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Filling dependence of a new type of charge ordered liquid on a triangular lattice system

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Abstract

We study the new characteristic gapless charge ordered state in a spinless fermion system on a triangular lattice under strong inter-site Coulomb interactions. In this state the charges are spontaneously divided into solid and liquid components, and the former solid part aligns in a Wigner crystal manner while the latter moves among them like a pinball. We show that such a charge ordered liquid is stable over a wide range of filling, $1/3 < n < 2/3$, and examine its filling dependent nature.

1. Introduction

Ever since the concept of frustration-induced ‘spin liquids’ has been introduced to the triangular lattice systems [1], the theoretical search for a special state without any types of long range ordering has proceeded in the strongly correlated systems under geometrical frustration [2, 3]. Such liquids are now being explored experimentally in materials like NiGa_2S_4 [4] and $\kappa\text{-ET}_2\text{Cu}_2(\text{CN})_3$ [5]. However, the competition among several orders towards their destruction often makes the system reconcile with another different type of ordering. Simplest examples are the spins on frustrated lattices forming dimers [6], plaquettes [7], etc. Most recent ones are reported on hard core bosons of a nematic ordering in a frustrated square lattice [8] as well as of supersolids in the triangular lattice [9]. We also proposed a frustration induced novel charge liquid in a triangular lattice denoted as a ‘pinball liquid’ [10], which turned out to have very similar character as the above supersolids despite the difference in the statistics. This state has a coexistence of a Wigner crystal type of solid and itinerant liquid type of charges so that a phase separation is expected without any domain structures. In this paper we examine the filling dependent nature of this liquid in detail in the spinless fermion system and confirm the strong coupling picture.

2. Model

The present spinless fermion system is described by the t - V model Hamiltonian,

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left(-tc_i^\dagger c_j + \text{h.c.} + Vn_i n_j \right), \quad (1a)$$

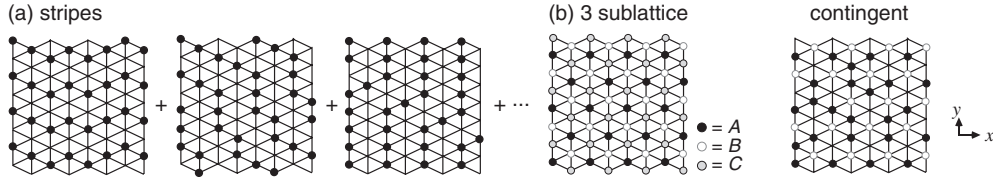


Figure 1. Schematic illustration of the representative classical ground states: (a) twofold stripes, (b) basic three sublattice structure and one of its contingents.

where c_j denotes the annihilation operator of fermions and $n_j (=c_j^\dagger c_j)$ is its number operator. The summation is given over the nearest neighbour (nn) pair sites on a triangular lattice with indices $\langle ij \rangle$. Together with the strong coupling argument, we perform the exact diagonalization on an $N = 4 \times 6$ cluster with periodic boundary conditions, which could fully describe both the threefold and twofold type of periodicity which reside in the present system. Since the size dependence of the energy is confirmed to be very small and also the correlation function shows a well converged character within a relatively short range in comparison with the parallel works [10, 9], the present results are sufficiently qualified to support the physical picture we present.

3. Strong coupling theory

In the strong coupling limit, $t = 0$, the system is identical with the classical Ising $S = 1/2$ spin system on a triangular lattice. The ground state is disordered due to a macroscopic number of degenerate states [12] which are classified into two groups according to their periodicity as shown in figure 1; one portion is composed of twofold striped states which have staggered alignment of charges in any one of three directions but is disordered in other two directions. This state has an order \sqrt{N} degeneracy. The others have a three sublattice structure represented by figure 1(b). Here, as long as A and C sublattices are filled and empty, respectively, the configuration of the B sites is chosen arbitrarily. In addition, there are a large number of contingents which include the irregular structure on A and B sublattices as shown in figure 1(b) but still have the same binding energy. Including all of them, the three sublattices can afford any fillings over $1/3 < n < 2/3$ without changing the binding energy, in sharp contrast to the strictly half-filled stripes.

The introduction of $t \neq 0$ drives the classical disordered system to a new ordered phase, which we call a pinball liquid [10]. For simplicity, we start from the $n = 1/3$ case, which has a well known unique ground state, where only the A-sublattice is filled. Then the extra binding energy $2V$ is required to move a single charge from one of the A sites, thus the ‘pins’ on the A site form a solid. Next we add a single extra charge on one of the empty sites. This charge can move to another nearest empty site without losing the binding energy. Therefore once the filling is off $n = 1/3$, the system discontinuously becomes gapless. The simplest picture of the pinball liquid is that the extra charge moves around like a ‘ball’ avoiding the ‘pins’ on the A sublattice. The kinetic energy gain per single ‘ball’ corresponds to the bandwidth of the honeycomb lattice which is obtained after depleting the A sublattice (pinned sites) from the original lattice. With increasing filling the energy gain will be affected by the correlation among ‘balls’. We plot in figure 2 the estimation of $E_1 = (E_Q - E_C)/N$, where E_Q is numerically obtained by the diagonalization of equation (1a) and the classical binding energy is given by $E_C = 3V N_e$, where N_e denotes the electron number. The kinetic energy gain, $|E_1|$,

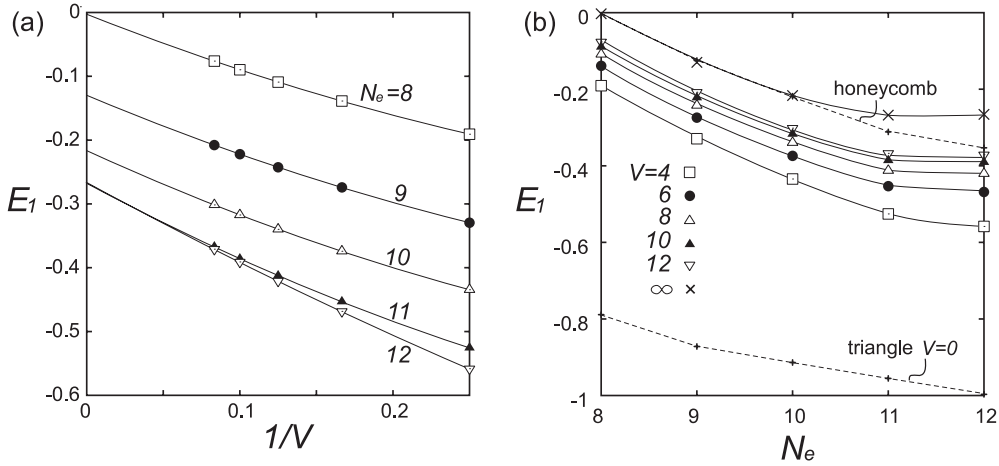


Figure 2. Kinetic energy gain, $E_1 = (E_Q - E_C)/N$, in the formation of a pinball liquid at $N = 24$ with $t = 1$ as a function of (a) $1/V$ and (b) N_e , where $N_e = 8, 12$ corresponds to $n = 1/3, 1/2$, respectively. The fitting by the power of $1/V$ is given in (a), whose results are reflected in (b) as those of $V = \infty$. The band energy gains of the free electrons on corresponding honeycomb ($N = 16$) and triangular ($N = 24$) lattices are shown together for comparison.

increases with increasing filling, i.e. the number of ‘balls’ that can move. In figure 2(a) we fit the data by the power of $1/V$ as $E_1 = c_0 + c_1/V + c_2/V^2$, where c_j are fitting constants and c_0 gives the kinetic energy gain in the strong coupling limit. The obtained results at $V = \infty$ are given as a function of filling in figure 2(b) together with E_1 at finite V . In the strong coupling limit, $E_1(V = \infty)$ seems to follow the band energy of the honeycomb lattice at $N_e < 10$, which supports the simplest pinball liquid picture we discussed above in the dilute case. As the filling approaches $n = 1/2$, E_1 deviates from the honeycomb one and saturates. This is because the correlation among ‘balls’ increases to avoid the loss of V as they become dense. Then the balls can no longer move independently of each other and the wavefunctions become relatively localized so that the kinetic energy gain does not increase much with N_e .

Although we see shortly that the pinball liquid is dominant over $1/3 < n \leq 1/2$, its stability is still the most difficult to be guaranteed at half-filling because the largest number of contingents exists that might destroy the ‘pins’ to some extent. We remind that the charges on B and C sites can hop by t to its neighbouring site as in figure 3(a) without the loss of binding energy when the neighbouring population number of that charge remains unchanged. The example is given in figure 3(b) where some of the balls can move in the direction indicated by arrows. This rule also holds for the charges on the A site in the irregular contingent states, e.g. when three neighbouring hexagons have special kind of configuration as shown in figure 3(c). Fortunately, in this case the contingent cannot destroy the ‘pins’ completely. This is because the charges which were originally a ‘pin’ cannot go more than one site away without freezing the configuration of the original two neighbours. Otherwise, one of these neighbours refills the original ‘pin’ and the ‘balls’ can move again smoothly. Therefore, although the local fluctuations squeeze the amplitude of the ‘pins’ they remain relatively stable [10] and the collective destruction of ‘pins’ does not take place. Considering the particle–hole symmetry, the same discussion holds by regarding the C sublattice (holes) as ‘pins’. Therefore, the ‘pins’ and ‘balls’ are not completely fixed and free, respectively, at half-filling.

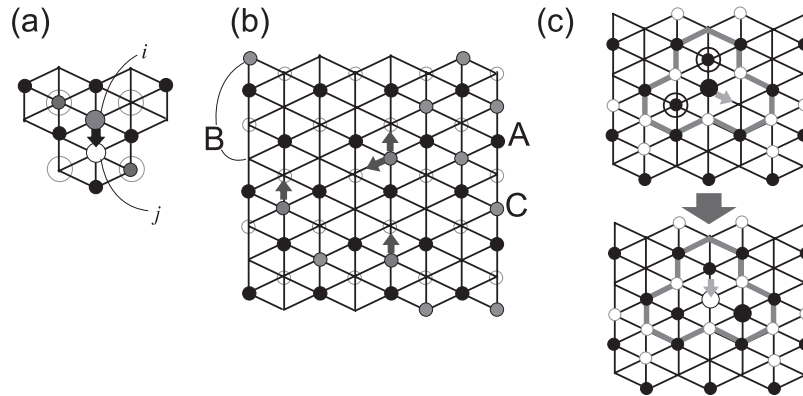


Figure 3. (a) Example of two bases that are allowed to mix by t . The ball can move from site i to j when the extra two neighbours of site i with big circles together have the same number of balls as those of site j . (b) Representative basis of the three sublattice states at $n = 0.5$. Filled black circles and gray or red circles denote the ‘pin’ and ‘ball’, respectively, and the open circle the empty C sites. The ‘balls’ on the C site can move to the neighbouring B site and vice versa when condition (a) is fulfilled. Arrows show the possible movement. (c) Example of the case when the ‘pin’ (big black circle) on the A site moves to its neighbour. When the black circle moves away from the configuration shown at the bottom, the two ‘balls’ marked with the big circle can no longer move. If one of these ‘balls’ refills the original ‘pin’, then other balls can move away.

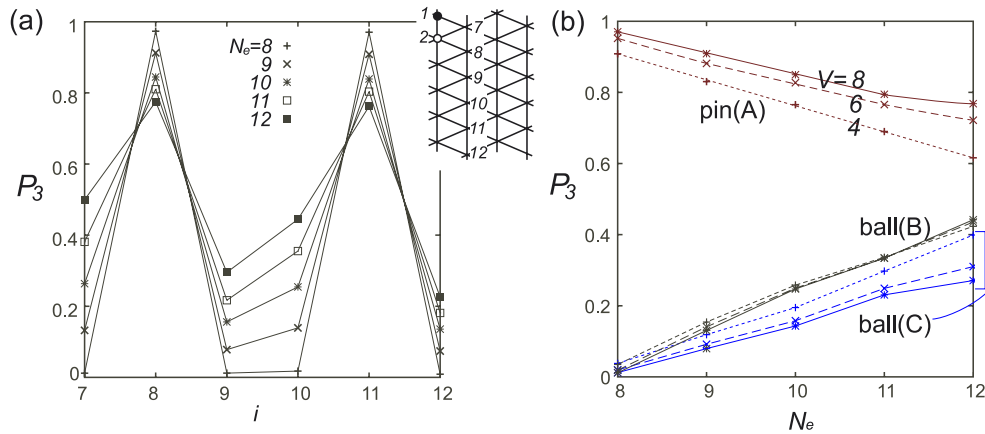


Figure 4. (a) Three-body correlation function, $P_3(i) = \langle n_1(1 - n_2)n_i \rangle$, along the second chain at several fillings between $1/3 \leq n \neq 1/2$. $N_e = 8, 12$ correspond to $1/3$ and $1/2$ fillings, respectively. (b) Amplitude of P_3 as a function of N_e at sites $i = 4, 5, 6$ which belong to the A, B, C sublattices, respectively. The difference between pins and balls becomes small near half-filling.

(This figure is in colour only in the electronic version)

4. Correlation functions

To further compare the stability of the pinball liquid under different fillings, we present the numerical estimation of order parameters for several number of charges $N_e = 8-12$ at $N = 24$, which correspond to the fillings, $n = 1/3-1/2$. As discussed elsewhere, the pinball liquid is characterized by a three-body correlation [10]. Figure 4 shows such a function,

$P_3(i) = \langle n_1(1 - n_2)n_i \rangle$, at $t = 1$. As we see in figure 4(a), the amplitude of ‘pins’ (A) near $n = 1/3$ is almost 1 which decays only little with distance. This sturdily supports the strong coupling picture and is also consistent with the fact that the kinetic energy gain in figure 2(a) at low fillings is almost identical with the honeycomb lattice band energy. With increasing N_e the oscillation amplitude of P_3 becomes suppressed and has larger decay. It is more clearly displayed in figure 4(b) as a function of N_e for several choices of V . However, the amplitudes of ‘pins’ are always larger for larger V , and we expect a long range order in the bulk limit at least in the very strong coupling region even at half-filling.

5. Summary

We have displayed the process of formation and the detailed nature of the new gapless charge liquid denoted as the pinball liquid at $1/3 < n \leq 1/2$, which was reported very recently at half-filling [11]. Due to the particle–hole symmetry, the same results are obtained for $1/2 \leq n < 2/3$ by just regarding holes as ‘pins’. Despite the anticipation that the increasing number of particles towards half-filling might drive the ‘pins’ towards destruction, the kinetic energy gain and the correlation function indicate that the pinball picture still holds while the balls become strongly correlated.

Acknowledgments

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