MESOSCOPIC WIGNER CRYSTALLIZATION IN TWO DIMENSIONAL LATTICE MODELS

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The quantum-classical crossover from the Fermi liquid towards the Wigner solid is numerically revisited, considering small square lattice models where electrons interact via a Coulomb $U/r$ potential. The studies of models without disorder and spin and including disorder and spin show that the electron solid is formed in two stages, giving rise to an intriguing solid-liquid regime at intermediate couplings.

1 Lattice model

We consider $N$ electrons on $L \times L$ square lattice with periodic boundary conditions (BCs). The Hamiltonian reads

$$\mathcal{H} = \sum_{i,\sigma} (-t \sum_{i',\sigma} c_{i',\sigma}^\dagger c_{i,\sigma} + v_i n_{i,\sigma}) + \frac{U}{2} \sum_{i,\sigma, i'\sigma'} n_{i,\sigma} n_{i',\sigma'} + 2U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

where $c_{i,\sigma}$ ($c_{i,\sigma}^\dagger$) destroys (creates) an electron of spin $\sigma$ at the site $i$ and $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$. The first terms describe the kinetic energy $(\propto -t)$ and the random substrate energy ($\propto v_i$ uniformly distributed inside $[-W/2, W/2]$). The interaction consists of a $U/|i-i'|$ Coulomb repulsion plus a $2U$ Hubbard repulsion. $|i-i'|$ is the smallest distance between the sites $i$ and $i'$ on a square lattice with periodic BCs. In our model, the Coulomb energy to kinetic energy ratio $r_s = U/(2t\sqrt{\pi n_e})$ for a filling factor $n_e = N/L^2$.

$S$ and $S_z$ are the total spin and its component along an arbitrary direction $z$. $\mathcal{H}$ can be written in a block-diagonal form, with $N + 1$ blocks where $S_z = -N/2, \ldots, N/2$ respectively. Assuming $N = 4$ and $L = 6$, the three blocks with $S_z \geq 0$ are diagonalized using Lanczos algorithm to obtain the minimum eigenenergy $E_0(S_z)$ of each block.

2 Spinless fermions without disorder

We begin by studying the ground state (GS) of the block $\mathcal{H}(S_z = 2)$ when $W = 0$. When $U = 0$, the states are $N_H$ plane wave Slater determinants (SDs) $\prod_{p=1}^4 d^\dagger_{k(p)} |0\rangle$, where $d^\dagger_{k(p)}$ creates a particle in a state of momentum $k(p) = 2\pi(p_x, p_y)/L$ and $|0\rangle$ is the vacuum state. The low energy eigenstates are given by: (A) 4 degenerate ground states (GSs) $|K_0(\beta)\rangle > (\beta = 1, \ldots, 4)$ of energy $E_0(U = 0) = -13t$ and of momenta $K_0 \neq 0$; (B) 25 first excitations of energy $E_1(U = 0) = -12t$. (C) 64 second excitations $|K_2(\alpha)\rangle >$ of energy $E_2(U = 0) = -11t$; (D) 180 third excitations $|K_3(\alpha)\rangle >$ of energy $E_3(U = 0) = -10t$ and (E) 384 fourth excitations of energy $E_4(U = 0) = -9t$. We define the 20 plane wave SDs useful to partly describe the intermediate GS. They are given by 4 plane wave SDs $|K_1(\beta)\rangle >$ of energy $-12t$ where the particles have energies $-4t, -3t, -3t, -2t$ respectively, and by 16 plane waves SDs $|K_4(\delta)\rangle >$ of energy $-9t$ where the particles have energies $-4t, -3t, -3t, -2t, 0t$ (first set of 8 SDs) and $-3t, -3t, -2t, -t$ (second set of 8 other SDs) respectively. Those 20 SDs are directly coupled by the pairwise interaction and their momenta are zero ($K = \sum_{p=1}^4 k(p) = 0$).

When $t = 0$, the states are $N_H$ Slater determinants $c^\dagger_{i_1} c^\dagger_{i_2} c_{k} c_{l} |0\rangle$ built out from the site orbitals. The low energy states are the following site SDs: (A) 9 squares $|S_0(I)\rangle > (I = 1, \ldots, 9)$
of side \(a = 3\) and of energy \(E_0(t = 0) \approx 1.80U\); (B) 36 parallelograms \(|S_1(I)\rangle\) of sides \((3, \sqrt{10})\) and of energy \(\approx 1.85U\); (C) 36 other parallelograms \(|S_2(I)\rangle\) of sides \((\sqrt{10}, \sqrt{10})\) and of energy \(\approx 1.97U\) and (D) 144 deformed squares \(|S_3(I)\rangle\) obtained by moving a single site of a square \(|S_I\rangle\) by one lattice spacing and of energy \(\approx 2U\).

Figure 1: UPPER LEFT: Low energy part of the spectrum exhibiting a GS level crossing at \(r_s^F\). Inset: two first level spacings \(\Delta_1/t\) (dashed) and \(\Delta_2/t\) (dotted) which become equal at \(r_s^W\) and the perturbative result \(\Delta_1/t = \Delta_2/t \approx 10392/r_s^3\) valid when \(r_s \to \infty\) (dot-dashed). UPPER RIGHT: GS projections \(P_0(r_s)\) onto a few plane wave SDs, given by the 4 \(|K_0(\beta)\rangle\) (empty circle), the 4 \(|K_1(\beta)\rangle\) (empty square), the 64 \(|K_2(\alpha)\rangle\) (filled diamond), the 180 \(|K_3(\delta)\rangle\) (\(\times\)), the 16 \(|K_4(\delta)\rangle\) (asterisk) respectively. LOWER LEFT: GS projection \(P_\infty(r_s)\) onto a few site SDs, given by the 9 squares \(|S_0(I)\rangle\) (filled square), the 36 parallelograms \(|S_1(I)\rangle\) (asterisk), the 36 parallelograms \(|S_2(I)\rangle\) (diamond), and the 144 deformed squares \(|S_3(I)\rangle\) (left triangle) respectively. LOWER RIGHT: GS projection \(P_0^F(r_s)\) (asterisk) and \(P_\infty^W(r_s)\) (empty square) and total GS projection \(P\) (filled circle) onto the re-orthonormalized basis using the low energy eigenvectors of the two limiting bases.

For the first low energy states, the crossover from the \(U = 0\) eigenbasis towards the \(t = 0\) eigenbasis is shown in Fig. 4 (upper left) when one increases the ratio \(r_s\). If we follow the 4 GSs \(E_0(r_s = 0)\) \((K_0 \neq 0)\), one can see a first level crossing at \(r_s^F \approx 9.3\) with a non degenerate state \((K_0 = 0)\) which becomes the GS above \(r_s^F\), followed by two other crossings with two other sets of 4 states with \(K_I \neq 0\). When \(r_s\) is large, 9 states coming from \(E_1(r_s = 0)\) have a smaller energy than the 4 states coming from \(E_0(r_s = 0)\). The degeneracies ordered by increasing energy become \((1, 4, 4, 4, \ldots)\) instead of \((4, 25, 64, \ldots)\) for \(r_s = 0\). These 9 low energy states give the 9 square molecules \(|S_0(I)\rangle\) when \(r_s \to \infty\). When \(r_s^{-1}\) is very small, the first 9 states correspond to a solid molecule free to move on a restricted \(3 \times 3\) lattice, with an effective hopping term \(T \propto tr_s^{-3}\). This gives 9 states of kinetic energy given by \(-2T(\cos K_I(I) + \cos K_I(I))\) with \(K_I(I) = 2\pi p_I/3\) and \(K_I(I) = 2\pi p_I/3\) \((p_I = 1, 2, 3)\). This structure with degeneracies 1, 4, 4 respectively and two equal energy spacings \(\Delta_1\) and \(\Delta_2\) appears (inset of Fig. 4 upper left) when \(r_s\) is larger than the crystallization threshold \(r_s^W \approx 28\). The two characteristic thresholds \(r_s^F\) (level crossing) and \(r_s^W\) (9 first states having the structure of the spectrum of a single solid molecule free to move on a
3 \times 3 \text{ square lattice) can also be detected by other methods given in Ref. [1].}

To understand further the nature of the intermediate GS between $r_s^F$ and $r_s^W$, we have projected the GS wave functions $|\Psi_0(r_s)\rangle$ over the low energy eigenvectors of the two eigenbases valid for $U/t = 0$ and for $t/U = 0$ respectively. Let us begin with the $U = 0$ eigenbasis. Below $r_s^F$, each of the 4 GSs $|\Psi_0^\alpha(r_s)\rangle$ with $K_0 \neq 0$ has still a large projection $P_0(r_s,0) = \sum_{\beta=1}^4 |<\Psi_0^\beta(r_s)|K_0(\beta)>|^2$ over the 4 non interacting GSs. There is no projection over the 25 first excitations and smaller projections $P_0(r_s,2)$ and $P_0(r_s,3)$ over the 64 second and 180 third excitations of the non interacting system. Above $r_s^F$, the non degenerate GS with $K_0 = 0$ has a large projection

$$P_0(r_s,1) = \sum_{\beta=1}^4 |<\Psi_0(r_s)|K_1(\beta)>|^2$$

which is equally distributed over the 4 excitations $|K_1(\beta)>$ of momentum $K_1 = 0$ and a second significant contribution

$$P_0(r_s,4) = \sum_{\delta=1}^{16} |<\Psi_0(r_s)|K_4(\delta)>|^2$$

given by its projection onto the 16 mentioned plane wave SDSs $|K_4(\delta)>$ of energy $-9t$. Above $r_s^F$, its projections onto the 4 $|K_0(\beta)>$, the 21 other first excitations and the second and third excitations of the non interacting system are zero or extremely negligible. The total GS projection $P_0^s(r_s) = P_0(r_s,1) + P_0(r_s,4)$ onto the 4 $|K_1(\beta)>$ and 16 $|K_4(\delta)>$ is given in Fig. 1 (lower right) when $r_s > r_s^F$. This shows us that a large part of the system remains an excited liquid above $r_s^F$.

We now study the GS projections $P_\infty$ onto the $t = 0$ eigenbasis. The GS projection

$$P_\infty(r_s,0) = \sum_{I=1}^9 |<\Psi_0^\alpha(r_s)|S_0(I)>|^2$$

onto the 9 square site SDSs $|S_0(I)>$ is given in Fig. 1 (lower left), together with the GS projection $P_\infty(r_s,J)$ onto the site SDSs corresponding to the $J^{th}$ degenerate low energy excitations of the $t = 0$ system. The total GS projection $P_\infty^s(r_s) = \sum_{p=0}^4 P_\infty(r_s,p)$ onto the 9 squares $|S_0(I)>$, the 36 parallelograms $|S_1(I)>$, the 36 other parallelograms $|S_2(I)>$ and the 144 deformed squares $|S_3(I)>$ is given in Fig. 1 (lower right) when $r_s > r_s^F$. This shows us that the ground state begins to be a floppy solid also above $r_s^F$.

The site SDSs and plane wave SDSs are not orthonormal. After re-orthonormalization, the total projection $P$ of $|\Psi_0(r_s)>$ over the subspace spanned by the 4 $|K_1(\beta)>$ and 16 $|K_4(\delta)>$ and 225 site SDSs of lower electrostatic energies are given in Fig. 1 (lower right), showing that $|\Psi_0(r_s)>$ is almost entirely located inside this very small part of a huge Hilbert space for intermediate $r_s$, spanned by low energy SDSs of different nature, and adapted to describe a solid entangled with an excited liquid.

3 Magnetization and polarization energies in presence of a random substrate

We now consider weakly disordered samples when the spin degrees of freedom are included. Their role and the consequences of an applied parallel magnetic field which aligns only the spins without inducing orbital effects, have been the subject of Ref. [2]. The study of a statistical ensemble of samples with $W = 5$, $N = 4$ and $L = 6$ provides complementary signatures of a particular intermediate behavior. Let us note $M$ the fraction of clusters with $S = 1$ at $B = 0$, $Q_2 = E_0(S_z = 2) - E_0(S_z = 0)$ and $Q_1 = E_0(S_z = 1) - E_0(S_z = 0)$ the Zeeman energies necessary to yield $S = 2$ and $S = 1$ respectively for a cluster with $S = 0$. 
In Fig. 2, $M$ is given as a function of $r_s$. One can see a first threshold at $r_s \approx 0.35$ where the interaction can drive $S = 1$ in certain samples. Above a second threshold $r_s^{FS}$, $M$ regularly decreases to reach a zero value at a third threshold $r_s^{WS} \approx 9$ where an antiferromagnetic square molecule is formed. The ensemble averages $<\log Q_1>$ and $<\log Q_2>$ (without taking into account the $S = 1$ spontaneously magnetized clusters) define the typical fields $B$ necessary to yield $S = 1$ or $S = 2$ in a $S = 0$ cluster. In Fig. 2, one can see an intermediate regime again for $r_s^{FS} < r_s < r_s^{WS}$ where $<\log Q_1>$ becomes roughly independent of $r_s$, while $Q_2 \propto r_s^{-2}$.

4 Conclusion

One concludes that mesoscopic Wigner crystallization proceeds in two stages. In a clean system, a minimal description of the intermediate GS requires to combine the low energy states of the two limiting eigenbases. In this sense, the intermediate GS is neither solid, nor liquid, but rather the quantum superposition of those two states of matter. This is strongly reminiscent of the conjecture proposed by Andreev and Lifshitz for the quantum melting of a solid. A path integral Monte Carlo approach has recently shown that a few electrons confined in a harmonic trap crystallize also in two stages, firstly via a radial ordering of electrons on shells and secondly via the freezing of the intershell rotation. As one can see, a two stage crystallization is not only characteristic of a mesoscopic harmonic trap, but also occurs in a mesoscopic 2$d$ torus. To add a random substrate defavors the liquid state. The magnetization gives also the signature of an intermediate regime where Stoner ferromagnetism is defavored by Wigner antiferromagnetism.

References

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