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Do electrons change their c-axis kinetic energy upon entering the superconducting state?*

S. Chakravarty[a]

Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, California 90095-1547, USA

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Abstract. The interlayer tunneling mechanism of the cuprate high temperature superconductors involves a conversion of the confinement kinetic energy of the electrons perpendicular to the CuO-planes (c-axis) in the normal state to the pair binding energy in the superconducting state. This mechanism is discussed and the arguments are presented from the point of view of general principles. It is shown that recent measurements of the c-axis properties support the idea that the electrons substantially lower their c-axis kinetic energy upon entering the superconducting state, a change that is nearly impossible in any conventional mechanism. The proper use of a c-axis conductivity sum rule is shown to resolve puzzles involving the penetration depth and the optical measurements.

PACS. 74.20.-z Theories and models of superconducting state – 74.25.Gz Optical properties – 74.72.-hHigh-T_c compounds

1 Introduction

There are abundant indications of a remarkable mechanism of superconductivity in cuprate high temperature superconductors, known as the interlayer tunneling mechanism [1]. At its simplest, the theory is that the confinement kinetic energy of the electrons in the normal state is converted into the superconducting binding energy. From the uncertainty principle, confinement implies a kinetic energy of order $\hbar^2/2md^2$, where d is the separation between the planes. It is as though the electrons were confined in a deep potential well perpendicular (c-axis) to the CuO-planes [2]. There is considerable experimental support for this idea, although theoretical controversy persists.

The very concept of confinement of the motion of the electrons is at odds with the time honored notion of a Fermi liquid. At issue is the concept of orthogonality catastrophe in a non-Fermi liquid, which posits that the motion along the c-axis is accompanied by the overlap of many particle wave functions of N electrons, vanishing as $N \to \infty$. In the absence of controlled non-perturbative methods to treat this inherently non-perturbative phenomenon, little has been settled. It is therefore necessary to present the arguments from the point of view of general principles.

Consider the question posed in the title of this paper: "Do electrons change their c-axis kinetic energy upon entering the superconducting state?" It is useful to expand on the precise meaning of this question. In a BCS superconductor, the kinetic energy of the superconducting state is *greater* than that of the normal state [3]. The reason is that the normal state is a Fermi liquid in which the kinetic energy is diagonal, the happiest possible situation from the point of view of the kinetic energy. Therefore, any change of state must necessarily increase the kinetic energy. This increase is, however, overwhelmed by the gain in the potential energy. Thus, a BCS superconductor becomes a superconductor despite the increase in the kinetic energy. In contrast, if we considered the transition to a superconducting state from a state in which the kinetic energy is not diagonal, the driving mechanism can be the saving in the kinetic energy. The interlayer mechanism capitalizes on the possibility that the c-axis kinetic energy is frustrated in a non-Fermi liquid. The question we ask is whether or not this frustration is relieved in the superconducting state, and whether or not the phenomenology of the cuprates support this theory.

How should we view the crossover from two to three dimensions in cuprate superconductors? In particular, what is the role of the fluctuations of the phase of the superconducting order parameter? It will be shown that the issues involving phase fluctuations are separate from the issues involving the microscopic superfluid stiffness. A striking characteristic of the interlayer mechanism is that the coupling between the layers can significantly enhance this stiffness, which is nearly impossible in a conventional BCS superconductor. The phase fluctuations should, however, be similar to those in a conventional superconductor. The prospect of unifying the concepts of phase fluctuations with the concepts of interlayer tunneling then becomes apparent.

* Dedicated to J. Zittartz on the occasion of his 60th birthday

[a] e-mail: sudip@physics.ucla.edu

How can we test the change of the c-axis kinetic energy? This question is answered using a powerful sum rule for the c-axis conductivity, which, it will be shown, leads to the resolution of an apparent paradox posed by the optical measurements in these materials over the years. The paradox has been that the c-axis penetration depth estimated from the change in the kinetic energy alone is apparently the same as that obtained ignoring this change.

2 Superconductivity as a 2D to 3D crossover phenomenon

Superconductivity in cuprates can be viewed as a dimensional crossover between two (2D) and three dimensions (3D). This is an experimental fact. While the charge transport perpendicular to the CuO-planes in the normal state is indicative of an insulator, there is perfect coherence in the superconducting state. Dimensional crossovers are known even for classical statistical mechanical problems involving phase transitions, or for quantum statistical mechanical problems that can be effectively viewed in terms of order parameters with only classical fluctuations at finite temperatures. What, then, is different here? To answer this question, it is necessary to probe it more carefully.

Phase transitions in classical statistical mechanics are independent of the kinetic energy; only the potential energy is relevant. The superconducting transition in BCS superconductors can be described by a classical complex order parameter theory, namely the Ginzburg-Landau theory; quantum mechanics determines merely the parameters of this model. Thus, the kinetic energy cannot play an explicit role in this phase transition. Low dimensional superconductors are known to exhibit considerable fluctuation effects at finite temperatures that are entirely classical in nature. In dimensions less than or equal to two, the fluctuations are so severe that the order parameter vanishes. In two dimensions, a topological phase transition to a superconducting state takes place, but with a vanishing order parameter [4]. In the low temperature state, there is a finite superfluid density as determined from the current response, but no long range order.

Imagine now that two dimensional planes are stacked to form a three dimensional superconductor. Conventionally, this is described by the Lawrence-Doniach (LD) model [5], which consists of the free energy functional

$$\mathcal{F} = \sum_n \int d^2x \Big[\alpha |\psi_n|^2 + \frac{1}{2}\beta |\psi_n|^4 + \frac{\hbar^2}{2m_{\rm ab}} |\nabla \psi_n|^2 + \frac{\hbar^2}{2m_c d^2} |\psi_n - \psi_{n+1}|^2 \Big], \quad (2.1)$$

where α, β, m_{ab}, and m_c are parameters that are in general temperature dependent. The order parameter in the plane labeled n, $\psi_n(x,y)$, is a function of the 2D coordinates x and y. The bending energy in the ab-plane is expressed in terms of a gradient energy, but the energy in the perpendicular direction is written in its discrete form. This is correct, because although the coherence length in the planes is frequently much larger than the lattice spacing, it is not so in the perpendicular direction, and therefore the continuum limit cannot be taken in this direction. The minimization of this functional determines the order parameter in mean field theory, but to incorporate fluctuations it is necessary to integrate over all possible order parameter configurations in the partition function.

This is emphatically a classical model [6]. What determines the coupling between the layers? It is argued that this is due to the Josephson effect [3]. Assume for the moment that the magnitude of the order parameter is independent of n, $\psi_n = |\psi| e^{i\phi_n}$. Then, the last term in equation (2.1) is

$$\frac{\hbar^2 |\psi|^2}{2m_c d^2} [1 - \cos(\phi_n - \phi_{n+1})] \geq 0. \quad (2.2)$$

This coupling can represent the Josephson effect only close to T_c, where the Josephson coupling energy is indeed proportional to the square of the order parameter in a conventional superconductor, while it is only proportional to the magnitude of the order parameter as $T \to 0$ [7]. This is not terribly disturbing because the Ginzburg-Landau functional is only supposed to be valid close to T_c. But it must be remembered that there is *no* LD model at low temperatures for conventional superconductors, which is a frequently misunderstood point [8]. In contrast, the Josephson effect between two superconductors with non-Fermi liquid normal states can be recast in the language of the LD model [7].

In mean field theory, the free energy functional is minimized by setting the order parameter to be the same everywhere, that is, both its magnitude and phase. If we apply this theory to equation (2.1), we are back to uncoupled layers and no enhancement of the mean field transition temperature, T_c^0. Sometimes, an enhancement is claimed, which is merely the result of considering the functional in equation (2.1) in which the coupling between the layers is taken to be $-(\psi_n^* \psi_{n+1} + c.c.)$ instead of $|\psi_n - \psi_{n+1}|^2$. For a conventional superconductor this is incorrect, because the Josephson energy in that case is proportional to $[1 - \cos(\phi_n - \phi_{n+1})]$ instead of $-\cos(\phi_n - \phi_{n+1})$. The only way to enhance T_c^0 would be to change the parameters of the LD model appropriately. This is difficult to achieve in a BCS superconductor, because the density of states is changed very little by the small hopping matrix elements of the electrons between the layers of a highly anisotropic superconductor.

So, what does the coupling between the layers do? It can suppress phase fluctuations by coupling the phases of the layers to raise the true T_c closer to T_c^0. Note that, in general, the true T_c is less than T_c^0. Thus, a dimensional crossover is driven by suppressing phase fluctuations, and unless the individual two dimensional layers have a high T_c^0, we gain little by suppressing phase fluctuations. Of course, phase coherence will be established in all three directions, and those properties that depend on this coherence will certainly be affected. The actual increase of

the true transition temperature due to interlayer coupling can be easily estimated from the XY-model [4].

A prominent feature of the interlayer tunneling theory is that T_c^0 can be enhanced by the coupling between the layers. Phrased in the language of the LD model, it means that the parameters of this model can be changed substantially. The phase fluctuations should, however, be similar to those in a conventional superconductor [9].

3 c-axis conductivity sum rule

For simplicity, consider a model [10] in which the microscopic Hamiltonian expressing hopping of electrons along the c-axis is

$$H_c = -t_\perp \sum_{jl,s} c^\dagger_{jl,s} c_{jl+1,s} + h.c., \tag{3.1}$$

where the label j refers to the sites of the two-dimensional plane, l refers to the layer index, and s refers to spin; $c^\dagger_{jl,s}$ is the electron creation operator. In this section, I focus only on single layer materials for which all CuO-planes are equivalent, such as LSCO, Tl2201, Hg1201, and Bi2201. In the next section, I shall also touch upon multilayer materials.

One can now derive a sum rule [11]. First, the frequency and the wavevector dependent c-axis conductivity can be written as

$$\sigma^c(q_c,\omega,T) = -\frac{1}{Ad}\left(\frac{ed}{\hbar}\right)^2 \frac{\langle -H_c(T)\rangle - \Lambda^c_{ret}(q_c,\omega,T)}{i(\omega+i\delta)}, \tag{3.2}$$

where q_c is the momentum transfer perpendicular to the plane, A is the two-dimensional area and d is the separation between the layers. The retarded current-current commutator is $\Lambda^c_{ret}(l,t,T) = -i\theta(t)\langle[j^c_H(l,t), j^c_H(0,0)]\rangle$. The paramagnetic current operator is defined by $j^c(l) = it_\perp \sum_j (c^\dagger_{jl,s} c_{jl+1,s} - h.c.)$, and the corresponding Heisenberg operator, j^c_H, is defined with respect to the full interacting Hamiltonian. The averages refer to the thermal averages and $\langle H_c(T)\rangle = -t_\perp \sum_{j,s}\langle c^\dagger_{jl,s} c_{jl+1,s} + h.c.\rangle$. For optical conductivity, one may set $q_c = 0$, and then, noting that the retarded current-current commutator is analytic in the upper-half of the complex ω-plane and that it vanishes at infinity, we arrive at the c-axis conductivity sum rule

$$\int_{-\infty}^{\infty} d\omega\ \Re\ \sigma^c(\omega,T) = \frac{\pi e^2 d^2}{\hbar^2 Ad}\langle -H_c(T)\rangle, \tag{3.3}$$

which is a variant of the well-known f-sum rule [12]. Note that it is necessary that the integral runs between the limits $-\infty$ and ∞ to arrive at this sum rule.

There are a number of noteworthy points.

- It was argued by Kohn [13] that the f-sum rule does not hold in a metal, because the unbounded position operator is not a valid hermitian operator. Indeed, all derivations of this sum rule involving the position operator in an extended system do look suspicious. However, the f-sum rule *is* satisfied [11]. The reason is that the f-sum rule can be derived by introducing the exponential operator $e^{i\mathbf{q}\cdot\mathbf{x}}$ and then taking the limit $\mathbf{q}\to 0$. Of course, there is no such sum rule if the interaction itself is velocity dependent.
- On occasions, this sum rule is written with finite limits, which is assumed to be some interband gap. This is incorrect [14].
- The right hand side of the sum rule is the average of the single particle hopping Hamiltonian. This may be deceptive because it is the true interacting kinetic energy.
- The sum rule is satisfied at any temperature T.
- The absence of Galilean invariance on a lattice allows the charge carrying effective mass to vary with temperature and interaction. In the continuum limit, such that $d\to 0$, but $t_\perp d^2$ fixed, the right hand side of equation (3.3) is $\frac{\pi n e^2}{m}$, where $\frac{\hbar^2}{2m} = t_\perp d^2$, and n is the density of electrons in the planes. In this limit, interactions cannot renormalize the effective mass because the current operator commutes with the Hamiltonian.

We shall now put this sum rule to good use. For a superconductor, we can write quite generally

$$\Re\ \sigma^{cs}(\omega,T) = D_c(T)\delta(\omega) + \Re\ \sigma^{cs}_{reg}(\omega,T). \tag{3.4}$$

The first term signifies the lossless flow of electrons in the superconducting state, while the second is the regular (nonsingular) part of the optical conductivity. The normal state optical conductivity is nonsingular; so, the sum rule can be cast into a more useful form:

$$\begin{aligned} D_c(T) \quad &= \quad \int_0^\infty d\omega \left[\Re\ \sigma^{cn}(\omega,T) - \Re\ \sigma^{cs}_{reg}(\omega,T)\right] \\ &\quad + \frac{\pi e^2 d^2}{2Ad\hbar^2}\left[\langle -H_c(T)\rangle_s - \langle -H_c(T)\rangle_n\right]. \end{aligned} \tag{3.5}$$

If the c-axis kinetic energy is unchanged between the normal and the superconducting states, as it should be in a conventional layered superconductor, we recover a variant of the Ferrell-Glover-Tinkham sum rule [3]. The missing area between the c-axis conductivities of the normal and the superconducting states is proportional to the c-axis superfluid density.

Frequently, the sum rule in equation (3.5) is not meaningfully applied to high temperature superconductors. Instead of the true sum rule in equation (3.5), the following missing area is considered:

$$D'_c(T) = \int_0^\infty d\omega[\Re\ \sigma^{cn}(\omega,T_c) - \Re\ \sigma^{cs}_{reg}(\omega,T)]. \tag{3.6}$$

Under what conditions can $D'_c(T)$ be related to the true c-axis penetration depth? It must be assumed that the c-axis kinetic energy must be the same for the normal

and the superconducting states and independent of temperature, with the implicit assumption that the normal state conductivity would change very little for all temperatures $T \leq T_c$, if superconductivity could be suppressed. For a conventional superconductor, these assumptions are justified, but not for cuprates. First, the change in the c-axis kinetic energy is strikingly evident. Second, the c-axis resistivity is generically semiconducting and strongly temperature dependent, at least in the underdoped and optimally doped regimes [15]. This temperature dependence should persist if superconductivity could be suppressed, say by applying a magnetic field, and therefore the equality of the conductivity at T_c and those at $T \leq T_c$ cannot be assumed. For LSCO, this has been demonstrated experimentally [16]. Even the ab-plane resistivity was found to be insulating and temperature dependent once superconductivity was suppressed by applying strong magnetic fields. These experiments bring into question theories that are based on the assumption that the $T = 0$ state is metallic [17]. Therefore, we conclude that the consideration of $D_c'(T)$ begs the interesting question "Do electrons change their c-axis kinetic energy upon entering the superconducting state?"

On general grounds, there is little we can say about $\Re\,\sigma^{cn}(\omega, T)$ for $T \leq T_c$. How do we overcome this impasse? To answer this question, consider the sum rule at zero temperature, which can be restated as

$$D_c(0) \geq \frac{\pi e^2 d^2}{2Ad\hbar^2}\Big[\langle -H_c(0)\rangle_s - \langle -H_c(0)\rangle_n\Big]. \tag{3.7}$$

I have assumed that the integral in equation (3.5) is positive definite. This could be a strict inequality, although I cannot find a rigorous argument. One can see, however, that at very high frequencies the two conductivites should approach each other, and, at low frequencies, $\sigma^{cn}_{reg}(\omega, T = 0) \geq \sigma^{cs}_{reg}(\omega, T = 0)$, if the superconducting state is at least partially gapped.

If the experiments of Ando *et al.* [16] are taken as an indication, the system, at $T = 0$, is insulating along the c-axis. It is plausible, therefore, that the integral in equation (3.5) is smaller than what one would have guessed for metallic conduction along the c-axis. This is because the frequency dependent c-axis conductivity in a non-Fermi liquid is expected to vanish as a power law in contrast to the Drude behavior. If this is indeed true, we can make the approximation

$$D_c(0) \approx \frac{\pi e^2 d^2}{2Ad\hbar^2}\Big[\langle -H_c(0)\rangle_s - \langle -H_c(0)\rangle_n\Big]. \tag{3.8}$$

Defining $n_s^c(0)$ by $D_c(0) = \dfrac{\pi n_s^c(0) e^2}{2m}$, and δT by $\delta T = [\langle -H_c(0)\rangle_s - \langle -H_c(0)\rangle_n]$, we get the simple equation

$$\frac{\hbar^2 n_s^c(0)}{md^2} \approx \frac{\delta T}{Ad}\,. \tag{3.9}$$

The precise definition of the mass, m, is irrelevant because the penetration depth depends only on $D_c(0)$, that is, only on the combination $\dfrac{n_s^c(0)e^2}{m}$. The left hand side of equation (3.9) is of the order of the confinement kinetic energy of a particle in an one dimensional potential well of width d, consistent with the uncertainty principle.

The c-axis penetration depth is given by [18]

$$\frac{1}{\lambda_c^2(0)} = \frac{8D_c(0)}{c^2}, \tag{3.10}$$

where c is the velocity of light. Therefore, it satisfies the inequality

$$\lambda_c(0) \leq \frac{\hbar c}{ed}\frac{1}{\sqrt{4\pi(\delta T/Ad)}}\,. \tag{3.11}$$

If we replace $(\delta T/Ad)$ by the condensation energy U of the electrons per unit cell per CuO-layer, including both spin orientations, and replace the inequality by the equality, we arrive at the approximate expression

$$\lambda_c(0) \approx \frac{\hbar c}{ed}\frac{1}{\sqrt{4\pi U}}, \tag{3.12}$$

which is twice as large as that of Anderson [19]. While Anderson equates the condensation energy to the Josephson coupling energy, E_c, I have equated it to the change in the kinetic energy. I believe that this is more appropriate because there can be situations in which the condensation energy of the superconductor is not derived from the change in the kinetic energy, but E_c is finite–conventional Josephson effect, for example.

Anderson [19] has observed that λ_c calculated from the procedure outlined above agrees well with the measured values. Actually, my expression for λ_c in equation (3.12) is a factor of 2 larger, but this may not be significant at this time, given the uncertainties involved in extracting the condensation energy from the measured specific heat [20]. In LSCO, the c-axis reflectivity exhibits a striking plasma edge in the superconducting state whose position is readily determined [21]. As there is little ambiguity in the measured background dielectric constant, which is approximately 25, the penetration depth can be easily read off from the plasma edge. In contrast, the analysis based on the missing area, if not properly carried out, will be flawed [22]. For all doping, the agreement found by Anderson is good. It is also reassuring to note that the penetration depth measured from the plasma edge is in agreement with the microwave measurements [23]. For the single layer Hg1201, the condensation energy is not known from experiments. Anderson estimated it from the assumption that it is proportional to T_c^2. This yields a penetration depth in good agreement with experiments [24]. It must be remembered, however, that this estimate is subject to a greater uncertainty.

The fly in the ointment is the measurement of Moler *et al.* [25] in the single layer Tl2201. The measured penetration depth is almost a factor of 20 too large [19]. Given the similarities between Tl2201 and Hg1201, this is surprising. However, the c-axis resistivity of Tl2201 is very anomalous; not only does it not show insulating behavior,

but it is linear in its temperature dependence; the magnitude of the resistivity near T_c is enormous, however. In addition, the material chemistry of Tl2201 is quite curious. The optimally doped materials contain significant interstitial oxygen defects between the two TlO planes, but more surprisingly, they also contain sizable Cu substitution at the Tl site [26]. It may be that there are metallic shorts connecting the CuO planes. Thus, it is unclear if this measurement reflects the true penetration depth of this material or not. The material chemistry of Hg1201 appear to be somewhat different [26].

It is interesting that the same sum rule can be turned on its ear to argue that conventional explanations of λ_c are implausible. In Fermi liquid based theories, the change in the c-axis kinetic energy must be zero. The penetration depth is then

$$\lambda_c(0) = \frac{c}{\left(8\int_0^\infty d\omega[\Re\ \sigma^{cn}(\omega,0) - \Re\ \sigma^{cs}_{reg}(\omega,0)]\right)^{1/2}}. \tag{3.13}$$

As argued above, the integral on the right hand side of the denominator is likely to be small. Consequently, the penetration depth obtained from this formula is likely to be too large to agree with experiments in LSCO and Hg1201. Note that this sum rule argument is independent of any microscopic details.

4 Interlayer enhancement of the mean field transition temperature

In this section we return to the enhancement of T_c^0 in multilayer materials to compare against the observed systematics, providing further support to the theory. The inequality derived in the previous section needs only small modifications. The idea is simple. The coupling between the layers was set by the energy scale $\dfrac{\hbar^2 n_s^c(0)}{md^2}$, but now we have to distinguish between the coupling between the close layers and the coupling between the distant layers. Let us define them to be $g_\perp$ and $g'_\perp$, respectively. Strictly speaking this is a simplification, because the tunneling matrix elements between the various layers in an unit cell and those in the neighboring cell are not all the same.

Imagine that not only the true transition temperature including fluctuations, but even T_c^0 of an individual layer is very small. I now show that if the coupling between the layers is included, the increase in T_c^0 is negligible in BCS theory. In contrast, the interlayer mechanism leads to a striking enhancement of T_c^0. The mean field equation for single layer materials, due to interlayer coupling, is

$$2g'_\perp \chi_{in-plane}(T_c^0) = 1, \tag{4.1}$$

where $\chi_{in-plane}$ is the in-plane pair susceptibility. For a n-layer material, $n \geq 2$, the mean field equation is

$$\frac{2(n-1)g_\perp + 2ng'_\perp}{n}\chi_{in-plane}(T_c^0) = 1. \tag{4.2}$$

We must now determine $\chi_{in-plane}(T)$. Our knowledge of the scale of the coupling energy is insufficient for this purpose [27]. To apply the mean field argument, it is necessary to know the nature of the coupling between the planes. In particular, it is necessary to know if the Josephson pair tunneling Hamiltonian is diagonal in the parallel momentum or not. One of the striking aspects of the interlayer tunneling theory is that it is approximately diagonal in the parallel momentum [1,28,29]. So, the $\chi_{in-plane}$ to be substituted in these mean field equations must correspond to the momentum for which this susceptibility is the largest. To see the striking difference caused by this assumption, it is necessary to consider only the BCS pair susceptibility. If the coupling Hamiltonian is not diagonal in the parallel momentum, it is the momentum integrated pair susceptibility that is relevant, which, however, is only logarithmically divergent because

$$\begin{aligned}\chi_{BCS}(T) &= N(0)\int_0^{\omega_c}\frac{d\varepsilon}{\varepsilon}\tanh(\frac{\varepsilon}{2T}),\\ &= N(0)\ln(1.14\omega_c/2T).\end{aligned} \tag{4.3}$$

where $N(0)$ is the density of states at the Fermi energy and ω_c is a cutoff of the order of the Debye energy. When substituted in equations (4.1, 4.2), the enhancement of T_c is negligible because $N(0)g'_\perp$, $N(0)g_\perp$ are small compared to unity. In contrast, if the Josephson pair tunneling is diagonal in the parallel momentum, it is the maximum susceptibility on the Fermi surface that is relevant. As $\varepsilon \to 0$,

$$\chi_{BCS}(\varepsilon \to 0, T) = \frac{1}{2T}, \tag{4.4}$$

diverges faster as $T \to 0$. When this susceptibility is substituted into equations (4.1, 4.2), it gives rise to far greater enhancements of the transition temperature. It can be shown from simple models of a non-Fermi liquid that the largest in-plane pair susceptibility (not momentum integrated) remains of the same order [30], that is, it is a/T, for T close to T_c^0, where a is a number of order unity. Then, the mean field transition temperatures T_{c1}^0, T_{c2}^0, T_{c3}^0, T_{c4}^0, for one, two, three, four, ... layer materials are given by $T_{c1}^0 = \dfrac{2g'_\perp}{a}$, $T_{c2}^0 = T_{c1}^0 + \dfrac{g_\perp}{a}$, $T_{c3}^0 = T_{c1}^0 + \dfrac{4}{3}\dfrac{g_\perp}{a}$, $T_{c4}^0 = T_{c1}^0 + \dfrac{3}{2}\dfrac{g_\perp}{a}$, *etc.*; the sequence $1, 4/3, 3/2, \ldots$ converges to 2. This pattern of the systematic enhancement of the transition temperatures of the multilayer materials is in accord with experiments.

5 Conclusion

The purpose of this paper has been to present some very general arguments in favor of the interlayer tunneling theory. There are two significant outcomes of the present paper. The first concerns the nature of the 2D to 3D crossover in the superconducting state. It was shown that the interlayer tunneling mechanism can enhance the microscopic superfluid stiffness in a way that is not possible

in conventional theories. This stiffness sets the scale at which the amplitude of the order parameter forms. On general grounds, it is difficult to settle whether or not phase fluctuations are important; experimental evidence on this question appears to be mixed. If, however, they are assumed to be present, as has been argued by Emery and Kivelson [9], they can be included by combining interlayer tunneling theory with the Lawrence-Doniach model. The pseudogap observed in the underdoped materials in that case would be the superconducting gap calculated within the interlayer tunneling theory, while the true T_c will be determined by the phase fluctuations.

The second outcome of the present paper is the resolution of the paradoxical interpretations of the c-axis optical measurements, universally evident in the literature. On the one hand, it appeared that one could obtain the correct estimates of the c-axis penetration depths only from the change in the kinetic energy of the electrons as they enter the superconducting state [19], on the other hand, the same results were apparently obtained from the c-axis conductivity sum rule ignoring the change in the kinetic energy [21]. The resolution is that, until now, the sum rule has not been meaningfully applied to high temperature superconductors. The paradox disappears with the correct interpretation of the sum rule. The evidence for the change in electron's kinetic energy, an essential element of the interlayer tunneling theory, appears to be strong in LSCO, reasonably convincing in Hg1201, and nonexistent in Tl2201 on the basis of the recent measurements [25]. In regard to Tl2201, important materials questions remain.

Future measurements of the c-axis optical conductivity and the penetration depth in both single and multilayer materials will be valuable. In particular, I would like to suggest that these experiments be carried out on the single layer Bi2201, which in many respects is as anomalous as its high-T_c cousins. If possible, the optical measurements should be carried out in the presence of a magnetic field necessary to suppress superconductivity. In this low T_c material, the required magnetic field should be considerably smaller than in the experiments of Ando *et al.* [16] Moreover, the normal state can be pursued and measured more precisely to lower temperatures.

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Note added in proofs

G. Boebinger has drawn my attention to their high magnetic field work (Y. Ando *et al.*, Phys. Rev. Lett. **77**, 2075 (1996)) on Bi2201 in which they have shown that a "metallic" in-plane resistivity coexists with the "semiconducting" c-axis resistivity. This is difficult to understand within Fermi liquid theory.

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12. See, for example, P.C. Martin, in *Many-Body Physics*, edited by C. De Witt, R. Balian (Gordon and Breach, New York, 1967).
13. W. Kohn, Phys. Rev. **133**, A171 (1964).
14. The hopping Hamiltonian is an effective model, where all the effects of higher energy bands are in principle downfolded by a method akin to a renormalization group procedure [10]. This implies that this effective Hamiltonian is applicable only to low energy processes below a cutoff presumably of the order of the interband transition. But once this model is determined, theoretically there are no more degrees of freedom left and mathematically the integral in equation (3.3) has to be between $-\infty$ and ∞ for the sum rule to be correct. This means that the conductivity $\sigma^c(\omega)$ calculated from this effective Hamiltonian cannot be the physical conductivity for scales of the order or larger

than the high energy cutoff implied in the effective Hamiltonian. This makes it problematic to accurately estimate the missing area as only the order of magnitude of the cutoff is known.

15. For a review, see Y. Iye, in *Physical properties of High Temperature Superconductors III*, edited by D.M. Ginsberg (World Scientific, Singapore, 1992). See also, H. Takagi *et al.*, Phys. Rev. Lett. **69**, 2975 (1992). Contrary to underdoped and optimally doped materials, the temperature dependence of the overdoped materials is not obviously semiconducting. That is not to say that they are metallic; on the contrary, the magnitude of the resistivities above T_c are enormous. There are other notable exceptions as well, such as optimally doped Tl2201 and YBCO for which the c-axis resistivity is approximately linear with temperature. Nonetheless, even in these exceptional cases, the temperature dependence can be assumed to persist if superconductivity could be suppressed.
16. Y. Ando *et al.*, Phys. Rev. Lett. **75**, 4662 (1995); G.S. Boebinger *et al.*, Phys. Rev. Lett. **77**, 5417 (1996).
17. M.J. Graf *et al.*, Phys. Rev. B **52**, 10588 (1995); P.J. Hirschfeld, S.M. Quinlan, D.J. Scalapino, Phys. Rev. B **55**, 12742 (1997).
18. It is useful to elaborate on this further. From the singular part of the real part of the conductivity, we conclude from the Kramers-Kronig relation that $\omega\Im\ \sigma(\omega) = \frac{2\mathrm{D}_c(T)}{\pi}$. Consider now the Josephson expression for the current density in its gauge invariant form, which is $J = J_c \sin(\delta\theta - \frac{2ed\mathcal{A}}{\hbar c})$, assuming a uniform vector potential $\mathcal{A}$ between the two layers separated by d; J_c is the critical current density. If we now set $\delta\theta = 0$ and take the limit $\mathcal{A} \to 0$, then we get $J = -\frac{2J_c ed}{\hbar c}\mathcal{A}$. Equating this to the defining equation for the penetration depth, $J = -\frac{c}{4\pi\lambda_c^2}\mathcal{A}$, we get $\lambda_c = \left(\frac{\Phi_0 c}{8\pi^2 J_c d}\right)^{1/2}$, which is a frequently used expression for layered superconductors described by the LD model. (See, for example, Moler *et al.* [25] and references therein.) The remaining task is to relate J_c to the imaginary part of the conductivity. This is easily done by choosing the vector potential to be time dependent, that is, $\mathcal{A}(t) = \mathcal{A}_\omega e^{-i\omega t}$. Then, following the same line of reasoning as above, we get $\omega\Im\sigma(\omega) = \frac{2edJ_c}{\hbar}$. The penetration depth can now be expressed as $\lambda_c = \frac{c}{\sqrt{4\pi\omega\Im\sigma(\omega)}}$. We can now substitute the expression for the imaginary part of the conductivity to find the desired expression for the penetration depth: $\lambda_c = c/(8D_c(T))^{1/2}$.
19. P.W. Anderson, Science **279**, 1196 (1998). For example, for doping level of 17-20% in LSCO, the calculated c-axis penetration depth is $3 \pm 1\mu$. Similarly, for Hg1201, it is $1 \pm 0.5\mu$.
20. J.W. Loram *et al.*, Physica C **235-240**, 134 (1994).
21. S. Uchida, K. Tamasaku, S. Tajima, Phys. Rev. B **53**, 14558 (1996); see also D.N. Basov *et al.*, Phys. Rev. B **52**, R13141 (1995).
22. Further elaboration on this point may be useful. Aside from the proper use of the sum rule in equation (3.5), there are two common mistakes. From the Lawrence-Doniach model, which is valid only close to T_c, the c-axis penetration depth is $\lambda_c = (c\Phi_0/8\pi^2 dJ_c)^{1/2}$ [18]. It is customary to assume the validity of the Ambegaokar-Baratoff formula [3]

$$J_c(T) = \frac{\pi\Delta(T)}{2eR_n}\tanh\frac{\Delta(T)}{2T}$$

with $R_n = \rho_c d$, ρ_c being the c-axis resistivity at T_c. First, this formula is valid for a special (SIS) Josephson tunnel junction, with a temperature independent Ohmic resistance. Moreover, the parallel momentum must not be conserved. Finally, the gap Δ must be an isotropic s-wave gap. None of these assumptions are pertinent to the present situation. In the case that the parallel momentum is assumed to be conserved, an expression for J_c due to L. Bulaevski (JETP **37**, 1133 (1973)) is used. This is a pathological formula that is independent of the gap and does not even vanish as the superconducting gap tends to zero. The flaw is that this formula is obtained from ordinary second order perturbation theory in a situation in which the correct treatment requires Brillouin-Wigner perturbation theory.
The second mistake is to apply equation (3.6) and to integrate up to 2Δ. It was already elaborated why $D_c'(T)$ cannot be simply related to the actual penetration depth. In addition, there is no known sum rules in which the frequency integral is integrated to a finite limit. The correct sum rule applicable to conventional superconductors is $\int_0^\infty d\omega[\Re\ \sigma^{cn}(\omega, T_c) - \Re\ \sigma^{cs}_{reg}(\omega, T)] = \frac{\pi edJ_c}{\hbar}$. It is true, however, that for an isotropic BCS superconductor most of the missing area is contained within an energy few times the gap, Δ. For high temperature superconductors, however, the difference between $\sigma^{cn}(\omega)$ and $\sigma^{cs}_{reg}(\omega)$ persists up to high energies [21], of order 1000 cm^{-1} in LSCO. Finally, because the gap is likely to be a d-wave gap, the specification of the finite upper limit of the integral in terms of the gap is ambiguous.
It is important to note that such redistribution of spectral weight over enormously large energy range is impossible in any Fermi liquid based theories, with or without impurities, because the c-axis single particle hopping bandwidth is small, especially in the single layer materials. The spectral weight redistribution must be due to strong correlation effects. All conventional theories that purportedly explains the experimental measurements of the c-axis penetration depth suffer from this criticism and cannot be trusted.
23. T. Shibauchi *et al.*, Phys. Rev. Lett. **72**, 2263 (1994).
24. C. Panagopoulos *et al.*, Phys. Rev. Lett. **79**, 2320 (1994).
25. K.A. Moler *et al.*, Science **279**, 1193 (1998).
26. For a brief review of the materials aspects, see J.D. Jorgensen *et al.*, Physica C **282-287**, 97 (1997) and references therein.
27. This is also true for classical statistical mechanical problems discussed in Section 2.
28. S. Chakravarty, A. Sudbø, P.W. Anderson, S. Strong, Science **261**, 337 (1993).
29. The momentum diagonal pair tunneling Hamiltonian is infinitely long ranged in real space and must be understood as a mean field Hamiltonian. The long ranged nature renders the mean field theory exact. The BCS reduced Hamiltonian has the same property in its real space form. S. Chakravarty, to be published.
30. See Ref. [1], and also L. Yin, S. Chakravarty, Int. J. Mod. Phys. B **10**, 805 (1996).