High-T_c superconductivity of iodine-intercalated $Bi_2Sr_2CaCu_2O_x$: An interlayer-coupling model

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A major problem in the theory of high-T_c superconductivity is to what extent the superconducting properties are bound to the two dimensionality of the CuO_2 planes, and how the extension into the third dimension is achieved by the coupling between adjacent CuO_2 planes. A theory, based on an interplane single-electron hopping between two-dimensional t-J lattices, is used to explain the T_c depression, recently observed in iodine-intercalated $Bi_2Sr_2CaCu_2O_x$. The effect of interlayer coupling on high-T_c superconductivity is discussed.

I. INTRODUCTION

In spite of the large efforts invested to understand the mechanism and the nature of high-T_c superconductors, the basic mechanism involved in superconducting pairing is still unknown. It is generally accepted that the microscopic superconducting mechanism takes place in the CuO_2 planes, which are a common feature of all copper oxides superconductors. Experiments have revealed a strong anisotropy between the in-plane and the off-plane directions in their physical properties such as the normal-state resistivity,[1] the upper critical field,[2] the thermal conductivity,[3] etc. These results suggest a weakly coupled layered structure for the above materials.

One of the central problems in the theory of high-T_c superconductivity is then to what extent the superconducting properties are bound to the two dimensionality of the CuO_2 planes, and how the extension into the third dimension is achieved by the coupling between adjacent CuO_2 planes. The role of interlayer coupling in high-T_c superconductivity has been studied within the framework of BCS-like models by several authors.[4] On the other hand, many of the microscopic models that have been proposed to describe the properties of the high-T_c copper oxides are based on the two-dimensional Hubbard model or the t-J model.

The t-J model was proposed by Anderson,[5] as the simplest model containing all details relevant to superconductivity. Such a model attempts to describe both magnetism and superconductivity within the same framework and successfully accounts for many of the unconventional transport and collective mode properties observed in the metallic phases of cuprate superconductors.[6] Approximated solutions of the t-J model can be obtained by means of a mean-field decoupling of the Hamiltonian, and several mean-field phases have been suggested.[7–14]

In a recent work,[15] I have shown that a single-electron hopping between two bidimensional t-J lattices can reduce the superconducting transition temperature to values that agree more with the experimental ones. In the present work, I show that the above model can be applied to the interpretation of the observed behavior of iodine-intercalated $Bi_2Sr_2CaCu_2O_x$.[16] Iodine intercalation in $Bi_2Sr_2CaCu_2O_x$ has allowed modification of the interlayer coupling, without affecting the electronic structure of the CuO_2 layers. This view is supported by measurements of the in-plane resistence before and after intercalation. Besides, both x-ray and electron-microscopy results indicate that iodine intercalates between the Bi-O bilayers, affecting the interlayer coupling but leaving the intrinsic CuO_2 plane structure intact.[16] The physical properties of iodine-intercalated $Bi_2Sr_2CaCu_2O_x$ are then very interesting in view of a full understanding of the relationship between dimensionality and high-T_c superconductivity.

II. THEORY

The t-J model is defined by the Hamiltonian

$$H = -t \sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + J \sum_{\langle i,j\rangle} (\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4} n_i n_j) - \mu_f \sum_i n_i \,, \tag{1}$$

where $\vec{S}_i = \frac{1}{2} c^\dagger_{iw} \hat{\vec{\sigma}}_{w\beta} c_{i\beta}$ and $n_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$. This Hamiltonian is under the constraint that no site is double occupied. Such a constraint can be satisfied by employing the slave-boson formalism,[17] in which the electron operator $c^\dagger_{i\sigma}$ is replaced by $c^\dagger_{i\sigma} = f^\dagger_{i\sigma} b_i$. The constraint of no double occupancy implies that $b^\dagger_i b_i + \sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} = 1$ at each site i; this request may be satisfied by adding to the Hamiltonian (1) a term $\sum_i \lambda_i (\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i - 1)$, where λ_i is a Lagrangian multiplier. A mean-field theory for the Hamiltonian (1) can be obtained by decoupling the four-fermion term $\vec{S}_i \cdot \vec{S}_j$. This leads to the introduction of the Hubbard-Stratonovich fields $\chi_{ij} = \langle \sum_\sigma f^\dagger_{i\sigma} f_{j\sigma} \rangle$ and $\Delta_{ij} = \langle f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} \rangle$. A mean-field theory is achieved by replacing the fields χ_{ij}, Δ_{ij}, b_i, and λ_i by their saddle-point values. The hopping term $t \sum_\sigma f^\dagger_{i\sigma} f_{j\sigma} b^\dagger_j b_i$ is replaced by $b_0^2 t \sum_\sigma f^\dagger_{i\sigma} f_{j\sigma}$, where b_0 is the saddle-point value of the boson field b_i. The mean-field Hamiltonian then becomes[13]

$$H^{\rm MF}=\frac{3J}{8}\sum_{\langle i,j\rangle}\left[|\chi_{ji}|^2+|\Delta_{ji}|^2-\chi^*_{ji}\sum_\sigma f^\dagger_{j\sigma}f_{i\sigma}-\text{c.c.}-\Delta^*_{ji}(f_{j\uparrow}f_{i\downarrow}-f_{j\downarrow}f_{i\uparrow})-\text{c.c.}\right]$$

$$-tb_0^2\sum_{\langle i,j\rangle}\left(\sum_\sigma f^\dagger_{j\sigma}f_{i\sigma}+\text{c.c.}\right)-\mu_0\sum_{i\sigma}f^\dagger_{i\sigma}f_{i\sigma}+\mu_b\sum_i\left(\sum_\sigma f^\dagger_{i\sigma}f_{i\sigma}+b_0^2-1\right)\,, \tag{2}$$

where $\mu_0=\mu_f-3J/4$. The decoupling in the particle-hole channel is supposed to be uniform, that is, $\chi_{ij}=\chi$ for all bonds $\langle i,j\rangle$. The decoupling in the particle-particle channel is instead chosen so that $\Delta_{ij}=+\Delta$ if $\mathbf{ij}\|\hat{x}$, $\Delta_{ij}=-\Delta$ if $\mathbf{ij}\|\hat{y}$: This choice corresponds to the d-wave phase.[8] The Hamiltonian (2) can be conveniently written in the Nambu formalism,

$$H^{\rm MF}=\sum_{\vec{k}}\psi^\dagger_{\vec{k}}H_{\vec{k}}\psi_{\vec{k}}+\frac{3J}{4}N(\chi^2+\Delta^2)+\mu_b b_0^2N-\mu_0N\,, \tag{3}$$

where $\psi^\dagger_{\vec{k}}\equiv(f^\dagger_{\vec{k}\uparrow},f_{-\vec{k}\downarrow})$ and N is the number of lattice points. The Hamiltonian matrix $H_{\vec{k}}$ is given by

$$H_{\vec{k}}=\begin{pmatrix}A_{\vec{k}} & B_{\vec{k}}\\ B_{\vec{k}} & -A_{\vec{k}}\end{pmatrix}\,, \tag{4}$$

where $A_{\vec{k}}=-2(tb_0^2+3J\chi/8)[\cos(k_x)+\cos(k_y)]+\mu_b-\mu_0$ and $B_{\vec{k}}=-(3J\Delta/4)[\cos(k_x)-\cos(k_y)]$.

I consider now the effect of a single-electron hopping among an array of bidimensional t-J lattices. I consider then the Hamiltonian

$$H=\sum_l H_l^{\rm MF}+\sum_{\vec{k}}\sum_{\substack{l,l'\\ l'=l\pm1}}w(l,l')\psi^\dagger_{l,\vec{k}}\hat{\sigma}_z\psi_{l',\vec{k}}\,, \tag{5}$$

where $\hat{\sigma}_z$ is the third Pauli matrix, $w(l,l')$ is the hopping constant between the lth and the l'th t-J lattice, and $\psi_{l,\vec{k}}$ is the Nambu spinor corresponding to the lth t-J lattice. I introduce two different values of w, corresponding to the interlayer hopping matrix element for nearest-neighbor CuO_2 planes (w_1) and next-nearest-neighbor CuO_2 planes (w_2). Such a model can be applied to materials such as $Bi_2Sr_2CaCu_2O_x$ that contain two CuO_2 planes in the unit cell. If periodic boundary conditions are considered, Eq. (5) can be written in the form

$$H=\sum_{\vec{k}}\Psi^\dagger_{\vec{k}}\tilde{H}_{\vec{k}}\Psi_{\vec{k}}+\frac{3J}{4}MN(\chi^2+\Delta^2)+\mu_b b_0^2MN-\mu_0MN\,, \tag{6}$$

where M is the total number of t-J layers, $\Psi^\dagger_{\vec{k}}\equiv(f^\dagger_{1,\vec{k}\uparrow},f_{1,-\vec{k}\downarrow},f^\dagger_{2,\vec{k}\uparrow},f_{2,-\vec{k}\downarrow},\ldots,f^\dagger_{M,\vec{k}\uparrow},f_{M,-\vec{k}\downarrow})$, and the Hamiltonian matrix $\tilde{H}_{\vec{k}}$ is given by

$$\tilde{H}_{\vec{k}}=\begin{pmatrix}
A & B & w_1 & 0 & 0 & 0 & \cdots & w_2 & 0\\
B & -A & 0 & -w_1 & 0 & 0 & \cdots & 0 & -w_2\\
w_1 & 0 & A & B & w_2 & 0 & \cdots & 0 & 0\\
0 & -w_1 & B & -A & 0 & -w_2 & \cdots & 0 & 0\\
0 & 0 & w_2 & 0 & A & B & \cdots & 0 & 0\\
0 & 0 & 0 & -w_2 & B & -A & \cdots & 0 & 0\\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot\\
w_2 & 0 & 0 & 0 & 0 & 0 & \cdots & A & B\\
0 & -w_2 & 0 & 0 & 0 & 0 & \cdots & B & -A
\end{pmatrix}\,. \tag{7}$$

The eigenvalues of the Hamiltonian (7) can be calculated analytically; for $M=4$ one finds

$$E=\pm\sqrt{(A_{\vec{k}}\pm w_1\pm w_2)^2+B^2_{\vec{k}}};$$

for $M=8$,

$$E=\pm\sqrt{(A_{\vec{k}}\pm w_1\pm w_2)^2+B^2_{\vec{k}}},$$

$$E=\pm\sqrt{(A_{\vec{k}}\pm\sqrt{w_1^2+w_2^2})^2+B^2_{\vec{k}}}$$

(doubly degenerate); for $M=16$,

$$E=\pm\sqrt{(A_{\vec{k}}\pm w_1\pm w_2)^2+B^2_{\vec{k}}},$$

$$E=\pm\sqrt{(A_{\vec{k}}\pm\sqrt{w_1^2+w_2^2})^2+B^2_{\vec{k}}}$$

(doubly degenerate); and

$$E=\pm\sqrt{(A_{\vec{k}}\pm\sqrt{w_1^2+w_2^2\pm\sqrt{2}w_1w_2})^2+B^2_{\vec{k}}}$$

(doubly degenerate). The mean-field parameters are determined by the condition of minimum of the thermodynamic potential

$$\Omega=MN\left[\frac{3J}{4}(\chi^2+\Delta^2)+\mu_b b_0^2-\mu_0-T\ln(4)\right]-2T\sum_{\vec{k},s}\ln\cosh\left(\frac{E_{\vec{k},s}}{2T}\right)\,, \tag{8}$$

where s indicates which energy eigenvalue is considered among the ones given above. Besides, the chemical potential μ_0 is determined by the condition $\partial\Omega/\partial\mu_0=\delta-1$, where the doping δ is the number of holes per plane, so that the average number of electrons in each site is $1-\delta$. The parameter δ must be related to the number

of holes per CuO_2 unit in the sample. Such a value can be obtained through different techniques: Hall coefficient measurements,[19] chemical methods,[20] or by assuming a given valence state for the ions in the compounds.[21]

Through a direct comparison of the self-consistent equations, one can easily obtain the values of $b_0^2 = \delta$ and $\mu_b = 4t\chi$. The critical temperature can be calculated by setting $\Delta = 0$ in the self-consistent equations.

III. RESULTS AND DISCUSSION

In a recent work,[15] I have shown that the critical temperature corresponding to the superconducting transition in a bilayer t-J model is sensibly reduced when a single-electron hopping between the two layers is considered. This can be seen in Fig. 1, where the critical temperature T_c is represented as a function of the doping δ. The solid curve refers to a single t-J layer, while the dashed and dotted curves correspond to two t-J layers with a hopping term $w = 0.5J$ and $w = 0.6J$, respectively. Superconductivity is suppressed at low doping, and the critical temperature is reduced to values that are in better agreement with the experimental ones.

In the case of an array of t-J layers, it is very important to study how the boundary conditions affect the final results. In Fig. 2, the critical temperature is represented as a function of the doping δ, for different values of the parameters. The dotted, dashed, and solid curves refer, respectively, to a system with 4, 8, and 16 layers. The curves corresponding to 8 and 16 layers are practically coincident, which proves that such results are independent of the boundary conditions and correspond to an infinite system.

The present theory can be compared with the observed behavior of iodine-intercalated $Bi_2Sr_2CaCu_2O_x$.[16] Iodine

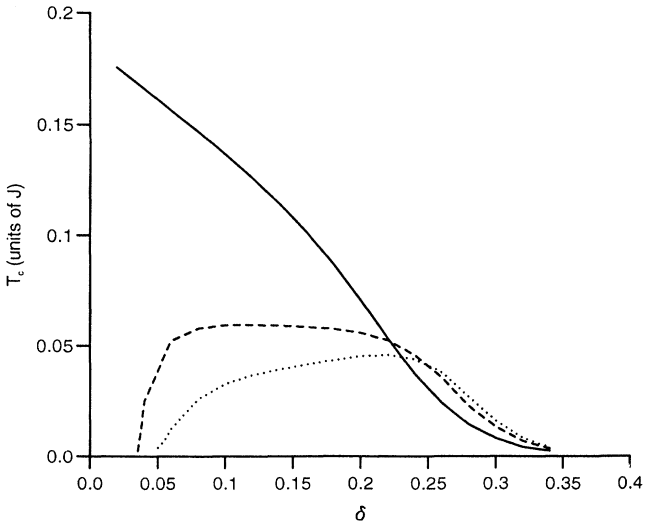

FIG. 1. The superconducting transition temperature T_c as a function of the doping δ for $t/J = 3$. The solid curves correspond to a single t-J layer. The dashed and dotted curves correspond to two t-J layers with a hopping term $w = 0.5J$ and $w = 0.6J$, respectively.

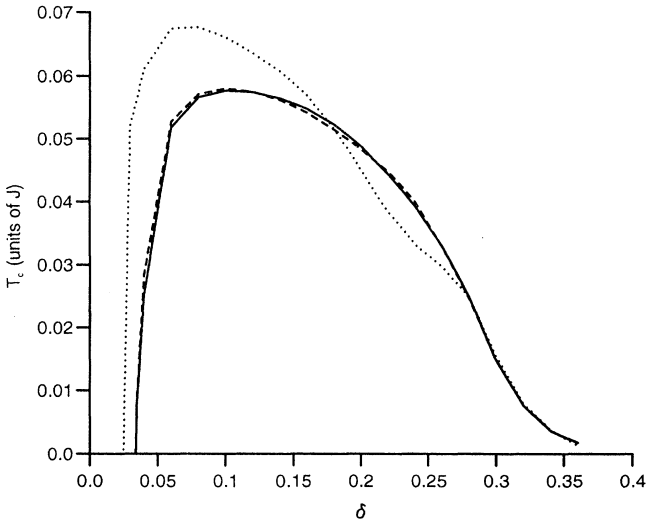

FIG. 2. The superconducting transition temperature T_c as a function of the doping δ for $t/J = 3$, $w_1 = 0.5J$, and $w_2 = 0.2J$. The solid, dashed, and dotted curves refer, respectively, to a system with 16, 8, and 4 layers.

intercalation gives origin to a suppression of the transition temperature by ≈ 10 K and to a sensible reduction of the out-of-plane resistivity $\rho_\perp$. Both x-ray and electron-microscopy results indicate that iodine intercalates between the Bi-O bilayers, thus affecting the interlayer coupling but leaving the intrinsic CuO_2 plane structure intact. This view is supported also by measurements of the in-plane resistance before and after intercalation.[16] Since the sample in-plane resistence is not modified by intercalation, one can reasonably assume that intercalation does not affect the electronic structure of the CuO_2 planes.

Conduction in the out-of-plane direction can be reasonably ascribed to a process of tunneling between CuO_2 layers, so that the resistivity assumes the form[22,16]

$$\rho_\perp \propto \frac{1}{\alpha|w_1|^2} + \frac{1}{\beta|w_2|^2}$$

where w is the interlayer hopping matrix element for nearest-neighbor CuO_2 planes (w_1) and next-nearest-neighbor planes (w_2). The reduction of $\rho_\perp$ can be ascribed to an enhancement of the interlayer coupling between next-nearest-neighbor planes, since it is reasonable to assume that w_1 is not affected by iodine intercalation.[16]

In Fig. 3 it is shown how the phase diagram is modified by a variation of w_2. The solid, dashed, and dotted curves correspond, respectively, to a hopping parameter $w_2 = 0.2J$, $w_2 = 0.1J$, and $w_2 = 0$. The critical temperature at optimal doping is reduced as w_2 is increased, in qualitative agreement with experiments. On the other hand, the experimental behavior of iodine-intercalated $Bi_2Sr_2CaCu_2O_x$ is inconsistent with the model proposed by Wheatly, Hsu, and Anderson,[18] which predicts an enhancement of the critical temperature if the interlayer

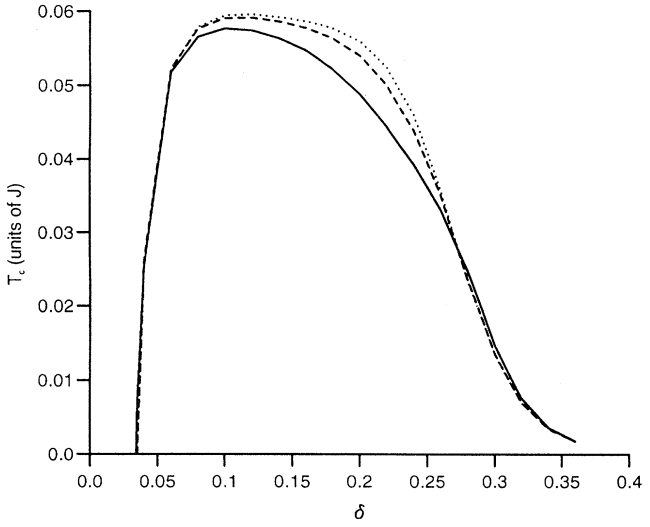

FIG. 3. The superconducting transition temperature T_c as a function of the doping δ for $t/J = 3$ and $w_1 = 0.5J$, for different values of w_2. The solid, dashed, and dotted curves refer, respectively, to $w_2 = 0.2J$, $w_2 = 0.1J$, and $w_2 = 0$.

coupling is increased (see Ref. 16).

In order to investigate the relationship between dimensionality and high-T_c superconductivity, many groups have studied the electrical transport properties of $YBa_2Cu_3O_7/PrBa_2Cu_3O_7$ (YBCO/PBCO) superlattices.[24,25] In these systems, insulating layers (PBCO) are interposed between superconducting layers (YBCO). The superconducting properties of the above systems are a function of both YBCO and PBCO layer thicknesses. The critical temperature T_c decreases as the YBCO layer thickness is decreased or as the PBCO layer thickness is increased, but for all YBCO layer thicknesses, including layers one unit cell thick, the superconducting transition temperature saturates at nonzero values.[24,25] Besides, the widths of the superconduction transitions are large, with $\Delta T_c \approx 37$ K for one unit cell thick YBCO layers isolated in a PBCO matrix.[25] Several different models have been proposed in order to explain such a behavior, which are based upon Kosterlitz-Thouless transition and charge redistribution effects,[26–30] interlayer coupling,[31,32] proximity effect,[33–36]and hole filling.[37] Unlike the case of iodine-intercalated $Bi_2Sr_2CaCu_2O_x$, the T_c depression in YBCO/PBCO superlattices cannot be ascribed only to an interlayer coupling effect. This has been shown by Norton *et al.*, who have studied the dependence of the superconducting transition of YBCO-based superlattices on the electronic properties of the barrier layers.[25] They used three different barrier materials, namely, $PrBa_2Cu_3O_7$, $Pr_{0.7}Y_{0.3}Ba_2Cu_3O_7$, and $Pr_{0.5}Ca_{0.5}Ba_2Cu_3O_7$, and found that the critical temperature T_c(onset) does not depend on the nature of the barrier layer. On the other hand, the electrical resistance above T_c changes strongly when the composition of the barrier layer is varied, and a strong dependence on the nature of the barrier layer is expected also for the interlayer coupling constant. From the above considerations, one can deduce that the T_c depression in YBCO-based superlattices cannot be explained in terms of interlayer coupling effects, so that the theory presented in this paper cannot be applied to that case.

The results obtained in this work contrast with the belief, shared by many authors, that interlayer coupling gives origin to an increase of the critical temperature in high-T_c superconductors. It is well known that materials with n CuO_2 planes within the unit cell show a critical temperature T_c^0 that increases with n, for $n \leq 3$, and drops for $n \geq 4$. This fact is generally ascribed to an interlayer coupling effect: The coupling between superconducting CuO_2 planes is believed to raise the critical temperature. On the other hand, if the charge distribution is nonhomogeneous among the various CuO_2 planes for $n \geq 3$, T_c is expected to decrease for large values of n, because of the depletion of hole density in the central layers.[23]

Even if the above model allows a consistent interpretation of the observed properties of multilayer systems, an alternative interpretation can be given. In fact, one can reasonably suppose that the pair-breaking effects induced by a coupling with an insulating layer are stronger with respect to the ones corresponding to a coupling with another superconducting layer. Such a view can explain the experimental enhancement of the critical temperature in multilayer systems. On the other hand, it does not exclude the possibility that coupling between superconducting planes could give origin to a depression of T_c with respect to the ideal bidimensional system.

In conclusion, I have shown that the T_c depression, recently observed in iodine-intercalated $Bi_2Sr_2CaCu_2O_x$, can be explained by a model based on an interplane single-electron hopping between two-dimensional t-J lattices. In addition, the effect of interlayer coupling in cuprate superconductors has been discussed.

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