PHYSICAL REVIEW B VOLUME 45, NUMBER 1 1 JANUARY 1992-I

Intralayer versus interlayer pairing in the copper oxide superconductors: The three- and four-layer problems

S. H. Liu
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6032

R. A. Klemm
Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439

(Received 20 May 1991)

We have analyzed the possible superconducting states of a model layered superconductor with N conducting layers in a unit cell, for $N=3$ and 4, in the presence of both intralayer and interlayer pairing interactions. In case all layers are identical, the system has the same behavior as one-layer and two-layer systems, namely that pure intralayer pairing interaction stabilizes an s-wave state with equal and isotropic gaps in all N quasiparticle bands, while interlayer pairing produces both singlet and triplet paired states with anisotropic gap functions. The singlet state is always energetically more stable than the triplet state. The analysis can be easily extended to nonidentical layers. As one example, a model for $YBa_2Cu_3O_{7-\delta}$ consisting of two CuO_2 layers in a unit cell separated by a layer of CuO chains is discussed. It is shown that the system reduces to an effective two-layer model, due to the large difference in electronic energy states between the planes and the chains. The chains are most likely nonsuperconducting. In another example, we show that $Bi_2Sr_2CaCu_2O_8$ can be reduced to an effective three-layer system. Recent tunneling data can be understood on the basis of this model.

I. INTRODUCTION

In two recent papers we have reported a series of analyses of the consequences of intralayer and interlayer pairing on the physical properties of layered superconductors.[1,2] In a material with one layer per unit cell, both intralayer and interlayer pairing produces isotropic gap functions, but the ordered states are entirely different in nature. The intralayer paired state is pure s wave, while the interlayer paired state is an equal mixture of singlet and triplet states. The two types of ordered states cannot coexist in a material where both interactions are present; the ordered state is dictated by which interaction gives the higher critical temperature. In a material with two layers per unit cell, intralayer pairing stabilizes an s-wave state with an isotropic gap function, while interlayer pairing favors a singlet state with an anisotropic gap function. The gap functions are associated with electron bands, not with layers. The competition between intralayer and interlayer interactions is more complex. In general, there is a three-way competition between intralayer s-wave, interlayer singlet, and interlayer triplet states in that the one that has the highest critical temperature tends to suppress the others. If intralayer pairing dominates, the system will have a conventional s-wave-paired state. If interlayer pairing dominates, the system, under suitable conditions, may allow either the intralayer s-wave or the interlayer triplet state to mix with the dominant interlayer state at a lower temperature.

In this paper we extend our analysis to a model with N layers per unit cell, $N=3$ and 4, for both intralayer and interlayer interactions. The investigation was motivated by the existence of the family of superconducting compounds. $Tl_2Ba_2Ca_{N-1}Cu_NO_{4+2N}$, which has N nearly identical CuO_2 layers in a unit cell. In addition, there may be other conducting layers in the system, such as TlO double layers, which participate in the superconducting properties. The analysis is more complex than the one-layer and two-layer cases, so we will limit ourselves to the discussion of intraband paired states because interband paired states are spontaneously pair broken, and their order parameters are suppressed in the ordered phase. We have shown that s-wave intralayer pairing produces equal and isotropic gap functions in all N quasiparticle energy bands. We exclude p- and d-wave intralayer pairing because there is no evidence for gap anisotropy within the ab plane in $YBa_2Cu_3O_{7-\delta}$ (Y 1:2:3) or other layered superconductors.[3,4] Interlayer pairing favors a singlet paired state with complex and anisotropic gap functions, at least one of which has a node. A triplet state is possible but is generally suppressed by the singlet state. The Ginzburg-Landau free energy is derived, and we deduce from its expression that the competition between different ordered states in complete analogy with the two-layer case.

There is also the question whether Y 1:2:3 should be regarded as a three-layer material because the CuO chains, which form a layer distinct from the CuO_2 layers, may participate in superconductivity. We will demonstrate that because the chains have electronic energy levels very different from the planes, the material reduces to an effective two-layer system. The observed gap anisotropy suggests that the dominant pairing interaction is interlayer. Under this condition the chains are nonsuperconducting. In a similar way, the compound $Bi_2Sr_2CaCu_2O_8$ (Bi 2:2:1:2), which has two CuO_2 layers and two BiO layers, can be reduced to a three-layer model. We will show that the recent tunneling data for this material can be understood on the basis of this model.

II. THE MODEL

The model under discussion is a straightforward extension of the two-layer model defined in Refs. 1 and 2. In Secs. III and IV we assume N identical conducting layers separated from each other by distances d within the unit cell and d' between unit cells such that $(N-1)d+d'=s$, where s is the edge of the unit cell perpendicular to the planes. Within each plane the quasiparticles have two-dimensional band energies $\xi_0(\mathbf{k})$, where $\mathbf{k}=(k_x,k_y)$ is the wave vector in the planes. The band energy is measured from the Fermi level E_F. The planes are insulated from each other except for electron hopping between nearest-neighbor planes, with hopping matrix elements J_1 within the unit cell and J_2 between adjacent unit cells. The band Hamiltonian is then

$$H_0=\sum_{jk\sigma}\sum_{n=1}^{N}\xi_0(\mathbf{k})\psi^\dagger_{jn\sigma}(\mathbf{k})\psi_{jn\sigma}(\mathbf{k})+\sum_{jk\sigma}\left[J_1\sum_{n=1}^{N-1}\psi^\dagger_{jn\sigma}(\mathbf{k})\psi_{j,n+1,\sigma}(\mathbf{k})+J_2\psi^\dagger_{jN\sigma}(\mathbf{k})\psi_{j+1,1\sigma}(\mathbf{k})+\text{H.c.}\right], \tag{1}$$

where $\xi_0(\mathbf{k})=\mathbf{k}^2/2m_0-E_F$, σ is the spin index, and the sum on j is over all unit cells normal to the planes ($\hbar=1$). The pairing interaction V consists of an intralayer pairing term V_0 and an interlayer pairing term V_1, where

$$V_0=-\sum_{jn}\sum_{k\sigma}\sum_{k'\sigma'}\lambda_{0n}\psi^\dagger_{jn\sigma}(\mathbf{k})\psi^\dagger_{jn\sigma'}(-\mathbf{k})\psi_{jn\sigma'}(-\mathbf{k}')\psi_{jn\sigma}(\mathbf{k}'), \tag{2}$$

and

$$V_1=-\tfrac{1}{2}\sum_{j}\sum_{k\sigma}\sum_{k'\sigma'}\left[\lambda_1\sum_{n=1}^{N-1}\psi^\dagger_{jn\sigma}(\mathbf{k})\psi^\dagger_{j,n+1,\sigma'}(-\mathbf{k})\psi_{j,n+1,\sigma'}(-\mathbf{k}')\psi_{jn\sigma}(\mathbf{k}')\right.$$
$$\left.+\lambda_2\psi^\dagger_{jN\sigma}(\mathbf{k})\psi^\dagger_{j+1,1\sigma'}(-\mathbf{k})\psi_{j+1,1\sigma'}(-\mathbf{k}')\psi_{jN\sigma}(\mathbf{k}')+\text{H.c.}\right]. \tag{3}$$

All intralayer coupling strengths λ_{0n} are cut off at $\omega_\parallel$. Interlayer coupling strengths are λ_1 between nearest-neighbor planes in the same unit cell and λ_2 between planes in adjacent cells. All interlayer interactions are cut off at $\omega_\perp$.

We have chosen to discuss the simplest possible N-layer problem at first in order to explore the mathematical structure of the theory. The N layers are assumed to be identical, with identical two-dimensional band structures. It will be shown that interlayer hopping will create N slightly split bands. This is in accord with band calculations, for instance, the system $YBa_2Cu_3O_{7-\delta}$ has two nearly degenerate bands associated with the two CuO_2 layers per unit cell. It will be demonstrated in Sec. V that the chain layer can be treated as a third, nonidentical layer by extending the same formalism. The assumption of interlayer pairing between nearest-neighbor layers is also the simplest possible. The formalism can be easily extended to include pairing between more distant neighbor layers, as shown in Sec. V.

In the following sections we will discuss the solution of the three- and four-layer problems. We will emphasize the limit of $J_1,J_2>T_c$ as found in real materials ($k_B=1$). As in the one- and two-layer problems, the proper starting point of the analysis is to diagonalize H_0 in the band representation first and then treat the pairing interactions in the mean field approximation using the three-dimensional band-wave functions as basis states. As a consequence of this procedure, the gap functions belong to the electronic bands and are not associated with individual layers.

III. THE THREE-LAYER PROBLEM

The band problem is solved in two steps. We first Fourier analyze the electron operators in the c direction, the direction normal to the planes. Defining the Fourier transforms of the electron operators by

$$\bar{\psi}_{n\sigma}(k)=M^{-1/2}\sum_{j}\psi_{jn\sigma}(\mathbf{k})e^{ik_x[js+(n-1)d]}, \tag{4}$$

where M is the number of units cells in the c direction, $k=(\mathbf{k},k_z)$, and k_z is the wave vector in the c direction, we obtain

$$\begin{aligned}H_0=&\sum_{nk\sigma}\xi_0(\mathbf{k})\bar{\psi}^\dagger_{n\sigma}(k)\bar{\psi}_{n\sigma}(k)\\&+\sum_{k\sigma}[J_1e^{ik_zd}\bar{\psi}^\dagger_{1\sigma}(k)\bar{\psi}_{2\sigma}(k)\\&\quad+J_1e^{ik_zd}\bar{\psi}^\dagger_{2\sigma}(k)\bar{\psi}_{3\sigma}(k)\\&\quad+J_2e^{ik_zd'}\bar{\psi}^\dagger_{3\sigma}(k)\bar{\psi}_{1\sigma}(k)+\text{H.c.}]\,.\end{aligned} \tag{5}$$

The diagonalization of the Hamiltonian in Eq. (5) is carried out by a canonical transformation to the band operators $\psi_{l\sigma}(k)$,

$$\psi_{l\sigma}(k)=\sum_{n}b_{ln}(k_z)\bar{\psi}_{n\sigma}(k), \tag{6}$$

where $l=1,2,3$ is the band index, and the matrix elements b_{ln} of the transformation are solutions of the eigenvalue problem:

$$\begin{bmatrix} -\varepsilon_l & J_1 e^{ik_x d} & J_2 e^{-ik_x d'} \\ J_1 e^{-ik_z d} & -\varepsilon_l & J_1 e^{ik_z d} \\ J_2 e^{ik_z d'} & J_1 e^{-ik_z d} & -\varepsilon_l \end{bmatrix} \begin{bmatrix} b_{l1} \\ b_{l2} \\ b_{l3} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} , \qquad (7)$$

where the eigenvalues $\varepsilon_l(k_z)$ are the roots of the cubic equation

$$\varepsilon^3-(2J_1^2+J_2^2)\varepsilon-2J_1^2J_2\cos(k_zs)=0 . \qquad (8)$$

If we define $\bar{J}^2=(2J_1^2+J_2^2)/3$ and $\eta(k_z)$ by

$$\cos(3\eta)=[J_1^2J_2/\bar{J}^3]\cos(k_zs) , \qquad (9)$$

we can write the solutions of Eq. (7) as

$$\varepsilon_l(k_z)=2\bar{J}\cos[\eta(k_z)+\tfrac{2}{3}\pi(l-1)] , \qquad (10)$$

for $l=1,2,3$. The diagonalized band Hamiltonian is

$$H_0=\sum_{lk\sigma}\hat{\xi}_l(k)\psi_{l\sigma}^\dagger(k)\psi_{l\sigma}(k) , \qquad (11)$$

where $\hat{\xi}_l(k)=\xi_0(\mathbf{k})+\varepsilon_l(k_z)$ is the energy of the band labeled by l. The Fermi surfaces generated by the bands are three concentric corrugated cylinders. In the superconducting state each band has its own gap function.

The coefficients $\{b_{ln}\}$ are solved from Eq. (7) plus the normalization condition, i.e., $\sum_n|b_{ln}|^2=1$, up to a common phase factor. For example, we may regard Eq. (7) as a set of three linear homogeneous equations, and solve the first two for the ratios of the coefficients b_{ln}. We then choose b_{l3} to be real for all l and use the normalization condition to obtain

$$\begin{aligned} b_{l1}&=|b_{l1}|e^{-ik_zd'+i\phi_{l3}(k_z)} , \\ b_{l2}&=|b_{l2}|e^{-ik_zd-i\phi_{l2}(k_z)} , \qquad (12)\\ b_{l3}&=|b_{l3}| , \end{aligned}$$

where

$$\begin{aligned} |b_{l1}|^2&=\left[\frac{\varepsilon_l^2-J_1^2}{3(\varepsilon_l^2-\bar{J}^2)}\right]^{1/2} , \\ |b_{l2}|^2&=\left[\frac{\varepsilon_l^2-J_2^2}{3(\varepsilon_l^2-\bar{J}^2)}\right]^{1/2} , \qquad (13)\\ |b_{l3}|&=|b_{l1}| . \end{aligned}$$

The expressions for the phase angles ϕ_{ln} will be given later. Alternatively, we may solve the last two equations for the ratios, choose b_{l1} to be real for all l and obtain

$$\begin{aligned} b_{l1}'&=|b_{l1}| , \\ b_{l2}'&=|b_{l2}|e^{-ik_zd+i\phi_{l1}(k_z)} , \qquad (14)\\ b_{l3}'&=|b_{l3}|e^{ik_zd'-i\phi_{l3}(k_z)} , \end{aligned}$$

where the phases are

$$\tan\phi_{l1}=\tan\phi_{l2}=\frac{J_2\sin(k_zs)}{\varepsilon_l+J_2\cos(k_zs)} \qquad (15)$$

and

$$\tan\phi_{l3}=\frac{J_1^2\sin(k_zs)}{\varepsilon_lJ_2+J_1^2\cos(k_zs)} . \qquad (16)$$

The two sets of results in Eqs. (12) and (14) must be equivalent to within a common phase factor. This requires that the phases ϕ_{ln} satisfy the following sum rule:

$$\sum_n\phi_{ln}(k_z)=k_zs . \qquad (17)$$

The orthogonality of the band states implies another useful sum rule:

$$\sum_l b_{ln}^*b_{ln'}=\delta_{nn'} . \qquad (18)$$

These result will be used to study the pairing interactions.

We first investigate the ordered state, which results from intralayer pairing alone. We transform V_0 in Eq. (2) to the band operators by applying the inverse transformations of Eqs. (4) and (6). This results in a host of pairing interaction terms; some involve electrons within the same band and others involve electrons in different bands. As discussed in detail in Ref. 2, interband pairing breaks the time-reversal symmetry and the resulting superconducting state is suppressed. Consequently, we need only keep the intraband pairing terms in V_0:

$$\begin{aligned} V_0'=-(M)^{-1}\sum_{ll'}\sum_{k\sigma}\sum_{k'\sigma'}&V_{ll'}(k_z,k_z')\psi_{l\sigma}^\dagger(k)\psi_{l\sigma'}^\dagger(-k) \\ &\times\psi_{l'\sigma'}(-k')\psi_{l'\sigma}(k') , \qquad (19) \end{aligned}$$

where

$$V_{ll'}(k_z,k_z')=\sum_n\lambda_{0n}u_{ln}(k_z)u_{l'n}(k_z') , \qquad (20)$$

and $u_{ln}(k_z)=|b_{ln}(k_z)|^2$.

Unlike the one-layer and two-layer problems, the symmetry of the order parameters is not obvious from the expression of the pairing matrix elements $V_{ll'}(k_z,k_z')$. A set of mathematical tools will be needed, and we will develop them presently. Given any three complex numbers c_l, $l=1,2,3$, we can uniquely resolve them into linear combinations of three other complex numbers $\bar{c}_m$, $m=0$, 1, 2 in terms of a unitary transformation:

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \bar{c}_0 \\ \bar{c}_1 \\ \bar{c}_2 \end{bmatrix} . \qquad (21)$$

The inverse transformation is given by the transpose matrix. The meaning of the transformation becomes clear if we write the column vectors as diagonal matrices. We introduce three 3×3 diagonal matrices $\underline{\mu}_j$, $j=0,1,2$, as follows:

$$\underline{\mu}_0=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix},$$

$$\underline{\mu}_1=\frac{1}{\sqrt{2}}\begin{bmatrix}2&0&0\\0&-1&0\\0&0&-1\end{bmatrix},\tag{22}$$

$$\underline{\mu}_2=\left[\frac{3}{2}\right]^{1/2}\begin{bmatrix}0&0&0\\0&1&0\\0&0&-1\end{bmatrix}.$$

The matrix $\underline{\mu}_0$ is simply the unit matrix, and $\underline{\mu}_1,\underline{\mu}_2$ are, aside from a numerical factor and some rearrangement of elements, the two diagonal generators of the SU(3) group.[5] The transformation in Eq. (21) can be written as

$$\begin{bmatrix}c_1&0&0\\0&c_2&0\\0&0&c_3\end{bmatrix}=\frac{1}{\sqrt{3}}(\bar{c}_0\underline{\mu}_0+\bar{c}_1\underline{\mu}_1+\bar{c}_2\underline{\mu}_2)\ .\tag{23}$$

We will call $\{\bar{c}_m\}$ the SU(3) components of $\{c_l\}$. As an example, the SU(3) components of the band energies $\{\varepsilon_l\}$ are $\bar{\varepsilon}_0=0$, $\bar{\varepsilon}_1=\sqrt{6}J\cos\eta(k_z)$, $\bar{\varepsilon}_2=\sqrt{6}J\sin\eta(k_z)$. The fact that the SU(3) symmetry becomes relevant in the three-layer problem is not surprising, in view of the importance of SU(2) symmetry in the two-layer problem.

The quasiparticle Green's functions are defined in the familiar way:

$$\begin{aligned}G^{ll'}_{\alpha\beta}(k,\tau-\tau')&\equiv-\langle T[\psi_{l\alpha}(k,\tau)\psi^\dagger_{l'\beta}(k,\tau')]\rangle\ ,\\F^{ll'}_{\alpha\beta}(k,\tau-\tau')&\equiv\langle T[\psi_{l\alpha}(k,\tau)\psi_{l'\beta}(-k,\tau')]\rangle\ ,\end{aligned}\tag{24}$$

etc. Since intralayer pairing only allows singlet pairs, the spin indices α and β must have the opposite signs. As discussed earlier, we will limit our discussion to intraband pairing, so only $l=l'$ components of the Green's functions will survive. In the mean-field approximation, the equations of motion of the Green's-function components can be written in a compact SU(2)×SU(3)×SU(2) matrix form:

$$\begin{aligned}\underline{\hat{G}}^{-1}(k,\omega)=&\,i\omega\underline{\rho}_0\otimes\underline{\mu}_0\otimes\underline{\sigma}_0-\xi_0(\mathbf{k})\underline{\rho}_3\otimes\underline{\mu}_0\otimes\underline{\sigma}_0\\&-\sqrt{2}\bar{J}\cos\eta(k_z)\underline{\rho}_3\otimes\underline{\mu}_1\otimes\underline{\sigma}_0\\&-\sqrt{2}\bar{J}\sin\eta(k_z)\underline{\rho}_3\otimes\underline{\mu}_2\otimes\underline{\sigma}_0\\&-\sum_{m=0}^{2}(\bar{\Delta}'_m\underline{\rho}_1-\bar{\Delta}''_m\underline{\rho}_2)\otimes\underline{\mu}_m\otimes\underline{\sigma}_2\ .\end{aligned}\tag{25}$$

In the above equation the Pauli matrices $\{\underline{\sigma}_j\}$, $j=1,2,3$ and its associated identity matrix $\underline{\sigma}_0$ identify the spin states of the quasiparticles, a second set of Pauli matrices $\{\underline{\rho}_j\}$ identify the four Green's function components $G,F,F^\dagger,-G^\dagger$, ω is the Matsubara frequency, and $\bar{\Delta}'_m$, $\bar{\Delta}''_m$, are the real and imaginary parts of the SU(3) component $\bar{\Delta}_m$ of the gap functions Δ_l for the bands $l=1,2,3$. The band gap functions are defined by

$$\Delta_l(k_z)=\sum_{k'}\sum_{l'}V_{ll'}(k_z,k_z')\langle\psi_{l'+}(k')\psi_{l'-}(-k')\rangle\ .\tag{26}$$

The self-consistent equations for the gap functions are

$$\begin{aligned}\bar{\Delta}_m=&-\tfrac{1}{12}T\sum_{\omega}\sum_{m'=0}^{2}\int\frac{d^3k'}{2\pi}\bar{V}^{(0)}_{mm'}(k_z,k_z')\\&\times\mathrm{Tr}[(\underline{\rho}_1-i\underline{\rho}_2)\otimes\underline{\mu}_m\otimes\underline{\sigma}_2\underline{\hat{G}}(k',\omega)],\end{aligned}\tag{27}$$

where

$$\bar{V}^{(0)}_{mm'}(k_z,k_z')=\sum_{n=1}^{3}\lambda_{0n}\bar{u}_{mn}(k_z)\bar{u}_{m'n}(k_z')\ ,\tag{28}$$

and $\{\bar{u}_{mn}\}$ are the SU(3) components of $\{u_{ln}\}$.

The matrix $\underline{\hat{G}}^{-1}$ is diagonal in three 4×4 blocks, each of which can be inverted. There are two ways to write the gap equations, either in the SU(3) representation as in Eq. (27) or in the band representation as in Eq. (26). The two sets of equations are related by the canonical transformation in Eq. (21). The SU(3) equations are more convenient for the purpose of determining the bare critical temperatures, but those in the band representation are simpler in form for deriving the Ginzburg-Landau free energy. Up to the third order of the gap function, the gap equations in the band representation are

$$\begin{aligned}\Delta_l(k_z)=&\,\pi TN(0)\sum_{\omega}\sum_{l'}\int\frac{s\,dk_z'}{2\pi}V_{ll'}(k_z,k_z')\\&\times\left[\frac{\Delta_{l'}(k_z')}{|\omega|}-\frac{\Delta^2_{l'}(k_z')\Delta^*_{l'}(k_z')}{2|\omega|^3}\right].\end{aligned}\tag{29}$$

In the above equation the gap function of the lth band is denoted by Δ_l, which is, in general, dependent upon k_z. The quantity $N(0)$ is the density of states per band at the Fermi level.

The linearized gap equation in the SU(3) representation has the form of an eigenvalue problem:

$$\begin{aligned}\bar{\Delta}_m(k_z)=&\,a_\parallel(T_{c0})N(0)\sum_{n}\lambda_{0n}\bar{u}_{mn}(k_z)\\&\times\sum_{m'}\int\frac{s\,dk_z'}{2\pi}\bar{u}_{m'n}(k_z')\bar{\Delta}_{m'}(k_z')\ ,\end{aligned}\tag{30}$$

where the quantity

$$a_\parallel(T_{c0})=\ln(2\gamma\omega_\parallel/\pi T)\ ,$$

and $\gamma=1.78$. Using the sum role on u_{ln} in Eq. (18), we can establish that $\bar{u}_{0n}=1/\sqrt{3}$ for all layer indices n and

$$\bar{u}_{m1}=\bar{u}_{m2}=-\tfrac{1}{2}\bar{u}_{m3}\ ,$$

for $m\neq0$. In the special case where all λ_{0n} are equal to λ_0, it is not difficult to establish that $\bar{V}^{(0)}_{00}=\lambda_0$, and $\bar{V}^{(0)}_{0m}=\bar{V}^{(0)}_{m0}=0$. Therefore, 3×3 matrix $(\underline{\bar{V}}^{(0)}_{mm'})$ is block diagonal, and one of the eigenvalues is λ_0. Numerical diagonalization of the 2×2 block shows that the other two eigenvalues are much smaller. As a result, the critical temperature T_{c0} is given by

$$1=\lambda_0 N(0)a_{\parallel}(T_{c0}) \ . \tag{31}$$

The corresponding eigenvector $\overline{\Delta}_0$ is independent of k_z, which means that the band gap functions Δ_l are equal and isotropic. The presence of the other two eigenfunctions can be neglected entirely because the dominant isotropic gap suppresses all other possible superconducting states.

In case the three layers do not have the same coupling constant, the matrix $\underline{V}_{mm'}$ is not block diagonal so that the gap functions must be found by diagonalizing Eq. (30). One finds that this results in nonvanishing $\overline{\Delta}_m$ components with $m=1,2$ and the band gap functions become slightly dependent on k_z. As an extreme example, we show in Fig. 1 the gap functions for $\lambda_{01}=\lambda_{03}$ and $\lambda_{02}=0$. In the top panel we show the results for $J_1/J_2=0.5$. The gap functions for bands 1 and 3 are nearly equal, and both are larger than that for band 2. In the bottom panel we show that for $J_2/J_1=0.5$ the middle band has a larger gap function than the other two bands. The density of states (DOS) of the two cases are shown in Figs. 2 and 3. In these and all other similar curves, the DOS in the superconducting state $N_s(\omega)$ is normalized to the to-

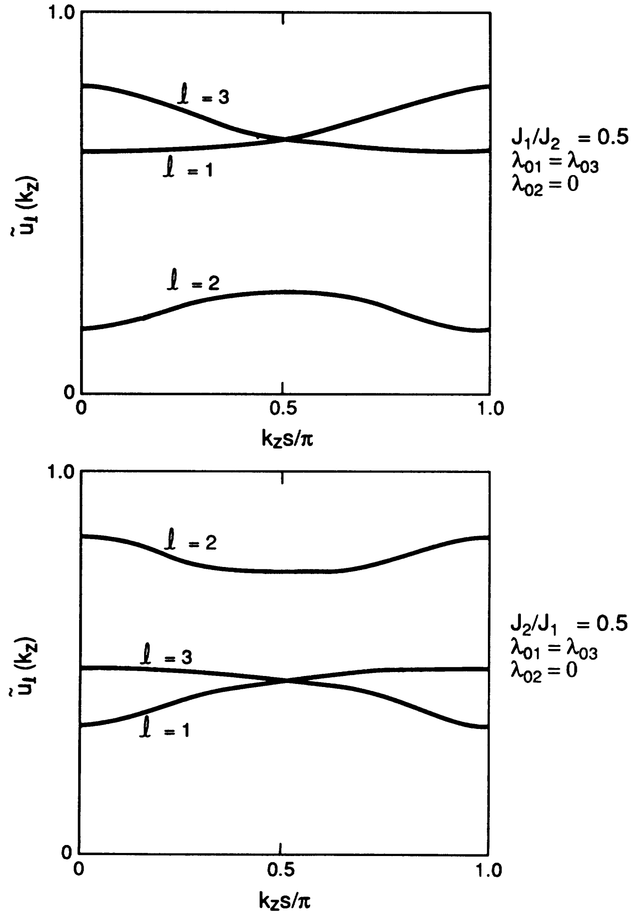

FIG. 1. Normalized gap functions for the superconducting state of a three-layer model with unequal intralayer pairing strengths. The coupling constants are $\lambda_{01}=\lambda_{03}$, $\lambda_{02}=0$. In the top panel the hopping matrix elements are such that $J_1/J_2=0.5$, whereas in the bottom panel $J_2/J_1=0.5$.

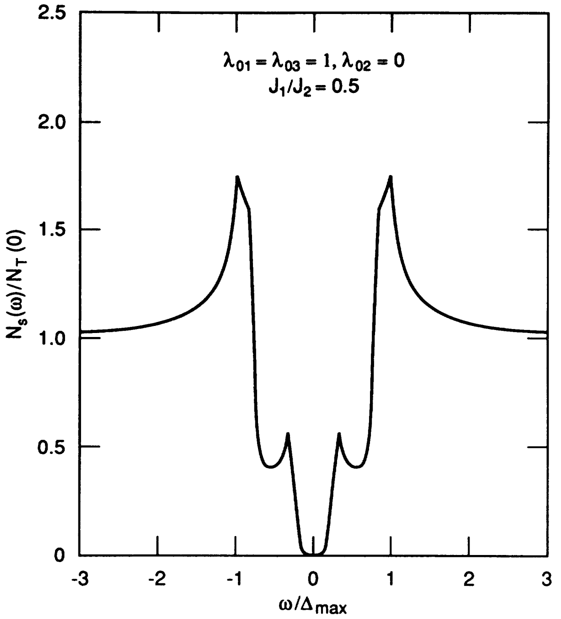

FIG. 2. The density of states (DOS) for the intralayer pairing model with $\lambda_{01}=\lambda_{03}$, $\lambda_{02}=0$, and $J_1/J_2=0.5$. The DOS $N_s(\omega)$ in the superconducting state is normalized by the total normal-state DOS $N_T(0)$, which is the number of bands N multiplied by the DOS $N(0)$ per band. The single band with the smaller gap gives rise to an inner structure between the main peaks. In this and later DOS plots a small broadening factor $\Gamma=0.03\Delta_{\max}$ is folded into the calculation to smooth out sharp cusps so that the curves resembled more closely the measured tunneling conductance curves.

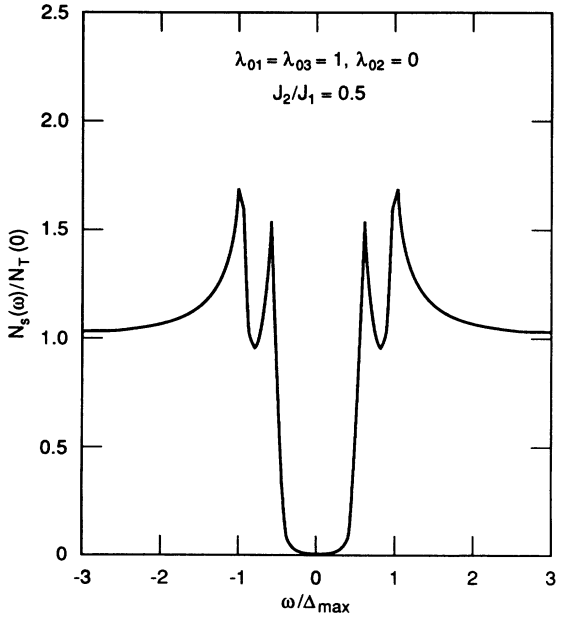

FIG. 3. The density of states for the intralayer pairing model with the same λ_{0n} values but $J_2/J_1=0.5$. The single band with the larger gap gives rise to structures outside of the main peaks.

tal DOS in the normal state $N_T(0)$ which is the product of the number of bands N and the DOS per band $N(0)$. A small broadening factor $\Gamma=0.03\Delta_{\max}$ is also folded into the DOS calculation to smooth out sharp cusps so that the curves more closely resemble the measured tunneling conductance curves. Both figures show multiple gap features, namely, additional peaks inside of the main peaks. In the limit of $J_1=J_2$ all three bands have equal and isotropic gaps for arbitrary values of λ_{0n}.

Returning to the case that all λ_{0n} are equal, we denote the band-gap functions Δ_l by $\Delta_0/\sqrt{3}$ and put them into the nonlinear gap equation, Eq. (29). After functionally integrating the resulting equation, we find the following expression for the Ginzburg-Landau free energy:

$$F_s-F_n=\tfrac{1}{2}N(0)f_0 \ , \tag{32}$$

with

$$f_0=|\Delta_0|^2\ln\left[\frac{T}{T_{c0}}\right]+\frac{1}{2}b_0|\Delta_0|^4 \ , \tag{33}$$

and $b_0=7\zeta(3)/[8(\pi T)^2]$. The quantity Δ_0 is the only order parameter for intralayer intraband s-wave pairing.

We now turn our attention to the consequences of interlayer pairing alone. As was done for intralayer pairing, we transform V_1 in Eq. (3) to band operators and keep only intraband pairing terms to obtain V_1' in analogy with Eqs. (19) and (20), with

$$\begin{aligned}V_{ll'}(k_z,k_z')=\lambda_1\sum_{n=1}^{2}\,&[u_{ln}(k_z)u_{l'n}(k_z')+v_{ln}(k_z)v_{l'n}k_z')]\\&+\lambda_2[u_{l3}(k_z)u_{l'3}(k_z')+v_{l3}(k_z)v_{l'3}(k_z')] \ ,\end{aligned} \tag{34}$$

where

$$\begin{aligned}u_{ln}&=|b_{ln}b_{ln'}|\cos\phi_{ln} \ ,\\ v_{ln}&=|b_{ln}b_{ln'}|\sin\phi_{ln} \ ,\end{aligned} \tag{35}$$

and $n'=n+1$ (mod 3). In deriving these results we have used the sum rule on phase angles in Eq. (17). Explicitly, we find

$$\begin{aligned}u_l(k_z)=u_{l2}(k_z)&=\frac{\varepsilon_l(k_z)J_1+J_1J_2\cos(k_zs)}{3(\varepsilon_l^2-\bar{J}^{\,2})} \ ,\\ u_{l3}(k_z)&=\frac{\varepsilon_l(k_z)J_2+J_1^2\cos(k_zs)}{3(\varepsilon_l^2-\bar{J}^{\,2})} \ ,\\ v_{l1}(k_z)=v_{l2}(k_z)&=\frac{J_1J_2\sin(k_zs)}{3(\varepsilon_l^2-\bar{J}^2)} \ ,\\ v_{l3}(k_z)&=\frac{J_1^2\sin(k_zs)}{3(\varepsilon_l^2-\bar{J}^{\,2})} \ .\end{aligned} \tag{36}$$

The functions u_{ln} are even functions of k_z, while v_{ln} are odd functions, and as a result interlayer pairing will allow both singlet and triplet states.

The 12×12 inverse Green's-function matrix is given by

$$\begin{aligned}\underline{\hat{G}}^{\,-1}(k,\omega)=i\omega\underline{\rho}_0\otimes\underline{\mu}_0\otimes\underline{\sigma}_0-\xi_0(\mathbf{k})\underline{\rho}_3\otimes\underline{\mu}_0\otimes\underline{\sigma}_0-\sqrt{2}\bar{J}\cos\eta(k_z)\underline{\rho}_3\otimes\underline{\mu}_1\otimes\underline{\sigma}_0-\sqrt{2}\bar{J}\sin\eta(k_z)\underline{\rho}_3\otimes\underline{\mu}_2\otimes\underline{\sigma}_0\\ -\sum_{m=0}^{2}\sum_{j=0}^{3}(\bar{\Delta}'_{mj}\underline{\rho}_1-\bar{\Delta}''_{mj}\underline{\rho}_2)\otimes\underline{\mu}_m\otimes\sigma_j \ ,\end{aligned} \tag{37}$$

where $\bar{\Delta}_{mj}=\bar{\Delta}'_{mj}+i\bar{\Delta}''_{mj}$ are the singlet ($j=2$) and triplet ($j=0,1,3$) order parameters. The self-consistent gap equations are

$$\bar{\Delta}_{mj}(k_z)=-\frac{1}{12}T\sum_{\omega}\sum_{m'}\int\frac{d^3k'}{(2\pi)^3}\bar{V}_{mm'}(k_z,k_z')\mathrm{Tr}[(\underline{\rho}_1-i\underline{\rho}_2)\otimes\underline{\mu}_{m'}\otimes\underline{\sigma}_j\underline{\hat{G}}(k',\omega)] \ , \tag{38}$$

where $\underline{\bar{V}}_{mm'}$ is the SU(3) representation of $\underline{V}_{ll'}$ in Eq. (34). Again, the inverse Green's function is block diagonal in 4×4 blocks and each block can be inverted without difficulty. We define a four-vector band-order parameter $\tilde{\Delta}_l(k_z)$ by

$$\tilde{\Delta}_l\equiv(i\Delta_{l0},\Delta_{l1},\Delta_{l2},\Delta_{l3}) \ . \tag{39}$$

Then the nonlinear gap equations in the band representation become, after a considerable amount of algebra,

$$\tilde{\Delta}_l(k_z)=\pi TN(0)a_\perp(T)\sum_{l'}\int\frac{s\,dk_z'}{2\pi}V_{ll'}(k_z,k_z')\tilde{\Delta}_{l'}(k_z')-N(0)b_0\sum_{l'}\int\frac{s\,dk_z'}{2\pi}V_{ll'}(k_z,k_z')[2\tilde{\Delta}_{l'}\tilde{\Delta}_{l'}\cdot\Delta_{l'}^{*}-\tilde{\Delta}_{l'}^{*}\tilde{\Delta}_{l'}\cdot\tilde{\Delta}_{l'}] \ , \tag{40}$$

where $a_\perp(T)=\ln(2\gamma\omega_\perp/\pi T)$, and $\omega_\perp$ is the cutoff energy of interlayer pairing interaction. The quantity b_0 has been defined under Eq. (33). We will use this equation later to deduce the Ginzburg-Landau free-energy expression. For the moment we will study the linearized gap equation in the SU(3) representation to deduce the equations for the bare critical temperatures. The equations are

$$\bar{\Delta}_{mj}(k_z)=a_\perp(T_c)\sum_{m'=0}^{2}\int\frac{s\,dk_z'}{2\pi}\bar{V}_{mm'}(k_z,k_z')\bar{\Delta}_{m'j}(k_z') \ , \tag{41}$$

where $j=2$ is for the singlet state, and the other three j's are for the triplet states.

It will be shown in the Appendix that $\sum_l u_{ln} = \sum_l v_{ln} = 0$. Hence, in the expression for $\bar{V}_{mm'}$ the components $\bar{u}_{0n}$ and $\bar{v}_{0n}$ are zero. Consequently, the gap-function component $\bar{\Delta}_{0j}$ vanishes for both singlet and triplet states. In complete analogy with the two-layer problem, we construct orthonormal bases from the remaining basis functions, $\bar{u}_{mn}$ and $\bar{v}_{mn}$ for $m=1,2$, and diagonalize the $\bar{V}$ matrix to obtain the eigenvalues and bare critical temperatures. Since $V_{ll'}$ contains no cross terms between the u and v functions, the $\bar{V}$ matrix is block diagonal in terms of singlet and triplet blocks, and each can be diagonalized separately. One can see from Eq. (36) that there are two linearly independent $\bar{u}_{mn}$ for each m. We define the transformation to orthonormal bases by

$$\bar{u}_{mn} = \sum_{p=1}^{2} \alpha_{mp}^{(n)} \hat{u}_{mp} \ . \tag{42}$$

It follows that the singlet part of the linearized gap equation reduces to the matrix eigenvalue problem:

$$\langle \hat{u}_{mp} | \bar{\Delta}_m \rangle = N(0) a_\perp(T_{cs}) \sum_{m'p'} \hat{V}^{s}_{mp,m'p'} \langle \hat{u}_{m'p'} | \bar{\Delta}_{m'} \rangle \ , \tag{43}$$

where the bracket notation represents the inner product of the two functions involved, and the interaction matrix element is

$$\hat{V}^{(s)}_{mp,m'p'} = \lambda_1 \sum_{n=1}^{2} \alpha_{mp}^{(n)} \alpha_{m'p'}^{(n)} + \lambda_2 \alpha_{mp}^{(3)} \alpha_{m'p'}^{(3)} \ . \tag{44}$$

We denote the largest eigenvalue of the 4×4 $\underline{\hat{V}}^{(s)}$ matrix by λ_s and the eigenvector by $\check{u}_m(k_z)$, then the bare critical temperature of the singlet state is solved from

$$1 = \lambda_s N(0) a_\perp(T_{cs}) \ , \tag{45}$$

and the SU(3) components of the gap functions are

$$\bar{\Delta}_{m2}(k_2) = \Delta_s \check{u}_m(k_z) \ , \tag{46}$$

where Δ_s is the order parameter. The functions $\check{u}_m$ are normalized such that

$$\int_{-\pi/s}^{\pi/s} \frac{s\, dk_z}{2\pi} [\check{u}_1^2(k_z) + \check{u}_2^2(k_z)] = 1 \ . \tag{47}$$

The band-gap functions $\Delta_l(k_z) = \Delta_s \tilde{u}_l(k_z)$ can be deduced from Eq. (46) by the canonical transformation in Eq. (21). The functions $\tilde{u}_l(k_z)$ are normalized according to

$$\sum_{l=1}^{3} \int \frac{s\, dk_z}{2\pi} \tilde{u}_l^2(k_z) = 1 \ . \tag{48}$$

In analogy with the two-layer problem, we will call $\tilde{u}_l(k_z)$ the normalized gap functions.

The gap functions for the triplet states satisfy an equation similar to Eq. (43) except that the matrix $\hat{V}^{(t)}$ is 2×2 because all v_{ln} functions are proportional to each other. We construct $\underline{\hat{V}}^{(t)}$ in the same way as $\underline{\hat{V}}^{(s)}$, and denote the largest eigenvalue by λ_t. The bare critical temperature for the triplet state is solved from

$$1 = \lambda_t N(0) a_\perp(T_{ct}) \ , \tag{49}$$

and the gap functions are

$$\begin{aligned} \bar{\Delta}_{m0}(k_z) &= \frac{1}{\sqrt{2}} (\Delta_{t+} + \Delta_{t-}) \check{v}_m(k_z) \ , \\ \bar{\Delta}_{m1}(k_z) &= \Delta_{t0} \check{v}_m(k_z) \ , \\ \bar{\Delta}_{m3}(k_z) &= \frac{-i}{\sqrt{2}} (\Delta_{t+} - \Delta_{t-}) \check{v}_m(k_z) \ , \end{aligned} \tag{50}$$

where $\check{v}_m(k_z)$ for $m=1,2$ are the normalized gap functions and the three components of the triplet order parameter form a vector $\mathbf{\Delta}_t$. Again, the band-gap functions $\mathbf{\Delta}_{lj}(k_z) = \mathbf{\Delta}_t \tilde{v}_l(k_z)$ are obtained from the results in Eq. (50) by the transformation in Eq. (21).

In Fig. 4 we show a set of typical band-gap functions $\tilde{u}_l(k_z)$ and $\tilde{v}_l(k_z)$ for both singlet and triplet states. The singlet gap functions for bands 1 and 3 reflect into the negative of each other at the point $k_z = \pi/2s$, while the one for band 2 reflects into the negative of itself. Except for a small region of the parameter space near $\lambda_1 \ll \lambda_3$ and $J_1 > J_3$ the singlet gap functions for the two outer bands are nodeless. For the middle band, however, the

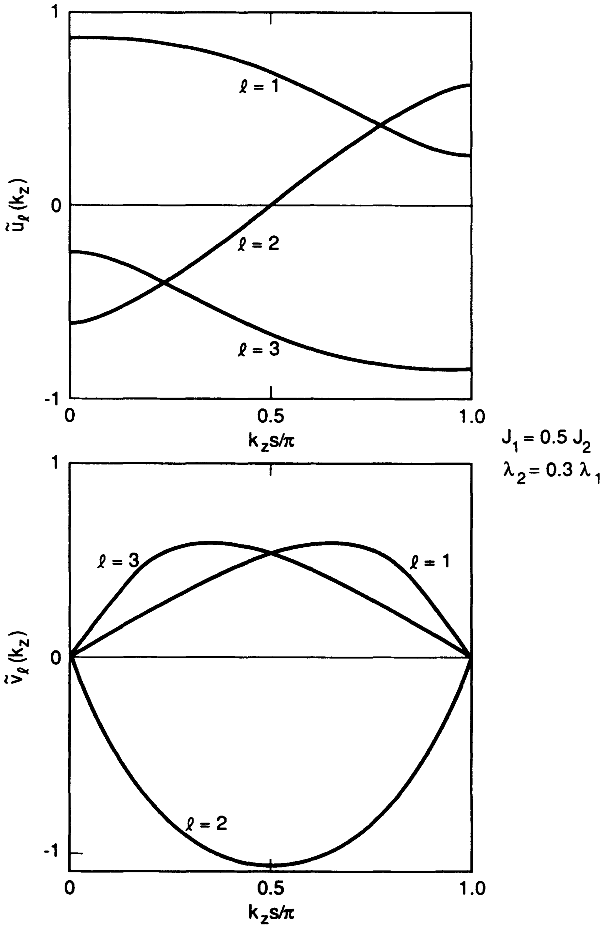

FIG. 4. Normalized gap functions for singlet (top) and triplet (bottom) states of a three-layer model with interlayer pairing interaction.

gap function always has a node. The triplet gap functions have nodes at $k_z=0$ and π/s, and the gap functions for bands 1 and 3 reflect into each other and the one for band 2 reflects into itself. The bare critical temperature for the triplet state is much less than that for the singlet state except when $J_1 \simeq J_2$, where the three-layer model reduces to the one-layer model.

Putting the results in Eqs. (46) and (50) into the nonlinear gap functions in Eq. (40) and functionally integrating the resulting equations with respect to the singlet and triplet order parameters, we find the Ginzburg-Landau free energy of the system has the form:

$$F_s - F_n = \tfrac{1}{2} N(0) f_1 \ ,$$

with

$$\begin{aligned} f_1 = {} & |\Delta_s|^2 \ln \left[\frac{T}{T_{cs}} \right] + \boldsymbol{\Delta}_t \cdot \boldsymbol{\Delta}_t^* \ln \left[\frac{T}{T_{ct}} \right] \\ & + \frac{1}{2} b_s |\Delta_s|^4 + \frac{1}{2} b_t (\boldsymbol{\Delta}_t \cdot \boldsymbol{\Delta}_t^*)^2 \\ & + b_{st} [2|\Delta_s|^2 \boldsymbol{\Delta}_t \cdot \boldsymbol{\Delta}_t^* - \mathrm{Re} \Delta_s^{*2} \boldsymbol{\Delta}_t \cdot \boldsymbol{\Delta}_t] \ . \end{aligned} \tag{51}$$

The coefficients b_s, b_t, and b_{st} are given by

$$\begin{aligned} b_s &= \frac{1}{2} b_0 \int \frac{s\,dk_z}{2\pi} [\check{u}_1^2(k_z) + \check{u}_2^2(k_z)]^2 \ , \\ b_t &= \frac{1}{2} b_0 \int \frac{s\,dk_z}{2\pi} [\check{v}_1^2(k_z) + \check{v}_2^2(k_z)]^2 \ , \end{aligned} \tag{52}$$

and

$$b_{st} = \frac{1}{2} b_0 \int \frac{s\,dk_z}{2\pi} [\check{u}_1^2(k_z) + \check{u}_2^2(k_z)][\check{v}_1^2(k_z) + \check{v}_2^2(k_z)] \ .$$

The free energy is obviously minimized by choosing the singlet and vector triplet order parameters to be in phase. Furthermore, since the free energy has the same structure as the two-layer problem, the competition and coexistence of singlet and triplet order parameters in the two systems are in complete analogy. For instance, since $T_{cs} \gg T_{ct}$ over most of the parameter space, the singlet order tends to suppress the triplet order. In the narrow region where the two bare critical temperatures are close, it is possible to have a second-order phase transition at $\tilde{T}_{ct} < T_{ct} < T_{cs}$ where triplet order begins to coexist with singlet order.

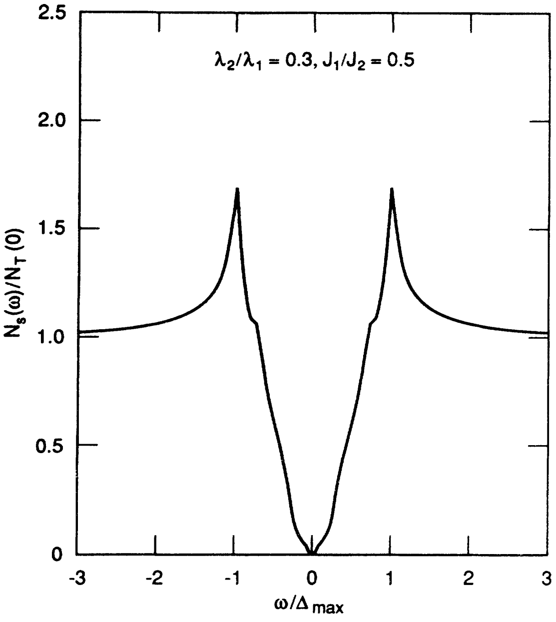

FIG. 5. The density of states of the three-layer interlayer interaction model whose gap functions are shown in Fig. 4.

One can also demonstrate that, as in the two-layer case, the gap functions change very little with temperature. The fact that the singlet gap function for the middle band has a pair of nodes gives rise to an interesting energy level structure as shown in the density-of-states curve in Fig. 5. In contrast to the standard s-wave superconductor, the DOS is zero at the point of zero quasiparticle energy and rises linearly on both sides of this point. There are also multiple peak structures coming from the flat regions of the gap functions at the center and the boundary of the Brillouin zone. In the narrow region of parameter space, where $J_1 \simeq J_2$, the emergence of the triplet state below $\tilde{T}_{ct}$ removes the nodes of the singlet gap function of the middle band as well as the linear portions of the DOS near zero energy. We are not aware of any tunneling data on the three-layer Tl compound to compare with, but the curve bears some resemblance to the observed tunneling characteristic of Y 1:2:3 material. However, there are other indications that Y 1:2:3 is better represented by the two-layer model, as we will discuss in detail in Sec. V. We also show in Sec. VI that Bi 2:2:1:2 can be reduced to an effective three-layer system with nonidentical layers, and this model can explain the recent tunneling data for this material.

Finally, we summarize very briefly the competing roles of intralayer and interlayer interactions. Recalling that the intralayer order parameter belongs to the $m=0$ representation of the SU(3) group and the interlayer singlet order parameter belongs to the $m=1,2$ representations, we immediately conclude that their bare critical temperatures completely separate. One interaction cannot help the other to boost the critical temperature of the system. Without showing any of the details, we write down here the total free energy of the system when both interactions are present:

$$F_s - F_n = \tfrac{1}{2} N(0) f \ ,$$

where

$$\begin{aligned} f = f_0 + f_1 + b_0 [& 2|\Delta_0|^2 |\Delta_s|^2 + \mathrm{Re} \Delta_0^{*2} \Delta_s^2 \\ & + 2|\Delta_0|^2 \boldsymbol{\Delta}_t^* \cdot \boldsymbol{\Delta}_t - \mathrm{Re} \Delta_0^{*2} \boldsymbol{\Delta}_t \cdot \boldsymbol{\Delta}_t] \ . \end{aligned} \tag{53}$$

The quantities f_0 and f_1 are given in Eqs. (32) and (51), respectively. Again, this expression has the same structures as that for the two-layer problem. An immediate consequence is that it is not possible to minimize the free energy by choosing the phases of intralayer singlet, interlayer singlet, and interlayer triplet order parameters with all three being nonvanishing. As a result, the three types

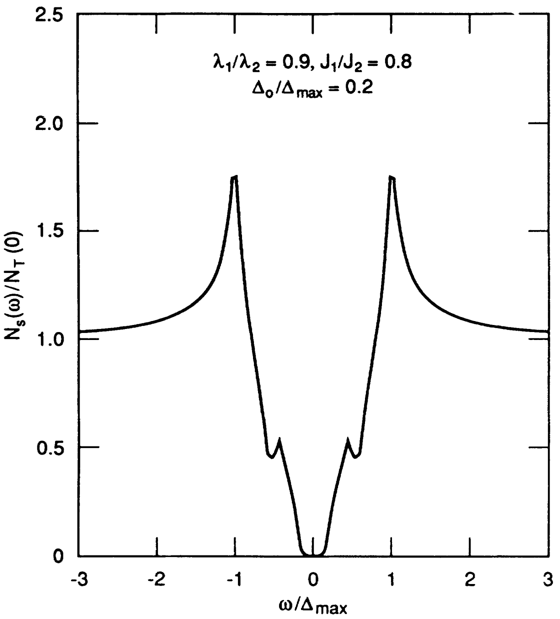

FIG. 6. The density of states of a three-layer model with mixed interlayer and intralayer order parameters. The node is removed by mixing with the isotropic intralayer gap function.

of order cannot exist in one system simultaneously. If intralayer pairing dominates, it will suppress the interlayer pairing effects completely. If interlayer pairing dominates, however, the system may suppress the interlayer triplet order but allow the intralayer order parameter to become nonvanishing below a temperature $\tilde{T}_{c0} < T_{c0}$, as discussed before for the two-layer system.[1,2]

One consequence of mixing the intralayer s-wave order parameter into the interlayer singlet order parameter is to remove the node in the gap function of the middle band. Just like the mixing of the interlayer singlet and triplet order parameters, a real gap appears in the DOS, as shown in Fig. 6.

IV. THE FOUR-LAYER PROBLEM

The solution of the four-layer problem follows substantially the same procedure as the three-layer problem. The band Hamiltonian is diagonalized by the same set of transformations in Eqs. (4) and (6), but with both layer index n and band index l ranging from 1 to 4. The band energies $\varepsilon_l(k_z)$, and the transformation matrix elements $b_{ln}(k_z)$ are solved from the eigenvalue problem:

$$\begin{bmatrix} -\varepsilon_l & J_1 e^{ik_z d} & 0 & J_2 e^{-ik_z d'} \\ J_1 e^{-ik_z d} & -\varepsilon_l & J_1 e^{ik_z d} & 0 \\ 0 & J_1 e^{-ik_z d} & -\varepsilon_l & J_1 e^{ik_z d} \\ J_2 e^{ik_z d'} & 0 & J_1 e^{-ik_z d} & -\varepsilon_l \end{bmatrix} \begin{bmatrix} b_{l1} \\ b_{l2} \\ b_{l3} \\ b_{l4} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} . \tag{54}$$

The band energies are the roots of the following quartic equation

$$\varepsilon^4 - (3J_1^2 + J_2^2)\varepsilon^2 + [J_1^4 + J_1^2 J_2^2 - 2J_1^3 J_2 \cos(k_z s)] = 0 . \tag{55}$$

If we denote $\bar{J}^2 = (3J_1^2 + J_2^2)/4$ and

$$A = [J_1^4 + J_1^2 J_2^2 - 2J_1^3 J_2 \cos(k_z s)]^{1/2} ,$$

we can write

$$\begin{aligned} \varepsilon_1 &= \tfrac{1}{2}(4\bar{J}^2 + A)^{1/2} + (4\bar{J}^2 - A)^{1/2}] , \\ \varepsilon_2 &= \tfrac{1}{2}(4\bar{J}^2 + A)^{1/2} - (4\bar{J}^2 - A)^{1/2}] , \\ \varepsilon_3 &= -\varepsilon_2, \quad \varepsilon_4 = -\varepsilon_1 . \end{aligned} \tag{56}$$

All four roots are real. The four bands generate four concentric cylindrical Fermi surfaces.

The elements of the transformation matrix are calculated in the same way as in the three layer case. The results are

$$\begin{aligned} b_{l1} &= |b_{l1}| , \\ b_{l2} &= |b_{l2}| e^{-ik_z d + i\phi_{l1}} , \\ b_{l3} &= |b_{l3}| e^{-2ik_z d + i(\phi_{l1} + \phi_{l2})} , \\ b_{l4} &= |b_{l4}| e^{-3ik_z d + i(\phi_{l1} + \phi_{l2} + \phi_{l3})} \\ &= |b_{l4}| e^{ik_z d' - i\phi_{l4}} , \end{aligned} \tag{57}$$

where

$$\begin{aligned} |b_{l1}| = |b_{l4}| &= \left[\frac{\varepsilon_l^2 - 2J_1^2}{4(\varepsilon_l^2 - \bar{J}^2)} \right]^{1/2} , \\ |b_{l2}| = |b_{l3}| &= \left[\frac{\varepsilon_l^2 - J_1^2 - J_2^2}{4(\varepsilon_l^2 - \bar{J}^2)} \right]^{1/2} , \end{aligned} \tag{58}$$

and

$$\begin{aligned} \tan\phi_{l1}(k_z) = \tan\phi_{l3}(k_z) &= \frac{J_1 J_2 \sin(k_z s)}{\varepsilon_l^2 - J_1^2 + J_1 J_2 \cos(k_z s)} , \\ \tan\phi_{l2}(k_z) &= \frac{J_1 J_2 \sin(k_z s)}{\varepsilon_l^2 - J_2^2 + J_1 J_2 \cos(k_z s)} , \\ \tan\phi_{l4}(k_z) &= \frac{J_1^3 \sin(k_z s)}{J_2(\varepsilon_l^2 - J_1^2) + J_1^3 \cos(k_z s)} . \end{aligned} \tag{59}$$

The following identities are satisfied:

$$\sum_l b_{ln}^* b_{ln'} = \delta_{nn'} , \tag{60}$$

$$\sum_n \phi_{ln}(k_z) = k_z . \tag{61}$$

The coefficients $\{b_{ln}\}$ are normalized according to $\sum_n |b_{ln}|^2 = 1$.

The symmetry of the order parameters is readily sorted out by considering the SU(4) symmetry. We define

$$\underline{\mu}_0=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix},\quad \underline{\mu}_1=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix},$$
$$\underline{\mu}_2=\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{bmatrix},\quad \underline{\mu}_3=\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{bmatrix}. \tag{62}$$

Then an arbitrary set of complex numbers $\{c_l\}$, $l=1,2,3,4$, can be resolved into the linear combinations of its SU(4) components $\{\bar{c}_m\}$, $m=0,1,2,3$:

$$\begin{bmatrix}c_1&0&0&0\\0&c_2&0&0\\0&0&c_3&0\\0&0&0&c_4\end{bmatrix}=\tfrac{1}{2}\sum_{m=0}^{3}\bar{c}_m\underline{\mu}_m . \tag{63}$$

In particular, the SU(4) components of the band energies are

$$\begin{aligned}&\bar{\varepsilon}_0=\bar{\varepsilon}_3=0 ,\\&\bar{\varepsilon}_1=(4\bar{J}^2+A)^{1/2} ,\\&\bar{\varepsilon}_2=(4\bar{J}^2-A)^{1/2} .\end{aligned} \tag{64}$$

We can work out all pertinent results of the superconductivity problem by drawing an analogy with the three-layer problem.

In case of pure intralayer pairing with all layers having the same coupling constant λ_0, the interaction matrix element has the expression

$$V_{ll'}(k_z,k_z')=\lambda_0\sum_n u_{ln}(k_z)u_{l'n}(k_z') . \tag{65}$$

where $u_{ln}=|b_{ln}(k_z)|^2$. As shown in the last section, the nature of the gap function can be deduced entirely from the SU(4) components of the basis functions u_{ln}. The following results are readily deduced from the expressions of b_{ln}:

$$\begin{aligned}&\bar{u}_{0n}=\tfrac{1}{2},\quad \bar{u}_{1n}=0,\quad \bar{u}_{2n}=0 ,\\&\sum_n\bar{u}_{3n}=0 .\end{aligned} \tag{66}$$

This is sufficient to demonstrate that the matrix $\bar{V}_{mm'}$ has one eigenvalue λ_0, and the corresponding eigenvector $\bar{\Delta}_0$ is independent of k_z. It can also be shown that this is the largest eigenvalue, and, as in the $N=3$ case, all other eigenstates have negligible effects. Thus, the critical temperature is given by Eq. (31) and the gap functions for all bands are equal and isotropic. Furthermore, if we define the gap functions by $\Delta_l=\Delta_0/2$, the Ginzburg-Landau free energy will have exactly the same form as the three-layer result in Eq. (33).

The interaction matrix element for pure interlayer pairing is given by

$$\begin{aligned}V_{ll'}(k_z,k_z')=\lambda_1\sum_{n=1}^{3}&[u_{ln}(k_z)u_{l'n}(k_z')+v_{ln}(k_z)v_{l'n}(k_z')]\\&+\lambda_2[u_{l4}(k_z)u_{l'4}(k_z')+v_{l4}(k_z)v_{l'4}(k_z')] ,\end{aligned} \tag{67}$$

where the basis functions are

$$\begin{aligned}&u_{ln}=|b_{ln}b_{ln'}|\cos\phi_{ln} ,\\&v_{ln}=|b_{ln}b_{ln'}|\sin\phi_{ln} ,\end{aligned} \tag{68}$$

where $n'=n+1$ (mod 4). The explicit expressions for u_{ln} and v_{ln} are readily worked out:

$$\begin{aligned}&u_{l1}(k_z)=u_{l3}(k_z)=\frac{J_1(\varepsilon_l^2-J_1^2)+J_1^2J_2\cos(k_zs)}{D_l} ,\\&u_{l2}(k_z)=\frac{J_1(\varepsilon_l^2-J_2^2)+J_1^2J_2\cos(k_zs)}{D_l} ,\\&u_{l4}(k_z)=\frac{J_2(\varepsilon_l^2-J_1^2)+J_1^3\cos(k_zs)}{D_l} ,\end{aligned} \tag{69}$$

$$\begin{aligned}&v_l(k_z)=v_{l2}(k_z)=v_{l3}(k_z)=\frac{J_1^2J_2\sin(k_zs)}{D_l}\\&v_{l4}(k_z)=\frac{J_1^3\sin(k_zs)}{D_l} ,\end{aligned} \tag{70}$$

with

$$D_l=4\varepsilon_l(\varepsilon_l^2-2\bar{J}^2) . \tag{71}$$

Since $\varepsilon_4=-\varepsilon_1$ and $\varepsilon_3=-\varepsilon_2$, we deduce immediately that $u_{1n}=-u_{4n}$, $u_{2n}=-u_{3n}$, and $\sum_l u_{ln}=0$. The same relations hold for triplet basis functions v_{ln}. Thus, when transformed into SU(4) bases, we have $\bar{u}_{mm}=\bar{v}_{mn}=0$ for $m=0$ and 3. The surviving SU(4) components are

$$\begin{aligned}&\bar{u}_{1n}=u_{1n}+u_{2n} ,\\&\bar{u}_{2n}=u_{1n}-u_{2n} .\end{aligned} \tag{72}$$

and similar relations for $\bar{v}_{mn}$, $m=1,2$. For the singlet state the remaining basis functions have the further degeneracy that $\bar{u}_{m1}=\bar{u}_{m3}$, as can be found from Eq. (69). Consequently, the Hilbert space for each m is three dimensional, and we only need to diagonalize a 6×6 matrix $\underline{\hat{V}}^{(s)}$ to obtain T_{cs} and the dominant singlet gap function $\check{u}_m(k_z)$. The triplet basis functions v_{ln} for the same l are proportional to each other. This enables us to diagonalize a 2×2 matrix $\underline{\hat{V}}^{(t)}$ and obtain T_{ct} and the dominant triplet gap function $\check{v}_m(k_z)$. The transformation to band gap functions is done in complete analogy with the three-layer problem. The Ginzburg-Landau free energy has the same expression as in Eq. (53), including the definitions for b_s, b_t, and b_{st}. Numerical calculations have revealed that $T_{cs}\geq T_{ct}$ over the entire parameter space. The equality signs holds only when $J_1=J_2$, i.e., when the system reduces to the one layer model, as for $N=2,3$. The gap functions are usually highly dispersive, and may or may not have nodes depending on the various

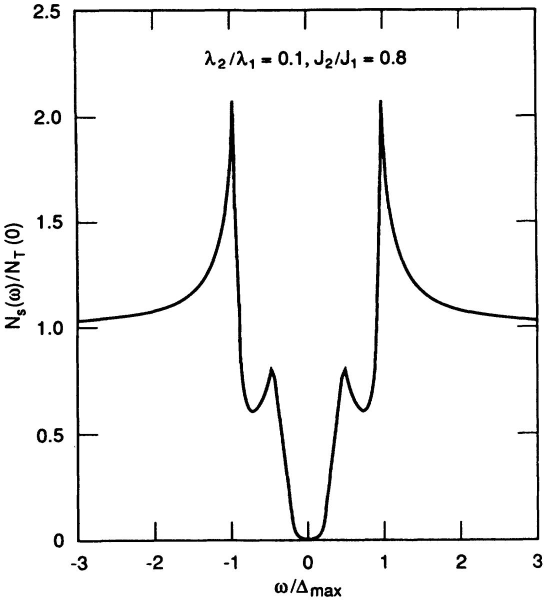

FIG. 7. The density of states of a four-layer model whose gap functions are all nodeless.

parameters. Like the three-layer system, the density of states generally has complex structure. In Fig. 7 we show the DOS of a four-layer system for which the singlet gap functions are all nodeless. A minimum gap is seen around the zero-energy point. When the gap functions of some bands have nodes, the DOS rises linearly around the zero-energy point, as illustrated in Fig. 8.

We have shown that the intralayer order parameter belongs to the $m=0$ representation of the SU(4) group, but the interlayer ones belong to the $m=1,2$ representations. It follows that if both interactions are present, they do not help each other to increase the critical temperature of the system. The Ginzburg-Landau free energy for such a system is given by Eq. (53), so the competition and coexistence of the different order parameters follow the same pattern as the two- and three-layer problems.

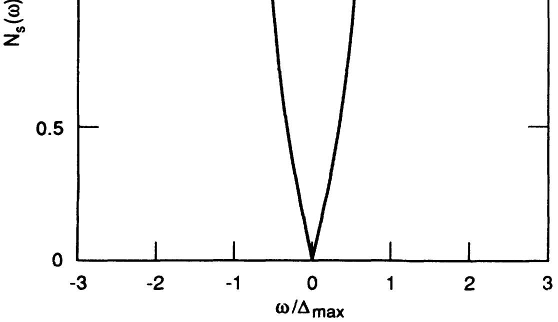

FIG. 8. The density of states of a four-layer model whose gap functions have nodes.

V. $YBa_2Cu_3O_{7-\delta}$ AS A THREE-LAYER SYSTEM

The unit of cell of Y 1:2:3 has two CuO_2 layers intervened by a CuO chain. There has always been the question whether the chain electrons are an integral part of the superconducting system because pairs of electrons can hop between the planes through the chain. In this section we carry out an analysis of this problem regarding the unit cell as a three-layer system, where the middle layer has a different two-dimensional band structure from the two other layers. It will be shown that, for band parameters representative of Y 1:2:3, hopping between the layers creates a pair of bands mainly associated with the planes and a third band mainly associated with the chains. For intralayer pairing the plane bands and the chain band form two separate superconducting systems. The interlayer pairing problem reduces to a two-band problem discussed in Refs. 1 and 2. The chain band is not superconducting although it participates in the interlayer hopping, and this may explain both the linear specific heat below T_c,[6] and the non-zero tunneling current in the center of the gap.[7]

The band Hamiltonian for a general three-layer system is given by

$$H_0=\sum_{jn\mathbf{k}\sigma}\xi_{0n}(\mathbf{k})\psi^{\dagger}_{jn\sigma}(\mathbf{k})\psi_{jn\sigma}(\mathbf{k})$$
$$+\sum_{j\mathbf{k}\sigma}[J_1\psi^{\dagger}_{j1\sigma}(\mathbf{k})\psi_{j2\sigma}(\mathbf{k})+J_2\psi^{\dagger}_{j2\sigma}(\mathbf{k})\psi_{j3\sigma}(\mathbf{k})$$
$$+J_3\psi^{\dagger}_{j3\sigma}(\mathbf{k})\psi_{j+1,1\sigma}(\mathbf{k})]\ , \qquad (73)$$

The two-dimensional band energies for the three layers are denoted by $\xi_{0n}(\mathbf{k})$, and the interlayer hopping constants are J_n. The layer $n=2$ is distinct from the other two layers, so we will set $\xi_{02}(\mathbf{k})\neq\xi_{01}(\mathbf{k})=\xi_{03}(\mathbf{k})$ and $J_1=J_2$ at the end of the calculation. The band Hamiltonian is diagonalized by the same set of transformations in Eqs. (2) and (4). The band energies $\hat{\xi}_l(k)$, $l=1,2,3$, and the transformation matrix elements $b_{\text{ln}}(k)$ are solved from the eigenvalue problem

$$\begin{bmatrix} \xi_{01}-\hat{\xi}_l & J_1e^{ik_zd} & J_3e^{-ik_zd'} \\ J_1e^{-ik_zd} & \xi_{02}-\hat{\xi}_l & J_2e^{-ik_zd} \\ J_3e^{ik_zd'} & J_2e^{-ik_zd} & \xi_{03}-\hat{\xi}_l \end{bmatrix} \begin{bmatrix} b_{l1} \\ b_{l2} \\ b_{l3} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} . \qquad (74)$$

The condition that the above equations have nonzero solutions for $\{b_{ln}\}$ is

$$(\hat{\xi}_l-\xi_{01})(\hat{\xi}_l-\xi_{02})(\hat{\xi}_l-\xi_{03})-J_1^2(\hat{\xi}_l-\xi_{01})-J_2^2(\hat{\xi}_l-\xi_{02})$$
$$-J_3^2(\hat{\xi}_l-\xi_{03})-2J_1J_2J_3\cos(k_zs)=0\ . \qquad (75)$$

This cubic equation has three real roots, which are the energies of the three bands. The elements of the transformation matrix are functions of $k=(\mathbf{k},k_z)$. They have the same expressions as in Eqs. (12) and (14) but with

$$|b_{ln}|^2=g_{ln}/\sum_{n'}g_{ln'}\ , \tag{76}$$

where

$$g_{l1}=(\hat{\xi}_1-\xi_{02})(\hat{\xi}_l-\xi_{03})-J_2^2\ , \tag{77}$$

and two other expressions obtained by cyclically permuting the layer indices. The new expressions for the phase angles are

$$\tan\phi_{l1}=\frac{J_2J_3\sin(k_zs)}{(\hat{\xi}_l-\xi_{03})J_1+J_2J_3\cos(k_zs)}\ , \tag{78}$$

and two other expressions obtained by cyclically permuting the layer indices. The sum rules in Eqs. (17) and (18) continue to hold.

We expect the electronic energy levels in the chain to be quite different from the two-dimensional band energies in the planes, at least over most of the two-dimensional Brillouin zone. In particular, if

$$|\xi_{01}-\xi_{02}|\gg\max(J_1,J_2,J_3)\ , \tag{79}$$

we can factorize the equation for $\hat{\xi}$ approximately to obtain

$$\hat{\xi}(k)\simeq\xi_{02}-2J_1'+2\zeta^2J_3\cos(k_zs)\ , \tag{80}$$

which is a one-dimensional band associated with the chain, and

$$(\hat{\xi}-\xi_{01})^2-2J_1'(\hat{\xi}-\xi_{01})-J_3^2-2J_1'J_3\cos(k_zs)\simeq0\ , \tag{81}$$

whose solutions are

$$\hat{\xi}(k)=\xi_{01}+J_1'\pm\varepsilon_\perp(k_z)\ . \tag{82}$$

In the above equations we have used the following shorthand notations $\zeta=J_1/(\xi_{01}-\xi_{02})$, $J_1'=\zeta J_1$, and

$$\varepsilon_\perp=[J_1'^2+J_3^2+2J_1'J_3\cos(k_zs)]^{1/2}\ . \tag{83}$$

The pair of bands are the same as those obtained in Refs. 1 and 2 for the two-layer system except that one of the hopping integrals is renormalized by the factor ζ. This factor is dependent on $\mathbf{k}$, but for simplicity we will approximate it by its average over the Fermi circle of the plane bands. Thus, the band problem of this three-layer system maps onto that of the two-layer system plus a separate chain band. The condition in Eq. (79) implies $|\zeta|\ll1$. We will label the ± bands by 1,2 and the chain band by 3.

The model band structure compares quite well qualitatively with the calculated bands, which consist of a pair of nearly one-dimensional bands associated with the chain and two two-dimensional (2D) bands that cross the Fermi level.[8,9] The chain band splits into two because the chain is populated by two atomic species, Cu and O. With oxygen deficiency as low as 0.1, the lower chain band is entirely filled and the upper one entirely empty. Thus, over the 2D Fermi surface of the planes, ξ_{01} and ξ_{02}, differ by amounts measured in eV. The dispersion of the plane bands in the c direction is much smaller, so the condition in Eq. (79) holds.

The intraband pairing matrix elements are given in Eq. (20). The following results are quite easy to establish by using the results in Eqs. (76) and (77):

$$|b_{l1}|^2=|b_{l3}|^2=\tfrac{1}{2}+O(\zeta)\ ,$$
$$|b_{l2}|^2=O(\zeta)\ ,$$

for $l=1,2$ and

$$|b_{3l}|^2=|b_{33}|^2=O(\zeta)\ ,$$
$$|b_{32}|^2=1+O(\zeta)\ . \tag{84}$$

Neglecting quantities of the order of ζ, we find that $V_{ll'}=\frac{1}{2}(\lambda_{01}+\lambda_{02})$, for $l,l'=1,2$, $V_{33}=\lambda_{03}$. All other matrix elements vanish. Hence, the plane and chain bands completely decouple into two superconducting systems. The gap functions of the plane bands are isotropic, so this model cannot explain the observed gap anisotropy.

We also generalize the interlayer pairing interaction by adding a new term to the interaction Hamiltonian in Eq. (3). The term is

$$-\frac{\lambda_4}{2}\sum_j\sum_{k\sigma}\sum_{k'\sigma'}[\psi_{j1\sigma}^\dagger(\mathbf{k})\psi_{j3\sigma'}^\dagger(-\mathbf{k})\psi_{j3\sigma'}(-\mathbf{k}')\psi_{j1\sigma}(\mathbf{k}')+\text{H.c.}]\ , \tag{85}$$

which represents a pairing interaction between the CuO$_2$ layers within the same unit cell mediated directly through the O(4) and Cu(1) link without involving chain electrons. The expression for $\hat{V}_{ll'}$ in Eq. (34) also acquires an added term:

$$\lambda_4[u_{l4}(k_z)u_{l'4}(k_z')+v_{l4}(k_z)v_{l'4}(k_z')]\ , \tag{86}$$

where

$$u_{l4}=|b_{l1}b_{l3}|\cos(k_zs-\phi_{13})\ ,$$
$$v_{l4}=|b_{l1}b_{l3}|\sin(k_zs-\phi_{13})\ . \tag{87}$$

In the Appendix we have worked out the explicit expressions for u_{ln} and v_{ln} in Eqs. (A3) and (A4). In the limit of Eq. (79), we can show that, to the zeroth order in ζ, the only surviving basis functions are

$$u_{13}=-u_{23}=[J_3+J_1'\cos(k_zs)]/2\varepsilon_\perp\ ,$$
$$v_{13}=-v_{23}=J_1'\sin(k_zs)/2\varepsilon_\perp\ ,$$
$$u_{14}=-u_{24}=[J_1'+J_3\cos(k_zs)]/2\varepsilon_\perp\ ,$$
$$v_{14}=-v_{24}=J_3\sin(k_zs)/2\varepsilon_\perp\ , \tag{88}$$

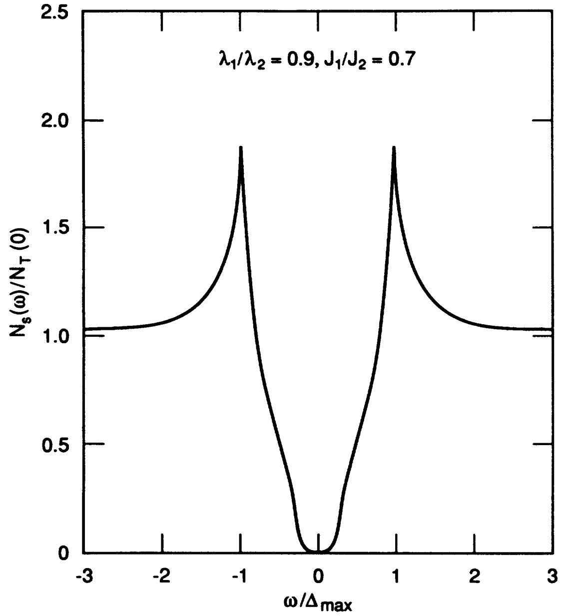

FIG. 9. The density of states of the two-layer interlayer interaction model discussed in Refs. 1 and 2.

where $\varepsilon_\perp$ is in Eq. (83). We have retained the renormalized hopping integral J_1' although it contains the factor ζ because otherwise the system would not be three dimensional. When we put these results into Eq. (34) we immediately obtain $V_{3l}=0$, which implies that there is no net pairing interaction in the chain. The basis functions u_{ln}, v_{ln} for $l=1,2$ and $n=3,4$ are identical in form to those for the two-layer model.[1,2] Thus, we have mapped the problem onto the now familiar two-layer problem plus a nonsuperconducting chain band. A typical density-of-states curve for the two-layer model is shown in Fig. 9. If we add a uniform background to represent the contribution of the chain band, we obtain a rather realistic looking tunneling characteristic for Y 1:2:3. The presence of normal chain electrons may also explain the linear specific heat in the superconducting state.[6] Our result that the chain and plane electrons form two independent Fermi fluids may give some justification to the recent effort by Schlesinger and Collins who analyzed the temperature dependence of the energy gap of Y 1:2:3 on the basis of a two-fluid model.[10]

VI. $Bi_2Sr_2CaCu_2O_8$ AS A THREE-LAYER PROBLEM

The unit cell of Bi 2:2:1:2 consists of two BiO layers and two CuO_2 layers. The band calculation for this system predicts two bands apiece for Cu-O and Bi-O layers, and the four hybridize where they cross such that two Cu-O bands and one Bi-O band cross the Fermi level.[11] This makes the material an effective three-layer system, with the two BiO layers counted as one. Over most of the Brillouin zone (BZ) the Bi-O and Cu-O bands are well separated. By the same principle discussed in the last section, the two sets of bands form two separate superconducting systems, provided that we ignore band hybridization. The Bi-O band is described by the one-layer model, while the Cu-O bands form a two-layer system. Each set would have its own T_c and order parameter, which we denote by T_{cn} and Δ_n for $n=1,2$. The effects of band hybridization can be studied in the same way outlined in Sec. III for identical layers. The crucial quantity is the pairing matrix element $V_{ll'}(k,k')$. When l and l' refer to different sets of bands, we find by following the same kind of argument presented in Sec. V that $V_{ll'}$ is negligible except over the small region of BZ where the bands hybridize. It can be seen in Eq. (29) that this gives rise to linear as well as higher-order mixing of parameters of the two bands. The linear mixing term is limited to order parameters of the same symmetry. For reasons to be discussed later, we will limit ourselves to interlayer pairing and will retain only the order parameters for the singlet states.

The Ginzburg-Landau free energy of the coupled-band system has the form

$$\begin{aligned} F_s - F_n = \frac{1}{2}\Bigg[& N_1(0)|\Delta_1|^2 \ln\left[\frac{T}{T_{c1}}\right] + \frac{1}{2} b_1 N_1(0)|\Delta_1|^4 \\ & + N_2(0)|\Delta_2|^2 \ln\left[\frac{T}{T_{c2}}\right] + \frac{1}{2} b_2 N_2(0)|\Delta_2|^4 \\ & - 2cN_{12}(0)\mathrm{Re}(\Delta_1^*\Delta_2)\Bigg] \; . \end{aligned} \tag{89}$$

In the above equation, $N_n(0)$, $n=1,2$ are the normal-state density of states of the two sets of bands, b_n differ from b_0 in Eq. (33) by numerical factors of the order unity, $N_{12}(0)=[N_1(0)N_2(0)]^{1/2}$, and c is a small number, which we use to parametrize the hybridization. The evaluation of the parameters b_n and c requires complicated calculations, but for the present discussion their precise values are unimportant. It is easy to see from Eq. (89) that the free energy is phase minimized when the two Δ's are in phase, so we will choose them as real.

The critical temperature of the coupled system is obtained by diagonalizing the quadratic part of the free energy. This gives, for T_{c1} sufficiently close to T_{c2}, that

$$T_c = \tfrac{1}{2}\{T_{c1}+T_{c2} \pm [(T_{c1}-T_{c2})^2 + 4c^2 T_{c1}T_{c2}]^{1/2}\} \; . \tag{90}$$

We denote the "+" solution by T_c, whose value is larger than the larger one of T_{cn}, and the minus solution by T_{ci}, whose value is smaller than the smaller one of T_{cn}. We do not know which band has the higher T_c. We will assume $T_{c1} > T_{c2}$ and $\Delta_1 > \Delta_2$ and investigate the consequences. In the range $T_{ci} < T < T_c$, the gaps of the two systems are given by

$$\Delta_1(T) = [(T_c - T)/b_1 T_c]^{1/2} \; ,$$

and

$$\begin{aligned} \Delta_2(T) &= c[N_1(0)/N_2(0)]^{1/2} T_{c2}\Delta_1(T)/(T_{c1}-T_{c2}) \\ &\ll \Delta_1(T) \; . \end{aligned} \tag{91}$$

Both gaps emerge at the same critical temperature T_c. For $T < T_{ci}$, the larger gap $\Delta_1(T)$ has nearly the same ex-

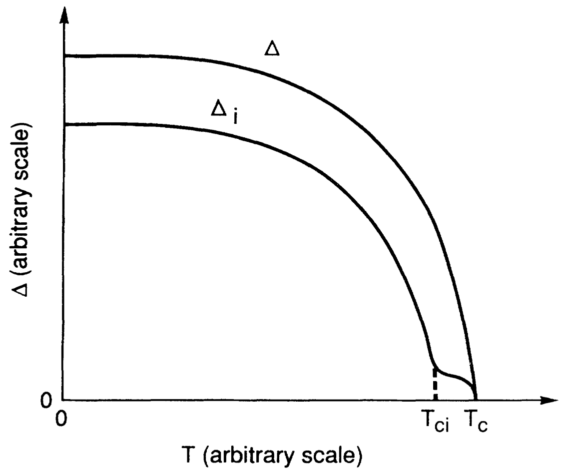

FIG. 10. Schematic representation of the temperature dependence of the two gaps of the coupled one-layer and two-layer model for Bi 2:2:1:2. The inner gap extrapolates to zero at T_{ci} but actually vanishes at T_c.

pression, but the smaller gap $\Delta_2(T)$ grows rapidly with decreasing temperature according to

$$\Delta_2(T)=[(T_{ci}-T)/b_2T_{ci}]^{1/2} . \tag{92}$$

The temperature dependence of the two gaps is shown qualitatively in Fig. 10.

The two coupled gap problem discussed here is isomorphic to the two-band problem investigated by Suhl, Matthias, and Walker.[12] What the authors of Ref. 12 had in mind is a transition metal with overlapping *s* and *d* bands. In reality the *s*-*d* hybridization matrix element is of the order of 1 eV, which is much higher than T_c. This has the effect of raising T_{c1} significantly and suppressing T_{c2} entirely. There is only one gap, which is shared by the strongly hybridized bands. The weak coupling case predicted in Ref. 12 and this paper have a better chance to be realized in layered systems because the bands are inherently weakly coupled.

The existence of two gaps and their distinct dependence on temperature may have been seen by tunneling measurements on cleaved *ab* planes of Bi 2:2:1:2. On three different samples with $T_c=90$ K, Tao *et al.*[13] reported $T_{ci}=80$, 7, and 58 K, respectively, and the temperature dependence of the inner gap has the shape given by the BCS theory. Between T_{ci} and T_c a small peak is seen at zero bias, which can be interpreted as the unresolved feature due to the small residual inner gap. In Fig. 11 we show a simulated tunneling characteristic of our two-layer plus one-layer model. The best fit to the experimental curve requires the larger gap to have a node and the smaller gap to have relatively weak k_z dependence. This would indicate the presence of interlayer pairing and that the larger gap belongs to the Bi-O layer because the interlayer singlet gap function of the one-layer model always has a node. This assignment of the relative sizes of the Cu-O and Bi-O band gaps is in agreement with the recent photoemission result.[14] The existence of a node also gives a natural explanation why the energy gap of Pb, which makes the counter electrode, is seen in some of the samples at sufficiently low temperatures.

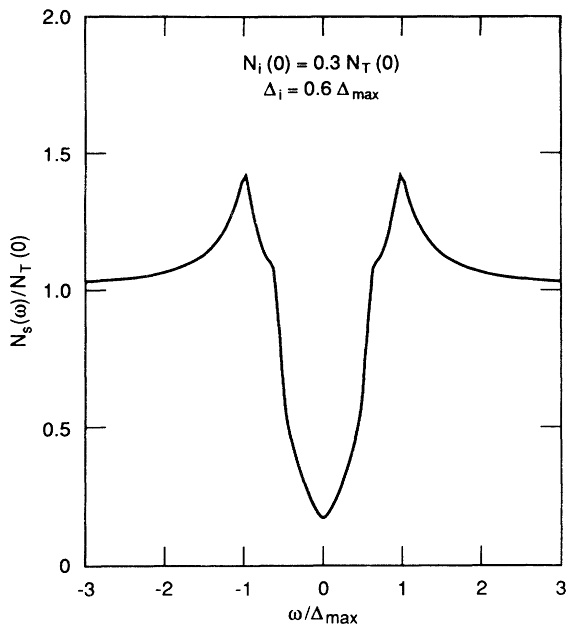

FIG. 11. Theoretical curve for the tunneling characteristic for the three-layer model for Bi 2:2:1:2 described in the text. The curve is broadened by a width parameter $\Gamma=0.08\Delta_{\max}$ to simulate all smearing effects.

The fitting parameters indicate that the band with the inner gap has only 30% of the total DOS, whereas band calculation shows that the Cu-O bands have much larger DOS than the Bi-O band. A plausible reason for this discrepancy is that the topmost surface of the crystal is known to be a Bi layer, so most of the tunneling current is contributed by electrons from this layer. The smaller contribution from the electrons in the CuO_2 layers renders their gap feature much weaker.

VII. SUMMARY AND DISCUSSION

In this paper we have analyzed the effects of intralayer and interlayer pairing in three- and four-layer models with identical layers and two three-layer models each with one distinct layer. In every case there are N energy bands, each has its own gap function. If the N conducting layers are identical, we have shown that intralayer pairing results in equal and isotropic gap functions for all bands, but interlayer pairing gives rise to different and anisotropic gap functions. The two types of pairing interactions do not help each other to boost the critical temperature of the system. The CuO chain layer in Y 1:2:3 presents a distinct middle layer in a three-layer system. It is shown that the chain band is well separated from the plane bands, and in the case of interlayer pairing, the chain band is not superconducting although it participates actively in electron motion along the *c* direction. The gap functions of the plane bands are equal in magnitude. In the case of intralayer pairing they are isotropic and have the same sign, but for interlayer pairing they are anisotropic and have the opposite sign. In Bi 2:2:1:2 the two BiO layers act like one distinct layer in addition to the two CuO_2 layers. The hybridization of the energy bands of these two sets of layered systems results in linear mixing of their superconducting order parameters. The recent tunneling data can be well described by this model.

We can extend the calculation to models with more than four identical layers in a unit cell. The symmetry of the N-layer problem is SU(N), and the results are qualitatively the same as systems with two to four layers in a unit cell.

ACKNOWLEDGMENTS

This work was supported by the U. S. Department of Energy, Division of Basic Energy Research under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc., and under Contract No. W-31-109-ENG-38 with Argonne National Laboratory. One of us (R.A.K.) was supported during part of the research by Oak Ridge National Laboratory under the same contract. Close collaboration with the experimental group of Professor E. L. Wolf is especially acknowledged.

APPENDIX

In this Appendix we will first derive explicit expressions for $\{u_{ln}\}$ and $\{v_{ln}\}$ for interlayer pairing in the general three-layer model and then show that the following sum rules are satisfied:

$$\sum_l u_{ln}=\sum_l v_{ln}=0 \ , \tag{A1}$$

for $n=1,2,3$. We begin by calculating $\cos\phi_{ln}$ and $\sin\phi_{ln}$ in the definition of u_{ln} and v_{ln} in Eq. (35), given that $\tan\phi_{ln}$ has the expression in Eq. (78) and others obtained by cyclically permuting the layer indices. The sum of squares of the numerator and the denominator of Eq. (78) gives

$$(J_2J_3\sin k_zs)^2+[(\hat{\xi}_l-\xi_{03})J_1+J_2J_3\cos(k_zs)]^2 \\ =(\hat{\xi}_l-\xi_{03})^2J_1^2+(\hat{\xi}_l-\xi_{03})2J_1J_2J_3\cos(k_zs)+J_2^2J_3^2 \ . \tag{A2}$$

Since $\hat{\xi}_l$ is a root of the cubic equation in Eq. (75), we can solve for $2J_1J_2J_3\cos(k_zs)$ and substitute the result into the right-hand side of Eq. (A2). After some algebra we reduce the resulting expressions into the product $g_{l1}g_{l2}$, where g_{ln} are defined in Eq. (77). It then follows by putting $\cos\phi_{ln}$ and $\sin\phi_{ln}$ into Eq. (35) that

$$u_{l1}=[(\hat{\xi}_l-\xi_3)J_1+J_2J_3\cos(k_zs)]\Big/\sum_n g_{ln} \ ,$$

and (A3)

$$v_{l1}=J_2J_3\sin(k_zs)\Big/\sum_n g_{ln} \ .$$

The expressions for u_{1n},v_{1n} for $n=2,3$ are obtained from cyclically permuting the layer indices. In case all ξ_n are equal, the above expressions reduce to Eq. (37). In a similar manner, the quantities u_{l4} and v_{l4} introduced in Eq. (86) are found to be

$$u_{l4}=[J_1J_2+(\hat{\xi}_l-\xi_2)J_3\cos(k_zs)]\Big/\sum_n g_{ln} \ , \\ v_{l4}=(\hat{\xi}_l-\xi_2)J_3\sin(k_zs)\Big/\sum_n g_{ln} \ . \tag{A4}$$

The fact that $\hat{\xi}_l$ for $l=1,2,3$ are roots of the cubic equation allows us to equate the left-hand side of Eq. (75) with the product $(\hat{\xi}-\hat{\xi}_1)(\hat{\xi}-\hat{\xi}_2)(\hat{\xi}-\hat{\xi}_3)$ for arbitrary values of $\hat{\xi}$. Differentiating both quantities with respect to $\hat{\xi}$ and setting $\hat{\xi}=\hat{\xi}_1$, we obtain

$$\sum_n g_{1n}=(\hat{\xi}_1-\hat{\xi}_2)(\hat{\xi}_1-\hat{\xi}_3) \ . \tag{A5}$$

The same proof applies to two similar relations for g_{ln}, $l=2$ and 3. This puts the denominators in Eqs. (A3) and (A4) in closed forms, e.g.,

$$u_{11}(k)=\frac{[(\hat{\xi}_1-\xi_{03})J_1+J_2J_3\cos(k_zs)]}{(\hat{\xi}_1-\hat{\xi}_2)(\hat{\xi}_1-\hat{\xi}_3)} \ , \\ v_{11}(k)=\frac{J_2J_3\sin(k_zs)}{(\hat{\xi}_1-\hat{\xi}_2)(\hat{\xi}_1-\hat{\xi}_3)} \ , \tag{A6}$$

and similar expressions for other values of l and n. These are used in Sec. V to derive the transformation coefficients in Eqs. (87).

The following identities involving three arbitrary real or complex numbers a,b,c are readily established by direct verification:

$$\frac{1}{(a-b)(a-c)}+\frac{1}{(b-a)(b-c)}+\frac{1}{(c-a)(c-b)}\equiv 0 \ , \tag{A7}$$

$$\frac{a}{(a-b)(a-c)}+\frac{b}{(b-a)(b-c)}+\frac{c}{(c-a)(c-b)}\equiv 0 \ . \tag{A8}$$

We put in $\hat{\xi}_l$ with $l=1,2,3$ for a,b,c in the above equations. We then multiply Eq. (A7) by $J_2J_3\cos(k_zs)-\xi_{03}J_1$ and Eq. (A8) by J_1 and add the results. This enables us to prove that

$$\sum_l u_{l1}(k)=0 \ .$$

In a similar manner, we multiply Eq. (A7) by $J_2J_3\sin(k_zs)$ to obtain the result

$$\sum_l v_{l1}(k)=0 \ .$$

The proof for other values of n follows.

Incidentally, the sum rule in Eq. (17), namely,

$$\sum_l |b_{ln}|^2 = 1 \ , \tag{A9}$$

can also be established in the same way using the additional identity

$$\frac{a^2}{(a-b)(a-c)} + \frac{b^2}{(b-a)(b-c)} + \frac{c^2}{(c-a)(c-b)} \equiv 1 \ .$$

---

[1] R. A. Klemm and S. H. Liu, Physica C **176**, 189 (1991).

[2] R. A. Klemm and S. H. Liu, Phys. Rev. B **44**, 7526 (1991); S. H. Liu and R. A. Klemm, Chinese J. Phys. (Taipei) **29**, 157 (1991).

[3] U. Welp, M. Grimsditch, H. You, W. K. Kwok, M. M. Fang, G. W. Crabtree, and J. Z. Liu, Physica C **161**, 1 (1989).

[4] Z. Schlesinger, R. T. Collins, F. Holtzberg, C. Feild, S. H. Blanton, U. Welp, G. W. Crabtree, Y. Fang, and J. Z. Liu, Phys. Rev. Lett. **65**, 801 (1990).

[5] M. Gell-Mann, in *The Eightfold Way,* edited by M. Gell-Mann and Y. Ne'eman (Benjamin, New York, 1964), p. 49.

[6] R. A. Fisher, J. E. Gordon, and N. E. Phillips, J. Supercond. **1**, 231 (1988); S. E. Stupp and D. M. Ginsberg, Physica C **158**, 299 (1989).

[7] M. Gurvitch, J. M. Valles, Jr., A. M. Cucolo, R. C. Dynes, J. P. Garno, L. F. Schneemeyer, and J. V. Waszezak, Phys. Rev. Lett. **63**, 1008 (1989).

[8] S. Massidda, J. Yu, A. J. Freeman, and D. D. Koelling, Physics Lett. **122**, 198 (1987).

[9] J. Yu, S. Massidda, A. J. Freeman, and D. D. Koelling, Phys. Lett. **122**, 203 (1987).

[10] Z. Schlesinger and R. T. Collins (private communication).

[11] S. Massida, J. Yu, and A. J. Freeman, Physica C **152**, 251 (1959).

[12] H. Suhl, B. Matthias, and L. R. Walker, Phys. Rev. Lett. **3**, 552 (1959).

[13] H. J. Tao, A. Chang, F. Lu, and E. L. Wolf (unpublished).

[14] D. S. Dessau, B. O. Wells, Z. X. Shen, W. E. Spicer, A. J. Arko, R. S. List, D. B. Mitzi, and A. Kapitulnik, Phys. Rev. Lett. **66**, 2160 (1991).