Four-band model for oxygen holes in copper oxide superconductors. II. Phase diagram

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Transport in the doped lamellar copper oxides is carried by quasiparticles, composed of holes which move on the oxygen ions on the CuO_2 planes, with strong magnetic coupling to the neighboring Cu spins. In the preceding paper, we calculated the bands of these quasiparticles. In the present paper, we use the lowest of these bands to obtain the critical temperature T_c as a function of the concentration of holes in these planes, using simple BCS equations. We find that the pairing interaction induced by the magnetic frustration model of Aharony *et al.* yields a phase diagram which is quite similar to the one observed experimentally, provided that one allows hopping between the planes, of order 0.03 eV. We discuss the variation of the phase diagram with the different hopping and interaction parameters. Some features should apply beyond the scope of our specific model.

I. INTRODUCTION

In the preceding paper,[1] we studied the properties of the charge carriers in the CuO_2 planes of the copper oxide high-temperature superconductors (HTSC). We assumed long-range AFM (antiferromagnetic) correlations, identified the form of the favored quasiparticle (which is composed of the eigenstates of the interaction between the oxygen hole and the spins of its two neighboring coppers) and calculated its spectrum using the tight-binding model. Since the hopping amplitude of the quasiparticles depends on the magnetic environment, we had tight-binding cells that consist of four oxygen sites and thus yielded four bands for the spectrum of the quasiparticles. For the actual calculation of the hopping amplitudes we used the effective Hamiltonian, which is derived from a three-band Hubbard model.[2] In the present paper, we use the lowest of these bands to obtain the dependence of T_c on the concentration of holes in the CuO_2 planes.

Original attempts to apply new models such as the resonating valence bond (RVB) or anyons were not very successful. On the other hand the basic assumptions of the BCS theory[3] were supported experimentally. Specifically, the existence of an energy gap was demonstrated by infrared absorption,[4] Andreev reflection,[5] Raman scattering, and tunneling.[5,6] Measurements of flux quantization and Josephson effect[7] show that the charge of the basic charge carrier is $(2e)$, which indicates the existence of Cooper pairs. These experiments and many others support the idea that the BCS theory is a reasonable starting point. Nevertheless, there have been suggestions to modify the simplified original solution of BCS. Suggested modifications included using band calculation methods to obtain the band spectrum and use it explicitly in the BCS equation,[2,8,9] evaluating a more realistic coupling instead of the simplified assumption of a constant coupling (e.g., due to enhanced Coulomb screening),[10] taking into account other channels of interactions such as a magnetic mechanism,[2,8] considering different quasiparticles,[2] and considering the consequences of the very short coherence length.[11] In our approach we use such modifications as well. We use the explicit form of the lowest band that we derived in the previous paper and we take into account the role of the magnetic interactions in the pairing mechanism. For these interactions, we use the expressions for the frustration model of Aharony and co-workers.[12] Although our results are presented in the context of that model, their qualitative significance is quite general. Particularly, we demonstrate how solutions of the BCS equations depend on variations in the band structure (e.g., the hopping between planes) and in the pairing interaction (e.g., as a result of varying the ratio between on-site and nearest-neighbor cell interactions).

As we have already mentioned in our previous paper, there are experimental indications that the phase diagrams of $La_{2-x}Sr_xCuO_4$ (Ref. 13), $YBa_2Cu_3O_{6+y}$ (Ref. 14), and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ref. 15), are similar when we measure T_c as a function of the concentration of holes in the CuO_2 planes. For $La_{2-x}CuO_4$, all additional holes (at least for $x \leq 0.15$) are introduced into the CuO_2 planes. Thus, since x is known, the phase diagram is measured directly. However, in the other two compounds not all the additional holes reside in the CuO_2 planes and the determination of x involves assumptions concerning their distribution. Thus, their phase diagrams are obtained in an indirect and less precise manner. Nevertheless, the different phase diagrams strongly support the suggestion that the concentration of holes in the CuO_2 planes is a key factor in the HTSC. Therefore, we calculate the dependence of the critical temperature on the concentration of holes in the CuO_2 planes. Our major result is that when we use a coupling that is induced by the magnetic frustration model, we obtain a phase diagram that has features, which are similar to those observed experimentally. The rest of the paper is organized as follows: in Sec. II we discuss the magnetic coupling, in Sec. III we solve the BCS equations to calculate the phase diagrams, and in Sec. IV we summarize.

II. THE MAGNETIC COUPLING

The existence of magnetic correlations in the superconducting phase of the HTSC may indicate that magnetic interactions have an important role in the pairing mechanism. The possibility that superconductivity in the HTSC is mainly due to magnetic interactions between holes in the CuO_2 planes, was one of the important results of the "magnetic frustration model" that was introduced by Aharony and co-workers.[12] They argued that a hole that resides on an oxygen site induces ferromagnetic coupling between its two copper neighbors. Since in the absence of oxygen holes the copper spins have nearest-neighbor AFM couplings, the additional holes frustrate the spin system. When two holes are added, it was found that it is energetically favored for the holes to be "close." Thus, one may say that there is an attractive potential between the two holes. It was also observed that holes that have antiparallel spins have larger attraction (taking into consideration also the Coulomb repulsion) than holes that have parallel spins. Therefore, we assume hereafter a singlet pairing of the superconducting holes.

The potential presented in Ref. 12 implies that two holes would prefer being on two neighboring tight-binding cells and they repel each other when they reside on the same cell. Therefore, in wave-vector space the magnetic coupling has the following form:

$$V_m(\mathbf{q})=-V_0-V_1(\cos q_x+\cos q_y+b\cos q_x\cos q_y)\ , \quad (2.1)$$

where V_0 is the constant coupling, which reflects the on-site coupling in real space, and V_1 is the coefficient of the q-dependent part of the coupling, due to the nonlocal magnetic interaction. The value of b is determined by the ratio between the attraction of two holes that reside on nearest-neighbor cells and that of two holes that reside on *next-* nearest-neighbor cells. For the simple case of Ising spins that was considered in Ref. 12, we compared the average attraction in both cases (we should average, since there are four possible locations in each cell) and we found it to be 4/9 thus $b=8/9$. This is only an approximation, since in our model the charge carriers are quasiparticles that are composed of three Heisenberg spins.

The form of the coupling implies that the gap may have the following general form

$$\Delta(\mathbf{q})=\Delta_0+\Delta_i\cos q_x+\Delta_1'\sin q_x+\Delta_2\cos q_y+\Delta_2'\sin q_y+2\Delta_3\cos q_x\cos q_y+\Delta_3'\cos q_x\sin q_y+\Delta_3''\sin q_x\cos q_y+\Delta_4\sin q_x\sin q_y\ . \quad (2.2)$$

As we mentioned before, the singlet pairing is favored. Therefore, we keep only the symmetric parts in the gap. Thus,

$$\Delta(\mathbf{q})=\Delta_0+\Delta_1\cos q_x+\Delta_2\cos q_y+\Delta_3\cos q_x\cos q_y+\Delta_4\sin q_x\sin q_y\ . \quad (2.3)$$

III. THE BCS EQUATION

In this section we solve the BCS equation for the assumed coupling and gap in order to obtain T_c as a function of the concentration of holes in the CuO_2 planes. In the preceding paper we calculated the bands in the plane, completely neglecting the hopping between the planes. This was justified for the properties that we calculated. However, for the use of the BCS equation we cannot neglect this coupling. To take it into account, we add a simple tight-binding hopping in the z direction and we obtain the following spectrum

$$\varepsilon_{\mathbf{k}}=\varepsilon_{\parallel}(k_{\parallel})+\varepsilon_z(k_z)\ , \quad (3.1)$$

where $\varepsilon_{\parallel}$ is the spectrum that we obtained from the four-band model in the plane and $\varepsilon_z(k_z)=c\cos k_z$. For the value of c we follow Schnieder and Frick[16] who used $c=0.03$ eV based on photoemission data. As we see in Fig. 1, the value of c greatly affects the shape of the density of states. It is clear that as c is increased we cross over from a typical two dimensional tight-binding model (including also the van Hove singularity) to a three-dimensional shape, and in the extreme limit of very large c we observe the shape that is typical to the one dimensional tight-binding model. The results of Figs. 2, 3, 4, and 6 were derived with $c=0.03$ eV.

In order to determine T_c we substitute $\Delta(\mathbf{q})$ in the BCS equation and since Eq. (2.3) has five parameters we obtain five equations (instead of one in the simple BCS case). For the first four parameters the equations may be written in a matrix form,

$$\begin{bmatrix} 1-V_0F_{0,0} & -V_0F_{1,0} & -V_0F_{0,1} & -V_0F_{1,1} \\ -V_1F_{1,0} & 1-V_1F_{2,0} & -V_1F_{1,1} & -V_1F_{2,1} \\ -V_1F_{0,1} & -V_1F_{1,1} & 1-V_1F_{0,2} & -V_1F_{1,2} \\ -bV_1F_{1,1} & -bV_1F_{2,1} & -bV_1F_{1,2} & 1-bV_1F_{2,1} \end{bmatrix} \begin{bmatrix} \Delta_0 \\ \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{bmatrix} =0\ , \quad (3.2)$$

where

$$F_{m,n}=\frac{1}{N}\sum_k \frac{\tanh(\beta\varepsilon_k/2)}{2\varepsilon_k}\cos^m k_x\cos^n k_y\ , \quad (3.3)$$

$\beta=1/k_BT$ (k_B is Boltzmann's constant and T is the temperature) and N is the number of sites. For the parameter Δ_4 we obtain

$$1=\frac{V_1}{N}\sum_k \frac{\tanh(\beta\varepsilon_k/2)}{2\varepsilon_k}\sin k_x\sin k_y\ . \quad (3.4)$$

We identify T_c as the highest temperature at which either the determinant of the matrix in Eq. (3.2) is zero or Eq. (3.4) is solved. We find that we always obtain lower temperatures for the latter case. Therefore, we consider only

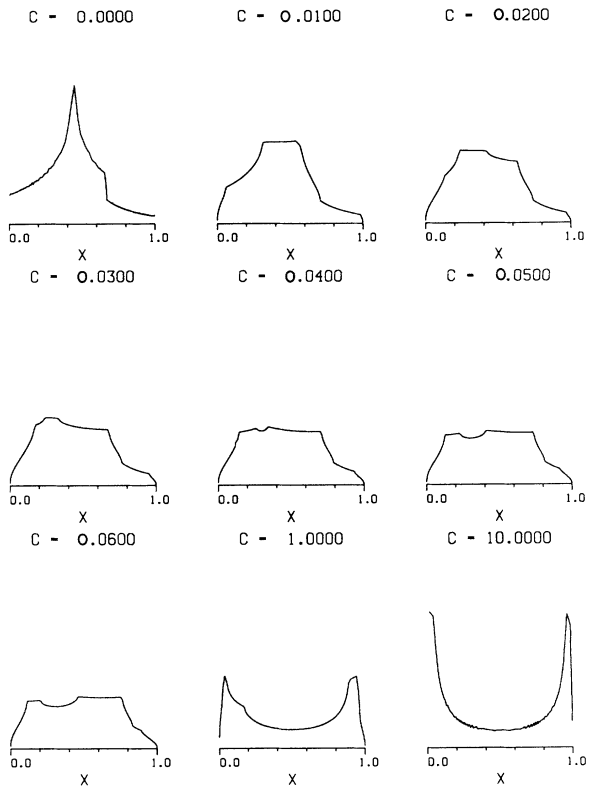

FIG. 1. The density of states for various values of c.

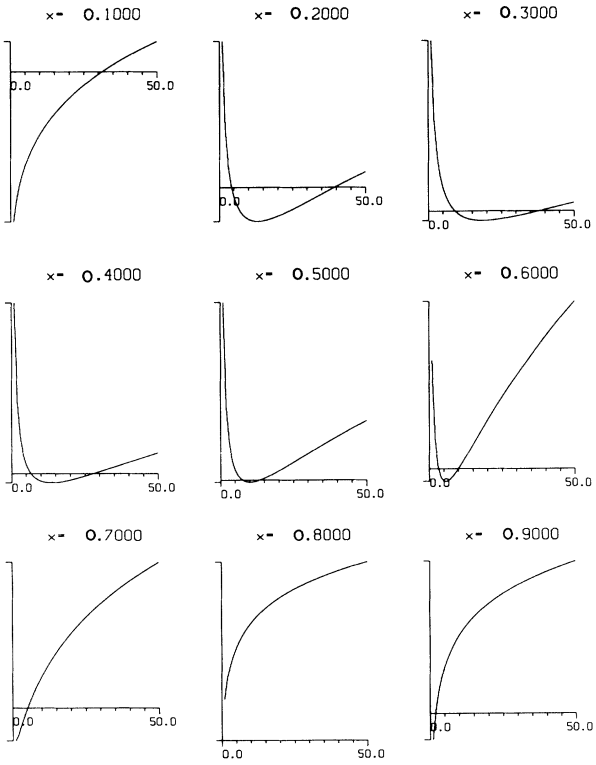

FIG. 2. The determinant of Eq. (3.2) as a function of temperature for various concentration values, where $V_0=0$ and $V_1=0.07$ eV.

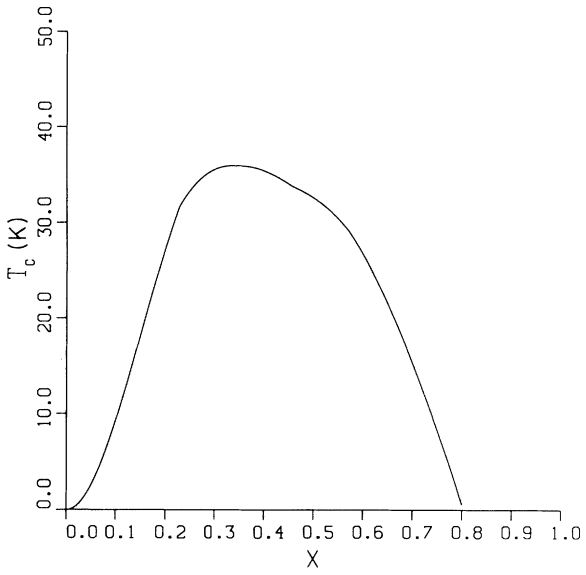

FIG. 3. The Phase diagram, where $V_0=0.04$ eV and $V_1=0$.

Eq. (3.2) (in Fig. 2 we present some examples of the dependence of the determinant on the temperature). The dependence of T_c on the concentration enters through the determination of the Fermi energy (which is chosen so that it yields the required concentration at low temperatures). Thus, since T_c clearly depends on the Fermi energy, we can calculate T_c as a function of x.

We first assume a constant coupling where $V_1=0$ and we adjust $V_0=0.04$ eV to fit the maximal T_c of $La_{2-x}Sr_xCuO_4$ (for this coupling we are still in the weak-coupling regime). It is clear that in this case the shape of the phase diagram (see Fig. 3) follows approxi-

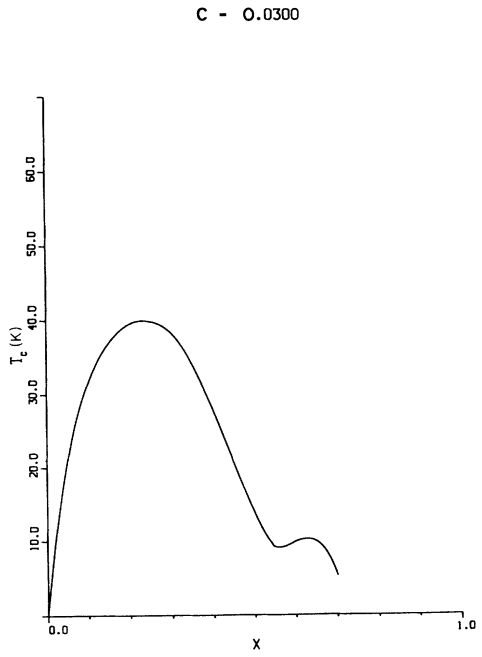

FIG. 4. The phase diagram, where $V_0=0$ and $V_1=0.07$ eV.

mately the shape of the density of states and it does not look similar to the experimental phase diagram. This similarity between the phase diagram and the density of states, in the case of constant coupling, holds also for the case where we sum over the entire Brillouin zone, since the states near ε_F have a dominant contribution, due to the $1/\varepsilon_k$ factor in the BCS equation.

We next assume a coupling where $V_0=0$ and adjust

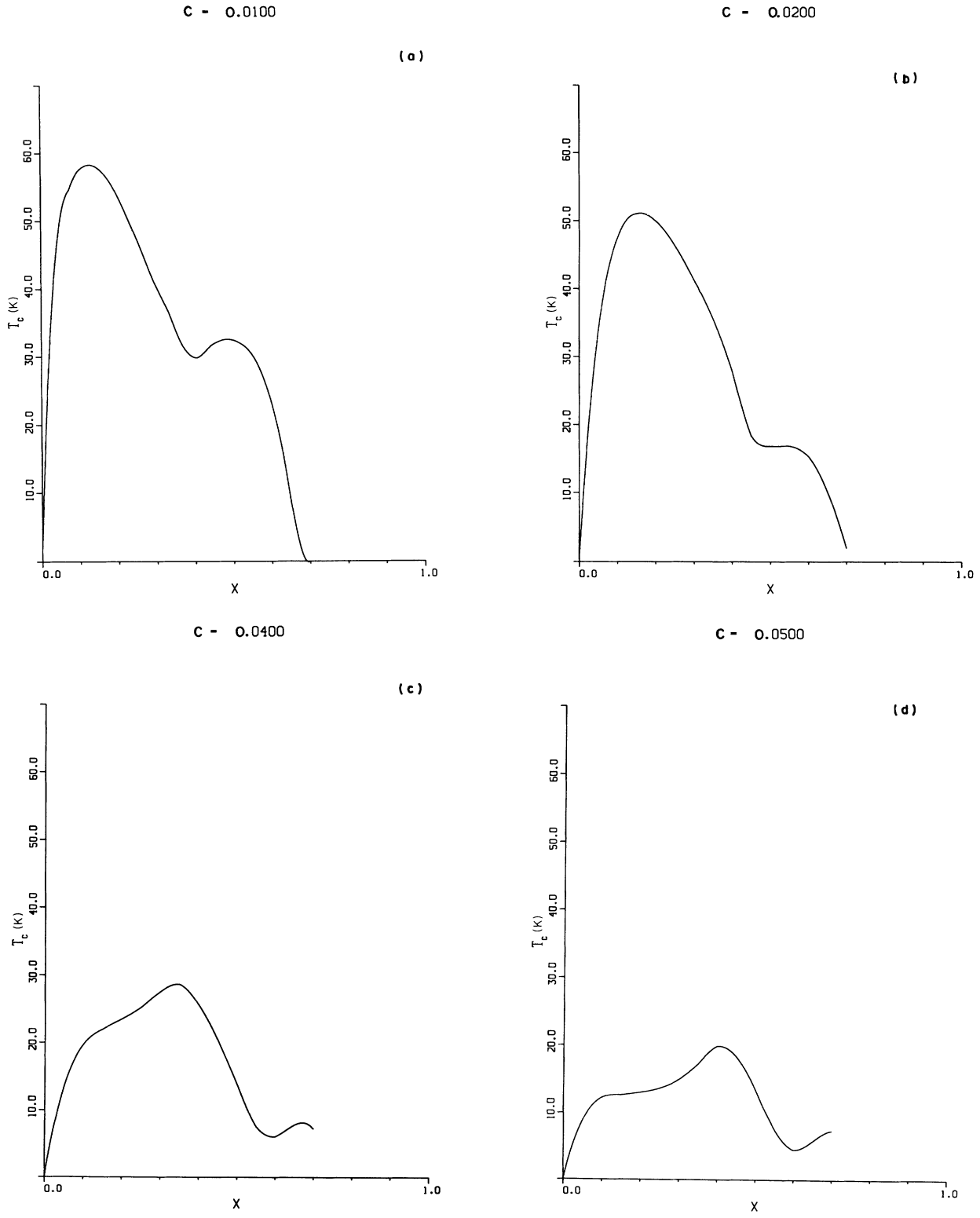

FIG. 5. The phase diagrams, where $V_0=0$ and $V_1=0.07$ eV for various values of c.

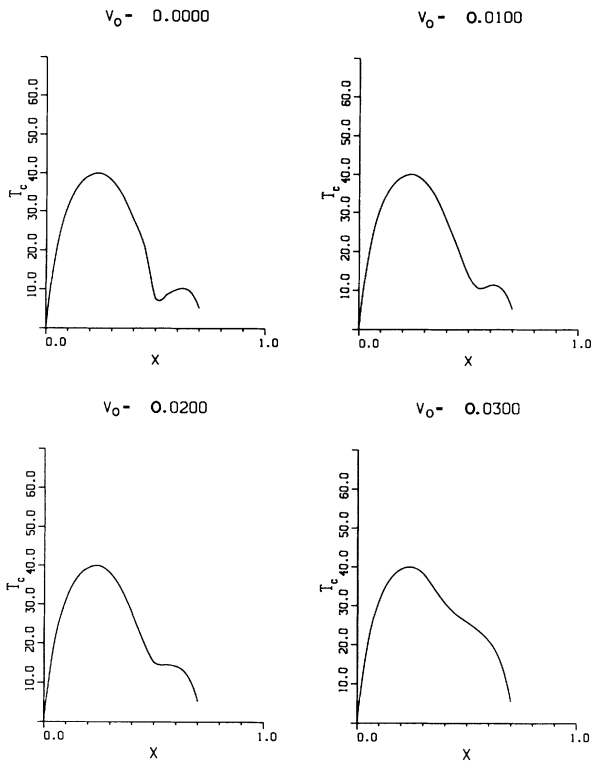

FIG. 6. The phase diagrams for $V_1=0.07$ eV and various values of V_0.

$V_1=0.07$ eV. This time the phase diagram (see Fig. 4) looks much more similar to the one observed experimentally. The value of V_1 that we choose corresponds to an attractive potential of order 0.035 eV between holes on neighboring cells. Aharony and co-workers[12] estimated an attractive potential of the order of the AFM coupling, which is about 0.13 eV. This is almost four times larger than the estimate that we use. However, the large estimate was made for Ising spins and a long-range order AFM background, whereas the spins are actually Heisenberg spins and the AFM correlations have finite range. Therefore, we should certainly assume an attractive potential that is lower than 0.13 eV. Moreover, it was noted by Birgeneau and co-workers[12] that as the concentration of the holes is increased the attractive potential should decrease, due to reduced AFM correlations, and thus we may obtain even a better fit with experimental data at high concentrations. On the other extreme of the phase diagram, we obtain nonvanishing T_c's for concentrations less than $x=0.05$, contrary to what is observed for $La_{2-x}Sr_xCuO_4$. However, it is believed that in this regime there is localization due to the random potential introduced by the Sr's and this effect is not considered in our tight-binding model.

Although we have not treated the parameter c as an adjustable parameter, we next checked how sensitive is the phase diagram to changes in its value. In Fig. 5 we present the phase diagrams for various values of c and we see that if we had to choose its value we could not have made a better choice. We also find that when we add a negative V_0 to the chosen V_1 (which reflects the on-site repulsion) it does not affect the phase diagram at all. However, when we consider an additional positive V_0, it has a big effect (see Fig. 6) when we approach $V_0=0.04$ eV.

IV. SUMMARY

We studied the phase diagram that is obtained when we consider the magnetic interactions between the holes in the CuO_2 planes. We solved the set of the BCS equations and calculated the phase diagram.

We obtained a phase diagram that fits experimental data quite well with one adjustable parameter, i.e., the strength of the magnetic interaction V_1. An even better fit is expected if effects of localization are considered at lower concentrations and effects of decreasing magnetic correlations are considered for the higher concentrations regime.

The implications of our results are not constrained to the specific model that we considered. The drastic effect of the strength of the coupling between planes, c, on the density of states and thus on the phase diagram, may be significant in other cases as well. Moreover, the form of V_1 may stem from other mechanisms that yield finite-range pairing interaction.

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