Variational Monte Carlo study of the supercondcuting condensation energy on the dependence of $\varepsilon_p - \varepsilon_d$ in the two-dimensional d-p model

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Abstract

The superconducting condensation energy and the numbers of the d- and p-holes as a function of the energy difference $(\varepsilon_p - \varepsilon_d)$ between the oxygen and copper sites in the two-dimensional d-p model have been estimated by use of the variational Monte Carlo method. We have found that the dependence on $\varepsilon_p - \varepsilon_d$ of the superconducting condensation energy in the two-dimensional d-p model seems to be interpreted well when we see from the view point of the numbers of the d- and p-holes.

Key words: superconducting condensation energy, d-p model, $\varepsilon_p - \varepsilon_d$ dependence, variational Monte Carlo method

1. Introduction

Field of the strongly correlated electron systems has been paid much attention since the discovery of the high temperature superconductivity (HTSC) in the cuprate-oxide materials. One important study on HTSC is to clarify the mechanism of the superconductivity of HTSC, and the other important study is to investigate how to find out the material with higher superconducting critical temperature (T_c). One of the most important findings based on the latter point is the relationship between the Madelung potential difference (ΔV_M) between the oxygen and the copper sites and T_c in the case of the optimal doping, first pointed out by Torrance and Metzger [1]. They estimated the values of ΔV_M for each cuprate superconductor. They found the clear correlation between ΔV_M and T_c for the case of the optimum doping.

In this paper we treat the energy difference $(\varepsilon_p - \varepsilon_d)$ between the oxygen and copper sites in the microscopic model, i.e., the two-dimensional d-p model. We are able to treat the effect of ΔV_M in this model. The calculations through this paper have been done for the absolute zero temperature. We estimate the superconducting condensation energy (ΔE) instead of T_c. The higher ΔE is obtained, the higher T_c is expected in general. ΔE was estimated by use of the variational Monte Carlo (VMC) technique [2].

2. Results and Discussion

We consider the $d_{x^2-y^2}$ BCS and SDW wave functions with the Gutzwiller projection operator as the trial wave functions. The energy expectation value is obtained through the Monte Carlo technique, then we optimize the variational parameters so that the lowest energy is obtained. All expectation values we want to obtain are given by this optimized variational wave function with the help of the Monte Calro procedure. The notations we used here are the same as those in the previous paper [3].

As was discussed in the pervious paper [3], we found that near half-filling the SDW state is most stable in a wide range concerning both hole and electron doping cases with $\varepsilon_p - \varepsilon_d = 2$, $t_{pp} = 0.4$, $U_d = 8$ and $U_p =$

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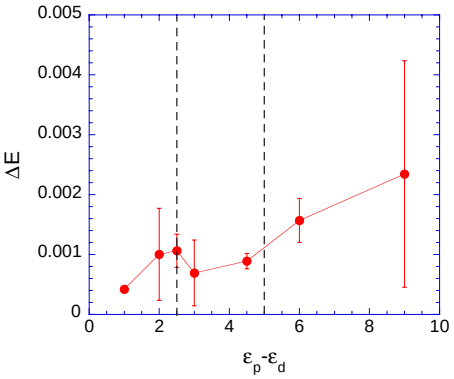

Fig. 1. The obtained superconducting condensation energy as a function of $\varepsilon_p - \varepsilon_d$ in the system of 8×8 lattices. The values of the model parameters are $t_{pp} = 0.4, U_d = 8$ and $U_p = 0$ in units of t_{pd}. The hole number is 80 which corresponds to the doping ratio $\delta = 0.25$.

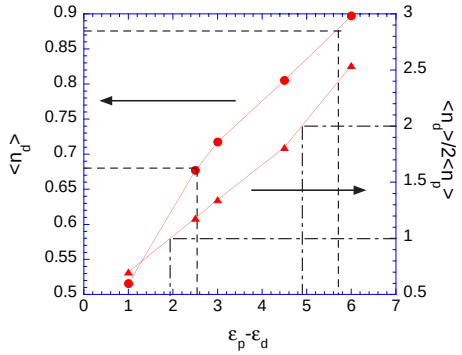

Fig. 2. The expectation values of $\langle n_d \rangle$ (circles) and $\langle n_d \rangle / 2\langle n_p \rangle$ (triangles) are displayed. These values are calculated using the optimized Gutzwiller projected BCS wave function. The values of the model parameters are the same to Fig. 1.

0 in units of t_{pd} for the system size of 8×8 lattices. The $d_{x^2-y^2}$ wave superconducting state turned out to be more favorable than the SDW state when the hole doping ratio is more than or almost equal to 0.2.

In this paper, we have calculated ΔE, the numbers ($\langle n_d \rangle$) of the holes at Cu sites and those ($\langle n_p \rangle$) at the O sites as a function of $\varepsilon_p - \varepsilon_d$. The result is shown by Figs. 1 and 2. We notice that $\langle n_d \rangle$ is less than one for $\varepsilon_p - \varepsilon_d \leq 6$. The inequality $U_d > \varepsilon_p - \varepsilon_d$ are required for HTSC materials, because these materials are considered to be the charge-transfer type insulators. In order to confirm whether $\varepsilon_p - \varepsilon_d$ dependences of ΔE, n_d and n_p are valid or not, we have also calculated ΔE and $\langle n_d \rangle$ in the case of $U_p = 4$ employing the Gutzwiller projection at the O sites with the system size being 6×6. Further, we have also employed the following modified trial function; $\psi = \prod_{<i,j>}(1 - (1 - g_n n_i n_j)) P_G \psi_{BCS}$, where $\langle i, j \rangle$ means nearest neighbor sites and P_G is the Gutziwiller projection operator. Here, g_n appears due to consideration of the nearest-neighbor correlation in the wave function. If the correlation between the long-range separated sites is important for the trial wave function, the large difference for the obtained results between these two trial wave functions is expected. The obtained results shared features qualitatively similar to Figs. 1 and 2. Thus the Gutzwiller projected BCS function is considered to be valid one for our calculation. Therefore, we consider that the results shown in Figs. 1 and 2 are revealing the essence of the superconducting state for the two-dimensional d-p model.

In the view point of the experimetal fact, Torrance and Metzger summarized the relationship between T_c for the case of the optimal doping and the energy difference between a hole on an oxygen and one on a copper site based on the ionic model for each cuprate superconductor [1]. They found the tendency that optimal T_c is raised up by reducing the energy difference. The energy difference they employed corresponds to $\varepsilon_p - \varepsilon_d$ in our model, therefore this seems to contradict with our obtained results for the two-dimensional d-p model at a glance, as is illustrated in Fig. 1. Let us consider whether the experimental facts really contradict with our results or not.

The values of n_d and $n_d/2n_p$ in the superconducting region obtained by NQR/NMR study are between 0.68 and 0.875 for n_d and between 1 and 2 for $n_d/2n_p$ [4]. From Fig. 2, we find that expected value for $\varepsilon_p - \varepsilon_d$ in HTSC materials should be between about 2.5 and 5. This region coincides with the region Ohta et al. have estimated based on the Madelung potential for the various cuprate oxides [5]. As is shown in Fig. 1, our result shows that ΔE is lowered with the increase of $\varepsilon_p - \varepsilon_d$ in this region, although it is quite small and more detailed study is needed. Incidentally, obtained ΔE for $\varepsilon_p - \varepsilon_d = 2$, which is consistent with the value obtained by the first principal calculation, is in fair agreement with the value estimated by the specific heat and critical field measurements for optimally doped samples, as in the case of the two-dimensional Hubbard model [6]. Therefore, it is possible that our obtained results are quite successful in reproducing the tendencies of the experimental facts.

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