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Physica B 281&282 (2000) 933–934

PHYSICA B

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SDW and d-wave states in the CuO_2 model by variational Monte Carlo simulations

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Abstract

The ground state of the Cu–O network in the oxide superconductors is investigated by using the variational Monte Carlo method. We employ the Gutzwiller-projected BCS, SDW and AF-BCS wave functions in search for a possible ground state with respect to dependences on electron density ρ and transfer t_{pp}, where the AF-BCS state is the coexistence state of antiferromagnetism and superconductivity. Near half-filling there is a large SDW phase for both the hole and electron doping cases. The d-wave state turns out to be stable away from half-filling. We have found that the AF-BCS state is most stable among the above wave functions near half-filling in the SDW region. It is also found that the extended s-wave state is possible for the electron doping case.

Keywords: High-T_c superconductors; Multi-band Hubbard model; Variational Monte Carlo method

1. Hamiltonian and wave functions

The ground state of the oxide high-T_c superconductors is investigated based on the three-band Hubbard model for the CuO_2 model. The Hamiltonian is given as [1]

$$H = \varepsilon_d \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + U_d \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow}$$
$$+ \varepsilon_p \sum_{i\sigma} (p^\dagger_{i+\hat{x}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^\dagger_{i+\hat{y}/2,\sigma} p_{i+\hat{y}/2,\sigma})$$
$$+ t_{pd} \sum_{i\sigma} [d^\dagger_{i\sigma}(p_{i+\hat{x}/2,\sigma} + p_{i+\hat{y}/2,\sigma} - p_{i-\hat{x}/2,\sigma} - p_{i-\hat{y}/2,\sigma}) + \text{h.c.}]$$
$$+ t_{pp} \sum_{i\sigma} [-p^\dagger_{i+\hat{y}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^\dagger_{i+\hat{y}/2,\sigma} p_{i-\hat{x}/2,\sigma} + p^\dagger_{i-\hat{y}/2,\sigma} p_{i+\hat{x}/2,\sigma} - p^\dagger_{i-\hat{y}/2,\sigma} p_{i-\hat{x}/2,\sigma} + \text{h.c.}]. \quad (1)$$

$\hat{x}$ and $\hat{y}$ represent unit vectors along x and y directions, respectively. $p^\dagger_{i\pm\hat{x}/2,\sigma}$ and $p_{i\pm\hat{x}/2,\sigma}$ denote the operators for the p electrons at site $R_i \pm \hat{x}/2$. Similarly $p^\dagger_{i\pm\hat{y}/2,\sigma}$ and $p_{i\pm\hat{y}/2,\sigma}$ are defined. Other notations are standard and energies are measured in units of t_{pd}. For simplicity we neglect the Coulomb interaction among p electrons.

We consider the following wave functions: normal-state Gutzwiller function, the Gutzwiller function with antiferromagnetic long-rang order, the Gutzwiller-projected BCS wave function, and the coexistence state of antiferromagnetism and superconductivity. These types of functions are standard ground state wave functions and have been investigated considerably for the Hubbard model [2–4]. The last one is written as $\psi_{\text{AF-BCS}} = P_{N_e} P_G \prod_k (u_k + v_k \alpha^\dagger_{k\uparrow} \alpha^\dagger_{-k\downarrow})|0\rangle$ where $\alpha_{k\sigma}$ is constructed as a linear combination of two wave numbers k and $k+Q$ for the commensurate vector $Q = (\pi, \pi)$. P_G is the Gutzwiller projection operator and P_{N_e} is a projection operator which extracts only the states with a fixed total electron number. The parameters in our calculations are the following: $\varepsilon_d = -2$, $\varepsilon_p = 0$, $U_d = 8$ and $0 \leqslant t_{pp} \leqslant 0.4$ in units of t_{pd} for the 6×6 square lattice.

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0921-4526/00/$ - see front matter
PII: S0921-4526(99)01093-5

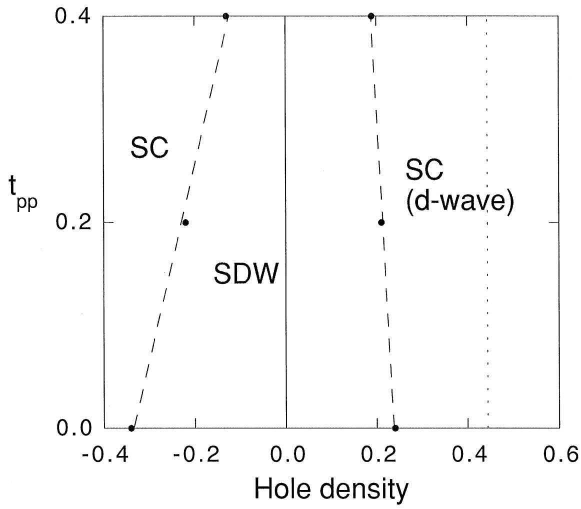

Fig. 1. Phase diagram in the plane of t_{pp} and δ. Parameters are given by $U_d = 8$ and $\varepsilon_p - \varepsilon_d = 2.0$ in units of t_{pd}.

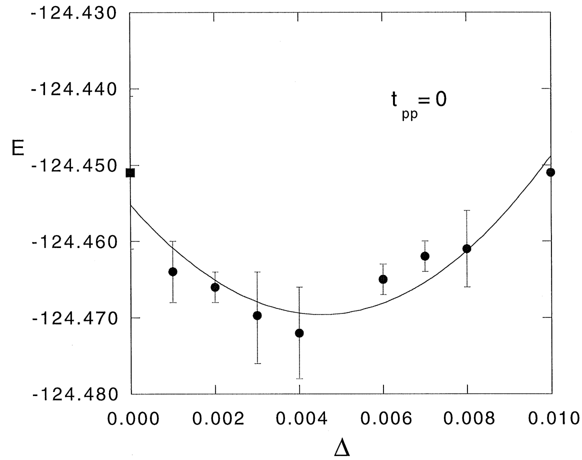

Fig. 2. Energy as a function of SC order parameter Δ for the AF-BCS state. AF order parameter is optimized for each value of Δ. The hole density is given by $\delta = 0.111$.

2. Results

First let us consider the BCS and SDW wave functions. In Fig. 1 we show the phase diagram in the plane of t_{pp} and δ where δ is the hole density. The negative δ denotes the electron-doping case. The energy is lowered considerably by the antiferromagnetic long-range order up to 20% hole doping. The d-wave state exists in a region where $0.2 < \delta < 0.44$ and $\delta < -0.2$ (for $t_{pp} = 0.2$). The extended s-wave state has higher energy than the d-wave state for the hole-doping case, while the extended s-wave state is more stable than the d-wave state for the electron-doping case near half-filling. This indicates a possibility of the extended s-wave superconductivity. Second, let us discuss the coexistence state near half-filling. We show the energy as a function of the superconducting order parameter Δ for $\psi_{\text{AF-BCS}}$ in Fig. 2, where $\delta = 0.111$ and the d-wave order parameter is assumed. The AF order parameter is given by $\Delta_{\text{AF}} = 0.41$ near the minimum. It is also found that the coexistence state is most stable among the variational wave functions shown above for the electron-doping case near half-filling. A possibility of the coexistence state will enlarge the superconducting region. We furthermore found that the antiferromagnetic state with spin modulations has possibly lower energy than the uniform AF and AF-BCS states near half-filling.

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