Interplay between electronic correlations
and quantum fluctuations in disordered square lattices

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Abstract

Using exact numerical studies of a few particles, the quantum melting of the Wigner crystal is revisited in two dimensions. The existence of an intermediate supersolid phase is suggested between the Fermi liquid and the Wigner crystal. The difference between lattice and continuum descriptions is clarified.

1 INTRODUCTION

After the discovery of an unexpected metal-insulator transition \cite{1} in two dimensions, it becomes necessary to revisit a fundamental issue: How does a Fermi liquid become a Wigner crystal as the carrier density decreases? We revisit this issue using exact numerical studies of the ground state (GS) of a few spinless fermions with Coulomb repulsion. Taking a square lattice with random potentials, three points are investigated: What are the lattice effects? How the different regimes detected without disorder are modified by weak random potentials? At zero temperature, how does the electron solid melt as the interaction strength decreases?

2 LATTICE AND CONTINUUM DESCRIPTIONS

For electrons in a background of positive ions, the continuum model is obtained after approximating the ionic lattice by a uniform positive jellium. The continuum model contains two scales: the inter-electron spacing \(a\) and the Bohr radius \(a_B\), and their ratio \(r_s = a/a_B\) is the scaling parameter. To keep the ionic lattice, one can use the tight-binding approximation, for getting a lattice model which has a third scale: the lattice spacing \(s\). If \(s\) is irrelevant, the lattice model keeps the same universal scaling than its continuum limit, if one uses the combination of lattice parameters which becomes \(r_s = a/a_B\) in the continuum.

The continuum model for \(N\) polarized electrons of mass \(m\) in a square of size \(D\) contains one body kinetic terms, two body interaction terms plus the constant term yielded by the uniform positive jellium. Measuring the energies in rydbergs (\(1\,\text{Ry} = me^4/2\hbar^2\)) and the lengths in units of the interparticle spacing \(a\), the continuum Hamiltonian \(H_c\) reads

\[
H_c = -\frac{1}{r_s^2} \sum_{i=1}^{N} \nabla_i^2 + \frac{2}{r_s} \sum_{1 \leq i < j \leq N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \text{const.} \quad (2.1)
\]
which only depends on the ratio $r_s = a/a_B$ and $N$. For large $r_s$ (strong coupling limit), the electrons form a Wigner crystal and the GS energy $E_0$ per particle in rydbergs can be expanded in powers of $r_s^{1/2}$, with the following factors in the thermodynamic limit:

$$E_0 = \frac{-2.2122}{r_s} + \frac{1.628}{r_s^{3/2}} + \frac{f_2}{r_s^2} + O(r_s^{5/2}), \quad r_s \gg 1. \quad (2.2)$$

The first term gives the Coulomb energy while the second represents the quantum zero point energy of the crystal in the harmonic approximation.

A square lattice model of spacing $s$, size $L = D/s$, nearest neighbor hopping element $t = \hbar^2/(2ms^2)$ and interaction strength $U = e^2/s$ is described by an Hamiltonian $H_1:

$$H_1 = t \left( 4N - \sum_{\langle j,j' \rangle} c_j^+ c_{j'} \right) + \frac{U}{2} \sum_{j \neq j'} \frac{n_j n_{j'}}{|d_{jj'}|} + \text{const}, \quad (2.3)$$

where $c_j^+$ creates a polarized electron at the site $j$, $n_j = c_j^+ c_j$. The boundary conditions (BCs) are periodic and $d_{jj'}$ is the distance [2] defined with those BCs between $j$ and $j'$ in unit of $s$. $\hbar R_y = U^2/4t$, $a_B = 2st/U$ and the ratio $r_s$ becomes:

$$r_s = \frac{a}{a_B} = \frac{UL}{2\sqrt{\pi N}} = \frac{r_1}{\sqrt{4\pi N}}, \quad (2.4)$$

where $r_1 = UL/t$. To include disorder, one can add $H_{dis} = W \sum_j c_j n_j$, the variables $c_j$ being taken at random between $[-1/2, 1/2]$.

In Fig. 1 (upper left), the regime of validity of the continuum approximation is given in the $(s/a_B^2, a/a_B^*)$ plane when $W = 0$, $a_B^*$ denoting the effective Bohr radius. The domain typically explored using 2d electron gases in different materials are indicated by double arrows. Different equivalent criteria can be used [3] to get this diagram. Let us discuss two of them when there is no disorder ($W = 0$).

### 2.1 Persistent current

Enclosing a flux $\Phi$ in the longitudinal $x$-direction yields a total longitudinal current $I_l(\Phi)$ which can be written in terms of the projections $\Psi_{k_1 \ldots k_N}$ of the GS wave-function $|\Psi_0\rangle$ onto the many particle eigenvectors $\prod_{n=1}^N d_{kn}^d|0\rangle$ characterizing the limit $U = W = 0$. $d_{kn}^d$ creates a particle in a state of momentum $k_n$. $\Phi_0$ being the flux quantum, one gets [2]:

$$I_l(\Phi) = \frac{2}{L} \sum_{k_1 \ldots k_N} |\Psi_{k_1 \ldots k_N}|^2 \sum_{i=1}^N \sin \left( k_{iN} + 2\pi \frac{\Phi}{L\Phi_0} \right). \quad (2.5)$$

If one can assume that $\sin k_s \approx k_s$ for all momenta $k$ where the projections $|\Psi_{k_1 \ldots k_N}|$ are significant, the lattice expression can be simplified by its continuum limit, giving:

$$I_l(\Phi) = \frac{2}{L} \left( \langle K_l \rangle + \frac{2\pi N \Phi}{L} \phi_0 \right) \quad (2.6)$$

$$\langle K_l \rangle = \sum_{k_1 \ldots k_N} \left( \sum_{i=1}^N k_{l,i} \right) |\Psi_{k_1 \ldots k_N}|^2. \quad (2.7)$$

$\langle K_l \rangle$ is the $l$-component of the total GS momentum $\langle \mathbf{K} \rangle$. A similar expression can be obtained [2] for the transverse component of $\mathbf{I}(\Phi)$. Since $\langle \mathbf{K} \rangle$ is conserved when $U$ varies for $W = 0$, $\mathbf{I}$ is
Fig. 1. Upper left: Lattice and continuum regimes without disorder (\(W = 0\)) in the \((s/a_B^i, a/a_B)\) plane. The lattice model behaves as in the continuum limit in the non-shaded part. \(r_r^* = 0.55(s/a_B^i)^{4/3}\) above \(r_r^* \approx 37\), and \(r_r^* = s/a_B^i + O(s/a_B^i)^3\) below \(r_r^*\). The double arrows correspond to typical Ga-As heterostructures, cuprate oxides and layered sodium cobalt oxides \(\text{Na}_x\text{CoO}_2\). Upper right: Change in \(E_0(r_\ell)/\Delta E_0(r_\ell = 0) \propto L_1\) of the GS energy after a twist \((\text{periodic} \rightarrow \text{antiperiodic})\) of the longitudinal SC for \(L = 6\) (\(\square\)), 9 (\(\circ\)), 12 (\(\triangle\)), 15 (\(\circ\)), 18 (\(\circ\)) and \(N = 3\) as a function of \(r_\ell\). Lower left: Energy ratio \(F_{N=3}(L, U, t)\) as a function of \(r_\ell = U L/t\) given for \(L = 6\) (\(\circ\)), 9 (\(\square\)), 12 (\(\triangle\)), 15 (\(\triangle\)), 18 (\(\circ\)). The dotted-dashed line \(0.2327 \sqrt{r_\ell}\) (behavior expected for a continuum Wigner molecule) intersects the limiting dashed lines \(12 L / (4t - 4t \cos(2\pi / L))\) at \(r_\ell^*(L)\). Inset: A GS configuration when \(t = 0\) and \(L = 24\). Lower right: Lattice and continuum regimes with disorder in the \((U/t, W/t)\) plane detected using \(N = 3\) spinless fermions. The shaded part gives the continuum regimes. The thick dashed lines give the threshold values \(W_{\text{stripe}}\) and \(W_{\text{loc}}\) and \(W_{\text{glass}}\) separating different lattice regimes.

**2.2 Lattice limit to the continuum zero point motion**

From the lattice GS energy \(E_0(L, U, t)\) of total momentum \(K = 0\), we define the dimensionless ratio:

\[
F_{N=3}(L, U, t) = \frac{E_0(L, U, t) - E_0(L, U, t = 0)}{E_0(L, U = 0, t)} ,
\]

Fig. 2. Sketches of the hopping processes characterizing the three lattice regimes of a weakly disordered lattice when $U > U^*$ ($L = 6$ and $N = 3$). From left to right: Ballistic Wigner molecule (BWM) for $U < U^*$; Coulomb Guided Stripe of Current (CGSC) for $U_{\text{stripe}} < U < U_{\text{loc}}$; and one particle motion out of a Localized Wigner Molecule (LWM) above $U_{\text{loc}}$.

which gives the change of the GS energy from the Coulomb energy due to the quantum effects, in units of the kinetic energy at $U = 0$. In Fig. 1 (lower left), one can see that the values of $F_{N=3}(L,U,t)$ calculated for different $L$ scale onto a universal continuum curve below a lattice threshold $r^*_L(L)$. For intermediate values of $r_L$, the lattice data agree with $F_{N=3} \approx 0.2327\sqrt{t}$ obtained [3] using a continuum strong coupling expansion (Eq. 2.2 with numerical factors re-calculated for $N = 3$), before saturating to $4Nt/E_0(L,U = 0,t)$ above $r^*_L(L)$ (dashed lines). Therefore $r^*_L$ corresponds also to the value of $UL/t$ where the quantum zero point energy of the crystal reaches the lattice limit $4Nt$. This criterion yields [3] $r^*_s = 0.55(s/a_0)^{2/3}$ (see Fig. 1 (upper left)) in the thermodynamic limit.

3 EFFECTS OF WEAK RANDOM POTENTIALS

3.1 Lattice regimes

When weak random potentials are added ($W \neq 0$), new regimes can be detected using the current $I$ driven by a flux $\Phi$ enclosed along the longitudinal $x$-direction. Fig. 1 (lower right) shows where these regimes are located in the plane $(U/t, W/t)$. Let us begin with three lattice regimes occurring when $U > U^*$. The corresponding processes yielding different effective hopping terms $t_{\text{eff}}$ are sketched in Fig. 2. The first one ($U^* < U < U_{\text{stripe}}$) characterizes the motion of the center of mass of a Ballistic Wigner molecule (BWM) in the clean limit. When $U_{\text{stripe}} < U < U_{\text{loc}}$, a different collective motion is yielded by disorder, where $I$ does not flow along the shortest path enclosing $\Phi$, but along the axes of the pinned Wigner molecule (a diagonal path when $N = 3$) enclosing $\Phi$. Above $U_{\text{loc}}$, a strongly Localized Wigner Molecule (LWM) gives mainly rise to exponentially small one particle currents enclosing $\Phi$ along the shortest paths. The dependence of the corresponding effective hopping terms $t_{\text{eff}} \propto I$ as a function of the lattice parameters $U, W, t, L$ reads [2] respectively:

\begin{align*}
    t^\text{BWM}_{\text{eff}} & \propto \frac{t^N}{U^{N-1}}L^{3N-3} \quad \text{for } U < U^* < U_{\text{stripe}} \quad (3.1) \\
    t^\text{CGSC}_{\text{eff}} & \propto \frac{(t^\text{BWM}_{\text{eff}})^{2L+3}}{\sqrt{NW}L^{2L+3-1}} \quad \text{for } U_{\text{stripe}} < U < U_{\text{loc}} \quad (3.2) \\
    t^\text{LWM}_{\text{eff}} & \propto \frac{t^LL^{3L-3}}{UL^{-1}} \quad \text{for } U > U_{\text{loc}}. \quad (3.3)
\end{align*}

The dependence of the total longitudinal current $I_{\text{eff}} \propto t_{\text{eff}}$ is shown as a function of $U$ in Fig. 3 (left), with the power-law decays implied by Eqs. 3.1, 3.2 and 3.3 when $N = 3$, $L = 6$, $t = 1$.
3.2 Continuum regimes

As shown in Fig. 3 (middle and right), the disorder induced CGSC-regime persists in the continuum limit, at a weaker value of $U \approx 50$ where one can see in Fig. 3 (left) that $I$ is independent of $U$ instead of exhibiting a lattice decay. The occupation numbers $n_0^j$ form an extended diagonal stripe, instead of being localized upon three main sites, as in the CGSC lattice regime.

4 SUPERSOLID

When we continue to decrease $U$, to eventually get a Fermi glass of three independent particles, the diamagnetic $I$ becomes paramagnetic below an interaction $U_{lc}$. Around $U_{lc}$, the local currents continue to exhibit a quasi 1d topology, as shown in Fig. 3 (middle) and in Fig. 4 (right). Extending Leggett’s 1d rule to quasi-1d, one can argue [2] that a diamagnetic current stripe is carried by an odd number of particles ($N = 3$), while the paramagnetic current stripe observed below $U_{lc}$ is due to a single delocalized pair ($N = 2$ even) in the background of an almost localized third particle. The quantum melting seems to proceed through an intermediate regime, where a correlated pair co-exists with an almost independent particle. This is reminiscent of the supersolid proposed in Ref. [4].

A supersolid regime can also be detected in the clean limit ($W = 0$) by the following argument. If the relative motions remain localized over scales smaller than $D = Ls$, one can show in the strong coupling limit that the continuum GS energy $E_0(K)$ depends on the total momentum $K$ only through a contribution $E_{cm}(K)$ coming from the motion of the center of mass. We show in Fig. 4 (right) the GS energies $E_0(K) - E_{cm}(K) - E_{Coul}$ as a function of $r_s$, for $W = 0$, $N = 3$, $L = 18$ and different momenta $K$. The solid line gives the behavior ($0.139 \sqrt{r_s}$) implied [2] by the continuum strong coupling expansion assuming small relative motions. This theory is only accurate for $r_s^W < r_s < r_s^*(L)$. Below $r_s^W \approx 50$, the $E_0(K)$ are roughly described above $r_s^* \approx 10$ by the previous theory, but with $K$-dependent corrections. This shows that
Fig. 4. Left: Map of currents for $\Phi = 0.05\Phi_0$ observed below the paramagnetic-diamagnetic crossover ($U < U_{lc}$) in a disordered sample with $N = 3$, $L = 9$, $W = 1$, $t = 1$ and $U = 7$. Middle: Corresponding site occupation numbers $n_0^j$. The left and middle figures are now disconnected, flowing mainly perpendicularly to the axis where the $n_0^j$ are maxima. Same conventions than in Fig. 3. Right: The GS-energies $E_0(K) - E_{cm}(K) - E_{Coul}$ for different total momenta $K$ as a function of $r_s$ ($W = 0$, $L = 18$ and $N = 3$). For $r_s^W < r_s < r_s^*$ the behavior is described by the usual strong coupling continuum expansion (solid line $0.139\sqrt{r_s}$).

the relative motions are delocalized over a scale $\approx D$ below $r_s^W$. Large zero-point motions are the signature of a supersolid [4, 7]. This intermediate supersolid was previously discussed in Ref. [5, 6] in a limit where the lattice effects play a role ($L = 6$). These results for $L = 18$, where the Wigner molecule can be described by a continuum theory give further support to the existence of a supersolid for $r_s^F < r_s < r_s^W$, i.e. for intermediate values of $r_s$ where a 2d-metal is observed [1]. In the continuum limit, the Wigner crystal is believed to become a quantum liquid below $r_s^W \approx 37$ (without disorder). This belief comes from fixed node quantum Monte-Carlo studies [8], where the GS nodal structure is given by an ansatz. Recently, a novel ansatz has been studied [9], built from the extended Bloch waves of an attractive potential having the symmetry of the Wigner crystal. This novel ansatz gives a more stable GS than those previously obtained [8] when $31 < r_s < 80$. If there is a supersolid, it is not surprising that a more delocalized ansatz than these previously used to describe a Wigner crystal allows to lower the fixed node GS energy. In conclusion, exact studies of a few particles and fixed node Monte-Carlo studies extrapolated towards the thermodynamic limit give complementary evidences supporting the existence of a new intermediate phase.

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References