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Plane-chain coupling in $YBa_2Cu_3O_7$: Impurity effect on the critical temperature

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We have studied the effect of impurities on the critical temperature for a model of Y-Ba-Cu-O involving pairing both in the CuO_2 planes and in the CuO chains. In this model pairing in the planes is due to phonons, while Coulomb repulsion induces in the chains an order parameter with opposite sign. Due to the anticrossing produced by hybridization between planes and chains, the order parameter changes sign on a single sheet of the Fermi surface, resulting in nodes in the gap. We find that, in our model, the critical temperature is much less sensitive to impurities than in standard d-wave models. One reason is that impurities produce essentially plane-plane and chain-chain scattering, which does not affect the critical temperature. T_c is reduced by the scattering between parts of the Fermi surface which have opposite signs for the order parameter, just as in standard d-wave models. In our model this is due to plane-chain scattering. We have found that this scattering, whatever its origin, will be smaller by a factor of order t/E_F (that is, hybridization coupling over the Fermi energy) compared to plane-plane and chain-chain scattering. Accordingly the sensitivity of T_c to impurities in our model is reduced by a similar factor, compared to the d-wave situation. In the specific case which we have studied in detail and which reduces to the two-band model, we have found a further reduction of the sensitivity of T_c to impurities with a behavior which can vary continuously from s-wavelike to d-wavelike depending on the parameters. We expect a similar behavior and reduction to occur in the general case. [S0163-1829(96)04730-3]

I. INTRODUCTION

The mechanism responsible for high-T_c superconductivity is still highly controversial.[1] While a large part of the theoretical effort is based on the hypothesis that Cooper pairs are formed in high-T_c compounds, there is no agreement on the physical origin of the pairing interaction or on the symmetry of the pair wave function. These two questions are actually intimately related. Indeed repulsive interactions, such as produced by spin fluctuations,[2] require an order parameter which changes sign on the Fermi surface in order to produce pairs. This leads, in the simplest hypothesis, to pairing with d-wave symmetry if we assume singlet pairing. On the other hand purely attractive interactions lead to pairing with s-wave symmetry since any change of sign is unfavorable in this case. Therefore an experimental determination of the order parameter symmetry should greatly help to identify the physical interaction responsible for pair formation: Although it would not be enough to provide a unique identification, it would strongly narrow the remaining possibilities. For this reason a large part of the recent experimental work has been aimed toward providing a clear signature for the symmetry of the order parameter.

Quite surprisingly recent experiments on $YBa_2Cu_3O_7$ (YBCO) designed with this purpose of identifying the symmetry have given clear-cut, but contradictory answers.[1] Indeed the observation of a sizable Josephson current[3] in a c-axis tunneling junction between $YBa_2Cu_3O_7$ and Pb is quite difficult to reconcile with a pure d-wave symmetry while it is in full agreement with s-wave symmetry. Similarly the fact that there is no angular dependence in the critical current of YBCO-YBCO grain boundary junctions in the a-b plane[4] goes clearly in the direction of an s-wave interpretation. On the other hand a number of experiments are in favor of a d-wave symmetry. Many experiments, including tunneling, NMR, Raman scattering, photoemission, and penetration depth,[1] have shown the existence of low-energy excited states. Actually these experiments are compatible with a strongly anisotropic s-wave order parameter. Or more simply one may look for extrinsic effects and wonder if these states do not arise from surface effects or defects, which would provide quasinormal regions. However, the existence of a linear T dependence of the penetration depth over a large range of temperature, simultaneously in crystals and films, with the same slope,[5] makes an extrinsic interpretation for all these experiments unlikely (while this kind of explanation may very well be valid for some of them). Moreover some experiments specifically designed to check if the order parameter changes sign over the Fermi surface have given positive answers. These are the corner superconducting quantum interference device (SQUID) experiments[6] which give a clear indication for a change of sign of the order parameter between the a and b axes, and the observation of a spontaneous magnetization corresponding to a half magnetic flux quantum in three grain-boundary Josephson junctions[7] which implies a π shift, in clear agreement with d-wave symmetry.

On the other hand the d-wave interpretation is not free of problems. For example recent experiments show that some thermodynamical superconducting properties are markedly anisotropic (the a- and b-axis results are different). Indeed the penetration depth in good YBCO crystals displays a strong anisotropy of the penetration depth,[8] and the specific heat anomaly at T_c of the parent compound $LuBa_2Cu_3O_7$ (with same T_c as YBCO) has a marked anisotropy as a function of the orientation of an applied magnetic field.[9] It is difficult to ascribe these anisotropies to the weak orthorhombic distortion, and it is more likely that the CuO chains play

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a significant role in the superconducting properties. One of the most conspicuous problems of the d-wave interpretation is the weak sensitivity of the critical temperature of $YBa_2Cu_3O_7$ to the presence of impurities. Indeed any kind of impurities, whether magnetic or not, produces in d-wave superconductors[10–12] an effect analogous to pair breaking by magnetic impurities in standard s-wave superconductors.[13] In particular the critical temperature[10,11] decreases rapidly with increasing impurity concentration following the Abrikosov-Gor'kov (AG) law,[13] and superconductivity disappears at a critical concentration. In contrast all samples of $YBa_2Cu_3O_7$ seem to have a T_c around 90 K. It is difficult to believe that all samples (including the earlier ones) are clean enough to affect only weakly the critical temperature, whereas all microscopic studies show that there are always more structural defects than what is generally admitted. Moreover, ion[14] or electron[15] irradiation experiments have shown a rather weak sensitivity of the critical temperature of $YBa_2Cu_3O_7$ on the inverse lifetime deduced from resistivity measurements.[11] Actually Zn impurities are known[16,17] to have a depressing effect on T_c, but this can be interpreted as a standard pair-breaking effect since the environment of a Zn impurity, located in the CuO_2 planes, is known to be magnetic.[18].

In order to solve these contradictions we have proposed recently[19] for $YBa_2Cu_3O_7$ a model which mixes s-wave and d-wave features. In our model, in addition to the CuO_2 planes, the CuO chains play an essential role. The pairing interaction within the planes is attractive (it can be, for example, produced by phonons). On the other hand the pairing interaction between planes and chains is repulsive (it can be produced by the Coulomb interaction). In this way the order parameter has opposite signs on the planes and on the chains. Moreover, we include the hybridization between planes and chains, which corresponds physically to taking into account the possibility for an electron to jump from planes to chains or vice versa. Naturally the coupling responsible for this hybridization is fairly small, but it is a well-known feature of all band structure calculations.[20] It is of importance only when the plane and the chain band intersect. In this case it leads to an anticrossing in the dispersion relations, and similarly to an anticrossing of the Fermi surfaces, wherever the (uncoupled) pieces of the Fermi surface related to plane and chain cross. As a result, when we move on a given sheet of the Fermi surface, we go from a part which corresponds physically to a plane electron, to a part which corresponds physically to a chain electron. Since the order parameter has opposite signs for plane and chain electrons, this implies that the order parameter changes sign on a given sheet of the Fermi surface and therefore has nodes on this sheet by continuity. Therefore our model provides an order parameter which is quite analogous to a d-wave order parameter and it can in this way explain[19] all the experiments in favor of d-wave symmetry. On the other hand it does not have a d-wave symmetry since the nodes, which occur at the intersection between plane and chain bands, have no reason to satisfy $k_x = k_y$, and the average of the order parameter has no symmetry reason to be zero. Hence there is, for example, no problem with the nonzero Josephson current in $YBa_2Cu_3O_7$-Pb junctions along the c axis.[3] Moreover, since the attractive in-plane interaction and the repulsive interaction between plane and chain help each other, there is no problem in explaining the high value of the critical temperature of $YBa_2Cu_3O_7$.[21] Naturally our model is specific of $YBa_2Cu_3O_7$, but we can think that it can be generalized to other compounds where the role of the chains can be played by other parts of the structure, such as the BiO planes in Bi-Sr-Ca-Cu-O. On the other hand there is no possibility of this kind in La-Sr-Cu-O and accordingly we do not expect experiments to display in this compound the same physical features as in YBCO.

Our model has common features with many other models. As a two-band model it is quite similar to the two-band models introduced by Suhl, Matthias, and Walker and others[22–26] to describe superconductivity in transition metals. The possibility of an interband repulsive interaction in two-band models was already introduced by Kondo.[24] More recently a two-band superconducting–normal-metal (SN) model has been introduced by Abrikosov and Klemm[27] to account for Raman scattering data. The idea of an interband repulsion has been put forward by various groups[28–31] recently in the context of high-T_c superconductivity in order to show that experiments displaying a change of sign of the order parameter did not necessarily imply a spin fluctuation mechanism. Our model is also similar to the one proposed by Abrikosov,[32] where there are attractive and repulsive interactions within a single band, leading to a change of sign of the order parameter within this band. Finally, as noted above, chain-plane hybridization is a standard feature of band structure calculations[20] and there have been various suggestions of the importance of the chains in the physics of $YBa_2Cu_3O_7$, whether for intrinsic or for extrinsic reasons,[33–35] these models allowing for the electron to jump between planes and chains.

In this paper we consider the effect of impurities on the critical temperature in our model. We will actually restrict ourselves to nonmagnetic impurities. Indeed magnetic impurities are easily included, but they will naturally lead to pair breaking and produce a T_c following the AG law as in other models. Hence magnetic impurities cannot discriminate between various models and we ignore them for simplicity. The conclusion of our study is that, in our model, for generic parameters, the critical temperature is much less sensitive to impurities than in standard d-wave models. Therefore we might say that, with respect to the sensitivity of the critical temperature to nonmagnetic impurities, our model behaves as a ''weak'' d-wave model. This happens for two independent reasons. First the reduction of T_c is due to plane-chain scattering, which is weak compared to plane-plane scattering. Next the fact that we have a two-band model provides further possibilities for a weak impurity sensitivity. In Sec. II we present our model and we calculate the critical temperature of the clean superconductor as a first step toward the calculation of the impurity dependence, which is dealt with in Sec. III. Finally Sec. IV is devoted to a comparison with experimental results and to our conclusion.

II. MODEL

Let us first define specifically our model. We will describe the motion of an electron in planes and chains by the following Hamiltonian:

$$H_0=\sum_k \varepsilon_k c_k^\dagger c_k+\sum_k \varepsilon'_k d_k^\dagger d_k+\sum_k t_k c_k^\dagger d_k+\text{H.c.}, \quad (1)$$

where $c_k^\dagger$ and $d_k^\dagger$ are creation operators in the plane and in the chain band, respectively. The first term corresponds to an isolated plane with dispersion relation ϵ_k, the second one to isolated chains with dispersion relation ϵ'_k, and the last term describes hopping between planes and chains. Actually this independent electron Hamiltonian does not correspond precisely to the situation found in $YBa_2Cu_3O_7$. Indeed $YBa_2Cu_3O_7$ is built by stacking up sets made of two CuO_2 planes and one CuO chains plane. Therefore a better description is obtained by the Hamiltonian

$$\begin{aligned}H_0=&\sum_n \varepsilon c_{1,n}^\dagger c_{1,n}+\sum_n \varepsilon c_{2,n}^\dagger c_{2,n}+\sum_n t_p(c_{1,n}^\dagger c_{2,n}+\text{H.c.})\\&+\sum_n \varepsilon' d_n^\dagger d_n+\sum_n t_c(c_{1,n}^\dagger d_n+\text{H.c.})\\&+\sum_n t_c(c_{2,n}^\dagger d_{n+1}+\text{H.c.}),\end{aligned} \quad (2)$$

where all quantities are understood to depend on k_x and k_y and summations run also over $k_{x,y}$. The indices 1 and 2 number the CuO_2 planes and the index n numbers the stacks. Introducing the even and odd plane band operators $c_\pm$ by $c_{1,2} = (c_+ \pm c_-)/\sqrt{2}$, and taking the Fourier transform in the z direction, we obtain

$$\begin{aligned}H_0=&\sum_k (\varepsilon+t_p)c_{+,k}^\dagger c_{+,k}+\sum_k (\varepsilon-t_p)c_{-,k}^\dagger c_{-,k}\\&+\sum_k \varepsilon' d_k^\dagger d_k+\sum_k t_+(c_{+,k}^\dagger d_k+\text{H.c.})\\&+\sum_k t_-(c_{-,k}^\dagger d_k+\text{H.c.}),\end{aligned} \quad (3)$$

where a dependence and summation on k_z is now understood, and $t_+=t_c\sqrt{2}\cos(k_zc/2)$ and $t_-=t_c\sqrt{2}\sin(k_zc/2)$, with c being the size of the unit cell along the z direction. Band structure calculations[20] give a crossing of the chain band Fermi surface with the odd plane band Fermi surface, whereas there is no crossing with the even plane band. Therefore the even plane band will not play an interesting physical role in our model and we will forget it for simplicity, but it should clearly be retained in a very realistic calculation. This leads us back to the Hamiltonian, Eq. (1), where the plane band is actually the odd plane band. The hopping term has a k_z dependence as given by t_-. However, if the even plane band happens to cross the chain band, we would have no problem in extending our model. This would be particularly easy in the two extreme cases where the even and odd plane bands are nearly degenerate ($t_p \ll t_c$) or well separated ($t_p \gg t_c$) since we would be led again to the Hamiltonian, Eq. (1).

With respect to pairing interactions, as we have already indicated, we take an attractive pairing interaction in the plane which can be, for example, due to phonon exchange. On the other hand we assume a repulsive pairing interaction between plane and chain. A natural physical origin for this term is the Coulomb repulsion, since screening is certainly not very efficient in YBCO because it is a weak metal. Moreover, screening is probably very ineffective along the z direction since hopping in this direction is small. We note, however, that hopping is physically necessary in order to have a pairing term between planes and chains. Finally there is little experimental evidence for an attractive pairing interaction in the chains. However, we will assume its existence for the sake of generality. We include also the standard intraband Coulomb repulsion.

Let us first consider the critical temperature of the clean superconductor. In a first step we ignore the hopping term t_k. The Eliashberg equations at the critical temperature are

$$\Delta_n Z_n=\pi T\sum_n \lambda_{n-m}\frac{\Delta_m}{|\omega_m|}-\pi T\mu\sum_n^{\omega_c}\frac{\Delta_m}{|\omega_m|}-\pi Tk\sum_n^{\omega_c}\frac{\Delta'_m}{|\omega_m|}, \quad (4)$$

$$\begin{aligned}\Delta'_n Z'_n=&\pi T\sum_n \lambda'_{n-m}\frac{\Delta'_m}{|\omega_m|}-\pi T\mu'\sum_n^{\omega_c}\frac{\Delta'_m}{|\omega_m|}\\&-\pi Tk'\sum_n^{\omega_c}\frac{\Delta_m}{|\omega_m|}.\end{aligned} \quad (5)$$

Here Δ_n and Z_n are the order parameter and the renormalization function at the Matsubara frequency ω_n. Primed quantities refer to the chains while unprimed ones correspond to the planes; λ_n and λ'_n are the effective frequency-dependent interactions due to phonon exchange while μ, μ' and k, k' are the intraband and interband Coulomb repulsion with cutoff ω_c of order of the Fermi energy. While the interactions that we consider here have certainly a wave vector dependence in the real superconductor, we have no precise idea of what they are and we do not have any physical reason to believe that this dependence is strong. Therefore, for the sake of simplicity and clarity, we have taken isotropic interactions within planes and chains. We can now proceed to the usual reduction of the cutoff from ω_c to a frequency ω_D a few times a typical phonon frequency. For $\omega_n > \omega_D$, the order parameters Δ_n and Δ'_n become constants Δ_∞ and Δ'_∞ while Z_n, $Z'_n \approx 1$. These constants are obtained from Eqs. (4) and (5) as

$$(1+\mu r)\Delta_\infty+kr\Delta'_\infty=-\pi T\mu\sum_n^{\omega_D}\frac{\Delta_m}{|\omega_m|}-\pi Tk\sum_n^{\omega_D}\frac{\Delta'_m}{|\omega_m|}, \quad (6)$$

$$(1+\mu' r)\Delta'_\infty+k'r\Delta_\infty=-\pi T\mu'\sum_n^{\omega_D}\frac{\Delta'_m}{|\omega_m|}-\pi Tk'\sum_n^{\omega_D}\frac{\Delta_m}{|\omega_m|}, \quad (7)$$

where $r=\ln(\omega_c/\omega_D)$. When these results are carried into Eqs. (4) and (5), one obtains the same equations, except that the cutoff is now ω_D and μ, μ' and k, k' are replaced by renormalized Coulomb interactions μ^*, μ'^* and k^*, k'^* given by

$$\mu^{*}=\frac{\mu+(\mu\mu'-kk')r}{(1+\mu r)(1+\mu' r)-kk'r^{2}},$$

$$k^{*}=\frac{k}{(1+\mu r)(1+\mu' r)-kk'r^{2}},\qquad(8)$$

and similar expressions for μ'^{*} and k'^{*} obtained by exchanging primed and unprimed quantities. Naturally one recovers the standard Coulomb pseudopotential when there is no interband interaction. It seems safe to assume $\mu\mu'-kk'>0$; otherwise we would have pairing from an ‘‘s-wave’’ Coulomb interaction alone (when pairing from the Coulomb interaction is considered, this is usually for higher ‘‘angular momenta’’). In this case renormalization does not change the sign of the various quantities. We see that, in addition to its direct effect, the interband interaction decreases the effective intraband repulsion, leading to an increase of the critical temperature, as it should.[36] In the following we will restrict ourselves to the weak-coupling limit where Δ_n and Δ'_n can be taken as constants and mass renormalization is negligible. Indeed, as will be clear in the following, we do not expect strong-coupling effects to modify qualitatively our conclusions. In this case T_c depends only on the combinations $\lambda^{*}\equiv\lambda_0-\mu^{*}$ and $\lambda'^{*}\equiv\lambda'_0-\mu'^{*}$, in addition to k^{*} and k'^{*}. From now on we will omit the asterisk for all the renormalized coupling constants. Then, if we let $x=\ln(\Omega/T_c)$ where Ω is a typical phonon frequency (or rather 1/4 of a typical phonon frequency[37]), T_c is obtained from

$$(x^{-1}-\lambda)(x^{-1}-\lambda')=kk',\qquad(9)$$

which is the standard two-band result.[22] Although one expects physically that the Coulomb interaction reduces the isotope effect, this is not obvious from Eqs. (8) and (9). This has been shown to be true by Kondo[24] in some limiting cases. We show in the Appendix that this property holds quite generally.

As a preliminary to the calculation with impurities, let us finally consider how the above calculation of the critical temperature is modified when we take into account the hybridization t_k between planes and chains. As indicated above, we take isotropic interactions and order parameters in the planes and in the chains. Corresponding to the effective interaction Hamiltonian

$$H_{\mathrm{int}}=-g\sum_{k,k'}c^{\dagger}_{k'}c^{\dagger}_{-k'}c_{-k}c_{k}+K\sum_{k,k'}d^{\dagger}_{k'}d^{\dagger}_{-k'}c_{-k}c_{k}+\mathrm{H.c.}$$
$$-g'\sum_{k,k'}d^{\dagger}_{k'}d^{\dagger}_{-k'}d_{-k}d_{k},\qquad(10)$$

the order parameter satisfies

$$\Delta=-g\sum_{k}\langle c_{-k}c_{k}\rangle+K\sum_{k}\langle d_{-k}d_{k}\rangle,\qquad(11)$$

$$\Delta'=K\sum_{k}\langle c_{-k}c_{k}\rangle-g'\sum_{k}\langle d_{-k}d_{k}\rangle.\qquad(12)$$

However, because of the hybridization, the plane and chain operators c_k and d_k do not correspond to the eigenstates of H_0. The unitary transformation

$$c_i=a_{ij}\gamma_j\qquad(13)$$

diagonalizes the Hamiltonian into $H_0=\Sigma\, e_i\,\gamma_i^{\dagger}\,\gamma_i$ where we have set for convenience $c_1\equiv c$ and $c_2\equiv d$. The energies e_1 and e_2 of the hybridized bands are given by $2e_{1,2}=\epsilon+\epsilon'\pm[(\epsilon-\epsilon')^2+4\,t^2\,]^{1/2}$ and $a_{11}=a_{22}=[(e_1-\epsilon')/(e_1-e_2)]^{1/2}\equiv\cos\theta$, $a_{21}=-a_{12}=[(e_1-\epsilon)/(e_1-e_2)]^{1/2}\equiv\sin\theta$, with again the k dependence understood everywhere. When we carry out this transformation in the mean field Hamiltonian

$$H=H_0+\Delta\sum_{k}c^{\dagger}_{k}c^{\dagger}_{-k}+\Delta'\sum_{k}d^{\dagger}_{k}d^{\dagger}_{-k}+\mathrm{H.c.},\qquad(14)$$

we will obtain interband pairing terms, such as $\gamma_{-k,1}\gamma_{k,2}$, coupling the hybridized bands. However, we will consider that t_k is large enough so that these bands are well separated. Specifically this means that we assume $\omega_D\ll t_k$ (otherwise we should make a much more careful strong-coupling treatment, which would probably not bring anything new qualitatively). In this case the above pairing terms will be negligible because we cannot have two electrons $(k,1)$ and $(-k,2)$ at the Fermi surface with opposite wave vectors, but belonging to different bands (we will justify more specifically this approximation in the next section). Therefore the transformation, Eq. (13), gives

$$H=H_0+\sum_{k}\delta_{1,k}\gamma^{\dagger}_{1,k}\gamma^{\dagger}_{1,-k}+\sum_{k}\delta_{2,k}\gamma^{\dagger}_{2,k}\gamma^{\dagger}_{2,-k}+\mathrm{H.c.}\qquad(15)$$

with $\delta_{1,k}=\Delta\cos^2\theta_k+\Delta'\sin^2\theta_k$ and $\delta_{2,k}=\Delta\sin^2\theta_k+\Delta'\cos^2\theta_k$. Naturally this band-diagonal expression for the Hamiltonian is obvious once the interband pairing terms are neglected, and we could have written it immediately. Our essential point is that, starting from isotropic interactions in planes and chains, we obtain a specific anisotropy for the order parameter $\delta_{1,k}$ and $\delta_{2,k}$. In particular we obtain nodes at the Fermi surface since we have managed to have Δ and Δ' with opposite signs, and $\cos^2\theta_k$ goes from 0 to 1 when we move at the Fermi surface of a given band. Therefore we have an order parameter which is d-wave like, although we have assumed an attractive pairing in the planes.

We have then as usual $\langle\gamma_{-i}\gamma_i\rangle=-(\delta_i/2e_i)\tanh(\beta e_i/2)$. From Eqs. (11), (12), and (13) this leads to

$$\Delta=\sum_{k}(g\cos^2\theta_k-K\sin^2\theta_k)\frac{\delta_{1,k}}{2e_{1,k}}\tanh\left(\frac{\beta e_{1,k}}{2}\right)$$
$$+(g\sin^2\theta_k-K\cos^2\theta_k)\frac{\delta_{2,k}}{2e_{2,k}}\tanh\left(\frac{\beta e_{2,k}}{2}\right),\qquad(16)$$

$$\Delta'=\sum_{k}(g'\sin^2\theta_k-K\cos^2\theta_k)\frac{\delta_{1,k}}{2e_{1,k}}\tanh\left(\frac{\beta e_{1,k}}{2}\right)$$
$$+(g'\cos^2\theta_k-K\sin^2\theta_k)\frac{\delta_{2,k}}{2e_{2,k}}\tanh\left(\frac{\beta e_{2,k}}{2}\right).\qquad(17)$$

Since the bands are well separated, the $\mathbf{k}$ summations will be around the Fermi surface of each band with cutoff ω_D for $e_{i,k}$. The integration perpendicular to the Fermi surface will give the standard factor $x=\ln(1.13\beta\omega_D)$ and we are left with summations along the Fermi surface:

$$\Delta = x\sum_{k} (g\cos^2\theta_k - K\sin^2\theta_k)\,\delta_{1,k}\,\delta(e_{1,k}) + (g\sin^2\theta_k - K\cos^2\theta_k)\,\delta_{2,k}\,\delta(e_{2,k}), \tag{18}$$

$$\Delta' = x\sum_{k} (g'\sin^2\theta_k - K\cos^2\theta_k)\,\delta_{1,k}\,\delta(e_{1,k}) + (g'\cos^2\theta_k - K\sin^2\theta_k)\,\delta_{2,k}\,\delta(e_{2,k}), \tag{19}$$

where the order parameter $\delta_{i,k}$ should not be confused with the Dirac function $\delta(e)$. For $e_{1,k} = 0$ we have $\cos^2\theta = \epsilon'/(\epsilon + \epsilon')$ and $\cos^2\theta = \epsilon/(\epsilon + \epsilon')$ for $e_{2,k} = 0$. Moreover, for most of the Fermi surface we have $\epsilon \ll \epsilon'$ or $\epsilon' \ll \epsilon$, leading to $\cos^2\theta = 0$ or 1. This corresponds merely to the result one obtains without hybridization. Subtracting from Eqs. (18) and (19) their counterpart without hybridization, we are left with summations over quantities which are essentially nonzero only in the anticrossing region. In this small region it is convenient to take, at fixed k_z, ϵ and ϵ' as new variables instead of k_x and k_y. The Jacobian of the transformation is $J = \partial(\epsilon,\epsilon')/\partial(k_x,k_y) = |\mathbf{v}_p \times \mathbf{v}_c|$ where $\mathbf{v}_p$ and $\mathbf{v}_c$ are the Fermi velocities of the plane and chain band at the crossing point. We are then led to evaluate

$$\int d\varepsilon\, d\varepsilon' \frac{f(\varepsilon,\varepsilon')}{(\varepsilon+\varepsilon')^2}[\delta(e_1) + \delta(e_2) - \delta(\varepsilon) - \delta(\varepsilon')],$$

with $f(\epsilon,\epsilon') = \epsilon^2$ or ϵ'^2 or $-\epsilon\epsilon'$. This is easily done by taking ϵ/t_k and ϵ'/t_k as new variables and extending the boundaries of the integrals to infinity. The result is the same for the three integrals, namely, $-\pi|t_k|$. When this result is carried into Eqs. (18) and (19) we find naturally the first-order correction to the coupling constants $\lambda = N_p g$, $\lambda' = N_c g'$, $k = N_c K$, and $k' = N_p K$, where N_p and N_c are the total density of states of the (uncoupled) plane and chain bands. The hybridization changes these coupling constants, respectively, into $\lambda - N_t(g+K)$, $\lambda' - N_t(g'+K)$, $k - N_t(g+K)$, and $k' - N_t(g'+K)$. Here N_t is an effective density of states due to the hybridization and given by $N_t = \overline{t}/(\pi J c)$, where $\overline{t}$ is the average of $|t_k|$ over k_z (we have taken into account that there are four crossings in the Brillouin zone). Naturally since we have $N_t \ll N_p$, N_c in our model these changes are small.

III. IMPURITY EFFECT ON THE CRITICAL TEMPERATURE

We consider now the effect on the critical temperature of impurities located in the planes and in the chains. We will assume that the impurity potential scatters electrons within the planes or within the chains, but that it does not scatter them from plane to chain. Our physical motivation is naturally that planes and chains are physically well separated, which corresponds to the fact that the hopping term t_k is small. Therefore the potential for scattering from plane to chain is reduced by a factor of order t_k/t_0 compared to the intraplane or intrachain scattering (where t_0 is a typical hopping term within planes or chains). This physical point is essential for the validity of our result. Including this small plane-chain scattering does not make any problem, but for sake of clarity and simplicity we will not do it explicitly and we will rather come back to this point after we have obtained the effect of intraplane and intrachain scattering. We will also take an isotropic scattering within planes and chains, consistently with what we have done for the interactions. This leads us to the following impurity potential:

$$V = U_1 \sum_{k,k'} c^\dagger_{1,k} c_{1,k'} + U_2 \sum_{k,k'} c^\dagger_{2,k} c_{2,k'}. \tag{20}$$

We treat this potential within the Born approximation since, for the calculation of the critical temperature, making use of the T-matrix approximation is merely equivalent to renormalizing the scattering potential. There is, however, another effect produced by going beyond the Born approximation, which will be considered at the end of this section.

Within the Born approximation and after impurity averaging, only contributions to the self-energy corresponding to scattering twice on the same impurity are retained.[38] Since the potential, Eq. (20), does not scatter electrons from plane to chain, the impurities contribution to the self-energy has only components within planes or chains. They are given by[39]

$$\Sigma_i = n_i U_i^2 \sum_k \tau_3 G_{ii} \tau_3, \tag{21}$$

where n_1 and n_2 are the number of impurities per unit volume in the planes and in the chains, τ_i are the Pauli matrices in Nambu space, and G is the temperature Green's function in plane-chain representation. The Green's function is related to the self-energy by

$$G^{-1} = G_0^{-1} - \Sigma, \tag{22}$$

where G_0 is the Green's function in the absence of the impurity self-energy. Explicitly we set

$$G^{-1}_{ij} = (i\tilde{\Omega}_i - \varepsilon_i \tau_3 - \tilde{\Delta}_i \tau_1)\,\delta_{ij} - t\tau_3\sigma_{x,ij}, \tag{23}$$

$$G^{-1}_{0,ij} = (i\omega - \varepsilon_i \tau_3 - \Delta_i \tau_1)\,\delta_{ij} - t\tau_3\sigma_{x,ij}, \tag{24}$$

where $\omega = (2n+1)\pi T$ is the Matsubara frequency (we omit systematically for clarity the index n in the Matsubara frequency and all frequency-dependent quantities), σ_x is the Pauli matrix in plane-chain space, and Δ_i is the off-diagonal self-energy due to the pairing interaction (we have set $\epsilon_1 \equiv \epsilon$ and $\epsilon_2 \equiv \epsilon'$). In order to invert G^{-1} it is convenient to go the hybridized band representation, or more precisely to make the transformation which diagonalizes G^{-1} when the off-diagonal part $\tilde{\Delta}_i$ of the self-energy is zero. For G_0^{-1} the transformation matrix is just $a_{ij}\tau_0$ where a_{ij} is the transformation considered in the preceding section. In the present case we have merely to formally generalize it by replacing ϵ_i by $\epsilon_i - i\tilde{\Omega}_i$ for the particle-particle part in Nambu space and by $\epsilon_i + i\tilde{\Omega}_i$ in the hole-hole part. We keep the same notation for this transformation, but the a_{ij} are now complex. The complete transformation matrix is now $A_{ij} = (a_{ij} + a^*_{ij})\,\tau_0/2 + (a_{ij} - a^*_{ij})\,\tau_3/2$. Actually we have Σ, $\Delta \ll t$, since we assume that the hybridized bands are well separated (Σ or Δ are typically of the same order of magnitude in the important cases as it will be clear below). Moreover, as usual we will be only concerned with Matsubara frequencies ω at most of order Σ and Δ and therefore negligible compared to t. This implies that, when it multiplies a quantity of order Σ or Δ, we can take for a_{ij} its zero order value, namely, the real value found in the preceding section. This leads to the expression $g^{-1} = {}^tA\ G^{-1}A$ for the full Green's function in the hybridized representation (${}^tA$ is the transpose of A):

$$g_{ij}^{-1} = -\tfrac{1}{2}[(\tilde{e}_i - \tilde{e}_i^*)\tau_0 + (\tilde{e}_i + \tilde{e}_i^*)\tau_3]\delta_{ij} - a_{ki}\tilde{\Delta}_k a_{kj}\tau_1, \tag{25}$$

where

$$\begin{aligned} 2\tilde{e}_{1,2} &= \varepsilon_1 + \varepsilon_2 - i(\tilde{\Omega}_1 + \tilde{\Omega}_2) \\ &\quad \pm[(\varepsilon_1 - \varepsilon_2 - i\tilde{\Omega}_1 + i\tilde{\Omega}_2)^2 + 4t^2]^{1/2} \\ &\approx 2e_{1,2} - 2i\tilde{\omega}_{1,2} \end{aligned} \tag{26}$$

and we have set

$$2\tilde{\omega}_{1,2} = \tilde{\Omega}_1 + \tilde{\Omega}_2 \pm \frac{(\tilde{\Omega}_1 - \tilde{\Omega}_2)(\varepsilon_1 - \varepsilon_2)}{[(\varepsilon_1 - \varepsilon_2)^2 + 4t^2]^{1/2}}. \tag{27}$$

Now the dominant contributions to the summations of G over the wave vector **k** will come from the vicinity of the Fermi surface of the hybridized bands. In this case either $\tilde{e}_1$ is large and all the other matrix elements of g^{-1} are small (of order Δ typically), or $\tilde{e}_2$ is large and the other elements are small. It is then easy to see that when $\tilde{e}_2$ is large, we obtain g by simply inverting the (1,1) block of g^{-1}; that is, we have $g_{ij} \approx [(g^{-1})_{11}]^{-1}\ \delta_{i,1}\ \delta_{j,1}$. The other terms of g_{ij} are smaller by a factor of order Δ over energy separation of the hybridized bands (for fixed **k**), that is, a factor of order Δ/t or less. We have a similar result when $\tilde{e}_1$ is large. Taken together this means that we can take g_{ij} as block diagonal, that is, $g_{ij} = g_{ii}\ \delta_{ij}$, with

$$g_{ii} = -\frac{1}{\tilde{e}_i\tilde{e}_i^* + \tilde{\delta}_i^2}\begin{pmatrix} \tilde{e}_i^* & \tilde{\delta}_i \\ \tilde{\delta}_i & -\tilde{e}_i \end{pmatrix}, \tag{28}$$

where $\tilde{\delta}_i = a_{ij}^2\ \tilde{\Delta}_j$, that is, explicitly $\tilde{\delta}_1 = \tilde{\Delta}_1\ \cos^2\theta + \tilde{\Delta}_2\ \sin^2\theta$ and $\tilde{\delta}_2 = \tilde{\Delta}_1\ \sin^2\theta + \tilde{\Delta}_2\ \cos^2\theta$.

We can now calculate the impurity self-energy Σ. Since g_{ij} is block diagonal, we have $G_{ii} = a_{ij}^2\ g_{jj}$. When we carry this result into Eq. (21), we can perform the integration perpendicularly to the Fermi surface (that is, integrate over e_1 or e_2) since it converges within an energy range of order Δ. We are then left with summations along the Fermi surface, just as in the calculation of the critical temperature in the preceding section. This leads to

$$\Sigma_i = -\pi n_i U_i^2 \sum_k\ a_{ij}^2\delta(e_j)\frac{i\tilde{\omega}_j\tau_0 - \tilde{\delta}_j\tau_1}{|\tilde{\omega}_j|}, \tag{29}$$

where we have taken into account that $\tilde{\delta}_i \ll \tilde{\omega}_i$ since we are only interested in the calculation of the critical temperature. We can then proceed as in the preceding section: For most of the Fermi surface we have $\epsilon_1 \ll \epsilon_2$ or $\epsilon_2 \ll \epsilon_1$, leading to $a_{ij}^2 = 0$ or 1. This corresponds to the result without hybridization, which is

$$\Sigma_i^0 = -\Gamma_i\left(i\tau_0\mathrm{sgn}\omega - \frac{\tilde{\Delta}_i}{|\tilde{\Omega}_i|}\tau_1\right), \tag{30}$$

where $\Gamma_i = \pi n_i N_i\ U_i^2$ with $N_1 \equiv N_p$ and $N_2 \equiv N_c$. When we calculate $\Sigma_i - \Sigma_i^0$ we are left with summations over nonzero quantities only in the anticrossing region. We take then $(\epsilon_1 - \epsilon_2)/t$ and $(\epsilon_1 + \epsilon_2)/2t$ as new variables and extend the boundaries of the integrals to infinity. The resulting expression simplifies under exchanging ϵ_1 and ϵ_2. We obtain that the diagonal parts of Σ_i and Σ_i^0 are equal, which implies $\tilde{\Omega}_i = \omega + \Gamma_i$ sgn ω. On the other hand we find from the off-diagonal part

$$\begin{aligned} \tilde{\Delta}_1 &= \Delta_1 + \Gamma_1\frac{\tilde{\Delta}_1}{|\tilde{\Omega}_1|} + \Gamma_1\frac{N_t}{N_1}\frac{2}{\pi}\int_0^1\frac{du}{(1-u^2)^{3/2}} \\ &\quad \times\left[\frac{(1+u)^2\tilde{\Delta}_1 + (1-u^2)\tilde{\Delta}_2}{|(1+u)\tilde{\Omega}_1 + (1-u)\tilde{\Omega}_2|} + \{u \to -u\} - \frac{2\tilde{\Delta}_1}{|\tilde{\Omega}_1|}\right], \end{aligned} \tag{31}$$

where $u = (\epsilon_1 - \epsilon_2)/[(\epsilon_1 - \epsilon_2)^2 + 4t^2]^{1/2}$ and a similar result for $\tilde{\Delta}_2$.

This equation displays explicitly an essential point for our result: The correction to the self-energy due to hybridization is small, of order $N_t\ /\ N_{1,2}$, compared to the self-energy in the absence of hybridization. This correction corresponds physically to the scattering from plane to chain induced by hybridization. However, without hybridization, we are in the standard s-wave situation and impurities do not change the critical temperature. The only effect on T_c will come from the correction due to hybridization. Since this correction is small, we expect the change of T_c to be small with respect to what one would get with a simple d-wave order parameter. Although the integration in Eq. (31) can be performed analytically in the general case, the result is not simple. Therefore, in order to obtain reasonably simple calculations, we will continue our quantitative investigation only in the particular case where $\Gamma_1 = \Gamma_2 \equiv \Gamma$, which implies $\tilde{\Omega}_1 = \tilde{\Omega}_2 \equiv \tilde{\Omega}$. Actually this equality is always valid when the Matsubara frequency ω is large enough compared to Γ_1 and Γ_2. This is in particular always valid when the impurity concentration is small enough so that $\Gamma_{1,2} \ll T_c$. Therefore the case we consider is quite reasonable.

In this case the equations for $\tilde{\Delta}_1$ and $\tilde{\Delta}_2$ simplify to

$$\tilde{\Delta}_1 = \Delta_1 + \Gamma\frac{\tilde{\Delta}_1}{|\tilde{\Omega}|} + \Gamma\frac{N_t}{N_1}\frac{\tilde{\Delta}_2 - \tilde{\Delta}_1}{|\tilde{\Omega}|}, \tag{32}$$

$$\tilde{\Delta}_2 = \Delta_2 + \Gamma\frac{\tilde{\Delta}_2}{|\tilde{\Omega}|} + \Gamma\frac{N_t}{N_2}\frac{\tilde{\Delta}_1 - \tilde{\Delta}_2}{|\tilde{\Omega}|}. \tag{33}$$

We have finally to calculate from Eqs. (12) and (13) the self-energies Δ_1 and Δ_2 due to the pairing interactions. We have already obtained the off-diagonal part of the Green's function, and the calculation is essentially the same as for the off-diagonal part of the impurity self-energy. One finds

$$\Delta_1 = N_1 g \pi T \sum_n \left[\frac{\tilde{\Delta}_1}{|\tilde{\Omega}|} + \frac{N_t}{N_1} \frac{\tilde{\Delta}_2 - \tilde{\Delta}_1}{|\tilde{\Omega}|} \right] - N_2 K \pi T \sum_n \left[\frac{\tilde{\Delta}_2}{|\tilde{\Omega}|} + \frac{N_t}{N_2} \frac{\tilde{\Delta}_1 - \tilde{\Delta}_2}{|\tilde{\Omega}|} \right], \tag{34}$$

$$\Delta_2 = N_2 g' \pi T \sum_n \left[\frac{\tilde{\Delta}_2}{|\tilde{\Omega}|} + \frac{N_t}{N_2} \frac{\tilde{\Delta}_1 - \tilde{\Delta}_2}{|\tilde{\Omega}|} \right] - N_1 K \pi T \sum_n \left[\frac{\tilde{\Delta}_1}{|\tilde{\Omega}|} + \frac{N_t}{N_1} \frac{\tilde{\Delta}_2 - \tilde{\Delta}_1}{|\tilde{\Omega}|} \right]. \tag{35}$$

However, these equations merely mean that we have to calculate the critical temperature with the coupling constants modified by the hybridization, as we have found at the end of the preceding section. With these coupling constants, Eqs. (34) and (35) take the simple form

$$\Delta_1 = \lambda \pi T \sum_n \frac{\tilde{\Delta}_1}{|\tilde{\Omega}|} - k \pi T \sum_n \frac{\tilde{\Delta}_2}{|\tilde{\Omega}|}, \tag{36}$$

$$\Delta_2 = \lambda' \pi T \sum_n \frac{\tilde{\Delta}_2}{|\tilde{\Omega}|} - k' \pi T \sum_n \frac{\tilde{\Delta}_1}{|\tilde{\Omega}|}. \tag{37}$$

From Eqs. (32) and (33) we have

$$\frac{\tilde{\Delta}_1}{|\tilde{\Omega}|} = \frac{\Delta_1}{|\omega|} + \frac{\gamma_1 (\Delta_2 - \Delta_1)}{|\omega| (|\omega| + \gamma_1 + \gamma_2)}, \tag{38}$$

$$\frac{\tilde{\Delta}_2}{|\tilde{\Omega}|} = \frac{\Delta_2}{|\omega|} + \frac{\gamma_2 (\Delta_1 - \Delta_2)}{|\omega| (|\omega| + \gamma_1 + \gamma_2)}, \tag{39}$$

where we have set $\gamma_1 = \Gamma N_t / N_1$ and $\gamma_2 = \Gamma N_t / N_2$. As expected the inverse lifetime Γ due to scattering within planes and chains has disappeared from the equations, and only are left γ_1 and γ_2 which describe physically the scattering from plane to chain due to hybridization. When this is carried into Eqs. (36) and (37) and the summations on the Matsubara frequency are carried out, one finds

$$\Delta_1 = \lambda \left[\Delta_1 x + (\Delta_2 - \Delta_1) \frac{k}{k + k'} K(\rho) \right] - k \left[\Delta_2 x + (\Delta_1 - \Delta_2) \frac{k'}{k + k'} K(\rho) \right], \tag{40}$$

$$\Delta_2 = \lambda' \left[\Delta_2 x + (\Delta_1 - \Delta_2) \frac{k'}{k + k'} K(\rho) \right] - k' \left[\Delta_1 x + (\Delta_2 - \Delta_1) \frac{k}{k + k'} K(\rho) \right] \tag{41}$$

where $x = \ln\,(1.13\omega_D / T_c)$ and $K(\rho) = \psi(1/2 + \rho) - \psi(1/2)$, with $\rho = (\gamma_1 + \gamma_2)/(2\pi T_c)$, and we have used the fact that in our case $k/k' = \gamma_1/\gamma_2$. Equations (40) and (41) are essentially what one obtains for the effect of the impurities in a two-band model.[26] This is easy to understand physically since, because of hybridization, the in-plane scattering potential allows effectively an electron to scatter from plane to chain, for example. However, our essential point is that the corresponding effective inverse scattering time $\gamma \equiv \gamma_1 + \gamma_2$ is strongly reduced, compared to plane-plane or chain-chain scattering, because the hybridization is small. We note also that, in the general case, our Eq. (31) does not reduce to a simple two-band model, although we expect the physics to be similar.

Let us briefly review the existing literature[26] for the consequences of Eqs. (40) and (41) for the critical temperature, and add some results for the case which is of interest for us, namely, the general situation with repulsive interactions. From Eqs. (40) and (41) one gets an equation for x which is more conveniently rewritten as

$$K(\rho) = \frac{(x - x_0)(x - x_1)}{x - x_2}. \tag{42}$$

Here x_0 and x_1 are the solutions of Eq. (9). More precisely Eq. (9) has two physically relevant solutions when $\lambda\lambda' > kk'$. The lower one, x_0, gives the physical critical temperature. The higher one, x_1, corresponds to an unstable superconducting state where the order parameter has the same sign in the two bands, and therefore the interband coupling decreases the critical temperature with respect to the uncoupled situation instead of increasing it [in the uncoupled limit $x_0 = 1/\lambda$ and $x_1 = 1/\lambda'$; we assume, for example, $\lambda > \lambda'$ (Ref. 41)]. When $\lambda\lambda' < kk'$, the interband coupling is too strong for the state with the ill-chosen signs of the order parameter to exist and the unstable solution disappears (there is still a mathematical solution with $x_1 < 0$ but it must be rejected physically because it does not satisfy the weak-coupling condition $x \gg 1$ anymore). Finally we have $(\lambda\lambda' - kk') x_2 = (\lambda k + \lambda' k' + 2kk')/(k + k')$ in Eq. (42). It is easy to see that one has always $x_0 < x_2 < x_1$ for $\lambda\lambda' > kk'$, while $x_1 < x_2 < x_0$ is satisfied for $\lambda\lambda' < kk'$. Now for fixed γ, $K(\rho)$ is a positive, increasing function of $x + \ln\,(\gamma/\omega_D)$, with $K(\rho) \to 0$ for $x \to -\infty$ and $K(\rho) \approx x + \ln\,(\gamma/\omega_D)$ for $x \to \infty$. Then it is easy to see graphically that, starting from x_0 for $\gamma = 0$, x as given by Eq. (42) is an increasing function of γ. Therefore, in all possible cases, the critical temperature decreases when the impurity concentration increases.

For $\lambda\lambda' > kk'$ the increase of x saturates at x_2, leading to a large concentration limit T_c^∞ for the critical temperature given, as found by Kusakabe,[26] by

$$\ln\left(\frac{1.13\omega_D}{T_c^\infty} \right) = \frac{2kk' + \lambda k + \lambda' k'}{(\lambda\lambda' - kk')(k + k')}. \tag{43}$$

This saturation corresponds physically to the situation where strong impurity scattering has made the order parameter completely isotropic, $\Delta_1 = \Delta_2$, while $(\Delta_1 - \Delta_2) K(\rho)$ takes an independent nonzero value. The result, Eq. (43), is then easily rederived directly from Eqs. (40) and (41). Therefore in this case the superconducting state survives very strong impurity scattering by becoming isotropic. This situation is analogous to the fate of very dirty anisotropic s-wave superconductors[40] and naturally quite different from the standard behavior of a d-wave superconductor. We note incidentally that, when one goes from the pure system to the very dirty one, one goes from $\Delta_1\ \Delta_2 < 0$ to $\Delta_1\ \Delta_2 > 0$, which implies that, if $\lambda + k' > \lambda' + k$, for example, the chains be-

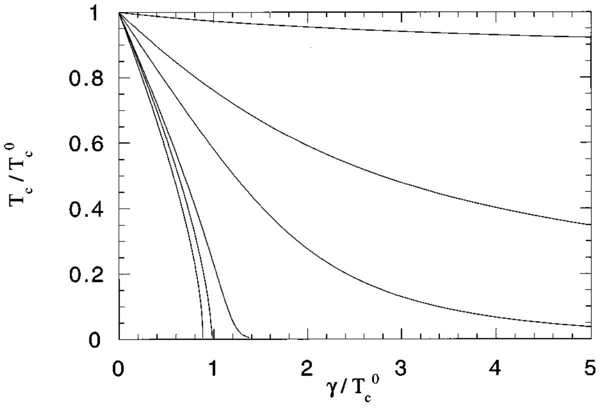

FIG. 1. Relative variation of the critical temperature from Eq. (42) as a function of our reduced effective relaxation rate γ/T_c^0 for the parameters $\lambda = 1$, $\lambda'=0$, and $k'=0.5$, and for k taking the values 0.01, 0.1, 0.2, 0.5, 1.5, and 5 ($k=1.5$ gives exactly an AG law).

come gapless $\Delta_2 = 0$ at some specific impurity concentration [given from Eqs. (40) and (41) by $K(\rho)=(k+k')/(\lambda\lambda'-kk')$ and $x=(\lambda'+k)/(\lambda\lambda'-kk')$]. However this case $\lambda\lambda'>kk'$ requires not too small coupling constants λ and λ' in both bands. In YBCO it is not clear at all that the CuO chains alone have a superconducting tendency. If we have $\lambda' \approx 0$, the condition $\lambda\lambda'>kk'$ cannot be satisfied.

For $\lambda\lambda'<kk'$ there is no saturation in the increase of x and the critical temperature goes to zero when the impurity concentration is increased, as found by Kusakabe.[26] However when we substitute in Eq. (42) the large x behavior of $K(\rho)$, we obtain

$$x-x_0=\ln\frac{T_c^0}{T_c}=\frac{(x_0-x_2)\ln(1.13\gamma/T_c^0)}{x_2-x_1-\ln(1.13\gamma/T_c^0)}, \tag{44}$$

where T_c^0 is the critical temperature without impurities. Therefore T_c goes to zero for a critical impurity concentration and we find in this case a behavior similar to the standard d-wave result. The corresponding critical value γ_c for γ is given by

$$\ln\frac{1.13\gamma_c}{T_c^0}=x_2-x_1=\frac{1}{2(kk'-\lambda\lambda')}\left[\sqrt{(\lambda-\lambda')^2+4kk'}-\frac{(\lambda-\lambda')(k-k')+4kk'}{k+k'}\right]. \tag{45}$$

The right-hand side (RHS) of Eq. (45) is positive and it goes from zero (for $\lambda-\lambda'=k-k'$ or $k'=0$) to infinity (for $\lambda\lambda'=kk'$). Therefore the lowest possible value of γ_c is the standard d-wave result $\gamma_c=0.88T_c^0$ but it can easily be much higher since it is given by the exponential of the rhs of Eq. (45). From this, one would conclude that, for a given γ, our model is much less sensitive to impurities than standard d waves. However, when one looks at the behavior of T_c as a function of γ, one sees that this large value of γ_c is obtained at the end of a long tail where the value of T_c is already quite small, as can be seen in Fig. 1. Therefore, in order to fully characterize the sensitivity of T_c to impurities, we have also to look at the initial slope found for low impurity concentration.

In this regime we have from Eq. (42)

$$1-\frac{T_c}{T_c^0}=\frac{\pi}{4}\frac{\gamma}{T_c^0}\frac{x_0-x_2}{x_0-x_1}=\frac{\pi}{4}\frac{\gamma}{T_c^0}\left[\frac{1}{2}+\frac{(\lambda-\lambda')(k-k')+4kk'}{2(k+k')\sqrt{(\lambda-\lambda')^2+4kk'}}\right], \tag{46}$$

which is the result of Moskalenko and Palistrant.[26] As they indicated, $(x_0-x_2)/(x_0-x_1)$ goes from 0 to 1, which implies that the decrease of T_c is always less than for the pure d-wave case. The d-wave result is obtained in the limiting case $\lambda-\lambda'=k-k'$ or $k'\to 0$. On the other hand for $k\to 0$ (and fixed k'), the critical temperature does not depend anymore on the impurity concentration [this result is actually valid whatever the impurity concentration as it can be seen from Eq. (42)]. This limiting case is not unphysical since it corresponds to a situation where the density of states N_c in the chains would be very small. We would still have a d-wave-type order parameter with change of sign and nodes, but the critical temperature would be completely controlled by the planes and the chains would simply follow. Therefore we have the surprising result of a superconducting phase with a d-wave-type order parameter which has a critical temperature insensitive to impurities just as an s-wave superconductor. However, it is fair to say that we do not expect such a limiting situation to occur in YBCO. Hence we believe that in our case Eq. (46) leads to a sensitivity to impurities which is always somewhat reduced with respect to the standard d-wave case, but not by a large factor. An example of the general behavior of T_c / T_c^0 as a function of our scattering rate γ is given in Fig. 1 where we have chosen the parameters $\lambda=1$, $\lambda'=0$, and $k'=0.5$, and k takes the values 0.01, 0.1, 0.2, 0.5, 1.5, and 5 ($k=1.5$ gives exactly an Abrikosov-Gor'kov law).

In order to conclude this section, let us now come back to the various terms we have omitted from the beginning. We did not take into account direct plane-chain scattering by impurities. As we mentionned, we expect physically this scattering to be reduced by a factor $N_t/N_{p,c}$ compared to plane-plane or chain-chain scattering which we have treated. Including this plane-chain term is just what is done in the standard two-band model when the effect of impurities on T_c is calculated. Since we have shown that our calculation leads us to the two-band model, including direct plane-chain scattering would just give us an additional term of the same order as the one we have found (it would appear as an additional term in Σ_0). Therefore our conclusions with respect to the sensitivity of T_c to impurities are unchanged. We have also omitted mixed plane-chain terms Δ_{12} for the order parameter. This is justified by our finding that, when the hybridized bands are well separated, the dominant contributions of g come from the block diagonal parts g_{11} and g_{22}. Hence we have, for example, $G_{12}=a_{11}g_{11}a_{21}+a_{12}g_{22}a_{22}$. However, the products $a_{11}a_{21}$ and $a_{12}a_{22}$ are significantly different from zero only in the anticrossing region. When we calculate the off-diagonal self-energy, we have to sum G_{12} over **k**. Accordingly the result Δ_{12} will be smaller by a factor of order $N_t/N_{p,c}$ compared to Δ_1 and Δ_2, which justifies our approximation. Finally we note that going beyond the Born approximation will not only renormalize the impurity cross section. It will also introduce plane-chain terms Σ_{12} in the impurity self-energy because, after scattering on a plane impurity, an electron can go to the chains through G_{12} and scatter on a chain impurity. But we have just seen that, after summation of G_{12} over **k**, one obtains a result which is smaller by a factor $N_t/N_{p,c}$. This leads to a Σ_{12} which is smaller than Σ_1 or Σ_2 by the same factor and hence negligible.

IV. DISCUSSION

The conclusion of our study is that, in our model, the critical temperature is much less sensitive to impurities than it is in standard d-wave models. One basic reason is that we expect physically impurities to produce essentially plane-plane and chain-chain scattering. Just as in s-wave superconductors, this scattering does not affect the critical temperature. On the other hand T_c is reduced by scattering between parts of the Fermi surface which have opposite signs for the order parameter, just as in standard d-wave case. In our model this is due to plane-chain scattering. We have found that this scattering, whatever its origin, will be smaller by a factor of order t/E_F (that is, hybridization coupling over Fermi energy) compared to plane-plane and chain-chain scattering. From the band structure calculations we expect this factor to be typically somewhere between 0.1 and 0.3. Therefore the sensitivity of T_c to impurities in our model is reduced by a similar factor, compared to the d-wave situation. In the specific case which we have studied in detail and which reduces to the two-band model, we have found a further reduction of the sensitivity of T_c to impurities with a behavior which can vary continuously from s-wave like to d-wave like depending on the parameters. From our discussion of its physical origin, we expect a similar behavior and reduction to occur in the general case.

It is unfortunately not possible to make a quantitative comparison with experiments. Indeed it seems surprisingly quite difficult[18] to avoid a magnetic character for substitutional impurities in YBCO. Naturally this occurs when the isolated impurity atom itself has a magnetic moment. But this happens also when a nonmagnetic impurity acquires a magnetic moment due to its interaction with the environment, as is the case for Zn, for example.[18] Naturally an impurity with a magnetic character will produce pair breaking, leading to an Abrikosov-Gor'kov like law in any model, in agreement with what is observed experimentally. Hence these kind of experiments cannot be used directly to eliminate theoretical models. Nevertheless, after these words of caution with respect to a simple-minded interpretation of impurity experimental results, we note that the reduction of T_c down to 13 K for 8% Zn is obtained by an increase of the residual resistivity[18] by a factor of order 10. The corresponding $\hbar/\tau$ should be then of order 20 T_c (see below). This is much more than what is necessary to destroy superconductivity within a d-wave model according to the Abrikosov-Gor'kov law. Moreover, it is useful to plot the results of Refs. 17 and 18 for the critical temperature as a function of the residual resistivity. This is done in Fig. 2. It can be seen that the behavior of some of our results found in Fig. 1 is quite similar to the experimental results (we assume naturally that the residual resistivity is proportional to the scattering rate due to impurities). We have naturally enough adjustable parameters to fit them nicely. However, such a fit would be rather meaningless because, in addition to the magnetic problem, the scatter in the data is rather important at low impurity content and the interpretation of the data for larger concentration is uncertain (localization effects which are not taken into account in our theory might play a significant role).

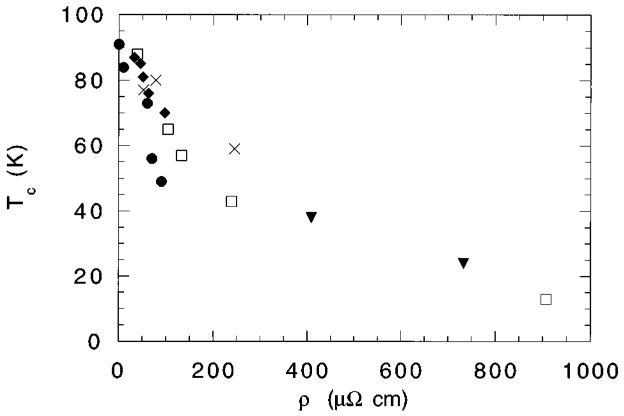

FIG. 2. Experimental results for the variation of the critical temperature of YBCO, due to Zn impurities, as a function of the residual resistivity. The solid circles are the results of Ref. 17, the open squares, the crosses, the solid diamonds, and the solid triangles are, respectively, the results for the batches 2, 3, 4, and 6 of Ref. 18.

If we turn to irradiation experiments, whether by electrons or by light ions, the interpretation is also not an easy one. It is known that high-T_c compounds have a critical temperature much more sensitive to irradiation than standard superconducting materials. However, although it is likely that most of the created defects do not have a magnetic character, we can not eliminate, from our knowledge on substitutional impurities, the possibility that some are magnetic. The experimental evidence is controversial in this respect.[15] Then there is some evidence that localization effects might be important since a metal-insulator transition is observed in YBCO under light ion irradiation, and there is no intermediate normal phase between the superconducting phase and the insulating one.[14] This sensitivity to localization is easy to understand because of the two-dimensional nature of the CuO_2 planes. Localization effects are not included in our theoretical study. It is also not clear at all that the created disorder can be considered as homogeneous[12] since the resistivity measurements do not always display a sharp drop at the critical temperature. Similarly one might expect that the defects created by irradiation are randomly distributed at the microscopic scale, but it is actually quite likely that the chains are more sensitive to irradiation than the planes. There is finally the obvious problem of having an experimental determination of the quasiparticle lifetime produced by disorder. Measuring the increase in resistivity appears the best way to do it[11] although it is far from perfect since, for example, it measures at best a transport lifetime which we expect to be somewhat larger than quasiparticle lifetime.

Notwithstanding the above problems let us try to interpret the irradiation experiments with our theoretical model, just to see what comes out. From Drude's law, with a typical resistivity of 100 $\mu\Omega$ cm at T_c and a plasma frequency of 1.1 eV,[15] we have a typical inverse lifetime $\hbar/\tau \approx 2T_c$. Since superconductivity disappears in the d-wave case when the inverse lifetime due to impurities is of order $2T_c$ we would expect that an increase of resistivity of 100 $\mu\Omega$ cm leads to the suppression of T_c.[11] This corresponds roughly to a decrease of T_c of 1 K per $\mu\Omega$ cm (the AG law is essentially linear). The experimental results of Ref. 15 give a linear decrease of T_c with respect to resistivity with a slope 0.3 K/$\mu\Omega$ cm. In Ref. 14 there is an upward curvature at low resistivity with a maximal initial slope of 0.1 K/$\mu\Omega$ cm. Since in our model a reduction by a typical factor 1/10 with respect to the d-wave result corresponds to a typical choice of our parameters, we see that this last experimental result agrees with our expectation. But the result of Ref. 14 could easily be explained, for example, by a larger value of the hybridization energy or by a suitable choice of the other parameters of our two-band model. Quite generally we have enough parameters to vary in our model and so we can easily get agreement with these various experimental results. However, it must also be kept in mind that, as discussed above, there are other possible physical processes which we have not taken into account and which will add up to produce a faster decrease of the critical temperature with the resistivity. A clear example of this is found in Ref. 14 where a more rapid decrease is found for a set of samples and attributed to extrinsic effects, while good samples show an average decrease of 0.03 K/$\mu\Omega$ cm. Therefore we can consider an experimental result as an upper bound for our theoretical result, but it may quite well be larger than what we find. Clearly it is more difficult to explain in a d-wave model the slow dependence of T_c on resistivity found in Ref. 14 than it is in our model to explain the somewhat stronger dependence found in Ref. 15.

In conclusion we have seen that our model is quite coherent with the present experimental evidence. Naturally, with respect to this problem of the effect of impurities on the critical temperature, it would be much better to have experiments providing stronger constraints on theoretical models, but this might prove difficult to achieve.

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APPENDIX

Let us vary Eq. (9) with respect to the phonon frequencies ω_D and Ω. We assume, for example, $\delta r = -\delta\omega_D/\omega_D = -\delta\Omega/\Omega < 0$. The variation of Eq. (9) gives

$$\delta y(2y-\lambda^*-\lambda'^*) = \delta(k^*k'^*) - \delta\mu^*(y-\lambda'^*) - \delta\mu'^*(y-\lambda^*), \tag{A1}$$

where $y = x^{-1}$. The isotope effect is reduced if we show that $\delta y < 0$. We set $D^{-1} = (1+\mu r)(1+\mu' r) - kk' r^2$. We have $\delta(k^*k'^*) = 2k^*k'^*\delta D/D$, and $\delta\mu^* = \mu^*\delta D/D + D(\mu\mu' - kk')\delta r > \mu^*\delta D/D$ (we assume $\mu\mu' - kk' > 0$, which implies $\mu^*\mu'^* - k^*k'^* > 0$). Since we have $y > \lambda^*$ and $y > \lambda'^*$, and $\delta D > 0$, it is enough to prove that

$$2k^*k'^* - \mu^*(y-\lambda'^*) - \mu'^*(y-\lambda^*) < 0. \tag{A2}$$

The left-hand side is zero when the variable y is equal to $Y = (2k^*k'^* + \mu^*\lambda'^* + \mu'^*\lambda^*)/(\mu^* + \mu'^*)$. We find that $y_1 < Y < y_0$, since we have

$$\begin{aligned}(\mu^*+\mu'^*)^2[(Y-\lambda^*)(Y-\lambda'^*) - k^*k'^*] \\ = -k^*k'^*[\lambda^*-\lambda'^*+\mu^*-\mu'^*]^2 - (\mu^*\mu'^* - k^*k'^*) \\ \times[(\lambda^*-\lambda'^*)^2 + 4k^*k'^*] < 0,\end{aligned} \tag{A3}$$

where $y_0 = 1/x_0$ and $y_1 = 1/x_1$. Since we have $y > y_0 > Y$, Eq. (A2) is satisfied and the isotope effect is indeed reduced. There is no reduction only in the limiting case $\mu\mu' = kk'$ and $\lambda^* + \mu^* = \lambda'^* + \mu'^*$.

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