Superconducting correlations in the two-band Hubbard model

K. P. Jain and R. Ramakumar
Laser Technology Research Programme, Department of Physics, Indian Institute of Technology, New Delhi, India 110016

C. C. Chancey
Department of Physics, Amherst College, Amherst, Massachusetts 01002
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A theoretical study of superconducting correlations in the two-band Hubbard model, corresponding to a narrow copper d band hybridized with a wide oxygen p band, is presented. Assuming that direct superconducting correlations have finite amplitude only in the narrow band, we have applied Hubbard-like decoupling approximations in deriving a generalized superconducting gap function for indirect singlet pairing in the oxygen band. We find this gap to be second order in the hybridization. This gap function interpolates between the weak-coupling (BCS) limit and the intermediate-interaction regime. In the intermediate regime, the gap function scales as the bandwidth of the correlated narrow copper d band. The magnitude of the gap increases with narrow band filling, and our analysis indicates a maximum value in the region of half filling.

INTRODUCTION

There exists a wide body of experimental evidence that indicates that holes induced by doping a high-T_c material are primarily of O($2p$) character.[1] This seems to suggest that pairing of oxygen holes may be the dominant mechanism for high-temperature superconductivity. A theoretical framework for the pairing of p holes in the oxygen band was first proposed by Emery.[2] He invoked a two-band Hamiltonian in which hybridization between the p and d bands played the key role and assumed that pairing was mediated by strong coupling to local spin configurations on the copper sites. The importance of oxygen bands also has been discussed by Varma *et al.*,[3] who have invoked charge-transfer excitations as the elementary excitations necessary for superconductivity. This approach has been emphasized recently by Chakraverty *et al.*[4] in a comprehensive review article. They conclude that the insulating cuprate oxides with a highly localized network of copper d spins ($3d^9$) are charge-transfer insulators; real-space pairing between oxygen holes leads to high-temperature superconductivity.

The basic model for investigating superconductive correlations in narrow-band systems is the Hubbard model. In particular, the one-band Hubbard model with an on-site attractive interaction has been studied extensively by a number of authors. Robasckiewicz *et al.*[5] have analyzed this model using a Hartree-Fock (HF) mean-field approach [and assuming a three-dimensional (3D) band structure] to obtain a phase diagram which is a function of both an on-site interaction (I) and an intersite interaction (V). They found that the ground state exhibits superconducting order for $I<0$ and $V<0$, independent of the band filling. (Various other phases also occur depending on the values of I and V.) Micnas *et al.*,[6] assuming weak coupling, have demonstrated a similar dependence for the ground state of the 2D system. Granted this interest in one-band models, it must be admitted that more realistic models must address the existence of two bands in the high-T_c materials: a narrow copper d band hybridized with a wider oxygen p band. Such a two-band model was first studied by Robasckiewicz *et al.*[7] in an attempt to understand small bipolaronic superconductivity in narrow-band systems. In their model, an attractive on-site interaction ($I<0$) arises as a result of the strong coupling between narrow-band electrons and lattice deformations; the phonon coupling to wide-band electrons is small in comparison and is neglected. Their model assumes the strong-coupling limit ($|I|$ much greater than the narrow bandwidth) to achieve small bipolaron formation; these charged bosons induce pairings in the wider band through hybridization. Detailed phase diagrams have been obtained in this limit.[7]

Electron pairing in the Hubbard narrow-energy-band model has been considered recently by the present authors.[8–10] In that work, an approximate expression is derived for the generalized energy gap function, $\Delta_{k\mu}$, for a system of interacting electrons in a narrow s band. This function has the virtue that it interpolates between the weak-interaction (BCS) limit and the intermediate-coupling regime and in doing this tracks the build up of pairing correlations in the order parameter beyond the weak-coupling regime.

Our purpose in this paper is to investigate the possibility of superconductivity in a system consisting of a wide band hybridized with a narrow band in which attractive electron (hole) pairing correlations exist. Applied to the high-T_c systems, the relevant bands are the oxygen p band and the copper d band. That attractive correlations in a narrow d band can arise by way of several physical mechanisms (polaronic, excitonic, plasmonic) underscores the generality of our starting model. Our principal aim will be to study the buildup of pairing correlations as the coupling progresses from weak to intermediate strength (from $|I| \ll W$ to $|I| \approx W$, where W is the bandwidth of the narrow band). Assuming that direct pairing

correlations have finite amplitude in only the narrow band and applying Hubbard-like decoupling approximations, we have derived a generalized gap function for hybridization-induced pairing of carriers in the wide band. This gap function reduces to a BCS-like result in the weak-coupling limit and is proportional to W in the intermediate-coupling regime.

Park *et al.*[11] have performed a local-density approximation band-structure calculation and find the O $2p$ bandwidth to be about 5 eV. Their estimate is supported by the analysis of Eskes, Tjeng, and Sawatzky,[1] in which the effects of correlation, multiplet structure, and hybridization on the electronic structure of the high-T_c compounds are considered. Sawatzky, in a recent review,[12] has emphasized the narrowness (about 1 eV) of the highly correlated Cu d band in these materials and has estimated the $t(p-d)$ matrix element as about 2.5 eV [$T_{p-d}(b_1)$ in Sawatzky]. Experimental studies like photo electron spectroscopy, core level x-ray photon spectroscopy, Auger spectroscopy, and x-ray absorption[13–16] provide estimates of the charge-transfer energy and U_{dd} energy of about 3 and 9 eV, respectively. The large value for U_{dd} and the relatively small charge-transfer gap make it reasonable to restrict our attention, in the first analysis, to a single narrow Cu d subband and a wider O $2p$ band. As a calculational aid, we shall restrict our analysis to considering the hybridization as a perturbation.

Current experimental estimates[17] of the parameter $k_F\xi_0$ (k_F, the Fermi wave vector; ξ_0, the coherence length) in the high-T_c materials support the relevance of analyses which include intermediate coupling strengths. For $YBa_2Cu_3O_7$, estimates for $k_F\xi_0$ vary from 5 to 10, while for $La_{1.85}Sr_{0.15}CuO_4$ the values range from 10 to 20. These numbers suggest that the high-T_c superconductors are in the intermediate interaction regime rather than the Cooper pairing or Bose limits ($k_F\xi_0 \ll 1$ and $k_F\xi_0 \gg 1$, respectively). Our investigation of superconducting correlations in the weak- to intermediate-coupling region should thus be of considerable interest.

THE HAMILTONIAN AND THE GENERALIZED GAP FUNCTIONS

We begin by writing a two-band Hubbard Hamiltonian for electrons (holes) in p and d bands as[4]

$$H = H_d + H_p + H_{pd} \ , \tag{1}$$

where H_d and H_p are Hamiltonians for electrons in d and p bands, respectively, and H_{pd} is an interaction term. Specifically,

$$H_d = \sum_{i\sigma} \varepsilon_d n_{i\sigma} + \sum_{\substack{ij \\ \sigma}} T_{ij}^d c_{i\sigma}^\dagger c_{j\sigma} + I \sum_i n_{i\uparrow} n_{i\downarrow} \ , \tag{2}$$

$$H_p = \sum_{i\sigma} \varepsilon_p n_{i\sigma}^p + \sum_{\substack{ij \\ \sigma}} T_{ij}^p p_{i\sigma}^\dagger p_{j\sigma} \ , \tag{3}$$

and

$$H_{pd} = \sum_{\substack{ij \\ \sigma}} h_{ij} (p_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger p_{i\sigma}) + V_{pd} \sum_{ij} \sum_{\sigma\sigma'} n_{i\sigma} n_{j\sigma'}^p \ . \tag{4}$$

In the preceding equations $c_i^\dagger$ (c_i) and $p_j^\dagger$ (p_j) are operators that create (destroy), respectively, an electron on copper site i and oxygen site j; ε_d and ε_p are the center-of-mass energies of the copper and oxygen bands and h_{ij} is the hybridization overlap integral between Cu and O nearest-neighbor sites. The function V_{pd} represents a Coulomb repulsion between two electrons on neighboring Cu and O sites, and $n_{i\sigma}^p = p_{i\sigma}^\dagger p_{i\sigma}$ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ are the appropriate number operators.

We introduce the $d_{i\sigma}^\alpha$ operators, following Refs. 5 and 18,

$$d_{i\sigma}^\alpha = n_{i,-\sigma}^\alpha c_{i\sigma} \ , \tag{5}$$

where $n_{i\sigma}^+ - n_{i\sigma}$ and $n_{i\sigma}^- = 1 - n_{i\sigma}$, and $\alpha = \pm$.

To obtain a first approximation for the equation of motion for $d_{i\sigma}^\alpha$ we begin by setting $V_{pd} = 0$. The resulting equation is

$$\begin{aligned} i\dot{d}_{i\sigma}^{\ \alpha} = {} & \varepsilon_\alpha d_{i\sigma}^\alpha + \sum_{j \neq i} T_{ij}^d n_{i,-\sigma}^\alpha c_{j\sigma} + \xi^\alpha S_{i,-\sigma} c_{i\sigma} \\ & - \sum_j h_{ij} [\xi^\alpha (p_{j,-\sigma}^\dagger c_{i,-\sigma} c_{i\sigma} + c_{i,-\sigma}^\dagger c_{i\sigma} p_{j,-\sigma}) \\ & - n_{i,-\sigma}^\alpha p_{j\sigma}] \ , \end{aligned} \tag{6}$$

where

$$\begin{aligned} & S_{i,+\sigma} = \sum_{j \neq i} T_{ij}^d (c_{i\sigma}^\dagger c_{j\sigma} - c_{j\sigma}^\dagger c_{i\sigma}) \ ; \\ & \varepsilon_+ = I + \varepsilon_d; \quad \varepsilon_- = \varepsilon_d; \quad \xi^+ = -\xi^- = 1 \ . \end{aligned} \tag{7}$$

The analogous Heisenberg equation of motion for $p_{i\sigma}$ is

$$i\dot{p}_{i\sigma} = \varepsilon_p p_{i\sigma} + \sum_{k \neq i} T_{ki}^p p_{k\sigma} + 2 \sum_j h_{ij} c_{j\sigma} \ . \tag{8}$$

Solutions of the coupled Eqs. (6) and (8) will lead to generalized gap functions for pairing in both the p and d bands. We shall carry out a derivation for the approximate p-band energy gap Δ_k^p treating the hybridization as a perturbation. Following this, we obtain the analogous generalized energy gap function for pairing in the d band, $\Delta_{k\mu}^d$, using the same approximation.

We begin our derivation for Δ_k^p by linearizing so as to keep terms linear in $n_{i\sigma}$, $c_{i\sigma}$, and $p_{i\sigma}$. In doing this we neglect all terms involving combinations of these three operators, thus limiting the heirarchy of the equations of motion. Doing this we obtain,

$$\begin{aligned} & p_{j,-\sigma}^\dagger c_{i,-\sigma} c_{i\sigma} \approx \langle c_{i,-\sigma} c_{i\sigma} \rangle p_{j,-\sigma}^\dagger + \langle p_{j,-\sigma}^\dagger c_{i,-\sigma} \rangle c_{i\sigma} \ , \\ & n_{i,-\sigma}^\alpha p_{j\sigma} \approx \langle n_{i,-\sigma}^\alpha \rangle p_{j\sigma} \ , \end{aligned}$$

and

$$c_{i,-\sigma}^\dagger c_{i\sigma} p_{j,-\sigma} \approx -\langle c_{i,-\sigma}^\dagger p_{j,-\sigma} \rangle c_{i\sigma} \ .$$

Following the same mean-field approximations for $n^{\alpha}_{i,-\sigma}c_{i\sigma}$ and $S_{i,-\sigma}c_{i\sigma'}$ given in Refs. 9 and 18, we have in addition the following:

$$n^{\alpha}_{i,-\sigma}c_{j\sigma}\approx\langle n^{\alpha}_{i,-\sigma}\rangle c_{j\sigma}+\xi^{\alpha}\langle c_{i,-\sigma}c_{j\sigma}\rangle c^{\dagger}_{i,-\sigma}\ ,$$

$$S_{i,-\sigma}c_{i\sigma}\approx\langle S_{i,-\sigma}\rangle c_{i\sigma}+\sum_{j\neq i}\langle c_{j,-\sigma}c_{i\sigma}\rangle T_{ij}c^{\dagger}_{i,-\sigma}-\sum_{j\neq i}\langle c_{i,-\sigma}c_{i\sigma}\rangle T_{ij}c^{\dagger}_{j,-\sigma}\ .$$

In the absence of hybridization, the d-band Hamiltonian leads to two energy levels which in the atomic limit are separated by I. In the band limit these levels spread out to form two bands whose centers are separated by energy I. The preceding approximations introduced correctly lead to these Hubbard band energies and thus extend our analysis beyond that obtainable through the usual Hartree-Fock mean-field approach. In using the preceding approximations, we have not considered spin-flip or singlet Kondo-type terms. Further, it should be noted that we have neglected fluctuations in any of the order parameters. Inclusion of fluctuations in the spin-order parameter is straightforward in the weak-coupling regime.[17] However, in the intermediate-coupling region the equations become quite complicated.

The decoupling approximations just outlined can lead to erroneous conclusions when applied in the strong interaction limit ($|I|\gg W$). This is because they do not represent the case of a Heisenberg antiferromagnet for the condition of a half-filled band. It can be shown, however,[19] that a more sophisticated decoupling scheme does lead to a result which is correct to order (W/I) in the strong-coupling regime (for example, in calculating the energy of the lower Hubbard subband[20]). This latter point is amplified by Harris and Lange[21] who have discussed the conditions necessary for ferromagnetism in the case of a nearly half-filled band.[22] Negative spectral weights, which can arise from decoupling approximations such as are used here, again are a problem only in the strong-coupling limit. Our analysis is limited to the weak- and intermediate-coupling regions and should thus be unaffected.

Applying the decoupling approximations, Eq. (6) reduces to

$$i\dot{d}^{\alpha}_{i\sigma}=\varepsilon_{\alpha}d^{\alpha}_{i\sigma}+\sum_{j\neq i}T_{ij}\langle n^{\alpha}_{i,-\sigma}\rangle c_{j\sigma}+\xi^{\alpha}\sum_{j\neq i}Y_{ij}c^{\dagger}_{i,-\sigma}+\xi^{\alpha}Z_{i,-\sigma}c_{i\sigma}+\lambda\xi^{\alpha}\sum_{j}T_{ij}c^{\dagger}_{j,-\sigma}+\sum_{j}h_{ij}(\langle n^{\alpha}_{i,-\sigma}\rangle p_{j\sigma}+\lambda\xi^{\alpha}p^{\dagger}_{j,-\sigma})\ , \tag{9}$$

where

$$\lambda=-\langle c_{i,-\sigma}c_{i\sigma}\rangle\ , \tag{10}$$

$$Y_{ij}=T_{ij}(\langle c_{i,-\sigma}c_{j\sigma}\rangle+\langle c_{j,-\sigma}c_{i\sigma}\rangle)\ , \tag{11}$$

$$Z_{i,-\sigma}=\langle S_{i,-\sigma}\rangle-\sum_{j}h_{ij}(\langle p^{\dagger}_{j,-\sigma}c_{i,-\sigma}\rangle-\langle c^{\dagger}_{i,-\sigma}p_{j,-\sigma}\rangle)\ . \tag{12}$$

As Hubbard and Jain[18] have shown,

$$\langle n^{\alpha}_{i\sigma}\rangle\approx n_{\alpha}+O(\delta n)\ ,$$

where $n_{+}=n$ and $n_{-}=1-n$, while $\langle S_{i\sigma}\rangle\approx O(\delta S)$. Here n is defined to be the number of electrons (holes) of spin σ at site i, assuming the paramagnetic case: $\langle n_{i\uparrow}\rangle=\langle n_{i\downarrow}\rangle=n$. Both δn and δS are of order h and thus may be neglected in the first approximation. Fourier transforming we get

$$i\dot{d}^{\alpha}_{k\sigma}=\varepsilon_{\alpha}d^{\alpha}_{k\sigma}+(n_{\alpha}\varepsilon_{k}+\xi^{\alpha}Z_{k,-\sigma})c_{k\sigma}+\xi^{\alpha}(\lambda\varepsilon_{k}+2\tilde{\varepsilon}_{0})c^{\dagger}_{-k,-\sigma}+n^{\alpha}h_{k}p_{k\sigma}+\xi^{\alpha}\lambda h_{k}p^{\dagger}_{-k,-\sigma}\ , \tag{13}$$

where $\tilde{\varepsilon}_{0}=\sum_{k}\varepsilon^{d}_{k}\Lambda_{-k}$ and $\Lambda_{-k}=\langle c_{-k,-\sigma}c_{k\sigma}\rangle$. Here h_{k} is the Fourier transform of the hybridization matrix element h_{ij}, and $\lambda=-\sum_{k}\Lambda_{-k}$. The last two terms on the right-hand side of Eq. (13) contain the effects of hybridization in terms of h_{k}. An analogous expression for the equation of motion for $p_{k\sigma}$ is

$$i\dot{p}_{k\sigma}=\varepsilon^{p}_{k}p_{k\sigma}-h_{k}c_{k\sigma}\ . \tag{14}$$

Equations (13) and (14) form a simultaneous pair of differential equations.

We now introduce the Hubbard subband destruction operators $D^{\mu}_{k\sigma}$ ($\mu=1,2$) to describe correlation of electrons in the d band.[18] As previously defined in terms of $d^{\alpha}_{k\sigma}$,

$$D^{\mu}_{k\sigma}=\frac{N_{k\mu}}{\varepsilon^{d}_{k}}\left[\frac{d^{+}_{k\sigma}}{(E_{k\mu}-I)}+\frac{d^{-}_{k\sigma}}{E_{k\mu}}\right]\ , \tag{15}$$

where E_{k1} and E_{k2} are the energies of the upper and lower Hubbard subbands, respectively:

$$E_{k\mu}=\tfrac{1}{2}(I+\varepsilon^{d}_{k})+\tfrac{1}{2}(-1)^{\mu+1}[(I-\varepsilon^{d}_{k})^{2}+4nI\varepsilon^{d}_{k}]^{1/2}\ .$$

Using the $D^{\mu}_{k\sigma}$, Eq. (13) becomes

$$i\dot{D}^{\mu}_{k\sigma}=\tilde{E}_{k\mu}D^{\mu}_{k\sigma}+\Delta^{d}_{k\mu}D^{\dagger\mu}_{-k,-\sigma}+N_{k\mu}h_{k}(\varepsilon^{d}_{k})^{-2}p_{k\sigma}+N_{k\mu}(\varepsilon^{d}_{k})^{-1}T_{k\mu}h_{k}\lambda p^{\dagger}_{-k,-\sigma}\ , \tag{16}$$

where

$$T_{k\mu}=\frac{I}{E_{k\mu}(E_{k\mu}-I)}\ , \tag{17}$$

$$\tilde{E}_{k\mu}=E_{k\mu}+Z_{k,-\sigma}\ , \tag{18}$$

and

$$\Delta^{d}_{k\mu}=\left[\lambda+\frac{2\tilde{\varepsilon}_{0}}{\varepsilon^{d}_{k}}\right]T_{k\mu}N_{k\mu} \tag{19}$$

with

$$N_{k\mu}=\left[\frac{n}{(E_{k\mu}-I)^{2}}+\frac{1-n}{(E_{k\mu})^{2}}\right]^{-1}\ .$$

Equation (16), as expressed, neglects the pairing of elec-

trons in different Hubbard subbands. Similarly, Eq. (14) gives

$$i\dot{p}_{k\sigma}=\varepsilon_k^p p_{k\sigma}+h_k(D_{k\sigma}^1+D_{k\sigma}^2)\ . \tag{20}$$

The approximate solution of the two simultaneous equations, (16) and (20), is outlined in Appendix A. Using Eq. (A6) and writing the time dependence of the oxygen band operators as

$$p_{k\sigma}(t)=\exp(-i\varepsilon_k^p t)p_{k\sigma}(0) \tag{21}$$

allows us to give an approximate equation of motion for the $p_{k\sigma}(t)$ which involves only the oxygen band operators explicitly:

$$\dot{p}_{k\sigma}(t)+i(\varepsilon_k^p-\alpha_k h_k^2)p_{k\sigma}(t)+i\beta_k h_k^2 p^{\dagger}_{-k,-\sigma}$$
$$=-i\sum_{\mu}[h_k e^{-i\bar{E}_{k\mu}t}D_{k\sigma}^{\mu}(0)+i\alpha_k h_k^2 e^{-i\bar{E}_{k\mu}t}p_{k\sigma}(0)$$
$$-i\beta_k h_k^2 e^{-i\bar{E}_{k\mu}t}p^{\dagger}_{-k,-\sigma}(0)]\ , \tag{22}$$

where

$$\alpha_k=(\varepsilon_k^d)^{-2}\sum_{\mu}\frac{N_{k\mu}}{\bar{E}_{k\mu}-\varepsilon_k^p} \tag{23}$$

and

$$\beta_k=-\lambda(\varepsilon_k^d)^{-1}\sum_{\mu}\frac{N_{k\mu}T_{k\mu}}{\bar{E}_{k\mu}+\varepsilon_k^p}\ . \tag{24}$$

Equation (22) is the effective equation of motion for p-band electrons, and it enables us to define a new generalized gap equation for p-band superconducting pairing, due to p-d hybridization, as

$$\Delta_k^p=-\lambda h_k^2\sum_{\mu}\frac{(\varepsilon_k^d)^{-1}N_{k\mu}T_{k\mu}}{\bar{E}_{k\mu}+\bar{\varepsilon}_k^p}\ , \tag{25}$$

where the corresponding quasiparticle energies are

$$E_k^p=[(\varepsilon_k^p-\alpha_k h_k^2)^2+(\Delta_k^p)^2]^{1/2}\ . \tag{26}$$

Looking at Eq. (25) we note that $\Delta_k^p\to 0$ as $h_k\to 0$, underlining our assumption that pairing in the p band is a result of p-d hybridization. Furthermore, $N_{k\mu}T_{k\mu}\approx I$ for $I\approx 0$ so that $\Delta_k^p\to 0$ as $I\to 0$, emphasizing the importance of correlation in our model. The possibility of superconductivity due to electron-electron correlations in the p bands is expected to be small due to the weakness of the correlation and has been neglected.

It is appropriate to point out that by using an analogous method to that adopted in Appendix A in solving for $D_{k\sigma}^{\mu}(t)$, one can approximately solve Eq. (20) for $p_{k\sigma}(t)$ first. Substituting this result into Eq. (16) gives an effective equation of motion for electrons in the d band:

$$i\dot{D}^{\mu}_{k\sigma}(t)-\bar{\bar{E}}_{k\mu}D_{k\sigma}^{\mu\dagger}(t)-\alpha_{k\mu}h_k^2 D^{\mu}_{-k,-\sigma}(t)$$
$$=-A_{\mu}h_k\sum_{\nu}\frac{e^{-i\varepsilon_k^p}D_{k\sigma}^{\nu}(0)}{\bar{E}_{k\nu}-\varepsilon_k^p}$$
$$-B_{\mu}h_k\sum_{\nu}\frac{e^{i\varepsilon_k^p}D^{\nu\dagger}_{-k,-\sigma}(0)}{\bar{E}_{k\nu}-\varepsilon_k^p}$$
$$+A_{\mu}e^{-i\varepsilon_k^p}p_{k\sigma}(0)+B_{\mu}h_k e^{i\varepsilon_k^p}p_{-k,-\sigma}(0)\ , \tag{27}$$

where

$$\bar{\bar{E}}_{k\mu}=\tilde{E}_{k\mu}+[\varepsilon_k^d]^{-2}N_{k\mu}h_k^2\sum_{\nu}\frac{1}{\bar{E}_{k\nu}-\varepsilon_k^p} \tag{28}$$

with

$$A_{\mu}=N_{k\mu}h_k(\varepsilon_k^d)^{-2}$$

and

$$B_{\mu}=\lambda N_{k\mu}T_{k\mu}h_k(\varepsilon_k^d)^{-1}\ .$$

From this we can write an expression for the generalized gap function for electrons in the d band, modified by the hybridization:

$$\bar{\Delta}^d_{k\mu}=\Delta^d_{k\mu}+\lambda h_k^2(\varepsilon_k^d)^{-1}\sum_{\nu}\frac{N_{k\mu}T_{k\mu}}{\bar{E}_{k\nu}-\varepsilon_k^p}\ . \tag{29}$$

where

$$\bar{E}_{k\mu}=[(\tilde{E}_{k\mu})^2+(\Delta^d_{k\mu})^2]^{1/2}$$

are the quasiparticle energies, including the effects of hybridization, as given in Appendix A. Equations (25) and (29) are the main results of this paper; in the remainder we will discuss the characteristics of the energy gaps. Thus far, we have made use of several energies: $E_{k\mu}$, $\tilde{E}_{k\mu}$, and $\bar{E}_{k\mu}$. For clarity we now review their differences. The energies $E_{k\mu}$ are the Hubbard subband energies; modifying them so as to include the hybridization produces the $\tilde{E}_{k\mu}$ and the related energies $\bar{\bar{E}}_{k\mu}$. The energies $\bar{E}_{k\mu}$ are the quasiparticle energies due to pairing of electrons (holes) in the d band, including the effects of hybridization. Note that as $h_k\to 0$ or $I\to 0$, then $\bar{\Delta}^d_{k\mu}$ reduces to $\Delta^d_{k\mu}$ as expected since the two bands completely decouple.

Expressing λ in terms of the destruction operators of the d-band electrons, as shown in Appendix B, allows us to reexpress the generalized gap in the p band, Eq. (25), as

$$\Delta_k^p=-h_k^2\sum_{\mu}\sum_{\nu k'}\frac{N_{k\mu}T_{k\mu}(\varepsilon_k^d)^{-1}}{[(\tilde{E}_{k\mu})^2+(\Delta^d_{k\mu})^2]^{1/2}+\varepsilon_k^p}$$
$$\times\left|(\varepsilon_{k'}^d)^{-2}N_{k'\nu}\frac{\Delta^d_{k'\nu}}{\tilde{\bar{E}}_{k'\nu}}[f(\tilde{\bar{E}}_{k'\nu})-f(-\tilde{\bar{E}}_{k'\nu})]\right|, \tag{30}$$

where the thermal averages have been taken from Appendix B and

$$\tilde{\bar{E}}_{k\mu}=[(\bar{\bar{E}}_{k\mu})^2+(\bar{\Delta}^d_{k\mu})^2]^{1/2}\ . \tag{31}$$

The corresponding gap for electrons (holes) in the d band is

$$\bar{\Delta}^{d}_{k\mu}=\Delta^{d}_{k\mu}+h_k^2\sum_{k'\nu}\sum_{\nu'}\frac{(\varepsilon^{d}_{k})^{-1}N_{k\mu}T_{k\mu}(\varepsilon^{d}_{k'})^{-2}N_{k'\nu}}{[(\tilde{E}_{k\nu'})^2+(\Delta^{d}_{k\nu'})^2]^{1/2}-\varepsilon^{p}_{k}}\frac{1}{2}\frac{\Delta^{d}_{k'\nu}}{\tilde{\tilde{E}}_{k'\nu}}[f(\tilde{\tilde{E}}_{k'\nu})-f(-\tilde{\tilde{E}}_{k'\nu})]\ . \tag{32}$$

The number of electrons (holes) is given by

$$N=2n=\frac{1}{2}\sum_{k\sigma\mu}\sum(\varepsilon^{d}_{k})^{-2}N_{k\mu}\left[\left[1+\frac{\tilde{\bar{E}}_{k\mu}}{\tilde{\tilde{E}}_{k\mu}}\right]f(\tilde{\tilde{E}}_{k\mu})+\left[1-\frac{\tilde{\bar{E}}_{k\mu}}{\tilde{\tilde{E}}_{k\mu}}\right]f(-\tilde{\tilde{E}}_{k\mu})\right]$$
$$+\frac{1}{2}\sum_{k}\left[\left[1+\frac{(\varepsilon^{p}_{k}-\alpha_k h_k^2)}{E^{p}_{k}}\right]f(E^{p}_{k})+\left[1-\frac{(\varepsilon^{p}_{k}-\alpha_k h_k^2)}{E^{p}_{k}}\right]f(-E^{p}_{k})\right]\ . \tag{33}$$

Equations (30), (32), and (33) must be solved self-consistently for Δ^{p}_{k}, $\bar{\Delta}^{d}_{k\mu}$, and N.

The generalized gap function for the p band shows that the pairing of the wide p-band electrons (holes) occurs indirectly through hybridization with the narrow band (where pairing correlations exist). The basic idea is that narrow-band electron pairs will induce pairing among wide-band electrons through hybridization; as a consequence, a superconducting energy gap appears in the single-particle spectrum of the wide-band electrons. The gap function for the p band, (30), is directly related to the gap function for the narrow d band, where pairing correlations are assumed to have finite amplitude. Naturally, this indirect pairing in the p band is second order in the hybridization matrix element. These gap functions are quite general in that they are representative of any mechanism which can lead to attractive correlations in the narrow band. Although we have assumed that there is no direct pairing in the p band, it would be straightforward, however, to introduce a weak phonon-assisted pairing in the p band in our theory.

Modification of the direct d-band pairing amplitude as a result of hybridization leads to the new gap $\bar{\Delta}^{d}_{k\mu}$. Using the p-band gap function, we can infer its dependence on the particle number $n=n_p+n_d$. For a fixed n, increasing n_d will lead to an increase in the magnitude of the p-band gap since more narrow-band electron pairs will be able to induce pairing in the wide band. For $n_d=0$ or 2, pairing in the p band will be zero since in the first case no pairs exist in the narrow band while in the second case the narrow band is completely filled.

Until now the interaction V_{pd} has been neglected. The simplest mean-field theory approximation to this term is

$$V_{pd}\sum_{ij}\sum_{\sigma\sigma'}c^{\dagger}_{i\sigma}c_{i\sigma}p^{\dagger}_{j\sigma'}p_{j\sigma'}\approx V_{pd}\sum_{ij}\sum_{\sigma\sigma'}(c^{\dagger}_{i\sigma}c_{i\sigma}\langle p^{\dagger}_{j\sigma'}p_{j\sigma'}\rangle+\langle c^{\dagger}_{i\sigma}c_{i\sigma}\rangle p^{\dagger}_{j\sigma'}p_{j\sigma'}-c^{\dagger}_{i\sigma}p_{j\sigma'}\langle c_{i\sigma}p^{\dagger}_{j\sigma'}\rangle-\langle c^{\dagger}_{i\sigma}p_{j\sigma'}\rangle c_{i\sigma}p^{\dagger}_{j\sigma'}+\langle c^{\dagger}_{i\sigma}c_{i\sigma}\rangle)\ , \tag{34}$$

where terms of the form $\langle c^{\dagger}_{i\sigma}p^{\dagger}_{j\sigma'}\rangle$ and $\langle c_{i\sigma}p_{j\sigma'}\rangle$ corresponding to p-d singlet (Kondo-type) superconductivity have been neglected. The terms corresponding to $\langle c^{\dagger}_{i\sigma}c_{i\sigma}\rangle$ and $\langle p^{\dagger}_{j\sigma}p_{j\sigma}\rangle$ can be absorbed into a modification of ε_d and ε_p in the original expression for the Hamiltonian given in Eqs. (1)–(4). Those of the form $\langle c^{\dagger}_{i\sigma}p_{j\sigma'}\rangle=\langle c_{i\sigma}p^{\dagger}_{j\sigma'}\rangle\approx O(h_{ij})$ when $\sigma'=\sigma$; consequently, they can be amalgamated into the hybridization integral. The $\sigma\neq\sigma'$ terms represent spin-flip interactions which have been previously neglected in our approximations. Therefore, in this approximation all our previous results can be carried over by an appropriate redefinition of ε_d, ε_p, and h_{ij}.

PROPERTIES OF THE GENERALIZED GAP FUNCTION

Consider the generalized gap function for pairing of electrons (holes) in the p band as given by Eq. (25). In the weak interaction limit ($I\ll W$), $N_{k1}T_{k1}\approx I$ and $N_{k2}T_{k2}\approx 0$ so that $\Delta^{d}_{k1}\approx I(\lambda+2\tilde{\varepsilon}_0/\varepsilon^{d}_{k})$ and $\Delta^{d}_{k2}\approx 0$. Substituting these into Eq. (25) gives

$$\Delta^{p}_{k}=\frac{h_k^2 I\lambda}{[(\tilde{E}_{k1})^2+(\Delta^{d}_{k1})^2]^{1/2}+\varepsilon^{p}_{k}}\frac{1}{\varepsilon^{d}_{k}}\ , \tag{35}$$

where in this limit, $E_{k1}=\varepsilon^{d}_{k}+Z_{k,-\sigma}$ using Eq. (18). Equation (35) consists of a product of two terms: $I\lambda$ which is the BCS gap and a prefactor which has a complicated dependence on hybridization. We note that $\Delta^{p}_{k}\to 0$, as $h_k\to 0$ and as $I\to 0$, as expected. In the intermediate interaction regime ($I\approx W$), $0\le E_{k1}\le O(\varepsilon_k)$ and $-W\le E_{k2}\le -W+O(\varepsilon_k)$, which leads to

$$\Delta^{d}_{k1}=-\Delta^{d}_{k2}=-(\lambda+\tilde{\varepsilon}_0/\varepsilon_k)O(W)\ ,$$

so that

$$\Delta^{p}_{k}=-h_k^2\frac{\lambda}{\varepsilon^{d}_{k}}\left[\frac{1}{[\tilde{E}^{\,2}_{k1}+(\Delta^{d}_{k1})^2]^{1/2}+\varepsilon^{p}_{k}}-\frac{1}{[\tilde{E}^{\,2}_{k2}+(\Delta^{d}_{k2})^2]^{1/2}+\varepsilon^{p}_{k}}\right]O(W)\ , \tag{36}$$

where

$$\tilde{E}_{k\mu}=E_{k\mu}+X+Z_{k,-\sigma}\ . \tag{37}$$

In the dilute limit when the number of electrons (holes), $2n$, is small and $T_{k\mu}N_{k\mu}=\xi^{\mu}I_{\text{eff}}$, where

$$I_{\text{eff}}=\left[\frac{I}{1-I/W}\right]\ . \tag{38}$$

Then, since $E_{k1}=\varepsilon^{d}_{k}$ and $E_{k2}=I$ and

$$\Delta^d_{k\mu}=(\lambda+2\tilde{\varepsilon}_0/\varepsilon^d_k)\xi^\mu I_{\rm eff}\ ,$$

one gets

$$\Delta^p_k=-h^2_k(\varepsilon^d_k)^{-1}\lambda I_{\rm eff}\left[\frac{1}{[\tilde{E}^{\,2}_{k1}+(\Delta^d_{k1})^2]^{1/2}+\varepsilon^p_k}-\frac{1}{[\tilde{E}^{\,2}_{k2}+(\Delta^d_{k2})^2]^{1/2}+\varepsilon^p_k}\right], \quad (39)$$

where $E_{k1}=\varepsilon^d_k+O(h)$ and $E_{k2}=I+O(h)$.

CONCLUSIONS

The two-band Hubbard model presented here has invoked hybridization between a narrow copper d band and an uncorrelated oxygen p band as a mechanism for superconducting pairing between oxygen holes. This analysis is valid in any general system which hybridizes wide and narrow bands, and in which direct pairing correlations have finite amplitude only in the narrow band. Many experiments on high-T_c systems, including x-ray absorption,[23] electron-energy-loss spectroscopy,[24] and photoelectron spectroscopic studies,[16] have shown further that doping the Cu-O planes produces essentially no change in the electronic configuration of the copper ions and that holes appear in what are principally the $2p$ levels of oxygen. The appropriateness of including a Cu-O hybridization term has been well borne out by a number of experiments,[25] particularly the photoemission studies on $YBa_2Cu_3O_{6.9}$ by List *et al.*[26] There is also evidence to show that doping produces an increase in density of unoccupied states having d symmetry.[23] This delocalization is a consequence of the hybridization of overlapping p and d bands, which in our model permits pairing in the less than half-filled Cu d band. We also note that for weakly coupled systems ($|I|\ll W$), pairing of holes in O($2p$) states is necessarily weak and the high T_c must be a consequence of strongly correlated d electrons.

In this paper we have derived self-consistent gap and band-filling equations for the two-band Hubbard model. We have assumed superconducting pairing correlations for the narrow Cu d electrons (holes) and have included the additional interaction of Cu-O hybridization. In doing this we have been principally interested in obtaining gap functions which are valid in both the weak- and intermediate-coupling regimes ($|I|\ll W$ and $|I|\approx W$, respectively). The generalized gap functions given in Eqs. (30) and (32) for s-wave pairing in the p and d bands are the principal results of the present work. We have detailed the route through which superconducting pairing correlations in a narrow band indirectly induce pairing in an uncorrelated wide band via hybridization. The gap function for the p band reduces to a BCS-like result in the weak-coupling regime but increases as the correlation strength ($|I|$) is increased. As I becomes larger, pairing correlations beyond the Hartree-Fock (BCS) mean-field regime begin to dominate. They significantly affect the gap structure in the p band through an alteration of the indirect pairing mechanism. The indirect pairing in the p band also shows a strong dependence on the narrow-band filling. The gap increases as the number of narrow-band electrons increases (starting from zero) and appears to reach a maximum near half filling. As stated, our analysis is applicable for any system in which an uncorrelated wide band is hybridized with a narrow band of electrons (holes) in which pairing correlations exist (possibly due to the exchange of plasmons, excitons or medium-sized bipolarons, for example). Our main aim has been to consider the behavior of the pairing functions as the interaction in the narrow band is increased beyond the BCS regime. Recent estimates of the parameter $k_F\xi_0$ (k_F, the Fermi momentum; ξ_0, the coherence length) for high-T_c systems are given as 5–10 for $YBa_2Cu_3O_7$ and about 10–20 for $La_{1.85}Sr_{0.15}CuO_4$.[17] This implies that these systems are neither in the BCS limit ($k_F\xi_0\gg 1$) nor in the strong-coupling Bose limit ($k_F\xi_0\ll 1$), but are rather in an intermediate regime. Since it seems unlikely that there is any but a negligible direct-pairing amplitude for O p holes, we believe that our two-band analysis should be of some interest in understanding the high-T_c superconductors. Numerical, self-consistent solutions of the coupled equations for $\bar{\Delta}^{\,d}_{k1}$, $\bar{\Delta}^{\,d}_{k2}$, Δ^p_k, and N [the band filling, Eq. (33)] are currently underway and are planned to form the topic of a future report.

APPENDIX A

The simultaneous equations to be solved are

$$i\dot{p}_{k\sigma}(t)=\varepsilon^p_k p_{k\sigma}(t)+h_k(D^1_{\mu\sigma}+D^2_{\mu\sigma}) \quad (A1)$$

and

$$i\dot{D}^\mu_{k\sigma}(t)=\tilde{E}_{k\mu}D^\mu_{k\sigma}(t)+\Delta^d_{k\mu}\tilde{D}^{\,\mu\dagger}_{-k,-\sigma}(t)+Ap_{k\sigma}(t)+Bp^\dagger_{-k,-\sigma}(t) \quad (A2)$$

using Eqs. (16) and (20), with

$$A=N_{k\mu}h_k(\varepsilon^d_k)^{-2} \text{ and } B=\lambda N_{k\mu}T_{k\mu}h_k(\varepsilon^d_k)^{-1}\ .$$

We begin our approximate solution by writing

$$i\dot{D}^{\,\mu}_{k\sigma}(t)=\tilde{E}_{k\mu}D^\mu_{k\sigma}(t)+\Delta^d_{k\mu}D^{\mu\dagger}_{-k,-\sigma}(t) \quad (A3)$$

and the analogous equation for $D^{\mu\dagger}_{-k,-\sigma}(t)$. We can solve this simplified system of equations to obtain the quasiparticle energies

$$\bar{E}_{k\mu}=[(E_{k\mu})^2+(\Delta^d_{k\mu})^2]^{1/2}\ .$$

Writing the time dependence of $D^\mu_{k\sigma}(t)$ as

$$D^\mu_{k\sigma}(t)=e^{-i\bar{E}_{k\mu}t}D^\mu_{k\sigma}(t)$$

we can write Eq. (A2) as

$$i\dot{D}^{\,\mu}_{k\sigma}(t)=\bar{E}_{k\mu}\tilde{D}^{\,\mu}_{k\sigma}(t)+Ap_{k\sigma}(t)+Bp^\dagger_{-k,-\sigma}(t)\ . \quad (A4)$$

Multiplying Eq. (A4) by $e^{-i\bar{E}_{k\mu}t}$, we obtain

$$ie^{i\bar{E}_{k\mu}t}\dot{D}^{\,\mu}_{k\sigma}(t)=\bar{E}_{k\mu}e^{i\bar{E}_{k\mu}t}D^\mu_{k\sigma}(t)+Ae^{i\bar{E}_{k\mu}t}p_{k\sigma}(t)+Be^{i\bar{E}_{k\mu}t}p^\dagger_{-k,-\sigma}(t)\ . \quad (A5)$$

The aim now is to express $D^{\mu}_{k\sigma}(t)$ in terms of $p_{k\sigma}(t)$ and $p^{\dagger}_{-k,-\sigma}(t)$. For this purpose we solve Eq. (A1) approximately by neglecting the inhomogeneous part. Then, using the solution of the homogeneous part of Eq. (A1) we have

$$i\frac{d}{dt}[e^{i\bar{E}_{k\mu}t}D^{\mu}_{k\sigma}(t)]=[Ap_{k\sigma}(t)+Bp^{\dagger}_{-k,-\sigma}(t)]e^{i\bar{E}_{k\mu}t}$$
$$=Ae^{i(\bar{E}_{k\mu}-\varepsilon^{p}_{k})t}p_{k\sigma}(0)$$
$$+Be^{i(\bar{E}_{k\mu}+\varepsilon^{p}_{k})t}p^{\dagger}_{-k,-\sigma}(0)\ . \quad \text{(A6)}$$

Equation (A6) can now be integrated to obtain

$$D^{\mu}_{k\sigma}(t)=e^{-i\bar{E}_{k\mu}t}D^{\mu}_{k\sigma}(0)-A\frac{p_{k\sigma}(t)}{\bar{E}_{k\mu}-\varepsilon^{p}_{k}}-B\frac{p^{\dagger}_{-k,-\sigma}(t)}{\bar{E}_{k\mu}+\varepsilon^{p}_{k}}$$
$$+A\frac{e^{-i\bar{E}_{k\mu}t}p_{k\sigma}(0)}{\bar{E}_{k\mu}-\varepsilon^{p}_{k}}+B\frac{e^{-i\bar{E}_{k\mu}t}p^{\dagger}_{-k,-\sigma}(0)}{\bar{E}_{k\mu}+\varepsilon^{p}_{k}}\ . \quad \text{(A7)}$$

In a similar way, $p_{k\sigma}(t)$ can also be expressed in terms of $D^{\mu}_{k\sigma}(t)$. The result is

$$p_{k\sigma}(t)=e^{-\varepsilon^{p}_{k}t}p_{k\sigma}(0)-h_k\sum_{\mu}\frac{e^{-i\bar{E}_{k\mu}t}D^{\mu}_{k\sigma}(0)}{\bar{E}_{k\mu}-\varepsilon^{p}_{k}}$$
$$+h_k\sum_{\mu}\frac{e^{-i\varepsilon^{p}_{k}t}D^{\mu}_{k\sigma}(0)}{\bar{E}_{k\mu}-\varepsilon^{p}_{k}}\ . \quad \text{(A8)}$$

APPENDIX B

In order to calculate the thermal averages $\langle p^{\dagger}_{k\sigma}p_{k\sigma}\rangle$ and $\langle p_{-k,-\sigma}p_{k\sigma}\rangle$, we follow Zubarev.[27] For this, we define double time Greens functions $\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle$ and $\langle\langle p_{-k,-\sigma};p_{k\sigma}\rangle\rangle$. The function $\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle$ satisfies the following equation of motion:

$$E\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle=\frac{1}{2\pi}\langle[p^{\dagger}_{k\sigma},p_{k\sigma}]\rangle+\langle\langle[p^{\dagger}_{k\sigma},H];p_{k\sigma}\rangle\rangle\ . \quad \text{(B1)}$$

Using the equation of motion for $p_{k\sigma}$, Eq. (22), Eq. (B1) can be written as

$$E\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle=\frac{1}{2\pi}+\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle+\Delta^{p}_{k}{}^{\dagger}\langle\langle p_{-k,-\sigma};p_{k\sigma}\rangle\rangle \quad \text{(B2)}$$

or

$$\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle=\frac{1}{2\pi(E-\tilde{\tilde{\varepsilon}}^{p}_{k})}+\frac{\Delta^{p}_{k}}{E-\tilde{\tilde{\varepsilon}}^{p}_{k}}\langle\langle p_{-k,-\sigma};p_{k\sigma}\rangle\rangle\ . \quad \text{(B3)}$$

A similar equation where $\tilde{\varepsilon}^{k}_{p}=\varepsilon^{k}_{p}-\alpha_k h^2_k$ can be derived for $\langle\langle p_{-k,-\sigma};p_{k\sigma}\rangle\rangle$. The result is

$$\langle\langle p_{-k,-\sigma};p_{k\sigma}\rangle\rangle=\frac{\Delta^{p}_{k}}{E+\tilde{\tilde{\varepsilon}}^{p}_{k}}\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle\ . \quad \text{(B4)}$$

Now solving Eqs. (B3) and (B4), we obtain,

$$\langle\langle p^{\dagger}_{k\sigma};p_{k\sigma}\rangle\rangle=\frac{(E+\tilde{\tilde{\varepsilon}}^{p}_{k})}{2\pi(E^2-\tilde{\tilde{\varepsilon}}^{p}_{k}{}^2-|\Delta^{p}_{k}|^2)} \quad \text{(B5)}$$

and

$$\langle\langle p_{-k,-\sigma};p_{k\sigma}\rangle\rangle=\frac{\Delta^{p}_{k}}{2\pi(E^2-\tilde{\tilde{\varepsilon}}^{p}_{k}{}^2-|\Delta^{p}_{k}|^2)}\ . \quad \text{(B6)}$$

In an analogous manner,

$$\langle\langle D^{\dagger\mu}_{k\sigma};D^{\nu}_{k\sigma}\rangle\rangle=\frac{(E+\bar{\bar{E}}_{k\mu})(\varepsilon^{d}_{k})^2N_{k\mu}\delta_{\mu\nu}}{2\pi(E^2-\bar{\bar{E}}^{2}_{k\mu}-\bar{\Delta}^{d^2}_{k\mu})} \quad \text{(B7)}$$

and

$$\langle\langle D^{\mu}_{-k,-\sigma};D^{\nu}_{k\sigma}\rangle\rangle=\frac{\bar{\Delta}^{d}_{k\mu}(\varepsilon^{d}_{k})^2N_{k\mu}\delta_{\mu\nu}}{2\pi(E^2-\bar{\bar{E}}^{2}_{k\mu}-\bar{\Delta}^{d^2}_{k\mu})}\ . \quad \text{(B8)}$$

Again following Zubarev[27] the thermal averages, and hence the particle number, can be calculated in a straightforward fashion. Using Eqs. (B4)–(B8), we obtain for the total number of particles in the system,

$$N=2n=\sum_{k}\sum_{\mu}(\varepsilon^{d}_{k})^{-2}N_{k\mu}\left[\left[1+\frac{\bar{\bar{E}}_{k\mu}}{\tilde{\bar{E}}_{k\mu}}\right]f(\tilde{\bar{E}}_{k\mu})+\left[1-\frac{\bar{\bar{E}}_{k\mu}}{\tilde{\bar{E}}_{k\mu}}\right]f(-\tilde{\bar{E}}_{k\mu})\right]$$
$$+\frac{1}{2}\sum_{k}\left[\left[1+\frac{\tilde{\tilde{\varepsilon}}^{p}_{k}}{E^{p}_{k}}\right]f(E_k)+\left[1-\frac{\tilde{\tilde{\varepsilon}}^{p}_{k}}{E^{p}_{k}}\right]f(-E_k)\right]\ . \quad \text{(B9)}$$

Also, noting that

$$\lambda=\sum_{k\mu\nu}\langle D^{\mu}_{k\sigma}D^{\nu}_{-k,-\sigma}\rangle\ ,$$

and using Eq. (B8), we have

$$\lambda=\frac{1}{2}\sum_{k\mu}(\varepsilon^{d}_{k})^{-2}N_{k\mu}\frac{\Delta^{d}_{k\mu}}{\tilde{\bar{E}}_{k\mu}}[f(\tilde{\bar{E}}_{k\mu})-f(-\tilde{\bar{E}}_{k\mu})]\ , \quad \text{(B10)}$$

where $f(E)$ is the Fermi function. This last equation is used in Eq. (29) in the main text.

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