Inhomogeneous d-wave state and lattice distortions in the three-band Hubbard model of high-T_c cuprates

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Abstract

Striped superconductivity (SC) with lattice distortions is investigated based on the three-band Hubbard model of high-T_c cuprates. A stable inhomogeneous striped state is determined in the low-temperature tetragonal (LTT) phase using a quantum variational Monte Carlo method. The ground state has vertical or horizontal hole-rich arrays coexisting with incommensurate magnetism and SC. The SC order parameter oscillates according to the inhomogeneity in the antiferromagnetic background with its maximum in the hole-rich region.

Key words: stripes, incommensurate SDW, lattice distortion, LTT phase, d-wave pairing

Introduction Over the last decade the oxide high-T_c superconductors have been investigated intensively. The mechanism of superconductivity (SC) has been extensively studied using various two-dimensional (2D) models of electronic interactions. Studies of these models over the last decade indicated that the d-wave SC is induced from the electronic repulsive interaction[1–7]; significantly it has been established that the SC condensation energy and the magnitude of order parameter are in reasonable agreement with the experimental results in the optimally doped case.[8,9]

In the underdoped region many physical properties remain unresolved. A striped state has been proposed based on incommensurate SDW and CDW correlations observed in the neutron-scattering measurements.[10,11] The linear doping dependence of incommensurability in the underdoped region supports a striped structure and suggests a relationship between magnetism and SC.[11] A relationship between the SDW, CDW orders and a crystal structure has also been suggested; in the LTT phase, the CDW order is stabilized, while no well defined incommensurate CDW peaks were observed for the orthorhombic systems.[12]

Lattice distortions and superconductivity The Hamiltonian is given by the three-band Hubbard model for d and p orbitals with the modulated transfer terms:

$$
\begin{aligned}
H = H^0_{pd} &+ t_{pp}\sum_{i\sigma} v_i[p^\dagger_{i+\hat{y}/2,\sigma}p_{i+\hat{x}/2,\sigma} - p^\dagger_{i+\hat{y}/2,\sigma}p_{i-\hat{x}/2,\sigma} \\
&- p^\dagger_{i-\hat{y}/2,\sigma}p_{i+\hat{x}/2,\sigma} + p^\dagger_{i-\hat{y}/2,\sigma}p_{i-\hat{x}/2,\sigma} + h.c.]. \\
&+ t_{pd}\sum_{i\sigma}[u_{i\hat{x}}d^\dagger_{i\sigma}p_{i+\hat{x}/2,\sigma} - u_{i,-\hat{x}}d^\dagger_{i\sigma}p_{i-\hat{x}/2,\sigma} \\
&+ u_{i\hat{y}}d^\dagger_{i\sigma}p_{i+\hat{y}/2,\sigma} - u_{i,-\hat{y}}d^\dagger_{i\sigma}p_{i-\hat{y}/2,\sigma} + h.c.] \\
&+ \frac{K_{pd}}{2}\sum_i(u^2_{i\hat{x}} + u^2_{i,-\hat{x}} + u^2_{i\hat{y}} + u^2_{i,-\hat{y}}) + \frac{K_{pp}}{2}\sum_i 4v^2_i \\
&+ U_d\sum_i d^\dagger_{i\uparrow}d_{i\uparrow}d^\dagger_{i\downarrow}d_{i\downarrow}. \qquad (1)
\end{aligned}
$$

H^0_{pd} is the kinetic term, and $\hat{x}$ and $\hat{y}$ represent unit vectors in the x- and y-direction, respectively.

The wave function with the inhomogeneous spin structure is made from solutions of the Hartree-Fock Hamiltonian with the potential $\sum_{i\sigma}[\delta n_{di} - \sigma(-1)^{x_i+y_i}m_i]d^\dagger_{i\sigma}d_{i\sigma}$ where δn_{di} and m_i are expressed

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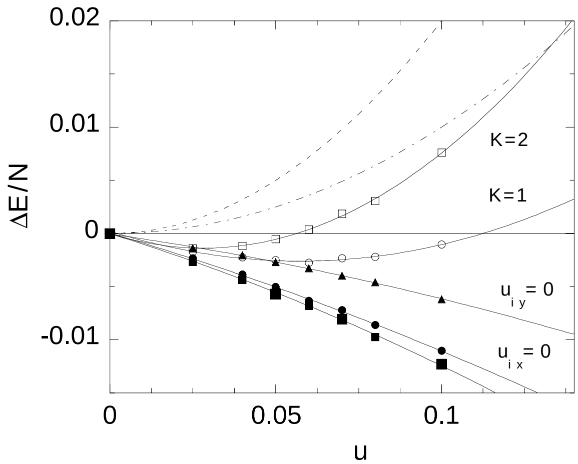

Fig. 1. $\Delta E = E(u=0) - E(u)$ per site as a function of transfer deformation in t_{pd} units. The parameters are $t_{pp} = 0.4$ and $U_d = 8$. The hole-rich stripes are in the y-direction. The energy gains for (A) $u_{i\hat{x}} = 0$ (solid circles), (B) $u_{i\hat{y}} = 0$, (triangles) and (C) (solid squares) are shown. The elastic energy $Ku^2/2$ is shown by the dashed line ($K = 1$) and dash-dotted line ($K = 2$). The open symbols display the summations of ΔE and the elastic energy corresponding to solid symbols. $K = 1$ is assigned for (A) and $K = 2$ for (C).

by modulation vectors Q_s and Q_c representing the spin and charge part, respectively.[9,13,14] The wave function is constructed from the solution of Bogoliubov-de Gennes equation for the SC order parameters in the d-electron part: $\Delta_{i,i+\hat{x}} = \Delta_s \cos(Q_x(x_i + \hat{x}/2))$, $\Delta_{i,i+\hat{y}} = -\Delta_s \cos(Q_x x_i)$, where $Q_x = \pi/4$ at 1/8-filling. The SC order parameter oscillates so that the amplitude has a maximum in the hole-rich region and is suppressed in the hole-poor region. The wave function is taken to be Gutzwiller.[15,16]

In the low-temperature tetragonal (LTT) phase, there is a tilting axis on which the copper and oxygen atoms never move.[17] When the tilting axis is in the μ-direction, the deformation of t_{pd} in the μ-direction vanishes: $u_{i\hat{\mu}} = 0$. We consider the following cases assuming that the stripes are parallel to the y-axis:

(A) $u_{i\hat{x}} = 0, u_{i\hat{y}} = u\cos(2Q_x x_i), v_i = u\cos(2Q_x x_i)$,
(B) $u_{i\hat{x}} = u\cos(2Q_x x_i), u_{i\hat{y}} = 0, v_i = u\cos(2Q_x x_i)$,
(C) $u_{i\hat{x}} = u_{i\hat{y}} = u\cos(2Q_x x_i), v_i = u\cos(2Q_x x_i)$,

where $Q_x = 2\pi\delta$, u is the amplitude of deformation of t_{pd} and t_{pp} and $u_{i\hat{\mu}} = u_{i,-\hat{\mu}}$. The energy gain per site defined as $\Delta E/N = (E(u=0) - E(u))/N$ is presented in Fig.1 as a function of u in t_{pd} units. According to Harrison's rule, t_{pd} is expected to vary as d^{-n} with $n \approx 7/2$, d being the Cu-O bondlength. The elastic energy is estimated as $E_{el} = \frac{1}{2}Cd^3(\frac{\delta d}{d})^2 = \frac{1}{2}Cd^3\frac{1}{n^2}u^2 \equiv \frac{K}{2}u^2$. The constant C is estimated as $C \approx 1.7 \times 10^{12}$ dyne/cm^2= 1.7 eV/$\AA^3$,[18] and then K is of the order of 1eV: $K \approx$ 1eV since $d \approx 2\AA$. As shown in Fig.1 the energy is lowered when the stripes are perpendicular to the tilting axis. Although the state in the case (C) has a lowest energy for fixed u, its total energy may be higher than that for (A) since the elastic energy will increase due to complex lattice distortions. We show schematically stable striped state in Fig.2.

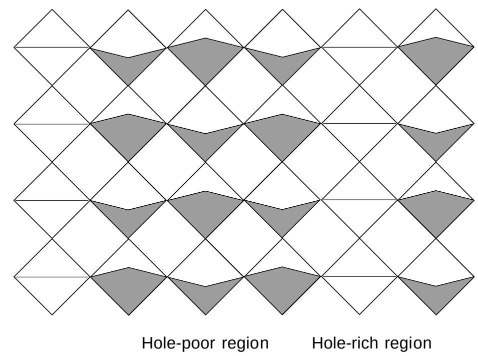

Fig. 2. Schematic structure of lattice distortions and stripes obtained by the present evaluations where the hole-rich arrays are perpendicular to the tilting axis. The shaded square represents distorted CuO unit cell.

Summary In this paper we have investigated the inhomogeneous ground state with the lattice distortions based on the three-band model. The stable striped state has hole-rich arrays being perpendicular to the tilting axis of the lattice distortions in the LTT phase.

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