Density of states of a layered S/N d–wave superconductor

W. A. Atkinson, J. P. Carbotte

Department of Physics and Astronomy, McMaster University,
Hamilton, Ontario, Canada L8S 4M1

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Abstract

We calculate the density of states of a layered superconductor in which there are two layers per unit cell. One of the layers contains a d–wave pairing interaction while the other is a normal metal. The goal of this article is to understand how the d–wave behaviour of the system is modified by the coupling between the layer–types. This coupling takes the form of coherent, single particle tunneling along the c–axis. We find that there are two physically different limits of behaviour, which depend on the relative locations of the Fermi surfaces of the two layer–types. We also discuss the interference between the interlayer coupling and pairing interaction and we find that this interference leads to features in the density of states.

74.20.-z, 74.20.Fg, 74.50.+r
I. INTRODUCTION

One of the most interesting developments in the study of high-temperature ($HT_c$) superconductors has been the idea that the gap is not isotropic within the copper-oxide planes. There is considerable experimental evidence that this is the case; angle resolved photoemission experiments\(^1\), for example, have directly observed an anisotropic gap in the $ab$-plane spectrum of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Furthermore, there have been a number of recent experiments\(^2\) in which the behaviour of the system can be explained by gaps which have at least one node on the Fermi surface. There have also been a number of controversial tunneling experiments (for example Wollman \textit{et al.}\(^3\)) in which the sign of the gap has been shown to change across the nodes. These experimental results have been taken as strong support for a gap with d-wave symmetry within the copper-oxide planes.

The d-wave symmetry of the gap is an integral part of a number of theories of superconductivity, such as RVB\(^4\) and spin-fluctuation\(^5\)–\(^8\) models. There are also a large number of BCS-like calculations\(^9\)–\(^14\) (of which we have only mentioned a few) in which the ansatz is made that the gap has a d-wave structure. The one feature which is common to all of these calculations is that they are 2-dimensional, and it is assumed that the effects of the third dimension will be weakly perturbative. This assumption reflects the belief that the superconductivity of the $HT_c$ materials occurs within the copper-oxide planes.

The goal of this work is to consider the effect that the third dimension will have on the properties of an otherwise d-wave system. In particular, we will calculate the superconducting density of states (DOS) of a layered S/N system. In this model, there are two layers in the unit cell. One of the layers (S) contains a d-wave pairing interaction which drives the superconducting transition. The second layer (N) is intrinsically normal in the sense that it contains no pairing interaction, although it still becomes superconducting because of its proximity to the S layer. Of the $HT_c$ materials, this model has the most in common with YBa$_2$Cu$_3$O$_7$, where it is considered that the copper-oxygen planes contain a superconducting pairing mechanism and the copper-oxygen chains are intrinsically normal.
Our particular version of the layered S/N model is based on one studied previously\textsuperscript{15}–\textsuperscript{18}, although the focus of these authors was somewhat different than here. In all cases, the authors considered the gap of the isolated superconducting plane to be isotropic, and the discussion focussed on the anisotropy introduced by the interplane coupling. Abrikosov and Klemm\textsuperscript{15} were interested in how the interplane coupling affects the density of states, the isotropy of the Raman spectrum and the behaviour of \( T_c \) and the gap. Buzdin \textit{et al.}\textsuperscript{16} calculated the density of states, while Bulaevskii\textsuperscript{17} considered various properties of a layered S/N model in the limits of very weak and very strong interlayer coupling. Tachiki \textit{et al.} have calculated a number of observable quantities (tunneling conductance, optical conductivity, knight shift and nuclear magnetic relaxation rate) for a more complicated model in which there are five layers per unit cell. In this paper, the pairing in the S layer is chosen to have a \( d_{x^2-y^2} \) symmetry and we are interested in how the interplane coupling will change the density of states from the 2–dimensional case\textsuperscript{9,10}.

The layout of the paper is as follows: In section \textbf{II} we introduce a model for a layered S/N superconductor and derive a formula for the density of states. In section \textbf{III} we calculate the DOS for different choices of model parameters. The discussion is broken up into two physically different limits. In one case, the Fermi surfaces of the two bands (which result from the two layer types) are far apart in the Brillouin zone, while in the second case they coincide. The difference between these two limits is that, in the second case, there are important (non–perturbative) interference effects between the mean field and the interplane coupling. In section \textbf{IV} we present a summary and discussion of our results.

\textbf{II. THE MODEL}

In this section we introduce a model for a layered superconductor, which is based on one proposed by Abrikosov\textsuperscript{15}. In this model we consider two types of metallic layers, stacked alternately one above the other in the z direction. These layers form two sublattices which we will assume are weakly coupled to each other. There is a BCS–like pairing potential localized
about the layers of the first sublattice which is responsible for the superconductivity of the sample. The Hamiltonian for such a system can be written

\[ H = \sum_{\sigma} \int d^3r \Psi^\dagger_\sigma(r)(H_0 + V_1 + V_2)\Psi_\sigma(r) \]
\[ + \sum_{\sigma\sigma'} \int d^3r \int d^3r' \Psi^\dagger_\sigma(r)\Psi^\dagger_{\sigma'}(r') I_1(r, r') \Psi_{\sigma'}(r')\Psi_\sigma(r) \]

(1)

where \( \Psi_\sigma \) is the field operator of spin \( \sigma \). The operator \( H_0 \) is the free particle Hamiltonian, \( p^2/2m \), while \( V_1 \) and \( V_2 \) are the potentials associated with each of the sublattices. The BCS–like pairing potential is

\[ I_1(r, r') = -1/2 \sum_Z V(x, y, x', y') \delta(z - Z) \delta(z' - Z), \]

where \( Z \) are the \( z \)–values of the planes in the first sublattice.

If the electrons are tightly bound to their planes, then the eigenstates of \( H_0 + V_1 + V_2 \) are well approximated by eigenstates of the sublattice Hamiltonians \( H_0 + V_1 \) and \( H_0 + V_2 \) (which are assumed known). Eigenstates of \( H_0 + V_1 \) and \( H_0 + V_2 \) are not orthogonal to each other, but may be orthogonalised to form a new set of states, \( \phi_{ik}(r) \), \( i = 1, 2 \), which are no longer eigenstates of the sublattice Hamiltonians but which satisfy \( \int d^3r \phi_{1k}^\ast(r)\phi_{2k}(r) = 0 \). The orthogonalisation procedure will conserve the Bloch–like properties of the original eigenstates. If we define

\[ a_{ik\sigma} = \int d^3r \phi_{ik}^\ast(r)\Psi_\sigma(r) \]

then the Hamiltonian may be written

\[ H - N\mu = \sum_{k\sigma} \left[ a_{1k\sigma}^\dagger a_{1k\sigma}\xi_1(k) + a_{2k\sigma}^\dagger a_{2k\sigma}\xi_2(k) \right] \]
\[ + \sum_{k\sigma} \left[ t(k)a_{1k\sigma}^\dagger a_{2k\sigma} + t^*(k)a_{2k\sigma}^\dagger a_{1k\sigma} \right] \]
\[ - \sum_k \left[ \Delta_k a_{1k\uparrow}^\dagger a_{1k\downarrow} + \Delta^*_k a_{1k\downarrow}^\dagger a_{1k\uparrow} \right] \]

(2)

where

\[ \xi_j(k) = \int d^3r \phi_{jk}^\ast(r)(H_0 + V_1 + V_2 - \mu)\phi_{jk}(r) \]
\[ t(k) = \int d^3r \, \phi_{1k}^*(r) \left( H_0 + V_1 + V_2 \right) \phi_{2k}(r) \]

and

\[ \Delta_k \equiv \frac{1}{\Omega} \sum_{k'} V_{kk'} \langle a_{1-k'} \downarrow a_{1k'} \uparrow \rangle. \tag{3} \]

Here \( \Omega \) is the volume of the sample and \( \langle \rangle \) denotes a thermal average. Equation (3) is the self-consistent equation which follows from making a mean field approximation for the pairing interaction in equation (1). The form of the potential, \( V_{kk'} \), comes from assuming a singlet pairing of electrons of opposite \( k \). We find that

\[
\begin{align*}
V_{kk'} &= \sum_Z \int dx dy dx' dy' \phi_{1k}^*(x, y, Z) \phi_{1-k'}^*(x', y', Z) \\
&\quad \times V(x, y, x', y') \phi_{1-k'}(x', y', Z) \phi_{1k}(x, y, Z),
\end{align*}
\]

which, in the limit in which the electrons are tightly bound to the planes, has no \( k_z \) or \( k'_z \) dependence. The interplane hopping term, \( t \), has been chosen to conserve \( k \), which makes sense if \( V_1 \) and \( V_2 \) have the same periodicity and we have a clean metal.

In the Nambu formalism, the Hamiltonian can be written

\[
H - N \mu = \sum_k A^\dagger(k) Q(k) A(k) + \text{const} \tag{4}
\]

where

\[
A(k) = \begin{bmatrix}
  a_{1k}^\uparrow \\
a_{1-k}^\downarrow \\
a_{2k}^\uparrow \\
a_{2-k}^\downarrow
\end{bmatrix}
\]

and

\[
Q = \begin{bmatrix}
  \xi_1(k) & -\Delta_k & t(k) & 0 \\
  -\Delta_k^* & -\xi_1(-k) & 0 & -t^*(-k) \\
t^*(k) & 0 & \xi_2(k) & 0 \\
0 & -t(-k) & 0 & -\xi_2(-k)
\end{bmatrix}. \tag{6}
\]
The diagonalisation of the matrix, $Q(k)$, will be simplified if we note that the symmetries $t(k) = t^*(-k)$ and $\xi_i(k) = \xi_i(-k)$ follow from time reversal symmetry. Then the energy eigenvalues are $E_1 = E_+,$ $E_2 = E_-$, $E_3 = -E_-$, $E_4 = -E_+$, with

$$E_\pm^2 = \frac{\xi_1^2 + \xi_2^2 + \Delta_k^2}{2} + t^2$$

$$\pm \sqrt{\left[\frac{\xi_1^2 - \xi_2^2 + \Delta_k^2}{2}\right]^2 + t^2[(\xi_1 + \xi_2)^2 + \Delta_k^2]}$$

$$= \frac{\xi_1^2 + \xi_2^2 + \Delta_k^2}{2} + t^2$$

$$\pm \sqrt{\left[\frac{\xi_1^2 + \xi_2^2 + \Delta_k^2}{2} + t^2\right]^2 - (t^2 - \xi_1\xi_2)^2 - (\xi_2\Delta_k)^2}$$

(7)

(8)

(we simplify our notation by understanding $t^2$ to mean $|t|^2$ and $\Delta_k^2$ to mean $|\Delta_k|^2$ throughout this paper). The first expression for $E_\pm$, given by equation (7), is useful for describing the weakly coupled (small $t$) limit, while the second, equation (8), is useful for describing $E_-$ near its minima.

The Hamiltonian now becomes

$$H - N\mu = \sum_k \sum_{i=1}^4 \hat{A}_i^\dagger(k)\hat{A}_i(k)E_i(k) + \text{const}$$

(9)

where $\hat{A}_i(k)$ is the quasiparticle annihilation operator associated with the $i^{th}$ energy band. The operator, $\hat{A}_i(k)$, is defined by

$$\hat{A}_i(k) = \sum_{j=1}^4 U^\dagger_{ij}(k)A_j(k),$$

(10)

and $U(k)$ is the $4 \times 4$ matrix which diagonalises $Q$: $U_{ij} = U_i(E_j)$ with

$$U_i(E_j) = \frac{1}{\sqrt{C}} \begin{pmatrix}
(E_j - \xi_2)A \\
-(E_j + \xi_2)B \\
tA \\
tB
\end{pmatrix}$$

(11)

$$A = t^2 - (\Delta_k + E_j + \xi_1)(E_j + \xi_2)$$
\[
B = t^2 - (\Delta_k^* + E_j - \xi_1)(E_j - \xi_2)
\]

\[
C = A^2[t^2 + (E_j - \xi_2)^2] + B^2[t^2 + (E_j + \xi_2)^2].
\]

We are now in a position to solve for the temperature dependence of the gap, \(\Delta_k\). We do this by writing equation (3) in terms of the quasiparticle operator \(\hat{A}_j(k)\). We get

\[
\Delta_k = \frac{1}{\Omega} \sum_{i=1}^{4} \sum_{k'} V_{kk'} U_{1i}(k') U_{2i}(k') f(-E_i(k'))
\]

where \(f(x) = [1 + \exp(\beta x)]^{-1}\) is the Fermi distribution function. Equation (12) is a self-consistent equation which can be solved numerically for the gap as a function of temperature.

Once the gap at \(T = 0\) is known, then the density of states (DOS) may be calculated. The density of states is

\[
\rho(\omega) = -\frac{2}{N\pi} \int d^3r \text{Im} G_{\uparrow\uparrow}^R(r, r, \omega)
\]

where the factor 2 is because we are only counting spin up electrons and \(N\) is the number of unit cells in the crystal. \(G_{\sigma\sigma'}^R\) is the retarded Green’s function:

\[
G_{\sigma\sigma'}^R(r, r', \omega) = \lim_{\delta \to 0^+} \int_{-\infty}^{\infty} dt e^{i(w+i\delta)t} \\
\times \langle\{\Psi_\sigma(r, t), \Psi_\sigma^\dagger(r', 0)\}\rangle \theta(t)
\]

where \(\theta(t)\) is the step function and \(\{ \}\) are anticommutating brackets. If we write

\[
\Psi_\uparrow(r, t) = \sum_{i=1}^{2} a_{ik\uparrow}(t) \phi_{1k}(r)
\]

\[
= \sum_{i=1}^{4} \left\{U_{1i}(k) \hat{A}_i(k, t) \phi_{1k}(r) \right. \\
\left. + U_{3i}(k) \hat{A}_i(k, t) \phi_{2k}(r) \right\}
\]

and

\[
\hat{A}_i(k, t) = e^{-iE_i(k)t} \hat{A}_i(k, 0)
\]

then
\[
\rho(\omega) = \frac{2}{N} \sum_{i=1}^{4} \sum_{k} \left[ U_{1i}(k)^2 + U_{3i}(k)^2 \right] \delta(w - E_i(k)).
\] (14)

The term proportional to \(U_{1i}(k)^2\) \((U_{3i}(k)^2)\) gives the contribution to the density of states of the first (second) sublattice made by the \(i^{th}\) band. It is therefore possible to write the DOS as the sum of the two sublattice densities of states

\[
\rho(\omega) = \rho_1(\omega) + \rho_2(\omega).
\] (15)

We will evaluate both the DOS and the gap equation, (12), in the following section.

III. A DISCUSSION OF NUMERICAL RESULTS

A. Specification of the Model

The goal of this section is to discuss the density of states of our model. We will do this by examining the features of our quasiparticle energy dispersions. To begin with however, we must choose a specific form for our Hamiltonian (equation (2)). We take

\[
\xi_i(k) = -2\sigma_i[\cos(k_x) + \cos(k_y)] - \mu_i, \ i = 1, 2
\] (16)

which comes from assuming that the electrons are described by tight binding dispersions within the planes. The Brillouin zone is \(-\pi < k_x, k_y \leq \pi, -\pi/d < k_z \leq \pi/d\) where \(d\) is the lattice constant in the \(z\)-direction. Since \(\xi_i\) describes the energy of an electron in a Bloch state of one of the sublattices, it will have a weak \(k_z\) dependence. However, a much larger \(k_z\) dependence will come from \(t(k)\), which describes the nearest neighbour hopping of electrons between layers of different types. The two chemical potentials in (16) allow the two bands to be offset from each other. The most significant feature of this choice of \(\xi_i\) is that there are saddle points at \((k_x, k_y) = (0, \pi)\) (at which \(\xi_i = -\mu_i\)) and other symmetry related points. A great deal has been written about model systems in which the saddle points lie at the Fermi surface where they play an important role in the dynamics of the system [2]. We wish to avoid this case since the aim of this paper is to understand the role of the interlayer coupling. For all of the results presented in this paper, then, we have taken \(|\mu_1|, |\mu_2| > \max(|t(k)|, |\Delta_k|).
The form of the interlattice coupling follows from the assumption that the electrons are tightly bound to the planes:

\[ t(k) = t_1 e^{ik_zd_1} + t_2 e^{-ik_zd_2}. \]  

(17)

Here \( t_1 \) and \( t_2 \) are complex constants, and the planes are alternately a distance \( d_1 \) and \( d_2 \) apart so that \( d = d_1 + d_2 \). The condition \( t(k) = t^*(-k) \) will be satisfied if \( t_1 \) and \( t_2 \) have the same phase. For our numerical calculations we reduce the number of free parameters by setting \( d_1 = d_2 = d/2 \), \( t_1 = t_2 = t_0/2 \) so that

\[ t(k) = t_0 \cos(k_zd/2). \]  

(18)

One of the things which will become apparent is that, although the fine structure of certain features of the DOS depend on the specific form we choose for \( t(k) \), the existence and important properties of these features are independent of this choice.

The pairing potential is taken to be separable so that \( V_{kk'} = V \eta_k \eta_{k'} \), with \( \eta_k = 1 \) for \( s \)-wave superconductors and \( \eta_k = \cos(k_x) - \cos(k_y) \) for \( d \)-wave superconductors. In this case we can define \( \Delta_0 \) by

\[ \Delta_0 = \frac{V}{\Omega} \sum_k \eta_k \langle a_{1-k\downarrow} a_{1\uparrow} \rangle, \]  

(19)

and equation (12) will simplify to

\[ \Delta_0 = \frac{V}{\Omega} \sum_{i=1}^4 \sum_k \eta_k U_{1i}(k) U_{2i}(k) f(-E_i(k)), \]  

(20)

with \( \Delta_k = \Delta_0 \eta_k \). We solve equation (20) for \( T_c \) and graph the results in Fig. 1. We can see that the critical temperature decreases rapidly with increasing \( t_0 \) which suggests that a weak coupling of the planes is necessary for any reasonable description of a \( HT_c \) superconductor. It has been suggested, however, that the inclusion of phonon mediated interlayer coupling may actually lead to an increase in \( T_c \) with coupling strength. We also calculate \( \Delta_0(T = 0) \) from equation (20) and plot \( \Delta_0(T = 0)/T_c \) in Fig. 1. We can see that \( \Delta_0(T = 0)/T_c \) increases rapidly for \( t_0 \) larger than .4\( \sigma_1 \). For YBCO the value of \( 2\Delta_{\text{max}}/T_c \) depends on the
experiment from which it is determined, but it is generally found to be less than 8. It is important to remember that the experimentally measured value of the gap is typically the lowest energy peak in the quasiparticle excitation spectrum, which is not necessarily related in any simple fashion to the order parameter. However, as a rough estimate, we can limit \( \max(2\Delta_k) = 4\Delta_0 < 8 \) so that, from Fig. 1, \( t_0/\sigma_1 < .5 \).

Once \( \Delta_0(T = 0) \) is determined, we can proceed to calculate the DOS for our Hamiltonian. Our discussion of the DOS will be aided by two observations. The first is that equation (16) implies that

\[
\xi_2 = \frac{\sigma_2}{\sigma_1} \xi_1 + \frac{\mu_1 \sigma_2 - \mu_2 \sigma_1}{\sigma_1}
\]

and the second is that the Brillouin zone boundary, \( k_x, k_y = \pm \pi \) maps into the diamond shaped boundary

\[
|\Delta_k| = 2\Delta_0 \left[1 - \frac{|\mu_i + \xi_i|}{4\sigma_i}\right]
\]

with \(-4\sigma_i - \mu_i < \xi_i < 4\sigma_i - \mu_i\) and \( i = 1 \) or 2. Equations (21) and (22) allow us to discuss the system using \( \xi_1 \) (or \( \xi_2 \) for that matter) and \( \Delta_k \), rather than \( k_x \) and \( k_y \), as independent variables.

We will consider two limiting cases of Eqn. (21). In the first case \( |\mu_1 \sigma_2 - \mu_2 \sigma_1|/\sigma_1 \gg \Delta_0 \) so that \( \xi_1^2 + \xi_2^2 \gg \Delta_k^2 \) everywhere in the Brillouin zone. In the second case, we take the Fermi surfaces of the sublattices to coincide, so that \( \mu_1 \sigma_2 - \mu_2 \sigma_1 = 0 \). The fundamental difference between the two cases is that it is possible to distinguish band structure effects from superconductivity effects in the first case, while in the second case the interplane coupling plays an important role at the Fermi surface.

**B. Case I: Distinct Fermi Surfaces**

We begin by discussing the quasiparticle energy dispersions. First of all, for most regions of the Brillouin zone \( \xi_1^2 + \Delta_k^2 - \xi_2^2 \gg t^2, \Delta_k^2 \) and we see from Eqn. (7) that \( E_\pm \) approaches the limiting form
\[ E_+ \sim \max(\sqrt{\xi_1^2 + \Delta_k^2}, |\xi_2|) \]
\[ E_- \sim \min(\sqrt{\xi_1^2 + \Delta_k^2}, |\xi_2|). \]  

(23)

In Fig. 2 we plot \( E_{\pm} \) along the line \( k_x = k_y, k_z = 0 \) and compare it with \(|\xi_2|\) and \( \sqrt{\xi_1^2 + \Delta_k^2} \). We have chosen an s–wave gap for illustrative purposes in the figure, since a d–wave gap would vanish along this line. In regions of the Brillouin zone where (23) is approximately true, the effect of the matrix elements \( U_{ij} \) will be to associate \( \sqrt{\xi_1^2 + \Delta_k^2} \) with the first sublattice and \(|\xi_2|\) with the second sublattice, so that the integrands in equation (14) will become

\[
\frac{1}{2} \left[ 1 + \frac{\xi_1}{\sqrt{\xi_1^2 + \Delta_k^2}} \right] \delta(\omega - \sqrt{\xi_1^2 + \Delta_k^2}) \\
+ \frac{1}{2} \left[ 1 - \frac{\xi_1}{\sqrt{\xi_1^2 + \Delta_k^2}} \right] \delta(\omega + \sqrt{\xi_1^2 + \Delta_k^2})
\]

for \( \rho_1 \) and

\[
\delta(\omega - \xi_2)
\]

for \( \rho_2 \). For most energies, then, the DOS will simply look like the DOS of the decoupled \( \rho_{10} \) \( \rho_{10} \) (small \( t \)) limit, which we show in Fig. 3.

It is the regions where the interlayer coupling has an important effect which we will discuss in the most detail. In Figs. 4, 5 and 6 we show the densities of states for nonzero interlayer coupling. These have a number of features that are absent in the uncoupled case, and we will discuss these features in turn.

The first thing which is clear is that, as \( t_0 \) is increased and the system goes from being 2–dimensional to 3–dimensional, the logarithmic divergences associated with the van Hove singularities (both the superconducting one and those intrinsic to \( \xi_1 \) and \( \xi_2 \)) become broadened peaks. This process is particularly clear in Figs. 4 and 5 where the intrinsic singularities at \( \omega = .8 \) in \( \rho_1 \) and \( \omega = -.4 \) in \( \rho_2 \) are broadened considerably by \( t_0 \).

The interlayer coupling is also important in regions of the Brillouin zone where \( t^2 \) is of the order of \( \xi_1^2 + \Delta_k^2 - \xi_2^2 \). The effect of the coupling is to create avoided band crossings wherever
\[ \xi_1^2 + \Delta_k^2 - \xi_2^2 = 0. \tag{26} \]

In Fig. 2, for example, we can see that there are two avoided crossings, one at \( k_x = k_y = 1.57 \), and one at \( k_x = k_y = 1.32 \).

At one of the avoided crossings (\( k_x = k_y = 1.57 \) in Fig. 2), \( \xi_1 \) and \( \xi_2 \) have the same sign and (expanding \( E_\pm \) in powers of \( \Delta_0 \))

\[ E_\pm \sim |\xi'| \pm |t(k)| + O(\frac{\Delta_0^2}{\xi'}), \tag{27} \]

where \( \xi_1 = \xi' \) is the solution to Eqns. (26) and (21) for which \( \xi_1 \) and \( \xi_2 \) have the same sign. The energy difference of the bands at the avoided crossing is \( \sim 2|t(k)| \). We can see from Fig. 2 that this avoided crossing does not introduce a van Hove singularity and, as a result, we do not find any feature in the DOS of Figs. 4 and 5 at this energy. On the other hand, in Fig. 6, we find that, because we have let \( \mu_1 = \mu_2 \), the avoided crossing occurs at the intrinsic van Hove singularities of \( \xi_1 \) and \( \xi_2 \). The result of this is that the logarithmic peaks evident in Fig. 3 at \( \omega \sim .8 \) are reduced far more than in Fig. 5, where the avoided crossing is far from the singularities. This is an important result because it shows that models in which the van Hove singularity plays an important role (i.e. it is near the Fermi surface) cannot also have a band crossing near the Fermi surface.

For the second avoided band crossing (at \( k_x = k_y = 1.32 \) in Fig. 2), \( \xi_1 \) and \( \xi_2 \) have opposite sign. Again we can expand \( E_\pm \) in powers of \( \Delta_0 \), and we find that the avoided crossing occurs at

\[ E_\pm = \sqrt{\xi''^2 + t(k)^2} \pm \frac{|t(k)|\Delta_k}{\sqrt{\xi''^2 + t(k)^2}} + O(\frac{\Delta_0^2}{\xi''}) \tag{28} \]

(\( \xi_1 = \xi'' \) is the solution to (26) and (21) for which \( \xi_1 \) and \( \xi_2 \) have opposite sign). We can see from Fig. 2 that there is actually a band gap of width

\[ E_+ - E_- \sim \frac{2|t(k)|\Delta_k}{\sqrt{\xi''^2 + t(k)^2}} + O(\frac{\Delta_0^2}{\xi''}) \tag{29} \]

at this point. What is interesting about this gap is that it only exists in the superconducting state (since it is proportional to \( \Delta_k \)) and that it forms away from the Fermi surface. This is
unusual since the effects of superconductivity normally manifest themselves near the Fermi surface. In Fig. 4, these structures are clearly visible at $\omega \sim \xi'' = 0.55$ in the first sublattice and $\omega \sim -\xi''$ in the second sublattice. In Fig. 5, the larger value of $t_0$ shifts the location of the minima slightly to $\omega = \pm 0.65$. In Fig. 6, the structures are clearly visible at $\omega = \pm 0.4$.

The widths of the gap–like structures are given approximately by

$$ E_+ - E_-|_{\text{max}} \sim \frac{4t_0 \Delta_0}{\sqrt{\xi''^2 + t_0^2}} \left[ 1 - \frac{|\mu_1 + \xi''|}{4\sigma_1} \right] $$

(30)

since the maximum value of $\Delta_k$ allowed for $\xi_1 = \xi''$ is given by Eqn. (22). The source of this gap is not immediately obvious, but the proportionality of Eqn. (30) to $t_0 \Delta_0$ suggests that it results from an interference of interlayer coupling and the mean field. In section III D we will show that this is in fact the case, and we will discuss why these gaps appear on opposite sides of the Fermi surface in each of the sublattices.

The final place where the interlayer coupling is important is near the Fermi surface, where it influences the superconducting properties of the system. In Fig. 2 we see that $E_-$ has two local minima which are related to the superconducting gaps of the two sublattices. We expand $E_-$ (Eqn. (8)) in $(t^2 - \xi_1 \xi_2)$ and $\Delta_k^2$ to get

$$ E_-^2 \sim \frac{(t^2 - \xi_1 \xi_2)^2 + (\Delta_k \xi_2)^2}{\xi_1^2 + \xi_2^2 + 2t^2}. $$

(31)

Equation (31) will vanish whenever $\Delta_k = 0$ and $t(k)^2 = \xi_1 \xi_2$. This happens for two values of $\xi_i$, which we denote by $\xi^{(j)}_i$ with $j = 1, 2$. From Eqn. (21) it is straightforward to show that

$$ \xi^{(j)}_1 = \frac{\mu_2 \sigma_1 - \mu_1 \sigma_2}{2\sigma_2} + (-1)^j \sqrt{\frac{(\mu_2 \sigma_1 - \mu_1 \sigma_2)^2 + 4\sigma_1 \sigma_2 t^2(k)}{2\sigma_2}} $$

(32a)

$$ \xi^{(j)}_2 = -\frac{\mu_2 \sigma_1 - \mu_1 \sigma_2}{2\sigma_1} + (-1)^j \sqrt{\frac{(\mu_2 \sigma_1 - \mu_1 \sigma_2)^2 + 4\sigma_1 \sigma_2 t^2(k)}{2\sigma_1}}. $$

(32b)

We then estimate the sizes of the superconducting gaps by substituting the equations (22), $\xi_i = \xi^{(j)}_i$ and $t = t_0$ into Eqn. (31):
\[ E_- \sim 2\Delta_0 \left| \frac{\xi_2^{(j)}}{\xi_1^{(j)} + \xi_2^{(j)}} \right| \left[ 1 - \frac{|\mu_1 + \xi_1^{(j)}|}{4\sigma_1} \right] \]  

In the limit that \( t_0 \) becomes small, the gap sizes become

\[ E_- \sim 2\Delta_0 \left[ 1 - \frac{|\mu_1|}{4\sigma_1} \right] + \frac{\Delta_0 t_0(k)^2}{2(\mu_2\sigma_1 - \mu_1\sigma_2)} \left[ \text{sgn}(\mu_1) - \frac{\sigma_1(4\sigma_1 - |\mu_1|)}{\mu_2\sigma_1 - \mu_1\sigma_2} \right] \]  

and

\[ E_- \sim 2\Delta_0 \left[ \frac{\sigma_2 t_0}{\mu_2\sigma_1 - \mu_1\sigma_2} \right]^2 \left[ 1 - \frac{|\mu_2|}{4\sigma_2} \right]. \]

Equation (34) shows how a weak interlattice coupling affects the gap in the intrinsically superconducting sublattice. One interesting point is that whether \( t_0 \) increases or decreases the gap size depends on the details of the band structure. When \( t_0 = 0 \) we have an approximate expression for the location of a logarithmic singularity in a two–dimensional d–wave superconductor. The exact expression is \( \Delta_0 (4\sigma_1 - |\mu_1|) / \sqrt{4\sigma_1^2 + \Delta_0^2} \). Equation (35) shows the size of the induced gap in the intrinsically normal sublattice.

The gaps described by equations (34) and (35) will appear in both \( \rho_1 \) and \( \rho_2 \) (this has also been pointed out for a similar model). The magnitudes of the contributions are determined by the matrix elements, \( U_{ij} \), in Eqn. (14). In the appendix, we derive the low energy DOS and can see explicitly how the matrix elements behave. In particular, Eqns. (A9) describe the strength with which each of the minima of \( E_- \) (labelled by \( i = 1, 2 \)) is reflected in \( \rho_1 \) (from \( U_1^2 \)) and \( \rho_2 \) (from \( U_2^2 \)). In the weakly coupled (small \( t_0 \)) limit, for example, equations (B2) tell us that \( U_1^2 \sim 1, U_2^2 \sim (\sigma_1 t)^2/(\mu_2\sigma_1 - \mu_1\sigma_2)^2 \) for the intrinsic gap given by (34), while \( U_1^2 \sim (\sigma_2 t)^2/(\mu_2\sigma_1 - \mu_1\sigma_2)^2, U_2^2 \sim 1 \), for the induced gap given by (35). In other words, features associated with one sublattice are reflected in the other sublattice with a strength proportional to \( t_0^2 \). We can see quite clearly in Fig. 6, for example, that both gaps are reflected in both densities of states.

The main results of the appendix are expressions for the low energy DOS in which a) two of the three k–space integrations have been performed approximately (Eqn. A10) and
b) the final integration is performed in a crude approximation in the small $t_0$ limit to find $\rho_1$ (Eqns. (A16)) and $\rho_2$ (Eqns. (A17)). The important features of these expressions can be summarised simply. First of all, the quantity $t^*(\omega)$ (Eqn. (A15)) gives the energy scale of the induced gap. In fact, the equation $t(k_z) = t^*(\omega)$ is just a rearrangement of the expression (33) for the induced gap. Eqn. (A16a) (with $\lambda_\pm$ given by Eqns. (A11a) and (A11b)) is an approximate expression for the d–wave gap in the S sublattice. Eqns. (A16b) and (A16c) are the corrections (of order $t_0^2$) to $\rho_1$ inside and outside the induced gap respectively. Similarly, Eqns. (A17a) and (A17b) give $\rho_2$ inside and outside the induced gap respectively.

One of the most important features of the induced gap is that, since both $t(k_z)$ and $\Delta_k$ have nodes, there are a large number of low energy excitations. The density of states still vanishes inside the induced gap but instead of vanishing linearly, it vanishes with a divergent slope. We can see this in Fig. 7 where we compare the low $\omega$ DOS, calculated numerically from Eqn. (14), with the approximate expressions derived in the appendix.

C. Case II: Coincident Fermi Surfaces

We will now consider the case where the Fermi surfaces of the two sublattices coincide, which requires that $\mu_1\sigma_2 = \mu_2\sigma_1$ so that Eqn. (21) becomes

$$\xi_2 = \frac{\sigma_2\xi_1}{\sigma_1}. \quad (36)$$

Away from the Fermi surface, the structure of the DOS is that of the uncoupled ($t_0 = 0$) limit for exactly the same reasons as in the previous case. Near the Fermi surface, however, the DOS behaves quite differently and is somewhat more complicated to describe, though a partially quantitative understanding is still possible. In Fig. 8 we can see that $E_-$ still has a double minimum structure throughout much of the Brillouin zone but that it is no longer possible to associate either of the minima with a particular sublattice. In Figs. 9 and 10, we show the DOS for two different strengths of interlayer coupling. In Fig. 9, the density of states exhibits a nested gap structure at the Fermi surface. For larger values of $t_0$ (Fig. 10),
the outer structure is no longer identifiable as a gap and the DOS is similar in appearance to that of a 2-dimensional d-wave material. However, as we shall see, the dependence of the gap width on the order parameter, $\Delta_0$, is vastly different than in the 2-dimensional case. The complicated structure of Figs. 9 and 10 is due to the mixing of band structure and superconductivity effects at the Fermi surface. Because of this, it is not possible to replicate the analysis of the last section where we were able to identify gap-like structures in the DOS with features of the energy spectrum. Instead, it is necessary to resort to the brute-force method of identifying saddle point singularities in $E_\pm$, and determining which features in the figures they are responsible for. The method used below is approximate and works well provided that $\Delta_0/\sigma_1 \ll 1$.

Since finding the zeros of $\nabla_k E_\pm$ is difficult, our approach is to set $\partial E_\pm/\partial \xi_1 = 0$ to find the surfaces of extrema of $E_\pm$ with respect to $\xi_1$, and then to assume that the van Hove singularities are at the extremal values of $|t(k)|$ and $|\Delta_k|$ on this surface. The extremal values of $|t|$ are simply zero and $t_0$, which is actually what we would find by setting $\nabla_k E_\pm = 0$ anyway. On the other hand, the extremal values of $|\Delta_k|$ are either zero, or given by Eqn. (22). Since this last constraint depends on $\xi_1$, it is wrong to treat $\Delta_k$ as independent when taking $\partial E_\pm/\partial \xi_1$. Providing that $\Delta_0$ is small, however, the approximation is good and introduces an error of $O(\Delta_0^3/\sigma_1^2)$ to the energies of the van Hove singularities.

We begin by substituting equation (36) into the expression for $E_\pm$ (equation (7)) and setting $\partial E_\pm/\partial \xi_1 = 0$. We find that there are two solutions:

$$\xi_1 = 0 \quad \text{(37)}$$

(for both $E_+$ and $E_-$), and

$$\xi_1^2 = \frac{\sigma_1(\sigma_1^2 + \sigma_2^2)|t(k)|\sqrt{t(k)^2(\sigma_1 + \sigma_2)^2 + 2\sigma_2^2\Delta_k^2(\sigma_1 - \sigma_2) - \sigma_1^2\sigma_2[\Delta_k^2(\sigma_1 - \sigma_2) + 2t(k)^2(\sigma_1 + \sigma_2)]}}{\sigma_2(\sigma_1 + \sigma_2)(\sigma_1 - \sigma_2)^2} \quad \text{(38)}$$

(for $E_-$ only). This second equation gives the location of the two minima of $E_-$ and only has positive solutions for $\xi_1^2$ if
\[ t(k)^2 > \frac{\sigma_2 \Delta_k^2 \left[(\sigma_1 + \sigma_2)(\sigma_1^2 + \sigma_2^2) - 2\sigma_1^3 + (\sigma_1^2 + \sigma_2^2)\sqrt{\sigma_1^2 + 2\sigma_1\sigma_2 + 2\sigma_1^2}\right]}{(\sigma_1 + \sigma_2)^4}. \]  

(39)

The important difference, then, between Figs. 8(a) and 8(b) is the size of \(|t(k)|\). This crossover in behaviour was noted previously \[3\], for the slightly simpler model in which \(\xi_1 \equiv \xi_2\) and \(\Delta_k \equiv \Delta_0\). Now at \(\xi_1 = 0\),

\[ E_{\pm} = \sqrt{\left(\frac{\Delta_k}{2}\right)^2 + t^2} \pm \left|\frac{\Delta_k}{2}\right|, \]

(40)

while when \(\xi_1\) is given by (38),

\[ E_\pm = \frac{2|t(k)|\sigma_1\sigma_2\sqrt{t(k)^2(\sigma_1 + \sigma_2)^2 + 2\sigma_2\Delta_k^2(\sigma_1 - \sigma_2) - \sigma_2[\Delta_k^2\sigma_2(\sigma_1 - \sigma_2) + 2t(k)^2\sigma_1(\sigma_1 + \sigma_2)]}}{(\sigma_1 + \sigma_2)(\sigma_1 - \sigma_2)^2}. \]

(41)

We first describe the saddle points at which \(\xi_1 = 0\). The extremal values of \(|t|\) are \(|t| = 0\) and \(|t| = t_0\), and the extremal values of \(\Delta_k\) are zero and (from (22))

\[ \Delta' = 2\Delta_0 \left[1 - \frac{\mu_1}{4\sigma_1}\right]. \]

(42)

Of the four points in the Brillouin zone just described, only two are actually saddle points (as opposed to band minima). There will be a saddle point in \(E_+\) at \(\Delta_k = \Delta', t(k) = 0\) at which

\[ E_+ = \Delta'. \]

(43)

There will also be saddle points in \(E_+\) and \(E_-\) at \(\Delta_k = \Delta', t(k) = t_0\) at which

\[ E_- = \sqrt{\left(\frac{\Delta'}{2}\right)^2 + t_0^2} - \frac{\Delta'}{2}; \]

\[ E_+ = \sqrt{\left(\frac{\Delta'}{2}\right)^2 + t_0^2} + \frac{\Delta'}{2}. \]

(44)  (45)

The double minimum, with energy given by (11) will also have two saddle points, though they are somewhat more complicated to describe. First of all, there will only be saddle points if the inequality (39) is satisfied for \(t = t_0\) and \(\Delta = \Delta''\). The quantity, \(\Delta''\) is the
solution to the pair of equations, (38) and (22) with \( t(k) = t_0 \). These equations can be solved iteratively in a straightforward fashion, and will yield two closely spaced solutions corresponding to the two slightly different energies at which the minima of \( E \) intersect the Brillouin zone boundary. The energy of the saddle point is then given by Eqn. (41).

In Fig. 9, \( \Delta' = 0.14 \), and the singularities at \( \pm \Delta' \) can be associated with the outer gap in the nested gap structure. If we recall Eqn. (34) and the discussion which follows, we will recognize that \( \Delta' \) is approximately the energy of the gap in a 2–dimensional d–wave superconductor. In Fig. 10, however, the nested gap structure is no longer clear and, although there are features at \( \pm \Delta' = \pm 0.23 \), they do not appear as a gap–like structure. In Fig. 10, the gap width is actually given by Eqn. (41) which gives the closely spaced sets of singularities \( \omega = \pm 0.072 \) and \( \omega = \pm 0.096 \). Eqn. (41) makes it clear that the structure in the DOS which we naively associate with the superconducting gap is, in fact, due to a complicated mixing of the gap and the interlayer coupling. It is an important point that a tunneling experiment might not be able to distinguish between Fig. 10 and the density of states of a 2–dimensional d–wave superconductor (\( \rho_1 \) in Fig. 3). In this case, then, a tunneling experiment would reveal very little about either the interlayer coupling or the nature of the pairing interaction.

In Fig. 9, the singularities due to Eqn. (41) are at \( \omega = \pm 0.0431 \) and \( \omega = \pm 0.0426 \). They are responsible for the inner gap in the nested gap structure. There is also a van Hove singularity nearby, at \( \omega = 0.05 \), which comes from Eqn. (44). It is difficult to see because of its close proximity to the other singularities, but in Fig. 10, this feature is clear and is at \( \omega = \pm 0.30 \). Once again, this feature is the result of the interference of interplane coupling with the mean field and it cannot be considered a perturbation of either a superconducting gap or a band gap. In Fig. 9, Eqn. (45) describes the smearing of the logarithmic singularity due to the intrinsic superconductivity of the first sublattice. It gives van Hove singularities at \( \omega = \pm 0.195 \). This should be compared with the second term of Eqn. (34), whose \( k_z \) dependence also smears the logarithmic singularity associated with the intrinsic gap. The difference is that, in (34), \( t \) appears as a perturbation, while in (45), the smearing is inherently non–
perturbative. In Fig. 10, the van Hove singularities are at \( \omega = \pm 0.534 \). The large broadening of the logarithmic singularity has caused it to overlap adjacent features so that it is not obvious that it is related to the singularity at \( \Delta' \). The remaining features in the DOS of Figs. 9 and 10 are due to the inherent structure of \( \xi_1 \) and \( \xi_2 \).

D. Discussion of the Superconducting Band Gap

In section III B we discussed the sublattice densities of states in the limit \(|\mu_1\sigma_2 - \mu_2\sigma_1| \gg \Delta_0\sigma_1\). We found that, in addition to the expected band and superconducting gaps, there were gap–like structures which appeared in the superconducting state away from the Fermi surface. This is surprising since the effects of superconductivity normally manifest themselves at the Fermi surface. A further property of these structures is that, if in one sublattice a gap–like structure should appear at some energy, \( \omega \), then there will be a similar structure in the other sublattice at energy \(-\omega\). The purpose of this section is to understand the source of these unusual gap–like structures.

The first clue to the nature of the structures is in the expression (30), which shows that the gap width is proportional to \( \Delta_0 t_0 \). This suggests that there is an interference between the interlayer coupling and the mean field. In order to examine this interference further, we will write out an equation for the Green’s function in which the interlayer coupling and the mean field are treated as perturbations. The Hamiltonian, Eqn. (4), can be written as

\[
H - N\mu = \sum_k A^\dagger(k)\{Q^0 + Q^1\}A(k) + \text{const} \tag{46}
\]

where

\[
Q^0 = \begin{bmatrix}
\xi_1(k) & 0 & 0 & 0 \\
0 & -\xi_1(-k) & 0 & 0 \\
0 & 0 & \xi_2(k) & 0 \\
0 & 0 & 0 & -\xi_2(-k)
\end{bmatrix} \tag{47}
\]

and
\( Q^1 = \begin{bmatrix} 0 & -\Delta_k & t(k) & 0 \\ -\Delta^*_k & 0 & 0 & -t^*(-k) \\ t^*(k) & 0 & 0 & 0 \\ 0 & -t(-k) & 0 & 0 \end{bmatrix}. \) 

(48)

Equation (48) is treated like a perturbation. The temperature Green’s function is defined as \( G_{ij}(k; \tau) = -\langle T A_i(k, -i\tau), A_j^\dagger(k, 0) \rangle \), where \( T \) is the time–ordered product and the time dependence of \( A_i(k, t) \) is determined by the full Hamiltonian, \( Q \). It is straightforward to show that

\[
G_{ij}(i\zeta_n) = G_{ij}^0(i\zeta_n) + \sum_{l,m=1}^4 G_{il}^0(i\zeta_n) Q^1_{lm} G_{mj}(i\zeta_n).
\] 

(49)

where \( G(i\zeta_n) \) and \( G^0(i\zeta_n) \) are the Fourier components of \( G(\tau) \) and \( G^0(\tau) \) and \( \zeta_n = \pi(2n + 1)/\beta \) are the Matsubara frequencies. The uncoupled Green’s function, \( G_{ij}^0 \), is the full Green’s function with \( t_0 = \Delta_0 = 0 \). It is easy to show that \( G_{ij}^0(i\zeta_n) = \delta_{ij}[i\zeta_n - Q^0_{ii}]^{-1} \).

With a little work we are able to write out equation (49) for \( G_{11} \) explicitly:

\[
G_{11} = G_{11}^0 + G_{11}^0 \Delta_k G_{22}^0 \Delta^*_k G_{11} + G_{11}^0 t G_{33}^0 t^* G_{11} + G_{11}^0 \Delta_k G_{22}^0 t^* G_{41}.
\] 

(50a)

\[
G_{41} = G_{44}^0 t G_{22}^0 \Delta^*_k G_{11} + G_{44}^0 t G_{22}^0 t^* G_{41}.
\] 

(50b)

The Green’s functions, \( G_{11} \) and \( G_{33} \), describes the propagation of spin–up electrons in the first and second sublattices respectively. On the other hand, \( G_{22} \) and \( G_{44} \) describe the propagation of spin–down holes in the first and second sublattices. The unusual term, \( G_{41} \), is essentially defined by Eqn. (50b) and it describes an electron which both hops between the planes and interacts with the mean field.

In Figs. (11a) and (11b) we write Eqns. (50a) and (50b) out in diagrammatic form. In part (a) we see that there are three processes which modify the propagation of an electron. The first of these processes, which simply describes the hopping of electrons between adjacent
layers, would appear in any band structure calculation involving two atoms per unit cell. The effect of this term is to cause the two bands, $\xi_1$ and $\xi_2$, to repel each other wherever they cross so that we have avoided band crossings whenever $\xi_1 = \xi_2$. The second process in Fig. 11(a) describes the intrinsic superconductivity of the first sublattice. It is useful, however to interpret this in the same way we interpreted the first process: as a coupling of two bands. The important point here, however, is that the two bands which are coupled by the mean field are not the two sublattice bands, but are, instead, the spin–up and spin–down components of the band in the first sublattice. Moreover, the coupling is actually between spin–up electron states and spin–down hole states. The terms in the Hamiltonian responsible for the superconductivity can be interpreted as describing transitions between the electron and hole bands in exactly the same way that the terms responsible for interlayer coupling describe transitions between electron bands. This is clear in Fig. 11(a) where an interaction with the mean field changes an electron into a hole. The second term in Fig. 11(a), then, will cause an avoided crossing in the quasiparticle energies wherever the original electron and hole bands cross. Since the dispersion of the original hole band is just $-\xi_1$, the superconducting band gap will open up at $\xi_1 = -\xi_2 = 0$. We can see that the reason that the effects of superconductivity normally manifest themselves at the Fermi surface is that the interaction between the hole and electron bands is largest there.

The final term in Fig. 11(a) is interesting because it describes the interference of the mean field and interlayer coupling. In (c) we have iterated this once, using Fig. 11(b), to show the lowest order contribution to the mixing. The diagram in (c) describes an electron of energy $\xi_1$ which interacts with the mean field to become a hole of energy $-\xi_1$ and then hops to the second sublattice before reversing the process. The effect of this diagram is simply to couple electron states in the first sublattice with hole states in the second sublattice. Exactly as before then, we should expect avoided crossings in our quasiparticle energy dispersions whenever $\xi_1 = -\xi_2$. As we discussed in section III B, this avoided crossing is responsible for the gap–like structures which appear away from the Fermi surface in Figs. 4, 5 and 6.

In section III C we discussed the case of coincident sublattice Fermi surfaces. In this case,
Fig. 11(a) still describes the system, but all three processes will contribute to the avoided band crossings at the same time. In particular, the final process in (a) will be responsible for the complicated nature of the gap at the Fermi surface.

IV. CONCLUSION

In this paper we have presented results on the density of states of a layered S/N system. The inherently superconducting sublattice was presumed to have a gap with d-wave structure. We investigated how the (coherent) coupling between the two types of layers changed the DOS from the usual 2-dimensional case. Our chosen Hamiltonian, Eqn. (2), led to a relatively complicated quasiparticle energy dispersion (Eqn. (7) or (8)), which we examined in an attempt to understand our numerical results for the DOS. We found that the behaviour of our model could be summarised by two limiting cases, distinguished by the relative positions of the sublattice Fermi surfaces.

In the first case, the Fermi surfaces of the S and N sublattices were far enough apart in the Brillouin zone that the interlayer coupling did not cause them to interfere with each other. In this limit it was clear that the effect of the interlayer coupling was to shift the usual 2-dimensional d-wave gap in the S sublattice perturbatively (Eqn. (34)) and to induce a small gap at the Fermi surface of the N sublattice (Eqn. (35)). The gaps in each of the sublattices were also weakly reflected in the DOS of the other sublattice, with a magnitude proportional to $t_0^2$. In the appendix, we derived an approximate expression for the density of states within the induced gap (Eqn. A17a), and we found that the behaviour is much different from the linear behaviour found in the unperturbed d-wave case. The most interesting features, though, of the DOS in this case were the gap-like structures which appeared away from the Fermi surface in the superconducting state (this was clearly visible in Fig. 4 and we gave an expression for the gap widths in Eqn. (29)). In section III D, we discussed this matter in some detail. Essentially, the point was that there is an interference of the interplane coupling and the mean field. Since the mean field can be viewed as an interaction between
holes and electrons within the superconducting sublattice, and the interplane coupling is an interaction between electrons in the two sublattices, the interference of the terms results in an interaction of holes and electrons in different sublattices. It is this interaction which resulted in the gap–like structures.

In the second case we considered, the sublattice bands ($\xi_1$ and $\xi_2$) crossed at their Fermi surfaces. In this case, there was a nontrivial mixing of mean field and superconductivity effects at the Fermi surface. In Fig. 9, we showed that, for weak interlayer coupling, the system has a nested gap structure, where the outer gap is associated with the usual d–wave gap, and the inner gap is a complicated function of the coupling and order parameter (Eqn. (41)). As the coupling was increased, however (Fig. 10), the outer gap became unrecognizable and the total DOS became very similar to that for a single layer system in which there is only one gap.

Perhaps the most important generalization which follows from this paper, then, is that the interference of the interlayer coupling and the superconducting mean field can produce surprising behaviour. One implication of this is that for a system like YBa$_2$Cu$_3$O$_7$, where gap–like features have been observed in tunneling and Raman scattering experiments, it could be very wrong to simply associate these features directly with the order parameter.

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APPENDIX: LOW ENERGY DOS

In this section we will derive the low energy approximation for the density of states in the case in which $|\sigma_1\mu_2 - \sigma_2\mu_1|/(\sigma_1 + \sigma_2) \gg \Delta_k, \omega$. One immediate consequence of this condition is that we can ignore terms in the DOS (equation (14)) containing $\delta(w \pm E_\pm)$ since
\[ E_+^2 \geq \max(\xi_1^2, \xi_2^2) \geq \left[ \frac{\sigma_1\mu_2 - \sigma_2\mu_1}{\sigma_1 + \sigma_2} \right]^2. \]  

This leaves us to consider the contributions to the DOS made by \( E_- \). Eqn. (31) is our first approximation to \( E_- \) at low energies and we recall that it is zero whenever \( \xi_1 = \xi_1^{(i)}, \xi_2 = \xi_2^{(i)} \), and \( \Delta_k = 0 \) with \( i = 1, 2 \) and \( \xi_j^{(i)} \) given by Eqn. (32). We will proceed by considering the contributions from the neighbourhoods of the two zeros of \( E_- \) separately, and we break the integral in Eqn. (14) into a sum of two integrals which are centred about each of these zeros. We define the coordinates

\[ \eta^{(i)} = \xi_1 - \xi_1^{(i)} \quad (A2) \]

and expand \( E_- \) to lowest order in \( \eta^{(i)} \) and \( \Delta_k \):

\[ E_-^2 \sim a^{(i)2}\eta^{(i)2} + b^{(i)2}\Delta_k^2 \quad (A3) \]

with

\[
a^{(i)} = \frac{\sigma_1\xi_2^{(i)} + \sigma_2\xi_1^{(i)}}{\sigma_1(\xi_1^{(i)} + \xi_2^{(i)})} \\
b^{(i)} = \frac{\xi_2^{(i)2}}{t^2 + \xi_2^{(i)2}}.
\]

The Jacobian for the transformation \((k_x, k_y) \to (\eta^{(i)}, \Delta)\) (where \( \Delta \equiv \Delta_k \)) is

\[
J = \frac{1}{4\sigma_1\Delta_0 \sin(k_x) \sin(k_y)} = \frac{\Delta_0}{\sigma_1\sqrt{[\Delta_+^2 - \Delta^2][\Delta_-^2 - \Delta^2]}} \quad (A4)
\]

with

\[
\alpha_\pm = 2\Delta_0 \left[ 1 \pm \frac{\eta^{(i)} + \mu_1 + \xi_1^{(i)}}{4\sigma_1} \right].
\]

This transformation maps the square \( 0 < k_x, k_y \leq \pi \) into a diamond shaped region whose boundaries are given by the lines \( \Delta = \pm \alpha_- \), \(-4\sigma_1 - \mu_1 - \xi_1^{(i)} \leq \eta^{(i)} \leq 4\sigma_1 - \mu_1 - \xi_1^{(i)} \). Then

\[
\int_0^\pi dk_x \int_0^\pi dk_y \to \int_{-4\sigma_1 - \mu_1 - \xi_1^{(i)}}^{4\sigma_1 - \mu_1 - \xi_1^{(i)}} d\eta^{(i)} \int_{\alpha_-}^{\alpha_+} d\Delta J(\eta^{(i)}, \Delta). \quad (A5)
\]
Since we are interested in small $\omega$, we make the further approximation that

$$\alpha_\pm \sim 2\Delta_0 \left[1 \pm \frac{|\mu_1 + \xi_1^{(i)}|}{4\sigma_1} \right]. \quad \text{(A6)}$$

We can now interchange the order of integration in (A5) so that for small positive $\omega$, 

$$\rho_j(\omega) = \frac{16}{N} \sum_{k_x,k_y=0}^{\pi} \sum_{j=0}^{\pi/d} U_{(2j-1)2}^2 \delta(w - E_-) \approx \frac{2\Delta_0 d}{\sigma_1 \pi^3} \sum_{i=1}^{\pi/d} dk_z \int_{-\alpha_-}^{\alpha_+} d\Delta \int_{-4\sigma_1-\mu_1}^{4\sigma_1-\mu_1} d\eta^{(i)} \frac{U_{(2j-1)2}^2 \delta(w - E_-)}{\sqrt{[\alpha_+^2 - \Delta^2][\alpha_-^2 - \Delta^2]}}. \quad \text{(A7)}$$

Finally, in the limit of small $\omega$,

$$U_{12}^2 \sim \frac{1}{2} \frac{\xi_2^{(i)2}}{t^2 + \xi_2^{(i)2}} \left[1 - \frac{a^{(i)}\eta^{(i)}}{\omega} \right], \quad \text{(A8a)}$$

$$U_{32}^2 \sim \frac{1}{2} \frac{t^2}{t^2 + \xi_2^{(i)2}} \left[1 + \frac{a^{(i)}\eta^{(i)}}{\omega} \right]. \quad \text{(A8b)}$$

The term $a^{(i)}\eta^{(i)}/\omega$ is not small but it is odd in $\eta^{(i)}$ and will vanish in the integration.

We perform the integral over $\eta^{(i)}$ in (A7) to get 

$$\rho_j(\omega) = \frac{4d\Delta_0 \omega}{\sigma_1 \pi^3} \sum_{i=1}^{\pi/d} dk_z \frac{U_j^2}{|a^{(i)}b^{(i)}|} \int_{-\Delta_{\text{max}}}^{\Delta_{\text{max}}} d\Delta \int_{-4\sigma_1-\mu_1}^{4\sigma_1-\mu_1} d\eta^{(i)} \frac{U_{(2j-1)2}^2 \delta(w - E_-)}{\sqrt{[\alpha_+^2 - \Delta^2][\alpha_-^2 - \Delta^2][(\omega/b)^2 - \Delta^2]}} \quad \text{(A10)}$$

where $\Delta_{\text{max}} = \min(\alpha_-, \omega/b^{(i)})$ and 

$$U_{1}^2 = \frac{\xi_2^{(i)2}}{t^2 + \xi_2^{(i)2}} \quad \text{(A9a)}$$

$$U_{2}^2 = \frac{t^2}{t^2 + \xi_2^{(i)2}} \quad \text{(A9b)}$$

If $\Delta_{\text{max}} = \omega/b^{(i)}$ then the energy surface $E_- = \omega$ is completely contained within the Brillouin zone. The integral over $\Delta$ can also be done analytically to give 

$$\rho_j(\omega) = \frac{4d\Delta_0 \omega}{\sigma_1 \pi^3} \sum_{i=1}^{\pi/d} dk_z \frac{U_j^2}{|a^{(i)}|} \frac{1}{\sqrt{\lambda_+}} K \left[ \frac{\lambda_+ - \lambda_-}{\lambda_+} \right]. \quad \text{(A10)}$$

The function, $K(x)$, is the complete elliptic integral. If $\omega < \alpha_+ b^{(i)}$ then 

$$\lambda_\pm = \alpha_+^2 [(\alpha_- b^{(i)})^2 + \omega^2] - 2(\omega \alpha_-)^2$$

$$\pm 2\omega \alpha_- \sqrt{[(\alpha_+ b^{(i)})^2 - \omega^2][\alpha_+^2 - \alpha_-^2]} \quad \text{(A11a)}$$
while if $\omega > \alpha + b(i)$ then
\[
\lambda_\pm = \omega^2(\alpha_+^2 + \alpha_0^2) - 2(\alpha_+\alpha_-b(i))^2 \
\pm 2(\alpha_+\alpha_-)\sqrt{[\omega^2 - (\alpha_+b(i))^2][\omega^2 - (\alpha_-b(i))^2]}.
\]

(A11b)

There is nothing special about $\omega = \alpha + b(i)$ and the integrand in (A10) is featureless at these points. On the other hand, $\lambda_-$ vanishes at $\omega = \alpha - b(i)$ and $K[(\lambda_+ - \lambda_-)/\lambda_+]$ diverges logarithmically. The integration over $k_z$ reduces the divergence to a peaked structure. The magnitude of these peaks in each of the densities of states is dictated by $U^2_j$.

The complexity of (A10) prevents us from performing the final integral analytically without further assumptions. So far we have used the fact that $\Delta_0$ and $\omega$ are small and we now add to this the assumption that $t_0$ is small. For one value of $i$,
\[
(-1)^i \text{sgn}(\mu_2\sigma_1 - \mu_1\sigma_2) = 1,
\]
and
\[
\xi_1^{(i)} \sim (\mu_2\sigma_1 - \mu_1\sigma_2)/\sigma_2, \quad \xi_2^{(i)} \sim \sigma_2 t^2/(\mu_2\sigma_1 - \mu_1\sigma_2), \quad a^{(i)} \sim \sigma_2/\sigma_1, \quad b^{(i)} = U_1^2 \sim (\sigma_2 t)^2/(\mu_2\sigma_1 - \mu_1\sigma_2)^2, \quad U_2^2 \sim 1, \quad \text{and} \quad \alpha^\pm \sim 2\Delta_0[1 \pm |\mu_2|/4\sigma_2].
\]
For the remaining value of $i$,
\[
(-1)^i \text{sgn}(\mu_2\sigma_1 - \mu_1\sigma_2) = -1,
\]
and
\[
\xi_1^{(i)} \sim -\sigma_1 t^2/(\mu_2\sigma_1 - \mu_1\sigma_2), \quad \xi_2^{(i)} \sim -(\mu_2\sigma_1 - \mu_1\sigma_2)/\sigma_1, \quad a^{(i)} \sim b^{(i)} = U_1^2 \sim 1, \quad U_2^2 \sim (\sigma_1 t)^2/(\mu_2\sigma_1 - \mu_1\sigma_2)^2, \quad \text{and} \quad \alpha^\pm \sim 2\Delta_0[1 \pm |\mu_1|/4\sigma_1].
\]
Substituting this into (A10) gives
\[
\rho_1 \sim \frac{4\Delta_0\omega}{\sigma_1\pi^2} \frac{1}{\sqrt{\lambda_+}} K \left[ \frac{\lambda_+ - \lambda_-}{\lambda_+} \right] 
+ \frac{4d\Delta_0\omega}{\pi^3} \frac{\sigma_2}{[\mu_2\sigma_1 - \mu_1\sigma_2]^2} \int_0^{\pi/d} dk_z \frac{1}{\sqrt{\lambda_+}} K \left[ \frac{\lambda_+ - \lambda_-}{\lambda_+} \right].
\]

(A14)

The first term is for $i$ given by (A13) and has $\lambda_\pm$ given by (A11a) since $b^{(i)} \sim 1$. The second term is for $i$ given by (A12) and, since $b^{(i)}$ is a function of $k_z$, $\lambda_\pm$ will be given by (A11a).
when \( t(k_z) > t^* \) and by (A11b) when \( t(k_z) < t^* \). The value of \( t^* \) comes directly from the condition \( \omega = \alpha_+ b^{(i)} \):

\[
t^* (\omega) = \frac{2 \omega}{\Delta_0 \sigma_2 [4 \sigma_2 + |\mu_2|]} |\mu_2 \sigma_1 - \mu_1 \sigma_2|.
\] (A15)

In order to solve the final integral in (A14), we make the crude approximation that \( \lambda_\pm \) can be replaced by the limiting forms \( \lambda_\pm (t \ll t^*) = \omega^2 [\alpha_+ \pm \alpha_-] \) when \( t < t^* \), and \( \lambda_\pm (t \gg t^*) = \alpha_+ \alpha_- b^{(i)} \) when \( t > t^* \). Essentially, the point of this approximation is that in regions of the Brillouin zone where the induced gap is smaller than \( \omega \), the second sublattice is treated as normal, while in the remaining regions, \( \omega \) is treated as much smaller than the induced gap.

We find that \( \rho_1 (\omega) \sim \rho_1' (\omega) + \rho_1'' (\omega) \) with

\[
\rho_1' (\omega) = \frac{4 \Delta_0 \omega}{\sigma_1 d \pi^2} \frac{1}{\sqrt{\lambda_+}} K \left[ \frac{\lambda_+ - \lambda_-}{\lambda_+} \right]
\] (A16a)

and

\[
\rho_1'' (\omega) = \frac{\sigma_2 t_0^2}{\pi^3 |\mu_2 \sigma_1 - \mu_1 \sigma_2|^2} K \left[ 1 - \frac{\mu_2^2}{16 \sigma_2^2} \right]
 \times \left[ \frac{\pi}{2} - \cos^{-1} \left( \frac{t^*}{t_0} \right) - \frac{t^*}{t_0} \sqrt{1 - \left( \frac{t^*}{t_0} \right)^2} \right]
 \times \left[ \frac{4 \sigma_2 t_0^2}{\pi^2 |\mu_2 \sigma_1 - \mu_1 \sigma_2|^2} \right]^{1 - \cos^{-1} \left( \frac{t^*}{t_0} \right)} (A16b)
\]

when \( t^*(\omega) < t_0 \), and

\[
\rho_1'' = \frac{\sigma_2 t_0^2}{2 \pi^2 |\mu_2 \sigma_1 - \mu_1 \sigma_2|^2} K \left[ 1 - \frac{\mu_2^2}{16 \sigma_2^2} \right]
\] (A16c)

when \( t^*(\omega) < t_0 \). Equation (A16a) is just the DOS which would result in the decoupled \( t_0 = 0 \) limit. Equation (A16b) shows that the interlayer coupling induces an inner gap for \( t^*(\omega) < t_0 \) (which is the prediction made in Eqn. (35)). The width of this gap is proportional to \( t_0^2 \) and is difficult to see for weak interlattice coupling.

We can find the DOS in the second sublattice, \( \rho_2 \), in an analogous manner:

\[
\rho_2 (\omega) \sim \frac{2}{\sigma_2 \pi^3} K \left[ 1 - \frac{\mu_2^2}{16 \sigma_2^2} \right] \left[ \frac{\pi}{2} - \cos^{-1} \left( \frac{t^*}{t_0} \right) \right]
\]
\[ + \frac{4t^*}{\sigma^2 \pi^2 t_0^2} \left[ 1 - \frac{|\mu_2|}{4\sigma_2} \right]^{-1} \sqrt{\left( \frac{t_0}{t^*} \right)^2 - 1} \]
\[ + \frac{\omega t_0^2\sigma_1}{4\pi \Delta_0} [\mu_2\sigma_1 - \mu_1\sigma_2]^{-2} \left[ 1 - \frac{\mu_1^2}{16\sigma_1^2} \right]^{-1} \]  
\[ (A17a) \]

when \( t^* < t_0 \) and

\[ \rho_2(\omega) \sim \frac{1}{\sigma_2^2} K \left[ 1 - \frac{\mu_2^2}{16\sigma_2^2} \right] \]
\[ + \frac{\omega t_0^2\sigma_1}{4\pi \Delta_0^2} [\mu_2\sigma_1 - \mu_1\sigma_2]^{-2} \left[ 1 - \frac{\mu_1^2}{16\sigma_1^2} \right]^{-1} \]  
\[ (A17b) \]

when \( t^* > t_0 \). Again we see that there is an induced gap for \( t^*(\omega) < t_0 \), due to the interactions of the sublattices. For \( t^*(\omega) > t_0 \), \( \rho_2(\omega) \) is just the normal state DOS at the Fermi surface with corrections of order \( t_0^2 \) due to the adjacent layers. In Fig. 7 we graph the low energy DOS calculated from equations (11), (A10) and from our analytical approximations. We see that, although our analytic expressions for \( \rho_1 \) and \( \rho_2 \) tend to overestimate the size of the inner gap, they contain the essential description of the DOS.
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FIGURES

FIG. 1. $T_c$ and $\Delta_0(T = 0)/T_c$ vs $t_0$. The model parameters are $\sigma_1 = 1$, $\sigma_2 = 0.6$, $\mu_1 = -0.8$, $\mu_2 = 0.4$

FIG. 2. Quasiparticle energy dispersion along the line $k_x = k_y$, $k_z = 0$. We have chosen an s–wave gap for purposes of illustration since a d–wave gap vanishes along this line. The features which are important for our discussion of the density of states are the two minima of $E_-$, which are related to the intrinsic and induced gaps, and the two avoided band crossings. The parameters are $\sigma_1 = 1$, $\sigma_2 = 0.6$, $\mu_1 = \mu_2 = -0.8$, $t_0 = 0.2$, $\Delta_0 = 0.1$

FIG. 3. Density of states in the normal and superconducting sublattices for the uncoupled limit. There are logarithmic divergences at $\omega \sim -\mu_1, -\mu_2$ due to the intrinsic van Hove singularities of $\xi_1$ and $\xi_2$. There is also a d–wave gap at the Fermi surface in the first sublattice. The choices of parameters are $\sigma_1 = 1$, $\sigma_2 = 0.6$, $\mu_1 = \mu_2 = 0.8$, $t_0 = 0.01$, $\Delta_0 = 0.1$, $T_c = 0.086$

FIG. 4. Density of states in the normal and superconducting sublattices. Here the bands $\xi_1$ and $\xi_2$ cross away from their van Hove singularities. In addition to the intrinsic singularities at $\omega \sim -\mu_1, -\mu_2$ and the d–wave gap in $\rho_1$ there are two gap–like structures at $\omega \sim \pm 0.55$. There is also an induced gap at the Fermi surface in $\rho_2$ which is too small to show on this plot. The parameters are $\sigma_1 = 1$, $\sigma_2 = 0.6$, $\mu_1 = -0.8$, $\mu_2 = 0.4$, $t_0 = 0.1$, $\Delta_0 = 0.09$, $T_c = 0.086$

FIG. 5. Density of states in the normal and superconducting sublattices. This figure shows the effect of increasing the interlayer coupling on Fig. 4. The smearing of the logarithmic singularities by the third dimension is clearly evident. The induced gap at the Fermi surface is now visible (although the fact that $\rho_2(0) = 0$ is not clear in the plot), and the gap–like structures away from the Fermi surface are much larger, and shifted slightly, as we would expect from Eqn. (28). Here we have $\sigma_1 = 1$, $\sigma_2 = 0.6$, $\mu_1 = -0.8$, $\mu_2 = 0.4$, $t_0 = 0.4$, $\Delta_0 = 0.15$, $T_c = 0.086$
FIG. 6. Density of states in the normal and superconducting sublattices. In this case, the van Hove singularities intrinsic to the sublattice dispersions at \( \omega \sim 0.8 \) are strongly suppressed by an avoided band crossing. This should be compared with Fig. 3, where the interlayer coupling is the same, but the intrinsic van Hove singularities of \( \xi_1 \) and \( \xi_2 \) can still be identified. The other interesting feature of this figure is that we can see clearly that the induced gap is reflected in \( \rho_1 \). We should also note again that \( \rho_2 \) actually vanishes at \( \omega = 0 \). Here \( \sigma_1 = 1, \sigma_2 = 0.6, \mu_1 = \mu_2 = -0.8, t_0 = 0.4, \Delta_0 = 0.15, T_c = 0.086 \).

FIG. 7. Low frequency densities of states: (a) Determined numerically from the exact expression, Eqn. (14) (b) Determined numerically from the approximate expression, Eqn. (A10) (c) Determined from the approximate analytical expressions (A16) and (A17). The model parameters are \( \sigma_1 = 1, \sigma_2 = 0.6, \mu_1 = \mu_2 = -0.8, t_0 = 0.2, \Delta_0 = 0.15 \).

FIG. 8. Quasiparticle energy dispersion along the lines (a) \( k_x = k_y, k_z = 0 \) and (b) \( k_x = k_y, k_z = \pi \) for an s–wave gap. In this case, the Fermi surfaces of \( \xi_1 \) and \( \xi_2 \) coincide. Whether or not \( E_- \), has a single minimum or double minimum structure depends on the value of \( t(k) \) (see eqn. (39)). The parameters are \( \sigma_1 = 1, \sigma_2 = 0.6, \mu_1 = -0.8, \mu_2 = -0.48, t_0 = 0.2, \Delta_0 = 0.1 \).

FIG. 9. Density of states. The Fermi surfaces of \( \xi_1 \) and \( \xi_2 \) are coincident. In addition to the intrinsic singularities at \( \omega \sim -\mu_1, -\mu_2 \), there is a nested gap structure at the Fermi surface. The outer gap is related to the usual d–wave gap in a 2–dimensional superconductor while the inner gap comes from a mixture of band structure and superconductivity effects. The parameters are \( \sigma_1 = 1, \sigma_2 = 0.6, \mu_1 = -0.8, \mu_2 = -0.48, t_0 = 0.1, \Delta_0 = 0.09, T_c = 0.086 \).

FIG. 10. Density of states. Again the Fermi surfaces of \( \xi_1 \) and \( \xi_2 \) are coincident. The increased interlayer coupling has changed the appearance of the DOS considerably from Fig. 3. The outer gap no longer exists and the gap which remains has a complicated dependency on both \( t_0 \) and \( \Delta_0 \). This DOS would not be simple to distinguish from that of a 2–dimensional d–wave superconductor in a tunneling experiment, even though the physics of the two systems is different. The parameters are \( \sigma_1 = 1, \sigma_2 = 0.6, \mu_1 = -0.8, \mu_2 = -0.48, t_0 = 0.4, \Delta_0 = 0.15, T_c = 0.086 \).
FIG. 11. Feynman diagram representation of the equations for $G_{11}$: (a) and (b) are diagrammatic forms of Eqns. (50a) and (50b) respectively. These equations form a self consistent set. In (c), the final term in (a) is iterated once, using (b), to give the lowest order effect of the mixing of interlayer coupling and the mean–field. Thick lines represent full Green’s functions, thin lines represent uncoupled Green’s functions, rightward pointing arrows represent spin up electrons, leftward pointing arrows represent spin down holes and vertical dashed lines represent interlayer hopping.
