## Solid versus fluid, and the interplay between fluctuations, correlations, and exchange in the fractional quantized Hall effect

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In this paper, we examine a series of solid wave functions for electrons moving in two dimensions under a magnetic field, with all of them staying in the lowest Landau orbital. We discover that whereas the direct energy of the system is almost optimized by the correlated motion of electrons as in the magnetophonons, the effect of exchange is to soften the transverse branch, allowing larger fluctuations of the electrons from their lattice sites. These fluctuations are large enough to destroy the true translational long-range order of the solid and change it into mere algebraic long-range order. Thus our phonons possess a gap without violating Goldstone's theorem. This gap is of the same order of magnitude as that exhibited by Laughlin's fluid wave function, but the ground-state energy for the algebraic solid turns out to be slightly lower. Finally, we suggest a plausible connection between the odd-denominator rule and fractional statistics, which does not require long-range positional order and is applicable both to the solid and the fluid.

### I. INTRODUCTION

Wigner first pointed out that electrons would crystallize into a solid at low densities, contrary to the behavior of most other materials.<sup>1</sup> This is due to the predominance of the Coulomb potential energy over kinetic energy when the average distance between electrons is large. However, in the presence of an extremely strong magnetic field, all the electrons would be coerced into having the same kinetic energy of zero-point motion, and only the Coulomb energy would remain effective in governing their distribution in space. The electrons would then assume a configuration that would minimize the mutual repulsion, presumably a regular lattice. A strong magnetic field could, therefore, be expected to facilitate the formation of a crystal from an electron fluid.

Recently, experiments corresponding to these conditions were carried out.<sup>2</sup> Two new phenomena, the integral and the fractional quantized Hall effects (QHE), were discovered. Much interesting work<sup>3</sup> has been done on the former so that it now seems fairly well understood. Here, we are mainly interested in the latter.

To explain the fractional quantized Hall effect (FQHE) Laughlin<sup>4</sup> proposed that the electrons form a fluid. He wrote down a trial wave function

$$
\phi_{\mathbf{L}} = \prod_{i > j} (z_i - z_j)^m \exp\left[-\sum_i r_i^2/4\right] \tag{1a}
$$

with probability density

$$
|\phi_{\mathbf{L}}|^2 = \exp\left[2m \sum_{i > j} \ln r_{ij} - \sum_{i} r_i^2/2\right],
$$
 (1b)

which provided good estimates of both the ground-state

energy as well as the magnitude of the gap. Here

$$
z_{(i,j)} = x_{(i,j)} + iy_{(i,j)}.
$$
 (1c)

 $r_i$  is the distance of the point  $(x_i, y_i)$  from some origin of coordinates, and  $r_{ij}$  is the distance between the points  $(x_i,y_i)$  and  $(x_j,y_j)$ .

In this paper we shall study the effect of exchange and correlations by exploring a series of possible solid wave functions. Solids and charge-density waves were among the first ideas examined as a plausible explanation, but were found insufficient in the absence of a sizable commensuration energy, at rational filling factors, in the Hartree-Fock approximation,<sup>5</sup> and their ground-state energy estimates were soon superseded by the fluid wave function mentioned above. The next improvement is to introduce correlations. In the harmonic approximation, this yields the magnetophonon solid wave function that we will be discussing in more detail later. It has also been discussed long ago.<sup>6</sup> One can improve upon this by going to self-consistent magnetophonons, but a glaring defect remains in that exchange effects have not yet been included. At this stage, if we try to increase the correlation between the motion of the electrons in some direction, they would tend to correlate less in the other direction. Let us take the liberty of quoting wave functions that we will introduce later, to illustrate this point. For example, we have looked at wave functions  $|\phi\rangle$  of the form

$$
|\phi\rangle = \exp\left[\sum_{q} V_q \delta z_q \delta z_{-q}\right] |\phi_{\mathrm{HF}}\rangle.
$$

Here  $z = x + iy$ ,  $\delta z_q$  is the Fourier component of the displacements from lattice positions with wave vector  $q$  and  $|\phi_{HF}\rangle$  is the Hartree-Fock ground state to be defined in detail in Eqs. (2) in the next section. We have assumed

that the electrons lie in the lowest Landau level, so that functions of z only, and not of its complex conjugate, can appear in the first factor. This ensures that the wave function so constructed lies in the lowest Landau level. As a consequence,  $\delta z_q \delta z_{-q} = |x_q|^2 - |y_q|^2$  plus purely imaginary terms.  $|x_q|^2$  and  $|y_q|^2$  occur with opposite signs! Hence no optimum correlations can be introduced in both directions simultaneously. However, exchange effects come in to counteract this and keep the electrons apart from each other. In other words, if we are going to increase correlation of electron motion in one direction, the electrons would then come closer together on the average due to decreased correlation in the other direction, and would be able to lower their energy from exchange. The direct Coulomb energy would suffer only a relatively small increase, since the correlations were first optimized with respect to this aspect. This effect, we think, is the reason why fluctuations are so large here. In this sense our solid wave function is very similar to the Laughlin wave function. However, by looking at systematic trends, we are able to gain a deeper understanding of the nature of the ground state. Indeed we have found a trial quasi solid wave function which has a slightly lower energy  $(-0.412)$  (Ref. 7) than that of Laughlin's  $(-0.410)$ .<sup>8</sup> The probability density of this wave function looks like the partition function of a two-dimensional (2D) solid at a  $fi$ nite temperature. It only possesses "algebraic" long-range translational order, and therefore is not subject to the dictates of Goldstone's theorem. In fact, the phonons of this wave function exhibit a gap of the same magnitude (0.076) as that of the Laughlin-type wave function  $(0.106)$ .<sup>9</sup> Our wave function brings up two interesting points which have not been appreciated previously. First, it provides an interesting example of evading Goldstone's theorem while retaining a solid like behavior which is a peculiar feature in 2D. It brings back all the interesting questions of longrange order versus rigidity and melting in that case. Secondly, it demonstrates that the solid energy may not be that different from the fluid energy when correlation effects are introduced. The fact that we can lower the sohd energy to one comparable to Laughlin's seems to suggest that there is a lot of similarity between the two. On the other hand, we can also compare our wave function with the magnetophonon solid wave function which still has true translational long-range order. Our wave function is stabilized with respect to it by benefiting from a much larger exchange while retaining a comparable direct energy. This effect is purely of quantum-mechanical origin and, to the best of our knowledge, has not been observed in other quantum solids such as the rare-gas crystals. Presumably the difference lies in the absence of a hard core in the present case.

### II. CHOICE OF WAVE FUNCTION

Let us motivate how we pick our wave function. The Hamiltonian,  $H$ , of the system can be written as  $H = H_0 + \sum_{i > j} e^2/r_{ij}$ , where  $H_0$  is the free-electron Hamiltonian in a magnetic field. In the large-field limit, one tries to minimize the Coulomb energy with a linear combination of the infinitely many degenerate eigenstates of  $H_0$  with all particles in the lowest Landau level. To achieve this, the electrons have to be kept apart as much as possible. The Laughlin fluid constitutes one way of doing this. Alternatively, one can start out with the idea of the Wigner solid that we mentioned. There are two complementary ways of describing the Wigner solid, either via the charge-density-wave  $(CDW)$  formalism,  $^{10}$  or by using the charge-density-wave (CDW) formalism,<sup>10</sup> or by using a non-orthogonal basis set.<sup>11</sup> We have chosen the latter because it is physically more direct and transparent, and also includes higher order harmonics not considered in CDW's. Specifically, we take Landau orbitals  $g_R(r)$  located at the sites R given by

$$
g_{\mathbf{R}}(\mathbf{r}) = \exp(-\left|\mathbf{r} - \mathbf{R}\right|^2/4 + i\mathbf{n} \times \mathbf{R} \cdot \mathbf{r}/2), \tag{2a}
$$

where **n** is a unit vector in the direction of the magnetic field,<sup>12</sup> and construct a Wigner-solid wave function  $\phi_{\text{HF}}$ as

$$
\phi_{HF} = \det(M) \tag{2b}
$$

where  $M$  is a matrix with components

$$
M_{ij} = g_{\mathbf{R}_i}(r_j) \tag{2c}
$$

with the  $\mathbf{R}_i$  forming a triangular Wigner lattice. The variational energy per particle of this wave function can 'variational energy per particle of this wave function can<br>be easily calculated.<sup>5</sup> For filling factors of  $\frac{1}{3}$  and  $\frac{1}{5}$ , the energy is dominated by the Hartree term and one obtains the same result  $(-0.389, -0.322)$  as the CDW calculation to within the significant figures quoted.<sup>13</sup>

It is now possible to combine the Wigner-solid wave function with correlations. The wave function  $\phi_R$  given by

$$
\phi_{\mathbf{R}} = \sum_{P} \prod_{i > j} (-1)^P (z_{Pi} - z_{Pj})^m \prod_i g_{R_i}(r_{Pi}) \tag{3}
$$

is still an eigenfunction of  $H_0$ . However, the first factors have introduced a correlation by attempting to force the electrons apart. This same type of correlation was also used by Laughlin. This wave function is discussed in detail in Appendix A. We found that it may produce a smooth interpolation from Laughlin's fluid wave function to one representing a solid, by varying the lattice spacing. To further simplify matters we shall here only consider these correlations up to harmonic terms only. Let us define the wave function  $\phi_{HMC}$  by

$$
\phi_{\text{HMC}} = \sum_{P} (-1)^{P} f(r_{P}), \qquad (4a)
$$
\n
$$
f(r) = \exp\left(-0.5m \sum_{i > j} \delta z_{ij}^{2} (d^{2} \ln z_{ij} / dz_{ij}^{2})_{z_{ij} = Z_{ij}}\right)
$$
\n
$$
\times \prod g_{R_{i}}(r_{j}). \qquad (4b)
$$

Here  $Z_i = X_i + iY_i$ ,  $(X_i, Y_i) = R_i$  are the lattice positions; r stands collectively for the set of variables and parameters  $(...,r_i,...;...,R_i,...)$  and  $r_p$  stands for the permuted set  $(...,r_{Pi},...;...;R_{Pi},...)$ . We sum over all possible permutations P.  $\delta z_i = z_i - Z_i$  corresponds to the displacement from the lattice positions.  $\phi_{HMC}$  can be obtained from  $\phi_L$ by writing  $(z_i-z_i)^m$  as an exponential and expanding the exponent about the lattice points, keeping only terms that

are second order in  $\delta z_i$ .<br>*f* belongs to a general class of functions  $f_G$  given by

$$
f_{\mathcal{G}}(r,h) = \exp\left(-\sum h_{qi} |\delta r_{qi}|^2 - i \sum (h_{q1} - h_{q2})\delta r_{q1} \delta r_{-q,2}\right)
$$
 (5a)

with

$$
h_{q1} + h_{q2} = \frac{1}{2} \tag{5b}
$$
 Let

$$
\phi = \sum_{P} (-1)^P f_G(r_P). \tag{5c}
$$

 $\phi$  is the most general wave function that (a) is translationally invariant, (b) contains only quadratic terms in the exponent, and (c) belongs to the lowest Landau level. To obtain f we set  $h_{qi} = \omega_{qi}^2/2$ .  $\omega_{qi}$  comes from the Fourier transform of the exponent in (4} and corresponds to the harmonic phonon frequencies of a one-component plasma in a solid phase.

The magnetophonon (MP) wave functions are also very similar to (3). These are eigenstates of the Hamiltonian  $H_{\text{MP}}$  which is obtained from the full Hamiltonian H by treating its Coulomb interaction term in the harmonic approximation. The spectrum of  $H_{MP}$  was first derived by Chaplik.<sup>6</sup> By using different elliptical gauges at different values of  $q$ , his results can be simplified quite a bit algebraically. This is discussed in detail in Appendix B, where the full SU(2) symmetry of the problem is displayed. We found the magnetophonon frequencies

$$
E = N_{+}E_{+} + N_{-}E_{-} + E_{0}
$$
 (6)

where  $E_+ = E_0 + E_1$ ,  $E_- = E_0 - E_1$ , where<br>  $E_0 = 0.5[(\omega_1 + \omega_2)^2 + \omega_0^2]^{0.5}$  is the zero-point energy<br>  $E_1 = 0.5[(\omega_1 - \omega_2)^2 + \omega_0^2]^{0.5}$ ;  $\omega_{1,2}$  are the phonon frequencies of the Wigner solid in the absence of a magnetic field, and  $\omega_c$  is the cyclotron frequency. It is straightforward to work out the corresponding wave function  $\phi_{\infty}$  in the high-field limit and we found

$$
\phi_{\infty} = \sum_{P} f_{G} [r_{P}, \nu_{qi}/2(\nu_{q1} + \nu_{q2})]. \tag{7}
$$

 $v_{qi}$  are the phonon frequencies of the  $1/r$  potential. In this case,  $f_G$  can also be written more explicitly as

$$
f_{\mathbf{G}} = \exp \left[ -\sum_{i} \delta r_{i}^{2} / 4 + i \mathbf{n} \times \mathbf{R}_{i} \cdot \mathbf{r}_{i} / 2 + \sum_{i > j} V_{ij} \delta z_{i} \delta z_{j} \right]
$$

where  $V_{ij}$  has the same behavior as the second derivative where  $V_{ij}$  has the same behavior as the second derivative<br>of ln  $\mathbf{R}_{ij}$  as  $\mathbf{R}_{ij} \rightarrow \infty$ . This wave function has been derived by Lam and Girvin<sup>14</sup> via a different method. Note that the exponent contains a correlation  $(\ln r)$  that has a longer range than the interaction potential  $(1/r)$  between the particles. Furthermore, the coefficient of this term is exactly the same as that obtained from a Taylor expansion of the exponent in (lb). This long-range correlation is also present in the Laughlin fluid wave function. It is a common feature among all the wave functions considered here, whether solid or fiuid. It is actually independent of the details of the potential one starts off with. It basically comes from the Anderson-Higgs idea<sup>15</sup> if we demand the presence of a gap  $(\hbar \omega_c)$  at zero wave vector.

### III. EXCITED STATES

We next discuss the excited states of our trial wave functions. The one-phonon states  $\psi_q$  can be easily constructed as

$$
\psi_{\mathbf{q}} = \delta z_{\mathbf{q}} \phi \tag{8}
$$

where  $\phi$  is the generic wave function defined in Eqs. (5). This wave function lies in the lowest Landau level and is orthogonal to the ground state. For  $\phi=\phi_{\infty}$ , defined in Eqs. (7),  $\psi_q$  is the exact one-magnetophonon state in the high-field limit. For a general  $\phi$  defined in Eqs. (3) and (5), the excitation energy  $\Delta_q$  can be evaluated as follows:

$$
\Delta_q = \sum_{i,j} \langle \psi_q | 1/| R_{ij} + \delta r_{ij} | |\psi_q \rangle / \langle \psi_q | \psi_q \rangle
$$
  
-  $\langle \phi | 1/| R_{ij} + \delta r_{ij} | |\phi \rangle / \langle \phi | \phi \rangle.$  (8a)

We have neglected the exchange contribution to the excitation. Let us use the symbols  $\psi_q$  and  $\phi$  to represent the normalized wave functions from this point onwards. The integral  $\langle \psi_q | 1/| R_{ij} + \delta r_{ij} | |\psi_q \rangle = I_q$  can be evaluated in an analogous manner as the direct integral by expressing the Coulomb potential in its Fourier representation as

$$
I_q = \int d^2k \exp \left[i \mathbf{k} \cdot \mathbf{R}_{ij} - \sum_{\alpha,\beta} k_{\alpha} k_{\beta} \right] \times \langle \psi_q | \delta r_{ij\alpha} \delta r_{ij\beta} | \psi_q \rangle / 2 \Bigg).
$$

It is straightforward to show that

$$
\langle \psi_q | \delta r_{ij\alpha} \delta r_{ij\beta} | \psi_q \rangle = \langle \phi_q | \delta r_{ij\alpha} \delta r_{ij\beta} | \phi \rangle + A_{\alpha\beta}
$$

where

$$
A_{ij} = \left(\sum_{l} e_{lqi} e_{lqj} [1 - \cos(\mathbf{q} \cdot \mathbf{R})] / h_{lq}^2 \right) / N \sum_{l'} (2h_{l'q})^{-1}
$$

We note that A is of the order of  $1/N$ ; hence

$$
\exp\left[\sum_{\alpha,\beta} k_{\alpha} k_{\beta} \langle \psi_q | \delta r_{ij\alpha} \delta r_{ij\beta} | \psi_q \rangle / 2\right]
$$
  
= 
$$
\begin{bmatrix} 1 - 0.5 \sum_{\alpha,\beta} k_{\alpha} k_{\beta} A_{\alpha\beta} \\ \times \exp\left[\sum_{\alpha,\beta} k_{\alpha} k_{\beta} \langle \phi | \delta r_{ij\alpha} \delta r_{ij\beta} | \phi \rangle / 2\right] \end{bmatrix}
$$

Substituting this back into equation (8a), we finally obtain

$$
\Delta_q=0.5\sum_{R,\alpha,\beta}A_{\alpha\beta}\partial_{R_{\alpha}}\partial_{R_{\beta}}\langle\phi\mid1/|R_{ij}+\delta r_{ij}| \mid\phi\rangle.
$$

Recalling the definition of  $A$ , we find

$$
\Delta_q = \sum_l \left[ \left( \nu' \right)_{lq}^2 / h_{lq}^2 \right] / \left[ \sum_l \left( 2h_{l'q} \right)^{-1} \right]
$$

Here

$$
\nu' = 0.5 \sum_{l,i} e_{lqi} e_{lqj} [1 - \cos(\mathbf{q} \cdot \mathbf{R})] \partial_{R_{\alpha}} \partial_{R_{\beta}}
$$

$$
\times \langle \phi | 1 / | R_{ij} + \delta r_{ij} | |\phi \rangle
$$

is a "finite temperature" phonon frequency for the  $1/r$  potential. At a small wave vector q,  $\Delta_q$  is proportional to  $v_{qt}^2/h_{qt}$ . For the MP,  $h_{qt}$  is proportional to  $q^{1/2}$ . Since  $v_{qt}$ , the transverse-phonon frequency of the  $1/r$  potential, is proportion to q,  $\Delta_q \approx q^{3/2}$ , as is well known. For  $\phi_{HMC}$ ,  $h_{qt} \approx q^2$ . Hence  $\Delta_q$  remains finite as  $q \to 0$ . From this the phonon gap quoted to q,  $\Delta_q \approx q^3$ . above for  $\phi_{HMC}$  can be obtained.

### IU. NUMERICAL CALCULATION

We now turn our attention to the evaluation of the Coulomb energy of the  $\phi$ 's. First the direct integral  $I_{ij} = \langle e^2/r_{ij} \rangle$ . As the wave function is quadratic in the exponent, the energy can be reduced to a sum of two-dimensional integrals, which can then be calculated numerically. Specifically, we write  $r_{ij}$  in terms of the equilibrium spacing  $R_{ij}$  and the deviwhich can then be calculated numerically. Specifically, we write  $r_{ij}$  in terms of the equilibrium spacing  $K_{ij}$  and the deviation  $\delta r_{ij}$  from these positions, viz.,  $r_{ij} = R_{ij} + \delta r_{ij}$ . The deviation  $\delta r_{ij}$  is then  $\delta r_{q,\alpha}$ . The integral  $I_{ij}$  can be written as

$$
I_{ij} = \int \prod_{q,\alpha} d^2 \delta r_{q\alpha} |R_{ij} + \delta r_{ij}|^{-1} \exp \left[-\sum_{q\alpha} 2h_{q\alpha} |\delta r_{q\alpha}|^2\right] \times \left[\int \prod_{q,\alpha} d^2 \delta r_{q\alpha} \exp \left[-\sum_{q\alpha} 2h_{q\alpha} |\delta r_{q\alpha}|^2\right]\right]^{-1}.
$$
\n(9a)

After the Gaussian integration over  $\delta r_q$  has been carried out, we obtain

$$
I_{ij} = \left[ (2\pi)^2 \mid a \mid ]^{-1/2} \int d^2 \delta r_{ij} \mid R_{ij} + \delta r_{ij} \mid^{-1} \exp \left[ - \sum_{\alpha, \beta} 0.5 \delta r_{ij\alpha} \delta r_{ij\beta} a_{\alpha\beta}^{-1} \right]. \tag{9b}
$$

I

Here

$$
a_{\alpha\beta} = \sum_{m=i,l} \int d\mathbf{q} [1 - \exp(i\mathbf{q} \cdot \mathbf{R})] e_{m\alpha} e_{m\beta} / 2h_{mq}. \qquad (9c)
$$

 $|a|$  is the determinant of the matrix a. The same calculation occurs in the self-consistent phonon calculation for quantum crystals. We have converted such a program by Glyde<sup>16</sup> from three to two dimensions, and included the effect of the magnetic field as well.

One can show that  $1/R_{ij} - (1/r_{ij}) = E_{1d,ij}$  goes as  $\ln R/R^3$  as R approaches  $\infty$ . We have evaluated this difference up to the 20th shell. The details of this for  $m = 3$  are shown in Table I. In this table  $\ln R/R^3$  is also

**TABLE I.** Details of the calculation of the direct Coulomb energy for  $\frac{1}{3}$ -filled,  $m = 3$ .  $0.5 \sum (\langle 1/r \rangle - 1/R) = 0.07297590$ ; energy equals  $-0.3773240$ .

$\boldsymbol{R}$	$\langle 1/r \rangle$	$\Sigma\langle 1/r \rangle$	$\langle 1/r \rangle - 1/R$	$2\ln R/R^3$
1	0.2225	1.335	$8.14\times10^{-3}$	0.00
1.7321	0.1285	2.106	$4.74 \times 10^{-3}$	$2.08\times10^{-3}$
$\mathbf{2}$	0.1091	2.7606	$1.92\times10^{-3}$	$1.71 \times 10^{-3}$
2.6458	0.0824	3.255	$1.38\times10^{-3}$	$1.03 \times 10^{-3}$
2.6458	0.0824	3.7494	$1.38 \times 10^{-3}$	$1.03\times10^{-3}$
3	0.0722	4.1826	$7.46\times10^{-4}$	$8.02\times10^{-4}$
3.4641	0.0626	4.5582	$7.19\times10^{-4}$	$5.89\times10^{-4}$
3.6055	0.06	4.9182	$5.46 \times 10^{-4}$	$5.39\times10^{-4}$
3.6055	0.06	5.2782	$5.46\times10^{-4}$	$5.39\times10^{-4}$
4	0.054	5.6022	$4.09\times10^{-4}$	$4.27\times10^{-4}$
4.3589	0.0496	5.8998	$4.22\times10^{-4}$	$3.50\times10^{-4}$
4.3589	0.0496	6.1974	$4.22\times10^{-4}$	$3.50\times10^{-4}$
4.5826	0.0471	6.48	$3.23\times10^{-4}$	$3.12\times10^{-4}$
4.5826	0.0471	6.7626	$3.23\times10^{-4}$	$3.12\times10^{-4}$
5.	0.0431	7.0212	$2.28\!\times\!10^{-4}$	$2.54\times10^{-4}$
5.1962	0.0415	7.2702	$2.46\times10^{-4}$	$2.31\times10^{-4}$
5.2915	0.0407	7.5144	$1.89\times10^{-4}$	$2.22\times10^{-4}$
5.2915	0.0407	7.7586	$1.89\times10^{-4}$	$2.22\times10^{-4}$
5.5678	0.0387	7.9908	$2.00\times10^{-4}$	$1.96\times10^{-4}$
5.5678	0.0387	8.223	$2.00\times10^{-4}$	$1.96 \times 10^{-4}$
6	0.0359	8.4384	$1.73 \times 10^{-4}$	$1.63 \times 10^{-4}$
6.0828	0.0354	8.6508	$1.59\times10^{-4}$	$1.58\times10^{-4}$
6.0828	0.0354	8.8632	$1.59\times10^{-4}$	$1.58\times10^{-4}$
6.245	0.0345	9.0702	$1.75 \times 10^{-4}$	$1.48 \times 10^{-4}$
6.245	0.0345	9.2772	$1.75\!\times\!10^{-4}$	$1.48 \times 10^{-4}$
6.5574	0.0328	9.474	$1.10\times10^{-4}$	$1.31 \times 10^{-4}$
6.5574	0.0328	9.6708	$1.10\times10^{-4}$	$1.31 \times 10^{-4}$

displayed. As can be seen, this asymptotic behavior is approximately followed. The total direct energy  $E_d$  is given proximately followed. The total direct energy  $E_d$  is given<br>by  $E_d = 0.5 \sum_{i,j} E_{1d,ij} + E_0$ , where  $E_0 = 0.5 \sum_{i,j} 1/R_{ij}$  is the energy of the undistorted Wigner lattice. This is equal to  $-0.78v^{0.5}$  for a triangular lattice. (v is the filling factor from this point on.) In evaluating the matrix  $a$  in Eq. (9c), we have experimented with mesh sizes  $\Delta qR = 0.174$ , 0.348, 0.87 and found no difference for our final result to within the significant figures quoted. For the integral over  $\delta r_{ij}$  we have used a mesh size such that the error is less than  $10^{-5}$ . Table II shows the contributions from the various shells for different values of m.

We next looked at the exchange energy  $\langle \phi | 1/r | \phi_P \rangle$ . This can be written as an infinite series involving increasing numbers of "linked" exchange particles. In fact, a linked-cluster expansion can be developed for this integral. The lowest-order term involves two-particle exchanges. We have evaluated this two-particle exchange integral for the three nearest neighbors as well as the threeparticle exchange integral in the same way that we evaluated the direct integrals. We found the three-particle exchange to be much smaller. This is discussed in detail in Appendix C. We summarize our results here. Both the normalization integral  $I_a = \langle \phi | \phi_P \rangle$  and the exchange  $I_b = \langle \phi | 1/r | \phi_P \rangle$  can be evaluated in the same fashion and we find

TABLE II. The direct Coulomb energy for different values of m. Values for different shells are displayed.

Sum	0.1241	0.1069	0.1052	0.146
R	$m = 0$	$m=1$	$m=2$	$m=3$
1.0000	0.0135	0.0106	0.0089	0.0082
1.7321	0.0020	0.0020	0.0024	0.0048
2.0000	0.0013	0.0013	0.0015	0.0019
2.6458	0.0006	0.0006	0.0007	0.0014
2.6458	0.0006	0.0006	0.0007	0.0014
3.0000	0.0004	0.0004	0.0005	0.0008
3.4641	0.0002	0.0003	0.0003	0.0007
3.6055	0.0002	0.0002	0.0003	0.0006
3.6055	0.0002	0.0002	0.0003	0.0006
4.0000	0.0002	0.0002	0.0002	0.0004
4.3589	0.0001	0.0001	0.0002	0.0004
4.3589	0.0001	0.0001	0.0002	0.0004
4.5826	0.0001	0.0001	0.0001	0.0003
4.5826	0.0001	0.0001	0.0001	0.0003
5.0000	0.0001	0.0001	0.0001	0.0003
5.1962	0.0001	0.0001	0.0001	0.0002
5.2915	0.0001	0.0001	0.0001	0.0002
5.2915	0.0001	0.0001	0.0001	0.0002
5.5678	0.0001	0.0001	0.0001	0.0002
5.5678	0.0001	0.0001	0.0001	0.0002
6.0000	0.0000	0.0000	0.0001	0.0002
6.0828	0.0000	0.0000	0.0001	0.0002
6.0828	0.0000	0.0000	0.0001	0.0002
6.2450	0.0000	0.0000	0.0001	0.0002
6.2450	0.0000	0.0000	0.0001	0.0002
6.5574	0.0000	0.0000	0.0003	0.0001
6.5574	0.0000	0.0000	0.0003	0.0001

TABLE III. Two-particle exchange integrals up to thirdnearest neighbor for various values of m.

<b>Shell</b>	$m=1$	$m=2$	$m=3$	
First	0.0082	0.0036	0.0287	
Second	0.0014	0.00083	0.0051	
Third	0.000061	0.000022	0.0002	
Total	0.0097	0.0045	0.034	

$$
I_a = \int d^2 u \exp(X)/2\pi (a_{xx} a_{yy})^{0.5},
$$
  
\n
$$
I_b = \int d^2 u \exp(X)/2 |u| \pi (a_{xx} a_{yy})^{0.5}
$$

where

$$
X = -u_y^2(1 - 1/a_{xx})/2 - u_x^2(1 - 1/a_{yy})/2
$$
  
+  $i (R_y u_x/a_{yy} - R_x u_y/a_{xx})$   
-  $R_y^2/2a_{yy} - R_x^2/2a_{xx}.$ 

The integration over k in  $I_a$  can be carried out analytically and we have

$$
I_a = \exp[-R_y^2/2(a_{yy} - 1) + R_x^2/2(a_{xx} - 1)]
$$
  
×[(a\_{xx} - 1)(a\_{yy} - 1)]<sup>-0.5</sup>.

The two-particle exchange for  $m = 3$  for the three nearest neighbors are shown in Table III. As can be seen, the third is much smaller than the first two. The threeparticle exchange contribution for different values of  $m$  is shown in Table IV. As we have mentioned, it is much larger for  $m = 3$ .

Our estimates for the ground-state energy of some of the trial wave functions are shown in Table V. We found the exchange energy for  $\phi_{\text{HMC}}$  (-0.034) to be lower than the exchange energy for  $\phi_{HMC}$  (-0.034) to be lower that that for  $\phi_{\infty}$  (-0.0031) for  $v=\frac{1}{3}$ . This happens probabl because the mean-square vibration is larger for  $\phi_{HMC}$  and the overlap is increased. The direct energy is not strongly affected since part of the time the particles move further apart and this compensates for the energy loss when they get closer together.

The total energy for  $\phi_{\text{HMC}}$  is now -0.412. This is slightly lower than that of the fluid  $(-0.410)^8$  Our result does not show conclusively that a solid phase is more stable since there may be other fiuid wave functions of lower energy. However it demands further research into this problem.

TABLE IV. Three-particle exchange integrals for  $m = 1, 2$ and 3.

m	$\langle \phi   1/r   \phi_P \rangle$	$\langle \phi   \phi_P \rangle$	
	0.00001	0.000018	
	0.00079	0.0000083	
	$< 10^{-7}$	$~10^{-7}$	

				$\phi_1(m)$		
Wave function	Fluid	CDW	$m = 1$	$m=2$	$m = 3$	MP
Total energy	0.41	0.390	0.399	0.400	0.412	0.397
Exchange		0.001	0.001	0.001	0.034	0.0031

TABLE V. Table of the direct energy of different variational wave functions for a filling factor of  $\frac{1}{3}$ . Variational energies  $\langle e^2/l \rangle$ .

# **V.** THE QUESTION OF  $\frac{1}{3}$

Let us now briefly address the question of "why  $\frac{1}{3}$ ." It has been pointed out that an *n*-particle exchange leads to a phase change of  $in\pi/\nu$  (Ref. 17) and hence may lead to a commensuration energy. Unfortunately, the energy involved in such a process in the Hartree-Fock approximation is so small that, at first sight, it is not very helpful since it would not be able to account for the gap. However, our phonons are not gapless! Our present picture is that these terms do indeed stabilize the solid at  $\frac{1}{3}$ -filled; but the gap is not caused by these  $n$ -particle exchanges alone. This explanation of the  $\frac{1}{3}$  for the solid is very similar to that based on the fluid recently discussed by Tao who focused on the question of fractional statistics and found a similar phase factor for the interchange of clusters. It is quite likely that the explanation of the odd-denominator rule is independent of the quasi longrange order of the system but is only an effect of fractional statistics.

#### VI. CONCLUSION

In conclusion, we have found a solid wave function, describing electrons moving in a plane under a magnetic field, that is competitive with fluid ones in energy, for the field, that is competitive with fluid ones in energy, for the interesting case of a filling factor of  $\frac{1}{3}$ . The phonons of this wave function exhibit a gap of the magnitude  $-0.072$ . Our wave function only has algebraic long-range order; hence Goldstone's theorem is not violated.

It is also possible to calculate the shear modulus of this wavefunction. We found a value of 0.061  $e^2/l^3$ 

### ACKNOWLEDGMENT

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### APPENDIX A

The probability density  $|\phi_{\mathbf{R}}|^2$  can also be written in the form of a partition function if the exchange terms are neglected as

$$
|\phi_{\mathbf{R}}|^2 = \exp\left[-2m \sum_{i > j} \ln r_{ij} + \sum_{i} |\mathbf{r}_{i} - \mathbf{R}_{i}^0|^2/2\right].
$$
 (A1)

If we look at the classical statistical mechanics problem that this describes as a partition function, we find that, in general, the equilibrium positions of the particle  $\mathbf{R}_i$  will not be at  $\mathbf{R}_i^0$ , but at

$$
\mathbf{R}_i = \mathbf{R}_i^0 / (1 - \nu m). \tag{A2}
$$

For  $vm = 1$ , our formula makes sense only if  $\mathbb{R}^0 = 0$ . In that case,  $\phi_R$  reduces to  $\phi_L$ . However, as one goes away from the commensurate situation by decreasing  $vm$ ,  $\phi_R$ provides a smooth interpolation away from a fiuid wave function to one describing a solid lattice.

Better still, the condition imposed by Eq. (A2) can be circumvented. As we mentioned  $\phi_{HMC}$  is obtained from  $\phi_R$  by expanding the exponent in Eq. (A1) about the lattice points, keeping only terms that are second order in  $\delta z_i$ . Because the linear terms are also discarded, the condition (A2) no longer applies.

### APPENDIX 8

In this appendix, we will present our derivation of the magnetophonon spectrum and the corresponding wave functions for a two-dimensional solid composed of identical charged particles, in terms of its plasmon spectrum in the absence of a magnetic field.

The Hamiltonian that we have to solve is

$$
H = \sum_{i} [p_i - e \mathbf{A}_i(\mathbf{r}_i)/c]^2 / 2m + \sum_{i > j} e^2 / r_{ij}.
$$
 (B1)

If we expand this expression in small displacements,  $x_i$ , from lattice points in the usual manner of harmonic approximations, we would get the magnetophonon Hamiltonian

$$
H_{\text{MP}} = \sum_{i} [\mathbf{p}_i - e \mathbf{A}_i(\mathbf{x}_i)/c]^2 / 2m + \sum_{i,j} V_{ij} \mathbf{x}_i \cdot \mathbf{x}_j, \quad \text{(B2)}
$$

where  $V_{ij}$  are the appropriate second derivatives of the Coulomb interaction about the equilibrium lattice configuration.

Let us split  $H_{MP}$  into a part,  $H_B$ , that depends on the magnetic field and a part,  $H_C$ , that does not. Explicitly,

$$
H_{\rm MP} = H_{\rm C} + H_{\rm B},
$$

where

$$
H_{\rm C} = \sum_{i} \mathbf{p}_i^2/2m + \sum_{i,j} V_{ij} \mathbf{x}_i \cdot \mathbf{x}_j,
$$

and

$$
H_{\rm B} = \sum_{i} [e^2 {\bf A}_i^2({\bf x}_i)/c^2
$$
  
\n
$$
/2 \Bigg| \qquad (A1)
$$
\n
$$
-{\bf p}_i \cdot e {\bf A}_i({\bf x}_i)/c - e {\bf A}_i({\bf x}_i) \cdot {\bf p}_i/c^2
$$

On applying the canonical transformation

$$
\mathbf{x}_{i} = N^{-1} \sum_{k} \mathbf{x}_{k} \exp(i\mathbf{k} \cdot \mathbf{R}_{i}),
$$

$$
\mathbf{p}_{i} = N^{-1} \sum_{k} \mathbf{p}_{k} \exp(-i\mathbf{k} \cdot \mathbf{R}_{i}),
$$

 $H<sub>C</sub>$  separates into phonon modes in the normal way, as

$$
H_{\rm C} = N^{-1} \sum_{k} \{ \mathbf{p}_{k}^{\dagger} \mathbf{p}_{k} / 2m + m \left[ \omega_{l0}(\mathbf{k})^{2} x_{kl}^{\dagger} x_{kl} + \omega_{l0}(\mathbf{k})^{2} x_{kl}^{\dagger} x_{kl} \right] / 2 \}.
$$

Here  $x_{kl}$  and  $x_{kt}$  are, respectively, the longitudinal and transverse components of  $x_k$ , with respect to the wave vector k;  $\omega_{l0}(\mathbf{k})$ ,  $\omega_{l0}(\mathbf{k})$  are the corresponding frequencies of the vibrating modes, assumed to be known henceforth; and  $N$  is the total number of particles comprising the solid. Following  $x_i$  and  $p_i$ , if we write

$$
\mathbf{A}_i(\mathbf{x}_i) = N^{-1} \sum_{k} \mathbf{A}_k \exp(i\mathbf{k} \cdot \mathbf{R}_i)
$$

as well, we would also get

$$
H_{\rm B}=N^{-1}\sum_{k}(e^2{\bf A}_k^{\dagger}{\bf A}_k/c^2-{\bf p}_k\cdot e{\bf A}_k/c-e{\bf A}_k\cdot{\bf p}_k/c)/2m.
$$

Now that the magnetophonon Hamiltonian has been explicitly separated in  $k$  space, let us denote each separated piece with an additional subscript of  $k$ . The followin serves to establish the notation:

$$
H_{\rm MP} = N^{-1} \sum_{k} h_{\rm MPk},
$$
  
\n
$$
H_{\rm C} = N^{-1} \sum_{k} h_{\rm C_k},
$$
  
\n
$$
H_{\rm B} = N^{-1} \sum_{k} h_{\rm B_k},
$$
  
\n
$$
h_{\rm MPk} = h_{\rm C_k} + h_{\rm B_k},
$$
  
\n
$$
h_{\rm C_k} = p_{k}^{\dagger} p_{k} / 2m + m [\omega_{l0}(\mathbf{k})^{2} x_{kl}^{\dagger} x_{kl} + \omega_{l0}(\mathbf{k})^{2} x_{kl}^{\dagger} x_{kl}] / 2,
$$
  
\n
$$
h_{\rm B_k} = (e^{2} \mathbf{A}_{k}^{\dagger} \mathbf{A}_{k} / c^{2} - p_{k} \cdot e \mathbf{A}_{k} / c - e \mathbf{A}_{k} \cdot p_{k} / c) / 2m.
$$

Our next chore is to pick a gauge. It turns out that we cannot settle on one, but have to deal with a whole class. With a coordinate system oriented so that  $\mathbf{k}=(k, 0)$ , let us consider

$$
\mathbf{A}_{i} = B(fy_{i},gx_{i})
$$

with  $g-f=1$ , so as to yield the required magnitude of the imposed magnetic field, but otherwise arbitrary. It is also clear that, with any of these choices, we are free to permute p's and A's in their scalar products, whether they are subscripted  $i$  or  $k$ . Thus,

$$
\mathbf{p}_i \cdot \mathbf{A}_i = \mathbf{A}_i \cdot \mathbf{p}_i
$$

and

$$
\mathbf{p}_k \cdot \mathbf{A}_k = \mathbf{A}_k \cdot \mathbf{p}_k.
$$

Now we can proceed to diagonalize  $h_{MPk}$  with this broad choice of vector potentials. Once again, we partition  $h_{MPk}$ into an anisotropic two dimensional harmonic oscillator, and an interaction between the orbit and the magnetic field, as follows:

$$
h_{\text{MP }k} = h_{0k} + h_{uk},
$$
  
\n
$$
h_{0k} = h_{C_k} + e^2 \mathbf{A}_k^{\dagger} \mathbf{A}_k / 2mc^2,
$$
  
\n
$$
h_{uk} = e \mathbf{A}_k \cdot \mathbf{p}_k / mc.
$$

Next we define the usual ladder operators

$$
a_{kj}^{\dagger} = x_{kj}^{\dagger}/x_{kj0} - ip_{kj}/p_{kj0},
$$
  
\n
$$
a_{kj} = x_{kj}/x_{kj0} + ip_{kj}^{\dagger}/p_{kj0}
$$

with

$$
x_{kj0} = [2\hbar / m\omega_j(\mathbf{k})]^{1/2},
$$
  

$$
p_{kj0} = [2\hbar m\omega_j(\mathbf{k})]^{1/2},
$$

where  $j$  can be either  $l$  or  $t$ .

Here,  $\omega_i$ , for  $j=l$  or t, are the longitudinal and transverse frequencies for the harmonic oscillator Hamiltonian  $h_{0k}$ :

$$
\omega_l^2 = \omega_{l0}^2 + g^2 \omega_c^2,
$$
  

$$
\omega_t^2 = \omega_{l0}^2 + f^2 \omega_c^2,
$$

where  $\omega_c$  is the cyclotron frequency

$$
\omega_c = eB/mc.
$$

The corresponding number operators are

$$
n_{kj} = a_{kj}^\top a_{kj}
$$

With the reality condition implying

$$
\mathbf{Z}_k^{\intercal} = \mathbf{Z}_{-k}
$$

where  $Z$  can be  $A$ ,  $x$ , or  $p$ , we have

$$
p_{kj} = ip_{kj0}(a_{kj} - a_{-kj})/2,
$$
  

$$
x_{kj} = x_{kj0}(a_{kj} + a_{-kj}^{\dagger})/2.
$$

Let us introduce the average of quantities over  $k$  and  $-k$ , and denote this by an underscore, thus, for instance

$$
\underline{h}_{0k} = (h_{0k} + h_{0-k})/2.
$$

It is a familiar result that

$$
\underline{h}_{0k} = (\underline{n}_{kl} + 1/2)\hbar\omega_l + (\underline{n}_{kt} + 1/2)\hbar\omega_t.
$$

Furthermore, if we set

$$
F_k = (\omega_l / \omega_t)^{1/2} f + (\omega_t / \omega_l)^{1/2} g,
$$
  
\n
$$
G_k = (\omega_l / \omega_t)^{1/2} f - (\omega_t / \omega_l)^{1/2} g,
$$
  
\n
$$
L_k = (a_{kt}^{\dagger} a_{kl} - a_{kl}^{\dagger} a_{kt}) / i,
$$
  
\n
$$
R_k = (a_{kl} a_{-kl} - a_{kt}^{\dagger} a_{-kl}^{\dagger}) / i,
$$

we would have

$$
\underline{h}_{uk} = G_k \underline{L}_k + F_k \underline{R}_k \hbar \omega_c / 2
$$

At this stage, we can eliminate the averaging of operators by writing

$$
H_{\text{MP}} = N^{-1} \sum_{k} h'_{\text{MP } k},
$$
  
\n
$$
h'_{\text{MP } k} = h'_{0k} + h'_{uk},
$$
  
\n
$$
h'_{0k} = (n_{kl} + \frac{1}{2})\hbar\omega_l + (n_{kt} + \frac{1}{2})\hbar\omega_t,
$$
  
\n
$$
h'_{uk} = (G_k L_k + F_k R_k)\hbar\omega_c/2.
$$

Let us now define the formal angular momentum operators

$$
J_{1k} = (a_{ki}^{\dagger} a_{kl} + a_{kl}^{\dagger} a_{ki})/2
$$
  
\n
$$
J_{2k} = L_k/2,
$$
  
\n
$$
J_{3k} = (n_{kl} - n_{kt})/2,
$$

obeying

$$
[J_{ik},J_{jk}] = ie_{ijk}J_{kk}.
$$

It is straightforward to verify that all of these operators commute with the total number operator

$$
N_k = n_{kl} + n_{kt},
$$

 $[J_{ik}, N_k] = 0,$ 

and in fact

$$
J_k^2 = (N_k/2 + 1)N_k/2
$$

In terms of these operators,

$$
h'_{0k} = (N_k + 1)\hslash(\omega_l + \omega_t) + J_{3k}\hslash(\omega_l - \omega_t),
$$
  

$$
h'_{uk} = (G_k J_{2k} + F_k R_k / 2)\hslash(\omega_c).
$$

We can bring the terms with the  $J$  operators together by the following rotation about the 1 axis,

$$
J'_{1k} = J_{1k},
$$
  
\n
$$
J'_{2k} = J_{2k} \cos \theta - J_{3k} \sin \theta,
$$
  
\n
$$
J'_{3k} = J_{3k} \cos \theta + J_{2k} \sin \theta,
$$

where

$$
\cos\theta = \hbar(\omega_l - \omega_t)/u_k
$$

$$
\sin\theta = G_k \hbar \omega_c / u_k,
$$

and

$$
u_k = \hslash [(\omega_l - \omega_t)^2 + \omega_c^2 G_k^2]^{1/2}.
$$

All we said about  $J$  is still true of  $J'$ , but we now have

$$
h'_{\text{MP }k} = (N_k + 1)\hslash(\omega_l + \omega_t)/2 + J'_{3k}u_k + F_k R_k \hslash\omega_c/2.
$$

Thus, provided that  $F_k = 0$ ,  $h'_{MPk}$  is diagonalized, since

$$
[J_{3k}^{\prime},N_k]=0.
$$

However, this last condition requires that  $f/g = -\omega_t / \omega_l$ . Bearing in mind that all frequencies must be positive, this then fixes the values of  $f$  and  $g$  to be

$$
f = -\omega_{t0}/(\omega_{l0} + \omega_{t0}),
$$
  

$$
g = \omega_{l0}/(\omega_{l0} + \omega_{t0}).
$$

As a consequence of this, we find

$$
\omega_j^2 = \omega_{j0}^2 \left[ 1 + \omega_c^2 / (\omega_{l0} + \omega_{t0})^2 \right],
$$

where  $j=l$  or t.

$$
G_k = -2(\omega_{l0}\omega_{t0})^{1/2}/(\omega_{l0}+\omega_{t0}),
$$

and since

$$
\omega_l/\omega_t = \omega_{l0}/\omega_{t0},
$$

we have

$$
G_k = -2(\omega_l \omega_t)^{1/2} / (\omega_l + \omega_t)
$$

also. To exhibit the energy spectrum more succinctly, we use the number operators

$$
n_{k+} = J'_{3k} + N_k / 2
$$
  

$$
n_{k-} = J'_{3k} - N_k / 2
$$

to rewrite  $h'_{MPk}$  as

$$
h'_{\text{MP }k} = \hslash (\omega_l + \omega_t)/2 + n_{k+1} E_{k+1} + n_{k-1} E_{k-1}
$$

with

$$
E_{k\pm} = \hslash (\omega_l + \omega_t) \pm [(\omega_l - \omega_t)^2 + 4\omega_c^2 \omega_l \omega_t / (\omega_l + \omega_t)^2]^{1/2}/2.
$$

In terms of the plasma frequencies in the absence of the external magnetic field, this becomes

$$
E_{k\pm} = \hbar [(\omega_{l0} + \omega_{t0})^2 + \omega_c^2]^{1/2} \pm [(\omega_{l0} - \omega_{t0})^2 + \omega_c^2]^{1/2}/2.
$$

Note that this never vanishes, unless one or both the plasma frequencies themselves vanish; and when one of them does vanish, only  $E_{-}$  vanishes.  $E_{+}$  is always positive and non-zero. Only when both modes in the plasma have zero frequency will an external magnetic field create a stable oscillation, but it has no effect on stability otherwise. If we square our expression for  $E_{k\pm}$ , we get

$$
(E_{k\pm}/\hbar)^2 = (\omega_l^2 + \omega_t^2 + \omega_c^2)/2 \pm S
$$

where

$$
4S^{2} = (\omega_{I}^{2} - \omega_{t}^{2})^{2} + \omega_{c}^{4} + 2\omega_{c}^{2}(\omega_{I}^{2} + \omega_{t}^{2}).
$$

This is identical with previous results.

To calculate the eigenfunctions of  $h'_{MPk}$ , let us go back to the rotation that transformed  $J$  to  $J'$ . The corresponding transformation on the spinor operators  $a_l$  and  $a_t$  that accomplished this is

$$
a'_{kl} = a_{kl} \cos(\theta/2) + i a_{kt} \sin(\theta/2),
$$

$$
a'_{kt} = a_{kt} \cos(\theta/2) + i a_{kl} \sin(\theta/2).
$$

The eigenfunctions are, in a straightforward manner,

$$
| n_{kl}, n_{kt} \rangle = (n_{kl}!)^{-1/2} (n_{kt}!)^{-1/2}
$$
  
 
$$
\times (a_{kl}^{\dagger})^{n_{kl}} (a_{kt}^{\dagger})^{n_{kt}} | 0 \rangle
$$

where  $|0\rangle$  is the ground state of  $h'_{0k}$ , which is also the ground state of  $h'_{\text{MP }k}$ .

However, we have still not, at this stage, diagonalized  $H_{MP}$  itself. We have diagonalized every one of its Fourier components  $h'_{MPk}$ , but with a different choice of the gauge for each. To make this legitimate, we would have to perform a gauge transformation for each  $h'_{MPk}$  to a common vector potential, which we would choose to be that given by the circular gauge, with  $f=-\frac{1}{2}, g=\frac{1}{2}$ . This gauge has the advantage of being invariant under rotation, so that all the vector potentials used in diagonalizing  $h'_{MPk}$  are now the same irrespective of the direction of k. The energy spectra remain unchanged, of course; and the eigenfunctions all acquire an extra phase factor, thus

 $\left| n_{kl}n_{kt}\right\rangle _{0}$ 

$$
=\exp[-i(\omega_{l0}-\omega_{t0})x_{kl}x_{kt}/2(\omega_{l0}+\omega_{t0})b^2]|n_{kl}n_{kt}\rangle
$$

where  $b$  is the magnetic length

$$
b^2 = \hslash / m \omega_c.
$$

In summary, the eigenstates of  $H_{MP}$  are

$$
\prod_k |n_{kl}n_{kt}\rangle_0
$$

with energies

$$
\sum_k n_{kl} E_{k} + n_{kt} E_{k} -
$$

### APPENDIX C

In this appendix the evaluation of the exchange integral will be discussed. The integral we are interested in is

$$
I = \sum_{P} (-1)^{P} \langle \phi | 1/r | \phi_{P} \rangle / \sum_{P} (-1)^{P} \langle \phi | \phi_{P} \rangle.
$$
 (C1)

A linked cluster expansion can be developed for the integrals in increasing number of exchanged particles. Let us illustrate this for the normalization integral  $I_a = \langle \phi | \phi_{P_i} \rangle$ . We first define the two-particle and threeparticle exchange integrals  $J_i$  as

$$
J_i = \langle \phi | \phi_{P_i} \rangle,
$$

where  $P_i$  corresponds to an *i*-particle exchange. Our aim is to write  $I_a$  as an infinite series of the J's, viz.,

$$
I = \left[1 + \sum_{l=2} J_l n_l\right]^N, \tag{C2}
$$

Here N is the total number of particles,  $n<sub>l</sub>$  is the number of bonds per particle. This factor comes from a counting of the multiplicity of the exchange terms. For example, for a hexagonal lattice  $n_2 = 3$ . Comparing Eq. (C2) with the definition of  $I$ , it is now possible to define all the higher order integrals recursively in terms of the lower order integrals. For example

$$
J_4 = \phi_{P_4} \langle \phi | \phi_{P_4} \rangle - N(N-1) n_2^2 (\langle \phi | \phi_{P_2} \rangle)^2.
$$

Our trial wave function  $\phi$  can be written as

$$
\phi = \exp\left(-\sum_{q} \omega_{1q}^{2} |\delta x_{q}|^{2} + \omega_{2q}^{2} |\delta y_{q}|^{2} + i(\omega_{1q}^{2} - \omega_{2q}^{2})\delta x_{q} \delta y_{-q}/2 - i\sum_{j} \mathbf{r}_{j} \times \mathbf{R}_{j} \cdot \mathbf{z}/2\right),\tag{C3}
$$

where  $\omega_{1q}^2 + \omega_{2q}^2 = 1$ .

We have looked at both the two- and the three-particle exchange integrals in detail and found the three-particle exchange to be much smaller; let us illustrate our calculation with the two-particle exchange and quote the corresponding result for the three-particle exchange at the end.

Both the normalization integral  $I_a = \langle \phi | \phi_P \rangle$  as well as both the normalization integral  $I_a = \langle \psi | \psi_P \rangle$  as well as<br>the exchange  $I_b = \langle \phi | 1/r | \phi_P \rangle$  can be expressed in term of the function  $A(u)$  defined by

$$
A(u) = \langle \phi_P | \delta(r_{12} - u) | \phi \rangle
$$
  
=  $\int d^2k \langle \phi_P | \exp[ik (R_{12} + \delta r_{12} - u)] | \phi \rangle / (2\pi)^2$ , (C4)

where we have represented the delta function in exponential form:

 $\phi_P = \phi(\delta r')$ 

with the set  $\{r'\}$  corresponding to the permuted coordinates. Its Fourier transform can be written in terms of the unpermuted coordinates as

$$
\delta r'_{q} = r_{12} [\exp(-i\mathbf{q} \cdot \mathbf{R}_{2}) - \exp(-i\mathbf{q} \cdot \mathbf{R}_{1})]/N^{0.5} + \delta r_{q}.
$$

Define  $c$  by

$$
\delta r'_q = c_q + \delta r_q. \tag{C5}
$$

Then

$$
c_q = u[\exp(-iq \cdot \mathbf{R}_2) - \exp(-iq \cdot \mathbf{R}_1)]/N^{0.5}.
$$
 (C6)

Substituting  $(C5)$  and  $(C3)$  into  $(C4)$ , we find that

$$
A = \int d^2k \exp(-B + C + i\mathbf{k} \cdot \mathbf{R}_{12})/(2\pi)^2
$$

where

$$
B = -\ln(\phi \times \phi_P^*)
$$
  
= 
$$
\sum_{j,q_x>0} \{2\omega_j^2 (|\text{Re}\delta r_{jq}|^2 + |\text{Im}\delta r_{jq}|^2) + 2\omega_{jq}^2 [\text{Re}(\delta r_{jq}) \text{Re}(c_{jq}) + \text{Im}(\delta r) \text{Im}(c)]
$$
  

$$
-i(\omega_1^2 - \omega_2^2) [\text{Re}(\delta r_{jq}) \text{Re}(c_{3-j,q}) + \text{Im}(\delta r) \text{Im}(c)] + \omega_j^2 |c_{jq}|^2\}
$$
  

$$
-i(\omega_1^2 - \omega_2^2) [\text{Re}(c_{xq}) \text{Re}(c_{yq}) + \text{Im}(c_{xq}) \text{Im}(c_{yq})] - F.
$$
 (C7)

 $F$  comes from the phase factors and is given by

$$
F = i \sum_{j} (\mathbf{r}_{pj} - \mathbf{r}_j) \times \mathbf{R}_j \cdot \mathbf{z}/2 = i (\mathbf{r}_{12} \times \mathbf{R}_{21}) \cdot \mathbf{z}/2.
$$
 (C8)

C comes from the delta function and is given by

$$
C = i\mathbf{k} \cdot \delta \mathbf{r}_{12}
$$
  
= 2*i*  $\sum_{q_x > 0} \mathbf{k} \cdot [\cos(qR_1) - \cos(qR_2)] \text{Re}(\delta \mathbf{r}_q) - [\sin(qR_1) - \sin(qR_2)] \text{Im}(\delta \mathbf{r}).$  (C9)

On completing squares in this exponent, one finds that

$$
B - C + F = \sum_{q_x > 0} \sum_{j} 2\omega_{jq}^2 [\text{Re}(\delta r_{jq}) + D]^2 + G,
$$
 (C10)

$$
G = -2\omega_{jq}^2 D^2 + \omega_j^2 \text{Re}(c_j)^2 - 2i(\omega_1^2 - \omega_2^2)[c_1(q)c_2(-q)],
$$
\n(C11)

where  $D$  is given by

$$
D = \text{Re}(c_{jq})/2 - i(\omega_1^2 - \omega_2^2)\text{Re}(c_{3-j,q})/4\omega_{jq}^2 - ik_j[\cos(qR_1) - \cos(qR_2)]/2\omega_{jq}^2
$$
  
+ corresponding imaginary part. (C12)

The integration over  $\delta r_q$  can now be carried out. The final result is then proportional to  $\exp(G)$ . To facilitate the remain-<br>ing integration over k and u, we now rewrite G by grouping  $2\omega_2 D^2$  into terms involving  $c^$  $(C_1, D_1)$ . We find that there is a cancellation of the cross product of the first two terms of D and  $i(\omega_1^2 - \omega_2^2)[\text{Re}(c_1)\text{Re}(c_2) + \text{imaginary roman parts}]$  in calculating  $A_1$ . More precisely,  $G = A_1 + B_1 + C_1 + D_1 + F$  where

$$
A_1 = \sum_{q_x > 0} [(0.5 - 1)\omega_{jq}^2 - (\omega_1^2 - \omega_2^2)^2 / 8\omega_{j-jq}^2] \text{Re} |c_{jq}|^2 + \text{corresponding imaginary part}
$$
  
= 
$$
- \sum_{j,q_x > 0} |c_{jq}|^2 / (8\omega_{j-j,q}^2)
$$
  
= 
$$
- \sum_{i,j} g_{i,j} u_i u_j,
$$
 (C13)

with

$$
g_{ij}(R) = \sum_{ql} e_{qli} e_{qlj} [1 - \cos(q \cdot R)] / (8\omega_{q,3-l}^2 N),
$$
  
\n
$$
B_1 = - \sum_{j,q_x>0} k_j [\cos(qR_1) - \cos(qR_2)]^2 / 2\omega_{jq}^2 N
$$
  
\n
$$
= -0.5 \sum_{i,j} k_i k_j a_{i,j}
$$
 (C14)

where  $a$  was defined in Eq. (9c) as

$$
a_{ij}(R) = \sum_{ql} e_{qli} e_{qlj} [1 - \cos(q \cdot R)] / (\omega_{ql}^2 N),
$$
  
\n
$$
C_1 = -i \left[ \sum_{j,q_x > 0} \text{Re}(c_j) k_{aj} [\cos(qR_1) - \cos(qR_2)] + \text{corresponding imaginary part} \right]
$$
  
\n
$$
= i \mathbf{u} \cdot \mathbf{k}.
$$
 (C15)

This is canceled out by an identical term already present in the exponent;

$$
D_1 = -\sum_{q_x > 0} (\omega_1^2 - \omega_2^2) \sum_j \text{Re}(c_{3-j}) k_j [\cos(qr_1) - \cos(qr_2)] / 2\omega_{jq}^2 + \text{corresponding imaginary part}
$$
  
= 
$$
\sum_{i,j} t_{i,j} k_i u_j,
$$
 (C16)

where

$$
t_{ij}(R) = \sum_{ql} e_{qli} e_{q,3-l,j} \left[1 - \cos(q \cdot R)\right] (\omega_1^2 - \omega_2^2)/(2\omega_{ql}^2 N).
$$

Note that, since  $e_{2x} = -e_{1y}$ , and  $e_{2y} = e_{1x}$ ,

$$
g_{yx} = g_{xy} = -a_{xy}/8, g_{xx} = a_{yy}/8, g_{yy} = a_{xx}/8,
$$
  
\n
$$
t_{xx} = -t_{yy} = a_{xy}/2 = a_{yx}/2,
$$
  
\n
$$
t_{yx} = a_{yy}/2 - 1, t_{xy} = -a_{xx}/2 + 1.
$$
\n(C17)

For example

$$
t_{xx} = \sum_{q} e_{q1x} e_{q1y} [1 - \cos(q \cdot \mathbf{R})] (\omega_1^2 - \omega_2^2) (\omega_{q1}^{-2} + \omega_{q2}^{-2})/(2N)
$$
  
= 
$$
\sum_{q} [1 - \cos(q \cdot \mathbf{R})] (e_{q1x} e_{q1y} \omega_{q1}^{-2} + e_{q2x} e_{q2y} \omega_{q2}^{-2})/(2N) = a_{xy}/2
$$

where we have used  $\omega_1^2 + \omega_2^2 = 1$ . To summarize, we have

$$
A = \int \frac{d^2k}{(2\pi)^2} \exp \left[ - \sum_{i,j} (g_{i,j} u_i u_j - t_{i,j} k_i u_j + 0.5 k_i k_j a_{i,j}) + i \mathbf{k} \cdot \mathbf{R}_{12} - i \mathbf{u} \times \mathbf{R}_{12} / 2 \right].
$$

On carrying out the  $k$  integration, we get

$$
I_a = \int d^2 u \exp(X) / 2\pi (a_{xx} a_{yy})^{0.5},
$$
 (C18)

$$
I_b = \int d^2 u \exp(X)/2 |u| \pi (a_{xx} a_{yy})^{0.5},
$$
 (C19)

where

$$
X = -u_y^2(1 - 1/a_{xx})/2 - u_x^2(1 - 1/a_{yy})/2 + i(R_y u_x/a_{yy} - R_x u_y/a_{xx}) - R_y^2/2a_{yy} - R_x^2/2a_{xx}.
$$
 (C20)

Note that  $\sum_{q_x > 0}$  = 0.5  $\sum_{q}$ . The k integration for  $I_q$  can be carried out analytically and we have

$$
I_{a} = \exp[-R_{y}^{2}/2(a_{yy}-1) + R_{x}^{2}/2(a_{xx}-1)] / [(a_{xx}-1)(a_{yy}-1)]^{0.5}.
$$
 (C21)

We now quote the corresponding formulas for the three-particle exchange. Assume  $P 1 = 3$ ,  $P 2 = 1$ ,  $P 3 = 2$ , A is now given by  $5(n-1)$  $5(n-1)$  $\mathbf{r}$ 

$$
A = \langle \phi_P | \delta(r_{31} - u_a) \delta(r_{12} - u_b) | \phi \rangle
$$
  
=  $\int d^2 k_a d^2 k_b \langle \phi_P | \exp[i k_a (R_{31} + \delta r_{31} - u_a) + k_b (R_{12} + \delta r_{12} - u_b)] | \phi \rangle / (2\pi)^4.$  (C22)

Let  $u_a = r_{31}$ ,  $u_b = r_{12}$ , then  $-u_a - u_b = r_{23}$  and

$$
c_q = [u_a \exp(-i\mathbf{q} \cdot \mathbf{R}_1) + u_b \exp(-i\mathbf{q} \cdot \mathbf{R}_2) - (u_a + u_b) \exp(-i\mathbf{q} \cdot \mathbf{R}_3)]/N^{0.5}.
$$
 (C23)

The exponent of A is now given by  $-B + C + i k_a \cdot R_{31} + i k_b \cdot R_{12}$ .

$$
F = i (u_a \times \mathbf{R}_{13} + u_b \times \mathbf{R}_{23}) \cdot z / 2,
$$
\n(C24)  
\n
$$
C = 2i \sum_{q_x > 0} \mathbf{k}_a \cdot [\cos(qR_3) - \cos(qR_1)] \cdot \text{Re}(\delta r_q) - [\sin(qR_3) - \sin(qR_1)] \cdot \text{Im}(\delta r) + \text{corresponding } k_b \text{ term},
$$
\n(C25)

$$
D = \text{Re}(c_{jq})/2 - i(\omega_1^2 - \omega_2^2)\text{Re}(c_{3-j,q})/4\omega_{jq}^2
$$
  
-  $ik_{aj}[\cos(qR_3) - \cos(qR_1)] + k_{bj}[\cos(qR_1) - \cos(qR_2)]/2\omega_{jq}^2 + \text{corresponding imaginary part,}$  (C26)

$$
G = -\sum_{i,j=1,2} (f_{ij}k_i u_j + h_{ij}k_i k_j + b_{ij}u_i u_j) + iH(u,k),
$$
\n(C27)

$$
iH(u,k) = i(\mathbf{k}_a \cdot \mathbf{R}_{31} + \mathbf{k}_b \cdot \mathbf{R}_{12} + u_a \times \mathbf{R}_{13}/2 + u_b \times \mathbf{R}_{23}/2),
$$
 (C28)

where the *buu* terms comes from  $A_1$ ; hkk, from  $B_1$ ; fku, from  $D_1$ ;

*buu* = 
$$
\sum_{i,j=x,y} g_{i,j}(13)u_{a,i}u_{a,j} + g_{i,j}(23)u_{b,i}u_{b,j} + [g_{i,j}(23) + g_{i,j}(13) - g_{i,j}(12)]u_{a,i}u_{b,j},
$$
 (C29)

$$
hkk = \sum_{i,j=x,y} 0.5a_{i,j}(13)k_{ai}k_{aj} + 0.5a_{i,j}(12)k_{bi}k_{bj} + 0.5[a_{i,j}(23) - a_{i,j}(12) - a_{i,j}(31)]k_{ai}k_{bj},
$$
 (C30)

$$
fuk = \sum_{i,j=x,y} -t_{i,j}(13)k_{ai}u_{aj} + 0.5[t_{i,j}(12) - t_{i,j}(13) - t_{i,j}(23)]k_{ai}u_{bj}
$$
  
+ 0.5[t\_{i,j}(13) + t\_{i,j}(12) - t\_{i,j}(23)]k\_{bi}u\_{aj} + 0.5[t\_{i,j}(13) - t\_{i,j}(23) - t\_{i,j}(12)]k\_{bi}u\_{bj}  
+ i(k\_b \cdot u\_b + k\_b \cdot u\_a - k\_a \cdot u\_b)/2. (C31)

The integral for the three particle exchange can be evaluated as follows. We defined a vector v by  $v = (u_a, u_b, k_a, k_b)$ , then G can be written as  $G = \sum_{i,j} z(i,j)v(i)v(j)$  where the matrix  $z = z 1 + iz 2$ , z 1 is given by

$$
\begin{vmatrix}\n2s_{13} & s_{13} + s_{23} - s_{12} & -2\omega_{13} & \omega_{12} + \omega_{13} - \omega_{23} \\
\overline{s}_{13} + \overline{s}_{23} - \overline{s}_{12} & 2s_{23} & \omega_{12} - \omega_{13} - \omega_{23} & \omega_{13} - \omega_{12} - \omega_{23} \\
-2\overline{\omega}_{13} & \overline{\omega}_{12} - \overline{\omega}_{13} - \overline{\omega}_{23} & 2v_{13} & v_{23} - v_{12} - v_{31} \\
\overline{\omega}_{12} + \overline{\omega}_{13} - \overline{\omega}_{23} & \overline{\omega}_{13} - \overline{\omega}_{12} - \overline{\omega}_{23} & \overline{v}_{23} - \overline{v}_{12} - \overline{v}_{31} & 2v_{12}\n\end{vmatrix}
$$

where  $s = 0.5g$ ,  $\omega = 0.25\bar{t}$ ,  $v = 0.25a$ , a bar denotes the transpose of the matrix. z 2 is given by



Similarly H can be written as  $H = \sum h(i)v(i)$ . The overlap integral is then equal to

$$
\exp(-\hslash z^{-1}h/4)/[16\det(z)^{1/2}].
$$

We have evaluated the two-particle exchange up to the third neighbor; the result is shown in Table III. As can be seen, the third-neighbor exchange is already quite small. We have also evaluated the three-particle exchange and found that it is an order of magnitude smaller.

To include the two-particle exchange in the total energy, we note that the exchange energy  $E_{ex}$  per particle is

given by

$$
E_{\text{ex}} = n \left[ -\langle \phi | 1/r | \phi_P \rangle \right.+ \langle \phi | \phi_P \rangle \langle \phi | (1/r - U_0) | \phi \rangle \right]. \tag{C32}
$$

Here *n* is the average number of bonds and  $U_0$  denotes the contribution to the potential due to the background. For a hexagonal lattice it is 3.

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will not be explicitly specified from now on.

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