Wigner crystal versus fermionization for one-dimensional Hubbard models with and without long-range interactions

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Abstract

The ground state properties of the Hubbard model with or without long-range interactions in the regime with strongly repulsive on-site interactions are investigated by means of the exact diagonalization method. We show that the appearance of \(N\)-crests in the density profile of a trapped \(N\)-fermion system is a natural result of ‘fermionization’ between antiparallel-spin fermions in the strongly repulsive limit and cannot be taken as the only signature of the Wigner crystal phase, as the static structure factor does not show any signature of crystallization. In contrast, both the density distribution and the static structure factor of the Hubbard model with strong long-range interactions display clear signatures of the Wigner crystal phase. Our results indicate the important role of long-range interaction in the formation of the Wigner crystal phase.

(Some figures may appear in colour only in the online journal)

1. Introduction

The Hubbard model has been widely used as a minimal model to describe strongly interacting electrons in a solid and plays a particularly important role in understanding the physics related to the quantum magnetism and high-temperature superconductivity. Recent experimental progress in trapping the quantum gas in an optical lattice [1–3] has renewed the interest in this basic model [4, 5]. In comparison with real materials in solid form, the fermionic quantum gas trapped in an optical lattice is a more ideal realization of the Hubbard model [2], which provides a laboratory to simulate and study this basic quantum many-body system from different aspects. In particular, current experimental techniques have also prompted intensive study of quantum many-body systems in reduced one-dimensional (1D) systems, among which important benchmarks include the experimental realization of Tonks–Girardeau (TG) gases [6, 7], and the Mott transition in 1D tight tubes [8]. Furthermore, the recent experimental realization of two-component Fermi gases in a quasi-1D geometry with tunable interaction strengths by Feshbach resonance [9] provides a unique possibility to experimentally study the 1D Hubbard model even in the strong interaction limit. The good tunability of optical lattices enables us to experimentally elucidate the subtleties of 1D quantum many-body systems, for example, the physical properties in the strongly interacting limit. Due to recent experimental progress on chromium atoms [10, 11] and heteronuclear polar molecules produced by the stimulated Raman adiabatic passage technique [12, 13], dipolar atomic systems with strong long-range dipole–dipole interactions (DDIs) have also attracted intensive studies [14–19]. In addition, schemes to create Coulomb-like interactions in cold atom systems have also been proposed [20, 21].

In the presence of long-range repulsive interaction, an interesting issue for the 1D fermionic system is the existence of the Wigner crystal phase [22]. For a 1D gas of electrons with long-range Coulomb interaction,
which has been investigated by Schulz in the scheme of bosonization [22], the extremely slow decay of density correlations at wavevector $4k_F$ has been used as a signature for the appearance of the Wigner crystal phase. Here $k_F = \pi n$ is the Fermi wavevector with $n$ the particle density. After that, exploration of the Wigner crystal phase in short-range interacting fermion systems, for example the Hubbard model, has also been carried out [23–26]. By using bosonization and density matrix renormalization group methods to study one-dimensional finite Hubbard chains with hard-wall boundaries, a crossover from $2k_F$- to $4k_F$-density oscillations with increasing repulsion has been found [23, 24], and sometimes the $4k_F$ density oscillations have been taken as a signature of the emergence of the Wigner crystal phase. In the limit of infinitely strong interactions, the on-site repulsion imposes an effective Pauli principle between fermions with different spins. Consequently, the ground state in the strong repulsion limit is degenerate for states with different spin configurations [27–29], and thus the ground state density distribution of an equally mixed trapped system is identical to the fully polarized system with the appearance of doubling of the crests in the density profiles. Such a phenomenon, which is also referred to as fermionization, was recently observed by an experiment in a two-particle system with tunable interaction using two fermionic $^6$Li atoms [30].

As the density distribution is not solely a convincing criterion for the Wigner crystal phase, the density–density correlation function plays an important role in characterizing it [31]. In this work, we shall study both the density distribution and the density correlation function of the Hubbard model either without or with long-range interactions. For the Hubbard model with only short-range interactions, we find that the density correlation function does not show any signature of Wigner crystal correlations in spite of the fact that the ground state density profile displays pronounced $4k_F$ Wigner oscillations in the strong repulsion limit. To unveil the role of the interaction range, we then study the Hubbard model with additional long-range interactions and compare the calculated results with those of the Hubbard model. We find that the system with long-range interactions indeed exhibits quite different behavior from that of the short-range Hubbard model. In particular, clear evidence in the static structure factor indicates the important role of the long-range interactions in the formation of the Wigner crystal phase.

The remainder of the paper is organized as follows. In section 2, we introduce our studied models and main conclusions based on the calculation of models. In section 3, we present our calculation results for density distributions and static structure factors, in sections 3.1 and 3.2 for the Hubbard model and the Hubbard model with additional long-range interactions, respectively. A summary is given in section 4.

2. Model Hamiltonian

The basic model describing the short-range interacting fermions in a 1D lattice is the Hubbard model [32]

$$H = -t \sum_{n} \hat{c}^\dagger_{i\sigma} \hat{c}_{i+1\sigma} + \text{H.c.} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$  

(1)

where $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) is the creation (annihilation) operator of the fermion with the spin $\sigma$, $\hat{n}_{i\sigma} = (\hat{c}_{i\sigma} \hat{c}^\dagger_{i\sigma})$ is the spin-up (down) particle number operator, $t$ is the hopping strength which is set to unity, and $U$ is the on-site interaction strength. The 1D Hubbard model can be realized by trapping a two-component Fermi gas in a deep 1D optical lattice.

To study the long-range interactions, we consider the following Hamiltonian:

$$H = -t \sum_{n} \hat{c}^\dagger_{i\sigma} \hat{c}_{i+1\sigma} + \text{H.c.} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \frac{1}{2} V \sum_{i \neq j} \frac{\hat{n}_{i} \hat{n}_{j}}{|i-j|^\alpha},$$  

(2)

with $V$ the strength of the long-range interaction and $\alpha$ the decaying exponent. For dipolar atoms confined in a 1D optical lattice, the dipole–dipole interaction decays as $1/|i-j|^3$ with the exponent $\alpha = 3$ [19], whereas $\alpha = 1$ corresponds to an electron system with long-range Coulomb interaction. In this work, we consider the case with a repulsive on-site interaction $U > 0$ and a repulsive long-range interaction $V > 0$.

In the following section, we shall first calculate the density distribution and the density–density correlation function for the Hubbard model (1) with the on-site interaction strength varying from the weak to the strong repulsion limit by an exact diagonalization method. In order to see the oscillation of the density profile, we shall use an open boundary condition (OBC) in the calculation of the density distribution, whereas a periodic boundary condition (PBC) will be used in the calculation of the structure factor, where for the case of the PBC, the distance of the long-range interaction should be $\min(|i-j|, L-|i-j|)$. In the limit of $U \to \infty$, the total ground state density distribution with different spin configurations is identical to that of the polarized noninteracting fermions, despite the fact that the spin-dependent densities are different. This is consistent with the exact result obtained via the exact construction of the many-body wavefunction [29]. Our numerical diagonalization results also show that the structure factor, which is the Fourier transform of the density–density correlation function, in the infinite repulsion limit also displays the same behavior as the fully polarized fermions. These results suggest that the appearance of the doubling of peaks of the equally mixing system (or $4k_F$ Wigner oscillation) in the infinite repulsion limit cannot be taken as a hallmark of the emergence of the Wigner crystal phase. It is just a kind of ‘fermionization’ between fermions with different spins as a result of the effective Pauli principle imposed by the infinite repulsion.

The absence of the Wigner crystal phase in the short-range Hubbard model implies that the long-range interaction may play a very important role in the formation of the Wigner crystal phase. To unveil its role, we then calculate the density distribution and the density–density correlation function for the Hubbard model with the additional long-range interaction described by the Hamiltonian (2). For convenience, we shall focus our calculation on the case with $\alpha = 1$ for which the long-range interaction decays more slowly than the dipole–dipole interaction. Keeping the
on-site interaction fixed, we find that the Wigner crystal phase emerges with increase of the long-range interaction strength $V$. Finally, we also calculate the case with $\alpha = 3$, which exhibits similar behavior to the case of $\alpha = 1$.

3. Results and discussion

3.1. The Fermi–Hubbard model

We first calculate the ground state density distribution $n_i = n_{\uparrow i} + n_{\downarrow i}$ of the Fermi–Hubbard model (1) under the OBC, where $n_{\sigma i} = \langle \hat{n}_{\sigma i} \rangle$ is the spin-dependent ground state density distribution. In figure 1, we show the density profiles $n_i$ and $n_{\sigma i}$ versus different $U$ for the balanced Fermi–Hubbard model (1) with $N_\uparrow = N_\downarrow = 3$ and the lattice size $L = 24$. For the balanced case, we always have $n_\uparrow = n_\downarrow = n_i/2$. In the limit of $U \to 0$, we have $n_{\sigma i} = \sum_{\nu}^{N_{\sigma}} |\psi_{\nu}(i)|^2$, where $\psi(i) = \sqrt{\frac{2}{L+1}} \sin(\frac{\pi L + 1}{L+1} i)$ is the $i$th single particle wavefunction of the open tight binding chain [33], which fulfils the OBC $\psi(0) = \phi_L(L+1) = 0$. It is obvious that there are three crests in the density distribution of $n_i$ for $N_\uparrow = N_\downarrow = 3$ in the weakly interacting limit. As the interaction strength $U$ keeps increasing, the density distribution clearly displays six crests for $U = 10$. In the limit of $U \to \infty$, we have $n_i = \sum_{\nu}^{N} |\psi_{\nu}(i)|^2$ with $N = N_\uparrow + N_\downarrow$ for different spin configurations according to the exact construction of the many-body wavefunctions [29] due to the induced Pauli exclusion principle between antiparallel spins. As shown in figure 1, the total density profile for $U = 200$ obtained by the exact diagonalization method is completely overlapped with the exact result in the strongly interacting limit. For the imbalanced case with $N_\uparrow = 2, N_\downarrow = 4$ and $L = 24$, we show the change of density profiles of the Hubbard model with the increase of $U$ in figure 2. Despite the fact that we now have $n_\uparrow \neq n_\downarrow$, the total density distribution also clearly displays six crests for $U = 10$. Also, the total density profile for $U = 200$ coincides with the density profile of the fully polarized system. Our numerical results clearly show that the total density distributions of the interacting fermion systems with different spin configurations are identical in the limit of infinite repulsion [29].

Next we calculate the static structure factor, which is defined as the Fourier transform of the density–density correlation function,

$$S(k) = \frac{1}{L} \sum_{i,j \neq i} e^{i(k-j)} \langle [\hat{n}_i \hat{n}_j] - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle \rangle,$$

(3)

where $k = 2m\pi/L$ with $m = 0, 1, \ldots, L$. In general, the Wigner crystal phase can be characterized by the enhancement of the $4k_F$ peak in the static structure factor. In figure 3(a), we show the change of the static structure factor with the increase of the interaction strength $U$ for the case of $N_\uparrow = N_\downarrow = 3$ and $L = 24$ under the PBC. The imbalanced case of $N_\uparrow = 2$ and $N_\downarrow = 4$ is shown in figure 3(b). For both cases, when $U$ is large enough (for example, $U = 200$), the distribution of the static structure factor approaches the distribution function of a fully polarized $N$-particle free fermion system, as shown in figure 3(c). Except for the drops at $kL/(2\pi) = N, L - N$, no obvious peaks in the static structure factor are detected. Our numerical results clearly indicate that just the appearance of $N$ peaks in the ground state density profile of the finite trapped Hubbard system shown in [23–26] cannot be taken as a mark of the emergence of the Wigner crystal phase in the strongly
Figure 2. The density distribution of the Hubbard model for different $U$ with $N^\uparrow = 2, N^\downarrow = 4$ confined in a lattice with $L = 24$ under the open boundary condition. Here, the square is for $n_i$, the circle is for $n_i^\uparrow$, and the triangle is for $n_i^\downarrow$. The density $n_i$ for $U \to \infty$ is shown in (d) marked by hollow inverted triangles.

Figure 3. The static structure factor $S(k)$ versus $kL/(2\pi)$ for different $U$ with the periodic boundary condition: (a) is for $N^\uparrow = N^\downarrow = 3, L = 24$; (b) is for $N^\uparrow = 2, N^\downarrow = 4, L = 24$; and (c) is for the polarized free fermion system with $N = 6$ and $L = 24$.

3.2. The Hubbard model with long-range interaction

Now we study the Hamiltonian of the Hubbard model with long-range interaction (2). For the case of $V = 0$, the ground state properties of the system have almost no change with increase of the on-site interaction strength when the $U$ is large enough. In order to explore the effect of the long-range interaction, we shall keep $U$ fixed as $U = 200$ and change $V$ in the following calculation. For simplicity, we focus our discussion on the case of $\alpha = 1$, and finally discuss the case of $\alpha = 3$ briefly.

In figure 4, we show the density distribution for the long-range Hubbard model with $\alpha = 1, N^\uparrow = N^\downarrow = 3$, and $L = 24$ under the OBC. At $V = 0$, six crests have already appeared for $U = 200$. Nevertheless, with the increase of $V$, the particles move away from each other as far as possible to minimize the total energy. As shown in figure 4, very sharp peaks have emerged for $V = 50$ and the height of the peaks increases with increase of $V$. In contrast to the case of $V = 0$ with only small oscillations, the density profile of the system with large $V$ resembles six well-separated localized wave packets which are uniformly distributed. The density oscillation in [23–26] corresponds to the density distribution with $V = 0$ shown in figure 4, which shows no sharp peaks and is very similar to the density distribution of fully polarized fermions.

To characterize the Wigner crystal phase, we further calculate the static structure factor of the system with $L = 24, N^\uparrow = N^\downarrow = 3$ under the PBC. As shown in figure 5(a), obvious peaks have already emerged at $kL/(2\pi) = N, L - N$ for $V = 5$. As $V$ keeps increasing, the height of the peaks increases further and a new peak emerges at $kL/(2\pi) = 2N$. In figure 5(b), we calculate the static structure factor for a system with $L = 32, N^\uparrow = 1, N^\downarrow = 3$ under the PBC. Similarly, as the long-range interaction keeps increasing, a series of peaks emerges at $kL/(2\pi) = mN$ with $m$ an integer. We also
Figure 4. The density distribution of the Hubbard model with long-range Coulomb interaction for different $V$ with $U = 200$, $N_\uparrow = N_\downarrow = 3$, and $L = 24$ under the open boundary condition.

Figure 5. The static structure factor $S(k)$ versus $kL/2\pi$ for systems with $U = 200$ and different $V$ under the periodic boundary condition: (a) is for $L = 24$, $N_\uparrow = N_\downarrow = 3$; (b) is for $L = 32$, $N_\uparrow = 1, N_\downarrow = 3$.

demonstrate data for the static structure factor $S(k)$ versus $k/(n\pi)$ in figure 6 for systems with $L = 24$, $N_\uparrow = N_\downarrow = 3$ under the OBC. The static structure factors of the same system with the PBC are plotted in figure 7(b). It is obvious that both the density profiles and the static structure factors display very similar behavior to that of the system with $\alpha = 1$. A quantitative difference is that the height of the peaks in figures 7(a) and (b) is lower than that of the corresponding system with Coulomb interaction shown in figures 4 and 5(a), as the long-range dipole–dipole interaction decays much faster than the Coulomb interaction. Despite the minor differences, our calculated results indicate the existence of the Wigner crystal phase for the Hubbard model with strong dipole–dipole interactions.

As a comparison, we also study the extended Hubbard model described by

$$H = -t \sum_{\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{i+1\sigma} + \text{H.c.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i+1,\downarrow},$$

(4)

where only the nearest neighbor short-range interaction is considered. The density profiles and static structure factors of the extended Hubbard model with $L = 24$, $N_\uparrow = N_\downarrow = 3$ are shown in figures 7(c) and (d), respectively. For $V = 50$, we observe that the oscillations in the density distribution of the extended Hubbard model are enhanced, but the wave packets are still overlapping, which is quite different from the density profile of the dipolar system with well-separated localized wave packets. With further increase of the nearest neighbor interaction, no obvious change is found. The static structure factors also exhibit different behavior from the long-range interacting system. As shown in figure 7(d), only small peaks emerge at $kL/2(\pi) = N, L - N$ for $V = 50$ and the height of the peaks does not change obviously with further increase of $V$. The absence of peaks at $kL/(2\pi) = 2N$ implies that the crystal phase is not detectable. The different behavior exhibited in systems with short-range and long-range interactions indicates the important role of the long-range interaction in the formation of the Wigner crystal phase. Incidentally, the phase diagram for the extended Hubbard model is...
model with half filling is studied widely [34–38]. The phase transition point between the spin density wave (SDW) and the charge density wave (CDW) is $2V = U$ for large $U$, $V$. Also, we can find that for large $U$, the quarter-filled system undergoes a transition from a Luttinger-liquid phase to a CDW under the open boundary condition. At a lower filling factor, a good approximation for a large repulsive interaction $U$, $V$, it is equivalent to the $N$ spinless fermions moving at $L - N$ lattice sites [40].

To get a straightforward understanding of the crystal phase of the Hubbard model with long-range interactions, we consider the atomic limit ($t = 0$) of the system with $L/N = 1/n = \gamma$ under the PBC. In the atomic limit, for the case of $V < U$ and $\gamma$ being an integer larger than 1, the ground states $|\psi_{0\alpha}\rangle$ correspond to the configurations with no more than two particles in the consecutive $\gamma$ sites, where \( \alpha = 1, 2, \ldots, \gamma C_N^{N/\gamma} \) is for the different configurations of the degenerate ground states. The degeneracy is derived from two parts, one is the translation invariance due to the PBC and the other comes from indistinguishable spin configurations. The eigenenergy of $H_0 = U\sum_{\alpha}n_{\alpha}n_{\alpha} + \frac{1}{2}V\sum_{\alpha\neq \beta}n_{\alpha}n_{\beta}(|i - j|^\alpha)$ is $E_0 = V/\{(N/2)^{\gamma - 1}\gamma^{\alpha}\} + NV\sum_{\beta=1}^{N/\gamma - 1}/(\beta \gamma)^{\alpha}$ for even $N$ and $E_0 = NV\sum_{\beta=1}^{(N-1)/2}/(\beta \gamma)^{\alpha}$ for odd $N$. To account for the first order perturbation of the hopping term, we also consider the states $|\psi_{0\mu\nu}\rangle$ that are obtained from $|\psi_{0\alpha}\rangle$ with one of the particles hopping to the next sites and $m = 1, 2, \ldots, 2N$. The expected value of $H_0$ in $|\psi_{0\mu\nu}\rangle$ is $E_1 = \langle \psi_{0\mu\nu} | H_0 | \psi_{0\mu\nu} \rangle = \delta_{\mu1}\delta_{\nu1}(E_0 + E')$, where for $N = \text{even}$

$$E' = \frac{V}{(N/2 \gamma - 1)^{\alpha}} \left( \frac{V}{(N/2 \gamma)^{\alpha}} \right) + NV\sum_{\beta=1}^{N/2 - 1}/(\beta \gamma)^{\alpha} + \frac{1}{(\beta \gamma - 1)^{\alpha}} - \frac{2}{(\beta \gamma)^{\alpha}},$$

and for $N = \text{odd}$

$$E' = NV\sum_{\beta=1}^{(N-1)/2}/(\beta \gamma + 1)^{\alpha} + \frac{1}{(\beta \gamma)^{\alpha}}.$$

The states of $\{ |\psi_{0\mu}\rangle, |\psi_{0\nu}\rangle \}$ form a reduced space. The Hamiltonian $H = H_0 + H'$ in this reduced space is block diagonalization, and the dimension of each block is $2N + 1$, where $H' = -t\sum_{\alpha}(c_{i+1\alpha}^\dagger c_{i\alpha} + \text{H.c.})$ is the perturbation term. We compare the approximate results with the one of exact diagonalization for $N_1 = N_1 = 3$, $L = 24$, $t = 1$, $U = 200$, $V = 150$. The relative error in the energy is about 0.88% for $\alpha = 1$. The obvious peaks are observed at $k/(\pi N) = 2m$ by calculating the static structure factor using the perturbation wavefunctions, characterizing the system in the Wigner crystal regime. However, the approximation does not work well with the same parameters for $\alpha = 3$ (the relative error in the energy is about 27.03%), due to the faster decay
of the dipole–dipole interaction\(^3\). Here, the strength of the interactions between particles with the distance \(\gamma\) has the same order of magnitude as the hopping amplitude, so larger \(U, V\) are needed for our perturbation approach.

4. Summary

In summary, we have studied the ground state properties of finite Hubbard systems either with or without long-range interactions by using the exact diagonalization method. We find that the appearance of \(N\)-crests in the density profile of the Hubbard model in the strongly repulsive limit cannot be taken as the only signature of the Wigner crystal phase, as it is induced by the effective Pauli principle between antiparallel-spin fermions enforced by the infinite repulsion.

The absence of the Wigner crystal phase is clearly verified by the calculation of the static structure factor, which shows the same behavior as the polarized free fermion system with no \(4k_F\) peaks. If the long-range interaction is considered, the Hubbard model with long-range interaction can form a perfect crystalline phase in the regime with strong long-range repulsions. The existence of the Wigner crystal phase can be well characterized by its density distribution and the emergence of a series of peaks in the static structure factor. Our study unveils the important roles of the long-range interactions in the formation of the Wigner crystal phase. In view of the rapid progress in manipulating dipolar atomic systems with tunable interactions, it should be possible to test our results using potential cold atom experiments.

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References

[1] Greiner M, Mandel O, Esslinger T, Hänsch T W and Bloch I 2002 Nature (Lond.) 415 39
[2] Jördens R, Strohmaier N, Günter K, Moritz H and Esslinger T 2008 Nature (Lond.) 455 204–7
[3] Köhl M, Moritz H, Stöferle T, Günter K and Esslinger T 2005 Phys. Rev. Lett. 94 080403
[4] Jakobs D, Bruder C, Cirac J I, Gardiner C W and Zoller P 1998 Phys. Rev. Lett. 81 3108
[5] Hofstetter W, Cirac J I, Zoller P, Demler E and Lukin M D 2002 Phys. Rev. Lett. 89 220407
[6] Paredes B, Widera A, Murg V, Mandel O, Fölling S, Cirac I, Gavrielides P, Mandel O, Nascimbène S and Bloch I 2004 Nature 429 277

\(^3\) For 1D fermionic models, the case of interactions with the \(1/p^2\)-tails has been studied by using the bosonization method [41, 42]. Treating the long-range forward scattering as a perturbation, it is found that the long-range forward scattering for \(\alpha > 1\) is an irrelevant perturbation. We note that the above conclusion is based on the perturbation analysis of the low-energy effective Luttinger-liquid theory with linear dispersion and it does not exclude the possibility of the existence of the Wigner crystal phase in the limit of strong dipole–dipole interaction. Roughly speaking, if \(V/|t| > 3|\gamma|\), the long-range repulsion tends to push the particles away from each other as far as possible and the hopping term cannot destroy the crystal phase.