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Cluster Calculation of CuO_2 in High-T_c Superconductors

by

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Cluster Calculation of CuO_2 in High-T_c Superconductors

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Abstract

The eigenvalues of a small cluster in the CuO_2 plane are obtained by exactly diagonalizing the extended Hubbard Hamiltonian. This eigenenergy spectrum is used for the grand partition function. The magnetic and thermodynamic quantities such as the magnetic susceptibility and specific heat are calculated with different occupation numbers and discussed in terms of the excited states of the system.

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I. Introduction

Since the discovery of superconductivity in oxide compounds [1], many theoretical and experimental studies were carried out for the pairing mechanism on these compounds. For most crystalline solids, the electronic properties are well described by the band theory in terms of a one-body Hamiltonian. But it is now generally believed that the superconducting oxide compound do not fit this description. In this case, the excitations of these systems are totally beyond the description of the band-structure approximation. Therefore, in this paper, we study the magnetic and thermodynamic properties in a small cluster with an appropriate extended Hubbard Hamiltonian, because those properties mainly depend on the excitation spectrum of the system.

Even though the high-temperature oxide superconductors have some similarities with conventional superconductors, there seems to be a fundamental difference for pairing mechanism. In conventional superconductors, the attraction between two electrons arises from the phonon exchange, where the retarded phonon attraction is able to overcome the screened Coulomb repulsion between two electrons. However it is very hard to consider a similar mechanism for high-temperature oxide superconductors with short coherent length $\xi_x \sim d$, where d is the interparticle distance between electrons. The wide range of energy gap instead of a sharp gap observed in most tunneling measurements [2] seems due to the fluctuation effect, which is expected to be considerably large due to the short coherent length. More recently discovered n-type superconductors[3], which have similar crystal structures to the p-type, provide additional information about these compounds: (1) the superconducting pairs occur in purely two dimensions, and (2) there must be electron-hole symmetry for whatever band is used in the Hamiltonian.

Ⅱ. Theory

The central physics in the theory of high-temperature superconductivity centers on which effective Hamiltonian one should take to describe the electrons in the CuO_2 plane. The high-T_c compounds can be explained well by the extended Hubbard Hamiltonian. In previous papers[4], we have pointed out two important physical features of the pairing of electrons and holes in n-type and p-type oxide superconductors, respectively: (i) the vacuum level must be defined as (d^9p^6) for the copper and oxygen sites instead of the closed orbit configuration ($d^{10}p^6$) used by other [5]. x-ray absorption spectra show that the charge carriers (electrons) are mostly located on the copper sites (Cu^{+}) in n-type superconductors[6], while the charge carriers (holes) are located on oxygen sites (O^{1-}) in p-type superconductors [7]. By this observation, it is appropriate to define the vacuum level to be (d^9p^6), which is an undoped configuration for both types and plays a critical role for fixing the electron and the hole energy levels. (2) Since holes are not true particles but are the empty states which represent the absence of electrons, we have to be more careful in setting up the Hubbard Hamiltonian. Generally the on-site Coulomb repulsion is introduced in the Hubbard Hamiltonian when two electrons occupy the same orbit. This cannot be the case for the hole states. If one electron is removed from two electron states of the given orbit, i. e., one hole is created, the on-site Coulomb repulsion disappears.

In other words, the on-site Coulomb repulsion, which is usually the largest parameter in the Hubbard Hamiltonian, appears whenever a hole is created from the given closed shell orbit instead of when two holes are created.

Considering the above two features, the extended Hubbard Hamiltonian can be written as [4]

$$\begin{aligned} H = {} & t_{pd} \sum_{\langle i,j \rangle}{}' \left(d^{h+}_{i\sigma} p_{j\sigma} + d^{e+}_{i\sigma} p^{+}_{j\sigma} + h.c. \right) \\ & - \sum_{j,\sigma} (E_d + U_d)\, d^{e+}_{j\sigma} d^{e}_{j\sigma} + \sum_{j,\sigma} E_d\, d^{h+}_{j\sigma} d^{h}_{j\sigma} \\ & - \sum_{j,\sigma} (E_p - U_p)\, p^{+}_{j\sigma} p_{j\sigma} - \sum U_p\, n_{j\sigma} n_{j\sigma'} \\ & - \sum_{\substack{i,j \\ \sigma,\sigma'}} U_{pd}\, n^{e}_{i\sigma} n^{h}_{j\sigma'} \quad , \end{aligned} \tag{1}$$

where t_{pd} is the hopping integral between neighboring Cu and O sites, and the $d_i\sigma$'s and $p_i\sigma$ are second quantization operators related to the Cu and O sites, respectively. The superscripts h and e on the Cu site operators represent the holes $Cu^{3+}(d^8)$ and electrons $Cu^{1+}(d^{10})$, explicitly. The prime on a summation indicates $i \neq j$, and $<i, j>$ indicates nearest neighbors between the Cu and O sites. E_d and E_p are the diagonal kinetic energies of the 3d and 2p orbitals, respectively. The electron-hole pair creation potential U_{pd} in the last term of the Hamiltonian is introduced to account for the largest valence change difference when an electron on an O site moves to a neighboring Cu site, ie. e., $Cu^{2+}(d^9) + O^{2-}(p^6) \rightarrow Cu^{1+}(d^{10}) + O^{1-}(p^5)$. As mentioned earlier, the on-site Coulomb repulsions U_d and U_p appear when an electron is created on a Cu site or a hole is created on an O site. With the condition $E_d + U_d > E_p - U_p$, the undoped La_2CuO_4 and Nb_2CuO_4 nominally consist of $Cu^{2+}$and O^{2-}, and the holes introduced by doping with the divalent Sr in La_2CuO_4 occupy the oxygen orbitals in p-type superconductors, while the electrons introduced by doping with the tetravalent Th in Nd_2CuO_4 occupy the copper orbitals in n-type superconductors. Clearly this observation is due to the presence or absence of electrons in the antibonding states of $Cu(d_{x^2-y^2})$ and $O(p_x$ or $p_y)$ orbitals.

We believe this hybridization is strongly related to the quick disappearance of the antiferromagnetic background on the Cu sites with a small amount of doping. Even though the direct hopping integral (t_{oo})between neighboring oxygen sites is not negligible, the direct oxygen band is supposed to be much lower than the antibonding states of the Cu and O orbitals[8] due to the condition $E_d + U_d > E_p + U_p$. Therefore, the direct oxygen hopping integral is not included in the Hamiltonian.

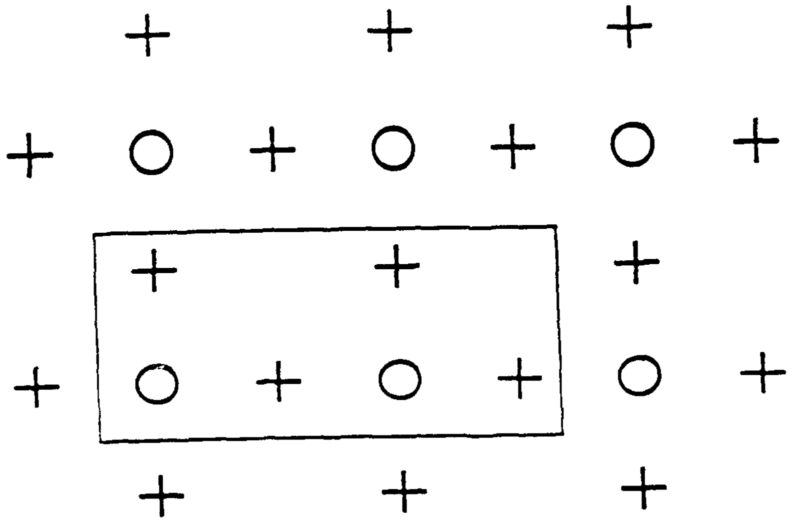

Fig 1.The cluster considered in the calculation includes two unit cells in the CuO_2 square lattice. The copper sites and oxygen sites are represented by the circles and plus signs, respectively.

Based on the above arguments, we have proposed a local pairing mechanism and estimated the binding energy of two carriers in a previous paper[4]. In the present study, we examine the magnetic and thermodynamic quantities such as the magnetic susceptibility and specific heat by exact diagonalization on small two-dimensional clusters of two unit cells on a CuO_2 lattice as shown in Fig. 1. By introducing the chemical potential μ into the Hamiltonian, we can allow the number of electrons to vary in this system. In this case, all the second quantization operators in Eq.(1) can be changed to the true electron representation without the hole picture. Information on the interaction between the cluster and the rest of the system is also included in the chemical potential. The Hubbard Hamiltonian, Eq.(1), of this system is now modified in the presence of a uniform magnetic field as

$$
\begin{aligned}
H = {} & t_{pd} \sum_{\langle i,j \rangle}{}' (d^{+}_{i\sigma} p_{j\sigma} - h.c.) \\
& - \sum_{i,\sigma} E_d\, d^{+}_{i\sigma} d_{i\sigma} - \sum U_d\, n_{i\sigma} n_{i\sigma'} \\
& - \sum_{j,\sigma} E_p\, p^{+}_{j\sigma} p_{j\sigma} - \sum_{j} U_p\, n_{j\sigma} n_{j\sigma'} \\
& - \sum_{\substack{\langle i,j \rangle \\ \sigma,\sigma'}} U_{pd}\, n_{i\sigma} n_{j\sigma'} - \mu \sum_{i,\sigma} n_{i\sigma} - \gamma B \sum_{i} (n_{i\sigma} n_{i\sigma'})
\end{aligned}
\qquad (2)
$$

where γ is the magnetic moment of the electron, and the uniform magnetic field B is perpendicular to the CuO_2 plane.

The eigenvalues of the above Hamiltonian can be obtained by diagonalizing exactly in a small cluster system. The grand partition function Z can be written immediately with the eigenvalues. To calculate the magnetic and thermodynamic quantities, we have to first evaluate the chemical potential of the system for the given occupation numbers. The chemical potential can be determined by inverting the expression

$$
\langle N \rangle = K_B T \left[\frac{\partial \, \ell n Z}{\partial \mu} \right]_{T,V} \qquad (3)
$$

in terms of the occupation number N and the other parameters in the Hamiltonian. The magnetic susceptibility χ and the specific heat C_v can be calculated with a knowledge of the grand partition function and the chemical potential in the usual manner.

Ⅲ. Numerical Calculations and Discussion

Considering four possible states per site, the given clusters has 4^N eigenvalues and eigenvectors. Since the Hamiltonian is isotropic in spin space, the total spin S and its z-component S_z are good quantum numbers. Then the $4^N \times 4^N$ Hamiltonian matrix can be reduced to many blocks with different number of occupations. In the following calculations, we have used these reported parameters, which are in the most acceptable range [8]: $\Delta E = 1.5$ eV, $t_{pd} = 1.2$ eV, $U_d = 9.0$ eV, $U_p = 6.0$ eV and two different values of (1) $U_{pd} = 0.0$eV, (2) $U_{pd} = 1.5$ eV. In all cases, it is found that the ground state in the state is the state with minimal $|S_z|$. This result is due to the relatively large hopping integral t_{pd} and more degree of freedom with less $|S_z|$. The behavior of the magnetic and thermodynamic quantities in the cluster model can be understood from the excitation spectra. In Figs. 2 and 3, we have shown the magnetic susceptibility and specific heat curves of the two unit-cell model for $N = 10$, which is a vacuum cofiguration in our definition. The low-temperature peaks in these figures are due to the transition from the ground state of singlet spin configuration on two copper sites to the triplet spin configuration which is the first excited state. By contrast, these peaks disappear for $N = 9$ and $N = 8$, which are shown in Figs. 4 through 7.

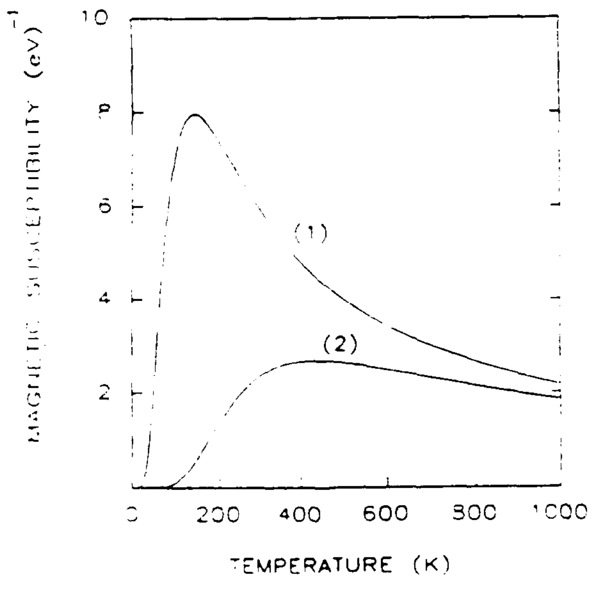

Fig 2. **Magnetic susceptibility curves** $(x/2r^2)$ for $N = 10$ with (1) $U_{pd} = 0.0$eV and (2) $U_{pd} = 1.5$eV.

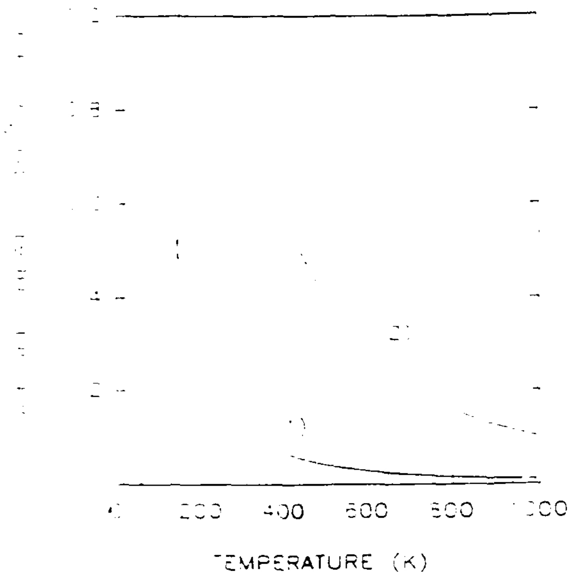

Fig. 3 **Specific heat curve** (C_V/N) for N= 10 with (1) U_{pd}= 0.0eV and (2) U_{pd}= 1.5eV.

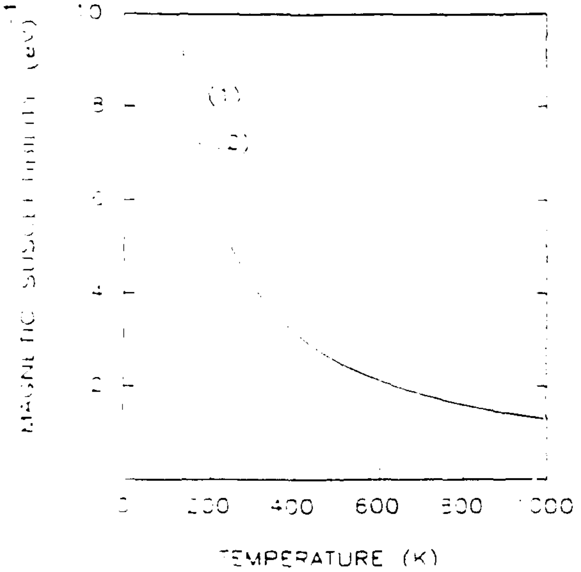

Fig. 4 **Magnetic susceptibility curves** ($\chi/2r^2$) for N= 9 with (1) U_{pd}= 0.0 eV and (2) U_{pd}= 1.5eV.

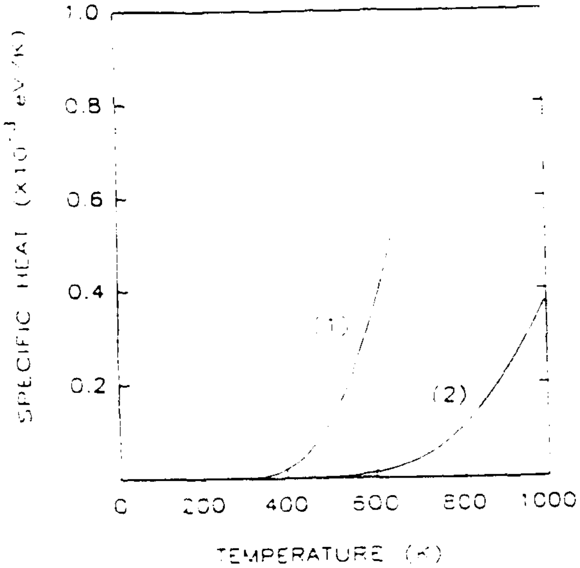

Fig. 5 **Specific heat curves** (C_v/N) for N= 9 with (1) U_{pd}= 0.0eV and (2) U_{pd}= 1.5eV.

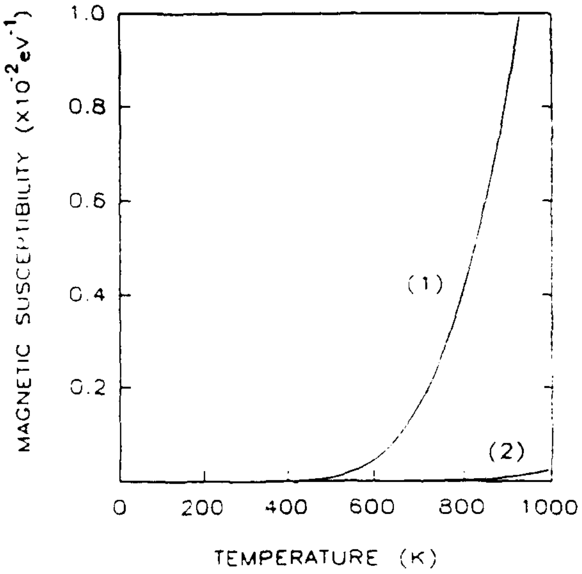

Fig. 6 **Magnetic susceptibility curves** ($x/2r^2$) for N= 8 with (1) U_{pd}= 0.0 eV and (2) U_{pd}= 1.5eV.

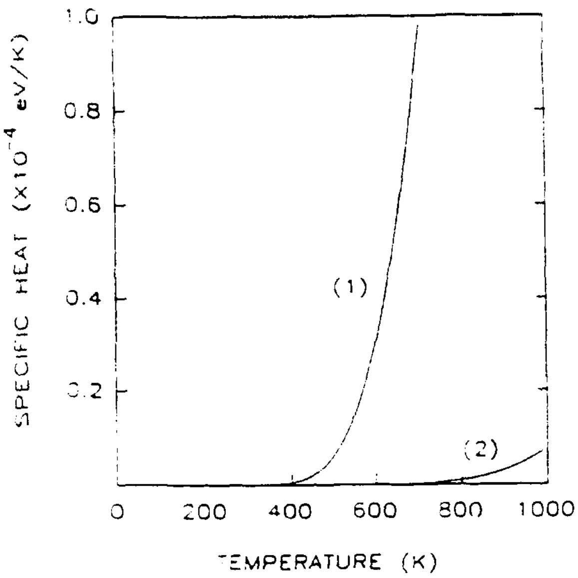

Fig. 7. **Specific heat curves** (C_V/N) for $N= 8$ with (1) $U_{pd}= 0.0$eV and (2) $U_{pd}= 1.5$eV.

For more than half-filling cases ($N>6$), the energy spectrum can roughly be divided into some groups with spacings of on-site Coulomb repulsion U_d or U_p, and the spacings between successive levels within the same group are expected to be on the order of t^2_{pd}/U_d or t^2_{pd}/U_p. As it turns out in our numerical calculations, the energy spacings between the ground state and the first excited state are greater than 0.5 eV for all cases except the vacunm configuration $N= 10$. The energy difference between the ground state ($S_t= 0$) and first-excited state ($S_t= 1$) results in 30 meV~60meV for $N= 10$ with various parameters in the Hamiltonian. This energy difference gives the superexchange parameter J between neighboring copper sites in the Heisenberg representation,

$$H= J\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j \qquad (4)$$

which is a good approximation for an undoped material[9]. J can be obtained alternatively by the fourth-order perturbation approximation to Eq.(1)[4],

$$J=\frac{4t^4_{pd}}{(\Delta E+U_d+U_{pd}+U_p)^2}\left[\frac{1}{U_d}+\frac{2}{2\Delta E+2U_d+4U_{pd}-U_p}\right] \qquad (5)$$

which has very good agreement with the above numerical result.

In Fig. 4, two magnetic susceptibility curves almost overlap and decreases monotonically as T increases because the ground level has a minimal $S_Z = 1/2$, which is different from the case of the $N = 8$ and $N = 10$. In Fig. 6, the magnetic susceptibility are increasing with increasing temperature as in Fig. 2, but no peaks appear under 1000 K due to the large excitation energy from the ground state, as explained earlier. These qualitatively different types of behavior of the magnetic susceptibility are merely caused by the smallness of the cluster. With the same explanation of large excitaiton energy from the ground state, the specific heat curves in Figs. 5 and 7 have no peaks in the low-temperature regime.

Ⅳ. Conclusions

The extended Hubbard Hamiltonian has been solved for clusters of two unit cells by an exact diagonalization. The ground states are always related to the minimal $|S_Z|$ configuration. The energy spectrum is grouped with the order of on-site coulomb repulsion U_p or U_d, and the successive levels in each group are separated at the order of t^2_{pd}/U_d or t^2_{pd}/U_p. But the first excited state in an undoped regime is the order of superexchange energy between nearest-neighbor copper sites, which agrees well with the result obtained by the fourth-order perturbation calculation. This small excitation energy contributes to the low-tempertaure peaks in the magnetic susceptibility and specific heat curves for $N = 10$. Due to the large excitation energy for the other configuration, no peaks appear in the magnetic susceptibility and specific heat curves in the low-temperature regime. From these results, we may conclude that the low-temperature physical anomalies appear only near the undoped regime. The magnetic susceptibility curve for the case of $N = 9$ is essentially of the Curie form, monotonically decreasing as temperture increases. This is due to the odd number of electrons in a small cluster. We believe that this kind of behavior will be diminshed if we increase the size of the cluster.

Finally, we would say that the results obtained in this calculation are all very stable with a wide range of parameters in the Hamiltonian.

Therefore, the qualitative nature of the results does not change within the acceptable parameter ranges, even though we have shown only two different values of U_{pd}, which is supposed to be the most uncertain.

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