Non-k-diagonality in the interlayer pair-tunneling model of high-temperature superconductivity

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I. INTRODUCTION

The interlayer pair-tunneling (ILT) model of high-temperature superconductivity has been the focus of much attention since it was introduced and later elaborated on quantitatively. Within the ILT model, the pairing of electrons in individual CuO$_2$-layers is considerably enhanced by the tunneling of Cooper pairs between neighbouring layers, giving critical temperatures which are substantially higher than those arising solely from a reasonable in-plane effective electron-electron attraction in a two-dimensional (2D) BCS-like theory.

The central underlying assumption of the ILT model is that the normal state of the cuprates is a strongly correlated non-Fermi liquid, where single-electron interlayer tunneling is incoherent or strongly damped, resulting in a frustrated $c$-axis kinetic energy. This kinetic energy is substantially lowered in the superconducting state, through tunneling of Cooper pairs between CuO$_2$ layers. Thus, contrary to the situation in conventional superconductors, it is the lowering of the kinetic energy, and not the potential energy, which drives the transition.

Recently, there have been extensive discussions in the literature about experimental tests of an unconventional relation, predicted by the ILT model, between the $c$-axis penetration depth $\lambda_c$ and the condensation energy $E_{\text{cond}}$. The agreement in LSCO seems quite good, but experiments on Hg-1201 and Tl-2201 give estimates for $\lambda_c$ which are 8-20 times larger than the predicted values. However, note that Chakravarty et al. have argued that this discrepancy between theory and experiment can be drastically reduced by taking more carefully into account the fluctuation contributions to the normal state specific heat when estimating $E_{\text{cond}}$.

It is not our purpose here to consider the microscopic foundations of the ILT mechanism. Instead, we will take it as a phenomenological starting point, and explore the effects of some modifications of the form of the pair tunneling term used in Ref. 3. There it was argued that, in order to obtain critical temperatures of the same order of magnitude as found in the high-$T_c$ cuprates, it was essential that the 2D momentum of the Cooper-pair electrons was conserved in the tunneling process. This momentum conservation was argued to follow from the momentum conservation of the single-electron tunneling Hamiltonian, in the absence of inelastic scattering. Translated to real space, this momentum conservation means that the electron-electron attraction associated with the interlayer tunneling has an infinite range.

A natural question to ask is then how sensitive the critical temperature $T_c$ is to a relaxation of this constraint. Specifically, what is the typical order of the interaction range below which $T_c$ will drop to values which are no longer comparable to critical temperatures in the high-$T_c$ cuprates? Moreover, several of the unusual $k$-space features of the gap predicted within the ILT mechanism have their origin in the assumed momentum conservation.

We will address this question phenomenologically, modelling the finite range by postulating modified functional forms of the pair tunneling term in which phenomenological parameters are introduced to measure the degree of “screening”. This will in turn lead to modifications of the original gap equations, which are then solved self-consistently to obtain the critical temperature and the superconducting gap. We expect that qualitatively correct conclusions may
be drawn from our modelling of the k-space broadening. Brief accounts of parts of this work have appeared in print elsewhere.

II. FORMULATION OF THE PROBLEM

For simplicity, we consider compounds with two CuO$_2$-layers per unit cell. The generalization to an arbitrary number of CuO$_2$-planes per unit cell is straightforward. Below the superconducting transition temperature, we will assume that the quasi-particle description is approximately valid. The total Hamiltonian is taken to be the sum of 2D BCS Hamiltonians for the individual layers, and an interlayer pair tunneling Hamiltonian, $H = H_{\text{layer}} + H_J$. When the zero-momentum pairing assumption is invoked, the intralayer part is given by

$$H_{\text{layer}} = \sum_{k,\sigma,i=1,2} \varepsilon_k c_{k\sigma}^{(i)\dagger} c_{k\sigma}^{(i)} + \sum_{k,k',i=1,2} V_{k,k'} c_{k\uparrow}^{(i)\dagger} c_{-k\downarrow}^{(i)} c_{-k'\downarrow}^{(i)} c_{k'\uparrow},$$  \hspace{1cm} (1)$$

while the interlayer pair-tunneling contribution to the Hamiltonian is given by the form

$$H_J = -\sum_{k,k'} T_J(k,k') c_{k\uparrow}^{(1)\dagger} c_{-k\downarrow}^{(1)} c_{-k'\downarrow}^{(2)} c_{k'\uparrow} + \text{h.c.}$$ \hspace{1cm} (2)$$

Here $c_{ka}^{(i)\dagger}$ is the creation operator of an electron in layer $i$ ($i = 1, 2$) with 2D in-plane wave vector $k$ and spin projection $\sigma$, $\varepsilon_k$ is the normal state dispersion measured relative to the Fermi level, and $V_{k,k'}$ is the inplane contribution to the pairing kernel.

An apparently pathological aspect of a particular version of $H_J$, namely with a $k$-diagonal tunneling term $T_J(k,k') = T_J \delta_{k,k'}$, becomes evident on Fourier-transforming back to real space, where it takes the form

$$-\frac{T_J}{N} \sum_{R_1,R_2,R} c_{R_1+r/2,\uparrow}^{(1)\dagger} c_{R_1-r/2,\downarrow}^{(1)} c_{R_2-r/2,\downarrow}^{(2)} c_{R_2+r/2,\uparrow} + \text{h.c.}$$ \hspace{1cm} (3)$$

where $N$ is the number of lattice sites per layer, and $R$ is the relative coordinate and $R_i$ the center of mass coordinate in layer $i$ of the two tunneling electrons. Note that there are no restrictions on $|R_1 - R_2|$ due to the zero-momentum pairing assumption, as in conventional superconductors. What is not conventional is that there is no restriction on the relative positions in each plane for which two electrons feel an attraction. Hence, $T_J \delta_{k,k'}$ represents an infinite-range attraction, contrary to the conventional case where it is a (retarded) contact-attraction. That such a version of the ILT-model then gives a large value of $T_c$ is perhaps not surprising, but it is difficult to understand how such an effective attraction is produced.

The $k$-diagonal model must therefore be viewed as an idealization, and the issue to adress is how representative this limit is, if at all. The more general model given in $H_J$ yields

$$-\frac{T_J}{N} \sum_{R_1,R_2,R} G(|r|) c_{R_1+r/2,\uparrow}^{(1)\dagger} c_{R_1-r/2,\downarrow}^{(1)} c_{R_2-r/2,\downarrow}^{(2)} c_{R_2+r/2,\uparrow} + \text{h.c.}$$ \hspace{1cm} (4)$$

The characteristic decay-length of the function $G(|r|) = \sum_k e^{ikr} f(k)$, with $f(k)$ defined via $T_J(k,k') = T_J f(k-k')$, represents the range of the effective interlayer tunneling attraction.

By assuming a layer-independent pair amplitude, the total Hamiltonian becomes decoupled in the layer indices, and the gap equation is seen to be the same as in the BCS case when one makes the replacement $V_{k,k'} \rightarrow V_{k,k'} - T_J(k,k')$, i.e.

$$\Delta_k = -\sum_{k'} V_{k,k'} \Delta_{k'} \chi_{k'} + \sum_{k'} T_J(k,k') \Delta_{k'} \chi_{k'},$$ \hspace{1cm} (5)$$

where $\Delta_k$ is the gap function, and $\chi_k$ is the pair susceptibility, given by $\chi_k = \tanh(\beta E_k/2)/E_k$, where $E_k = \sqrt{\varepsilon_k^2 + |\Delta_k|^2}$, $\beta = 1/k_B T$, $k_B$ is Boltzmann’s constant and $T$ is the temperature. We will consider $V_{k,k'}$ to be a separable function of $k$ and $k'$, i.e. $V_{k,k'} = -V g_k g_{k'}$, where $g_k$ belongs to the set of basis functions for irreducible representations of the point group of the underlying lattice, and $V > 0$ is an effective two-particle scattering matrix element.
III. GAP EQUATION IN ENERGY SPACE

Ref. 3 studied the case $T_J(k, k') = T_J \delta_{k, k'}$, i.e. the pair tunneling matrix element is both diagonal and $k$-independent. Using also the BCS approximation $g_k = \Theta(\omega_D - |\varepsilon_k|)$, where $\omega_D$ is an energy cutoff, the gap then depends on $k$ only through $\varepsilon_k$, so that the gap equation can be written in energy space as

$$\Delta(\varepsilon) = \Delta_0 \Theta(\omega_D - |\varepsilon|) + T_J \Delta(\varepsilon) \chi(\varepsilon),$$

where

$$\Delta_0 = \lambda \int_{-\omega_D}^{\omega_D} d\varepsilon \Delta(\varepsilon) \chi(\varepsilon).$$

The BCS coupling constant is $\lambda = VN(\varepsilon_F)$, where $N(\varepsilon_F)$ is the density of states per spin at the Fermi level $\varepsilon_F$ (i.e. here we have made the usual approximation of neglecting the variation of $\nabla_k \varepsilon$ inside the thin Debye shell around the Fermi energy). This gap equation can be regarded as the limit $\omega \to 0$ of the more general equation

$$\Delta(\varepsilon) = \Delta_0 \Theta(\omega_D - |\varepsilon|) + \frac{T_J}{2\omega} \int_{\varepsilon - \omega}^{\varepsilon + \omega} d\varepsilon' \Delta(\varepsilon') \chi(\varepsilon'),$$

where the parameter $\omega$ provides a measure of the amount of $k$-space broadening in the interlayer pairing kernel.

We have solved (8) self-consistently and show in Fig. 2 the results for $T_c$ as function of $\omega$ for $T_J = 30$ meV, $\omega_D = 20$ meV and $\lambda = 0.1$. The most important feature of this figure is the moderate reduction of $T_c$ as $\omega$ is increased from zero. To reduce $T_c$ by a factor 2 requires a broadening of $\omega \sim 40$ meV.

If we convert the energy broadening of the ILT term to a length using $\omega = \hbar^2 k^2/(2M)$, with $M$ equal to the electron mass, we obtain for the length $l = 1/k$

$$l \approx \left(\frac{62}{\sqrt{\omega}}\right) \text{Å},$$

where $\omega$ is to be measured in meV. Setting $\omega = 40$ gives an interaction range $l \approx 9.8$ Å.

IV. GAP EQUATION IN 1D $k$-SPACE

In this section, we will consider the gap equation (8) with a particular choice of $T_J(k, k')$. The main purpose of this paper is to establish a qualitative criterion for how robust the sharp $k$-space structures of the gap, obtained for a $k$-diagonal ILT term, are to momentum broadening. Given this limited purpose, it does make sense to simplify the problem by taking the $k$’s to be one-dimensional (1D). This simplification is purely mathematical, and of course does not imply anything about superconductivity with true off-diagonal long-range order in 1D systems, which is well-known not to exist for $T > 0$.

The first is the BCS approximation $g_k = \Theta(\omega_D - |\varepsilon_k|)$, also used in Sec. 1. It is analogous to isotropic $s$-wave pairing in 2D. The second form is $g_k = \cos(ka)$, which is most closely analogous to $s_{x^2+y^2}$ or $d_{x^2-y^2}$ pairing in 2D. The gap obtained for the first form does not change sign in the Brillouin zone, while the gap for the second form in general does.

For simplicity, we assume a simple tight-binding dispersion form for $\varepsilon_k$,

$$\varepsilon_k = -2t \left[\cos(ka) - \cos(k_F a)\right],$$

where $t$ is the single-electron intralayer tunneling matrix element, $a$ is the lattice constant and $k_F$ is the Fermi wave vector. The pair tunneling term is taken to be of the form $T_J(k, k') \equiv T_J f(k - k')$, where we have chosen $f(k)$ to have the particular form

$$f(k) = \frac{k_F a^2}{2L} \frac{1}{\sin^2 \left(\frac{k_F a}{2}\right) + \left(\frac{k_F a}{2}\right)^2}.$$
Thus the parameters $T_\epsilon$ and $k_0$ is a measure of the width of $f(k)$. The prefactor in (11) is chosen to ensure a $k$-diagonal ILT term in (3) in the limit $k_0 \to 0$. The sine function ensures that the scattering is periodic in the reciprocal lattice. One could construct infinitely many functions $f(k)$ which reduce to a delta function as $k_0 \to 0$, and hence our particular choice (3) is inevitably somewhat arbitrary. However, since our focus here is merely on the qualitative aspects of momentum broadening, the detailed form of $f(k)$ is of no concern to us; any function $f(k)$ which is “smeared out” as $k_0$ increases, would give the same qualitative results. Note that $G(r=0) = \sum_k f(k) = 1/\sqrt{1+(k_0a/2)^2}$, which means that the effective value of $T_J$ actually decreases as $k_0a$ is increased. In this respect, the effect of momentum broadening is at least not underestimated in our model.

Results and discussion

We have calculated the critical temperature $T_c$ and the zero-temperature gap function for various values of $k_0a$ by solving (3) self-consistently in the thermodynamic limit $L \to \infty$. In Fig. 2 we show the results for $T_c$ for $T_J = 30$ meV, $\omega_D = 20$ meV, $\varpi = 25$ meV, $k_Fa = \pi/4$ and $4/\varpi = 2.5$ meV. It is seen that $T_c$ is slightly more sensitive to $k_0a$ for $g_k = \cos(ka)$ than for $g_k = \Theta(\omega_D - |\varepsilon_k|)$. For $g_k = \cos(ka)$, $T_c$ is reduced by a factor 2 compared to the $k$-diagonal result when $k_0a/\pi \approx 0.25$. Only 1/10 of this broadening is required for a 50% reduction of $T_c$ if one instead chooses $T_J = 50$ meV, $t = 250$ meV and $LV/2\varpi = 25$ meV. The reason for this increased sensitivity to broadening is the large increase of $t$.

In Fig. 3 we show the gap at $T = 0$ for four values of $T_J$ and fixed $k_0 = 0$, the other parameter values being the same as used for Fig. 2. In this case, the gap is given implicitly by

$$\Delta_k = \frac{\Delta_0 g_k}{1 - T_J \chi_k},$$

where $\Delta_0 \equiv V \sum_k g_k \Delta_k \chi_k$. The maximum of the gap, and hence the critical temperature $T_c$, is determined by $T_J$ through the enhancement factor $1/(1 - T_J \chi_k)$, which has its maximum on the Fermi surface. However, as seen in Fig. 3, $T_J$ does not affect the sign of the gap, which is determined by $g_k$ alone. On a 2D square lattice, the analogous statement is that the transformation properties of the gap function under the symmetry operations of the point group of the square lattice, $C_{4v}$, is given entirely in terms of the intralayer contribution to the pairing kernel, which is expandable in terms of basis functions for the irreducible representations of $C_{4v}$.

In Fig. 4 we show the gap at $T = 0$ for four values of $k_0a$ and fixed $T_J = 30$ meV. Note how the $k$-space variation of the gap decreases with increasing $k_0a$. For large enough $k_0a$, $f(k)$ is essentially independent of $k$, so the ILT term in (3) essentially becomes a constant self-consistent shift of $\Delta_k$. The main contribution to the shift comes from the Fermi surface region, where $\Delta_k$ and $\chi_k$ are maximal. Therefore, the sign of the shift is essentially determined by the sign of $\Delta_k$ on the Fermi surface, which in turn is determined by the sign of $g_k$ on the Fermi surface, which for $g_k = \cos(ka)$ changes at half-filling. Thus, the qualitative form of the gap is given by $\Delta_k = \Delta_0 g_k + T_J \Delta_1$, where, for $g_k = \cos(ka)$, the sign of $\Delta_1$ is positive below half-filling and negative above half-filling. As a consequence of this shift, $\Delta_k$ eventually ceases to change sign in the Brillouin zone for $g_k = \cos(ka)$, as seen in Fig. 3.

We now discuss the criterion for how much broadening is needed to obtain a substantial reduction of the maximum value of the gap, thereby smoothing out the sharp $k$-space structures obtained in the $k$-diagonal case. For this purpose, it is instructive to consider how a slightly broadened $T_J(k,k')$ affects the maximum value of the gap. For $k_0a/\pi \ll 1$, $\Delta_k$ varies more rapidly in the Fermi surface region than $\chi_k$, because $1/(1 - T_J \chi_k)$ is sharply peaked at the Fermi surface. Thus the variation of $\Delta_k \chi_k$ in the Fermi surface region is essentially determined by $\Delta_k$. Furthermore, the main contributions to $\sum_{k'} T_J(k_F,k') \Delta_k \chi_k$ roughly come from the region $|k_F - k'| \ll k_0$. Temporarily denoting the gap calculated for $k_0 = 0$ as $\Delta_k(0)$, it follows that as long as $k_0$ is much smaller than the characteristic width of the peak of $\Delta_k(0)$, the broadened $T_J(k_F,k')$ essentially has the same effect as a $\delta$-function. Under such circumstances, the gap is little affected by the non-$k$-diagonality. A broadening of the order of the width of the peak of $\Delta_k(0)$ is therefore required for a substantial effect of the broadening to be felt. Fig. 3 shows that the width of the peak of $\Delta_k(0)$ increases with $T_J$. The detrimental effects on the gap of an increase of $k_0a$ will therefore be reduced with an increase of $T_J$. On the other hand, increasing $t$ will make the width of the peak of $\Delta_k(0)$ smaller, because the factor $1/(1 - T_J \chi_k)$ drops more abruptly away from its peak value as one moves away from the Fermi surface when the overall amplitude of the variation of $\varepsilon_k$ is increased, as seen from the fact that this drop is proportional to

$$\delta \varepsilon_k = 2ta \sin(k_Fa) \delta k.$$  

(13)

Thus the parameters $T_J$ and $t$ have opposite effects on the sensitivity of the gap to broadening of $T_J(k,k')$. Note that one may scale the parameter $t$ entirely out of (3) to obtain a gap equation in terms of the dimensionless parameters
$1/\beta t$, $T_J/t$, $\Delta_k/t$, $V/t$ and $k_0a$ (and $\omega_D/t$, when $g_k = \Theta(\omega_D - |\varepsilon_k|)$). It should also be mentioned that the ‘realistic’ values of $T_J/t$ are difficult to ascertain, because the model we have considered is one-dimensional, and because the experimentally relevant values of $T_J$ are hard to extract. For these reasons, we can only draw qualitative conclusions from our model.

Another interesting consequence of (13) is that the width of the peak of $\Delta_k(0)$ will increase as the Fermi level is moved towards the band edges where the dispersion flattens out, since then $\delta \varepsilon_k$ decreases. So in our 1D model the system becomes more robust to a finite $k_0$ for a nearly empty or nearly full conduction band.

We finally stress that our qualitative conclusions regarding the sensitivity to momentum broadening are valid also for a 2D model. This is because the arguments used to arrive at these conclusions depend on premises that will be present also in 2D: 1) in the $k$-diagonal case, the gap shows sharp enhancement at the Fermi surface, 2) the width (and height) of the peak of this gap is increased by increasing the amplitude $T_J$ of the interlayer tunneling matrix element, 3) there will be parameters in the 2D single-electron intralayer dispersion analogous to the bandwidth of the dispersion $\varepsilon_k$, and therefore affect the width of the peak of the $k$-diagonal gap in a manner similar to what occurs in the 1D case. Note also that in the 2D case, the tight-binding dispersion flattens out near the points $(\pm \pi/a,0)$ and $(0,\pm \pi/a)$, which lie on the Fermi surface when the band is half-filled (for nearest-neighbor hopping only) or close to half-filling (when next-nearest neighbor hopping is included). These are also the points where the $k$-diagonal gap is at its maximum for such filling factors $1$. Thus it appears that near half-filling in 2D, the maximum value of the gap should be fairly robust to moderate momentum broadening.

V. CONCLUSIONS

We have considered superconductivity within the ILT mechanism in the presence of non-$k$-diagonal interlayer tunneling. We find that the sensitivity to momentum broadening is larger the smaller the width of the peak of the gap obtained for $k$-diagonal tunneling. This width is increased by increasing the amplitude $T_J$ of the interlayer tunneling matrix element. The width is decreased by increasing the bandwidth of the single-electron intralayer dispersion. Finally, the width is larger at points on the Fermi surface where the dispersion is relatively flat as compared to points where the dispersion is steeper $2$. Although we illustrated these features by solving a model with one-dimensional intralayer wavevectors, these qualitative conclusions are also valid for the more experimentally relevant case of two dimensions.

Several unusual properties of the superconducting state of the cuprates are given an explanation with the ILT mechanism. The essential feature of the ILT mechanism is the sharp $k$-space structure of the gap that arises from an unusual enhancement factor $1/(1 - T_J\chi_k)$ for a $k$-diagonal interlayer tunneling. Conclusions based on these sharp structures ought therefore to be reexamined in the presence of a slightly broadened interlayer tunneling term. This pertains for instance to the explanation of the anomalies in the neutron scattering peaks observed in YBCO using the ILT mechanism. In this case, non-trivial Fermi surface kinematics almost unique to the mechanism are essential $2$.

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FIG. 1. The critical temperature $T_c$ of the gap equation (3) as a function of the energy broadening $\omega$.

FIG. 2. The critical temperature $T_c$ as a function of $k_0a/\pi$.

FIG. 3. The $T = 0$ gap function plotted for four values of $T_J$ with $k_0 = 0$. The two cases $g_k = \Theta(\omega_D - |\varepsilon_k|)$ and $g_k = \cos(ka)$ are shown in the upper and lower panel, respectively. As $T_J$ is increased, the maximum value of the gap, occurring on the Fermi surface, increases and the variation of the gap with $k$ is enhanced. Note how the sign of the gap is always determined by $g_k$.

FIG. 4. The $T = 0$ gap function plotted for four values of $k_0a/\pi$ with $T_J = 30$ meV. The two cases $g_k = \Theta(\omega_D - |\varepsilon_k|)$ and $g_k = \cos(ka)$ are shown in the upper and lower panel, respectively. As $k_0$ is increased, the maximum value of the gap and the variation of the gap with $k$ decreases. For large enough values of $k_0a/\pi$, this is reflected for $g_k = \Theta(\omega_D - |\varepsilon_k|)$ in a gap where the only $k$-space variation comes from the sharp discontinuity in $g_k$, while for $g_k = \cos(ka)$ the gap eventually ceases to change sign.
Fig. 1
$g_k = \Theta (\omega_D - |\varepsilon_k|)$

$g_k = \cos(ka)$

Fig. 2
$\Delta_k (\text{meV})$

$ka/\pi$

$T_J = 1 \text{ meV}$
$T_J = 5 \text{ meV}$
$T_J = 15 \text{ meV}$
$T_J = 30 \text{ meV}$

Fig. 3
Fig. 4