

The penetration depth in the interlayer tunnelling model for high-temperature superconductors

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1999 J. Phys.: Condens. Matter 11 9741

(<http://iopscience.iop.org/0953-8984/11/48/332>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.218

The article was downloaded on 15/05/2010 at 18:51

Please note that [terms and conditions apply](#).

The penetration depth in the interlayer tunnelling model for high-temperature superconductors

Melissa Castle and Božidar Mitrović[†]

Physics Department, Brock University, St Catharines, Ontario, Canada L2S 3A1

Received 6 September 1999, in final form 14 October 1999

Abstract. We investigate numerically the temperature dependence of the London penetration depth within the mean-field treatment of the interlayer pair tunnelling model for the copper oxide superconductors. It is found that the assumption that the pair tunnelling is the dominant pairing mechanism in YBCO (yttrium–barium–copper oxide) is not consistent with the experimental results on this material. We also consider the Knight shift and the dynamic spin susceptibility at a low temperature within the model. We find that the experimental results for these quantities are consistent with a relatively small contribution of the interlayer pair tunnelling to the pairing channel provided that, at least in the case of the dynamic susceptibility, the in-plane pairing produces a gap of $d_{x^2-y^2}$ -wave symmetry which is non-zero within at most a few tens of meV off the Fermi line.

1. Introduction

Chakravarty, Sudbø, Anderson, and Strong proposed [1] the interlayer pair tunnelling (ILPT) model as an alternative to the BCS (Bardeen–Cooper–Schrieffer) model for describing the properties of high- T_c copper oxide superconductors. They used the ILPT model in calculations of the Knight shift and the nuclear magnetic relaxation rates [2] and obtained results consistent with experiments. In a previous work [3] we put their model into the Eliashberg form and calculated the isotope effect and the effect of non-magnetic in-plane impurity scattering on T_c . We obtained good agreement with experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ for a reasonable choice of microscopic parameters. At the same time, Yin, Chakravarty, and Anderson [4] used the ILPT model to explain the appearance of a magnetic peak in neutron scattering experiments on optimally doped YBCO below the superconducting transition temperature. They stressed that $d_{x^2-y^2}$ -wave symmetry of the gap is essential for the appearance of a peak in the imaginary part of the spin susceptibility $\chi(\mathbf{Q}, \omega)$ at a wave vector $\mathbf{Q} = (\pi/a, \pi/a, \pi/c_b)$ below T_c (a is the lattice spacing of the square CuO lattice, and c_b is the distance between the layers within a bilayer). Moreover, on the basis of their numerical calculations, they argued that such a peak would be absent in the BCS model, and concluded that the pair tunnelling must be the dominant pairing mechanism in copper oxides.

In this work we calculate the ab -plane magnetic field penetration depth within the ILPT model. The penetration depth measurements of Hardy *et al* [5] on single-crystal samples of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ provided the first strong evidence that the gap function $\Delta(\mathbf{k})$ has $d_{x^2-y^2}$ -wave symmetry. Calculations within the BCS model [6] gave, after arbitrarily setting $2\Delta_{max}(0)/k_B T_c$ to a large value of 6–8, good qualitative agreement with experiments. Clearly,

[†] Author to whom any correspondence should be addressed.

it is important to find out whether the ILPT model can describe, at least qualitatively, the temperature dependence of the London penetration depth $\lambda(T)$.

The rest of the paper is organized as follows. In section 2 we summarize the ILPT model, give the expressions for the magnetic field penetration depth, and outline the numerical procedures used in the calculations. Section 3 contains our numerical results for the in-plane penetration depth as a function of temperature. In view of our results for $\lambda(T)$, we revisit the frequency dependence of $\text{Im } \chi(\mathbf{Q}, \omega)$ at zero temperature which was studied in [4], as well as the temperature dependence of the Knight shift below T_c [2]. In section 4 we give conclusions.

2. The model

In the interlayer pair tunnelling model the gap equation at a temperature T for an $N \times N$ lattice is given by [1–4]

$$\Delta_{\mathbf{k}}(T) = T_J(\mathbf{k}) \frac{\Delta_{\mathbf{k}}(T)}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right) + \frac{1}{N^2} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}(T)}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_B T}\right). \quad (1)$$

The first term in equation (1) arises from the pair tunnelling between the layers and is local in \mathbf{k} . The form of $T_J(\mathbf{k})$ proposed in [1] based on band-structure calculations [7] is

$$T_J(\mathbf{k}) = \frac{t_{\perp}^2}{16t} [\cos(k_x a) - \cos(k_y a)]^4 \quad (2)$$

where t_{\perp} characterizes the high-energy single-electron coherent hopping from layer to layer, and is estimated to be between 0.1 eV and 0.15 eV [1]. t is the nearest-neighbour hopping matrix element in the tight-binding model for the in-plane electron motion. The quasiparticle energy is given by

$$E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \quad (3)$$

where $\varepsilon_{\mathbf{k}}$ is the tight-binding dispersion for the electron motion within a layer:

$$\varepsilon_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a)] - 4t' \cos(k_x a) \cos(k_y a) - \mu \quad (4)$$

and μ is the chemical potential.

The second term in (1) comes from in-plane pairing due to an instantaneous interaction $V_{\mathbf{k},\mathbf{k}'}$. As in [4], we assume that $V_{\mathbf{k},\mathbf{k}'}$ leads to $d_{x^2-y^2}$ -wave symmetry of the gap and take

$$V_{\mathbf{k},\mathbf{k}'} = V g_{\mathbf{k}} g_{\mathbf{k}'} \quad g_{\mathbf{k}} = \frac{1}{2} [\cos(k_x a) - \cos(k_y a)] \Theta(\Omega_{max} - |\varepsilon_{\mathbf{k}}|) \quad (5)$$

where V and Ω_{max} are the magnitude and energy cut-off of the in-plane pairing interaction, respectively.

Equation (1) was solved self-consistently at any given temperature below the superconducting transition temperature. In the pure interlayer tunnelling limit ($V = 0$) at $T = 0$ the solution is trivial [4], and is given as

$$\Delta_{\mathbf{k}}(0) = \sqrt{\left(\frac{T_J(\mathbf{k})}{2}\right)^2 - \varepsilon_{\mathbf{k}}^2} \Theta\left(\frac{T_J(\mathbf{k})}{2} - |\varepsilon_{\mathbf{k}}|\right). \quad (6)$$

Thus, for a given \mathbf{k} -direction $\Delta_{\mathbf{k}}(0)$ is non-zero only within $T_J(\mathbf{k})/2$ off the Fermi line. We used this solution as an initial guess for $\Delta_{\mathbf{k}}$ when $V > 0$. Note that the in-plane pairing term is non-local in \mathbf{k} , and its contribution to $\Delta_{\mathbf{k}}$ is proportional to $g_{\mathbf{k}}$ for all \mathbf{k} . Therefore, the choice (6) for the initial guess does not force $\Delta_{\mathbf{k}}$ to be zero at a point \mathbf{k} at which the in-plane interaction produces a finite gap. At finite T we used for an initial guess the converged solution

at a lower temperature. In this way we obtained highly converged solutions for lattices as large as 1024×1024 .

The superconducting transition temperature T_c was obtained by viewing (1) as an eigenvalue problem when $E_k = |\varepsilon_k|$ and finding the highest temperature at which the maximum eigenvalue is 1. The maximum eigenvalue was determined using the power method [8]. We found that our self-consistent solutions for $T < T_c$ were in complete agreement with the T_c determined by solving for the maximum eigenvalue, in that Δ_k did not converge at temperatures exceeding T_c . This consistency gave us confidence in the overall accuracy of our numerical solutions.

The ab -plane London penetration depth is given by [9]

$$\frac{1}{\lambda(T)^2} = \frac{4\pi e^2}{c^2} 2 \frac{1}{(Na)^2 c} \sum_k v_{kx}^2 \left[\delta(\varepsilon_k) - \left(-\frac{\partial f(E_k)}{\partial E_k} \right) \right]. \quad (7)$$

Here, e is the electron charge, c is the speed of light in vacuum, c is the size of the unit cell along the c -axis, f is the Fermi function, and

$$v_{kx} = \frac{1}{\hbar} \frac{\partial \varepsilon_k}{\partial k_x} = 2ta \sin(k_x a) + 4t'a \sin(k_x a) \cos(k_y a) \quad (8)$$

is the x -component of the band velocity. The term in (7) containing the δ -function arises from the diamagnetic current density and is temperature independent. The term involving $-\partial f(E_k)/\partial E_k$ arises from the paramagnetic current density and is temperature dependent. Its size increases as the temperature increases and at T_c it completely cancels the diamagnetic part. The evaluation of (7) seems to be straightforward once the solution $\Delta_k(T)$ is known. However, since $-\partial f(E_k)/\partial E_k$ is sharply peaked near the Fermi line, a lattice (i.e. N) that is not large enough will not yield an accurate value for the paramagnetic term, in particular at low temperatures, because there are too few k -points in the important energy range. We found that a 64×64 lattice, which is commonly used in strong-coupling calculations involving antiferromagnetic spin-fluctuation models for high- T_c s, does not give accurate results for $\lambda(T)$. By comparing the values of $1/\lambda(T)^2$ obtained for 512×512 and 1024×1024 lattices we concluded that these lattices give accurate results for the penetration depth above 10 K in the case of the superconducting T_c of 94.55 K.

The lattice size problems could be reduced by rewriting (7) as

$$\frac{1}{\lambda(T)^2} = \frac{4\pi e^2}{c^2} 2 \frac{1}{c} \left(N_v^n(0) - \int_{-\infty}^{\infty} dE N_v^s(E) \left(-\frac{\partial f(E)}{\partial E} \right) \right) \quad (9)$$

where

$$N_v^n(E) = \frac{1}{(Na)^2} \sum_k v_{kx}^2 \delta(\varepsilon_k - E) \quad (10)$$

$$N_v^s(E) = \frac{1}{(Na)^2} \sum_k v_{kx}^2 \delta(E_k - E) \quad (11)$$

and evaluating these weighted densities of states using the tetrahedron method [10] adapted to a square lattice. While this method gave a vast improvement in $1/\lambda(T)^2$ calculated for smaller lattice sizes, it gave the same results as the direct k -summation method, equation (7), for a 512×512 lattice above 10 K ($T_c = 94.6$ K). However, we found that even for the largest lattice sizes considered, the tetrahedron method introduces a tiny gap in $N_v^s(E)$ for Δ_k with $d_{x^2-y^2}$ -wave symmetry. Thus, we did not trust the accuracy of $1/\lambda(T)^2$ calculated at very low temperatures and we present here only the results which could be reproduced by either of the two calculational methods on a 512×512 lattice.

In conclusion of this section we point out that $v_{k_x}^2$ is not invariant under the transformations from the C_{4v} point group, and therefore $v_{k_x}^2$ has to be replaced by $(v_{k_x}^2 + v_{k_y}^2)/2$ when the k -sums in (7), (10), and (11) are restricted to the irreducible wedge of the first Brillouin zone.

3. Numerical results

To fix the ideas, we choose the same band parameters as in [1–4], namely $t = 250$ meV and $t'/t = -0.45$. Also, we take the same value for the chemical potential, $\mu = -315$ meV, as in [2, 4]. This value of μ corresponds to a band filling factor of $n = 0.856$. As in [2], Ω_{max} was fixed at 20 meV (the energy cut-off for in-plane interaction was not specified in [4]), and the lattice size was fixed to 512×512 .

Next, we choose the parameters in the (t_{\perp}, V) -plane, or (T_J, V) -plane, where $T_J = t_{\perp}^2/t$, such that the superconducting transition temperature T_c is the same in all cases considered. We find that for $t_{\perp} = 104.62$ meV ($T_J = 43.78$ meV) and $V = 0$, corresponding to the case of an infinitesimal in-plane pairing, a T_c of 94.55 K is obtained—a value comparable to what is observed for optimally doped YBCO. In the opposite limit, when $t_{\perp} = 0$, i.e. for no interlayer pair tunnelling, an in-plane pairing interaction of $V = 2442.15$ meV ($\lambda \equiv N(0)V = 2.25$, $N(0) = 9.2 \times 10^{-4}$ states meV $^{-1}$ /(cell spin)) is needed to produce the same T_c . The additional values of t_{\perp} considered were 100 meV, 70 meV, 50 meV, and 30 meV (i.e. $T_J = 40$ meV, 19.6 meV, 10 meV, 3.6 meV, respectively), and the corresponding values of V were 824.745 meV, 1790.65 meV, 2125.23 meV, and 2331.04 meV (i.e. $\lambda = 0.76$, 1.65, 1.96, 2.15), respectively. We note that without the interlayer pair tunnelling these values of in-plane pairing interaction and $\Omega_{max} = 20$ meV give transition temperatures of 10.96 K, 61.3 K, 78.6 K, and 89.0 K, respectively. Thus, only for the two largest values of T_J can one say that the ILPT is the dominant pairing mechanism.

The results for the penetration depth are shown in figure 1 (for the c -axis lattice parameter

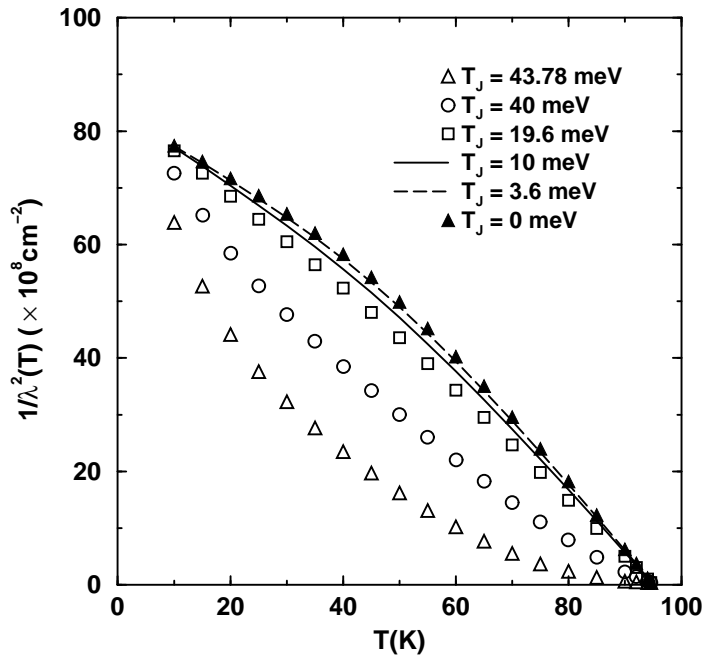


Figure 1. The temperature dependence of $1/\lambda(T)^2$ calculated for various values of $T_J = t_{\perp}^2/t$. The two largest values of T_J give curves that have a convex shape, which is not observed experimentally [5].

we took $c = 11.6802 \text{ \AA}$ [11]). Only the data obtained for $t_{\perp} \leq 70 \text{ meV}$ resemble qualitatively the experimental results of Hardy *et al* [5]. The values for $t_{\perp} \geq 100 \text{ meV}$ produce a convex shape of $1/\lambda(T)^2$ which is not observed experimentally. Thus, our results suggest that a scenario for superconductivity in YBCO in which the interlayer pair tunnelling is the dominant [4] pairing mechanism cannot be correct. We note that if the calculated values in figure 1 are linearly extrapolated to $T = 0 \text{ K}$ we find $\lambda(0) \approx 1100 \text{ \AA}$ —of the right order of magnitude for YBCO [12].

To understand the difference in shape of the curves in figure 1 obtained in the large- T_J limit (i.e. $t_{\perp} \geq 100 \text{ meV}$) from those that were obtained for smaller values of T_J it is necessary to examine the temperature dependence of the gap function $\Delta_k(T)$. In figure 2 we show the temperature dependence of the maximum gap $\Delta_{max}(T)$. It is interesting that the temperature dependence of the maximum gap for the case of no in-plane interaction is essentially the same as that which is calculated by Mühlischlegel [13] from the BCS theory for an isotropic s-wave superconductor (the dotted line in figure 2, which was obtained by scaling the numerical results of Mühlischlegel so that $\Delta(0)$ and T_c agree with our numerical results). Clearly, the variation of $\Delta_{max}(T)$ with temperature cannot account for the difference in shape of the $1/\lambda(T)^2$ curves in figure 1. However, the reason for the difference in shape can be deduced from figures 3–5 where the momentum dependence of the gap is plotted at $T = 0 \text{ K}$, 50 K , and 94 K (just below the critical temperature) for $T_J = 43.78 \text{ meV}$, 40 meV , and 10 meV , respectively. $\Delta_k(T)$ is more sharply peaked for smaller in-plane interaction V , and the relative sharpness increases with increasing temperature. In the extreme case of $V = 0$ (figure 3), the region of k -space in which $\Delta_k(T) \neq 0$ decreases with increasing temperature. This should be contrasted with

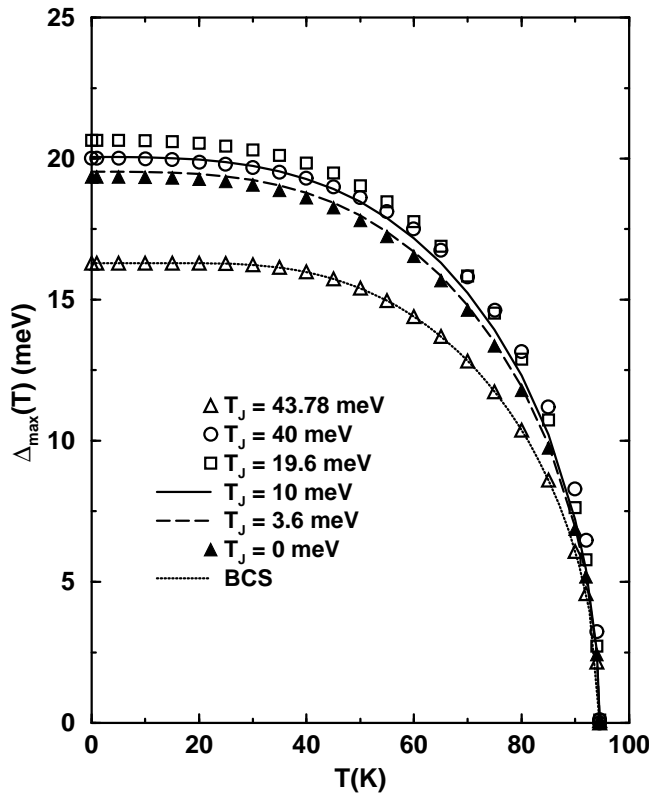


Figure 2. The temperature dependence of the maximum gap calculated for the same set of values of T_J as were used to obtain the curves in figure 1. The dotted curve (BCS) is obtained by scaling the numerical results of Mühlischlegel [13] for the BCS case so that $\Delta(0)$ and T_c agree with our numerical results for zero in-plane interaction ($T_J = 43.78 \text{ meV}$).

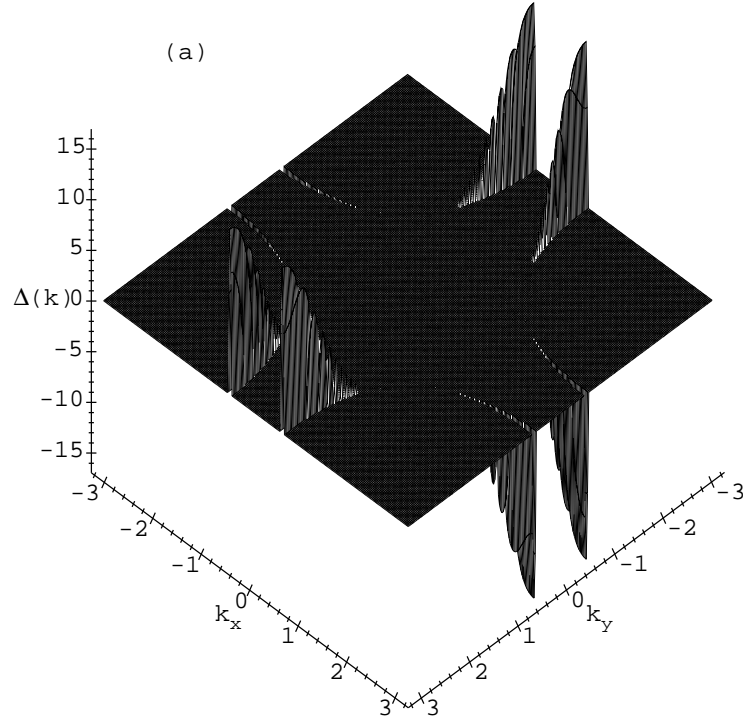


Figure 3. The gap $\Delta_k(T)$ (in meV) as a function of k_x and k_y (the lattice spacing a of the square CuO lattice is set equal to 1) for $T_J = 43.78$ meV. (a) $T = 0$ K, (b) $T = 50$ K, and (c) $T = 94$ K. In the case of no in-plane interaction the gap collapses to eight sharp spikes just below $T_c = 94.55$ K. The solutions in figures 3–5 were obtained for a 512×512 lattice, but in order to obtain clear graphs we show the solutions on a 256×256 mesh.

the case where $T_J = 10$ meV for which the larger in-plane interaction ensures that $\Delta_k(T)$ shrinks uniformly with increasing T . As a result, the cancellation of the diamagnetic term by the paramagnetic term in (7) occurs over a larger region of momentum space when T_J is large. Since this cancellation is not complete until a *common* T_c is reached, $1/\lambda(T)^2$ must be convex in the case of small in-plane pairing.

We note that the ratio $2\Delta_{max}(0)/k_B T_c$ is 4.0, 4.9, 5.1, 4.9, 4.8, and 4.75 for t_\perp equal to 104.62 meV ($V = 0$), 100 meV, 70 meV, 50 meV, 30 meV, and 0 meV, respectively. In fact, it is easy to prove analytically that $2\Delta_{max}(0)/k_B T_c$ is exactly 4 for no in-plane interaction as long as the maximum in $\sqrt{[(T_J(\mathbf{k})/2)^2 - \varepsilon_k^2]}$ is on the Fermi line $\varepsilon_k = 0$, *regardless* of the precise form of $T_J(\mathbf{k})$ and ε_k . These values of $2\Delta_{max}(0)/k_B T_c$ are larger than the canonical BCS value 3.53 for an isotropic s-wave superconductor. At the same time, they are about a factor of two smaller than what was obtained in the self-consistent studies [14, 15] of the two-dimensional Hubbard model. The retardation and damping effects associated with spin-fluctuation-mediated pairing suppress the value of transition temperature more than the zero-temperature gap, resulting in an enhanced value of $2\Delta_{max}(0)/k_B T_c$. Since the interlayer pair tunnelling term is local in both \mathbf{k} and the Matsubara frequency $i\omega_n$ (see reference [3]), it is not expected that these retardation and damping effects will change qualitatively the shape of $1/\lambda(T)^2$ in the case where the interlayer pair tunnelling is the dominant pairing mechanism. Our preliminary results [16] on a 64×64 lattice for a model [17] of in-plane pairing via antiferromagnetic spin fluctuations confirm this expectation.

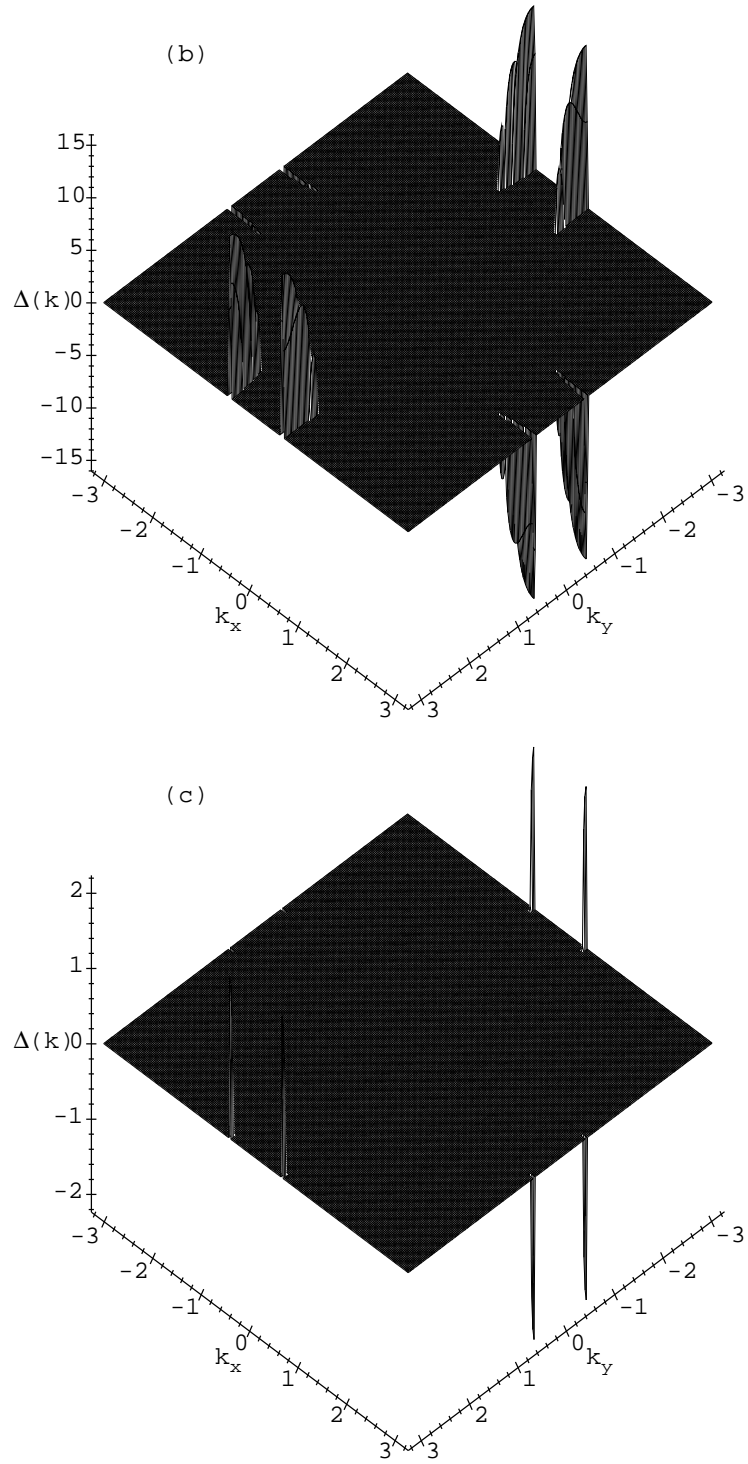


Figure 3. (Continued)

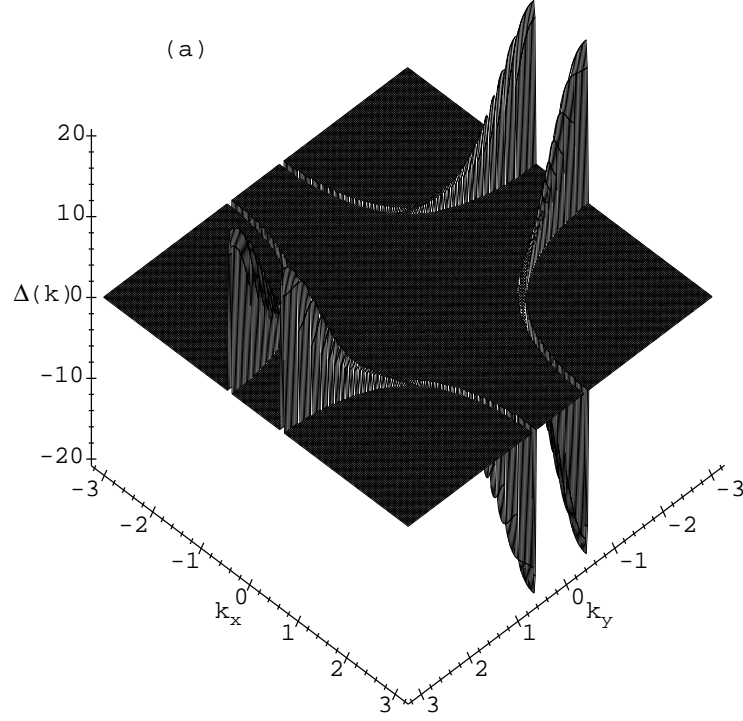


Figure 4. The gap $\Delta_k(T)$ (in meV) as a function of k_x and k_y for $T_J = 40$ meV at the three different temperatures used in figure 3: (a) $T = 0$ K, (b) $T = 50$ K, and (c) $T = 94$ K. Note that with a finite in-plane interaction, $\Delta_k(T)$ always has a component which is proportional to $g_k = (V/2)[\cos(k_x a) - \cos(k_y a)]\Theta(\Omega_{max} - |\varepsilon_k|)$. Here $\Omega_{max} = 20$ meV and $\lambda \equiv N(0)V = 0.76$.

Since we find that the experimentally observed temperature dependence of the penetration depth in YBCO is not consistent with the notion that the ILPT is the dominant pairing mechanism in this material, which contradicts the findings in [2] and [4], we calculate the Knight shift and the imaginary part of the spin susceptibility at $T = 0$ K for the parameters used in figure 1 to further investigate the model. In [2] the Knight shift was calculated assuming that the in-plane interaction yields s-wave symmetry of the gap. Our solutions for a 512×512 lattice, assuming $d_{x^2-y^2}$ -wave symmetry of the gap and using the same Fermi-liquid correction parameter $U = 2t$ as was used in [2] (see equation (8) in [2]), led to the temperature-dependent Knight shifts shown in figure 6. As in the case of the penetration depth, the two largest values of T_J give poor agreement with the experimental results (open and filled diamonds in figure 6) [18, 19]. At the same time, the results obtained for the cases when the in-plane pairing is the more dominant pairing channel are in reasonable qualitative agreement with the experiments.

At zero temperature the imaginary part of the spin susceptibility in the superconducting state is given by [4, 9]

$$\text{Im } \chi(\mathbf{Q}, \omega) = \pi \frac{1}{N^2} \sum_{\mathbf{k}} \frac{1}{2} \left(1 - \frac{\varepsilon_{\mathbf{k}} \varepsilon_{\mathbf{k}+\mathbf{Q}} + \Delta_{\mathbf{k}} \Delta_{\mathbf{k}+\mathbf{Q}}}{E_{\mathbf{k}} E_{\mathbf{k}+\mathbf{Q}}} \right) \delta(E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{Q}} - \omega). \quad (12)$$

In figure 7 we show our results for $\text{Im } \chi(\mathbf{Q}, \omega)$ calculated at the wave vector $\mathbf{Q} = (\pi/a, \pi/a)$ and at zero temperature for a 1024×1024 lattice using the tetrahedron method [10]. The larger lattice size was needed to avoid a spurious peak (single point) near the steep rise in $\text{Im } \chi$ for $T_J < 40$ meV. While the two largest values for T_J yield the sharpest peaks, all the values

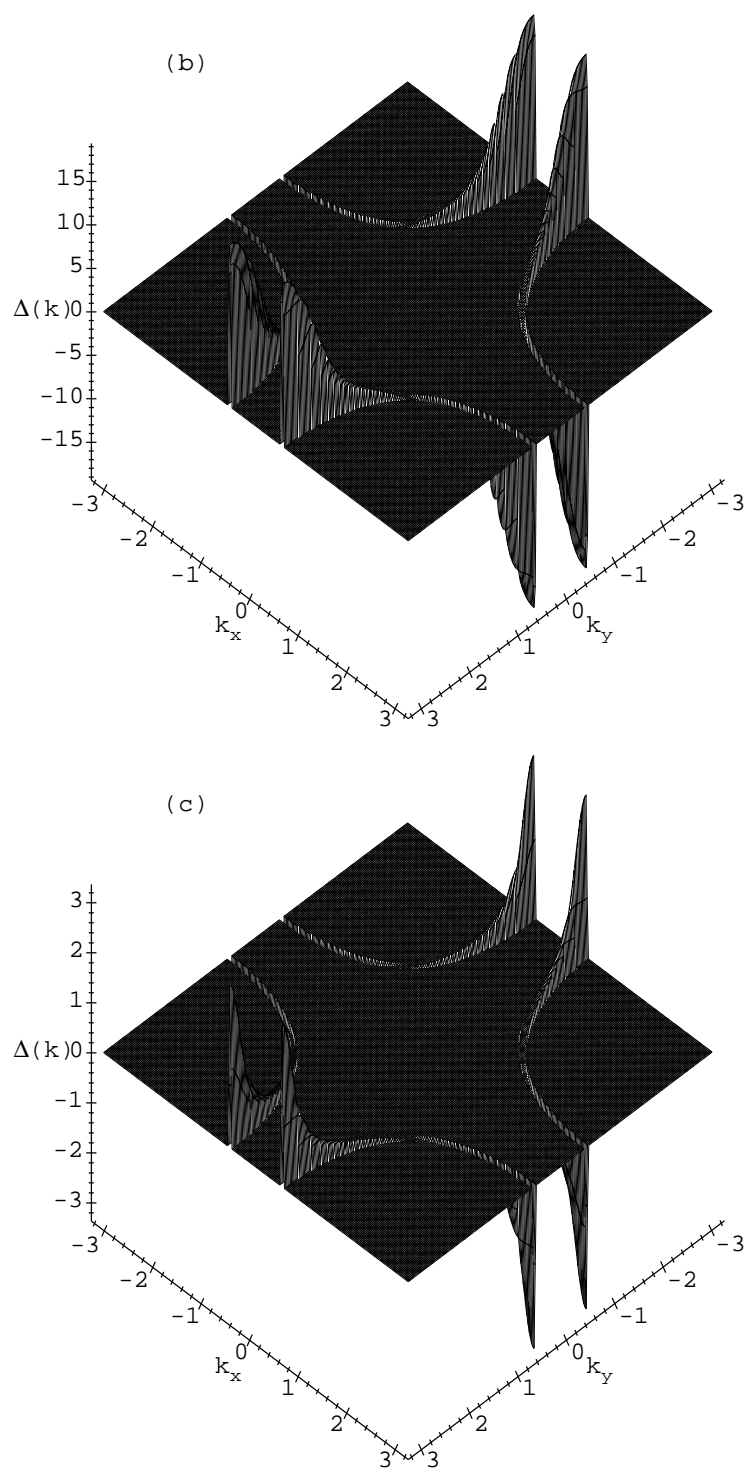


Figure 4. (Continued)

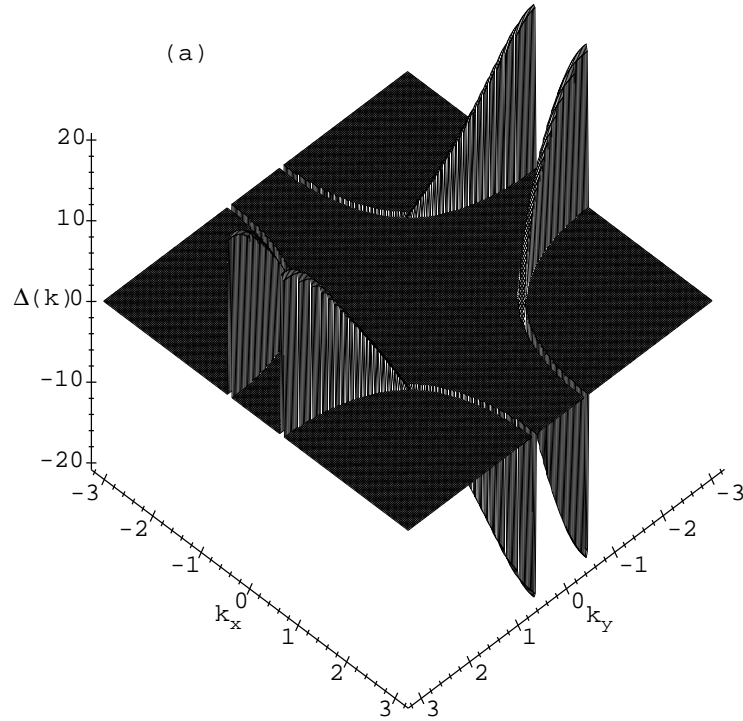


Figure 5. The gap $\Delta_k(T)$ (in meV) as a function of k_x and k_y for $T_J = 10$ meV. (a) $T = 0$ K, (b) $T = 50$ K, and (c) $T = 94$ K. This value of T_J is in the range where the size and the momentum dependence of the gap are dominated by in-plane interaction. In this case, unlike the two cases shown in figures 3 and 4 where the pair tunnelling dominates, the relative sharpness of the gap function does not increase with increasing temperature.

of T_J , including $T_J = 0$, produce peaks in $\text{Im } \chi(\mathbf{Q}, \omega)$. In fact, for $T_J < 40$ meV the peaks are located near 40 meV as found in the experiments [20, 21]. In [20], the intrinsic width of the magnetic peak was found to be at most 3 meV, while in [21], which had a slightly better energy resolution (4.7 meV compared to 5.5 meV), the magnetic peak was found to extend from 32 meV to 46 meV—a range comparable to what we find for $T_J < 40$ meV. Our results for $\text{Im } \chi(\mathbf{Q}, \omega)$ for small values of T_J contradict the findings in [4], in particular the claim by Yin *et al* that $T_J = 0$ produces no peak in the imaginary part of the spin susceptibility. We found that their $T_J = 0$ result is a consequence of their assumption that the $T_J = 0$ case corresponds to $\Delta_k = (\Delta_0/2)[\cos(k_x a) - \cos(k_y a)]$ for *all* \mathbf{k} in the first Brillouin zone, as indicated by the dash-dot curve in figure 7. Our result for $T_J = 0$ in figure 7 was obtained by cutting off the in-plane interaction (i.e. the gap) at $\Omega_{max} = 20$ meV off the Fermi line. This dependence of the shape of $\text{Im } \chi(\mathbf{Q}, \omega)$ on Ω_{max} prompted us to question whether our results for the London penetration depth, the Knight shift and the spin susceptibility would change if we chose a different value for the energy cut-off of the in-plane interaction, since the choice $\Omega_{max} = 20$ meV was rather arbitrary.

We recalculated $1/\lambda(T)^2$, $K(T)/K(T_c)$, and $\text{Im } \chi(\mathbf{Q}, \omega)$ for $T_J = 40$ meV, 19.6 meV, and 0 meV using an energy cut-off $\Omega_{max} = 200$ meV (an order of magnitude larger) and values of the in-plane interaction V that produce a superconducting transition temperature of 94.55 K, as before. The corresponding values of V were 403.07 meV, 595.36 meV, and 696.5 meV, respectively (i.e. $\lambda = N(0)V = 0.37, 0.55, \text{ and } 0.64$, respectively). For both the penetration

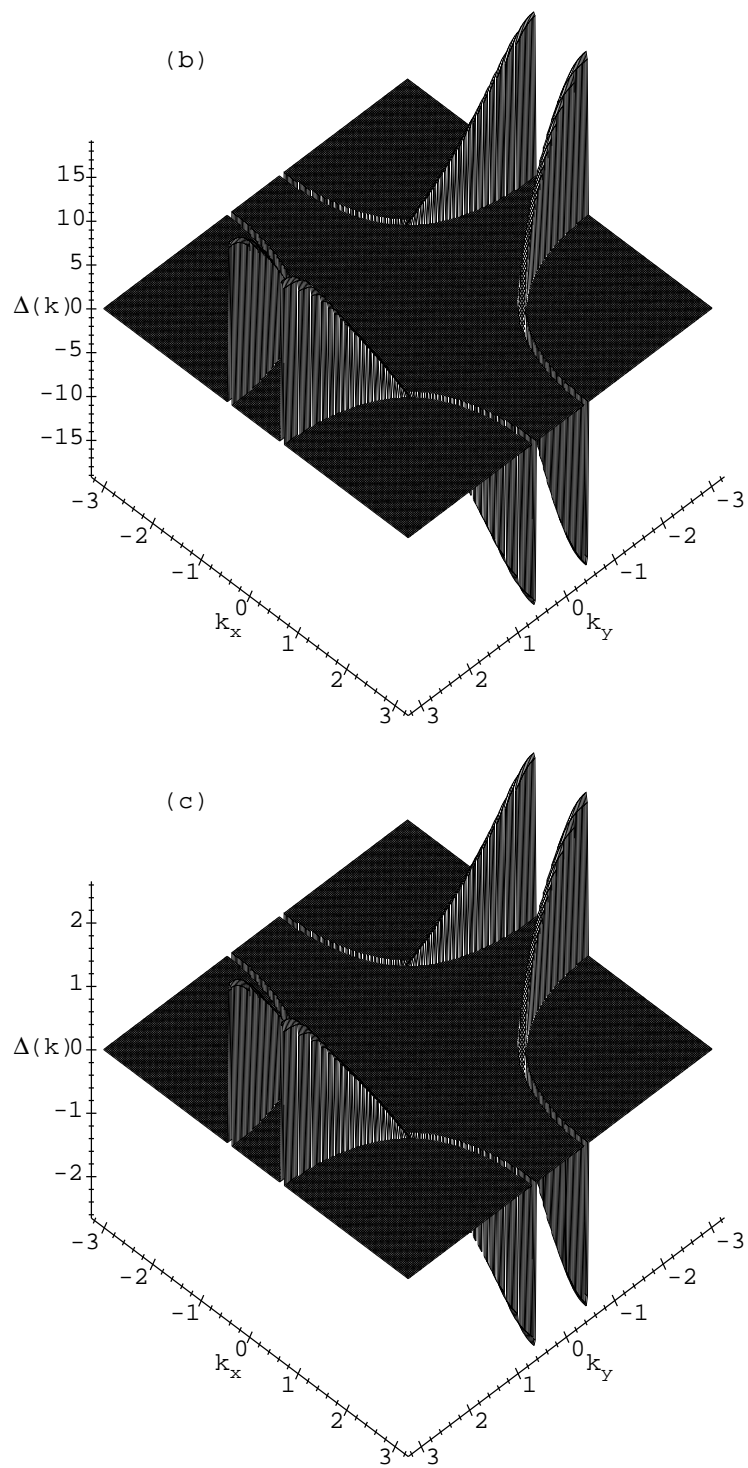


Figure 5. (Continued)

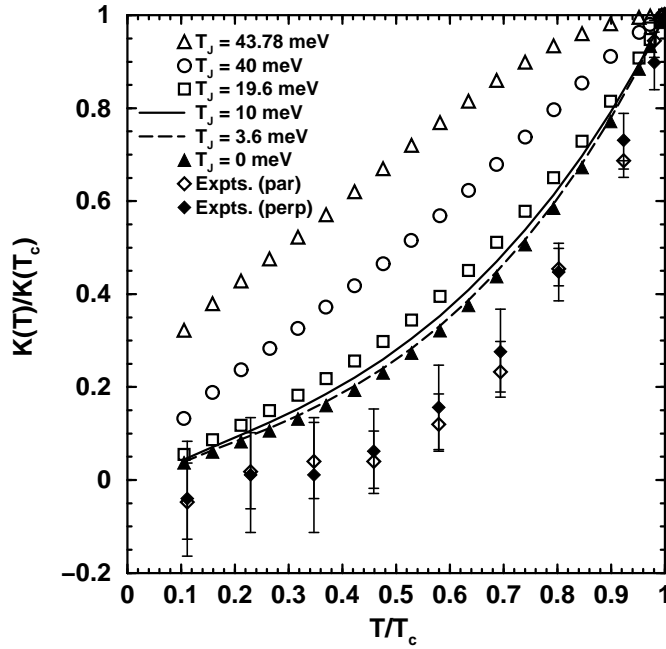


Figure 6. The Knight shift normalized to its value at T_c as a function of temperature for the values of T_J used in figure 1. The experimental values (open and filled diamonds) were obtained for YBCO for O(2, 3) [18, 19].

depth and the Knight shift we obtained virtually the same results as those in figures 1 and 6. We explain this result by the fact that these quantities probe the gap $\Delta_k(T)$ only to within about $k_B T$ off the Fermi line because of the factor $-\partial f(E)/\partial E$ (see equation (7)). The size and the shape of the gap in this energy range are determined by the requirement that T_c be fixed and by the form of $T_J(k)$ and/or by the form of $V_{k,k'}$ (equation (5)). However, as illustrated in figure 8, increasing the range of in-plane interaction from 20 meV to 200 meV has a dramatic effect on $\text{Im } \chi(Q, \omega)$ for $T_J < 40$ meV (i.e. for the case when T_J no longer dominates and the in-plane interaction becomes essential to produce a transition temperature of 94.55 K). The fairly sharp peak in figure 7 which was obtained for $T_J = 19.6$ meV is substantially reduced by increasing the range around the Fermi line in which $\Delta_k \neq 0$, and the peak in figure 7 obtained for $T_J = 0$ and $\Omega_{max} = 20$ meV is completely destroyed by increasing the cut-off to 200 meV. These results are in agreement with the argument given in [4] that the gap (of $d_{x^2-y^2}$ -wave symmetry) has to be non-zero in a fairly narrow region around the Fermi line in order to obtain a peak in $\text{Im } \chi(Q, \omega)$ [4]. However, our results for the penetration depth and the Knight shift assuming $d_{x^2-y^2}$ -wave symmetry of the gap rule out the scenario in which the narrowness of the gap is a consequence of the fact that the interlayer pair tunnelling is the dominant pairing mechanism in YBCO.

4. Conclusions

Our numerical results for the temperature dependence of the magnetic field penetration depth and for the Knight shift show that the interlayer pair tunnelling cannot be the dominant pairing mechanism in YBCO, at least within the mean-field-like description proposed in [1]

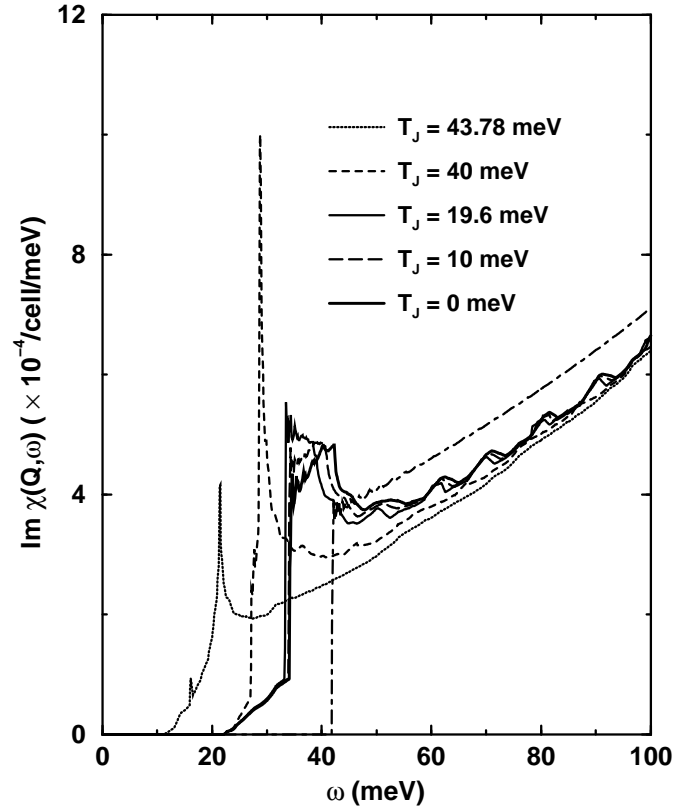


Figure 7. The imaginary part of the zero-temperature spin susceptibility $\chi(Q, \omega)$ at the wave vector $Q = (\pi/a, \pi/a)$ for the values of T_J used in figure 1, except for $T_J = 3.6$ meV which is nearly identical to the one obtained for $T_J = 0$ meV. The dash-dot curve was obtained for $\Delta_k = (\Delta_0/2)[\cos(k_x a) - \cos(k_y a)]$, $\Delta_0 = 25$ meV, for all k in the first Brillouin zone. The energy cut-off of in-plane interaction is $\Omega_{max} = 20$ meV.

(see also [3] which extends the mean-field model to the case of time-dependent in-plane interaction). While our results do not rule out the ILPT as an additional pairing channel in copper oxide superconductors, they do clearly show that the in-plane pairing interaction must play a significant role in these materials. The best agreement with the experimental results on YBCO for the penetration depth, the Knight shift, and for the peak in the spin susceptibility at a low temperature was obtained for $T_J \leq 19.6$ meV, assuming that the contribution to the gap from the in-plane interaction is significant only within a few tens of meV off the Fermi line. We emphasize that these conclusions hinge on the mean-field-like description of the interlayer pair tunnelling and in-plane interactions. It was pointed out in [1] that due to the locality in k -space of the pair tunnelling contribution to the gap, one should expect the fluctuations to play an important role when T_J is large. In the opposite limit, i.e. in the usual BCS theory, the number of pair states k' which interact with a given pair state k is large, and thus the mean-field treatment is valid. The quantity $1/\lambda(T)^2$ is proportional to the helicity modulus of a superconductor which measures the stiffness of the superconductor with respect to twists in phase of the order parameter. Roddick and Stroud have shown [22] that phase fluctuations in a nodeless order parameter can produce a low-temperature penetration depth $\lambda(T)$ which varies linearly with T in an isotropic, three-dimensional superconductor. Thus, it would be

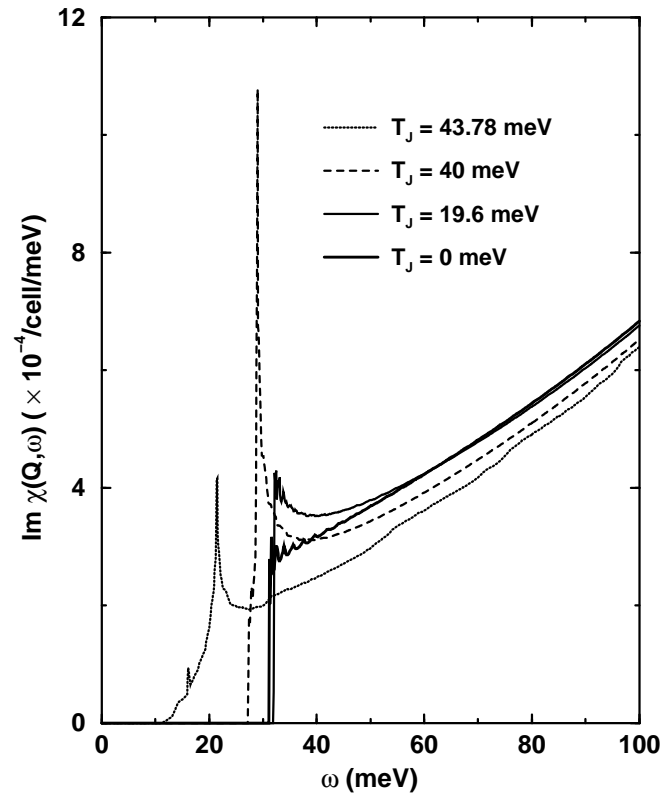


Figure 8. The imaginary part of the zero-temperature spin susceptibility $\chi(Q, \omega)$ at the wave vector $Q = (\pi/a, \pi/a)$ for the larger energy cut-off of in-plane interaction $\Omega_{max} = 200$ meV. Only several representative values of T_J from figure 7 are considered.

interesting to study the effects of fluctuations on $1/\lambda(T)^2$ within the ILPT model in the large- T_J limit. We leave this problem to a future investigation.

Finally, we note that our results are consistent with several recent experiments [23–25] which also conclude that the interlayer pair tunnelling cannot be the dominant pairing mechanism in high- T_c copper oxide superconductors.

Acknowledgments

This work was supported by the Natural Sciences and Engineering Research Council of Canada through a graduate scholarship awarded to MC and through an operating grant to BM.

References

- [1] Chakravarty S, Sudbø A, Anderson P W and Strong S 1993 *Science* **261** 337
- [2] Sudbø A, Chakravarty S, Strong S and Anderson P W 1994 *Phys. Rev. B* **49** 12 245
- [3] Mitrović B and Castle M 1997 *J. Phys.: Condens. Matter* **9** 9007
- [4] Yin L, Chakravarty S and Anderson P W 1997 *Phys. Rev. Lett.* **78** 3559
- [5] Hardy W N, Bonn D A, Morgan D C, Liang R and Zhang K 1993 *Phys. Rev. Lett.* **70** 3999
- [6] Scalapino D J 1993 *J. Phys. Chem. Solids* **54** 1433
- [7] Andersen O K, Liechtenstein A I, Jepsen O and Paulsen F 1996 *J. Phys. Chem. Solids* **56** 1573

- [8] Gentzsch W 1984 *Vectorization of Computer Programs with Applications to Computational Fluid Dynamics* (Braunschweig: Vieweg) pp 120–1
- [9] Schrieffer J R 1964 *Theory of Superconductivity* (New York: Benjamin)
- [10] Lehmann G and Taut M 1972 *Phys. Status Solidi b* **54** 469
Lehmann G and Taut M 1973 *Phys. Status Solidi b* **57** 815
- [11] Jorgensen J D, Veal B W, Paulikas A P, Nowicki L J, Crabtree G W, Claus H and Kwok W K 1990 *Phys. Rev. B* **41** 1863
- [12] Basov D N, Liang R, Bonn D A, Hardy W N, Dabrowski B, Quijada M, Tanner D B, Rice J P, Ginsberg D M and Timusk T 1995 *Phys. Rev. Lett.* **74** 598
- [13] Mühlischlegel B 1959 *Z. Phys.* **155** 313
- [14] Monthoux P and Scalapino D J 1994 *Phys. Rev. Lett.* **72** 1874
- [15] Pao C-H and Bickers N E 1995 *Phys. Rev. B* **51** 16 310
- [16] Castle M and Mitrović B 1999 unpublished
- [17] Kostur V N and Mitrović B 1995 *Phys. Rev. B* **51** 6064
- [18] Takigawa M, Hammel P C, Heffner R H, Fisk Z, Ott K C and Thompson J D 1989 *Physica* **162–164** 853
- [19] Takigawa M, Hammel P C, Heffner R H and Fisk Z 1989 *Phys. Rev. B* **39** 7371
- [20] Fong F H, Keimer B, Anderson P W, Reznik D, Doğan F and Aksay I A 1995 *Phys. Rev. Lett.* **75** 316
Fong F H, Keimer B, Reznik D, Milius D L and Aksay I A 1996 *Phys. Rev. B* **54** 6708
- [21] Bourges P, Regnault L P, Sidis Y and Vettier C 1996 *Phys. Rev. B* **53** 876
- [22] Roddick E and Stroud D 1995 *Phys. Rev. Lett.* **74** 1430
- [23] Yurgens A, Winkler D, Cleason T, Murayama T and Ando Y 1999 *Phys. Rev. Lett.* **82** 3148
- [24] Schützmann J, Somal H S, Tsvetkov A A, van der Marel D, Koops G E J, Kolesnikov N, Ren Z F, Wang J H, Brück E and Menovsky A A 1997 *Phys. Rev. B* **55** 11 118
- [25] Gagnon R, Pu S, Ellman B and Taillefer L 1997 *Phys. Rev. Lett.* **78** 1976