Phase diagram of the Cu–O model in the oxide superconductors: Variational Monte Carlo study

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Abstract

A variational Monte Carlo method is formulated to study the ground state of the model for the Cu–O plane in the oxide superconductors. The possibility of superconductivity is investigated employing the Gutzwiller-projected BCS and SDW wave functions with respect to dependences on electron density $\rho$ and transfer $t_{pd}$ between neighboring oxygen orbitals. Near half-filling the SDW state is most stable for both the hole and electron doping cases. Away from half-filling when hole doping ratio $\delta \sim 0.2$, the d-wave superconducting state turns out to be more favorable than the SDW state. The superconducting condensation energy is in reasonable agreement with the experimental value obtained from the critical magnetic field $H_c$. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: d–p model; Gutzwiller approximation; Variational Monte Carlo method

1. Introduction

We examine the phase diagram of the oxide high-$T_c$ superconductors based on the three-band Hubbard model for the CuO$_2$ plane, which is called the d–p model in this paper. The Hamiltonian is written as

$$H = e_d \sum_{ia} d_{ia}^\dagger d_{ia} + U_d \sum_{i} d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow}$$

$$+ e_p \sum_{ia} (p_{i+\hat{x}/2,\sigma}^\dagger p_{i+\hat{x}/2,\sigma} + p_{i+\hat{y}/2,\sigma}^\dagger p_{i+\hat{y}/2,\sigma})$$

$$+ t_{pd} \sum_{ia} [d_{i\sigma}^\dagger (p_{i+\hat{x}/2,\sigma} + p_{i+\hat{y}/2,\sigma} - p_{i-\hat{x}/2,\sigma})$$

$$- p_{i-\hat{y}/2,\sigma}) + h.c.]$$

$$+ t_{pp} [- p_{i+\hat{y}/2,\sigma}^\dagger p_{i+\hat{y}/2,\sigma} + p_{i+\hat{y}/2,\sigma}^\dagger p_{i-\hat{y}/2,\sigma}$$

$$+ p_{i-\hat{y}/2,\sigma}^\dagger p_{i+\hat{x}/2,\sigma} - p_{i-\hat{y}/2,\sigma}^\dagger p_{i-\hat{x}/2,\sigma} + h.c.].$$ (1)

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2. Wave functions and results

The wave functions considered in this paper are given by the normal-state Gutzwiller function, the Gutzwiller function with antiferromagnetic long-range order and the Gutzwiller-projected BCS wave function. These types of functions are standard ground state wave functions and have been investigated considerably for the Hubbard orbitals.
Fig. 1. Ground state energy versus doping ratio $\delta$. Parameters are given by $t_{pp} = 0$, $U_d = 8$ and $\epsilon_p - \epsilon_d = 2.0$ in units of $t_{pd}$. Energies for the normal Gutzwiller state, d-wave state and SDW state are shown.

model [1,2]. The parameters in our calculations are the following: $\epsilon_d = -2$, $\epsilon_p = 0$, $U_d = 8$ and $t_{pp} = 0$ or 0.2 in units of $t_{pd}$ for the $6 \times 6$ square lattice.

We show the energy for $t_{pp} = 0$ as a function of the hole doping ratio $\delta$ in Fig. 1. The energy is lowered considerably by the antiferromagnetic long-range order up to 20% hole doping. The energy of the d-wave state is slightly lower than the normal state. In Fig. 2 the phase diagram is shown in the plane of the energy gain $\Delta E/N$ per site and doping ratio. The d-wave state exists in a region for $0.2 < \delta < 0.5$ where the energy gain due to the superconducting order parameter is of the order of $0.0004$–$0.0007$ per site in units of $t_{pd}$. This value is comparable to the value for the Hubbard model [2] and is in reasonable agreement with the experimental superconducting condensation energy estimated from the expression $H_c^2/8\pi$ for the condensation energy [3]. Our preliminary calculations for larger systems suggest that the size dependence of the condensation energy is weak. The extended s-wave state has higher energy than the d-wave state, which is consistent with the large distance behavior of d-wave and ext-s pairing correlation functions in Ref. [4]. The strength of $U_d$ is also important to determine the phase boundary between the SDW and superconducting phases. If $U_d$ is extremely large, the SDW region extends near $\delta \sim 0.5$ for which the d-wave region hardly exists [5]. Our results indicate that the superconducting phase exists for an intermediate value of $U_d$.

References