Physica C 481 (2012) 125–131

Contents lists available at SciVerse ScienceDirect

Physica C

journal homepage: www.elsevier.com/locate/physc

Stripe states in t–t'–J model from a variational viewpoint

Masao Ogata *

Department of Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

ARTICLE INFO

Article history:
Accepted 22 March 2012
Available online 11 April 2012

Keywords:
Stripe
High-T_c cuprates
Variational Monte Carlo
Spatially oscillating superconductivity order parameter

ABSTRACT

The stripe states discussed in the variational Monte Carlo simulations are reviewed. The interplay between stripes and $d_{x^2-y^2}$-wave superconductivity in the two-dimensional t–t'–J model is emphasized. The next-nearest-neighbor hopping $t' < 0$ stabilizes the stripe states around the hole doping rate, $\delta = 1/8$. It is found that the stripes and spatially oscillating superconductivity coexist depending on parameters. The superconductivity order parameter is enhanced at the hole stripe regions, and its sign becomes opposite on the adjacent hole stripes (i.e., antiphase). It is also found that the energy differences between homogeneous states and the stripe states with and without superconductivity are relatively small. We consider the possibility that the antiphase coexistence may explain the weakness of the c-axis Josephson couplings in some of the high-T_c cuprates.

1. Introduction

As extensively discussed in this special volume, the stripe state is one of the interesting states realized in high-T_c cuprate superconductors [1–3]. The stripe state consists of one-dimensional charge modulation (hole stripe) and antiphase antiferromagnetic domains. Theoretically it is quite interesting to study whether such an inhomogeneous state can be realized in some strongly correlated electron systems. In this article we focus on the theoretical calculations based on variational Monte Carlo simulation which enables us to study possible inhomogeneous states with coexisting charge-order, antiferromagnetic-order and superconductivity. We also discuss the important effects of the next-nearest-neighbor hopping (t'-term). Although the lattice degrees of freedom may contribute to the stability of stripe states [1–3], in this review we focus on the stability of stripe states purely from the electronic origin.

Since high-T_c cuprates belong to the strongly correlated regime [4–6], conventional theoretical approaches such as perturbation, mean-field theories, and random phase approximation are not justified. Thus some numerical techniques should be used in order to study models with strong correlation. Among various numerical methods, density-matrix renormalization group calculations will be intensively described in the article by White and Scalapino in this volume [3]. Thus in this article we describe the results obtained in the variational Monte Carlo simulations. As another numerical method, exact diagonalization of small clusters has also been often used. However, this method is not appropriate for the study of stripe states, since the small clusters with up to 20 lattice sites are not large enough for studying long-range structures like stripes.

In Section 2, we first describe the t–J model (and its generalization) which is the canonical model for high-T_c cuprate superconductors [4–6]. We review the uniform states realized in the t–J model and explain its phase diagram. Then in Section 3, we discuss the coexistence of antiferromagnetism and superconductivity near half-filling. Since one of the important features of the stripe state is its antiferromagnetic domain structure, the relation between antiferromagnetism and superconductivity has to be understood even in the uniform state. In Section 4, we summarize the results for the stripe state obtained in the variational Monte Carlo method. Section 5 is devoted to the summary and discussions. Our present conclusion is that the stripe state can be realized in the t–t'–J model in particular for the case with $t' < 0$ [7]. Here t' represents the hopping integral between the next-nearest-neighbor Cu sites on a square lattice. The important point which we can extract from the existing numerical results is that the stripe state and other uniform states have very similar variational energies to each other. Therefore, the stripe state will be easily stabilized when some small perturbations, such as lattice structure deformation or local impurity potentials, give some favorable situation for the stripe states. (See for example, Adachi and Koike in this volume [3]). Another interesting feature of the stripe obtained in the variational Monte Carlo is that it can coexist with superconductivity. In such cases, superconducting order parameter has a spatial oscillation in accordance with the period of the underlying stripe structure. It is found that even the sign of the $d_{x^2-y^2}$-wave order parameter changes as a function of the position, which lead to unique properties [7].

* Tel.: +81 3 5841 4184.
E-mail address: ogata@phys.s.u-tokyo.ac.jp

0921-4534/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.physc.2012.03.047

2. *t–J* model and its uniform states

The *t–J* model is the canonical model for high-T_c cuprate superconductors which represents the "doped Mott insulator" [4]. Firstly, in the mother compound, e.g., La_2CuO_4, or without doping of carriers, the cuprate systems are Mott insulators. This is apparent from the resistivity measurements, i.e., the resistivity shows an insulating behavior above the Neel temperature, T_N. This means that the antiferromagnetic transition at T_N is not a spin-density-wave (SDW) phase transition but a magnetic phase transition of the localized spins inside the Mott insulator. (If this phase transition is an SDW transition, the system should behave as an Fermi liquid above T_N, and the resistivity should be metallic.)

Starting from this fact of the Mott insulator, it is natural to consider the *t–J* model on a two-dimensional square lattice [6]

$$H = -\sum_{\langle i,j\rangle\sigma} P_G\left(t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} + \text{h.c.}\right)P_G + J\sum_{\langle i,j\rangle}\boldsymbol{S}_i\cdot\boldsymbol{S}_j, \tag{1}$$

where the summation over (i, j) in the first term represents the summation over the bonds connected by hopping integrals, t_{ij}. In the so-called *t–t′–J* model, we have the nearest-neighbor hopping, t, and the next-nearest-neighbor hopping, t'. P_G represents the Gutzwiller projection operator [8] defined as $P_G = \prod_i(1 - n_{i\uparrow}n_{i\downarrow})$, which vanishes when there is at least one doubly occupied site, i.e., P_G excludes the double occupancy from the Hilbert space. The strong electron correlation prohibits the double occupancy. The second term in Eq. (1) represents the superexchange interaction between the localized spins on the Cu sites, and the summation over $\langle i, j\rangle$ represents the summation over the nearest-neighbor bonds. Typical parameters in the *t–t′–J* model are $t = 0.4$ eV, $t'/t \sim -0.1$ for LSCO and $t'/t \sim -0.3$ for YBCO and BSCCO, and $J = 0.13$ eV ($J/t = 0.3$) [9–12], which are obtained so as to reproduce the Fermi surface observed experimentally in ARPES [13,14] or in the band calculations [15].

It is apparent that, without doping ($\delta = 0$) or at half-filling, this model reduces to the two-dimensional Heisenberg model which describes the Mott insulator in the mother compounds. The effect of the doped holes just appears as the correlated hopping terms without disturbing the superexchange interactions away from the doped holes. Actually Zhang and Rice [16] showed in the early stage of the high-T_c research that the doped holes form so-called Zhang-Rice singlets by using a model with oxygen orbitals on which the doped holes are mainly located [17–19]. The Zhang–Rice singlet is a singlet pair formed between a localized spin on one of the Cu sites and a doped-hole on the neighboring oxygen sites. The stabilization energy is so large (about 5 eV [6]) that we can understand that every doped-hole definitely forms a Zhang–Rice singlet. This singlet behaves as a hole in the *t–J* model, and the Cu site is singly occupied unless a Zhang–Rice singlet is located. This fact is essential for high-T_c cuprates which are doped Mott insulator.

The most important and nontrivial effects in the Hamiltonian (1) is that the double-occupancy is strictly forbidden in the Hilbert space by the Gutzwiller projection, P_G. Due to this constraint, the theoretical tool for investigating this model is restricted. As we described in Section 1, the numerical methods which can be applied to the *t–J* model are exact diagonalization, density-matrix renormalization group and variational Monte Carlo simulations.

For the *t–J* model, it has been established that its ground-state will be a $d_{x^2-y^2}$-wave superconductivity near half-filling and for $J/t = 0.3$–0.4 (see Fig. 1) [20–24]. This situation is very different from that in the weak-coupling Hubbard model. In the variational point of view, we use the Anderson's Gutzwiller-projected BCS function for the *t–t′–J* model [4],

$$|\Psi\rangle = P_G|\text{BCS}\rangle, \tag{2}$$

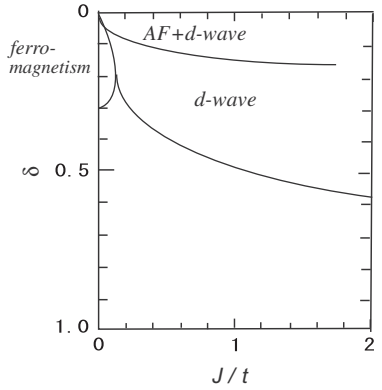

Fig. 1. Phase diagram obtained in the variational Monte Carlo simulations for the ground state of the two-dimensional *t–J* model as a function of J/t and δ. (From Ref. [23,28]).

where the projection operator P_G excludes the double occupancy in the wave function $|\text{BCS}\rangle$. $|\text{BCS}\rangle$ is a BCS mean-field wave function with $d_{x^2-y^2}$-wave superconducting order parameter.

$$|\text{BCS}\rangle = \prod_{\boldsymbol{k}}\left[u_{\boldsymbol{k}} + v_{\boldsymbol{k}}c^{\dagger}_{\boldsymbol{k},\uparrow}c^{\dagger}_{-\boldsymbol{k},\downarrow}\right]|0\rangle, \tag{3}$$

with

$$u_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 + \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)}, \qquad v_{\boldsymbol{k}} = \frac{\Delta_{\boldsymbol{k}}}{|\Delta_{\boldsymbol{k}}|}\sqrt{\frac{1}{2}\left(1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)}, \tag{4}$$

$E_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}$, and $\Delta_{\boldsymbol{k}} = \Delta(\cos k_x - \cos k_y)$ for the $d_{x^2-y^2}$-wave superconductivity. Here Δ is one of the variational parameters and $\xi_{\boldsymbol{k}}$ can be chosen as the original dispersion relation,

$$\xi_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y - \mu. \tag{5}$$

However, it is natural to choose t' and μ as variational parameters, t'_{var} and μ_{var}, which are to be optimized so as to minimize the variational energy. The variational parameter t'_{var} controls the shape of the Fermi surface [25]. t is chosen as a unit of energy and we need not to treat t as a variational parameter. Actually, the wave function (2), when normalized, depends only on Δ/t, t'_{var}/t, and μ_{var}/t. It can be easily shown that at $\delta = 0$ the variational state (2) is equivalent to the resonating-valence-bond (RVB) state proposed by Anderson for frustrated spin systems [26] due to the Gutzwiller projection P_G [4,6].

In the variational Monte Carlo simulation, we calculate the variational energy

$$E_{\text{var}} = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{6}$$

by using a Monte Carlo updates of the real-space electron configurations. Since there is no sign problem, the variational energy can be evaluated quite accurately. By optimizing the variational parameters, we obtain a phase diagram as shown in Fig. 1 where the coexistence of the antiferromagnetism and superconductivity discussed in the following section [27,28] is also included. As shown in Fig. 1, when we fix $J/t = 0.3$, the $d_{x^2-y^2}$-wave superconductivity is stabilized for $\delta < 0.4$. The doping dependence of the variational parameter, Δ/t, is shown in Fig. 2 for $J/t = 0.3$. Δ decreases monotonically with increasing δ. The phase boundary of the $d_{x^2-y^2}$-wave superconductivity is determined by the doping rate at which Δ vanishes. For $\delta < 0.1$, a coexistent state between antiferromagnetism and $d_{x^2-y^2}$-wave superconductivity is realized, This state is discussed in the following section. Furthermore, for the small values of J/t ($J/t < 0.1$) in Fig. 1, Nagaoka's ferromagnetic state [29,30] is found, which is consistent with the high-temperature expansion study [31].