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Quasiparticle energies for a two-band interlayer-coupling model of a high-T_c superconductor

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Much of the recent literature on the high-T_c, layered, cuprate superconductors emphasizes the necessity of including in theoretical models of these materials both oxygen and copper bands and, more recently, interlayer correlations. Accordingly, we construct a Hamiltonian that takes into account these requirements, and use it, together with existing decoupling methods and extensions thereof, to calculate the superconducting-state quasiparticle energies. Our result is a generalization, which contains corrections due to the interlayer parameters, of the quasiparticle energies for the corresponding equivalent one-layer model. These corrections indicate the presence of two superconductor gaps in the wide oxygen band and provide a starting point for obtaining self-consistent gap equations.

I. INTRODUCTION

With the discovery[1] of the $YBa_2Cu_3O_{7-\delta}$ superconductors, it was soon realized that even the strong-coupling approach to electron-phonon superconductivity is inadequate for explaining the higher transition temperatures of these compounds.[2] In an early paper[3] Tešanović showed that, for such two-layer per primitive cell structures, interlayer coupling due to interactions not only increases the stability of the long-range order, but also enhances the critical temperature. His calculation (which is a BCS-like calculation) features a single effective O band; he left the mechanisms for the net attractive interactions unspecified and he assumed the interlayer hopping integrals to be vanishingly small.

Subsequently, Bishop *et al.*[4] examined the underlying mechanisms in the two-layer compounds. They ascribed the enhancement of the critical temperature to charge-transfer excitations between the two copper oxide layers by showing that the pairing arises from the ease with which the chains can be polarized both in the transverse (intraplane pairing) and longitudinal (intraplane and interplane pairing) directions because of the proximity of the $Cu^{3+}O^{2-}$ and $Cu^{2+}O^{-}$ energy levels. They further pointed out that there is a phonon contribution to the transition temperature, because of the lattice deformations which typically occur in such materials, as a result of charge transfer between the layers.

Earlier, following the publication of data[5] showing the preference of the doping-induced holes in the lanthanum compounds for the oxygen sublattice, Emery[6] used a Hamiltonian for O($2p$) holes moving through a background of localized Cu($3d$) spins and oxygen sites, with the interactions restricted to on-site and nearest-neighbor repulsions, to model a single copper oxide layer. This model is known as the "extended Hubbard model" since, for a monatomic lattice and with the neglect of nearest-neighbor interactions and the approximation of constant on-site repulsion, the Hamiltonian reduces to the original Hubbard[7] Hamiltonian. Emery reduced the two-band Hamiltonian to an effective oxygen-band Hamiltonian and showed that the consequent effective bandwidth would be small. He then established that there would be a net attraction between two holes due to Cu($3d$)-O($2p$) exchange interactions and he conjectured that this interaction is the main source of pairing.

Long[8] analyzed the Emery model for different limits of the interband and intraband hopping and interaction parameters. He found that if the nearest-neighbor Coulomb repulsion is much larger than the p-d hybridization, then clustering of the oxygen holes occurs, which prevents superconductivity. Since this limit is inconsistent with a tight-binding Hamiltonian, Long concluded that the Emery model is valid provided that the hybridization dominates the nearest-neighbor repulsion.

Several authors[9–11] have emphasized the importance of explicitly including interband and intraband parameters in model calculations with extended Hubbard Hamiltonians. The resulting Hamiltonians are intractable if all the Cu and O bands are retained. Thus it is expedient to neglect enough of the parameters to reduce the problem to that of an effective two-band extended Hubbard Hamiltonian. Subsequent work has led to conclusions that the oxygen on-site repulsion can be neglected because of the delocalization of oxygen holes[12] and their comparatively low density on these sites.[13] Nevertheless, because the physical role of the various parameters is not well understood, the prudent strategy[10] for model pairing calculations is to retain all but the obviously irrelevant terms, pending further data.

In the light of a better understanding of interlayer mechanisms, various authors[14–17] have performed calculations to examine the effects upon pairing of interlayer hopping and correlations. These calculations feature a single tight-binding oxygen band with two or more layers. Few computational details are given in the paper by Schneider, De Raedt, and Frick.[14] However, the calculations of Hofmann and co-workers[15,16] employ the Gor'kov-Nambu formalism; the implicit assumption of a Fermi-liquid normal state for the layered compounds is now fairly well vindicated.[18]

Recently Jain, Ramakumar, and Chancey[19,20] (hereaf-

ter referred to as JRC) published two calculations of generalized energy-gap functions in negative-U Hubbard and extended Hubbard models. The first of these calculations[19] is for a one-band model and makes use of a formalism and an ingenious transformation of operators which was originally developed by Hubbard and Jain[21] (hereafter referred to as HJ) to treat both the weak-interaction and strong-interaction limits in metals. The second JRC calculation[20] extends this work to a two-band model. JRC again assume an attractive on-site interaction, i.e., $U<0$, in the narrow d band, along with hopping of holes between the d band and the wide oxygen band (p-d hybridization). As for most such calculations, the cause of the attractive correlations is not spelled out because, as yet, there is no consensus on the relative contributions of phonons, antiferromagnetic coupling, and charge-transfer excitations.

Using techniques from the HJ paper[21] and equation-of-motion methods, JRC calculated the quasiparticle energies for the p-band holes and found a p-band superconductor gap stemming from p-d hybridization; in turn, they found that the p-d hybridization modifies the d-band superconductor gap. In addition, using appropriate Zubarev[22] double-time Green's functions, they derived self-consistent equations for the p-band and d-band superconductor gaps and the hole number; they stated that they were attempting to obtain numerical, self-consistent solutions of the equations.

The purpose of this paper is to present a two-band, two-layer extension of the two-band, one-layer calculation reported by JRC.[20] We carry out the calculation of the copper- and oxygen-band quasiparticle energies for a two-layer per unit cell superconducting oxide. The two-layer, single-tight-binding-band model of Hofmann and co-workers[15] was offered as a theoretical explanation of evidence indicating two distinct superconductor gaps in $YBa_2Cu_3O_{7-\delta}$; we expect our model to show a similar feature. Typically, one must resort to numerical computations to estimate the values[14,17] and ratios[16] of the various coupling parameters. In this paper, we content ourselves with obtaining the theoretical corrections, stemming from the interlayer parameters, to the quasiparticle energies and superconductor gaps calculated by JRC. We expect that these results will be useful for subsequent computational work.

II. MODEL HAMILTONIAN AND EQUATIONS OF MOTION

We begin with the simplest two-layer generalization of the one-layer Hamiltonian for copper d and oxygen p bands. We adopt the notation of JRC,[19,20] label interlayer parameters with primes, and use the Hofmann *et al.*[15] notation for layer indices. Accordingly, our Hamiltonian is

$$H=\sum_{r=1}^{2}\left[\sum_{j,\sigma}\mathcal{E}^{d}n^{d}_{rj\sigma}+\sum_{j,\sigma}\mathcal{E}^{p}n^{p}_{rj\sigma}+\sum_{j,k,\sigma}t^{d}_{jk}c^{\dagger}_{rj\sigma}c_{rk\sigma}+\sum_{j,k,\sigma}t^{p}_{jk}p^{\dagger}_{rj\sigma}p_{rk\sigma}+\sum_{j,k,\sigma}h_{jk}(p^{\dagger}_{rj\sigma}c_{rk\sigma}+c^{\dagger}_{rk\sigma}p_{rj\sigma})+\frac{1}{2}U\sum_{j,\sigma}n^{d}_{rj\sigma}n^{d}_{rj-\sigma}\right]$$
$$+\sum_{r\neq s=1}^{2}\left[\sum_{j,k,\sigma}t^{d'}_{jk}c^{\dagger}_{rj\sigma}c_{sk\sigma}+\sum_{j,k,\sigma}t^{p'}_{jk}p^{\dagger}_{rj\sigma}p_{sk\sigma}+\sum_{j,k,\sigma}h'_{jk}(p^{\dagger}_{rj\sigma}c_{sk\sigma}+c^{\dagger}_{sk\sigma}p_{rj\sigma})+\frac{1}{4}U'\sum_{j,\sigma,\sigma'}n^{d}_{rj\sigma}n^{d}_{sj\sigma'}\right]. \tag{1}$$

Here r and s are layer indices and j and k are (position space) lattice site indices. We assume that U and U' are negative, following the suggestions of Bishop *et al.*[4] The operators c, $c^{\dagger}$, and n^{d} refer to Cu holes; the operators p, $p^{\dagger}$, and n^{p} refer to O holes. Also, t^{d}_{jk} ($t^{d'}_{jk}$), t^{p}_{jk} ($t^{p'}_{jk}$), and h_{jk} (h'_{jk}) are Cu-Cu, O-O, and Cu-O intralayer (interlayer) transfer integrals, respectively. (For simplicity, we have assumed the transfer intergrals to be symmetric under exchange of their subscripts; note, however, that this assumption is not necessary, since the same equations result after Fourier transformation when this simplification is not made.) A double sum over j and k is over nearest-neighbor sites only.

We see that there is considerable symmetry between the intralayer and interlayer terms in this Hamiltonian. The most striking difference is between the interaction terms; the Pauli principle limits the on-site intralayer interaction to holes of opposite spin, but there is no such restriction for the interlayer interaction.

The Heisenberg equations of motion for the O-hole annihilation operators are

$$i\frac{\partial p_{ri\sigma}}{\partial t}=\mathcal{E}^{p}p_{ri\sigma}+\sum_{j}h_{ij}c_{rj\sigma}+\sum_{j}t^{p}_{ij}p_{rj\sigma}+\sum_{j}t^{p'}_{ij}p_{sj\sigma}+\sum_{j}h'_{ij}c_{sj\sigma}\,, \tag{2}$$

where, here and henceforth, when $r=1$ (2), then $s=2$ (1). (We also take $\hbar=1$ throughout the paper.) Similarly, the Heisenberg equations of motion for the Cu-hole annihilation operators are

$$i\frac{\partial c_{ri\sigma}}{\partial t}=\mathcal{E}^{d}c_{ri\sigma}+\sum_{j}t^{d}_{ij}c_{rj\sigma}+\sum_{j}h_{ji}p_{rj\sigma}+Uc_{ri\sigma}n^{d}_{ri-\sigma}+\sum_{j}t^{d'}_{ij}c_{sj\sigma}+\sum_{j}h'_{ji}p_{sj\sigma}+\frac{1}{2}U'\sum_{\sigma'}n^{d}_{si\sigma'}c_{ri\sigma}\,. \tag{3}$$

We endow the intralayer HJ operators[21] with a layer index, and thus define them by

$$d^{\alpha}_{ri\sigma} \equiv c_{ri\sigma} n^{d\alpha}_{ri-\sigma} \ , \quad \alpha \equiv \pm \ , \qquad n^{d+}_{ri\sigma} \equiv n^{d}_{ri\sigma} \ , \quad n^{d-}_{ri\sigma} \equiv 1 - n^{d}_{ri\sigma} \ . \tag{4}$$

(Henceforth, $n^{d\alpha}_{ri\sigma} \equiv n^{\alpha}_{ri\sigma}$ and $n^{d}_{ri\sigma} \equiv n_{ri\sigma}$.) We also extend the JRC decoupling operators[20] to our two-layer model with the definitions

$$\mathcal{E}^{\alpha}_{r} \equiv \mathcal{E}^{\alpha} + \frac{1}{2} U' \sum_{\sigma'} n^{d}_{si\sigma'} \ , \tag{5}$$

$$\mathcal{E}^{+} \equiv \mathcal{E}^{d} + U \ , \quad \mathcal{E}^{-} \equiv \mathcal{E}^{d} \ , \tag{6}$$

$$S_{rri\sigma} \equiv \sum_{j} t^{d}_{ij} (c^{\dagger}_{ri\sigma} c_{rj\sigma} - c^{\dagger}_{rj\sigma} c_{ri\sigma}) \ , \tag{7}$$

$$S_{rsi\sigma} \equiv \sum_{j} t^{d\prime}_{ij} (c^{\dagger}_{ri\sigma} c_{sj\sigma} - c^{\dagger}_{sj\sigma} c_{ri\sigma}) \ , \tag{8}$$

and

$$\xi_{\alpha} = \pm 1 \ . \tag{9}$$

Then, with the use of Eqs. (3) and (4)–(9) we obtain

$$\begin{aligned} i \frac{\partial d^{\alpha}_{ri\sigma}}{\partial t} = {} & \mathcal{E}^{\alpha}_{r} d^{\alpha}_{ri\sigma} + \sum_{j} t^{d}_{ij} c_{rj\sigma} n^{\alpha}_{ri-\sigma} + \xi_{\alpha} c_{ri\sigma} S_{rri-\sigma} \\ & - \sum_{j} h_{ji} [\xi_{\alpha} (p^{\dagger}_{rj-\sigma} c_{ri-\sigma} c_{ri\sigma} + c^{\dagger}_{ri-\sigma} c_{ri\sigma} p_{rj-\sigma}) - p_{rj\sigma} n^{\alpha}_{ri-\sigma}] + \sum_{j} t^{d\prime}_{ij} c_{sj\sigma} n^{\alpha}_{ri-\sigma} + \xi_{\alpha} c_{ri\sigma} S_{rsi-\sigma} \\ & - \sum_{j} h'_{ji} [\xi_{\alpha} (p^{\dagger}_{sj-\sigma} c_{ri-\sigma} c_{ri\sigma} + c^{\dagger}_{ri-\sigma} c_{ri\sigma} p_{sj-\sigma}) - p_{sj\sigma} n^{\alpha}_{ri-\sigma}] \ . \end{aligned} \tag{10}$$

We now linearize this equation according to the HJ prescription,[21] which mandates that all terms be rendered linear in one of the n, c, $c^{\dagger}$, p, $p^{\dagger}$, and d operators at a time. For the mixed layer terms, we make the replacements

$$c_{sj\sigma} n^{\alpha}_{ri-\sigma} \rightarrow \langle n^{\alpha}_{ri-\sigma} \rangle c_{sj\sigma} + \xi_{\alpha} \langle c_{ri-\sigma} c_{sj\sigma} \rangle c^{\dagger}_{ri-\sigma} \ , \tag{11}$$

$$c_{ri\sigma} S_{rsi-\sigma} \rightarrow \langle S_{rsi-\sigma} \rangle c_{ri\sigma} + \sum_{j} t^{d\prime}_{ij} (\langle c_{sj-\sigma} c_{ri\sigma} \rangle c^{\dagger}_{ri-\sigma} - \langle c_{ri-\sigma} c_{ri\sigma} \rangle c^{\dagger}_{sj-\sigma}) \ , \tag{12}$$

$$p^{\dagger}_{sj-\sigma} c_{ri-\sigma} c_{ri\sigma} \rightarrow \langle c_{ri-\sigma} c_{ri\sigma} \rangle p^{\dagger}_{sj-\sigma} + \langle p^{\dagger}_{sj-\sigma} c_{ri-\sigma} \rangle c_{ri\sigma} \ , \tag{13}$$

$$c^{\dagger}_{ri-\sigma} c_{ri\sigma} p_{sj-\sigma} \rightarrow - \langle c^{\dagger}_{ri-\sigma} p_{sj-\sigma} \rangle c_{ri\sigma} \ , \tag{14}$$

and

$$p_{sj\sigma} n^{\alpha}_{ri-\sigma} \rightarrow \langle n^{\alpha}_{ri-\sigma} \rangle p_{sj\sigma} \ . \tag{15}$$

We make similar replacements for the intralayer terms. To linearize the term $\mathcal{E}^{\alpha}_{r} d^{\alpha}_{ri\sigma}$, consider

$$\frac{1}{2} U' \sum_{\sigma'} n_{si\sigma'} d^{\alpha}_{ri\sigma} = \frac{1}{2} U' \sum_{\sigma'} n_{si\sigma'} n^{\alpha}_{ri-\sigma} c_{ri\sigma} \equiv \tilde{U}' \ . \tag{16}$$

Following HJ, we assume a paramagnetic situation, so that to good approximation

$$\langle n^{\alpha}_{ri\sigma} \rangle = n^{\alpha}_{r} \ , \quad \langle S_{rri\sigma} \rangle \approx 0 \ , \quad \langle S_{rsi\sigma} \rangle \approx 0 \ . \tag{17}$$

Our linearization scheme then leads to the replacement

$$\begin{aligned} \tilde{U}' = U' [& n_s d^{\alpha}_{ri\sigma} + n^{\alpha}_{r} n_s c_{ri\sigma} + \tfrac{1}{2} n^{\alpha}_{r} \langle c_{si-\sigma} c_{ri\sigma} \rangle c^{\dagger}_{si-\sigma} + n_s \xi_{\alpha} \langle c_{ri-\sigma} c_{ri\sigma} \rangle c^{\dagger}_{ri-\sigma} \\ & - \tfrac{1}{2} \xi_{\alpha} \langle c^{\dagger}_{si\sigma} c^{\dagger}_{ri-\sigma} \rangle \langle c_{si\sigma} c_{ri-\sigma} \rangle c_{ri\sigma} - \tfrac{1}{2} \xi_{\alpha} \langle c^{\dagger}_{si\sigma} c^{\dagger}_{ri-\sigma} \rangle \langle c_{ri-\sigma} c_{ri\sigma} \rangle c_{si\sigma} \\ & - \tfrac{1}{2} \langle c^{\dagger}_{si\sigma} c_{ri\sigma} \rangle n^{\alpha}_{r} c_{si\sigma} - \tfrac{1}{2} \xi_{\alpha} \langle c^{\dagger}_{si\sigma} c_{ri\sigma} \rangle \langle c_{ri-\sigma} c_{si\sigma} \rangle c^{\dagger}_{ri-\sigma} - \tfrac{1}{2} \xi_{\alpha} \langle c^{\dagger}_{ri-\sigma} c_{si-\sigma} \rangle \langle c_{ri-\sigma} c_{ri\sigma} \rangle c^{\dagger}_{si-\sigma} \\ & - \tfrac{1}{2} \xi_{\alpha} \langle c^{\dagger}_{si-\sigma} c_{ri-\sigma} \rangle \langle c_{si-\sigma} c_{ri\sigma} \rangle c^{\dagger}_{ri-\sigma} - \tfrac{1}{2} \xi_{\alpha} \langle c^{\dagger}_{si-\sigma} c_{ri-\sigma} \rangle \langle c^{\dagger}_{ri-\sigma} c_{si-\sigma} \rangle c_{ri\sigma}] \ . \end{aligned} \tag{18}$$

We now simplify the notation by defining

$$\lambda_{rr} \equiv - \langle c_{ri-\sigma} c_{ri\sigma} \rangle \ , \tag{19a}$$

$$\lambda_{rs} \equiv - \langle c_{ri-\sigma} c_{si\sigma} \rangle \ , \tag{19b}$$

$$W_{rs} \equiv \langle c^{\dagger}_{ri\sigma} c_{si\sigma} \rangle \ , \tag{20}$$

$$Y_{rrij} \equiv t^{d}_{ij} (\langle c_{ri-\sigma} c_{rj\sigma} \rangle + \langle c_{rj-\sigma} c_{ri\sigma} \rangle) \ , \tag{21}$$

$$Y'_{rsij} \equiv t^{d\prime}_{ij} (\langle c_{ri-\sigma} c_{sj\sigma} \rangle + \langle c_{sj-\sigma} c_{ri\sigma} \rangle) \ , \tag{22}$$

$$Z_{rri-\sigma} \equiv - \sum_{j} h_{ji} (\langle p^{\dagger}_{rj-\sigma} c_{ri-\sigma} \rangle - \langle c^{\dagger}_{ri-\sigma} p_{rj-\sigma} \rangle) \ , \tag{23}$$

and

$$Z'_{rsi-\sigma} \equiv - \sum_{j} h'_{ji} (\langle p^{\dagger}_{sj-\sigma} c_{ri-\sigma} \rangle - \langle c^{\dagger}_{ri-\sigma} p_{sj-\sigma} \rangle) \ . \tag{24}$$

Then the linearized form of the equation of motion, Eq. (10), is

$$i\frac{\partial d^{\alpha}_{ri\sigma}}{\partial t}=(\mathcal{E}^{\alpha}+U'n_s)d^{\alpha}_{ri\sigma}+\sum_j t^d_{ij}n^{\alpha}_r c_{rj\sigma}+\lambda_{rr}\xi_{\alpha}\sum_j t^d_{ij}c^{\dagger}_{rj-\sigma}+\sum_j t^{d'}_{ij}n^{\alpha}_r c_{sj\sigma}$$
$$+\lambda_{rr}\xi_{\alpha}\sum_j t^{d'}_{ij}c^{\dagger}_{sj-\sigma}+\xi_{\alpha}\sum_j Y_{rrij}c^{\dagger}_{ri-\sigma}+\xi_{\alpha}\sum_j Y'_{rsij}c^{\dagger}_{ri-\sigma}+\sum_j h_{ji}(n^{\alpha}_r p_{rj\sigma}+\xi_{\alpha}\lambda_{rr}p^{\dagger}_{rj-\sigma})$$
$$+\sum_j h'_{ji}(n^{\alpha}_r p_{sj\sigma}+\xi_{\alpha}\lambda_{rr}p^{\dagger}_{sj-\sigma})+\xi_{\alpha}Z_{rri-\sigma}c_{ri\sigma}+\xi_{\alpha}Z'_{rsi-\sigma}c_{ri\sigma}$$
$$+U'(n^{\alpha}_r n_s+\tfrac{1}{2}\xi_{\alpha}\lambda^2_{rs}-\tfrac{1}{2}\xi_{\alpha}W_{sr}W_{rs})c_{ri\sigma}+U'(\tfrac{1}{2}\xi_{\alpha}W_{sr}\lambda_{rs}+\tfrac{1}{2}\xi_{\alpha}W_{sr}\lambda_{sr}-\xi_{\alpha}n_s\lambda_{rr})c^{\dagger}_{ri-\sigma}$$
$$-\frac{U'}{2}(\xi_{\alpha}\lambda_{rs}\lambda_{rr}+n^{\alpha}_r W_{sr})c_{si\sigma}-\frac{U'}{2}(n^{\alpha}_r\lambda_{sr}-\xi_{\alpha}W_{rs}\lambda_{rr})c^{\dagger}_{si-\sigma}\ . \tag{25}$$

Our next step is to calculate the Fourier transforms of Eqs. (2) and (25). We define the lattice Fourier transforms as usual by

$$c_{rj\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_j}c_{r\mathbf{k}\sigma}\ , \tag{26}$$

and

$$M_{ij}=\frac{1}{N}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}M_{\mathbf{k}}\ , \tag{27}$$

where M stands for any one of the transfer integrals. Of course, the normalization factors are a direct consequence of the identity

$$\sum_j e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}=N\,\delta_{\mathbf{k},\mathbf{k}'}\ , \tag{28}$$

where N is the number of primitive cells in the crystal.

We further define

$$\Lambda_{rr}\equiv-\frac{1}{N}\sum_{\mathbf{k}}\langle c_{r-\mathbf{k}-\sigma}c_{r\mathbf{k}\sigma}\rangle\ , \tag{29a}$$

$$\Lambda_{rs}\equiv-\frac{1}{N}\sum_{\mathbf{k}}\langle c_{r-\mathbf{k}-\sigma}c_{s\mathbf{k}\sigma}\rangle\ , \tag{29b}$$

$$\Omega_{rs}\equiv\frac{1}{N}\sum_{\mathbf{k}}\langle c^{\dagger}_{r\mathbf{k}\sigma}c_{s\mathbf{k}\sigma}\rangle\ , \tag{30}$$

$$\mathcal{E}_{rs}\equiv-\frac{1}{N}\sum_{\mathbf{k}}\mathcal{E}'_{\mathbf{k}}(\langle c_{s\mathbf{k}-\sigma}c_{r-\mathbf{k}\sigma}\rangle+\langle c_{r-\mathbf{k}-\sigma}c_{s\mathbf{k}\sigma}\rangle)\ , \tag{31}$$

$$\mathcal{E}_{0r}\equiv-\frac{1}{N}\sum_{\mathbf{k}}\mathcal{E}_{\mathbf{k}}\langle c_{r-\mathbf{k}-\sigma}c_{r\mathbf{k}\sigma}\rangle\ , \tag{32}$$

$$Z_{rr}\equiv Z_{rr-\sigma}\equiv-\frac{1}{N}\sum_{\mathbf{k}}h_{\mathbf{k}}(\langle p^{\dagger}_{r\mathbf{k}-\sigma}c_{r\mathbf{k}-\sigma}\rangle-\langle c^{\dagger}_{r\mathbf{k}-\sigma}p_{r\mathbf{k}-\sigma}\rangle)\ , \tag{33}$$

and

$$Z'_{rs}\equiv Z'_{rs-\sigma}\equiv-\frac{1}{N}\sum_{\mathbf{k}}h'_{\mathbf{k}}(\langle p^{\dagger}_{s\mathbf{k}-\sigma}c_{r\mathbf{k}-\sigma}\rangle-\langle c^{\dagger}_{r\mathbf{k}-\sigma}p_{s\mathbf{k}-\sigma}\rangle)\ . \tag{34}$$

Then we find that the Fourier transforms of Eqs. (2) and (25) are

$$i\frac{\partial p_{r\mathbf{k}\sigma}}{\partial t}=h_{\mathbf{k}}c_{r\mathbf{k}\sigma}+\mathcal{E}^{p}_{\mathbf{k}}p_{r\mathbf{k}\sigma}+\mathcal{E}^{p'}_{\mathbf{k}}p_{s\mathbf{k}\sigma}+h'_{\mathbf{k}}c_{s\mathbf{k}\sigma}\ , \tag{35}$$

and

$$i\frac{\partial d^{\alpha}_{r\mathbf{k}\sigma}}{\partial t}=\mathcal{E}^{\alpha}_{r}d^{\alpha}_{r\mathbf{k}\sigma}+\left[n^{\alpha}_r\mathcal{E}_{\mathbf{k}}+U'n^{\alpha}_r n_s+\xi_{\alpha}\left[Z_{rr}+Z'_{rs}+\frac{U'}{2}(\Lambda^2_{rs}-\Omega_{rs}\Omega_{sr})\right]\right]c_{r\mathbf{k}\sigma}$$
$$+\xi_{\alpha}\left[\Lambda_{rr}\mathcal{E}_{\mathbf{k}}+2\mathcal{E}_{0r}+\mathcal{E}_{rs}-n_sU'\Lambda_{rr}+\frac{U'}{2}\Omega_{sr}(\Lambda_{rs}+\Lambda_{sr})\right]c^{\dagger}_{r-\mathbf{k}-\sigma}+h_{\mathbf{k}}n^{\alpha}_r p_{r\mathbf{k}\sigma}$$
$$+\xi_{\alpha}\Lambda_{rr}h_{\mathbf{k}}p^{\dagger}_{r-\mathbf{k}-\sigma}+\left[\mathcal{E}'_{\mathbf{k}}n^{\alpha}_r-\frac{U'}{2}(\xi_{\alpha}\Lambda_{rr}\Lambda_{rs}+n^{\alpha}_r\Omega_{sr})\right]c_{s\mathbf{k}\sigma}$$
$$+\left[\xi_{\alpha}\mathcal{E}'_{\mathbf{k}}\Lambda_{rr}+\frac{U'}{2}(\xi_{\alpha}\Lambda_{rr}\Omega_{rs}-n^{\alpha}_r\Lambda_{sr})\right]c^{\dagger}_{s-\mathbf{k}-\sigma}+h'_{\mathbf{k}}n^{\alpha}_r p_{s\mathbf{k}\sigma}+\xi_{\alpha}\Lambda_{rr}h'_{\mathbf{k}}p^{\dagger}_{s-\mathbf{k}-\sigma}\ . \tag{36}$$

Here we have used the notation

$$t^d_{\mathbf{k}}\equiv\mathcal{E}_{\mathbf{k}}\ ,\quad t^{d'}_{\mathbf{k}}\equiv\mathcal{E}'_{\mathbf{k}}\ ,\quad t^{p}_{\mathbf{k}}\equiv\mathcal{E}^{p}_{\mathbf{k}}\ ,\quad t^{p'}_{\mathbf{k}}\equiv\mathcal{E}^{p'}_{\mathbf{k}}\ . \tag{37}$$

In the next section, we shall attempt to solve our set of equations by using the JRC decoupling method. However, this method requires the equations of motion for the adjoint operators.

We can see that the quantities defined in Eqs. (29), (31), and (32) are real, by recalling the BCS ground state;[23] these quantities will still be real at nonzero temperatures, as long as we are not considering the full electron-phonon

interaction.[24] In addition, from Eqs. (33) and (34) it is obvious that

$$(Z_{rr-\sigma})^* = -Z_{rr-\sigma} \ , \quad (Z'_{rs-\sigma})^* = -Z'_{rs-\sigma} \ . \tag{38}$$

Moreover, $Z_{rr\sigma}$ and $Z'_{rs\sigma}$ are the time reverses[25,26] of $Z_{rr-\sigma}$ and $Z'_{rs-\sigma}$, respectively, so that

$$(Z_{rr\sigma})^* = Z_{rr-\sigma} \ , \quad (Z'_{rs\sigma})^* = Z'_{rs-\sigma} \ . \tag{39}$$

It then follows from Eq. (36) that the equation of motion of $d^{\alpha\dagger}_{r-\mathbf{k}-\sigma}$ is

$$\begin{aligned} i\frac{\partial d^{\alpha\dagger}_{r-\mathbf{k}-\sigma}}{\partial t} = &-\mathcal{E}^{\alpha}_{r} d^{\alpha\dagger}_{r-\mathbf{k}-\sigma} - \left[n^{\alpha}_{r}\mathcal{E}_{\mathbf{k}} + U' n^{\alpha}_{r} n_{s} + \xi_{\alpha}\left(Z_{rr} + Z'_{rs} + \frac{U'}{2}(\Lambda^2_{sr} - \Omega_{rs}\Omega_{sr}) \right) \right] c^{\dagger}_{r-\mathbf{k}-\sigma} \\ &+ \xi_{\alpha}\left[\Lambda_{rr}\mathcal{E}_{\mathbf{k}} + 2\mathcal{E}_{0r} + \mathcal{E}_{rs} - n_{s}U'\Lambda_{rr} + \frac{U'}{2}\Omega_{rs}(\Lambda_{rs} + \Lambda_{sr}) \right] c_{r\mathbf{k}\sigma} - h_{\mathbf{k}} n^{\alpha}_{r} p^{\dagger}_{r-\mathbf{k}-\sigma} \\ &+ \xi_{\alpha}\Lambda_{rr} h_{\mathbf{k}} p_{r\mathbf{k}\sigma} - \left[\mathcal{E}'_{\mathbf{k}} n^{\alpha}_{r} - \frac{U'}{2}(\xi_{\alpha}\Lambda_{rr}\Lambda_{sr} + n^{\alpha}_{r}\Omega_{rs}) \right] c^{\dagger}_{s-\mathbf{k}-\sigma} \\ &+ \left[\xi_{\alpha}\mathcal{E}'_{\mathbf{k}}\Lambda_{rr} + \frac{U'}{2}(\xi_{\alpha}\Lambda_{rr}\Omega_{sr} - n^{\alpha}_{r}\Lambda_{rs}) \right] c_{s\mathbf{k}\sigma} - h'_{\mathbf{k}} n^{\alpha}_{r} p^{\dagger}_{s-\mathbf{k}-\sigma} + \xi_{\alpha}\Lambda_{rr} h'_{\mathbf{k}} p_{s\mathbf{k}\sigma} \ . \end{aligned} \tag{40}$$

We have also derived Eq. (40) directly, in the same way that we have derived Eq. (36).

III. HUBBARD-JAIN/JRC DECOUPLING APPLIED TO TWO LAYERS

Let us now consider the d operators in Eqs. (36) and (40). The necessary modification[20] to the original Hubbard-Jain transformation[21] can be written as

$$\sum_{\alpha} \frac{d^{\alpha}_{r\mathbf{k}\sigma}}{E^{\mu}_{r\mathbf{k}} - \mathcal{E}^{\alpha}} \equiv \frac{\mathcal{E}_{\mathbf{k}} D^{\mu}_{r\mathbf{k}\sigma}}{N^{\mu}_{r\mathbf{k}}} \ , \tag{41}$$

and

$$(N^{\mu}_{r\mathbf{k}})^{-1} \equiv \sum_{\alpha} \frac{n^{\alpha}_{r}}{(E^{\mu}_{r\mathbf{k}} - \mathcal{E}^{\alpha})^2} \ , \tag{42}$$

where $E^{\mu}_{r\mathbf{k}}$ ($\mu = 1,2$) are the energies of the upper and lower Hubbard bands for each layer, i.e., the solutions of

$$\sum_{\alpha} \frac{n^{\alpha}_{r}}{E_{r} - \mathcal{E}^{\alpha}} = \frac{1}{\mathcal{E}_{\mathbf{k}}} \ . \tag{43}$$

Here, $\mathcal{E}_{\mathbf{k}}$ is the overlap integral in the one-band Hubbard Hamiltonian. Some algebra yields the inversion formula

$$d^{\alpha}_{r\mathbf{k}\sigma} = \sum_{\mu} \frac{\mathcal{E}_{\mathbf{k}} n^{\alpha}_{r} D^{\mu}_{r\mathbf{k}\sigma}}{E^{\mu}_{r\mathbf{k}} - \mathcal{E}^{\alpha}} \ , \tag{44}$$

and, with the use of Eq. (43), the result

$$c_{r\mathbf{k}\sigma} = \sum_{\mu} D^{\mu}_{r\mathbf{k}\sigma} \ . \tag{45}$$

We now write the two-layer equations of motion, Eqs. (35), (36), and (40), in terms of the D operators. This is accomplished by multiplying each of the equations of motion by

$$F^{\alpha\mu}_{r\mathbf{k}} = \frac{N^{\mu}_{r\mathbf{k}}}{\mathcal{E}_{\mathbf{k}}} \frac{1}{E^{\mu}_{r\mathbf{k}} - \mathcal{E}^{\alpha}} \tag{46}$$

and summing over α. To harness the full power of the Hubbard-Jain decoupling, it is necessary to neglect[20] pairing between different Hubbard subbands. With the extended and modified definitions

$$A^{\mu}_{r\mathbf{k}} \equiv N^{\mu}_{r\mathbf{k}} h_{\mathbf{k}} / \mathcal{E}^2_{\mathbf{k}} \ , \tag{47}$$

$$B^{\mu}_{r\mathbf{k}} \equiv \Lambda_{rr} N^{\mu}_{r\mathbf{k}} T^{\mu}_{r\mathbf{k}} h_{\mathbf{k}} / \mathcal{E}_{\mathbf{k}} \ , \tag{48}$$

$$T^{\mu}_{r\mathbf{k}} \equiv \sum_{\alpha} \frac{\xi_{\alpha}}{E^{\mu}_{r\mathbf{k}} - \mathcal{E}^{\alpha}} \ , \tag{49}$$

$$\begin{aligned} \tilde{E}^{\mu}_{r\mathbf{k}} \equiv &E^{\mu}_{r\mathbf{k}} + n_{s}U' \\ &+ \frac{N^{\mu}_{r\mathbf{k}} T^{\mu}_{r\mathbf{k}}}{\mathcal{E}_{\mathbf{k}}} \left[Z_{rr} + Z'_{rs} + \frac{U'}{2}\Lambda^2_{rs} - \frac{U'}{2}\Omega_{rs}\Omega_{sr} \right] \\ &+ U' n_{s} \frac{N^{\mu}_{r\mathbf{k}}}{\mathcal{E}^2_{\mathbf{k}}} \ , \end{aligned} \tag{50}$$

$$\begin{aligned} \Delta^{d}_{r\mathbf{k}\mu} \equiv &\left[\Lambda_{rr} + \frac{2\mathcal{E}_{0r}}{\mathcal{E}_{\mathbf{k}}} + \frac{\mathcal{E}_{rs}}{\mathcal{E}_{\mathbf{k}}} - \frac{n_{s}U'\Lambda_{rr}}{\mathcal{E}_{\mathbf{k}}} \right. \\ &\left. + \frac{U'}{2\mathcal{E}_{\mathbf{k}}}\Omega_{sr}(\Lambda_{rs} + \Lambda_{sr}) \right] T^{\mu}_{r\mathbf{k}} N^{\mu}_{r\mathbf{k}} \ , \end{aligned} \tag{51}$$

$$A^{\mu'}_{r\mathbf{k}} \equiv N^{\mu}_{r\mathbf{k}} h'_{\mathbf{k}} / \mathcal{E}^2_{\mathbf{k}} \ , \tag{52}$$

$$B^{\mu'}_{r\mathbf{k}} \equiv \Lambda_{rr} N^{\mu}_{r\mathbf{k}} T^{\mu}_{r\mathbf{k}} h'_{\mathbf{k}} / \mathcal{E}_{\mathbf{k}} \ , \tag{53}$$

$$Q^{\mu}_{r\mathbf{k}} \equiv \frac{N^{\mu}_{r\mathbf{k}}}{\mathcal{E}^2_{\mathbf{k}}} \left[\mathcal{E}'_{\mathbf{k}} - \frac{U'}{2}\Omega_{sr} \right] - \frac{U'}{2\mathcal{E}_{\mathbf{k}}} \Lambda_{rr}\Lambda_{rs} N^{\mu}_{r\mathbf{k}} T^{\mu}_{r\mathbf{k}} \ , \tag{54}$$

and

$$R^{\mu}_{r\mathbf{k}} \equiv \frac{\Lambda_{rr} N^{\mu}_{r\mathbf{k}} T^{\mu}_{r\mathbf{k}}}{\mathcal{E}_{\mathbf{k}}} \left[\mathcal{E}'_{\mathbf{k}} + \frac{U'}{2}\Omega_{rs} \right] - \frac{U'}{2}\Lambda_{sr} \frac{N^{\mu}_{r\mathbf{k}}}{\mathcal{E}^2_{\mathbf{k}}} \ , \tag{55}$$

we obtain

$$i\frac{\partial p_{r\mathbf{k}\sigma}}{\partial t}=\mathcal{E}^{p}_{\mathbf{k}}p_{r\mathbf{k}\sigma}+h_{\mathbf{k}}(D^{1}_{r\mathbf{k}\sigma}+D^{2}_{r\mathbf{k}\sigma}) +\mathcal{E}^{p'}_{\mathbf{k}}p_{s\mathbf{k}\sigma}+h'_{\mathbf{k}}(D^{1}_{s\mathbf{k}\sigma}+D^{2}_{s\mathbf{k}\sigma}) , \tag{56}$$

$$i\frac{\partial D^{\mu}_{r\mathbf{k}\sigma}}{\partial t}=\tilde{E}^{\mu}_{r\mathbf{k}}D^{\mu}_{r\mathbf{k}\sigma}+\Delta^{d}_{r\mathbf{k}\mu}D^{\dagger\mu}_{r-\mathbf{k}-\sigma}+A^{\mu}_{r\mathbf{k}}p_{r\mathbf{k}\sigma} +B^{\mu}_{r\mathbf{k}}p^{\dagger}_{r-\mathbf{k}-\sigma}+Q^{\mu}_{r\mathbf{k}}D^{\mu}_{s\mathbf{k}\sigma}+R^{\mu}_{r\mathbf{k}}D^{\dagger\mu}_{s-\mathbf{k}-\sigma} +A^{\mu'}_{r\mathbf{k}}p_{s\mathbf{k}\sigma}+B^{\mu'}_{r\mathbf{k}}p^{\dagger}_{s-\mathbf{k}-\sigma} , \tag{57}$$

and

$$i\frac{\partial D^{\dagger\mu}_{r-\mathbf{k}-\sigma}}{\partial t}=-\tilde{E}^{\mu}_{r\mathbf{k}}D^{\dagger\mu}_{r-\mathbf{k}-\sigma}+\Delta^{d}_{r\mathbf{k}\mu}D^{\mu}_{r\mathbf{k}\sigma}-A^{\mu}_{r\mathbf{k}}p^{\dagger}_{r-\mathbf{k}-\sigma} +B^{\mu}_{r\mathbf{k}}p_{r\mathbf{k}\sigma}-Q^{\mu}_{r\mathbf{k}}D^{\dagger\mu}_{s-\mathbf{k}-\sigma}+R^{\mu}_{r\mathbf{k}}D^{\mu}_{s\mathbf{k}\sigma} -A^{\mu'}_{r\mathbf{k}}p^{\dagger}_{s-\mathbf{k}-\sigma}+B^{\mu'}_{r\mathbf{k}}p_{s\mathbf{k}\sigma} . \tag{58}$$

Here we have assumed, on physical grounds, that

$$\Lambda_{rs}=\Lambda_{sr}\equiv\Lambda' , \quad \Omega_{rs}=\Omega_{sr}\equiv\Omega' . \tag{59}$$

We shall now attempt to solve Eqs. (56)–(58), using the JRC approximation methods. If we had not made the assumptions of Eqs. (59), there would be four different R quantities, which would make a solution prohibitively difficult to obtain.

We first consider Eq. (56). As a first approximation, we neglect the inhomogeneous portion, which amounts to treating the hybridization as a perturbation.[20] We thereby obtain

$$i\frac{\partial p_{r\mathbf{k}\sigma}}{\partial t}=\mathcal{E}^{p}_{\mathbf{k}}p_{r\mathbf{k}\sigma}+\mathcal{E}^{p'}_{\mathbf{k}}p_{s\mathbf{k}\sigma} . \tag{60}$$

This system is easily solved with

$$p_{r\mathbf{k}\sigma}(t)=p_{s\mathbf{k}\sigma}(t) =e^{-i(\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}})t}p_{r\mathbf{k}\sigma}(0) , \tag{61}$$

which corresponds to the p operators in the two layers being in phase, and

$$p_{r\mathbf{k}\sigma}(t)=-p_{s\mathbf{k}\sigma}(t) =e^{-i(\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}})t}p_{r\mathbf{k}\sigma}(0) , \tag{62}$$

which corresponds to the p operators in the two layers being exactly out of phase.

We next attempt to solve the equations for D, Eqs. (57) and (58). We follow JRC in setting all the p-operator coefficients in Eqs. (57) and (58) to zero. For notational convenience, for the time being, we suppress band, wave vector, and spin indices and omit tildes. We then have

$$i\frac{\partial \underline{D}}{\partial t}=\underline{K}\,\underline{D} , \tag{63}$$

where

$$\underline{D}=(D_1 \;\; D_2 \;\; D_1^{\dagger} \;\; D_2^{\dagger})^{T} , \tag{64}$$

and

$$\underline{K}=\begin{bmatrix} E_1 & Q_1 & \Delta_1 & R_1 \\ Q_2 & E_2 & R_2 & \Delta_2 \\ \Delta_1 & R_1 & -E_1 & -Q_1 \\ R_2 & \Delta_2 & -Q_2 & -E_2 \end{bmatrix} . \tag{65}$$

To solve this system, we assume

$$\underline{D}=\underline{\eta}e^{\chi t} . \tag{66}$$

For a nontrivial solution, we must have

$$\det(\underline{K}-i\chi\underline{1}_4)=0 , \tag{67}$$

where $\underline{1}_4$ is the 4×4 unit matrix. Straightforward algebraic manipulations leave us with

$$\chi^4+a\chi^2+b=0 , \tag{68}$$

with

$$a=E_1^2+E_2^2+2Q_1Q_2+2R_1R_2+\Delta_1^2+\Delta_2^2 , \tag{69}$$

and

$$b=(E_1E_2-Q_1Q_2+R_1R_2-\Delta_1\Delta_2)^2 +(E_1\Delta_2-R_2Q_1+E_2\Delta_1-R_1Q_2)^2 . \tag{70}$$

Accordingly,

$$\chi^2=\frac{-(E_1^2+E_2^2+2Q_1Q_2+2R_1R_2+\Delta_1^2+\Delta_2^2)}{2} \pm\frac{\{[(E_1^2-E_2^2)+(\Delta_1^2-\Delta_2^2)]^2+J\}^{1/2}}{2} , \tag{71}$$

where

$$J=4R_1R_2[(E_1-E_2)^2+(\Delta_1+\Delta_2)^2] +4Q_1Q_2[(E_1+E_2)^2+(\Delta_1-\Delta_2)^2] -4(R_1Q_2-R_2Q_1)^2 +8(R_1Q_2+R_2Q_1)(E_1\Delta_2+E_2\Delta_1) . \tag{72}$$

Upon letting the interlayer parameters vanish in Eq. (71), we obtain the four roots

$$\chi_1^{\pm}=\pm i\sqrt{E_1^2+\Delta_1^2} , \quad \chi_2^{\pm}=\pm i\sqrt{E_2^2+\Delta_2^2} . \tag{73}$$

Thus, in this limiting case, the two layers are decoupled and the eigenenergies appearing in Eqs. (73) are the narrow-band quasiparticle energies of the one-layer model.

For the two-layer case, we write the four roots as

$$\chi=\pm\left[\frac{-(a\mp\sqrt{a^2-4b})}{2}\right]^{1/2} =\pm i\left[\frac{a\mp\sqrt{a^2-4b}}{2}\right]^{1/2}\equiv\pm i\bar{E}^{\mp}_{\mathbf{k}\mu} . \tag{74}$$

With these four distinct roots, we can write the general solution of Eq. (63) as

$$\underline{D}=\sum_{j=1}^{4}\underline{\eta}_j e^{\chi_j t} , \tag{75}$$

where the χ_j are given by Eq. (74). Since E_1 and E_2 in Eq. (71) are complex numbers [see Eq. (50)], the solutions given by Eq. (75) decay with time, corresponding to finite quasiparticle lifetimes.

We now attempt to find a p-band gap, using the JRC method and a single root, $-i\bar{E}^{+}_{\mathbf{k}\mu}\equiv -i\bar{E}_{\mathbf{k}\mu}$, given by Eq. (74). We rewrite Eq. (57) as

$$i[\partial D^{\mu}_{r\mathbf{k}\sigma}(t)/\partial t]=\bar{E}_{\mathbf{k}\mu}D^{\mu}_{r\mathbf{k}\sigma}(t)+A^{\mu}_{r\mathbf{k}}p_{r\mathbf{k}\sigma}(t)+B^{\mu}_{r\mathbf{k}}p^{\dagger}_{r-\mathbf{k}-\sigma}(t)+A^{\mu'}_{r\mathbf{k}}p_{s\mathbf{k}\sigma}(t)+B^{\mu'}_{r\mathbf{k}}p^{\dagger}_{s-\mathbf{k}-\sigma}(t)\ . \tag{76}$$

We place Eq. (61) as the solution to the homogeneous part of the full p problem given by Eq. (56) into Eq. (76), and integrate, to obtain

$$\begin{aligned}D_r(t)=&-\frac{A_rp_r(t)}{\bar{E}-\mathcal{E}^{p}_{\mathbf{k}}\mathcal{E}^{p'}_{\mathbf{k}}}-\frac{B_rp^{\dagger}_r(t)}{\bar{E}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}-\frac{A'_rp_s(t)}{\bar{E}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\\&-\frac{B'_rp^{\dagger}_s(t)}{\bar{E}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}+\frac{A_rp_r(0)e^{-i\bar{E}t}}{\bar{E}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\\&+\frac{B_rp^{\dagger}_r(0)e^{-i\bar{E}t}}{\bar{E}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}+\frac{A'_rp_s(0)e^{-i\bar{E}t}}{\bar{E}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\\&+\frac{B'_rp^{\dagger}_s(0)e^{-i\bar{E}t}}{\bar{E}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}+D_r(0)e^{-i\bar{E}t}\ .\end{aligned} \tag{77}$$

Here we have temporarily suppressed the indices $\mathbf{k}$, σ, and μ. We can now rewrite Eq. (56) so that the only implicit time dependence is in the p-band operators. We define

$$\alpha_{r\mathbf{k}}\equiv\frac{1}{\mathcal{E}^{2}_{\mathbf{k}}}\sum_{\mu}\frac{N^{\mu}_{r\mathbf{k}}}{\bar{E}_{\mathbf{k}\mu}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}=\frac{1}{h_{\mathbf{k}}}\sum_{\mu}\frac{A^{\mu}_{r\mathbf{k}}}{\bar{E}_{\mathbf{k}\mu}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\ , \tag{78}$$

and

$$\beta_{r\mathbf{k}}\equiv-\frac{\Lambda_{rr}}{\mathcal{E}_{\mathbf{k}}}\sum_{\mu}\frac{N^{\mu}_{r\mathbf{k}}T^{\mu}_{r\mathbf{k}}}{\bar{E}_{\mathbf{k}\mu}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}=-\frac{1}{h_{\mathbf{k}}}\sum_{\mu}\frac{B^{\mu}_{r\mathbf{k}}}{\bar{E}_{\mathbf{k}\mu}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}\ , \tag{79}$$

analogously to JRC. We then see from Eqs. (52) and (53) that

$$\alpha_{r\mathbf{k}}=\frac{1}{h'_{\mathbf{k}}}\sum_{\mu}\frac{A^{\mu'}_{r\mathbf{k}}}{\bar{E}_{\mathbf{k}\mu}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\ , \tag{80}$$

and

$$\beta_{r\mathbf{k}}=-\frac{1}{h'_{\mathbf{k}}}\sum_{\mu}\frac{B^{\mu'}_{r\mathbf{k}}}{\bar{E}_{\mathbf{k}\mu}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}\ . \tag{81}$$

Upon using Eq. (77) to substitute into Eq. (56), and using Eqs. (78)–(81), we obtain

$$\begin{aligned}i[\partial p_r(t)/\partial t]=&\mathcal{E}^{p}_{\mathbf{k}}p_r(t)+\mathcal{E}^{p'}_{\mathbf{k}}p_s(t)-h^{2}_{\mathbf{k}}\alpha_{r\mathbf{k}}p_r(t)+h^{2}_{\mathbf{k}}\beta_{r\mathbf{k}}p^{\dagger}_r(t)-h_{\mathbf{k}}h'_{\mathbf{k}}\alpha_{r\mathbf{k}}p_s(t)\\&+h_{\mathbf{k}}h'_{\mathbf{k}}\beta_{r\mathbf{k}}p^{\dagger}_s(t)-h'_{\mathbf{k}}h_{\mathbf{k}}\alpha_{s\mathbf{k}}p_s(t)+h'_{\mathbf{k}}h_{\mathbf{k}}\beta_{s\mathbf{k}}p^{\dagger}_s(t)-h'^{2}_{\mathbf{k}}\alpha_{s\mathbf{k}}p_r(t)+h'^{2}_{\mathbf{k}}\beta_{s\mathbf{k}}p^{\dagger}_r(t)\\&+\sum_{\mu}[h_{\mathbf{k}}D_r(0)e^{-i\bar{E}t}+\alpha_{r\mathbf{k}}h^{2}_{\mathbf{k}}p_r(0)e^{-i\bar{E}t}-h^{2}_{\mathbf{k}}\beta_{r\mathbf{k}}p^{\dagger}_r(0)e^{-i\bar{E}t}+h_{\mathbf{k}}h'_{\mathbf{k}}\alpha_{r\mathbf{k}}p_s(0)e^{-i\bar{E}t}\\&-h_{\mathbf{k}}h'_{\mathbf{k}}\beta_{r\mathbf{k}}p^{\dagger}_s(0)e^{-i\bar{E}t}+h'_{\mathbf{k}}D_s(0)e^{-i\bar{E}t}+h'_{\mathbf{k}}h_{\mathbf{k}}\alpha_{s\mathbf{k}}p_s(0)e^{-i\bar{E}t}\\&-h_{\mathbf{k}}h'_{\mathbf{k}}\beta_{s\mathbf{k}}p^{\dagger}_s(0)e^{-i\bar{E}t}+h'^{2}_{\mathbf{k}}\alpha_{s\mathbf{k}}p_r(0)e^{-i\bar{E}t}-h'^{2}_{\mathbf{k}}\beta_{s\mathbf{k}}p^{\dagger}_r(0)e^{-i\bar{E}t}]\ .\end{aligned} \tag{82}$$

As a first approximation, we neglect all terms summed over μ in Eq. (82), none of which contain time-dependent operators. In addition, we recall that the $p^{\dagger}$ operators have indices $r,-\mathbf{k},-\sigma$ and the p operators have indices $r,\mathbf{k},\sigma$. We need the equations for the $p^{\dagger}$ operators corresponding to Eqs. (82); these can be obtained by formally taking the adjoint of Eqs. (82) and effecting a $(\mathbf{k},\sigma)$ to $(-\mathbf{k},-\sigma)$ transformation in the complex-conjugated α and β coefficients. From Eqs. (78) and (79), via Eq. (38), we see that

$$\alpha^{*}_{r-\mathbf{k}-\sigma}=\alpha_{r\mathbf{k}\sigma}\ ,\quad \beta^{*}_{r-\mathbf{k}-\sigma}=-\beta_{r\mathbf{k}\sigma}\ . \tag{83}$$

We thus obtain the approximate set of equations

$$\begin{aligned}i[\partial p_r(t)/\partial t]=&(\mathcal{E}^{p}_{\mathbf{k}}-\alpha_{r\mathbf{k}}h^{2}_{\mathbf{k}}-\alpha_{s\mathbf{k}}h'^{2}_{\mathbf{k}})p_r(t)\\&+[\mathcal{E}^{p'}_{\mathbf{k}}-h_{\mathbf{k}}h'_{\mathbf{k}}(\alpha_{r\mathbf{k}}+\alpha_{s\mathbf{k}})]p_s(t)\\&+(h^{2}_{\mathbf{k}}\beta_{r\mathbf{k}}+h'^{2}_{\mathbf{k}}\beta_{s\mathbf{k}})p^{\dagger}_r(t)\\&+[h_{\mathbf{k}}h'_{\mathbf{k}}(\beta_{r\mathbf{k}}+\beta_{s\mathbf{k}})]p^{\dagger}_s(t)\ ,\end{aligned} \tag{84}$$

and

$$\begin{aligned}i[\partial p^{\dagger}_r(t)/\partial t]=&-(\mathcal{E}^{p}_{\mathbf{k}}-\alpha_{r\mathbf{k}}h^{2}_{\mathbf{k}}-\alpha_{s\mathbf{k}}h'^{2}_{\mathbf{k}})p^{\dagger}_r(t)\\&-[\mathcal{E}^{p'}_{\mathbf{k}}-h_{\mathbf{k}}h'_{\mathbf{k}}(\alpha_{r\mathbf{k}}+\alpha_{s\mathbf{k}})]p^{\dagger}_s(t)\\&+(h^{2}_{\mathbf{k}}\beta_{r\mathbf{k}}+h'^{2}_{\mathbf{k}}\beta_{s\mathbf{k}})p_r(t)\\&+[h_{\mathbf{k}}h'_{\mathbf{k}}(\beta_{r\mathbf{k}}+\beta_{s\mathbf{k}})]p_s(t)\ .\end{aligned} \tag{85}$$

To simplify the notation, let us define

$$\tilde{\mathcal{E}}_r\equiv\mathcal{E}^{p}_{\mathbf{k}}-\alpha_{r\mathbf{k}}h^{2}_{\mathbf{k}}-\alpha_{s\mathbf{k}}h'^{2}_{\mathbf{k}}\ , \tag{86}$$

$$\tilde{Q}\equiv\mathcal{E}^{p'}_{\mathbf{k}}-h_{\mathbf{k}}h'_{\mathbf{k}}(\alpha_{r\mathbf{k}}+\alpha_{s\mathbf{k}})\ , \tag{87}$$

$$\tilde{\Delta}_r\equiv h^{2}_{\mathbf{k}}\beta_{r\mathbf{k}}+h'^{2}_{\mathbf{k}}\beta_{s\mathbf{k}}\ , \tag{88}$$

and

$$\tilde{R}\equiv h_{\mathbf{k}}h'_{\mathbf{k}}(\beta_{r\mathbf{k}}+\beta_{s\mathbf{k}})\ . \tag{89}$$

We can then write Eqs. (84) and (85) as

$$i[\partial\underline{\mathcal{P}}(t)/\partial t]\equiv\underline{\mathfrak{K}}\,\underline{\mathcal{P}}\ , \tag{90}$$

where

$$\underline{\mathcal{P}}=(p_1(t)\ \ p_2(t)\ \ p_1^{\dagger}(t)\ \ p_2^{\dagger}(t))^T\ , \tag{91}$$

and

$$\underline{\mathfrak{K}}=\begin{bmatrix}\tilde{\mathcal{E}}_1 & \tilde{Q} & \tilde{\Delta}_1 & \tilde{R}\\ \tilde{Q} & \tilde{\mathcal{E}}_2 & \tilde{R} & \tilde{\Delta}_2\\ \tilde{\Delta}_1 & \tilde{R} & -\tilde{\mathcal{E}}_1 & -\tilde{Q}\\ \tilde{R} & \tilde{\Delta}_2 & -\tilde{Q} & -\tilde{\mathcal{E}}_2\end{bmatrix}\ . \tag{92}$$

Since Eq. (90) has precisely the same form as Eq. (63), we may immediately make use of the work done in arriving at Eqs. (71) and (74). Thus the matrix eigenvalues are given by

$$\chi=\pm\left[\frac{-(\tilde{\mathcal{E}}_1^{\,2}+\tilde{\mathcal{E}}_2^{\,2}+2\tilde{Q}^{\,2}+2\tilde{R}^{\,2}+\tilde{\Delta}_1^{\,2}+\tilde{\Delta}_2^{\,2})\pm\sqrt{(\tilde{\mathcal{E}}_1^{\,2}-\tilde{\mathcal{E}}_2^{\,2}+\tilde{\Delta}_1^{\,2}-\tilde{\Delta}_2^{\,2})^2+\tilde{J}}}{2}\right]^{1/2}\ , \tag{93}$$

where

$$\tilde{J}\equiv 4\tilde{R}^{\,2}[(\tilde{\mathcal{E}}_1-\tilde{\mathcal{E}}_2)^2+(\tilde{\Delta}_1+\tilde{\Delta}_2)^2]+16\tilde{R}\tilde{Q}(\tilde{\mathcal{E}}_1\tilde{\Delta}_2+\tilde{\mathcal{E}}_2\tilde{\Delta}_1)+4\tilde{Q}^{\,2}[(\tilde{\mathcal{E}}_1+\tilde{\mathcal{E}}_2)^2+(\tilde{\Delta}_1-\tilde{\Delta}_2)^2]\ . \tag{94}$$

Hence we can write

$$\tilde{E}_{\mathbf{k}}^{\rho\mp}=\left[\frac{(\tilde{\mathcal{E}}_1^{\,2}+\tilde{\mathcal{E}}_2^{\,2}+2\tilde{Q}^{\,2}+2\tilde{R}^{\,2}+\tilde{\Delta}_1^{\,2}+\tilde{\Delta}_2^{\,2})\mp\sqrt{(\tilde{\mathcal{E}}_1^{\,2}-\tilde{\mathcal{E}}_2^{\,2}+\tilde{\Delta}_1^{\,2}-\tilde{\Delta}_2^{\,2})^2+\tilde{J}}}{2}\right]^{1/2}\ . \tag{95}$$

First, let us note that setting Eq. (94) to zero is equivalent to decoupling the two layers. We thus have

$$\tilde{E}_{\mathbf{k}}^{\rho\mp}=\sqrt{\tilde{\mathcal{E}}_1^{\,2}+\tilde{\mathcal{E}}_2^{\,2}+\tilde{\Delta}_1^{\,2}+\tilde{\Delta}_2^{\,2}\mp(\tilde{\mathcal{E}}_1^{\,2}-\tilde{\mathcal{E}}_2^{\,2})\mp(\tilde{\Delta}_1^{\,2}-\tilde{\Delta}_2^{\,2})}\ , \tag{96}$$

and with Eqs. (86) and (88), we obtain

$$\tilde{E}_{1\mathbf{k}}^{\rho}=\sqrt{(\mathcal{E}_{\mathbf{k}}^{\rho}-\alpha_{1\mathbf{k}}h_{\mathbf{k}}^2)^2+(\beta_{1\mathbf{k}}h_{\mathbf{k}}^2)^2}\ , \tag{97}$$

and

$$\tilde{E}_{2\mathbf{k}}^{\rho}=\sqrt{(\mathcal{E}_{\mathbf{k}}^{\rho}-\alpha_{2\mathbf{k}}h_{\mathbf{k}}^2)^{p2}+(\beta_{2\mathbf{k}}h_{\mathbf{k}}^2)^2}\ . \tag{98}$$

In this limit, if we allow the interlayer parameters to vanish, the resulting quasiparticle energies, given by Eqs. (96) and (97), are simply the quasiparticle energies of the one-layer model. We have not found a factorization allowing us to eliminate the inner radical in Eq. (95). We can, however, convince ourselves that the energy-gap contribution due to interlayer-interband hopping, for example, is nontrivial, by considering the "worst-case scenario" in which Eqs. (86)–(89) are layer independent. Equation (94) thereupon becomes

$$\tilde{E}_{\mathbf{k}}^{\rho+}=\{[\mathcal{E}_{\mathbf{k}}^{\rho}+\mathcal{E}_{\mathbf{k}}^{\rho'}-\alpha_{\mathbf{k}}(h_{\mathbf{k}}+h'_{\mathbf{k}})^2]^2+\beta_{\mathbf{k}}^2(h_{\mathbf{k}}+h'_{\mathbf{k}})^4\}^{1/2}\ , \tag{99}$$

where we have chosen $\tilde{E}_{\mathbf{k}}^{\rho+}$ in Eq. (94), analogous to our use of Eq. (61) in obtaining Eq. (76). In view of Eqs. (53) and (81), we can identify the extra interlayer contribution to the p-band gap from

$$(\delta\tilde{\Delta}_{\mathbf{k}}^{\rho})^2=\beta_{\mathbf{k}}^2(h_{\mathbf{k}}+h'_{\mathbf{k}})^4-\beta_{\mathbf{k}}^2h_{\mathbf{k}}^4\ . \tag{100}$$

It should be noted that just as the one-layer quasiparticle energy for the p band, given by Eq. (97), contains d-band pairing contributions through the α and β coefficients, $\tilde{E}_{\mathbf{k}}^{\rho+}$ as given by Eq. (99) has pairing contributions from the d band, through Eq. (74), which enter into the α and β coefficients defined in Eqs. (78) and (79). It can be verified that

$$\lim_{U\to 0}[\tilde{\Delta}_{\mathbf{k}}^{\rho}]=\lim_{U\to 0}[\beta_{\mathbf{k}}(h_{\mathbf{k}}+h'_{\mathbf{k}})^2]=0\ , \tag{101}$$

as in the one-layer model. Additionally, we have

$$\lim_{U'\to 0}[\tilde{\Delta}_{\mathbf{k}}^{\rho}]=\Delta_{\mathbf{k}}^{\rho}\ , \tag{102}$$

where $\Delta_{\mathbf{k}}^{\rho}$ is the superconductor gap stemming from intralayer pairing alone. Furthermore, Eq. (100) has the property that

$$\lim_{h'_{\mathbf{k}}\to 0}[\delta\tilde{\Delta}_{\mathbf{k}}^{\rho}]=0\ . \tag{103}$$

We note that the intralayer anomalous average Λ enters into Eq. (99) through the α coefficients (implicitly) and through the β coefficients [explicitly, if we recall Eq. (53)]. However, the interlayer anomalous average Λ' enters into Eq. (99) implicitly only, through $\bar{E}_{\mathbf{k}\mu}$, in this model.

We must now attempt to make some sense of the different roots which have arisen in the various stages of this calculation. We recall that the calculation was begun from a particular solution to the two-layer Hubbard band problem, Eq. (63), with the energy given by one of the four choices in Eq. (74). Since $\tilde{E}_{\mathbf{k}}^{\rho}$ must be an improvement over the first approximation to the energy featured

in Eq. (61), we must choose $\tilde{E}^{p\,+}_{\mathbf{k}}$; furthermore, the assumption we made earlier that Eqs. (86)–(89) are layer independent yields, from Eq. (74), a simpler expression for the d-band quasiparticle energies:

$$\bar{E}^{\,+}_{\mathbf{k}\mu}=\sqrt{(\tilde{E}_{\mathbf{k}\mu}+Q_{\mathbf{k}\mu})^2+(R_{\mathbf{k}\mu}+\Delta_{\mathbf{k}\mu})^2}\equiv\sqrt{(E^d_{\mathbf{k}\mu})^2+(\tilde{\Delta}^{\,d}_{\mathbf{k}\mu})^2}\ , \tag{104}$$

where E^d includes all terms in Eqs. (50) and (54) except for the two terms featuring anomalous averages (the sum of which we denote by γ). These anomalous averages enter into the effective superconductor d-band gap, which is given by

$$\tilde{\Delta}^{\,d}_{\mathbf{k}\mu}=\sqrt{(\Delta_{\mathbf{k}\mu}+R_{\mathbf{k}\mu})^2+2\gamma_{\mathbf{k}\mu}E^d_{\mathbf{k}\mu}+\gamma^2_{\mathbf{k}\mu}}\ . \tag{105}$$

Note that we selected the positive superscript for the energy in Eq. (74), since our model must reflect the presence of a narrow-band gap in the absence of interlayer parameters.

The hybridization-induced superconductor gap in the p band is given by

$$\tilde{\Delta}^{\,p}_{\mathbf{k}}=-\frac{\Lambda}{\mathcal{E}_{\mathbf{k}}}(h_{\mathbf{k}}+h'_{\mathbf{k}})^2\sum_{\mu}\frac{N^{\mu}_{\mathbf{k}}T^{\mu}_{\mathbf{k}}}{\bar{E}^{\,+}_{\mathbf{k}\mu}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}}\ . \tag{106}$$

This equation gives the two-layer correction to the one-layer result. The interlayer coupling is embedded in $\bar{E}^{\,+}_{\mathbf{k}\mu}$, and in view of the smallness of the interlayer parameters relative to the intralayer ones, we can expect from this equation that the interlayer hopping contribution to the p-band gap will be smaller than the intralayer one.

Recalling Eqs. (47)–(55), we can write Eq. (106) more explicitly in terms of the hopping and Coulomb integrals, i.e.,

$$\tilde{\Delta}^{\,p}_{\mathbf{k}}=-\sum_{\mu}\Bigg[\Lambda(h_{\mathbf{k}}+h'_{\mathbf{k}})^2N^{\mu}_{\mathbf{k}}T^{\mu}_{\mathbf{k}}\mathcal{E}^{-1}_{\mathbf{k}}\Bigg\{\Bigg\{\Bigg[E^d_{\mathbf{k}\mu}+\frac{U'N^{\mu}_{\mathbf{k}}T^{\mu}_{\mathbf{k}}}{2\mathcal{E}_{\mathbf{k}}}(\Lambda'^2-\Lambda\Lambda')\Bigg]^2+\Bigg[\Bigg\{\mathcal{E}_{\mathbf{k}}\Lambda+2\mathcal{E}_{0r}+\mathcal{E}_{rs}-nU'\Lambda+U'\Omega'\Lambda'+\mathcal{E}'_{\mathbf{k}}\Lambda+\frac{U'}{2}\Lambda\Omega'\Bigg\}\frac{N^{\mu}_{\mathbf{k}}T^{\mu}_{\mathbf{k}}}{\mathcal{E}_{\mathbf{k}}}-\frac{U'\Lambda'N^{\mu}_{\mathbf{k}}}{2\mathcal{E}^2_{\mathbf{k}}}\Bigg]^2\Bigg\}^{1/2}+\mathcal{E}^{p}_{\mathbf{k}}+\mathcal{E}^{p'}_{\mathbf{k}}\Bigg]^{-1}\Bigg]\ . \tag{107}$$

As shown by JRC for the one-layer case, p-d hybridization not only induces a p-band superconductor gap, but it also modifies the effective d-band gap, as given by Eq. (105). Following the same method of approximation [Eqs. (77)–(82)], which leads to the coupled equations (84) and (85) in terms of wide-band operators only, but starting with Eqs. (56) and (61), one eventually obtains equations for the p operators in terms of time-dependent D operators only. When these equations are used to substitute into Eqs. (57) and (58), the result is a set of coupled equations expressed solely in terms of D operators, which are an improvement over Eqs. (57) and (58), to second order in the hybridization integrals. Complications arise, however, because both Hubbard subbands appear explicitly in the original Eq. (56) for the p-band operators, so that the new set of equations for the D operators is now not only coupled in the layers, but also in the Hubbard subbands. While the diagonalization of the resulting 8×8 matrix would be straightforward, it would undoubtedly be difficult to write a meaningful expression for the modified narrow-band gap, as our refined calculations for the one-layer problem have convinced us.

We therefore continue to use our simplifying assumption, which consisted of neglecting Hubbard subband coupling in arriving at Eqs. (57) and (58), thereby reducing the problem to the diagonalization of a 4×4 matrix resulting from the coupled layers. Then, making use of the assumption of layer independence of Eqs. (47)–(55), which allowed us to write a meaningful expression for the p-band gap, Eq. (106), we obtain the modification to the energies given by Eq. (104), namely,

$$\tilde{E}^{\,\mathrm{mod}}_{\mathbf{k}\mu}=E^d_{\mathbf{k}\mu}+(h_{\mathbf{k}}+h'_{\mathbf{k}})^2\frac{N^{\mu}_{\mathbf{k}}}{\mathcal{E}^2_{\mathbf{k}}}\frac{1}{\bar{E}^{\,+}_{\mathbf{k}\mu}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\ , \tag{108}$$

and the modified effective narrow-band superconductor gap,

$$\bar{\Delta}^{\,d}_{\mathbf{k}\mu}=\tilde{\Delta}^{\,d}_{\mathbf{k}\mu}+\frac{\Lambda(h_{\mathbf{k}}+h'_{\mathbf{k}})^2}{\mathcal{E}_{\mathbf{k}}}\frac{N^{\mu}_{\mathbf{k}}T^{\mu}_{\mathbf{k}}}{\bar{E}^{\,+}_{\mathbf{k}\mu}-\mathcal{E}^{p}_{\mathbf{k}}-\mathcal{E}^{p'}_{\mathbf{k}}}\ . \tag{109}$$

IV. DISCUSSION

Our Hamiltonian is an extension of the one-band and two-layer Hamiltonians[14–17] and the two-band and one-layer Hamiltonian[20] used in recent theoretical investigations of high-temperature superconductors. We have sought to construct a Hamiltonian that is tractable, yet includes the necessary hopping and interaction parameters.

We have noted the importance, as mentioned by several investigators,[9–11] of including the copper and the oxygen bands. We have also noted the potentially crucial role of interlayer coupling[3,4] in enhancing the transition temperatures of these superconducting materials. Accordingly, we have devised a Hamiltonian, given by Eq.

(1), which incorporates these features. Our goal has been to calculate the consequent quasiparticle energies and obtain information about the superconductor gap. Our calculational techniques are based on those developed by Hubbard and Jain,[21] and more recently by Jain, Ramakumar, and Chancey[19–20] for a one-layer and two-band model. Our task has been to extend these calculations to a two-layer and two-band model. The expressions we have obtained for the quasiparticle energies for our two-layer model are complicated, despite our approximations and notational simplifications. These complications are a manifestation of interlayer coupling in the equations of motion.

In order to obtain an understanding of our expressions for the quasiparticle energies and a meaningful expression for the gap, we have assumed that at some instant in time the parameters of the two layers were in phase. We find that the interlayer-interband hopping parameter $h'_{\mathbf{k}}$ contributes to the gap in much the same fashion as the p-d hybridization parameter $h_{\mathbf{k}}$ contributes to the one-layer gap. Our simplified expression, Eq. (100), for the interlayer-interband gap contribution suggests that even if $h_{\mathbf{k}}$ were an order of magnitude larger than $h'_{\mathbf{k}}$, the $h'_{\mathbf{k}}$ contribution to the gap would still be roughly 20% of the $h_{\mathbf{k}}$ contribution, which is not a negligible effect. Consequently, we have inferred the existence of two superconductor gaps in the wide oxygen band, in agreement with the results of Hofmann and co-workers.[15]

We note that even if we had omitted the $h'_{\mathbf{k}}$ terms in our Hamiltonian, the gap term in Eq. (106) would still contain corrections to the one-layer result; this is because $\beta_{\mathbf{k}}$ in Eq. (106) contains the interlayer hopping terms, $\mathcal{E}^{p\prime}_{\mathbf{k}}$ and $\mathcal{E}'_{\mathbf{k}}$, as well as the interlayer coupling, U'.

Relatively speaking, the gap equation (106) for this two-layer model is no more complicated than its one-layer counterpart, since it does not explicitly depend on Λ'; this was alluded to, following Eq. (103). Mathematically, the reason for the absence of the explicit appearance of such a term in Eq. (106) is that the Hubbard operators $d^{\alpha}_{ri\sigma}$ are purely intralayer operators. From a more physical viewpoint, the absence of such a term in Eq. (106) is, in our opinion, due to the fact that our model employs the two-dimensional one-layer Hubbard Hamiltonian, applied to each layer separately, plus intralayer and interlayer extensions. The rationale for such a feature in our model is, of course, the physical existence of these layers in high-T_c materials; to a great extent, this forces us to begin the construction of a model with the consideration of the physics within layer planes.

In the weak-coupling limit, the μ term in the numerator of Eq. (107) for the wide-band gap is approximately equal to the interaction U, as can easily be shown from Eqs. (42) and (49). The intralayer BCS gap for the narrow band then appears explicitly, along with its interlayer counterpart, $U'\Lambda'$, which is already present in Eq. (107). Again in the weak-coupling limit, the difference in the denominators of Eqs. (106) and (109) can be traced to the use of the Hubbard operators (which couple creation and annihilation operators in each band), defined in Eq. (4), and to the approximation methods we have used. We are attempting to extract more information on the relationship between the effective p-band and d-band gaps by examining the expressions for the quasiparticle energies which result from the inclusion of Hubbard subband coupling.

The next logical step in pursuing the work reported in this paper is the self-consistent evaluation of the p-band and d-band gaps and the hole number. The various thermal averages are most readily evaluated with the usual quantum-statistical methods[27] and the Zubarev[22] equations for the various anomalous averages appearing in Eqs. (107) and (109). With the added complexity resulting from the presence of two layers, such calculations amount, at the very least, to a challenging task.

In the spirit of JRC, we neglected V_{pd} and V'_{pd}, the intralayer and interlayer nearest-neighbor interaction terms, respectively, in our Hamiltonian; we, in effect, assumed that they can be taken account of by a renormalization of the overlap integrals. However, in the light of the crucial role played by nearest- and next-nearest-neighbor interactions in one layer,[4,10] we might have underestimated the importance of retaining such interaction terms. While we could approach the calculation of the quasiparticle energies, with the inclusion of these terms in the Hamiltonian, in the same manner as reported here, we have no indication at the outset that the linearized equations of motion can be decoupled to yield tractable expressions for the superconducting gaps.[28] Furthermore, we can be sure that a self-consistent calculation of these gaps would be even more laborious. To a first approximation, one could use existing self-consistent gap equations[19] for the narrow band as a starting point in an evaluation of the wideband gap function.

Note added in proof. Equations (99), (106), (108), and (109) in this paper correspond to the one-layer equations (26), (25), (28), and (29), respectively, in Ref. 20.

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