

Trial state for a two-dimensional hexatic

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We investigate a possible trial state for liquid crystalline phases with *hexatic* order in two dimensions using a generalization of Laughlin's wave function for a $1/7$ -filled lowest Landau level. This state has possible applications for the understanding of recent experiments showing melting at ca. 135 mK of the Wigner crystal to a fractional quantum Hall state at low filling factors [Phys. Rev. Lett. **88**, 176802 (2002)], and for other problems in two-dimensional crystallization of one-component plasmas like electrons on the surface of liquid helium.

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I. INTRODUCTION

It has been known for some time¹ that in a two-dimensional one-component plasma (2DOCP) a transition from a solid (usually a hexagonal lattice) to a liquid state occurs at finite temperature. However, the possibility of an intermediate *hexatic* phase, as first suggested by the (KTHNY) Kosterlitz, Thouless, Halperin, Nelson, and Young theory^{2–4} has never been experimentally realized. Although the 2D melting problem has been intensively studied for the past decades, the existence of a hexatic phase has long been debated and still remains poorly understood to date. The strongest evidence for the validity of the KTHNY theory of 2D melting was provided by the simulations of Chen *et al.*,⁵ who confirmed the existence of a hexatic phase in a 2D system interacting with a shifted Lennard-Jones (LJ) potential.

On these grounds it seems particularly interesting to investigate the possibility of a hexatic phase in 2D systems interacting with other potentials, such as Coulomb (or screened Coulomb, with 2D- or 3D-like radial dependence) as in the case of electrons in the partially filled Landau levels (LL) or on the surface of liquid Helium. Since there is a well-known analogy between the Laughlin state for the fractional quantum Hall effect (FQHE) and the 2DOCP,⁶ it may be interesting to see how ideas from these different viewpoints correlate to each other.

In the realms of FQHE, one of the oldest questions regards the transition point between the series of FQHE states and the Wigner crystal (WC).^{6–10} Initial estimations by Laughlin predicted the transition at $\nu_c \approx 1/10$,⁶ with subsequent improvements leading to an estimate of $\nu_c \approx 1/6.5$ (Refs. 9,10) or even at higher filling factors.^{8,10} The structure of the WC corresponds to a hexagonal lattice.

Recently, for very high mobility GaAs/Al_xGa_{1-x}As heterostructures, Pan *et al.*¹¹ have discovered evidence that for a window of temperatures above a filling-factor-specific temperature (e.g., ca. 135 mK for $\nu=1/7$) an apparent FQHE is observed, as evidenced by a dip in the longitudinal resistance

for various *very low* filling factors such as $\nu=2/11$, $3/17$, $3/19$, $2/13$, $1/7$, $2/15$, $2/17$, and $1/9$, corresponding to the hierarchical sequences of composite fermion (CF) states that originate from the $\nu=1/6$ and $\nu=1/8$ “Fermi seas”¹² (and which correspond to the attaching of 6 and 8 vortices to each electron, respectively). These recent experimental findings of an apparent FQHE state at finite temperatures corroborate earlier measurements showing a reentrant behavior at $\nu=1/7$ and $2/9$,^{13,14} although these features disappear as $T \rightarrow 0$. The general consensus is that the “true” ground state is, indeed, the WC and that the observations correspond to *melting* of such WC towards a correlated liquid state such as the FQHE's.

This explanation has shortcomings, however. Since the WC is the lowest *energy* state and it has a gapless excitation spectrum (for neutral excitations), it is difficult to see how the *free energy* $A=E-TS$ for the Laughlin state can be lower at finite temperatures, especially because the latter is gaped and hence should have lower entropy S , at least at very low temperatures. More refined arguments, which consider the entropy of the Laughlin state at temperatures high enough that there is a significant number of excitations across the gap, have shown that the FQHE state entropy may raise rapidly,¹⁵ which could explain the possibility of this WC to FQHE melting transition. The calculated transition temperature for the $\nu=1/7$ state should be 400–600 mK,¹⁵ considerably higher than the experimental result of ~ 135 mK (Ref. 11) (the difference is not necessarily unsatisfactory given the nature of the approximations needed for the calculation).

In this paper we propose many-body states, based on a broken rotational symmetry (BRS) generalization of Laughlin's with hexatic order. The motivation for these states has multiple origins: (i) Previous success of liquid crystalline approaches (“quantum Hall nematics”) to explain recently discovered anisotropic states and reentrant integer QHE states in partially filled LL's,^{16–21} moreover the characteristic transition temperatures are comparable;^{11,16,19} (ii) These

hexatic states are natural intermediaries between WC and FQHE states, or as the liquid crystalline intermediate phases between, e.g., hexagonal solid and liquid phases of electrons on the surface of liquid helium;¹⁻⁵ (iii) Due to the spontaneous broken symmetry of these BRS states, the existence of a Goldstone mode assures a gapless excitation spectrum, possibly leading to a lower free energy A at finite temperatures.

In Sec. II we describe the trial states that are considered in this paper. Section III describes the Monte Carlo (MC) procedure used to calculate expectation values of various operators with particular emphasis on the determination of the pair correlation function $g(\mathbf{r})$ and its Fourier transform, the static structure factor $S(\mathbf{q})$ (note that due to the BRS these acquire angular dependence). In Sec. IV we discuss the correlation energy of such states, in particular, how they compare to the relevant FQHE and WC states. The overall picture and discussion of results are presented in Sec. V.

II. HEXATIC TRIAL STATES

Consider Laughlin's⁶ many-body wave function for a $\nu = 1/(2m+1)$ FQHE state:

$$\Psi_\nu(\mathbf{r}_1, \dots, \mathbf{r}_N) = \left[\prod_{i<j}^N (z_i - z_j)^{2m} \right] \times \left[\prod_{i<j}^N (z_i - z_j) e^{-1/4 \sum_{k=1}^N |z_k|^2} \right], \quad (1)$$

where $z_i = x_i + iy_i$ is i th electron position in the xy plane (we work in units of the magnetic length $l_0^2 = \hbar/eB = 1$). In the CF picture,¹² this wave function corresponds to the attachment of $2m$ vortices to each electron by the Jastrow factor (the term between the first pair of brackets), and (in the mean field approximation) results in a $(2m+1)$ -fold reduction of the effective magnetic field for the CF's, which then completely fill the lowest LL (as represented by the term between the second set of brackets, which has the form of a Slater determinant). This state corresponds to a gaped, uniform and isotropic liquid, and is an excellent description of the state for the $\nu=1/3$ and $1/5$ FQHE. Note that for lower ν (e.g. $1/7$), as mentioned in Sec. I, a WC state is lower in energy.

There is no *a priori* reason why the vortices responsible for the CF transformation have to be attached precisely "on top" of the electrons, and variants of these states have been proposed in the past^{20,22-24} to deal with possible quantum Hall nematic states. The basic idea is to split the $2m$ nodes in a pattern around each electron. The only condition that needs to be satisfied is exchange antisymmetry (Fermi statistics), which imply that these zeros must be spread in symmetric pairs (and the single node in the Slater determinant must be "kept at the origin"). Recently, we have successfully used these ideas to explore possible quantum Hall *nematics* corresponding to the addition of two *off-center* vortices ($m=1$): at $\nu=1/3$ Refs. 20,22,23 and $\nu=1/2$ Ref. 24 (note however, that in this latter case the "base" CF state is different²⁵).

In this paper we are interested in studying possible quantum Hall hexatic states, which can be achieved by splitting the vortices in a regular hexagonal pattern, which can be

achieved for $\nu=1/(2m+1)$ for $m \geq 3$. We consider here the simplest of such states corresponding to filling factor $\nu=1/7$:

$$\Psi_{1/7}^\alpha(\mathbf{r}_1, \dots, \mathbf{r}_N) = \left\{ \prod_{i<j}^N \left[\prod_{\mu=0}^5 (z_i - z_j - \alpha_\mu) \right] \right\} \times \left[\prod_{i<j}^N (z_i - z_j) e^{-1/4 \sum_{k=1}^N |z_k|^2} \right], \quad (2)$$

where $\alpha_\mu \equiv \alpha \exp[i(2\pi\mu/6)]$, $\mu \in \{0,1,2,3,4,5\}$, and α can be taken to be real without loss of generality. This wave function represents a homogeneous liquid state, lies entirely in the lowest LL, and for $\alpha \neq 0$ has hexatic order (for $\alpha=0$ we recover Laughlin's wave function,⁶ which is obviously isotropic). This wave function represents, therefore, a good starting point to consider a quantum Hall *hexatic*.

III. MONTE CARLO SIMULATIONS

Given the many-body wave function $\Psi_{1/7}^\alpha$ [Eq. (2)], the probability density for some electron configuration $\{\mathbf{r}_1, \dots, \mathbf{r}_N\}$ is given by

$$P(\mathbf{r}_1, \dots, \mathbf{r}_N) \equiv |\Psi_\alpha|^2 = \exp[-U(\mathbf{r}_1, \dots, \mathbf{r}_N)], \quad (3)$$

where an irrelevant overall normalization constant has been omitted and

$$U(\mathbf{r}_1, \dots, \mathbf{r}_N) \equiv \frac{1}{2} \sum_{k=1}^N |z_k|^2 - \frac{1}{2} \sum_{i<j}^N \left[\left(\sum_{\mu=0}^5 \ln |z_i - z_j - \alpha_\mu|^2 \right) + \ln |z_i - z_j|^2 \right]. \quad (4)$$

It is interesting to note the analogy between Eqs. (3) and (4) and the Boltzmann distribution for a classical 2DOCP.⁶ For the hexatic state ($\alpha \neq 0$), the 2DOCP "particles" have additional higher-order multipole moments (which modify the short-range correlations but do *not* have any long-range effect).

From this probability distribution, it is possible to calculate the expectation value of any position-dependent operator in the usual form

$$\langle \mathcal{O} \rangle = \frac{\int d^2r_1 \cdots d^2r_N P(\mathbf{r}_1, \dots, \mathbf{r}_N) \mathcal{O}(\mathbf{r}_1, \dots, \mathbf{r}_N)}{\int d^2r_1 \cdots d^2r_N P(\mathbf{r}_1, \dots, \mathbf{r}_N)}. \quad (5)$$

It is easy to see that even for a modest number N of electrons, integrals such as those involved in Eq. (5) are essentially impossible to compute numerically unless the necessarily discrete sets of $2N$ -dimensional points is chosen appropriately, which is the essence of all MC methods. For each α under consideration, we start by uniformly distribut-

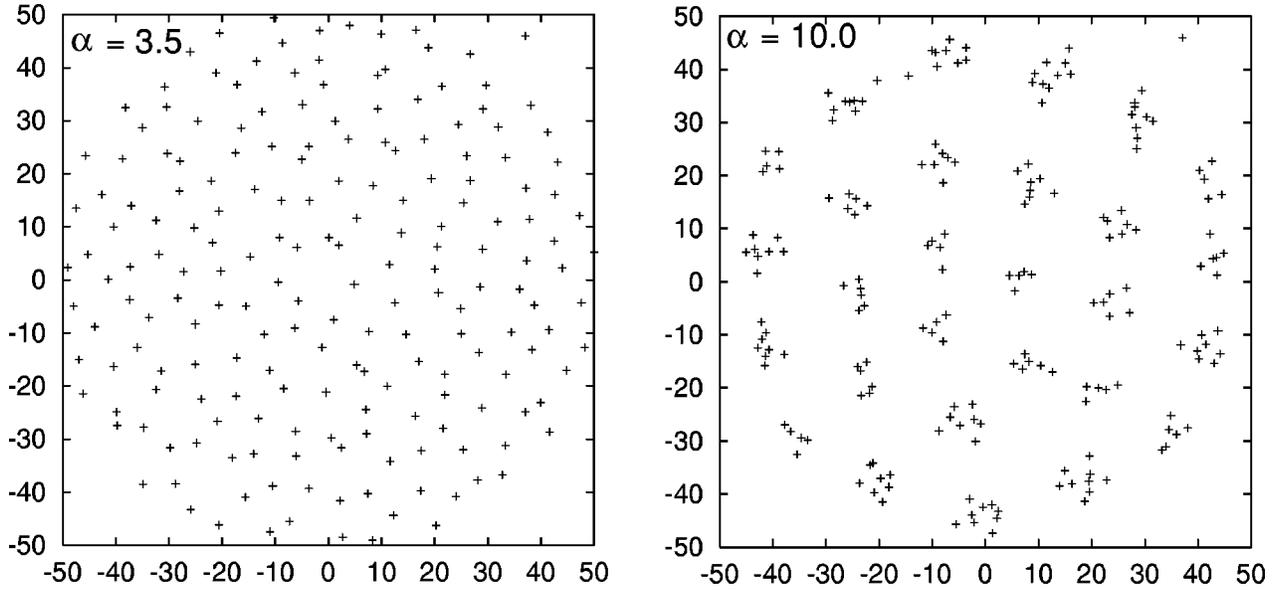


FIG. 1. A typical MC configuration of 200 electrons for $\alpha=3.5$ (left panel) and $\alpha=10.0$ (right panel). The picture for the lower α shows clearly how the system is uniform (the orientational order which is not visible in the picture is better seen from the pair correlation function plots in Fig. 2). The right picture for the unreasonably large α (the electron vortex separation is larger than typical electron-electron distances) is presented merely to aid the visualization of the underlying hexagonal symmetry of the state.

ing N electrons inside a disk of radius $R \approx \sqrt{2N/\nu}$. In each MC step, a random electron is moved a fixed distance d (chosen in the beginning of the run so that approximately 50% of the MC attempts are successful) in a random angle. Using the standard Metropolis algorithm,²⁶ we accept the move if the probability ratio between new and old electronic configurations, $P^{\text{new}}/P^{\text{old}}$, is bigger than a random number between 0 and 1, and otherwise reject it. The averages involved in Eq. (5) are approximated by

$$\langle \mathcal{O} \rangle \approx \frac{\sum_i \mathcal{O}_i}{\sum_i 1}, \quad (6)$$

where \mathcal{O}_i represents the operator evaluated at a given set of electron positions in a sequence of MC steps, i.e. $\mathcal{O}(\mathbf{r}_1^{(i)}, \dots, \mathbf{r}_N^{(i)})$. One should note that in order to improve the convergence, a large number of initial MC steps are discarded from the averages to allow the system to reach a “reasonable” state. For illustration, Fig. 1 shows typical snapshots of the electron configurations.

A quantity that is of particular interest is the pair correlation function $g(\mathbf{r})$. The importance of this function is that its knowledge permits the determination of the average of any two-particle position operator (e.g. a two-body interaction potential, see below), because $g(\mathbf{r})$ corresponds to the joint probability of finding a particle at position \mathbf{r} given that another particle is found at 0:

$$g(\mathbf{r}) \equiv \frac{1}{\rho^2} \left\langle \sum_{i \neq j}^N \delta(\mathbf{r}_i - \mathbf{r}') \delta(\mathbf{r}_j - \mathbf{r}'') \right\rangle, \quad (7)$$

where $\mathbf{r} \equiv \mathbf{r}' - \mathbf{r}''$, and ρ is the electron density ($\rho = \nu/2\pi$ for the state being considered). It is easy to see that

$$g(\mathbf{r}) = \frac{N(N-1)}{\rho^2} \frac{\int d^2r_3 \dots d^2r_N P(\mathbf{r}_1 \dots \mathbf{r}_N)}{\int d^2r_1 \dots d^2r_N P(\mathbf{r}_1 \dots \mathbf{r}_N)}, \quad (8)$$

where in this case $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. Furthermore $g(\mathbf{r})$ satisfies the *normalization condition* $\rho \int d^2r [g(\mathbf{r}) - 1] = -1$. In addition to its usual radial dependence, the pair correlation function acquires an angular dependence in the BRS states ($\alpha \neq 0$).

After an initial “thermalization” process of several million MC steps, we compute $g(\mathbf{r})$ by counting how many electrons are present in a discrete Cartesian array centered around each *other* electron,^{20,27} this counting process is averaged over several billion MC steps requiring several hours to a few days of computation in a fairly fast Alpha 21264 workstation. Roughly 200–800 electrons were used in the MC runs and the results were extrapolated to the thermodynamic limit.²⁸ Care is taken so that only electrons in the “bulk” of this system are counted (by excluding a ring near the periphery of the disk where the electron density and correlations are different from the bulk).

In Fig. 2 we show a plot of $g(\mathbf{r})$ for a state described by the modified (hexatic) Laughlin-like function [Eq. (2)] for a hexatic parameter $\alpha=3.5$. Approximately 10^9 MC steps were used for this determination. Similar features are observed for other finite α .

Another function of great interest is the static structure factor $S(\mathbf{q})$, which is essentially a reciprocal space version of $g(\mathbf{r})$,

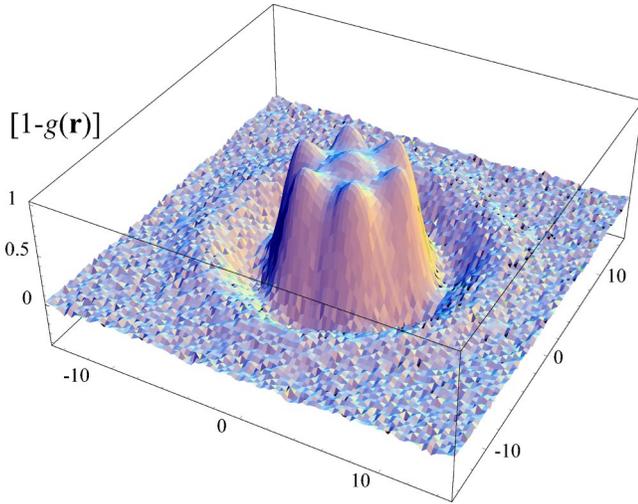


FIG. 2. Pair correlation function (plotted as $[1-g(\mathbf{r})]$ for clarity) for a state described by Eq. (2) for $\alpha=3.5$. Note the symmetric distribution of nodes of g .

$$S(\mathbf{q}) - 1 = \rho \int d^2r e^{-i\mathbf{q}\cdot\mathbf{r}} [g(\mathbf{r}) - 1]. \quad (9)$$

Fig. 3 presents a plot of $S(\mathbf{q})$ for a state described by the modified (hexatic) Laughlin-like function [Eq. (2)] for a hexatic parameter $\alpha=3.5$. Similar features are observed for other finite α .

IV. CORRELATION ENERGIES

It is interesting to compare the energies of the various trial states [Eq. (2)] as function of the anisotropic parameter α . Since wave function (2) lies entirely in the lowest LL, the kinetic energy per particle is quenched at the lowest cyclotron energy,

$$\frac{1}{N} \frac{\langle \Psi_\alpha | \hat{K} | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle} = \frac{1}{2} \hbar \omega_c, \quad (10)$$

where $\omega_c = eB/m_e$ is the cyclotron frequency. The potential, or correlation energy per electron is

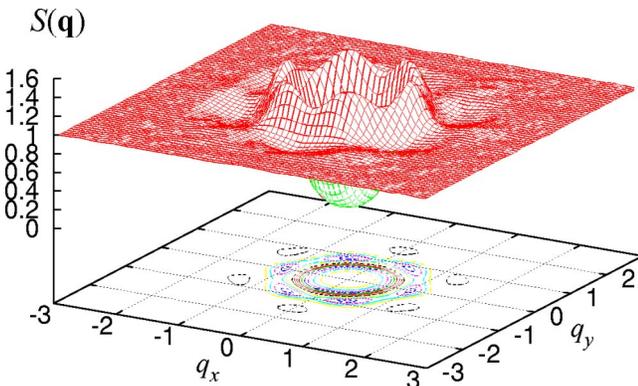


FIG. 3. Static structure factor for a state described by Eq. (2) for $\alpha=3.5$. Obtained from $g(\mathbf{r})$ using Eq. (9). Note the symmetric distribution of smooth peaks corresponding to a hexatic system.

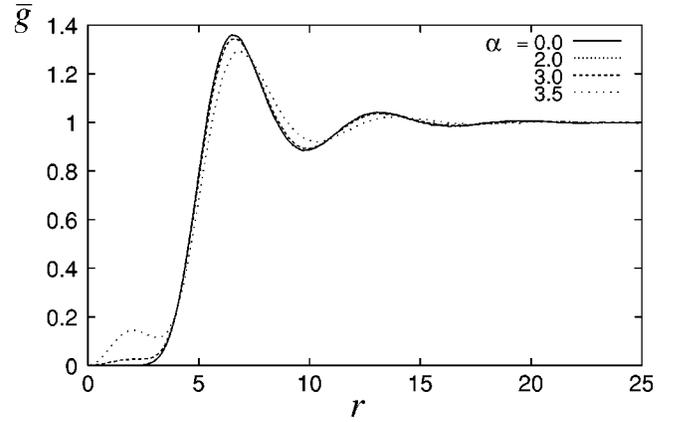


FIG. 4. Angle averaged pair distribution function $\bar{g}(r)$ for various values of α . See Eq. (15).

$$E_\alpha = \frac{1}{N} \frac{\langle \Psi_\alpha | \hat{V} | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle}, \quad (11)$$

where \hat{V} represents the electron-electron, electron-background, and background-background interactions.^{20,27} While this quantity can be computed directly using standard MC sampling (Sec. III), a new MC run has to be performed if the potential V needs to be changed (e.g. by considering a different sample width in the third dimension, or a particular screening length, etc). Fortunately, for two-body potentials, this correlation energy may also be written as

$$E_\alpha = \frac{\rho}{2} \int d^2r V(r) [g(\mathbf{r}) - 1]. \quad (12)$$

For an ideal 2D sample the interaction is a pure Coulomb potential $V(r) = e^2/(\epsilon r)$, while in samples with finite thickness a reasonable choice is the Zhang-Das Sarma (ZDS) potential $V(r) = e^2/(\epsilon \sqrt{r^2 + \lambda^2})$,²⁹ where λ is of the order of the sample thickness. Alternatively, the correlation energy can be computed in reciprocal space,

$$E_\alpha = \frac{1}{2} \int \frac{d^2q}{(2\pi)^2} \tilde{V}(q) [S(\mathbf{q}) - 1], \quad (13)$$

where $\tilde{V}(q)$ is the 2D Fourier transform (FT) of $V(r)$:

$$\tilde{V}(q) = \int d^2r e^{-i\mathbf{q}\cdot\mathbf{r}} V(r) = 2\pi \int_0^\infty dr r J_0(qr) V(r). \quad (14)$$

Although this paper focuses on the properties of electrons at very small filling factors of the lowest LL, for completeness we would like to remark that this second expression has the advantage of allowing for similar calculations of the correlation energy to be carried out at higher LL's, once static structure factor for the lowest LL is known by simply modifying the effective interaction potential $\tilde{V}(q) \rightarrow \tilde{V}_{\text{eff}}(q) \equiv \tilde{V}(q) \times [L_L(q^2/2)]^2$, where $L_L(x)$ are Laguerre polynomials and L corresponds to the LL index.^{20,23,24}

It is clear from Eq. (2) and Figs. 2 and 3 that both $g(\mathbf{r})$ and $S(\mathbf{q})$ are angle dependent for $\alpha \neq 0$. However, since the interaction potential is centrally symmetric, the energy E_α

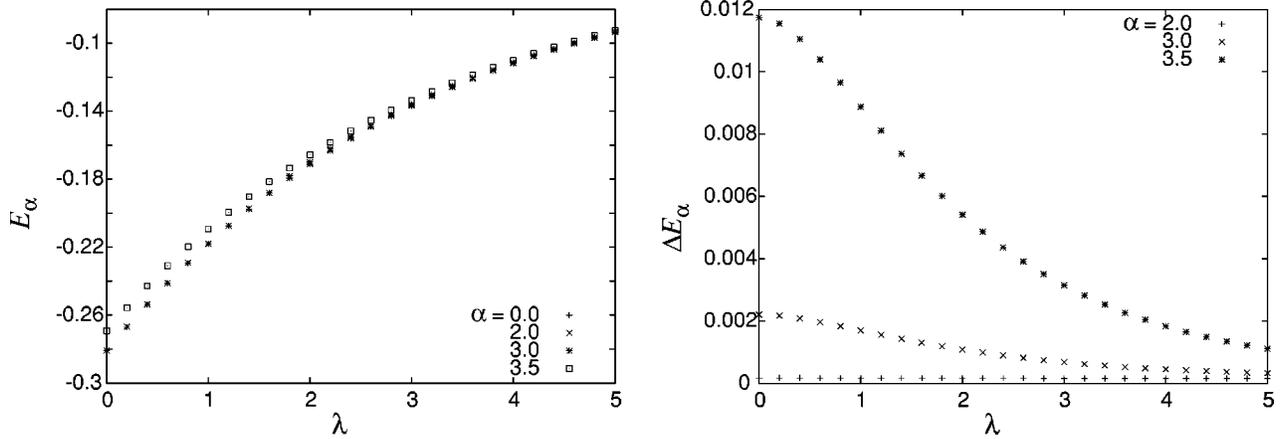


FIG. 5. Correlation energy per electron E_α (in units of $e^2/\epsilon l_0$) for various anisotropy parameters α and ZDS sample width parameters λ (Ref. 29). The right panel shows the difference in energy between a hexatic state and the isotropic Laughlin state $\Delta E_\alpha \equiv E_\alpha - E_0$. Notice that the Laughlin state is energetically favorable for all λ in the lowest LL.

depends only on the angle-averaged pair distribution function or static structure factor defined as

$$\bar{g}(r) = \int_0^{2\pi} \frac{d\theta}{2\pi} g(\mathbf{r}), \quad \bar{S}(q) = \int_0^{2\pi} \frac{d\theta}{2\pi} S(\mathbf{q}). \quad (15)$$

Figure 4 shows the angle-averaged pair correlation function $\bar{g}(r)$ for various values of α . The most remarkable feature is the change in the small- r behavior due to the splitting of the nodes of the wave function ($\bar{g} \sim r^{14}$ for $\alpha=0$, vs $\bar{g} \sim r^2$ for $\alpha \neq 0$).

In Fig. 5 (top panel) we show the correlation energy per electron E_α calculated from Eq. (12) using the angle-averaged $\bar{g}(r)$ (Fig. 4) for various values of α and the ZDS sample width parameter λ .²⁹ For comparison, the correlation energy per electron for a Wigner crystal is (for $\lambda=0$) $-0.3885e^2/\epsilon l_0$.⁹ The bottom panel of Fig. 5 shows the energy difference between hexatic and isotropic states $\Delta E_\alpha \equiv E_\alpha - E_0$. Notice that the Laughlin state is energetically favorable for all λ in the lowest LL. Similar conclusions were found for quantum Hall *nematics*, where anisotropic instabilities ($\Delta E_\alpha < 0$) were found only in *higher* LL's.^{20,23,24} The explanation for this seemingly universal behavior is easy to explain: in the lowest LL, the electron packets are simple Gaussians, and it is clear that the average distance between the electrons is largest when the vortices are at the electron's location ($\alpha=0$). For higher LL's, the wave packets take a more "ring like" shape, and a finite α permits a more optimal distribution of charge. In this work we focus on the physics of 2D electron systems at very low densities, the properties of possible hexatic phases in high LL's will be discussed elsewhere.³⁰

V. RESULTS AND DISCUSSION

In this work we applied MC methods to study BRS (hexatic) states at a $\nu=1/7$ filling factor. Although we find that the hexatic states proposed in this paper are slightly higher in energy than the isotropic Laughlin state, the fact that the BRS states are gapless (through their Goldstone mode) may make them a suitable candidate for a melting Wigner crystal at finite temperatures. Based on the analogy between the Laughlin-like states and the 2DOCP we can also interpret the proposed probability distribution as a candidate for a metastable hexatic phase of the 2D electrons trapped above a liquid helium surface and interacting with a Coulomb-like potential. Our results seem to suggest that, in contrast to LJ systems, this hexatic phase is not favorable for Coulomb-like interactions. It is evident that a calculation of the excitation spectrum (and resulting entropy) of these quantum Hall *hexatics* is highly desirable to settle the issue of melting observed at low filling factors by Pan *et al.*¹¹ We envision that the results obtained by for the static structure factor $S(\mathbf{q})$ will allow for the calculation of such spectrum, at least in the Girvin-MacDonald-Platzman single-mode approximation.³¹

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