Momentum Distributions of a Spinless Fermion $t$-$V$ Model on a Triangular Lattice in the Strong Coupling Region

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Abstract. Spinless fermion $t$-$V$ model on a triangular lattice has been studied. In the model, the presence of a novel metallic charge-ordered ground state named a pinball liquid state has been proposed. To clarify the metallic features in the pinball state, we calculate the momentum distribution function of the model. For comparison, we also analyze a corresponding model where charge ordering is strongly pinned. The results are consistent with the picture expected for the pinball liquid, where an insulating ordered state (pin) and a metallic state on the honeycomb lattice (ball) coexist.

1. Introduction

Strongly correlated systems have been attracted for decades. Recently, the effects of geometrical frustration have been paid attention to with an expectation that novel states are stabilized due to the frustration. As one of the simplest models where the effects of geometrical frustration play an important role, a spinless fermion $t$-$V$ model on a triangular lattice has been studied intensively [1, 2, 3]. The model without fermion hoppings is equivalent to the Ising model on the triangular lattice, where the ground state is macroscopically degenerate at particle densities $1/3 \leq \rho \leq 2/3$ [4]. The degeneracy should be lifted once the quantum effects of the hopping $t$ is taken into account.

Let us briefly introduce the pinball-liquid state which has been proposed as a ground state at $1/3 < \rho < 2/3$ of the model in the strong coupling region [1]. At $\rho = 1/3$, there exists a $\sqrt{3} \times \sqrt{3}$-type charge-ordered insulating state where particles occupy one of the three sublattices. As particles are further doped dilutely, i.e. at $\rho \gtrsim 1/3$, the particle-carriers move on the remaining two sublattices which form a honeycomb lattice, as shown in fig. 1(a). Thus, we see a coexistence of the insulating charge order states (pin) and metallic states (ball). We call this state the particle-pinned state. Similar state is realized at $\rho \lesssim 2/3$, where particles are replaced by holes in the above statements. The state is referred to as the hole-pinned state. The proposal in ref. [1] is that such states are realized in the entire range of the density $1/3 < \rho < 2/3$.

A variational Monte Carlo calculation has shown that, at half-filling, a long range charge-ordered state and a metallic state coexist in the strong coupling region [2]. Order parameters for
charge-ordered state as well as the quasi-particle spectral functions have been studied by exact diagonalizations, and various signs of coexistence of the charge-ordered states and metallic states are observed at $1/3 < \rho < 2/3$ [3].

For a comprehensive studies, we further introduce a strong pinned limit of the model. For the particle-pinned state on a triangular lattice, we consider a state where the particles on one of the three sublattices are artificially pinned so that fluctuations of the charge-ordered component is prohibited. The remaining particles act as carriers on the remaining sublattices, so that the pinball-liquid state is compelled to be realized.

Such pinning of the fermionic degrees of freedom can equivalently be realized by simultaneously depleting $1/3$ of the triangular lattice sites and the carrier particles, which leads to a $t$-$V$ model on a honeycomb lattice with reduced number of sites and particles. The particle density of the corresponding model $\rho'$ is given by $\rho' = (\rho - 1/3)/(2/3) = (3/2)\rho - 1/2$. For the hole-pinned state, we also define the limit similarly by replacing particles with holes.

In ref. [3], it is shown that the quasiparticle spectra of the model at various values of $\rho$ resemble those of the strong pin limit. Namely, the strongly pinned limit is an effective state for the metallic component of the original model. This gives another evidence for the validity of the pinball liquid.

In this paper, in order to make further studies for the metallic component of the pinball liquid state, we calculate the momentum distributions of the $t$-$V$ model on a triangular lattice in the strong coupling region. We also make comparisons with those for the corresponding model in the strongly pinned limit.

2. Model and Method
The Hamiltonian of the triangular spinless fermion $t$-$V$ model is defined as

$$\mathcal{H} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{h.c.}) + V \sum_{\langle ij \rangle} (n_i - 1/2)(n_j - 1/2),$$

(1)

where $t$ is a hopping amplitude and $V (>0)$ is a repulsive interaction between nearest-neighbor sites. $c_i^\dagger (c_i)$ is a $i$-th site spinless fermion creation (annihilation) operator and $n_i = c_i^\dagger c_i$. Second order perturbation theory with respect to $t/V$ is applied by projecting the Hilbert space within the macroscopically degenerate ground state at $t = 0$ [5]. Through this projection method, we can treat rather large cluster, i.e. up to 48 sites, although the calculations are limited to the strong coupling region $V/|t| \gg 1$. As a reference to discuss the metallic features in the pinball liquid state, we have calculated the strongly pinned limits as well.

In order to investigate metallic features in the pinball liquid state, we have calculated the momentum distribution $n_k$ defined as

$$n_k = \frac{1}{N} \sum_{i,j} e^{i k (r_i - r_j)} (c_i^\dagger c_j),$$

(2)
where $N$ and $r_i$ are number of sites and $i$-th sites coordinates, respectively. The calculation in refs. [1, 2, 3] indicates that symmetry broken state with a $\sqrt{3} \times \sqrt{3}$ type superstructure is realized in the strong coupling limit. Thus, we reconstruct Brillouin zone (BZ) assuming the $\sqrt{3} \times \sqrt{3}$ type superstructure as shown in fig. 1(b). Then, we calculate the momentum distribution defined on a folded BZ as

$$\tilde n_k = \sum_G n_{k+G},$$

where $G$ are the reciprocal lattice vectors. In order to check the $k$ dependence smoothly, we apply twisted boundary conditions.

Calculations are performed on 36-site and 48-site clusters. Since particle-hole symmetry is broken in the present model, hole-pinned states are energetically favored at half filling for the case $t > 0$ [2, 3]. Hereafter we define hole density as $\rho_h = 1 - \rho$, and analyze the model in the hole-pinned region $1/3 < \rho_h \leq 1/2$. We have also confirmed that, at sufficiently large $V/|t|$, features of particle-pinned states at $\rho < 1/2$ is quite similar to those of the hole-pinned states [3].

3. Results

Momentum distributions $\tilde n_k$ along $\Gamma-K-M-\Gamma$ lines (see fig. 1(b)) are calculated on 36-site and 48-site clusters for $V/t = 50$ at various densities. As typical cases, the results in the hole-pinned region $\rho_h = 3/8 (= 18/48), \rho_h = 5/12 (= 15/36 = 20/48), \rho_h = 11/24 (= 22/48)$ and $\rho_h = 1/2 (= 18/36 = 24/48)$ are shown in figs. 2(a)-(d). For comparison, we also show $\tilde n_k$ in the strongly pinned limits, which is calculated on 24-site and 32-site honeycomb lattices (corresponding to the 36-site and 48-site triangular lattices, respectively), with corresponding hole densities $\rho_h = 1/16$, $1/8$, $3/16$ and $1/4$.

We see that the results for the strongly pinned limits are quite similar to that for the original model. Let us note that similar results are obtained in the entire range of the density $1/3 < \rho < 2/3$. Thus we confirm that the strongly pinned limit gives a valid picture for the original model.

In the case that the density is away from the half-filling, (see figs. 2(a),(b) and (c)), it is likely that $\tilde n_k$ shows discontinuities, which is a typical Fermi liquid behavior. For the densities where Fermi liquid behavior is observed, we see weak system-size dependences. In addition, momentum distributions $\tilde n_k$ can be approximated well by those of free particles ($V = 0$) on the honeycomb lattice. On the other hand, the behaviors around $\rho = 1/2$ is more complicated. As shown in fig. 2(d), $\tilde n_k$ at $\rho = 1/2$ seems to be continuous and smooth. In addition, the system size effects can not be neglected. We give further discussions in the following section.

4. Summary and Discussions

We have calculated the momentum distributions $\tilde n_k$ on a triangular spinless Fermion $t$-$V$ model within projected subspaces in the strong coupling limits, and compared with those in the strongly pinned particles limits. The result is consistent with the pictures expected in the pinball liquid state [1, 2], where an insulating ordered state (pin) and an itinerant state on the honeycomb lattice (ball) coexist. Our results support the fact that the pinball liquid state is realized in a wide range of electron densities $1/3 < \rho < 2/3$. It seems that a typical Fermi liquid behavior appears for the metallic features of the pinball liquid in the particle densities away from the half-filling.

At and around half filling, we point out some possibilities for the ground state of the model: (i) Strongly correlated Fermi liquid behaviors. In this case, a small but numerically unclear jumps in $\tilde n_k$ should exist. (ii) The $\tilde n_k$ is connected smoothly and non-Fermi liquid behavior is realized. (iii) An insulator which presumably accompanies additional charge/bond orderings. The results in fig. 2(d) indicate that the strongly pinned particles limit pictures are equivalent to pin-ball liquid states even at half-filling. Thus, further investigation on the corresponding
Figure 2. Momentum distributions $\tilde{n}_k$ along $\Gamma$-$K$-$M$-$\Gamma$ lines at $V/t = 50$ on 36-site ($\triangle$) and 48-site ($\circ$) clusters are shown, for the hole densities of (a) $\rho_h = \frac{3}{8}$, (b) $\rho_h = \frac{5}{12}$, (c) $\rho_h = \frac{11}{24}$ and (d) $\rho_h = \frac{1}{2}$. The results in strongly pinned limits corresponding to 36-site (+) and 48-site ($\times$) clusters are also shown.

honeycomb lattice model at $\rho' = 1/4$ may give us some ideas about the features of the pinball liquid state around hall-filling.

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