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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 ρ and transfer t_{pp} 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

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

$\hat{x}$ and $\hat{y}$ represent unit vectors along the x and y directions, respectively. $d_{i\sigma}^\dagger$ and $d_{i\sigma}$ denote the creation and annihilation operators for the d electrons at site R_i. $p_{i\pm\hat{x}/2,\sigma}^\dagger$ and $p_{i\pm\hat{x}/2,\sigma}$ denote the operators for the p electrons at site $R_i \pm \hat{x}/2$. Similarly, $p_{i\pm\hat{y}/2,\sigma}^\dagger$ and $p_{i\pm\hat{y}/2,\sigma}$ are defined. Energies are measured in units of t_{pd}. U_d denotes the strength of the on-site Coulomb interaction among d electrons. For simplicity, we neglect the Coulomb interaction among p electrons. In this paper we examine the ground state properties of the d–p model using the variational Monte Carlo method. In order to understand the properties of superconductivity in the high-T_c oxide superconductors, we should investigate the d–p model taking into account the oxygen orbitals explicitly in the model.

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

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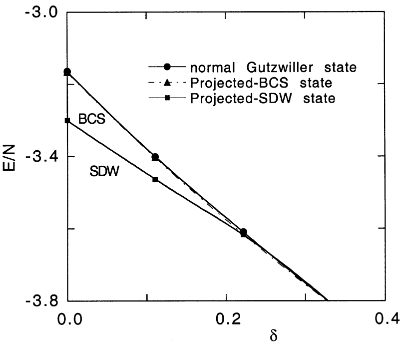

Fig. 1. Ground state energy versus doping ratio δ. Parameters are given by $t_{pp} = 0$, $U_d = 8$ and $\varepsilon_p - \varepsilon_d = 2.0$ in units of t_{pd}. Energies for the normal Gutzwiller state, d-wave state and SDW state are shown.

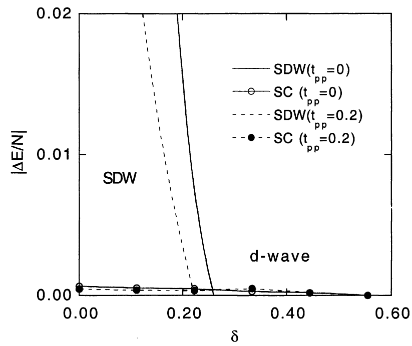

Fig. 2. Energy gain per site $\Delta E/N$ for $t_{pp} = 0$ (solid curves) and $t_{pp} = 0.2$ (dashed curves) as a function of doping ratio δ. The SDW and d-wave regions are shown in the figure.

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

We show the energy for $t_{pp} = 0$ as a function of the hole doping ratio δ 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.

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