the Fourier components of the density completely determine the whole one-particle density matrix. For this purpose, let us use the new variable $\mathbf{z}=\mathbf{x}-\mathbf{x}'$ in the one-particle density matrix, so that $\rho(\mathbf{x},\mathbf{x}')=\tilde{\rho}(\mathbf{x},\mathbf{z})$, where the tilde over ρ underlines the different functional expression of the new definition. It now transforms under spatial shifts as

$$\tilde{\rho}(\mathbf{x}-\mathbf{R},\mathbf{z}) = \exp\left(-\frac{ie}{\hbar c}\mathbf{A}(\mathbf{R})\cdot\mathbf{z}\right)\tilde{\rho}(\mathbf{x},\mathbf{z}). \qquad \text{(B8)}$$

Therefore, the function

$$\tilde{g}(\mathbf{x},\mathbf{z}) = \exp\left(-\frac{ie}{\hbar c}\mathbf{A}(\mathbf{x})\cdot\mathbf{z}\right)\tilde{\rho}(\mathbf{x},\mathbf{z}),$$

is fully periodic in the variable $\mathbf{x}$ under the lattice shifts. That is $\tilde{g}(\mathbf{x}-\mathbf{R},\mathbf{z})=\tilde{g}(\mathbf{x},\mathbf{z})$. Then, Fourier expanding $\tilde{g}$ leads to the following expression for $\tilde{\rho}$

$$\tilde{\rho}(\mathbf{x},\mathbf{z}) = \sum_{\mathbf{Q}} \exp\left(i\left(\mathbf{Q}-\frac{e}{\hbar c}\mathbf{A}(\mathbf{R})\right)\cdot\mathbf{x}\right)\tilde{\rho}(\mathbf{Q},\mathbf{z}),$$

where

$$\begin{aligned}
\tilde{\rho}(\mathbf{Q},\mathbf{z}) = \frac{1}{A_{\mathrm{cell}}}\int d\mathbf{x}'\ \exp(-i\mathbf{Q}\cdot\mathbf{x}')\\
\times\exp\left(i\frac{e}{\hbar c}\mathbf{A}(\mathbf{z})\cdot\mathbf{x}'\right)\tilde{\rho}(\mathbf{x}',\mathbf{z}).
\end{aligned} \qquad \text{(B9)}$$

Further, let us consider the density written as the sum

$$\begin{aligned}
&\sum_s \Psi_s(\mathbf{x})\Psi_s^*(\mathbf{x}')\\
&\quad= \sum_{\mathbf{p}}\sum_{r,\sigma,r',\sigma'} f_{r,\sigma}(\mathbf{p})\chi_{\mathbf{p}}^{(r,\sigma)}(\mathbf{x})f_{r',\sigma'}^*(\mathbf{p})\chi_{\mathbf{p}}^{(r',\sigma')}(\mathbf{x}')^*,
\end{aligned}$$

and the fact that each $\chi_{\mathbf{p}}^{(r',\sigma)}$ in the lower Landau level can be expanded as a linear combination of the complete basis functions $\{T_\ell\phi(\mathbf{x})\}$ defined over a lattice with one flux quantum per unit cell.[20] Then, a generic term in the integral in (B9) has the form

$$\widetilde{\rho_{\ell,\ell'}}(\mathbf{Q},\mathbf{z}) = \frac{1}{A_{\text{cell}}}\int d\mathbf{x}\,\exp(-i\mathbf{Q}\cdot\mathbf{x}) \times\exp\left(i\frac{e}{\hbar c}\mathbf{A}(\mathbf{z})\cdot\mathbf{x}\right)T_{\ell}\phi(\mathbf{x})(\,T_{\ell'}\phi(\mathbf{x}')|_{\mathbf{x}'=\mathbf{x}-\mathbf{z}})^{*}.$$

Since the function ϕ is a Gaussian, its magnetic translations (A3) have also this character, and thus the integrals in (B9) can be calculated explicitly. We obtain,

$$\widetilde{\rho_{\ell,\ell'}}(\mathbf{Q},\mathbf{z}) = \widetilde{\rho_{\ell,\ell'}}(\mathbf{Q},\mathbf{0})\exp\left(-\frac{\mathbf{z}^2}{4r_0^2}-\frac{1}{4r_0^2}\mathbf{Q}\cdot(\mathbf{n}\times\mathbf{z}+i\mathbf{z})\right).$$

But since the phase factor here is independent of the indices ℓ,ℓ', the summation of all the contributions in (B9) leads to the relation

$$\widetilde{\rho}(\mathbf{Q},\mathbf{z}) = \rho(\mathbf{Q})\exp\left(-\frac{\mathbf{z}^2}{4r_0^2}-\frac{1}{4r_0^2}\mathbf{Q}\cdot(\mathbf{n}\times\mathbf{z}+i\mathbf{z})\right), \tag{B10}$$

$$\widetilde{\rho}(\mathbf{Q},\mathbf{0}) = \rho(\mathbf{Q}),$$

which expresses the interesting result that the full one-particle density matrix is completely determined by the particle density.

We now consider the exchange term (B2). Using the above results the integrals in

$$\widetilde{\varphi}^{(e)}(\mathbf{x}) = -e^2\int d\mathbf{y}'P(\mathbf{x},\mathbf{y}')\int d\mathbf{z} \times\sum_{\mathbf{Q}}\exp\left(i\left(\mathbf{Q}-\frac{e}{\hbar c}\mathbf{A}(\mathbf{z})\right)\cdot\mathbf{y}'\right) \times\frac{\widetilde{\rho}(\mathbf{Q},\mathbf{z})}{|\mathbf{z}|}\varphi_{\mathbf{p}}(\mathbf{y}'-\mathbf{z}), \tag{B11}$$

can be calculated explicitly. For this purpose, let us consider again the integral of a generic term $T_{\ell}\,\phi$ in the sum over ℓ defining the functions $\varphi_{\mathbf{p}}$. The integral for this term is then reduced to two simple integrals, which after some algebra can be explicitly evaluated to obtain

$$\begin{aligned}L^{(e)}(\mathbf{x}) &= \sum_{\mathbf{Q}}v^{(e)}(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)\exp\left(i\frac{\mathbf{Q}\cdot\ell}{2}\right)T_{\ell+\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}\phi(\mathbf{x})\\ &= \sum_{\mathbf{Q}}v^{(e)}(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}T_{\ell}\phi(\mathbf{x}),\end{aligned} \tag{B12}$$

$$v^{(e)}(\mathbf{Q}) = -\frac{2\pi e^2 r_0}{\varepsilon_o}\sqrt{\frac{\pi}{2}}\widetilde{\rho}(\mathbf{Q},\mathbf{0})\exp\left(\frac{1}{4}r_0^2\mathbf{Q}^2\right)I_0\left(\frac{1}{4}r_0^2\mathbf{Q}^2\right). \tag{B13}$$

Henceforth, after adding all terms for different values of ℓ follows

$$H_{\text{HF}}^{(e)}\varphi_p(\mathbf{x}) = \left(\sum_{\mathbf{Q}}v^{(e)}(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}\right)\varphi_p(\mathbf{x}).$$

Using the independence and completeness of the basis formed by the φ_p's in the first Landau level, we thus obtain

$$H_{\text{HF}}^{(e)} = \sum_{\mathbf{Q}}v^{(e)}(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}.$$

Combining this results and the previous one (B6) the following representation for the one-particle Hartree-Fock Hamiltonian in the first Landau level follows,

$$\begin{aligned}H_{\text{HF}} &= \sum_{\mathbf{Q}}(v^{(d)}(\mathbf{Q})+v^{(e)}(\mathbf{Q}))\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}}\\ &= \sum_{\mathbf{Q}}v(\mathbf{Q})\exp\left(-\frac{1}{4}r_0^2\mathbf{Q}^2\right)T_{\mathbf{r}_0^2\mathbf{n}\times\mathbf{Q}},\end{aligned} \tag{B14}$$

with the coefficients defined by

$$v(\mathbf{Q}) = 2\pi r_0^2\rho(\mathbf{Q})\left(\frac{(1-\delta_{\mathbf{Q},\mathbf{0}})}{r_0|\mathbf{Q}|} - \sqrt{\frac{\pi}{2}}\exp\left(\frac{1}{4}r_0^2\mathbf{Q}^2\right)I_0\left(\frac{1}{4}r_0^2\mathbf{Q}^2\right)\right)\frac{e^2}{\varepsilon_o r_0}. \tag{B15}$$

APPENDIX C

In this Appendix we sketch the derivation of the formula (45) employed in the evaluation of the sample size dependence of the correction to the energy per particle. As before, we use the shorthand notation

$$\Phi_{\alpha} \equiv \Phi_{\mathbf{p}_{\alpha}}^{(b_{\alpha},\sigma_{\alpha})} = \sum_{r}g_r^{b_{\alpha}}(\mathbf{p}_{\alpha})\chi_{\mathbf{p}_{\alpha}}^{(r,\sigma_{\alpha})}(x) = \sum_{r}d_{\mathbf{p}_{\alpha}}^{(b_{\alpha},r,\sigma_{\alpha})}\varphi_{\mathbf{p}_{\alpha},r}(\mathbf{x}),$$

$$d_{\mathbf{p}_{\alpha}}^{(b_{\alpha},r,\sigma_{\alpha})} = \mathcal{F}(\mathbf{p}_{\alpha},r,\sigma_{\alpha})g_r^{b_{\alpha}}(\mathbf{p}_{\alpha}),$$

$$\mathbf{P}_{\alpha,r} \equiv \mathbf{P}^{(\mathbf{p}_{\alpha},r,\sigma_{\alpha})} = \mathbf{p}_{\alpha} - r\mathbf{s}_1 + \frac{\sigma_{\alpha}-1}{2}\frac{3}{2}\mathbf{s}_2.$$

The relations expressing the functions $\chi_{\mathbf{p}_{\alpha}}^{(r,\sigma_{\alpha})}$ in terms of $\varphi_{\mathbf{p}_{\alpha}}$ times a phase factor has also been employed in order to define the new coefficients $d_{\mathbf{p}_{\alpha}}^{(b_{\alpha},r,\sigma_{\alpha})}$. By representing the Coulomb potential by its Fourier transform, and substituting all the expansions of the functions $\varphi_{\mathbf{p}_{\alpha}}$ in terms of magnetic translations of the "seed" in the matrix elements (34), the resulting Gaussian integrals for each term can be evaluated. After some algebra it is possible to obtain the expression

$$
\begin{aligned}
M(\alpha,\alpha'|\beta',\beta) &= \int\int d\mathbf{x}d\mathbf{x}'\,\Phi^*_{\alpha}(\mathbf{x})\Phi^*_{\alpha'}(\mathbf{x}')\frac{1}{|\mathbf{x}-\mathbf{x}'|}\Phi_{\beta'}(\mathbf{x}')\Phi_{\beta}(\mathbf{x}) \\
&= \sum_{r_\alpha}\sum_{r_{\alpha'}}\sum_{r_{\beta'}}\sum_{r_\beta}(d^{(b_\alpha,r_\alpha,\sigma_\alpha)}_{\mathbf{p}_\alpha}d^{(b_{\alpha'},r_{\alpha'},\sigma_{\alpha'})}_{\mathbf{p}_{\alpha'}})^* d^{(0,r_{\beta'},\sigma_{\beta'})}_{\mathbf{p}_{\beta'}}d^{(0,r_\beta,\sigma_\beta)}_{\mathbf{p}_\beta} \\
&\quad\times\int\int d\mathbf{x}d\mathbf{x}'\,\varphi^*_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{x})\varphi^*_{\mathbf{P}_{\alpha',r_{\alpha'}}}(\mathbf{x}')\frac{1}{|\mathbf{x}-\mathbf{x}'|}\varphi_{\mathbf{P}_{\beta',r_{\beta'}}}(\mathbf{x}')\varphi_{\mathbf{P}_{\beta,r_\beta}}(\mathbf{x}), \\
&= N_{\phi_0}\sum_{r_\alpha}\sum_{r_{\alpha'}}\sum_{r_{\beta'}}\sum_{r_\beta}(d^{(b_\alpha,r_\alpha,\sigma_\alpha)}_{\mathbf{p}_\alpha}d^{(b_{\alpha'},r_{\alpha'},\sigma_{\alpha'})}_{\mathbf{p}_{\alpha'}})^* d^{(0,r_{\beta'},\sigma_{\beta'})}_{\mathbf{p}_{\beta'}}d^{(0,r_\beta,\sigma_\beta)}_{\mathbf{p}_\beta}\times\delta(\mathbf{P}_{\beta',r_{\beta'}}+\mathbf{P}_{\beta,r_\beta}-\mathbf{P}_{a,r_\alpha}-\mathbf{P}_{\alpha',r_{\alpha'}},0) \\
&\quad\times\frac{\varphi^*_{\mathbf{p}_\alpha}(\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2)\varphi^*_{\mathbf{p}_{\alpha'}}(-\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2)}{N^{(2,3)}_{\mathbf{P}_{\beta',r_{\beta'}}}N^{(2,3)}_{\mathbf{P}_{\beta,r_\beta}}}\times\sum_{\mathbf{Q}^*}\frac{2\pi}{|\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}}+\mathbf{Q}^*|} \\
&\quad\times\exp(-r_0^2(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}}+\mathbf{Q}^*)^2)\times\exp[-ir_0^2\mathbf{n}\times\mathbf{Q}^*\cdot(\mathbf{P}_{\alpha,r_\alpha}+\mathbf{P}_{\beta,r_\beta}-\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})],
\end{aligned}
\tag{C1}
$$

where the summation vectors $\mathbf{Q}^*$ and the norm functions are defined as follows:

$$
\mathbf{Q}^* = n_1\tfrac{3}{2}\mathbf{s}_1 + n_2\mathbf{s}_2, \tag{C2}
$$

$$
N^{(2,3)}_{\mathbf{P}} = \sqrt{N_{\phi_0}}\sqrt{\sum_{\ell}(-1)^{\ell_1\ell_2}\exp\left(i\mathbf{P}\cdot\ell-\frac{\ell^2}{4r_0^2}\right)},
$$

$$
\ell = \ell_1(2\mathbf{c}_1) + \ell_2(3\mathbf{c}_2),
$$

and, as before, $\delta(\mathbf{P}',\mathbf{P})$ equals one when the arguments are same modulo vectors of the class $\mathbf{Q}^*$ defined above, and zero otherwise. It is possible to show now that the ratio multiplying this latter function is simply a phase factor. For this purpose let us consider the definition of the $\varphi_{\mathbf{P}_{\alpha,r_\alpha}}$,

$$
\varphi_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{x}) = \frac{1}{N^{(2,3)}_{\mathbf{P}_{\alpha,r_\alpha}}}\sum_{\ell}(-1)^{\ell_1\ell_2}\exp(i\mathbf{P}_{\alpha,r_\alpha}\cdot\ell)T_\ell\phi(\mathbf{x}), \tag{C3}
$$

from which follows directly a connection between the value of this function at the origin and the norm functions appearing in (C1)

$$
\begin{aligned}
\varphi_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{0}) &= \sqrt{\sum_{\ell}(-1)^{\ell_1\ell_2}\exp\left(i\mathbf{P}_{\alpha,r_\alpha}\cdot\ell-\frac{\ell^2}{4r_0^2}\right)} \\
&= \frac{N^{(2,3)}_{\mathbf{P}_{\alpha,r_\alpha}}}{\sqrt{2\pi r_0^2 N_{\phi_0}}}.
\end{aligned}
$$

Further, let us recall the formula connecting a translated function of the basis $\varphi_{\mathbf{p}}$ and the same function for a shifted momenta (A8). After considering this relation evaluated at $\mathbf{x}=0$, the following expression can be obtained:

$$
\begin{aligned}
&\varphi_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2) \\
&\quad= \varphi_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{n}\times(\mathbf{P}_{\alpha,r_\alpha}-\mathbf{P}_{\beta,r_\beta})r_0^2) \\
&\quad= \mathcal{F}_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{n}\times(\mathbf{P}_{\beta,r_\beta}-\mathbf{P}_{\alpha,r_\alpha})r_0^2) \\
&\qquad\times\varphi_{\mathbf{P}_{\alpha,\mathbf{r}_\alpha}-(2e/\hbar c)A(\mathbf{n}\times(\mathbf{P}_{\alpha,\mathbf{r}_\alpha}-\mathbf{P}_{\beta,\mathbf{r}_\beta})r_0^2)}(\mathbf{0}).
\end{aligned}
$$

But the new momenta argument of the function in the rhs can be simplified as

$$
\begin{aligned}
-\frac{2e}{\hbar c}A(\mathbf{n}\times(\mathbf{P}_{\alpha,r_\alpha}-\mathbf{P}_{\beta,r_\beta})r_0^2) &= \frac{2}{r_0^2}\frac{\mathbf{n}}{2}\times(\mathbf{n}\times(\mathbf{P}_{\alpha,r_\alpha}-\mathbf{P}_{\beta,r_\beta})r_0^2) \\
&= \mathbf{P}_{\beta,r_\beta}-\mathbf{P}_{a,r_a},
\end{aligned}
$$

to produce

$$
\begin{aligned}
&\varphi_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2) \\
&\quad= \mathcal{F}_{\mathbf{P}_{\alpha,r_\alpha}}(\mathbf{n}\times(\mathbf{P}_{\beta,r_\beta}-\mathbf{P}_{\alpha,r_\alpha})r_0^2)\varphi_{\mathbf{P}_{\beta,r_\beta}}(0).
\end{aligned}
$$

Similarly it also follows

$$
\begin{aligned}
&\varphi_{\mathbf{P}_{\alpha',r_{\alpha'}}}(-\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2) \\
&\quad= \mathcal{F}_{\mathbf{P}_{\alpha',r_{\alpha'}}}(\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2)\varphi_{\mathbf{P}_{\beta',r_{\beta'}}}(\mathbf{0}),
\end{aligned}
$$

which finally leads to the desired results

$$\frac{\varphi^{*}_{\mathbf{P}_{\alpha,r_{\alpha}}}(\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2)\varphi^{*}_{\mathbf{P}_{\alpha',r_{\alpha'}}}(-\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2)}{N^{(2,3)}_{\mathbf{P}_{\beta',r_{\beta'}}}N^{(2,3)}_{\mathbf{P}_{\beta,r_{\beta}}}}$$

$$=\frac{\mathcal{F}^{*}_{\mathbf{P}_{\alpha,r_{\alpha}}}(\mathbf{n}\times(\mathbf{P}_{\beta,r_{\beta}}-\mathbf{P}_{\alpha,r_{\alpha}})r_0^2)\mathcal{F}^{*}_{\mathbf{P}_{\alpha',\mathbf{r}_{\alpha'}}}(\mathbf{n}\times(\mathbf{P}_{\beta',r_{\beta'}}-\mathbf{P}_{\alpha',r_{\alpha'}})r_0^2)}{2\pi r_0^2 N_{\phi_0}^2}. \tag{C4}$$

The expression for the matrix element (C1) allows us to directly write formula (45) employed in Sec. III for evaluating the correlation energy.

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