The Neutron Peak in the Interlayer Tunneling Model of High Temperature Superconductors

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Recent neutron scattering experiments in optimally doped YBCO exhibit an unusual magnetic peak that appears only below the superconducting transition temperature. The experimental observations are explained within the context of the interlayer tunneling theory of high temperature superconductors. [S0031-9007(97)03080-9]

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Many experimental observations in high temperature superconductors are commonly fit with a phenomenological model that derives from the original theory of Bardeen, Cooper, and Schrieffer (BCS). The model is characterized by a gap equation corresponding to a presumed symmetry of the order parameter, with an adjustable dimensionless coupling constant, and a given Fermi surface. Although a microscopic derivation of this effective model for the high temperature superconductors does not exist, the model is still used with a considerable degree of confidence. The main difficulties, to which we return below, are the unusual normal state properties of these materials and the enormously high transition temperatures, but there are many others. Such difficulties are extensively surveyed in the literature [1].

In the absence of a microscopic derivation, it is useful to ask if this phenomenological BCS model is unique and if an alternative phenomenological model exists that is capable of capturing features of these superconductors. One such physically motivated model, the interlayer tunneling model, was elaborated in a recent paper [2]. In the present Letter we use this model to interpret the startling neutron scattering experiments in optimally doped YBCO [3].

The experiments show that there are no sharp, or even broad, features in the magnetic excitation spectrum in the normal state. In contrast, the superconducting state exhibits a distinct magnetic feature located at an energy of 41 meV and near a wave vector $(\pi/a, \pi/a, \pi/c_b)$, where a is the lattice spacing of the square-planar CuO lattice, and c_b is the distance between the layers within a bilayer. While the peak is very sharp in energy, its momentum width is of the order of $0.1\pi - 0.2\pi$, more than the experimental resolution. The intensity under the peak vanishes at the transition temperature, but its frequency softens very little. Many explanations have been offered [4]. However, none of these explanations is fully microscopic, nor fully consistent with all the observed features.

In this Letter, we present quantitative but illustrative computations of the neutron scattering intensity and show that many of the experimental features are captured well. The theory discussed here has two important aspects: (1) The peak at $\mathbf{Q} = (\pi/a, \pi/a)$ is a combined effect of the coherence factor and the special geometry of the scattering surface in the interlayer tunneling model; (2) there is a preferential pairing in a state even in the interchange of the layers, which gives rise to the observed c-axis selection rule, that is, scattering from the even to the odd state.

The model Hamiltonian, motivated earlier [2], is that of a bilayer complex. It is

$$H = \sum_{k\sigma i} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma i} c_{\mathbf{k}\sigma i} - \sum_{\mathbf{q},\mathbf{k},\mathbf{k}',\sigma,\sigma',i} V_{\mathbf{q},\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\sigma i} c^{\dagger}_{-\mathbf{k}+\mathbf{q}\sigma' i} c_{-\mathbf{k}'+\mathbf{q}\sigma' i} c_{\mathbf{k}'\sigma i} - \sum_{\mathbf{q},\mathbf{k},\sigma,\sigma',i\neq j} T_J(\mathbf{q},\mathbf{k}) \times [c^{\dagger}_{\mathbf{k}\sigma i} c^{\dagger}_{-\mathbf{k}+\mathbf{q}\sigma' i} c_{-\mathbf{k}+\mathbf{q}\sigma' j} c_{\mathbf{k}\sigma j} + \mathrm{H.c.}]. \tag{1}$$

Here $i = 1, 2$ is the layer index. The fermion operators are labeled by the spin σ and the in-plane wave vector $\mathbf{k}$; V is the in-plane pairing interaction. This Hamiltonian incorporates the unique feature of the interlayer mechanism, that tunneling occurs with conservation of transverse momentum $\mathbf{k}$. Therefore, the momentum sum in the T_J term is only over $\mathbf{k}$ and $\mathbf{q}$. Disorder between the layers is weak, and even disorder would not affect this crucial difference between the tunneling and interaction terms.

Only in the subspace in which both the states $(\mathbf{k}\uparrow)$ and $(-\mathbf{k}\downarrow)$ are both simultaneously occupied or unoccupied, is the following reduced Hamiltonian sufficient:

$$H_{\mathrm{red}} = \sum_{\mathbf{k}\sigma i} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma i} c_{\mathbf{k}\sigma i} - \sum_{\mathbf{k},\mathbf{k}',i} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow i} c^{\dagger}_{-\mathbf{k}\downarrow i} c_{-\mathbf{k}'\downarrow i} c_{\mathbf{k}'\uparrow i} - \sum_{\mathbf{k},i\neq j} T_J(\mathbf{k}) [c^{\dagger}_{\mathbf{k}\uparrow i} c^{\dagger}_{-\mathbf{k}\downarrow i} c_{-\mathbf{k}\downarrow j} c_{\mathbf{k}\uparrow j} + \mathrm{H.c.}]. \tag{2}$$

This is because these are the only matrix elements that survive.

An important feature of our model Hamiltonian is the absence of the coherent single particle tunneling term that would lead to a splitting of the bands. The splitting and the corresponding c-axis velocity are not observed in experiments on transport in any cuprates. The definitive photoemission experiment has been carried out only on BISCO, where firm evidence for the absence of splitting is found [5]. Although observation of splitting was claimed in YBCO [6], the observed "splitting" does not resemble that predicted by band theory and is not confirmed by seeing superconducting coherence peaks at separate Fermi momenta, which are the only clean demonstrations of Fermi surfaces.

Incoherence does not preclude a particle-hole pair tunneling term [2,7], however, because it is generated by a second order *virtual* process. For underdoped materials exhibiting "spin gap" phenomena [8], this term is essential [9]. For mathematical convenience, we shall neglect the superexchange term for the moment and return to it below. Moreover, the electron operators will be treated as anticommuting fermion operators, which is only an approximation for a non-Fermi liquid [7].

The mean field analysis leads to the gap equation [2]

$$\Delta_{\mathbf{k}} = \frac{1}{1 - \chi_{\mathbf{k}} T_J(\mathbf{k})} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \chi_{\mathbf{k}'} \Delta_{\mathbf{k}'}, \tag{3}$$

where $\chi_{\mathbf{k}} = (1/2E_{\mathbf{k}})\tanh(E_{\mathbf{k}}/2T)$ is the pair susceptibility, with $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}$. Here μ is the chemical potential. Note that, until now, we have not specified the symmetry of the in-plane pairing kernel. In Ref. [2] this gap equation was solved with a s-wave in-plane kernel to accommodate the anomalous isotope effect measurements. However, it was stressed that the interlayer gap equation is indifferent to the actual in-plane pairing mechanism, and other mechanisms such as spin fluctuations could operate. From phase sensitive Josephson measurements, it appears that the gap is of $d_{x^2-y^2}$ symmetry. Therefore, for the purposes of the present Letter, we shall assume that $V_{\mathbf{k},\mathbf{k}'} = V g_{\mathbf{k}} g_{\mathbf{k}'}$, where $g_{\mathbf{k}} = \frac{1}{2}[\cos(k_x a) - \cos(k_y a)]$.

The point of our Letter is that the interlayer pair tunneling must dominate to account for the experimental observations, and, in this limit, the role of the in-plane pairing kernel is simply to anchor the symmetry of the order parameter in place. To see this, consider the solution of the gap equation at $T = 0$ when the in-plane pairing is precisely zero. Then it is possible to determine only the magnitude of the gap, and it is

$$|\Delta_k| = \sqrt{\frac{T_J^2(k)}{4} - (\varepsilon_k - \mu)^2}\, \theta\left(\frac{T_J(k)}{2} - |\varepsilon_k - \mu|\right). \tag{4}$$

Now consider the full gap equation at $T = 0$ and on the Fermi surface, assuming that the gap is real (time-reversal invariant). Then

$$\Delta_{\mathbf{k}_F} = g_{\mathbf{k}_F} \Delta_0 + \frac{T_J(\mathbf{k}_F)}{2} \operatorname{sgn}(\Delta_{\mathbf{k}_F}), \tag{5}$$

where Δ_0 is the positive definite integral over the in-plane pairing kernel, assuming that this kernel is attractive [10]. The solution is

$$\Delta_{\mathbf{k}_F} = \operatorname{sgn}(g_{\mathbf{k}_F}) |\Delta_{\mathbf{k}_F}|, \tag{6}$$

which holds regardless of the magnitude of Δ_0, even when $\Delta_0 \to 0$. By continuity, the symmetry is the same even away from the Fermi surface. Thus, the in-plane pairing kernel acts as a symmetry breaking field in the space of the symmetries of the order parameter. [The solution $\operatorname{sgn}(\Delta_{\mathbf{k}_F}) = -\operatorname{sgn}(g_{\mathbf{k}_F})$ cannot hold uniformly over the Fermi surface; the mixed solution has higher energy.]

For quantitative calculations, the in-plane one electron dispersion will be chosen to be $\varepsilon_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a)] + 4t' \cos(k_x a)\cos(k_y a)$. We adopt a representative set of parameters. These are $t = 0.25$ eV, $t' = 0.45t$, and $\mu = -0.315$ eV, corresponding to an open Fermi surface, with a hand filling of 0.86. The choice of these parameters is not critical to our theory, nor do we believe that the van Hove singularity is a prominent feature. The quantity $T_J(\mathbf{k})$ was first proposed to be $T_J(\mathbf{k}) = (T_J/16)[\cos(k_x a) - \cos(k_y a)]^4$ in Ref. [2] on the basis of symmetry and analyticity arguments. The validity of this expression is now strengthened by detailed electronic structure calculations [11].

The magnetic neutron scattering intensity is proportional to the imaginary part of the spin susceptibility $\chi(\mathbf{q}, \omega)$, which for the above model is simply the expression

$$\chi(\mathbf{q}, \omega) = \sum_{\mathbf{k}} \left[\frac{A^+_{\mathbf{k},\mathbf{q}} F^-_{\mathbf{k},\mathbf{q}}}{\Omega^1_{\mathbf{k},\mathbf{q}}(\omega)} + \frac{A^-_{\mathbf{k},\mathbf{q}}(1 - F^+_{\mathbf{k},\mathbf{q}})}{2} \times \left(\frac{1}{\Omega^{2+}_{\mathbf{k},\mathbf{q}}(\omega)} - \frac{1}{\Omega^{2-}_{\mathbf{k},\mathbf{q}}(\omega)} \right) \right], \tag{7}$$

where

$$A^{\pm}_{\mathbf{k},\mathbf{q}} = \frac{1}{2}\left[1 \pm \frac{(\varepsilon_{\mathbf{k}} - \mu)(\varepsilon_{\mathbf{k+q}} - \mu) + \Delta_{\mathbf{k}}\Delta_{\mathbf{k+q}}}{E_{\mathbf{k}} E_{\mathbf{k+q}}} \right], \tag{8}$$

$\Omega^1_{\mathbf{k},\mathbf{q}}(\omega) = \omega - (E_{\mathbf{k+q}} - E_{\mathbf{k}}) + i\delta$, $\Omega^{2\pm}_{\mathbf{k},\mathbf{q}}(\omega) = \omega \pm (E_{\mathbf{k+q}} + E_{\mathbf{k}}) + i\delta$, $F^{\pm}_{\mathbf{k},\mathbf{q}} = f(E_{\mathbf{k+q}}) \pm f(E_{\mathbf{k}})$, and $f(x)$ is the Fermi function.

Note that near $T = 0$ only the A^- term contributes, and this is negligible unless $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{k+q}}$ are of opposite sign, as noted in Ref. [13]. In fact, nothing is observed for $q \approx 0$ or 2π, as expected, and due to the coherence factor the peak is reasonably localized at $\mathbf{q} = \mathbf{Q}$, where $Q = (\pi/a, \pi/a)$. At higher temperatures, the A^+ term is temperature dependent, but almost independent of frequency for experimentally relevant frequencies. The χ with the A^+ term omitted will be denoted by $\bar{\chi}$.

At $T = 0$, Im $\bar{\chi}$ is calculated by solving the gap equation for a set of T_J, and with $\lambda \equiv N(0)V = 0.184$, where

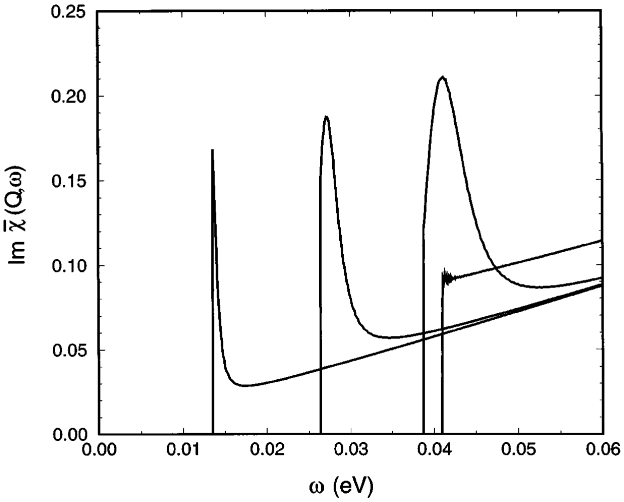

FIG. 1. Im $\bar{\chi}$ at $T = 0$. From left to right, $T_J = 0.025$, 0.05, and 0.075 eV. The curve corresponding to a step discontinuity at the edge is for BCS, with the d-wave gap $\Delta_{\mathbf{k}} = (\Delta_{\max}/2)[\cos(k_x a) - \cos(k_y a)]$, $\Delta_{\max} = 0.025$ eV.

$N(0)$ is the density of states per spin at the Fermi energy [$V = 0.2$ eV, $N(0) = 0.92$]. The intensities at $\mathbf{q} = \mathbf{Q}$, are shown in Fig. 1. While the interlayer model shows a peak at the threshold, the pure BCS case ($T_J = 0$) shows only a step discontinuity. For illustrative purpose, Im $\bar{\chi}$, for $T \neq 0$, was calculated for $\lambda = 0.184$ and $T_J = 0.075$ eV. No attempts were made to fit precisely the experimental data. The results are plotted in Fig. 2.

The intensities under the peak, calculated by fitting a linear background at high energies, are shown in Fig. 3. The results agree well with experiments. The softening of the position of the peak, shown in Fig. 3, is weaker than the falloff of the intensity; the experimental softening is even weaker, however.

We now address why Im $\bar{\chi}$ exhibits a peak in the interlayer tunneling model, while the BCS model exhibits only a step discontinuity at the threshold (see Fig. 1). An unusual feature of the interlayer gap [12] is that when T_J dominates, as is necessarily so for high T_c, the density of states is sharply peaked at $T_J/2$ and the electrons with $|\varepsilon_{\mathbf{k}} - \mu| > T_J(\mathbf{k})/2$ are unaffected by pairing [see Eq. (4)], in contrast to BCS where the effects of the gap extend out to high energies. Because the superconducting region around the Fermi line is very narrow, as shown in Fig. 4, the scattering surface is radically different from the BCS case. For simplicity, let $T = 0$, and set the coherence factor to unity. The image of the superconducting region including the Fermi line under $\mathbf{k} \to \mathbf{Q} - \mathbf{k}$ is shown in Fig. 4. The contributions come from the diamond shaped overlap regions in which both $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{Q}-\mathbf{k}}$ are finite. For the lower diamond, we can write $E_{\mathbf{k}} \approx (T_J/2)\cos^4(da/\sqrt{2})$, where d is the distance from $(\pi/a, 0)$. The corresponding constant ω contours are the arcs shown in Fig. 4. As ω increases, the length increases approximately linearly within the diamond, and then drops approximately linearly, hence the peak in the scattering intensity at $T_J(\mathbf{k}_0)$, where $\mathbf{k}_0$ denotes the center

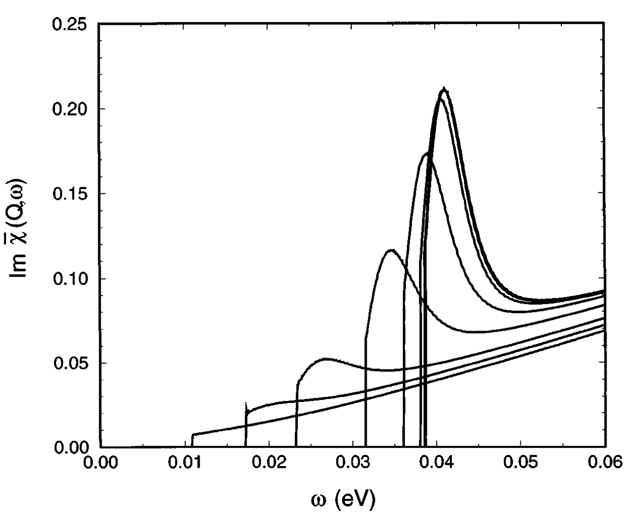

FIG. 2. Im $\bar{\chi}$ for $T_J = 0.075$ eV. From left to right, $T =$ 120, 110, 100, 80, 60, 40, 20, and 0 K. The results for $T = 0$ and 20 K are almost indistinguishable.

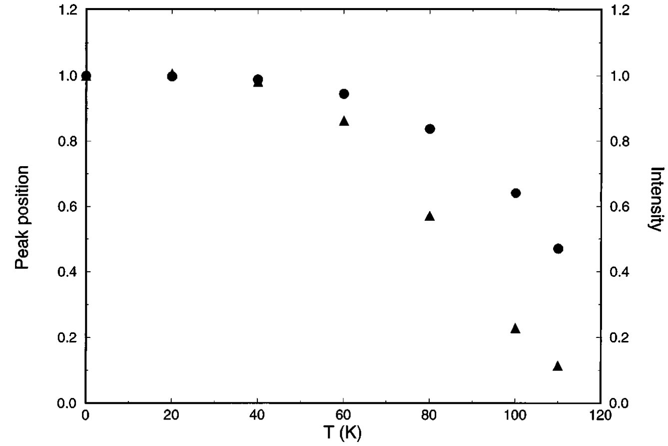

FIG. 3. The intensity (solid triangles) and the position of the peak (filled circles) normalized to the zero temperature values. The position of the peak is at 41.2 meV at $T = 0$.

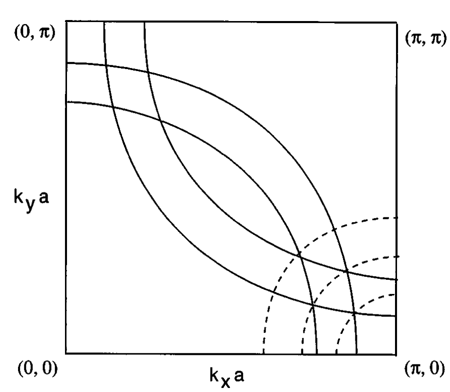

FIG. 4. The superconducting region and its mapping under $\mathbf{k} \to \mathbf{Q} - \mathbf{k}$. The diamond shaped overlap regions contribute to the peak of the imaginary part of the spin susceptibility. The dashed arcs are the constant ω contours centered at $(\pi, 0)$.

of the diamond. There are other momentum transfers for which the scattering intensity is finite for a gap of d symmetry. However, the intensities are considerably smaller. There are two interesting reasons for this. First, the phase space is a factor of 4 smaller. Second, for $\mathbf{q} = \mathbf{Q}$, the pairs are produced with zero center of mass momentum, because, in the interlayer model, $E_{\mathbf{k}+\mathbf{Q}} = E_{\mathbf{Q}-\mathbf{k}} = E_{-\mathbf{k}} = E_{\mathbf{k}}$. Therefore, the process is greatly enhanced over the case where the pair is produced with a finite center of mass momentum.

To understand the dependence of the scattering intensity on the momentum transfer perpendicular to the plane, it is necessary to consider the mixing of the electronic wave functions between the layers. This is a virtual mixing of the states due to second order processes and can be described by constructing the following operators [9]: $\alpha_{\mathbf{k},\sigma,1} = [c_{\mathbf{k},\sigma,1} + \eta(\mathbf{k})c_{\mathbf{k},\sigma,2}]/\sqrt{1+\eta^2(\mathbf{k})}$, and $\alpha_{\mathbf{k},\sigma,2} = [c_{\mathbf{k},\sigma,2} + \eta(\mathbf{k})c_{\mathbf{k},\sigma,1}]/\sqrt{1+\eta^2(\mathbf{k})}$, where $\eta(\mathbf{k})$ is the mixing parameter. The corresponding order parameter is $\Lambda_{\mathbf{k}} = \langle \alpha^\dagger_{\mathbf{k},\uparrow,1}\alpha^\dagger_{-\mathbf{k},\downarrow,1} + \alpha^\dagger_{\mathbf{k},\uparrow,2}\alpha^\dagger_{-\mathbf{k},\downarrow,2}\rangle$. It is also possible to *rewrite* this in terms of the operators $c^e_{\mathbf{k},\sigma} = \frac{1}{\sqrt{2}}(c_{\mathbf{k},\sigma,1} + c_{\mathbf{k},\sigma,2})$ and $c^o_{\mathbf{k},\sigma} = \frac{1}{\sqrt{2}}(c_{\mathbf{k},\sigma,1} - c_{\mathbf{k},\sigma,2})$. Thus, $\Lambda_{\mathbf{k}}$ will be a linear combination of $\langle c^{e\dagger}c^{-e\dagger}\rangle$ and $\langle c^{o\dagger}c^{-o\dagger}\rangle$, where $c^{e\dagger} \equiv c^{e\dagger}_{\mathbf{k},\uparrow}$, $c^{-e\dagger} \equiv c^{e\dagger}_{-\mathbf{k},\downarrow}$, etc.

The essential point [9] is that the consequences of the second order interaction Hamiltonian resulting from frustrated interlayer kinetic energy must reflect its origin. That is, the superconducting order parameter in a bilayer must be such as to reduce the interlayer kinetic energy $-\sum_{\mathbf{k}} t_\perp(\mathbf{k})(n^e_{\mathbf{k}} - n^o_{\mathbf{k}})$, where n are the occupancies. This reduction accounts for the pair binding energy [13]. However, there is also a superexchange interaction between the layers, analogous to, but formally quite different from that proposed by Millis and Monien [14]. Consider augmenting our Hamiltonian, Eq. (2), by this superexchange term [7]: $-\sum_{\mathbf{k},i\neq j} T_S(\mathbf{k})[c^\dagger_{\mathbf{k}\uparrow i}c_{\mathbf{k}\uparrow j}c^\dagger_{-\mathbf{k}\downarrow j}c_{-\mathbf{k}\downarrow i} + \text{H.c.}]$. If we ignore the in-plane interaction and assume that $T_S(k) = T_J(k)$, then, the total Hamiltonian is symmetric with respect to $(\mathbf{k},\uparrow,1) \leftrightarrow (\mathbf{k},\uparrow,2)$. The odd order parameter changes sign under this transformation and must vanish unless this symmetry is spontaneously broken. If $T_S(k) \neq T_J(k)$, and the in-plane interaction is present, the odd order parameter cannot, of course, vanish identically. It then becomes a dynamical question as to what the magnitudes of these order parameters are. However, if the symmetry is close, by perturbing around the symmetric Hamiltonian, it can be seen that the odd order parameter is small in comparison to the even order parameter, at least for states close to the Fermi surface. The argument for the combined Hamiltonian (pair tunneling and superexchange) goes through exactly as for the pair tunneling Hamiltonian alone.

If the above mentioned symmetry were exact, a hole would be excited only in the even state, and the corresponding electron will go into the odd state, for states which experience the gap. Note that in our theory coherent superposition of the single particle states of the layers is forbidden. This will give a perfect c-axis selection rule. However, because the symmetry is not exact, there can be some scattering at $(\pi,\pi,0)$, which is likely to be broad, and in the background, for the optimally doped YBCO, at the energies explored in current experiments. It is possible that for higher energies such scattering can rise above the background.

In conclusion, we find that these neutron results give us a surprisingly direct and complete picture of the nature of the pairing responsible for superconductivity, not only showing us the symmetry and approximate form of the gap, but even fixing the nature of the gap equation and the source of the pairing energy. In particular, the strong correlation between the layers excludes any purely interlayer mechanism for superconductivity, under our assumption—the singlet, and very plausible on other grounds—that the quasiparticle pairs do not have strong final state interactions.

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