# 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 $\rho$ 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 found that the AF-BCS state is most stable among 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$_c$ superconductivity, 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]

$$\begin{aligned}
H &= \epsilon_d \sum_{i\sigma} d^{\dagger}_{i\sigma} d_{i\sigma} + U_d \sum_i d^{\dagger}_{i\uparrow} d_{i\uparrow} d^{\dagger}_{i\downarrow} d_{i\downarrow} \\
&+ \epsilon_p \sum_{i\sigma} (p^{\dagger}_{i+\hat{x}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^{\dagger}_{i+\hat{y}/2,\sigma} p_{i+\hat{y}/2,\sigma}) \\
&+ t_{pd} \sum_{i\sigma} [d^{\dagger}_{i\sigma} (p_{i+\hat{x}/2,\sigma} + p_{i+\hat{y}/2,\sigma} - p_{i-\hat{x}/2,\sigma} \\
&- p_{i-\hat{y}/2,\sigma}) + h.c.] \\
&+ t_{pp} \sum_{i\sigma} [-p^{\dagger}_{i+\hat{y}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^{\dagger}_{i+\hat{y}/2,\sigma} p_{i-\hat{x}/2,\sigma} \\
&+ p^{\dagger}_{i-\hat{y}/2,\sigma} p_{i+\hat{x}/2,\sigma} - p^{\dagger}_{i-\hat{y}/2,\sigma} p_{i-\hat{x}/2,\sigma} + h.c.].
\end{aligned} \tag{1}$$

$\hat{x}$ 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 type of functions are standard ground state wave functions and have been investigated considerably for the Hubbard

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model[2–4]. The last one is written as $\psi_{AF-BCS} = P_{N_e} P_G \prod_k (u_k + v_k \alpha^\dagger_{k\uparrow} \alpha^\dagger_{-k\downarrow})|0\rangle$ 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: $\epsilon_d = -2$, $\epsilon_p = 0$, $U_d = 8$ and $0 \le t_{pp} \le 0.4$ in units of $t_{pd}$ for the $6 \times 6$ square lattice.

## 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 $\delta$ where $\delta$ is the hole density. The negative $\delta$ denotes the electron-doping case. The energy is lowered considerably by the antiferromagnetic long-range order up to 20 percent hole doping. The $d$-wave state exists in a region where $0.2 < \delta < 0.44$ and $\delta < -0.2$ (for $t_{pp} = 0.2$) where the energy gain due to the superconducting order parameter is of the order of $0.0004 \sim 0.0007$ per site in units of $t_{pd}$. This value is in reasonable agreement with the experimental superconducting condensation energy estimated from the expression $H_c^2/8\pi$ for the condensation energy[4,5]. 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 $\Delta$ for $\psi_{AF-BCS}$ in Fig.2, where $\delta = 0.111$ and the $d$-wave order parameter is assumed. The AF order parameter is given by $\Delta_{AF} = 0.5$ 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 near half-filling. We furthermore found that the antiferromanetic state with spin modulations has lower energy than the uniform AF and AF-BCS states near half-filling.

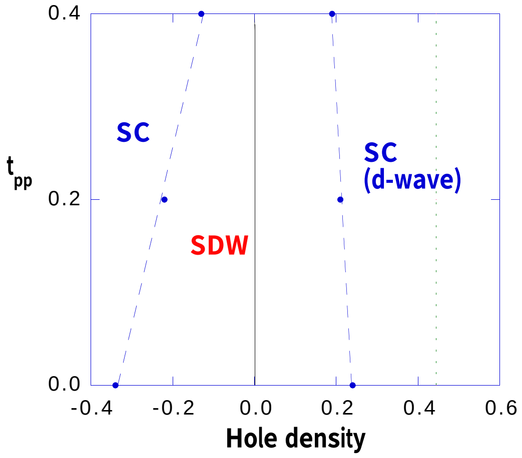


Fig. 1. Phase diagram in the plane of $t_{pp}$ and $\delta$. Parameters are given by $U_d = 8$ and $\epsilon_p - \epsilon_d = 2.0$ in units of $t_{pd}$.

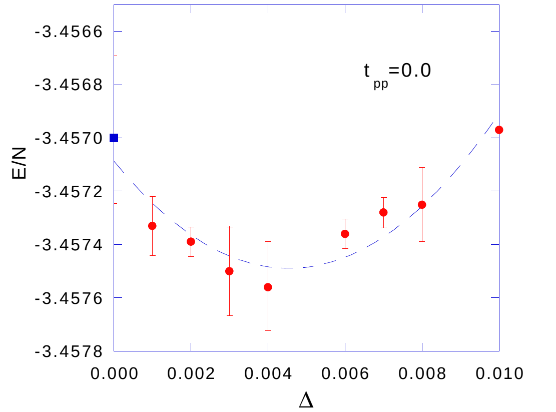


Fig. 2. Energy as a function of SC order parameter $\Delta$ for the AF-BCS state. AF order parameter is optimized for each value of $\Delta$. The hole density is given by $\delta = 0.111$.

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