Physica C 235-240 (1994) 2183-2184
North-Holland

PHYSICA C

Consistent Low-Energy Reduction of the Three-Band Model for Electrons and Holes in Copper Oxides to the Effective t−J Model

V.I. Belinicher, A.L. Chernyshev and L.V.Popovich [a] *

[a]Institute of Semiconductor Physics, 630090, Novosibirsk, Russia

A full three-band model for the CuO_2 plane with inclusion of all essential interactions - Cu-O and O-O hopping, repulsion at the copper and oxygen and between them - is considered. A general procedure of the low-energy reduction of the primary Hamiltonian to the Hamiltonian for holes and electrons is developed. For the purpose of fixing of the t-J model parameters we calculate the values of the superexchange constant J and the charge-transfer gap E_{gap} in the framework of the three-band model. Fitting values of J and E_{gap} to the experimental data allows to narrow the uncertainty region of the three-band model parameters. As a result the ratio t/J of the t-J model is fixed in the range $2.4 \div 2.7$ for holes and $2.5 \div 3.0$ for electrons.

1. INTRODUCTION

The problem a structure of the charge carriers remains as the key problem for the high-temperature superconductors on the base of copper oxides. Its complexity is caused by strong correlations in the motion of electrons and holes that can not be considered free in the framework of the band theory. Thus, the undoped copper oxides are the Mott dielectrics or, more rigorously, the charge-transfer dielectrics, in contrast with metal in an uncorrelated case. Doping of the CuO_2 planes by electrons or holes creates strongly doped semiconductor with either the long-range or short-range antiferromagnetic order. It follows from the band calculations and the spectroscopic data that the three-band Hubbard model or the Emery model incorporates in itself the most important characteristics of the electron excitations.

The purpose of our work [1] - [3] was finding the low-energy limit of the three-band model for the electron excitations in CuO_2 planes. The general case of the three-band model in the region of parameters consistent with the known band calculations and spectroscopic data was considered. We have taken into account all essential energy parameters in the framework of the three-band model: ϵ_p and ϵ_d are realistic values of the Cu and O energy levels; U_d, U_p and V_{pd} are Coulomb repulsions at Cu and O sites and between them, respectively; t_{pd} and t_{pp} are hopping integrals between Cu and O and between O and O, respectively. No parameters are supposed to be small.

Different experimental atomic and band calculations show that: $U_d = 5 \div 7$ eV, $7 \div 11$ eV, $U_p = 3 \div 8$ eV, $V_{pd} = 0 \div 1.7$ eV. U_p is always less than U_d. There is a general agreement for the $Cu-O$ system that $\Delta = \epsilon_p - \epsilon_d > 0$ and $< U_d$. It reflects the facts that first hole at unit cell is predominantly at Cu site and added hole has an oxygen's character. $t_{pd} = 1 \div 1.6$ eV (and it is unlikely that it less than 1 eV) , $t_{pp} = 0.5 \div 0.7$ eV. This set of magnitudes we will call hereafter as a realistic region of parameters.

2. THE LOW-ENERGY LIMIT OF THE THREE-BAND MODEL

Our method of the low-energy reduction has been based on construction of a set of local states with different number of holes over the filled atomic orbitals. The most essential states are:
1) The vacuum state or the vacancy which is simply

$$|v> = |0>, \qquad (1)$$

*This work was supported by the Council on Superconductivity of Russian Academy of Science, Grant N 93197; Russian Foundation for Fundamental Researches, Grant N 94-02-03235; The Competition Center for Natural Sciences at St.-Peterburg State University, Grant N 94-5.1-1060; The International Science Foundation by travel grant N 1490 1.

SSDI 0921-4534(94)01657-7

which is the state with filled Cu^+ and 0^{2-} orbitals in the elementary cell.

2) The one-hole states which represent the ground state of CuO_2 plane

$$|f\alpha> = U|d\alpha> - V|p\alpha>, \quad (2)$$

where $|d\alpha>$ and $|q\alpha>$ are the copper and symmetrical oxygen hole states with spin projection α, respectively.

3) The two-hole states which are the Zhang-Rice singlets:

$$|c> = U_1|d\uparrow d\downarrow> + V_1|q\uparrow q\downarrow> + W_1(|d\uparrow q\downarrow> - |d\downarrow q\uparrow>)/\sqrt{2}. \quad (3)$$

The coefficients U, V, U_1, V_1, W_1 are functions of the parameters . At half filling the Hamiltonian of the three-band model is reduced to the Heisenberg Hamiltonian with spin$-1/2$ (2) which are antiferromagnetically ordered due to the second-order virtual transitions through the set of two-hole states. Note, that above-named spins$-1/2$ are exactly states $|f\alpha>$ (2). It has been shown [2],[3] that for the case near to half filling the Hamiltonian of the three-band model is reduced to the Hamiltonian of the t-J like model of singlets, vacancies and spins. This model is characterized by five parameters E_v, E_c, t_e, t_h and J. The constants E_v and E_c are the local energies of a vacancy and singlet; t_e and t_h are the hopping integrals for a vacancy and singlet (electron and hole), respectively; J is the exchange constant. All these parameters are functions of the three-band model parameters. It has been shown that relative magnitudes of the omitted terms are of the order of ten percent [2],[3]. We believe that the three-band model describes many important properties of the cuprates. Therefore, the real values of its parameters are of great interest.

3. CALCULATION OF THE OBSERVABLE QUANTITIES

As was noted above the parameters of the primary model are known with low precision. In this situation calculation of observable quantities is an urgent issue since it provides a way to fix these parameters. The best defined experimental data which we can describe quite accurately are the superexchange constant J and the charge-transfer gap E_{gap}.

The expression for the AF coupling constant J in the framework of our approach is

$$J = -2h_1V^4U_p + \sum_n x_n \frac{|D_n|^2}{\Delta E_n}. \quad (4)$$

The first term in Eq.(4) represents the exchange energy between the two holes due to the repulsion at an oxygen. The second term in Eq.(4) represents the correction to energy due to the virtual transition of hole from state (2) into the two-hole state and back [3]. The expression for the change-transfer energy is:

$$E_{gap} = E^0_{gap} + \Delta E_e + \Delta E_h \quad (5)$$

Where E^0_{gap} is the difference in energies between a singlet and vacancy at local states separated by large distance and the ground state; ΔE_e and ΔE_h are depths of bands for an electron and hole (a vacancy and singlet). E^0_{gap} can be calculated in the framework of the three-band model, whereas for the calculation of ΔE_e and ΔE_h we use the t-J model: $\Delta E = -1.255t$. This formula is quite good up to $t/J \approx 5$.

In the framework of our approach we have calculated the exchange constant J = 0.14 eV (for lantan system) and the charge - transfer gap E_{gap} = 2.1 eV. The values of J and E_{gap} known from experiment give us possibility to fix with greater precision the hopping parameters t_e and t_h for electrons and holes. We have found that t_e = (2.4 ÷ 2.7)J, t_h = (2.5 ÷ 3.0)J. These values of t_e and t_h parameters are to be used for further calculations of the electrical and magnetic properties of copper oxides in the framework of the t-J model.

REFERENCES

1. V.I.Belinicher and A.L.Chernyshev, Phys. Rev., 1993, v. B47, p. 390.
2. V.I.Belinicher and A.L.Chernyshev, Physica C, 1993, v. 213, p. 298.
3. V.I.Belinicher and A.L.Chernyshev, Phys. Rev., 1994, B49, N14, p. 9746.