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Plane–chain coupling in $\text{YBa}_2\text{Cu}_3\text{O}_7$: temperature dependence of the penetration depth

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Abstract

We have studied the penetration depth for a model of $\text{YBa}_2\text{Cu}_3\text{O}_7$ involving pairing, both in the CuO_2 planes and in the CuO chains. In this model pairing in the planes is due to an attractive interaction, while Coulomb repulsion induces in the chains an order parameter with opposite sign. Due to the anti-crossing produced by hybridization between planes and chains, one obtains a d-wave like order parameter which changes sign on a single sheet of the Fermi surface and has nodes in the gap. We find that our model accounts quite well for the anisotropy of the penetration depth and for the absolute values. We reproduce fairly well the whole temperature dependence for both the a - and the b -directions, including the linear dependence at low temperature. We use a set of parameters which are all quite reasonable physically. Our results for the c -direction are also satisfactory, although the situation is less clear both experimentally and theoretically. © 1997 Elsevier Science B.V.

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1. Introduction

The debate about the mechanism of high- T_c superconductivity has recently seen marked progress by focusing on the symmetry of the superconducting order parameter. This question is intimately related to the mechanism but lends itself much more easily to experimental answers. A number of recent experiments, mostly on $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO), have shown that the order parameter displays lines of nodes on

the Fermi surface. The most spectacular ones are the phase sensitive experiments [1–3] which provide striking evidence for a change of sign of the order parameter at the Fermi surface. However these experiments are sensitive to the quality of the interfaces, which are not under perfect control. It is therefore important that other experiments, including tunnelling [4], Raman scattering [5] and penetration depth [6], have shown the existence of low energy excited states. Although these experiments are not phase sensitive and could be explained by a strongly anisotropic s-wave order parameter, this interpretation seems fairly unlikely in view of the linear slope of the penetration depth at low temperature, which is

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particularly striking and has been observed both in crystals [6] and in films [7].

A natural interpretation of the existence of nodes for the order parameter is the spin fluctuation mechanism [8–10] which predicted a $d_{x^2-y^2}$ symmetry. But this hypothesis remains controversial because it meets with experimental as well as theoretical difficulties. The most prominent experimental stumbling block is the observation of a sizeable Josephson current [11,12] in *c*-axis tunnelling between $\text{YBa}_2\text{Cu}_3\text{O}_7$ and Pb which contradicts a pure d-wave symmetry, and which is hard to interpret as being caused by the small orthorhombic distortion because of the large size of the effect. Other experiments display also a strong *ab*-plane anisotropy for the superconducting properties, such as the magnetic field dependence of the specific heat anomaly at T_c of the parent compound $\text{LuBa}_2\text{Cu}_3\text{O}_7$. Most strikingly, the penetration depth has a marked anisotropy [13] since, at zero temperature, the ratio between the superfluid densities $\lambda_b^{-2}(0)/\lambda_a^{-2}(0)$ is 2.3, in good agreement with the anisotropy of the normal state resistivity and of the square of the plasma frequency [13]. In $\text{YBa}_2\text{Cu}_4\text{O}_8$, which has an orthorhombic distortion of 0.8% (that is somewhat less than $\text{YBa}_2\text{Cu}_3\text{O}_7$ which has 1.6%) and where there are twice as many chains as in $\text{YBa}_2\text{Cu}_3\text{O}_7$, the superfluid density anisotropy [13] is as high as 6.2. In view of this evolution with increasing the number of chains, it is hard to escape the conclusion that the chains are conducting and that it is their direct contribution which is responsible for the superfluid density anisotropy. Now, the linear term in $\lambda_b^{-2}(T)$ at low T is typically 3 times the linear term in $\lambda_a^{-2}(T)$. If we attribute the linear term to the existence of nodes in the gap, this implies, roughly speaking, that there must be something like nodes on the chains. This does not fit easily in the spin fluctuation picture, and is rather a strong indication that chains must be explicitly taken into account for a proper description of the superconducting properties, even if it is believed that they are unlikely to be the place for the dominant driving force toward superconductivity.

Another conspicuous problem of the spin fluctuation interpretation is the weak sensitivity of the critical temperature of $\text{YBa}_2\text{Cu}_3\text{O}_7$ to the presence of impurities. Indeed, standard impurities produce in d-wave superconductors [14,15] an effect analogous

to pair-breaking by magnetic impurities in standard s-wave superconductors, with a rapid decrease of the critical temperature with increasing impurity concentration following the Abrikosov–Gorkov law. However, except for Zn which is likely to have a magnetic environment once in an YBCO matrix, impurities seem to have a rather weak effect on the T_c of $\text{YBa}_2\text{Cu}_3\text{O}_7$. Ion or electron irradiation have also shown a similarly weak sensitivity of the critical temperature.

In order to account for all these apparently contradictory experiments, recently we have proposed a model [16] where an order parameter with nodes is produced, not by in-plane repulsive interaction as in the spin fluctuation mechanism, but rather by a repulsive plane–chain pairing interaction which we attribute to mostly unscreened Coulomb repulsion. As a result the plane band and the chain band have order parameters with opposite sign. Since it is well known that these plane and chain bands hybridize because electrons are physically allowed to jump from planes to chains, this change of sign automatically gives rise to nodes of the gap in the region of the Brillouin zone where they anti-cross. In our model, although we do not exclude some pairing interaction coming from the chains, superconductivity arises primarily from an attractive interaction within the planes, due for example to phonon exchange. We can say that our order parameter is d-wave like because it is qualitatively similar [16] to the $d_{x^2-y^2}$ model: on each sheet of the Fermi surface there are four nodes. On the other hand, since the chains play an essential role in our model, it is meaningless to consider an approximate tetragonal symmetry. Rather, we have to consider only the orthorhombic symmetry, under which our order parameter is completely invariant (there is no symmetry breaking). Note that the $d_{x^2-y^2}$ order parameter is also invariant under this symmetry. We can also remark that our order parameter looks qualitatively like a d + s order parameter on each sheet of the Fermi surface, hence the difference with a distorted d-wave model is really more quantitative than qualitative.

Since the order parameter of our model changes sign, it accounts for all the experiments providing evidence for this. Actually, twinning complicates the interpretation of these experiments. In this respect

our model is in the same situation [16] as a $d + s$ model [17] and we will discuss it in this spirit. Indeed, because the chain electrons have their velocity along the b -axis, it is reasonable to assume that they give the dominant contribution to tunnelling in this direction. On the other hand, only plane electrons, which have an opposite sign for the order parameter, will contribute to tunnelling along the a -axis. With respect to twinning it has been shown [18] that the result of these experiments depends in an essential way on the relation between the order parameters on the two sides of the twin boundary. If one makes the assumption that the order parameter does not change sign when one crosses the boundary going straight along the a - or b -direction, the corner SQUID experiments would not meet any problem, but the c -axis tunnelling [11,12] should give a negative result by destructive interference of the twin domains (assumed to be in equal weight). If we make the opposite assumption for the sign of the order parameter on crossing the twin boundary, the c -axis tunnelling does not have any more problems, but the corner SQUID would be averaged out (assuming again equal weight for the twins). Clearly the best way (but not the easiest one) is to perform experiments on single crystals. Actually, this has been essentially done by now since corner SQUID experiments [1,2] have been performed on single crystals. On the other hand, it is known experimentally that c -axis tunnelling does not obey simple rules with respect to twins. This is well demonstrated in a very recent experiment [19] on c -axis tunnelling with a single twin boundary. It confirms the mixed (d and s) nature of the pairing, with evidence for a reversal of the sign of the s -wave component across the twin boundary. At the same time it shows that the perfect cancellation expected for two twins of equal weight is not found. A possible explanation is a non-uniformity in the twin boundary. This shows that a twin boundary might be a complex object.

Since our order parameter has nodes, our model accounts for the existence of low energy excitations. Because of the important role of the chains, it provides a simple explanation for the important anisotropy in the ab -plane mentioned above. The existence of two weakly coupled bands (plane and chain) in our model leads to the possibility of a weak sensitivity of the critical temperature to impurities, in agree-

ment with experiment, as we have shown very recently [20]. We note that our model has similarities with the two band S-N model, introduced by Abrikosov and Klemm [21–23] to account for Raman scattering data. It also has common features with single band models, where competing attractive and repulsive (Coulomb) interactions lead to a change of sign of the order parameter within the band, such as the ones proposed by Abrikosov [24] and by Santi et al. [25,26].

In this paper we will explore in detail the consequence of our model for the penetration depth. We note that, since it is a thermodynamic quantity, the penetration depth is less likely to be perturbed by extrinsic defects than a dynamical quantity. Moreover, since one explores the sample over typically 1000 Å, it is a bulk quantity. This is in contrast with surface experiments, such as photoemission or tunnelling, where only a few atomic layers are involved and which could give skewed information if the surface happens to be somewhat different from the bulk for some reason. All these features make the study of the penetration depth particularly interesting. Since our model naturally gives nodes in the gap, it is clear that it gives rise qualitatively to a linear dependence of the penetration depth $\lambda(T)$ at low temperature. However it is not obvious that our model can account quantitatively for the size of the slope nor for the experimentally observed temperature dependence and its anisotropy. The purpose of the present paper is to explore these points in detail. Here we will consider only $\text{YBa}_2\text{Cu}_3\text{O}_7$, since this compound is the best controlled and has been the most explored experimentally. The possible extension of our model to other compounds will be considered in another work [27].

Experiments on the penetration depth in YBCO, whether on crystals [6,28] or on films [7], are now in reasonable agreement. In particular they find a linear behaviour at low temperature with a typical slope of $4.3 \text{ \AA}/\text{K}$ for an average penetration depth λ_{ab} . More recently the anisotropy of the penetration depth has also been measured in untwinned single crystals [29]. Since these last experiments provide stronger constraints on theory, we will mostly take them for comparison with experimental results (note that the compound is more precisely $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$ but we will consider that it does not differ appreciably from

YBa₂Cu₃O₇). The $T=0$ values of the penetration depths are more difficult to obtain and we will make use of the results of Basov et al. [13] for comparison. However, experimental agreement is not complete and there might still be some progress in the future on this side, perhaps with some surprises [30].

2. The model

We first introduce the essential ingredients of our model. The non-interacting part of the Hamiltonian for the electrons in planes and chains is given [16] by:

$$H_0 = \sum_k \epsilon_k c_k^+ c_k + \sum_k \epsilon'_k d_k^+ d_k + \sum_k t_k c_k^+ d_k + h.c. \quad (1)$$

where c_k^+ and d_k^+ create electrons in the plane and in the chain band respectively. The first term corresponds to an isolated plane while the second one describes isolated chains with respective dispersion relations ϵ_k and ϵ'_k . The last term describes hopping between planes and chains. Actually, since YBCO is made of stacks containing two CuO₂ planes and one CuO-chains plane, this independent electron Hamiltonian does not correspond precisely to the situation found in YBCO. A more realistic description is obtained with the Hamiltonian:

$$\begin{aligned} H_0 = & \sum_n \epsilon c_{1,n}^+ c_{1,n} + \sum_n \epsilon c_{2,n}^+ c_{2,n} \\ & + \sum_n t_p (c_{1,n}^+ c_{2,n} + h.c.) + \sum_n \epsilon' d_n^+ d_n \\ & + \sum_n t_c (c_{1,n}^+ d_n + h.c.) \\ & + \sum_n t_c (c_{2,n}^+ d_{n+1} + h.c.). \end{aligned} \quad (2)$$

Here all quantities are understood to depend on k_x and k_y and summations run also over $k_{x,y}$. Indices 1 and 2 number the CuO₂ planes and the index n numbers the stacks. Introducing the even and odd plane band operators c_{\pm} by $c_{1,2} = (c_{+} \pm c_{-})/\sqrt{2}$, and taking the Fourier transform in the z -direction, we have:

$$H_0 = \sum_k (\epsilon + t_p) c_{+,k}^+ c_{+,k} +$$

$$\begin{aligned} & + \sum_k (\epsilon - t_p) c_{-,k}^+ c_{-,k} + \sum_k \epsilon' d_k^+ d_k \\ & + \sum_k t_+ (c_{+,k}^+ d_k + h.c.) \\ & + \sum_k t_- (c_{-,k}^+ d_k + h.c.). \end{aligned} \quad (3)$$

Now a dependence and summation on k_z is understood, and we have set $t_+ = t_{\delta}/2\cos(k_z c/2)$ and $t_- = t_{\delta}/2\sin(k_z c/2)$, with c being the size of the unit cell along the z -direction. From band structure calculations [31–33] the chain band Fermi surface crosses the odd plane band Fermi surface, whereas there is no crossing with the even plane band. Therefore the even plane band does not play an interesting physical role in our model. If it is omitted this leads back to the Hamiltonian Eq. (1) where the plane band is actually the odd plane band and $t_k = t_{\delta}/2\sin(k_z c/2)$. In order to simplify the discussion we will forget the even plane band. However, when we will come to realistic calculations we will take into account its contribution.

With respect to pairing interactions, we take an attractive pairing in the plane while we assume a repulsive pairing between plane and chain. On the other hand we have no precise indication on the pairing interaction within the chains (a simple and reasonable hypothesis would be to take the coupling constant equal to zero, but this is clearly somewhat arbitrary). This leads to the effective interaction Hamiltonian (with g and K positive):

$$\begin{aligned} H_{\text{int}} = & -g \sum_{k,k'} c_{k'}^+ c_{-k'}^+ c_{-k} c_k + K \sum_{k,k'} d_k^+ d_{-k'}^+ c_{-k} c_k \\ & + h.c. - g' \sum_{k,k'} d_k^+ d_{-k'}^+ d_{-k} d_k \end{aligned} \quad (4)$$

and the following mean field Hamiltonian:

$$H = H_0 + \Delta \sum_k c_k^+ c_{-k}^+ + \Delta' \sum_k d_k^+ d_{-k}^+ + h.c. \quad (5)$$

where the order parameter (Δ, Δ') satisfies:

$$\Delta = -g \sum_k \langle c_{-k} c_k \rangle + K \sum_k \langle d_{-k} d_k \rangle, \quad (6)$$

$$\Delta' = K \sum_k \langle c_{-k} c_k \rangle - g' \sum_k \langle d_{-k} d_k \rangle. \quad (7)$$

Because of hybridization, the plane and chain operators c_k and d_k do not correspond to the eigenstates

of H_0 and one has to perform a unitary transformation to diagonalize H_0 . The energies $e_{\pm}(\mathbf{k})$ are given by:

$$2e_{\pm}(\mathbf{k}) = \epsilon(\mathbf{k}) + \epsilon'(\mathbf{k}) \pm \left[(\epsilon(\mathbf{k}) - \epsilon'(\mathbf{k}))^2 + 4t^2(\mathbf{k}) \right]^{1/2}. \quad (8)$$

When this transformation is carried out in the pairing part of the Hamiltonian one obtains interband pairing terms coupling the hybridized bands. However, we will consider that t_k is large enough so that these bands are well separated. Specifically this means that we assume $\Delta, \Delta' \ll t_k$ (the parameters we use below do indeed satisfy this constraint, except for a small range around $k_z = 0$ which is quantitatively unimportant). In this case one can easily see [20] that these interband pairing terms are negligible. Therefore the transformation gives rise to a fully band-diagonalized Hamiltonian, with the order parameter in each band given explicitly by $\Delta_{\pm}(\mathbf{k}) = (\Delta\epsilon'(\mathbf{k}) + \Delta'\epsilon(\mathbf{k})) / (\epsilon(\mathbf{k}) + \epsilon'(\mathbf{k}))$ (\mathbf{k} being at the Fermi surface of the + or - band). The essential feature of our model is that, starting from isotropic interactions in planes and chains, we obtain a specific anisotropy for the order parameter ($\Delta_+(\mathbf{k}), \Delta_-(\mathbf{k})$). In particular we obtain an order parameter which changes sign and has nodes at the Fermi surface since we have managed to have Δ and Δ' with opposite signs, while $\epsilon(\mathbf{k}) / (\epsilon(\mathbf{k}) + \epsilon'(\mathbf{k}))$ goes essentially from 0 to 1 when we move at the Fermi surface of a given band. Therefore we have an order parameter which is d-wave like, although we have assumed an attractive pairing in the planes.

In order to obtain the temperature dependence of the penetration depth, we need the temperature dependence of the order parameter. This should be obtained as the solution of our two band model. As it is well known from the early work of Suhl et al. [34], the resulting temperature dependence can be appreciably different from the standard BCS result. However, we will not require in our calculations a ratio $|\Delta'|/\Delta$ between the chain and plane order parameters very different from unity (it will be typically 0.5). We have checked that, in the range of coupling constants which is of interest for us, within a weak

coupling calculation, the departure from the BCS temperature dependence is rather small.

Another complication is that, to obtain the order parameter and the penetration depth, we should perform a strong coupling calculation by solving Eliashberg equations. This is necessary to be consistent with the high value of the critical temperature (and indeed recent calculations of T_c within the spin fluctuation model are also performed in the strong coupling regime [35]). This is also consistent with the rather high values of $2\Delta/T_c$ whenever it has been measured experimentally, by tunnelling or Raman scattering for example. And indeed we will make use below of values for $2\Delta/T_c$ somewhat larger than the BCS one. Such calculations do not, in principle, cause any problem and they would be appropriate if we wanted precise quantitative results in order to fit experiment. However they have the disadvantage of introducing additional parameters — these would be the parameters necessary to describe the phonon spectrum [36,37], in addition to the coupling constants (including intraband Coulomb repulsion). However, our purpose in the present paper is not to perform refined calculations, but rather to show that our model can give a reasonable quantitative account for experiments without looking for perfect agreement (although as we will see we come already rather close to it). In addition we will find other sources of uncertainty. In this spirit we will take the following simplifying approach, as it is often done in the literature. We will perform a weak coupling calculation for the penetration depth and assume the weak coupling BCS result for the temperature dependence of the order parameter. We will take strong coupling effects into account only by a re-normalization of the ratio $2\Delta/T_c$. It is known that, for the moderate coupling constants we are interested in, strong coupling calculations do not give much different results. We will also invoke strong coupling effects when we will look for absolute values of the penetration depth since, because of mass re-normalization, they will modify the bare results. The advantage of this approach is that it leaves us with only two adjustable parameters, namely the ratio Δ'/Δ between the chain and plane order parameters (we assume each one isotropic for simplicity as in our original model) and the ratio $2\Delta/T_c$. Moreover, for both of these parameters we

do not have physically much freedom. The price is a quantitative inaccuracy, which we believe is rather small.

3. In-plane penetration depths, low temperature behaviour

Our calculations are made for clean superconductors. This limit seems appropriate for the experiments we consider, and more generally it seems to be the relevant one for high- T_c superconductors because of their short coherence length. It would naturally be of interest to study the effect of impurities on the low temperature behaviour of the penetration depth, since this can help to discriminate between various theories. However, since the physics is in this case controlled by the vicinity of the nodes of the gap, we do not expect much difference, at least qualitatively, with what is found for the standard d-wave model [38–40]. On the other hand, it is not clear that impurity effects can be entirely neglected in experiments, in particular for the penetration depth along the c -axis (we will take up this point again when we will look at this penetration depth). Nevertheless, we do not consider them in the present paper.

As we have already mentioned, in order to account for the experimental results we will need a fairly sizeable value of the hybridization parameter t_k , which will be much larger than a typical order parameter. In this case the two hybridized bands are well separated and we have to consider a multiband situation. In such a case, since we can not use a free electron description, one may worry about the contribution of interband terms to the paramagnetic current as in Ref. [41]. However one can check that the superfluid density is zero at T_c as it should (this results directly from the ‘effective mass theorem’ [42]), that is the paramagnetic current is exactly cancelled by the diamagnetic one. Below T_c the modification of the interband terms due to the superconducting condensation is small provided the separation between the bands (that is the difference between the energies of one-electron eigenstates with same wavevector) is large compared to the gap. More precisely, if D is a typical band separation and Δ is a typical gap, the correction is of order $(\Delta/D)^2$,

and should be neglected for consistency in our case (D is of order of the Fermi energy E_F except in the anti-crossing region where it is of order t_k , but since this region is small, the correction is of order $(\Delta/E_F)^2$ anyway).

The expression of the penetration depth in this case is just the sum of the contributions from each band. This leads to the standard result along the $i = x$ - or y -axis:

$$\frac{\lambda_i^{-2}(T)}{2e^2\mu_0} = \int_{\pm} \frac{d^3k}{(2\pi)^3} \delta(e_{\pm}) v_{i,\pm}^2 \times 2\pi T \sum_0^{\infty} \frac{\Delta_{\pm}^2(T)}{[\omega_n^2 + \Delta_{\pm}^2(T)]^{3/2}} \quad (9)$$

where the summation is over both the $+$ and the $-$ bands, and is limited to the Fermi surfaces by the Dirac function $\delta(e_{\pm})$. The gaps Δ_{\pm} , the energies e_{\pm} and the velocities $v_{i,\pm}$ are naturally all \mathbf{k} -dependent with the velocities $v_{i,\pm}(\mathbf{k}) = \partial e_{\pm}(\mathbf{k})/\partial k_i$. The discrete summation in Eq. (9) is over the Matsubara frequencies $\omega_n = (2n + 1)\pi T$.

We will first consider the low temperature behaviour of the penetration depth. Indeed on one hand the most striking feature of the recent experimental results is the linearity of the low T dependence. On the other hand, we can obtain in this regime explicit expressions in our model with a limited number of assumptions, because this dependence is controlled by the nodes of the gap which are located in the anti-crossing region. We will obtain an analytical expression for this low temperature behaviour in the limit of small hybridization. With this aim we note that there is no linear term at low temperature if hybridization is zero. Hence, if we subtract from Eq. (9) its counterpart with the hybridization parameter t_k set to zero, the low T behaviour is unchanged. Then we are left with summations over quantities which are essentially non-zero only in the anti-crossing region. If we assume t_k small enough, this region is small and we can perform a first order t_k expansion (since the unhybridized term does not contribute to the low T , we can forget it in the rest of the calculation). In this anti-crossing region the Fermi velocities $\partial\epsilon(\mathbf{k})/\partial\mathbf{k}$ and $\partial\epsilon'(\mathbf{k})/\partial\mathbf{k}$ of the plane and chain bands can be taken as constants, equal to their

value v_p and v_c at the crossing of the unhybridized Fermi surfaces.

It is more convenient to make a change of variables (at fixed k_z) and take $x = (\epsilon - \epsilon')/t_k$ and $y = (\epsilon + \epsilon')/2t_k$ as new variables instead of k_x and k_y . The Jacobian of the transformation is $J = \partial(x, y)/\partial(k_x, k_y) = |v_p \times v_c|/t_k^2$. The y integration is then easily performed. One can then see, by changing x into $-x$, that the contribution of the two bands $+$ and $-$ are identical, and we are thus left with the calculation on the $-$ band. The low T behaviour comes from the vicinity of the node x_0 of $\Delta_- = (1/2)[(\Delta + \Delta') - (\Delta - \Delta')x/(x^2 + 4)^{1/2}]$. This is given by $x_0 = (\Delta - |\Delta'|)/(\Delta|\Delta'|)^{1/2}$. Around this node, $\Delta_- = -2(x - x_0)(\Delta|\Delta'|)^{3/2}/(\Delta + |\Delta'|)^2$. In performing the x integration, we obtain the dominant T dependence by evaluating $v_{i,-}$ at the node x_0 . Since the gap Δ_- is now the only varying quantity, we are now led to a situation which is essentially identical to a d-wave calculation: after taking Δ_-/T as new variable, we are left with a purely numerical integral which turns out to be equal to $\pi \ln 2$. Taking into account the two bands \pm , we obtain for the low temperature dependence:

$$\lambda_i^{-2}(0) - \lambda_i^{-2}(T) = \frac{4 \ln 2}{\pi} \frac{e^2 \mu_0}{\hbar^2} \frac{\bar{t}}{c} T \frac{(\Delta + |\Delta'|)^2}{(\Delta|\Delta'|)^{3/2}} \left(\frac{v_{i,-}^2}{Jt_k^2} \right)_0 \quad (10)$$

where $c = 11.7 \text{ \AA}$ is the size of the cell along the c -axis, \bar{t} is the average of $|t_k|$ over k_z and the value of $(v_{i,-}^2/Jt_k^2)_0$ at the node is given by:

$$\left(\frac{v_{i,-}^2}{Jt_k^2} \right)_0 = \frac{(\Delta v_{c,i} + |\Delta'| v_{p,i})^2}{(\Delta + |\Delta'|)^2 |v_p \times v_c|} \quad (11)$$

This dimensionless quantity is typically of order unity. Expressing numerically all known physical constants, this can be rewritten as:

$$\lambda_i(T) - \lambda_i(0) = 1.76 \lambda_i^3(0) \frac{T}{T_c} \frac{T_c}{\Delta} \times \frac{(1 + |\Delta'|/\Delta)^2}{(|\Delta'|/\Delta)^{3/2}} \bar{t} \left(\frac{v_{i,-}^2}{Jt_k^2} \right)_0 \quad (12)$$

where all the penetration lengths are now expressed in units of 1000 \AA and the hybridization parameter \bar{t} is expressed in eV. We want now to compare this result with experiments [43] on $\text{YBa}_2\text{Cu}_3\text{O}_7$ which gives a slope of 4.7 \AA/K along the a -axis, and 3.6 \AA/K along the b -axis.

A first point to make is that our result contains the zero temperature value $\lambda_i(0)$ of the penetration depth. We can naturally perform a calculation for this quantity, as we will do below. However the necessary ingredients to obtain numerical results, namely band structure information and mostly re-normalization due to the interactions, are not precisely known. Moreover, $\lambda_i(0)$ is found by performing an averaging over the whole Fermi surface. Hence, its physical content is essentially unrelated to the other ingredients of Eq. (12) for which only the vicinity of the nodes is relevant: they give a very local information while $\lambda_i(0)$ contains a global one. Therefore, we might just take $\lambda_i(0)$ from experiment itself, which gives [13] the currently accepted values of $\lambda_a(0) = 1600 \text{ \AA}$ and $\lambda_b(0) = 1000 \text{ \AA}$. This is all the more reasonable as one sees that our result is fairly sensitive to the value of $\lambda_i(0)$ since it comes in the third power.

Even taking $\lambda_i(0)$ from experiment we have many parameters in our result which are not so well controlled. We can first consider the anisotropy of the linear term, since most of the factors in Eq. (12) are common to the two axes. We have:

$$\frac{\lambda_y(T) - \lambda_y(0)}{\lambda_x(T) - \lambda_x(0)} = \frac{\lambda_y^3(0)}{\lambda_x^3(0)} \frac{(\Delta v_{c,y} + |\Delta'| v_{p,y})^2}{(\Delta v_{c,x} + |\Delta'| v_{p,x})^2} \quad (13)$$

Since the chains are along the y -direction, it is quite reasonable to assume that the component $v_{c,x}$ of the chain electron velocity along x is essentially zero. Setting $v_{c,y} = v_c$, we obtain the following numerical condition between our parameters in order to agree with experiment: $\Delta/|\Delta'| + v_{p,y}/v_c = 1.77 v_{p,x}/v_c$. This relation is easily satisfied with gap ratios and velocity ratios of order unity, which is just what one would expect. It is therefore not a strong constraint. Just to give an example, the simplistic tight binding dispersion relations $\epsilon_k = -2t_1(\cos k_x + \cos k_y) - \mu$

and $\epsilon'_k = -2t'_1 \cos k_y - \mu'$ for the plane and the chain bands give $\Delta/|\Delta'| = (1.77 \sin k_x / \sin k_y - 1)t_1/t'_1$. This is satisfied with $t_1 \approx t'_1$, a crossing located [32] at $k_x \approx \pi/2$ and $k_y \approx \pi/4$, and $|\Delta'|/\Delta \approx 0.7$.

We consider now if we can account for the absolute value of the slope, say along the b -axis. We assume again $v_{c,x} = 0$ and make use of the above relation between parameters imposed by the experimental anisotropy. The result can be considered as an equation giving the hybridization parameter \bar{t} . Taking $T_c = 93$ K it reads (with \bar{t} in eV):

$$\bar{t} = 0.061 \frac{\Delta}{T_c} \left(\frac{\Delta}{|\Delta'|} \right)^{1/2} \frac{v_c}{v_{p,x}}. \quad (14)$$

Taking as an example the values we have chosen in Section 2, together with the BCS isotropic weak coupling value $\Delta/T_c = 1.75$, we obtain $\bar{t} = 0.09$ eV. However, anisotropy as well as strong coupling are expected to raise Δ/T_c , and if we rather take the average value found in experiments, namely $\Delta/T_c \approx 3$, this raises \bar{t} up to 0.16 eV. However we stress again that the low temperature slope is sensitive to the physical parameters in the vicinity of the nodes. If we consider that the gap Δ in the planes has actually some anisotropy, which is quite likely to happen, the gap value at the nodes can be lower than the maximum value that we have taken. Similarly, we should take into account the local value of the mass re-normalizations due to interactions, which would be quite hard to obtain. Hence, it should be clear that we cannot escape some appreciable uncertainty in our evaluations.

Nevertheless, the typical value required for the hybridization parameter in order to account for the experiments, namely $\bar{t} \approx 0.1$ eV, is quite satisfactory, taking into account that we have basically no adjustable parameters. Indeed, this parameter is small enough (compared to the full band width of the plane or chain bands which is of order 1.6 eV) to make our hybridization approach reasonable and consistent. In particular, it is small enough for our model to explain [20] the weak dependence of the critical temperature on impurity content, which is observed experimentally and which is one of the major problems of the spin fluctuation model. On the other hand, one might worry that the hybridization we find is too

large, although it is quite obvious from the start that we require a sizeable hybridization, since the linear dependence of the penetration depth at low temperature is a fairly strong effect. We will discuss later on this point together with our calculations of the penetration depth in the c -direction and see that this not the case.

4. Calculations of the penetration depth over the whole temperature range

In Section 3 we have discussed the low temperature behaviour of the penetration depth and we have found that our model can account for experiments in YBCO. The next interesting point is to know if it can do the same over the whole temperature range. A priori the answer is likely to be affirmative because the different components of this temperature dependence are controlled by different parameters of our model. Thus, in principle they can be adjusted independently to reproduce the experimental results. Indeed, the zero temperature value of the penetration depth is an average over the whole Fermi surface of band structure parameters (Fermi velocity, density of states), with proper re-normalization due to interactions. Therefore, it is a global quantity, which in particular does not depend on the values of the gaps. On the other hand, as we have already seen explicitly above, the low temperature slope of the superfluid density depends only on the band structure parameters and the gaps in the vicinity of the nodes, which makes it a local quantity. Finally, the slope of ρ_s near T_c is a global quantity which depends both on band structure parameters and on the gaps on the whole Fermi surface. Since we consider the possibility of strong coupling effects, the temperature dependence of the gaps near T_c is again an independent variable. The large number of parameters is an unpleasant feature of our model, but it is likely to be also an inescapable ingredient of the physics of $\text{YBa}_2\text{Cu}_3\text{O}_7$.

Having realized that our model is quite flexible, we can still wonder if we can account for experiment with reasonable values of the parameters. In order to explore this problem conveniently we reduce flexibility by making some reasonable simplifying as-

sumptions. We take the gaps constant within the plane band and the chain band. The ratio $R = |\Delta'|/\Delta$ between the gap Δ in the plane band and the gap Δ' in the chain band is one parameter of our calculation. We will assume that the temperature dependencies of these two gaps are the same and take for it a simple re-normalized BCS form: $\Delta(T) = (\Delta(0)/1.76k_B T_c) \Delta_{\text{BCS}}(T)$. The ratio $\Delta(0)/1.76k_B T_c$ is another parameter of our calculation. For the band structure we take a simple tight binding ansatz which reproduces reasonably well the results obtained by band structure calculations [32,33], and in particular the Fermi surface. We take for the plane band the simple tight-binding dispersion relation $\epsilon_k = -2t_1(\cos k_x + \cos k_y) + 2t_2 \cos k_x \cos k_y - \mu$, while we use naturally $\epsilon'_k = -2t'_1 \cos k_y - \mu'$ for the chain band. Actually, we find our best overall agreement for $t_2 \approx 0$. We note that the shape of the (uncoupled) odd plane band Fermi surface is indeed fairly well described by $t_2 \approx 0$, except for the vicinity of $(\pi, 0)$ and $(0, \pi)$ which are missed in our simple description (but since the velocities are small in these saddle point regions, this is likely to be unimportant for our purpose). On the other hand, for the even plane band a proper description of the Fermi surface requires a larger t_2 .

Finally, in order to make realistic calculations, we have also included a contribution to the penetration depth from this even parity plane band, which is uncoupled to the chains. We note that including this contribution makes agreement with experiment more difficult to reach. Indeed, since we have no nodes on this piece of the Fermi surface, the contribution of this part has an s-wave like temperature dependence and is essentially constant at low temperature. This makes it harder to account for the strong slope found experimentally. To perform the calculation, we need all the parameters characterizing this band as additional input. These parameters are not related in an obvious way to those of the odd parity plane band. Nevertheless we have made a simplifying assumption in order to avoid an increase in the number of parameters. The contribution of this plane band to λ_i^{-2} seems isotropic (from band structure calculations [32,33], its piece of the Fermi surface has essentially a tetragonal symmetry). In the a -direction there is no contribution from the chains in our model, and only the even and odd plane bands contribute. We have assumed for simplicity these

contributions equal at zero temperature. This means specifically that we have taken $\lambda_y^{-2}(0)|_{\text{even plane}} = \lambda_x^{-2}(0)|_{\text{even plane}} = \lambda_x^{-2}(0)|_{\text{odd plane + chain}}$. This fixes the $T=0$ contribution of the even plane band. With respect to its temperature dependence, we take the gap of the even plane equal to the one of the odd plane band, namely $\Delta(T)$. These assumptions are quite reasonable, but it is clear that the even plane band is an additional source of flexibility of our model, if required.

Given the large number of parameters still left in our model, we have not proceeded to a systematic exploration in the parameter space. We have just made use of our results, obtained in Section 3 in order to locate the region in parameter space for a proper description of the low temperature behaviour, and we have then adjusted empirically the parameters to obtain a good overall agreement with experiment. It is possible that better sets of parameters can be found. However our purpose in this paper was to check if our model could give a satisfactory account for experiment. Since our answer is positive we have not attempted an optimization of our parameters, which would be rather meaningless in view of the flexibility mentioned above. Later on we comment on the sensitivity of our results to the variation of our parameters. We find a good overall agreement, as shown in Fig. 1, with the set of parameters $t_1 = 0.5$ eV, $t_2 = -0.0$ eV, $t'_1 = 0.33$ eV, $\mu = -0.58$ eV, $\mu' = -0.46$ eV, $t_c = 0.2$ eV, $|\Delta'|/\Delta = 0.4$ and $2\Delta/T_c = 2.2$.

Let us first consider the $T=0$ values of the penetration depths. We find $\lambda_a = 800$ Å and $\lambda_b = 550$ Å. A priori our model is not designed to calculate the absolute values of the penetration depths, because it uses a rather primitive band structure. It is nevertheless interesting to compare our results to full band structure calculations [44] of the plasma frequencies Ω_{pi} which can be related to our penetration depths by $\lambda_i = c/\Omega_{\text{pi}}$. Their results give $\lambda_a = 730$ Å, $\lambda_b = 450$ Å and $\lambda_c = 2100$ Å. We see that our values are rather near these ab initio calculations, which proves that our model is quite reasonable. In particular, the anisotropy ratio they find is $\lambda_b/\lambda_a = 1.62$, while we obtain $\lambda_b/\lambda_a = 1.45$. Both are very near the experimental result of 1.6. This ratio does not vary much when we vary our parameters (in a reasonable range). This is easy to understand. This

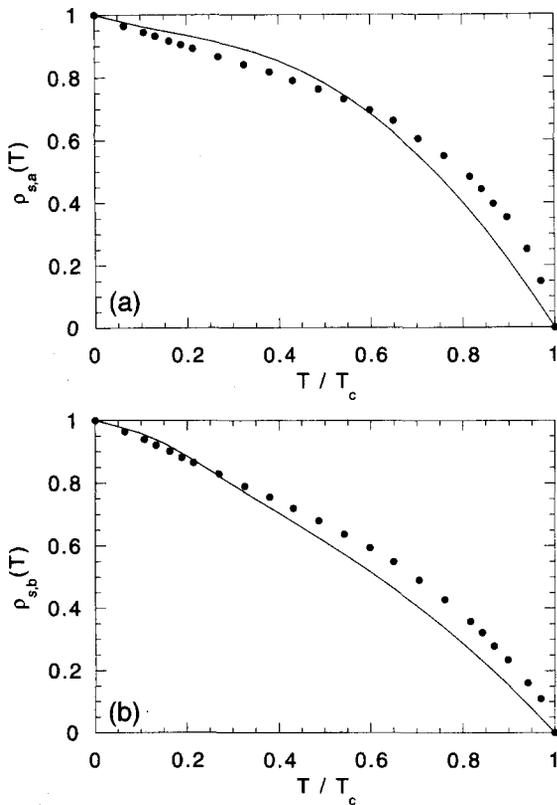


Fig. 1. (a) $\lambda_a^{-2}(T)/\lambda_a^{-2}(0)$ as a function of T/T_c . Full line: theory from Eq. (9) with parameters given in the text. Filled circles: experimental results from Ref. [24]. (b) Same as (a) for $\lambda_b^{-2}(T)/\lambda_b^{-2}(0)$ as a function of T/T_c .

ratio comes merely from the fact that a proper account has been made of the chain contribution to the penetration depth along the b -axis. This agreement with experiment is a strong indication that the chains have to be included in order to get a proper description of the superconducting properties of YBCO as we have discussed in the introduction. Nevertheless, both our calculation and Ref. [44] give absolute values for λ_i which are much lower than the experimental results. The obvious explanation for this is mass re-normalization, due to the interactions, which we have not taken into account. For an isotropic superconductor this would multiply the penetration depth by $(1 + \lambda)^{1/2}$, where λ is the coupling constant. In the present case this re-normalization factor is most likely rather anisotropic, but since we have unfortunately no precise idea of this

anisotropy, let us take it isotropic for the sake of this discussion. If we require for example that it pushes λ_a to the experimental value $\lambda_a = 1600 \text{ \AA}$, we find $\lambda_b = 1100 \text{ \AA}$, in quite good agreement with experiment. The corresponding value of λ is 3 which is reasonable for a strong coupling constant.

Let us turn now to our results for $\lambda^{-2}(T)/\lambda^{-2}(0)$ plotted in Fig. 1. As it can be seen we find a very reasonable agreement with the low temperature behaviour for both the a - and the b -directions. However, this requires the rather high value $t_c = 0.2 \text{ eV}$ which we will discuss later on. The low temperature slopes are naturally sensitive to the other band structure parameters because the Fermi velocities in the anti-crossing region must be high enough to account for experiment. This implies a proper location of the anti-crossing region. However, once the proper range for these parameters is found, the results are not particularly sensitive to their choice in this range. They are however sensitive to the choice of $|\Delta'|/\Delta$ because this parameter controls the position of the nodes, and the slopes are directly related to the orientation and the strength of the Fermi velocities at the nodes. We remark the value $|\Delta'|/\Delta = 0.5$ that we use is quite reasonable physically: since we expect superconductivity to arise mostly because of interactions in the planes, we should find the order parameter smaller in the chains than in the planes. We note also that the experimental results displays a linear behaviour over a remarkably large range of temperature since it goes almost up to $T/T_c = 0.5$. A natural explanation for this feature is strong coupling effects which, by increasing $2\Delta/T_c$, increase the scale for the low temperature behaviour (which is Δ) compared to the overall temperature scale (which is T_c). This effect is not fully accounted for by our calculations because we have a rather small $2\Delta/T_c = 2.2$. However, a larger value would lower the low temperature slopes and give a disagreement with experiment. This situation is due to our simplifying choice of an isotropic gap. Choosing an anisotropic gap would make it possible for us to have a large slope (related to the gap values near the nodes) and a large linear region (related to the gap values farther from the nodes). Finally, the agreement is not quite good when we get near T_c , but this was expected. Indeed, experimental results [45] give a $(1 - T/T_c)^y$ dependence for $\lambda(T)$ near T_c with $y \approx 1/3$, while

our mean field approach leads us naturally to the standard $(1 - T/T_c)^{1/2}$ dependence. If this experimental result is confirmed and the effect is due to a large domain for critical fluctuations [45], including this physics in our model will naturally bring us in better agreement with experiment.

5. *c*-Axis penetration depth

We come now to the calculation of the *c*-axis penetration depth. We note first that our simple model is intended to describe plane–chain coupling and is at the start a two-dimensional model. In order to make more realistic calculations, we have included a k_z dependent coupling in its simplest form. However this description is obviously very crude and we may fear that it gives a poor account of transport in the *c*-direction. For example our plane–chain coupling does not have any (k_x, k_y) dependence. Physically we forget that plane–chain hopping is likely to happen through the orbitals of the O4 apical oxygen. Similarly we do not take due account of plane–plane hopping which is obviously necessary for transport in the *c*-direction. Clearly a mismatch between plane–plane hopping and plane–chain hopping would strongly affect these transport properties (it has for example been suggested by Xiang and Wheatley [46] that the hopping along the *c*-axis vanishes at the nodes). It is nevertheless interesting to see what is the result of our model for the *c*-axis penetration depth, and we will see that it does not fare so badly.

Our raw value at $T=0$ is $\lambda_c = 2250 \text{ \AA}$. This result compares quite well with the result $\lambda_c = 2100 \text{ \AA}$ of band structure calculations given above. This is quite important because it validates the value of our plane–chain hopping parameter $t_c = 0.2 \text{ eV}$, which we might have feared to be too large. Therefore, this value of t_c is in reasonable agreement with what comes out of these band structure calculations. Next we have to re-normalize this result as we have done above for the *a*- and *b*-directions. Taking the same re-normalization factor, we obtain $\lambda_c = 4500 \text{ \AA}$. This is clearly smaller than the experimental result $\lambda_c \approx 10000 \text{ \AA}$, although this is not way off the mark. We note that this same problem is shared by band structure calculations.

It is perhaps not too difficult to understand this discrepancy. First the experimental side is probably less secure than for the in-plane measurements since λ_c is not obtained directly, but requires a subtraction of the *a*- or *b*-axis contributions which might be difficult to make precisely. Moreover, although experiments agree [28,47] to find $\lambda_c \approx 10000 \text{ \AA}$, they strongly disagree with respect to the temperature dependence. While Mao et al. [28] obtain at low temperature a linear decrease of λ_c^{-2} much stronger than in the *a*- or *b*-direction, Bonn et al. [47] find a much weaker dependence than for λ_a or λ_b . On the theoretical side our calculation is performed in the clean limit. While this sounds quite reasonable for the in-plane directions, one may reasonably think that transport along the *c*-axis is much more sensitive to any kind of scattering or disorder. The importance of incoherent hopping in the *c*-direction has been stressed for example by Graf et al. [48,49] and Radtke et al. [50,51]. Clearly the weakness of coherent hopping in the *c*-direction makes incoherent hopping much more relevant than for in-plane transport and this will lead to an increase in the penetration depth. Similarly, since *c*-axis transport implies electrons going through the chains, it will be much more sensitive to chain disorder than in-plane transport. This is confirmed by the strong dependence [52] of the *c*-axis resistivity on oxygen content in $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$ while the in-plane resistivity depends much less on *y*. Naturally, non-stoichiometry brings easily a strong oxygen disorder in the chains, and because of the one-dimensional nature of these chains, the electronic properties are much more perturbed by this disorder. A related explanation is the possible existence of layers of impurities or defects parallel to the planes, which would contribute to blocking *c*-axis transport. Such a situation would be similar to the one found in films for the *ab*-penetration depth [7], where extrinsic ‘weak links’ were shown to increase the penetration depth from the intrinsic value of 1700 \AA up to 3500 \AA . The ratio between these two values is similar to the discrepancy between our result and the experimental one for $\lambda_c(0)$. At the same time, these weak links make the low temperature dependence weaker than the intrinsic one. It is tempting to attribute the difference between the low temperature behaviour found by Mao et al. [28] and by Bonn et al. [47] to such an

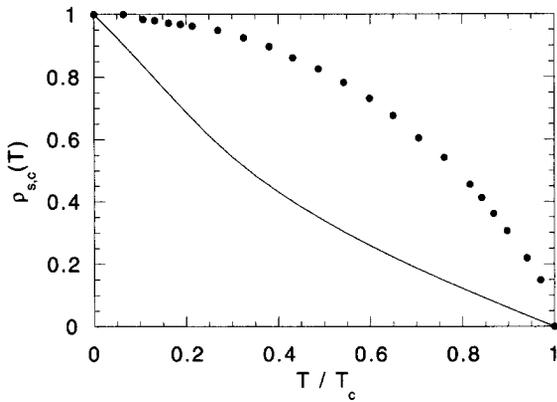


Fig. 2. $\lambda_c^{-2}(T)/\lambda_c^{-2}(0)$ as a function of T/T_c . Full line: theory from Eq. (9) with the same parameters as in Fig. 1. Filled circles: experimental results from Ref. [43].

effect, although this seems in contradiction with the fact that they find essentially the same value for $\lambda_c(0)$.

Let us now consider the temperature dependence that we find for $\lambda_c^{-2}(T)/\lambda_c^{-2}(0)$. It can be seen in Fig. 2 that it is quite strong. The physical explanation is quite clear. In our model all the k_z dependence of the band structure comes from hybridization, and hence it is stronger in the anti-crossing region. This implies that the largest $v_{k,z}$ comes from this region. Since the nodes of the gap are in this same region, their influence are particularly strong and in particular the low temperature slope is large. We notice that our result is very analogous to the one found experimentally by Mao et al. [28]. This is naturally satisfactory, but from the above discussion we should be careful not to draw any conclusion from this agreement.

We consider finally a slightly different version of our model which could correct for the discrepancy between our result and experiment for $\lambda_c(0)$. We may indeed wonder if the large value of $\lambda_c(0)$ is not due to a weak plane–plane coupling. This possibility has been suggested by Basov et al. [13]. In order to explore our model in this direction, we assume that the plane–plane coupling t_p is small. To zeroth order one combination of the plane bands is uncoupled and has energy ϵ_k while the orthogonal combination of the plane bands and the chain band are hybridized in the usual way with their dispersion relation given by Eq. (8) with $t_k = \sqrt{2}t_c$. The in-plane

penetration depths can be calculated to zeroth order. On the other hand, the velocity along the c -axis is zero at this order, and we have to go to first order in

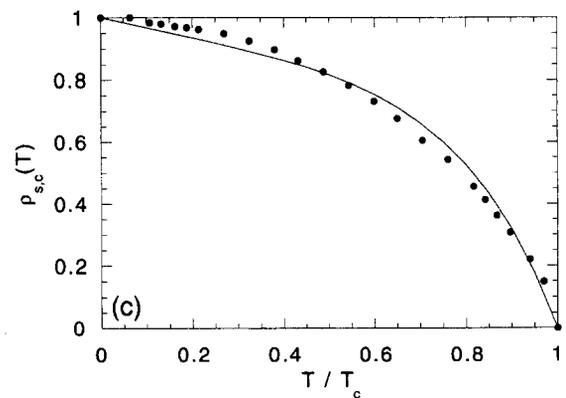
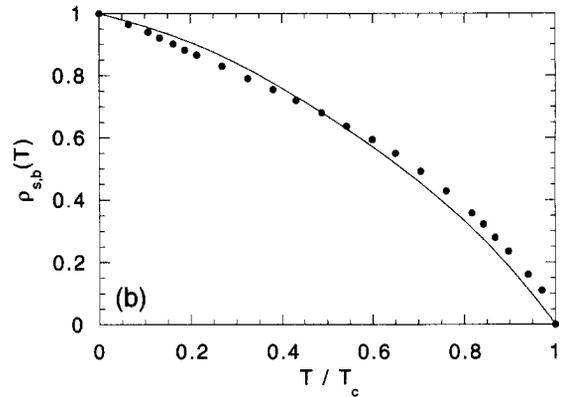
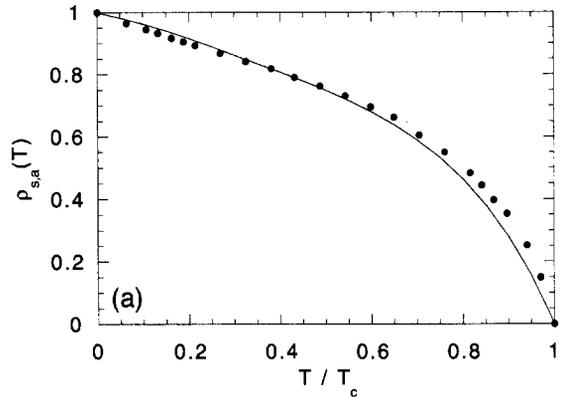


Fig. 3. (a) $\lambda_a^{-2}(T)/\lambda_a^{-2}(0)$ as a function of T/T_c . Full line: theory from Eq. (9) for small plane–plane hopping (see text), with parameters given in the text. Filled circles: experimental results from Ref. [24]. (b) Same as (a) for $\lambda_b^{-2}(T)/\lambda_b^{-2}(0)$ as a function of T/T_c . (c) Same as (a) for $\lambda_c^{-2}(T)/\lambda_c^{-2}(0)$ as a function of T/T_c . Filled circles: experimental results from Ref. [43].

t_p for the calculation of λ_c . This gives $\hbar v_{k,z}/c = t_p \sin(k_z c)$ for the even plane band, and $\hbar v_{k,z}/c = 2t_p t_c^2 \sin(k_z c) / [(e_{\pm} - \epsilon)^2 + 2t_c^2]$. Therefore, we can obtain the experimental value of $\lambda_c(0)$ by adjusting t_p . We show in Fig. 3 the result of our calculations for the set of parameters $t_1 = 0.33$ eV, $t_2 = -0.0$ eV, $t'_1 = 0.4$ eV, $\mu = -0.7$ eV, $\mu' = -0.56$ eV, $t_c = 0.2$ eV, $|\Delta'|/\Delta = 0.5$ and $2\Delta/T_c = 3$. As it can be seen the agreement with experiment is quite good. For the a -direction it is slightly better than in Fig. 1 because the average hybridization parameter is larger (in the present case it is constant while in the preceding case it is proportional to $\sin(k_z c/2)$) and the ratio Δ/T_c is larger. We note that we find for $\lambda_c(T)$ a temperature dependence which is now in good agreement with Bonn et al. [47] data. Turning now to the absolute values, our raw results at $T=0$ are $\lambda_a = 1300$ Å and $\lambda_b = 650$ Å. If for example we re-normalize λ_b to 1000 Å (and λ_a to 2000 Å), we find $\lambda_c = 10000$ Å if we take $t_p = 0.043$ eV. This small value justifies our first order expansion.

6. Conclusion

In this paper we have investigated the consequences of our coupled plane-chain model of $\text{YBa}_2\text{Cu}_3\text{O}_7$ for the penetration depth and compared them with experiments. We have found that our model accounts quite nicely for the anisotropy of the penetration depth in the ab -plane at $T=0$ (and also for the absolute values, when mass re-normalization is taken into account). This is obvious qualitatively since the chains contribute only in the b -direction. But the agreement with experiment is also quite good quantitatively. We reproduce fairly well the linear dependence at low temperature and more generally the whole temperature dependence for both the a - and the b -directions (except near T_c where experiments [45] do not give a mean field dependence). All this is obtained with a set of parameters which are all quite reasonable physically. In particular we require naturally a sizeable hopping term between plane and chain to account for experiment, but the value we use is in agreement with results from band structure calculations. Regarding the penetration depth along the c -axis, the situation is less satisfactory since two experiments strongly disagree with respect to the

temperature dependence. We can actually reproduce both temperature dependence by making slightly different choices for our model to describe hopping in the c -direction. The absolute value of the penetration depth disagrees typically by a factor 2 with experiments, but a natural explanation is the important effect of impurities and disorder on the transport properties along the c -axis.

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