Variational study on the cluster glass wave function for the 2D extended $t-J$ model

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Abstract. By using the variational Monte Carlo approach, we have demonstrated the existence of cluster glass states with a randomly-distributed short-ranged modulations is a natural outcome of the extended $t-J$ models. As shown in our recent paper [1], these glassy states have almost the same energy as the uniform superconducting ground state if the modulation is moderate. Also we show that there are many possible degenerate states within a wide range of variational parameters. Because of the unusual degeneracy in the extended $t-J$ models, random distribution of any defect or impurity in the materials could easily stabilize the glassy state. All these results obtained without introducing extra competing interactions or new order parameters seem to provide an appropriate framework to understand the experiments.

1. Introduction

In the context of the broad interest in challenging the properties of the high-$T_c$ superconductors, one of the most interesting properties is the possible existence of the stripe state consisting of one dimensional charge-density modulation coupled with spin order [2, 3, 4]. Many evidences of the presence of the non-superconducting stripe state as the ground state have been reported in several cuprate materials [5, 6, 7]. Very recently, the high-resolution scanning tunneling microscopy has observed unidirectional domains with periodic density of states modulation in two families of $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ [8, 9]. These bond-centered electronic patterns with a width of four lattice constants form the so called electronic cluster glass state with short-ranged modulations. In the theoretical side, Capello et al. [10] recently have found that the periodic resonating-valence-bond (RVB) stripe state could be a good candidate for the ground state in the extended $t-J$ models. In the mean time, we show that the antiferromagnetic (AF) modulation should be also included in the stripe state, and the randomly-distributed modulation could be another possible ground state due to high degeneracy in variational energy [1]. Furthermore, in this paper we will also show that the existence of cluster glass states could be a natural consequence of the extended $t-J$ models.

2. Variational approach

We consider the extended $t-J$ Hamiltonian,

$$H = - \sum_{i,j,\sigma} t_{ij} \left( \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + h.c. \right) + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j.$$  \hfill (1)
The hopping amplitude $t_{ij} = t$, $t'$, and $t''$ for sites $i$ and $j$ being the nearest-, the second-nearest, and the third-nearest-neighbors, respectively. The notations are standard. In the following, we mainly focus on the case $t'' = -t'/2$ and $J/t = 0.3$ at hole doping $1/8$.

We shall follow the work by Himeda et al. [11] to construct the variational wave functions. In the mean-field theory, we assume the staggered magnetization $m_i$ and the nearest-neighbor pairing order parameter $\Delta_{ij}$. Thus the effective mean-field Hamiltonian is reduced to

$$H_{MF} = \sum_{i,j} \left( c_{i\uparrow}^\dagger c_{i\downarrow} + H.c. \right) \left( \begin{array}{cc} H_{ij} & D_{ij} \\ D_{ji} & -H_{ji} \end{array} \right) \left( \begin{array}{c} c_{j\uparrow}^\dagger \\ c_{j\downarrow} \end{array} \right),$$

where the matrix elements

$$H_{ij\sigma} = -\left( t_v \sum_{\beta=NN} + t'_v \sum_{\beta=NN} + t''_v \sum_{\beta=NNN} \right) \delta_{j,i+\beta} + \left( \mu_i - \mu_v + \sigma(-1)^{x_i+y} m_i \right) \delta_{j,i}.$$  

Here $N, NN, NNN$ correspond to the nearest-, the next-nearest, and the third-nearest-neighbors, respectively, and $\sigma = \uparrow(1)$ or $\downarrow(-1)$. The local charge density is controlled by $\rho_i$ and $\mu_v$ is the chemical potential. For periodic stripes, we assume these spatially varying functions with simple forms:

$$\rho_i = \rho_v \cos[4\pi \delta \cdot (y_i - y_0)],$$

$$m_i = m_v \sin[2\pi \delta \cdot (y_i - y_0)],$$

$$\Delta_{i,i+\hat{x}} = \Delta_v^M \cos[4\pi \delta \cdot (y_i - y_0)] - \Delta_v^C,$$

$$\Delta_{i,i+\hat{y}} = -\Delta_v^M \cos[4\pi \delta \cdot (y_i - y_0) + 2\pi \delta] + \Delta_v^C.$$  

where $\delta(=1/8)$ is the doping density. Here we arrange the stripe to extend uniformly along the $x$ direction. $y_0 = 0 (1/2)$ corresponds to the site- (bond-) centered stripe. In this paper, we will only focus on the bond-centered stripe. If both $\Delta_v^M$ and $\Delta_v^C$ are positive, the hole density is maximum at sites with smallest pairing amplitude $|\Delta_{ij}|$ and smallest magnetization $|m_i|$. This is similar to the phase diagram [12, 13] predicted by the uniform RVB and AF states. Thus we will denote this state as the AF-RVB stripe state. Instead of the periodic stripe, we have also examined the stripe state with $4 \times 4$ patches on the $16 \times 16$ lattice system. For each patch, we randomly choose a direction of the stripe, $x$ or $y$. We consider this state as the random stripe state. There are total seven variational parameters $\mu_v, t_v, t_v', t_v'', \rho_v, m_v, \Delta_v^M$, and $\Delta_v^C$ with $t_v$ set to be 1. Once these parameters are given, we can diagonalize the mean-field Hamiltonian to construct the mean-field wave function. Finally, we optimize the variational energy by using the stochastic reconfiguration algorithm [14].

In addition, due to the large energy improvement [1], we have also introduced the hole-hole repulsive Jastrow factor [15, 16, 17]:

$$\prod_{i<j} \left( 1 - (1 - r_{ij}^{\alpha}) \cdot r_{ij}^{\beta} \cdot n_i^h \cdot n_j^h \right)$$

with

$$r_{ij} = \sqrt{\sin^2 \left( \frac{\pi}{L_x} (x_i - x_j) \right) + \sin^2 \left( \frac{\pi}{L_y} (y_i - y_j) \right)},$$

where $n_i^h = 1 - \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma}$. The parameters $v_{ij} = N, NN, NNN$ are for short-ranged hole-hole repulsion if these values are less than 1. The factor $r_{ij}^{\alpha}$ is for long-ranged correlations and it is repulsive if $\alpha$ is positive. $L_x$ and $L_y$ are the number of sites in the $x$ and $y$ direction, respectively.
3. Result and discussion

In this section, we first show the numerical results obtained by optimizing the random stripe states with the Jastrow factors for the extended $t-J$ model. As shown in the Fig.1 of Ref. [1], the energy differences among three states: the AF-RVB stripe, random stripe, and uniform $d$-wave RVB states are rather small. Here, in Figure 1 we illustrate further that the percentage of optimized energy difference between the random stripe and uniform RVB states are plotted as a function of $t'/t$. It is clear that random stripe states have the optimized energies about 0.3% higher than uniform $d$-wave RVB state. They are almost identical up to such a small percentage, even though we have not optimized parameters on every bond or site independently. These optimized random stripe states have finite $m_v$ and $\Delta^C_v$ but smaller $\Delta^M_v$.

In Figure 2, we show that the variational energies of the AF-RVB stripe states with different parameters $\Delta^M_v$ for some $\Delta^C_v$, and the other parameters are fixed. The variational energies for the case of $t'/t = -0.3$ are calculated on a $16 \times 16$ lattice system with the periodic and antiperiodic boundary conditions along the x and y directions, respectively. It is worthy to be noted that the energies with certain $\Delta^C_v$ are rather insensitive to $\Delta^M_v$ if $\Delta^M_v / \Delta^C_v < 34\%$. In other words, there exists many degenerate states with local minimal energy when $\Delta^M_v$ is less than around one third of $\Delta^C_v$. It leads to a fact that the AF-RVB stripe states can have many degenerate states in total energy competition. Therefore, one may say, many kinds of local arrangements for spin or hole configurations can have almost identical energy to the uniform wave functions [1].

The energy degeneracy has also been shown in the recent paper of other group [10]. We believe this energy degeneracy should be mainly caused by a fact that there is a very strong anti-correlated behavior between the kinetic energy and magnetic energy within local region (not shown). Even among different states, the energy competition between the kinetic energy and spin interaction is also robust. Their competition is enhanced by the no-doubly occupancy constraint as the presence of holes suppress the spin interaction to zero. Thus it is possible to have some of these local patterns with lower kinetic energy but higher magnetic energy than the

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**Figure 1.** Percentage of energy difference between the random stripe state and the uniform $d$-wave RVB state as a function of $t'/t$ on a $16 \times 16$ lattice system.

**Figure 2.** Variational energy of the AF-RVB stripe state as function of variational parameter $\Delta^M_v$ with the others fixed. Different symbols indicate different values of $\Delta^C_v$. 

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uniform $d$-wave RVB state and some other regions with opposite energetics.

4. Conclusion
In summary, we have used a variational Monte Carlo technique to examine the possibility of having inhomogeneous ground states within the extended $t-J$ model at 1/8 doping. We have considered states with spatial modulation of charge density, staggered magnetization and pairing amplitude, such as the AF-RVB stripe state and random stripe state. By improving these trial wave functions, we also introduced the hole-hole repulsive correlation. Most surprisingly, the random stripe state essentially has the same energy as the uniform state in spite of our oversimplified assumption that all the stripe domain has the same patterns of modulation instead of each site or bond with different values. Also we have shown that there are many local minimal energy for these proposed stripe wave functions. It is suggested that we could have many kinds of the inhomogeneous ground states with the energies almost close to the uniform solution in the extended $t-J$ model.

Due to the competition between the kinetic energy gain and magnetic interaction, it is very natural to have the spatial modulation, in periodic or random configuration, of charge density, magnetization and even pairing amplitude. The constraint of disallowing doubly occupation of electrons at each lattice site has significantly enhanced the competition. Thus, the presence of inhomogeneous or cluster glass states is apparently a very natural consequence of the $t-J$ model. There is no need for introducing additional interactions to generate such states. In a realistic material, other interactions such as impurity, disorder, and electron-phonon interactions, etc., may help to determine the most suitable local configuration of spins and holes. The confirmation of this speculation will be studied in the future.

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