Hybrid phase at the quantum melting of the Wigner crystal

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We study the quantum melting of the two-dimensional Wigner crystal using a fixed node quantum Monte-Carlo approach. In addition to the two already known phases (Fermi liquid at large density and Wigner crystal at low density), we find a third stable phase at intermediate values of the density. The third phase has hybrid behaviors in between a liquid and a solid. This hybrid phase has the nodal structure of a Slater determinant constructed out of the bands of a triangular lattice.

The physics of a system of $N$ electrons confined on a two dimensional surface $S$ is a textbook problem at the root of a very large body of literature. Two competing energies, electrostatic and kinetic, give rise to a rich phase diagram. The physics is controlled by the dimensionless parameter $r_s = m^* e^2 / (\hbar^2 e \sqrt{\pi n})$ which is the ratio of the average distance between electrons over the effective Bohr radius ($e$ is the electronic charge, $\epsilon$ the dielectric constant, $m^*$ the effective mass and $n = N/S$ the electronic density). At large density (low $r_s$), the kinetic energy dominates and the system is in a Fermi liquid phase [1]. Since the work of Wigner [2] in 1934, it is also known that at low density (large $r_s$), the Coulomb repulsion dominates and the electrons crystallize onto a (Wigner) triangular crystal [2, 3]. In their pioneering work in 1989, Tanatar and Ceperley [4] were able to locate that the quantum melting of the crystal occurs for a critical value of $r_s \approx 37 \pm 5$. Their work, which used a Fixed Node Quantum Monte-Carlo (FN-QMC) technique, was followed by more precise numerics [6] and a better description of the liquid phase [7, 8] that included backflow corrections.

This simple picture of a, presumably first order, direct transition between the solid and the liquid phase is to be contrasted with other aspects of the physics of the Wigner crystal which show more complex behaviors. For instance, its magnetism is believed to include a spin liquid phase in addition to the ferromagnetic phase found at very large $r_s$ [9]. The fermionic statistics of the electrons is also known to play a crucial role for $r_s \leq 60$ where the melting of the bosonic Wigner crystal occurs [10]. Also, the classical melting [11, 12, 13, 14] (as a function of temperature) occurs in two steps. The system first looses its translational order but retains some orientational order (hexatic phase [14]) while at higher temperature, all order disappears. The possibility that the melting of a quantum crystal would also take place in two steps, leading to a highly correlated intermediate phase has been discussed as early as 1969 by Andreev and Lifshitz [15], who proposed that a liquid of defects would exist together with the crystal state. This proposal has been revisited recently in small systems using exact diagonalization techniques [16, 17] as well as in screened systems [18].

In this letter, we study a new phase which is a hybrid of a liquid and a solid using a FN-QMC technique similar to the one used in [4]. The FN-QMC approach is a very powerful tool to tackle this problem, but it is of primary importance to understand the nature of the approximations which it involves. The method lies half way between a black box and a variational approach. Technically, the FN-QMC algorithm is fed with a wave-function called the guiding wave function (GWF) that has to be given explicitly, and that should be close to the ground state of the system. The FN-QMC algorithm modifies the GWF to become as close as possible to the ground state of the system, given the constraint that the sign of the wave function remains unchanged at every point of the Hilbert space. The method gives the best wave function for a given structure of the nodes of the GWF and is in this sense variational [19]. Our main result is summarized in the stability diagram Fig. 1 where the energies of the different phases (i.e. associated with the different GWFs) are plotted as a function of $r_s$. The hybrid phase is found to be stable in the (critical) region $r_s^* < r_s < r_s^{**}$

![Energy difference diagram](image-url)
with \( r_s^* \approx 30 \) and \( r_s^{*2} \approx 80 \).

**Model.** We consider a system of \( N \) spinless electrons on a square \( L_x \times L_y \) grid with periodic boundary conditions whose Hamiltonian is given by,

\[
H = -t \sum_{\langle \vec{r}, \vec{r}' \rangle} c_{\vec{r}}^\dagger c_{\vec{r}'} + \frac{U}{2} \sum_{\vec{r} \neq \vec{r}'} V(\vec{r} - \vec{r}') n_{\vec{r}} n_{\vec{r}'} + \lambda. \tag{1}
\]

The operator \( c_{\vec{r}}^\dagger \) (\( c_{\vec{r}} \)) creates (destroys) an electron on point \( \vec{r} \) with the standard anticommutation relation rules. The sum \( \sum_{\langle \vec{r}, \vec{r}' \rangle} \) is done on the nearest neighbor points on the grid and \( t \) is the corresponding hopping amplitude. The density operator reads \( n_{\vec{r}} = c_{\vec{r}}^\dagger c_{\vec{r}} \). \( U \) is the effective strength of the interaction. The two body interaction \( V(\vec{r}) \) is obtained from the bare Coulomb interaction using the Ewald summation techniques to avoid finite size effects, and reads

\[
V(\vec{r}) = \sum_{\vec{L}} \frac{1}{|\vec{r} + \vec{L}|} \operatorname{Erfc}(k_c|\vec{r} + \vec{L}|) \tag{2}
\]

\[
+ \frac{2\pi}{L_x L_y} \sum_{K \neq 0} \frac{1}{|K|} \operatorname{Erfc}(|\vec{K}|/(2k_c)) \cos(\vec{K} \cdot \vec{r}).
\]

In the previous equation, \( k_c \) is a (irrelevant) cut off. The vector \( \vec{L} \) takes discrete values \( \vec{L} = (n_x L_x, n_y L_y) \) with \( n_x \) and \( n_y \) integer numbers. The vector \( \vec{K} \) also takes discrete values, \( \vec{K} = \left( \frac{2\pi}{L_x} n_x, \frac{2\pi}{L_y} n_y \right) \) and \( (n_x, n_y) \neq (0, 0) \). The complementary error function is \( \operatorname{Erfc}(r) = \frac{2}{\sqrt{\pi}} \int_r^\infty e^{-t^2} dt \).

In order to assure electrostatic neutrality we add a positive continuous background (the positive background charges are not put on the grid but lie in the continuum). The constant term \( \lambda \) hence reads

\[
\lambda/N = 4t + UV(\vec{0}) - UV \frac{2\sqrt{\pi}}{k_c} - UV \frac{2k_c}{\sqrt{\pi}}. \tag{3}
\]

where \( \nu = \frac{N}{L_x L_y} \) is the average electronic density. All the energies in the problem are measured in unit of \( N 2\pi \nu t \).

The \( r_s \) parameter for this model reads, \( r_s = U/(2t\sqrt{\pi \nu}) \).

When \( \nu \ll 1 \) the role of the grid becomes irrelevant and Eq. 10 tends toward the continuous model studied in Ref \([14]\) provided our energies are multiplied by \( 2/r^2 \).

As we shall see however, the presence of the grid gives the possibility of constructing new types of GWF. In our numerics we have used \( \nu = 1/56 \) and \( \nu = 1/780 \). Standard two dimensional gas in GaAs heterostructures where the underlying grid is given by the Ga and As atoms correspond to \( \nu \approx 1/1000 \) or \( \nu \approx 1/10000 \) for the most diluted ones. In order for the Wigner crystal to fit into the system without distortion, we chose \( L_y = \sqrt{3} L_x \) and \( N = 2P^2 \) with \( P \) integer. The electrons in our study are fully spin polarized which corresponds to a system with a strong in plane magnetic field. However our results also extend to zero field systems since at \( r_s \geq 20 \) the polarized fluid is more stable than the non polarized one [6, 7].

Last, we have added a very small (irrelevant) disorder to the system in order to lift the degeneracies of the non interacting problem.

**FN-QMC Method.** The operator \( e^{-\beta H} \) is applied stochastically to an initial GWF in order to project it to the exact ground state. Our implementation is based on the Green Function Monte Carlo for lattice Hamiltonians introduced in \([20]\). Important sampling \([21]\) and Fixed Node are implemented as in \([13]\) by replacing \( H \) by an effective Hamiltonian \( H_{\text{FN}} \) that depends on the GWF. \( H_{\text{FN}} \) forbids the sign of the wave-function to change. The energies calculated with \( H_{\text{FN}} \) are larger than the one of the true ground state but smaller than the variational energy associated with the guiding wave-function \([14]\).

At \( \nu \ll 1 \) the technique is equivalent to the continuous fixed node diffusive Monte-Carlo used in \([4]\). The algorithm to update the Slater determinants can be found in \([22]\). By sampling directly the time spent by the walkers at one point of the Hilbert space using the algorithm described in \([24]\) we can use arbitrary small time steps and effectively work in continuous (imaginary) time. Instead of using branching, the control of the walkers population is done using a fixed number of walkers and the reconfiguration algorithm introduced by Sorella \([23]\). This algorithm allows to avoid the bias introduced in the branching technique by artificially controlling the walker population. Quantum averages of physical quantities \( \langle ... \rangle \) are calculated using the forward walking technique \([22]\), and hence do not suffer from the bias of mixed estimates.

A typical point for 72 particles involves 20 independent Monte-Carlo runs with 5000 walkers each.

**Guiding wave functions.** The GWFs used in our calculations are Slater determinants multiplied by Jastrow functions,

\[
\Psi(\vec{r}_1, \vec{r}_2...\vec{r}_N) = \text{Det} \left[ \phi_i(\vec{r}_j) \right] \times \prod_{i<j} J(|\vec{r}_i - \vec{r}_j|). \tag{4}
\]

The Jastrow part takes Coulomb interaction into account by introducing correlations between electrons. It has no nodes, and thus is irrelevant in the FN-QMC results. We use modified Yukawa functions \([24]\), \( J(r) = \Lambda(r_s)(1 - e^{-B(r_s)r}) \), where the distances are measured in unit of the average distance between nearest particles and \( \Lambda(r_s) \) and \( B(r_s) \) are (optimized) variational parameters.

We checked that the FN-QMC results are not sensitive to the choice of the Jastrow function. The Slater determinant of one-body wave functions, \( \text{Det} \left[ \phi_i(\vec{r}_j) \right] \) enforces the antisymmetric nature of the fermionic wave function and is responsible for the nodal structure of the GWF. The GWF used in the literature are constructed out of plane waves \( \phi_i(\vec{r}_j) \propto e^{-i\vec{k}_i \cdot \vec{r}_j} \) for the liquid GWF \( \Psi_{\text{liq}} \) and localized orbitals \( \phi_i(\vec{r}_j) \propto e^{-(\vec{r}_i - \vec{u}_i)^2}/\sigma_i^2 \) for the crystal GWF \( \Psi_{\text{cry}} \). Here the \( \vec{u}_i \) with \( i \in \{1...N\} \) stand for the...
positions of the electrons in the classical crystal and \( d_0 \) is a variational parameter. \( \Psi_{\text{liq}} (\Psi_{\text{cry}}) \) provides the exact ground state of \( H \) at very large (low) density.

Hybrid GWF. Below we give the detailed construction of a new GWF, \( \Psi_{\text{hyb}} \), such that the \( \phi_i(\vec{r}_j) \) are the Bloch states of a triangular crystal. First, an effective one-body Hamiltonian \( H_{\text{eff}} \) is constructed for an effective hole in a periodic potential given by a classical Wigner crystal,

\[
H_{\text{eff}} = -t \sum_{\langle \vec{r}, \vec{r}' \rangle} c_{\vec{r}}^\dagger c_{\vec{r}'} - U^* \sum_{\vec{r}} W(\vec{r}) n_{\vec{r}}
\]

where the one-body potential is \( W(\vec{r}) = \sum_{i=1}^{N} V(\vec{r} - \vec{u}_i) \). The singularity of \( W(\vec{r}) \) at \( \vec{r} = \vec{u}_i \) has been removed by setting \( W(\vec{u}_i) \equiv W(\vec{u}_i + (1,0)) \) and we checked that our results are unaffected by this choice. In a second step, we take advantage of the presence of the underlying grid and \( H_{\text{eff}} \) is numerically diagonalized using Lanczos algorithm. The \( N \) orbitals of lowest energy \( \phi_i(\vec{r}) \) \( (1 \leq i \leq N) \) are then used to construct the Slater determinant. \( U^* \) is a variational parameter.

The underlying idea behind the construction of \( \Psi_{\text{hyb}} \) is to put on the same level the melting of the Wigner crystal in real space (as the density is increased) and the destruction of the Fermi sea in momentum space (as the density is decreased). \( \Psi_{\text{hyb}} \) allows for an interpolation between momentum space \( (U^* = 0) \) and real space \( (U^* \gg 1) \). However, it never properly describes the Wigner crystal, since according to Bloch theorem, the \( \phi_i(\vec{r}) \) are always delocalized states (that can be concentrated around the \( \vec{u}_i \)'s but that are delocalized anyway). The available values of momentum \( \vec{k} \) are taken within the first Brillouin zone, and hence, the liquid-hybrid transition can be viewed as an instability of the shape of the Fermi surface that goes from a circular to a hexagonal form. The symmetry is broken at this transition, but it is only in a second step that larger values of \( |\vec{k}| \) will come into play, allowing the \( \phi_i(\vec{r}) \) to get localized and the actual crystallization to take place. This transition in two steps, where first the direction of \( \vec{k} \) and secondly its absolute value are affected, is reminiscent of the hexatic phase predicted in the classical melting.

Stability of the hybrid phase. Fig. 11 shows the energy differences \( E_{\text{liq}} - E_{\text{cry}} \) and \( E_{\text{hyb}} - E_{\text{cry}} \) as a function of \( r_s \) for a system of 72 electrons in a 48 \( \times \) 84 grid. These energy differences are very small, less than 0.1% of the total energy of the system. \( r_s \approx 40 \) where \( E_{\text{liq}} - E_{\text{cry}} \approx 0 \) would be the critical value or \( r_s \) in the absence of the hybrid phase. \( \text{Fig. 11} \). However, we find that for \( 30 < r_s < 80 \), the hybrid phase has a smaller energy than both the liquid and the solid phase. Around \( r_s^* \approx 30 \) we find a jump of \( U^* \) from zero to \( U^* = 0.3 \), see the inset of Fig. 2. \( U^*/U \approx 0.015 \) up to \( r_s^* \approx 80 \), above which the crystal phase become more stable than the hybrid phase. Finite \( N \) corrections shown in the inset of Fig. 11 at \( r_s \approx 42.2 \) do not perturb the previous picture. We note that although the variational energy of the hybrid phase is lower than the one of the liquid it is still higher than the crystal variational energy. The FN-QMC treatment is necessary to show the stability of the hybrid phase, as shown in Fig. 2. To make contact with the calculations of [4, 6], we have repeated these calculations for a more diluted system \( \nu = 1/78 \) where the role of the underlying grid is negligible. The results are plotted in Fig. 3 in the same way as Fig. 2 of [4] (with \( c_1 = -2.2122 \) ). In the inset of Fig. 3 we have reported the Wigner crystal data of \( \text{Fig. 4} \) and \( \text{Fig. 6} \) for comparison and find a good quantitative agreement with the latter. We note that finite \( N \) corrections would raise the energies by an amount \( \sim 0.01 \) (see the inset of Fig. 4) and are difficult to evaluate, especially in the absence of an analytical ansatz for the hybrid phase.

Nature of the hybrid phase. It is important to realize that, as described above, the nature of the intermediate phase is by construction something hybrid, being made of (delocalized) Bloch waves, yet having already the symmetry of the Wigner crystal. More insight can be gained by computing the electronic density \( n(\vec{r}) \) (not shown) which is the superposition of peaks at the classical positions (the \( \vec{u}_i \)'s) of the electrons in the crystal over a small background. The background is found to contain approximately 35% of the electrons while the rest lies in the peaks of the crystal. In that sense, the crystal part of the hybrid phase contains fewer electrons than sites, hence allowing exchange to take place. This is to be contrasted with the conjecture of Ref. [14] where a crystal with fewer sites than electrons was predicted. Although the total energy of the hybrid phase is below those of the liquid and crystal, both its kinetic and
electrostatic energies lie in between those of the liquid and solid. Fig. 4 shows the density-density correlation function (roughly measuring the probability of finding an electron at point \( \vec{r} \) knowing that an electron is at point \( \vec{0} \)),

\[
\langle \hat{c}^{\dagger}_{\vec{r}} \hat{c}_{\vec{r}} \rangle \approx L_x L_y \left| \frac{N(N-1)}{2} \right| \langle \hat{c}^{\dagger}_{\vec{0}} \hat{c}_{\vec{0}} \rangle
\]

for the three phases. \( g_{\text{hyb}}(\vec{r}) \) for the hybrid phase is intermediate between a liquid and a crystal. The value of \( g_{\text{hyb}}(\vec{r}) \) at its peaks is only twice as big as in the valley to be compared to a factor 15 at \( r_s = 100 \). In fact a very good fit is obtained with

\[
g_{\text{hyb}}(\vec{r}) \approx 0.35 g_{\text{liq}}(\vec{r}) + 0.65 g_{\text{cry}}(\vec{r})
\]

To conclude, we find that a new quantum phase is to be expected instead of a direct melting of the Wigner crystal. This intermediate phase, whose physical properties remain to be investigated in more depths, has hybrid behaviour between those of a solid and a liquid.

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FIG. 4: Density-density correlation function at for a system of 72 electrons in a 48 \( \times \) 84 grid. \( g(\vec{r}) \) measures the probability of finding a particle in \((X, Y)\) knowing that one electron lies in the middle of the sample. From left to right the liquid, crystal and hybrid phases are represented at \( U = 20 \) (\( r_s \approx 42.2 \)).

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