Thermal Fluctuations in d-wave Layered Superconductors

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Muriel Ney-Nifle\footnote{e-mail: ney@solrd.lps.u-psud.fr, permanent address: Laboratoire de Physique, Ecole Normale Supérieure, 46 allées d'ltalie, 69364 Lyon cedex 07, France} and Marc Gabay

Laboratoire de Physique des Solides \footnote{Laboratoire associé au CNRS}, Université de Paris-Sud, Bâtiment 510, 91405 Orsay Cedex, France

Abstract

We study the thermal fluctuations of anisotropic order parameters (OP) in layered superconductors. In particular, for copper oxides and a d-wave OP, we present some experimental consequences of fluctuations in the direction normal to the layers. It is shown that the c-axis penetration depth $\lambda_c$ can have a ”disorder-like” quadratic temperature dependence at low temperature.

The fluctuations are analyzed in the framework of a Lawrence-Doniach model with an isotropic Fermi surface. Anisotropies pin the orientation of the OP to the crystallographic axes of the lattice. Then we study an extended t-J model that fits Fermi surface data of bilayers $YBCO$ and $BSCCO$. This leads to a d-wave OP with two possible orientations and, including the thermal fluctuations, yields the announced temperature dependence of $\lambda_c$. Furthermore a reservoir layer is introduced. It implies a finite density of states at the Fermi energy which is successfully compared to conductance and specific heat measurements.

Keywords: d-wave superconductor, high-$T_c$ superconductors, fluctuation effects, London penetration depth.
1 Introduction

Despite an enormous amount of theoretical and experimental research devoted to High Temperature Superconductors (HTSC) in the past decade, many important issues still remain unsettled. In particular there is as yet no explanation for the pairing mechanism at work in these materials. Early on Anderson suggested [1] that spin fluctuations might play a critical role for the superconductivity of copper oxides. These fluctuations have been analyzed for instance in the framework of the t-J model [2] and a natural candidate to represent the superconducting state in that model is a d-wave order parameter (OP).

Many low temperature experiments seem to suggest that a d-wave symmetry is a strong possibility: the variation of the penetration depth with $T$ [3, 4] and $H$ [5], Knight Shift and $1/T_1 T$ data [6], angle resolved photoemission spectra [7], the variation of $C_V$ with $T$ and $H$ [8]. Yet these experiments do not probe directly the OP so that one cannot rule out other symmetries or mixtures of symmetries [9]. Precise measurements of the single particle density of state (DOS) near the Fermi energy in the superconducting state ought to give some clue about the pairing symmetry. Tunneling experiments however have been fairly inconclusive thus far, leading to s-wave, d-wave and, in the case of $YBCO$, to the conductance of a system with finite DOS at the Fermi surface [10, 11]. Materials issues have made it difficult to sort out genuine features from experimental artefacts. The observation of spin fluctuations well below $T_c$ seen by inelastic neutron scattering and a linear in $T$ dependence of $C_V$ once the phonon contribution is subtracted [12] have been interpreted as evidence for gapless superconductivity.

Despite the fact that a clear-cut answer still remains elusive for high $T_c$ materials, an interesting by-product of these studies has been a renewed interest in coherence effects in d-wave superconductors. Sigrist and Rice indeed suggested that d-wave superconducting currents would display a strong spatial anisotropy at a boundary [13]. This anisotropy should show up in Josephson experiment setups [14]. Ambiguous results have been obtained, although Tsuei-Kirtley’s experiment strongly supports a scenario where one has nodes for the OP (consistent with either d-wave or extended s-wave). Furthermore, the layer structure characterizing $CuO_2$ compounds should affect tunneling and Josephson currents as it does for vortex (thermo)-dynamics below $T_c$ and for superconducting fluctuations above $T_c$, where a Lawrence-Doniach model is used [15]. These reasons led us to investigate the issues of layering and of anisotropies in d-wave superconductors. Our results show that these effects may play a significant role in the interpretation of tunneling and penetration depth types of experiments.

Our paper is organized as follows: in section 2.1 we present the Landau-Ginzburg
free energy of a single layer of a d-wave superconductor with an isotropic Fermi surface by solving the Gorkov equations. We calculate the energy cost of the fluctuations in the orientation of the nodal lines, denoted \( \alpha \), of an OP with the \( d_{x^2-y^2} \) symmetry. These fluctuations can be seen as admixing \( d_{x^2-y^2} \) and \( d_{xy} \) terms and appear in gradient terms of the free energy. We also show that the d-wave symmetry results in anisotropies in gradients of \( \alpha \) and of the phase of the OP. These do not modify the critical behaviour near \( T_c \) but have an influence in the London regime at low \( T \). Then, introducing anisotropies in the Fermi surface, we see that this tends to orient the nodal lines at 45° with respect to crystallographic axes. We next consider the case of weakly coupled d-wave superconducting sheets and we derive the corresponding Lawrence-Doniach free energy (see section 2.2). The energy cost of the fluctuations of \( \alpha \) is once again computed and gives, in particular, the Josephson current perpendicular to the layers. We find that the fluctuations in the \( c \)-direction are limited to a coherence length.

In section 3 we consider a t-J model that reproduces a reasonable band structure for the bilayer compounds \( YBCO \) and also \( BSCCO \). It is found that the nodal lines can now take on two positions [13]. This seems in agreement with recent experiments on \( BSCCO \) [17]. We add a hopping energy \( t_n \) that couples two bilayers via a charge reservoir; depending on the strength of \( t_n \) one may go from a more 3D structure pertaining to \( YBCO \) to a more 2D structure relevant for \( BSCCO \). We show how these modify the DOS which is determined analytically near the Fermi surface. It starts linearly, as in case with pure \( d_{x^2-y^2} \) OP, with an offset that vanishes with \( t_n \). This offset is observed in specific heat measurements [18] that are in quantitative agreement with our result and also in conductance measurements [10, 11].

The existence of several orientations of the nodal lines enhances the effect of the thermal fluctuations pointed out above: they give a mechanism that permits the OP to change its orientation from one layer to another. This has experimental implications that we discuss in section 3.3, in particular in the case of \( c \)-direction penetration depth measurements. Fluctuations in the orientation of the OP in the \( c \)-direction can change the \( T \) dependence of \( \lambda_c \) from a linear to a quadratic behaviour at low \( T \), even in pure samples where it is linear in the \( a \)- and \( b \)-directions. This is consistent with experiments on \( YBCO \) [13, 20].

Section 4 is a brief conclusion.
2 Fluctuations of d-wave order parameters: phenomenology

The model under consideration is the one introduced by Lawrence and Doniach (LD) [15] for weakly coupled layered superconductors. Here we shall first study the motion of electrons within a layer and then consider the Josephson tunnel that couples adjacent layers.

We introduce the “nodal angle” which define the orientation of the nodes of the $d_{x^2-y^2}$ OP within a layer. It fluctuates both in the direction parallel and perpendicular to the layers and we determine the length scales of these fluctuations.

2.1 Free energy density in a layer

We consider a d-wave OP $\Delta_n(k, R)$ where $R$ is the center-of-mass coordinate of a Cooper pair, $n$ the layer’s number and $k$ the relative coordinate in the Fourier space, $k = (k_x, k_y) = (|k| \cos \theta, |k| \sin \theta)$. We choose for the $k$-dependence of $\Delta$ the form $\hat{k}_x^2 - \hat{k}_y^2 = \cos(2\theta)$ which has nodal lines, $k_x = \pm k_y$. If $\alpha_n(R)$ denotes the relative angle of these lines with respect to fixed axes one has

$$\Delta_n(k, R) = \Delta_0(T) \cos[2(\theta - \alpha_n(R))] e^{i\phi_n(R)} \quad (1)$$

This can be expanded as

$$\Delta_n(k, R) = \Delta_1^n(R) \psi_1(\theta) + \Delta_2^n(R) \psi_2(\theta) \quad (2)$$

where the $\Delta_i^n$ are two related gap functions

$$\left\{ \begin{array}{l} \Delta_1^n(R) = \Delta_0 \cos(2\alpha) e^{i\phi} \\ \Delta_2^n(R) = \Delta_0 \sin(2\alpha) e^{i\phi} \end{array} \right. \quad (3)$$

and the $\psi_i^n$ have the form of the d-wave pairing called $d_{x^2-y^2}$ and $d_{xy}$

$$\left\{ \begin{array}{l} \psi_1^n(\theta) = \cos(2\theta) = \hat{k}_x^2 - \hat{k}_y^2 \\ \psi_2^n(\theta) = \sin(2\theta) = 2k_x k_y \end{array} \right. \quad (4)$$

This is compatible with the factorized pairing potential $V(k-k') = V \sum \psi_i(k) \psi_i(k')$. The form (3) for the OP can be generalised to other symmetries or mixture of symmetries. A relevant example is the case with a $s + d$ OP (e.g. when one has orthorhombicity) which is given by (2) plus a term $\Delta_3 \psi_3$ having the desired s-wave symmetry. We mention later the resulting corrections to the free energy.
Then we shall write the GL equations for $\Delta_n$ where one integrates over $k$. We follow a method analogous to the one used previously for mixed OP [21] except that we introduce the nodal angle $\alpha_n(R)$ and we consider a different set of $\{\psi_i, \Delta_i\}$. The derivation of these equations may be done in two steps. The first concerns any OP and generalizes the s-wave pairing equations. Since this has been shown several times (see e.g. [22]) we only sketch the calculation in Appendix A. The second step specializes to the d-wave pairing considered above [1]. The whole procedure gives two coupled gap equations for the $\Delta_i^n$ in which, in the limit $T \to T_c$, we retain only the following terms $\Delta, \nabla^2 \Delta, \nabla^4 \Delta$ and $\Delta^3$. We get

$$\Delta_1^n = a <\psi_1^2> \Delta_1^n - \frac{b}{T_c^2} <\psi_1^4> |\Delta_1^n|^2 \Delta_1^n - 3 \frac{b}{T_c^2} <\psi_1^2 \psi_2^2> |\Delta_2^n|^2 \Delta_1^n$$

$$+ \eta v_F^2 (\psi_1^2 \hat{k}_x^2 <\nabla^2 \Delta_1^n> + \psi_1^2 \hat{k}_y^2 <\nabla^2 \Delta_1^n>)$$

$$+ c v_F^4 (\psi_1^2 \hat{k}_x^4 <\nabla^4 \Delta_1^n> + \psi_1^2 \hat{k}_y^4 <\nabla^4 \Delta_1^n> + 6 \psi_1^2 \hat{k}_x^2 \hat{k}_y^2 <\nabla^2 \nabla^2 \Delta_1^n>)$$

$$+ c v_F^4 (4 <\psi_1 \psi_2 \hat{k}_x \hat{k}_y> \nabla^3 \nabla \nabla + 4 <\psi_1 \psi_2 \hat{k}_x^3 \hat{k}_y> \nabla \nabla^3 \Delta_2^n)$$

In (5), $< ... >$ denotes an integration over $\theta$ and the various letters $a, b, ..., \eta$ denote the integration and summation $\int d[k] \sum \omega ...$. The Fermi surface being circular the energy only depends on $|k|$ and the integration on $\theta$ affects only the $\psi_i$ and the Fermi velocity [i.e. $(k_x, k_y) = m v_F (\cos \theta, \sin \theta)$]. One gets a similar equation, upon making the substitution $\Delta_1 \leftrightarrow \Delta_2$ (and $\psi_1 \leftrightarrow \psi_2$), which has the same coefficients $a, b, c$ and $\eta$. In these equations the d-wave pairing manifests itself in the $<\psi_i^2>$-dependence of the coefficients (while a non zero value of $\alpha_n$ introduced two gaps $\Delta_i^n$).

It appears that the contribution of the fourth order in $\nabla$ is anisotropic (see the $c$-terms in (5)). In the case of s-wave pairing these terms can be combined to give a single isotropic contribution to the free energy, as it should.

Finally the GL free energy density of the $n$th layer is given by

$$f_n = f_0 + f_{ani}$$

with

$$f_0 = -A (1 - \frac{T}{T_c}) (|\Delta_1^n|^2 + |\Delta_2^n|^2) + \frac{B}{2T_c^2} (|\Delta_1^n|^2 + |\Delta_2^n|^2)^2$$

$$+ E \left(\frac{hv_F}{T_c}\right)^2 (|\nabla R \Delta_1^n|^2 + |\nabla R \Delta_2^n|^2)$$

and the anisotropic part

$$f_{ani} = \sum_{i=1,2} \left(\frac{hv_F}{T_c}\right)^4 \left[C_i (|\nabla_x^2 \Delta_1^n|^2 + |\nabla_y^2 \Delta_1^n|^2) + C'_i |\nabla_x \nabla_y \Delta_1^n|^2 \right]$$
\[+\frac{C}{2} \left(\frac{\hbar v_F}{T_c}\right)^4 | \nabla_x \Delta_1^a \nabla_y^3 \Delta_2^\ast + \nabla_x \Delta_1^a \nabla_y^3 \Delta_2^a - \nabla_x \Delta_1^a \nabla_y \Delta_2^a - \nabla_x \Delta_2^a \nabla_y \Delta_2^a \right. \\
\left. + (\Delta_1 \leftrightarrow \Delta_2) \right] \]

where we used (4) and the circular model to calculate the integrations over \( \theta \) which we then incorporated in the coefficients \( A, B, \ldots \).

This free energy density has been obtained keeping only the leading term in the small-\(|k|\) expansion which yields the form (4) for the OP and an isotropic Fermi surface (FS). Within this restriction we got an expression that does not depend on \( \alpha_n(R) \) at the mean-field level. In other words, the free energy of one layer is minimised by any uniform \( \alpha_n \).

Let us now consider the anisotropy effects. They are two sources of anisotropy, one in the OP, the other in the Fermi energy. The effect of the first one is illustrated by the presence of \( f_{ani} \) which implies that the fluctuations of \( \alpha_n(R) \) (and also of \( \phi_n(R) \)) are anisotropic in a layer. The fact that this anisotropy appears to order \( \nabla_R^4 \Delta^2 \) is due to the particular form of the OP (another form yields another order, e.g. an additional s-wave OP gives anisotropic terms to order \( \nabla_R^2 \Delta^2 \) [9]).

One can verify that the anisotropic terms \( f_{ani} \) contain gradients of \( \alpha \) and of \( \phi \) which are coupled (this coupling being absent at lower orders). These terms are negligible in the high temperature region (near \( T_c \)) but come into play at lower \( T \). In the London regime, it could be interesting to study the implication of this coupling on the vortex state. As one replaces gradients by \( \nabla - \frac{e_i}{\hbar} A \) the term to the quadratic order takes on the form

\[\Delta_0^2 E\{(\frac{\hbar v_F}{T_c})^2 [4(\nabla_R \alpha_n)^2 + (A + \nabla_R \phi_n)^2] \} \tag{7}\]

In addition to the kinetic energy of the current one gets a rigidity term in the orientation of the OP, \( \alpha_n \). Thus the fluctuations of \( \alpha_n \) are relevant as long as \( \alpha_n \) is not fixed relatively to the crystallographic axes.

Indeed the introduction of an anisotropy in the FS due to a crystal structure can pin in the orientation \( \alpha_n \) and also generate anisotropic fluctuations of \( \alpha_n \). To show this on an example, we consider an elliptic FS, i.e. \( k_x^2 + k_y^2 + \epsilon k_y^2 \). To first order in \( \epsilon \) the anisotropic terms now come in to order \( \nabla^2 \Delta^2 \) while to order \( \epsilon^2 \) the terms \( |\Delta_1^a|^2 \) and \( |\Delta_2^a|^2 \) have different coefficients. This means that the term to order \( |\Delta|^2 \) now depends on \( \alpha_n \) which will be fixed by the minimisation of the free energy. In this case there are still anisotropic terms in the Free energy (in gradients of the phase of the OP) which are relevant in the London regime.
2.2 Free energy density for layered superconductors

Following [15] we now add a transverse component to the electron energy of the normal state

\[ \epsilon(k) = \frac{k_x^2 + k_y^2}{2m} + K \cos(k_zd) \]  

(8)

where \( d \) is the interlayer spacing. We performed an expansion of the gap equations in the limits \( T - T_c << 1 \) and \( K << T_c \) (see Appendix A). The free energy has the general form \( \Delta F = \sum_n \int d\mathbf{R}(f_n + f_{n,n+i}) \) with \( f_n \) given by (3) and

\[
\begin{align*}
    f_{n,n+i} &= E \frac{K^2}{T_c^2} (|\Delta_n^n - \Delta_{n+1}^{n+1}|^2 + |\Delta_n^n - \Delta_{n+1}^{n+1}|^2) \\
    &+ 12 C \frac{K^2}{T_c} \left( \frac{hv_F}{T_c} \right)^2 (|\nabla_{\mathbf{R}} (\Delta_1^n - \Delta_1^{n+1})|^2 + |\nabla_{\mathbf{R}} (\Delta_2^n - \Delta_2^{n+1})|^2) \\
    &+ \frac{3}{32} C \frac{K^4}{T_c^4} \sum_{i=1,2} (13|\Delta_i^n - \Delta_i^{n+1}|^2 \\
    &- 8|\Delta_i^n - \Delta_i^{n+2}|^2 + 3|\Delta_i^n - \Delta_i^{n+3}|^2 - 1/2|\Delta_i^n - \Delta_i^{n+4}|^2)
\end{align*}
\]  

(9)

Thus in this LD model thermal fluctuations give rise to variations of the value of the nodal angle \( \alpha_n \). One sees in (6) and (9) that \( \alpha_n \) fluctuates, both within a layer and from one layer to another, around a constant but arbitrary value (in \( f_0 \) the first two terms do not depend on \( \alpha_n \)). The energy cost of these fluctuations is given by

\[ \delta f = \Delta_0^2 E \left\{ 4 \left( \frac{hv_F}{T_c} \right)^2 (\nabla_{\mathbf{R}} \alpha_n)^2 + 2 \frac{K^2}{T_c^2} (1 - \cos[2(\alpha_n - \alpha_{n+1})] \cos(\phi_n - \phi_{n+1})) \right\} \]  

(10)

which was determined from the gradient terms of \( f_n \) and \( f_{n,n+i} \) with the simplifying assumption that \( \nabla_{\mathbf{R}} \phi_n = 0 \). We wrote only the dominant terms, that is, the first line in (9) and the part \( f_0 \) of \( f_n \) but one must keep in mind the presence of anisotropic terms. From (10) one gets a current density between two adjacent layers

\[ j_{n,n+1} \sim \cos[2(\alpha_n - \alpha_{n+1})] \sin(\phi_n - \phi_{n+1}) \]  

(11)

Although this is a current that flows perpendicularly to the layers, it has the same behaviour with \( \alpha_n - \alpha_{n+1} \) as the current across a tunnel junction in a layer [23]. Note that in a model where \( \alpha_n - \alpha_{n+1} \) can become arbitrarily large (i.e. when \( \alpha_n \) is not pinned by anisotropies in the FS), the fluctuations can suppress the tunneling in the c-direction (\( j_{n,n+1} \) vanishes on average).
Now to study the energetic balance of the fluctuations of $\alpha_n$ one has to compare the two characteristic lengths, $\xi_\parallel$ and $\xi_\perp$, that come from $\delta f$ and a third one, $\xi_{ani}$, from $f_{ani}$:

$$\frac{\xi_\perp^2}{\xi_\parallel^2} = \frac{K^2 d^2}{2 (hv_F)^2}$$

and

$$\frac{\xi_{ani}^2}{\xi_\parallel^2} = \frac{AC}{E^2} \frac{(hv_F)^2}{(1 - \frac{T}{T_c})^2}$$

where $AC/E^2$ is a numerical factor. The LD model is valid within a regime of temperature given by the limits

$$1 - \frac{T}{T_c} << 1 \quad \text{and} \quad \xi_\perp \sim (1 - \frac{T}{T_c})^{-1/2} << d$$

There, the intra-layer length $\xi_{ani}$ is of order of $\xi_\parallel$, while the inter-layer length, $\xi_\perp$, is much smaller yielding the fluctuations of the OP in the c-direction inexpensive. We study some experimental implications of the fluctuations in the c-direction in section 3.

The above analysis does not fix the value of $\alpha_n$ in the absence of anisotropies of the FS linked to the crystallographic structure of these materials. To remedy this one has to consider a microscopic model that specifies a reasonable band structure (a step in that direction was taken in section 2.1). We choose to start from the t-J model since it is a natural candidate for a d-wave superconducting phase [2].

### 3 The t-J model for bilayers coupled via a reservoir

In the usual t-J model one considers the pairing of nearest-neighbor fermions on a square lattice with an exchange energy $J_\parallel$ and a quasiparticle hopping energy $t_\parallel$. This leads [2, 20] to a normal state with a Fermi surface (FS) of square shape at half filling and favors a variational d-wave superconducting state (in fact the lowest energy state corresponds to an $s+id$ OP at half filling and to a d-wave OP away from half filling) There the OP has the $d_{x^2-y^2}$ symmetry of (1) with a nodal angle $\alpha = 0$, ( nodes lie at 45° with respect to the crystallographic axes ). Recently it was shown [16] that additional terms were needed to fit experimental data on BSCCO: Kuboki and Lee used a bilayer structure with an exchange energy between two layers, $J_\perp$, and a hopping term, $t_\perp$. In agreement with ARPES experiments [24] one gets a FS with two bands [16]. Furthermore the OP has two nodal angles at $\alpha = \pm \alpha_0$ which
may have been observed in \textit{BSCCO} \cite{17} \((\alpha_0 \sim 10^\circ)\). Here we shall go further by adding terms that describe the FS and the density of states (DOS) of \textit{YBCO}. We include a pairing along the diagonals in a layer, \(J_d\), and a hopping term, \(t_n\), that couples two bilayers via a charge reservoir, see figure 1.

### 3.1 Fermi surface and gap

The slave-boson mean-field Hamiltonian of the t-J model describes electrons with forbidden doubled occupancy on a site: the creation of an electron on site \(i\) in the layer \(s\) consists of the annihilation of a hole operator having the charge of the electron \(b^+_i\) and the creation of a fermion operator having the spin \(\sigma\) of the electron \(f^+_i\). To simplify we shall set \(b^+_i b^+_j = \delta\), i.e. the number of empty sites gives the doping rate.

The hamiltonian is given by

\[
\mathcal{H} = -\sum_{r,s} \sum_{i,j} \left[ \delta t_{ij} f^+_i f^+_{r} + J_{ij} (\vec{S}_r \cdot \vec{S}_s \ - \frac{1}{4} n_i n_j) \right]
\]

with the constraint \(\sum f^+_i f^{-}_i = 1 - \delta\) and \(\vec{S}_r = f^+_i \sigma \alpha \beta \sigma f^+_{j\beta} \), the \(t_{ij}\) and \(J_{ij}\) are shown in figure 1. Within mean-field approximation we introduce various OP, in particular we restrict our analysis to a d-wave coupling in the layers and to an s-wave coupling between layers:

\[
J_\parallel \sum_{\sigma} \sigma < f^+_i f^{-}_j > = (+) \Delta_\parallel \text{ with } j = i \pm x(\pm y) \text{ and } r = 1,2
\]

\[
J_d \sum_{\sigma} \sigma < f^+_i f^{-}_j > = (+) \Delta_d \text{ with } j = i \pm x \pm y(\mp x \mp y) \text{ and } r = 1,2
\]

\[
J_\perp \sum_{\sigma} \sigma < f^+_i f^{-}_j > = \Delta_\perp \text{ with } j = i + z
\]

in the particle-particle channel and

\[
\sum_{\sigma} < f^+_i f^{-}_j > = \chi_\parallel \text{ with } j = i \pm x \text{ or } \pm y
\]

\[
\sum_{\sigma} < f^+_i f^{-}_j > = \chi_d \text{ with } j = i \pm (x \pm y)
\]

\[
\sum_{\sigma} < f^+_i f^{-}_j > = \chi_\perp \text{ with } j = i + z
\]

\[
\sum_{\sigma} < f^+_i f^{-}_j > = \chi_n \text{ with } j = i + z
\]
in the particle-hole channel (here too \( r = 1, 2 \)).

As usual [2,26] we write the Hamiltonian terms depending on the OP in momentum space

\[
\mathcal{H}_\Delta = \sum_k F^+(k) M(k) F(k) + \frac{3N}{8} \left( \frac{\Delta_1^2}{J_{||}} + 2 \frac{\Delta_2^2}{J_d} + \frac{\Delta_3^2}{J_{\perp}} \right)
\]

with

\[
F(k) = ( f_{k,\uparrow}, f_{-k,\downarrow}, f_{k,\downarrow}, f_{-k,\uparrow}, f_{k,\uparrow}, f_{-k,\downarrow} ),
\]

\[
M = \begin{pmatrix}
\xi_1 & \Delta_1 & \tilde{t}_1 & \Delta_1 & \tilde{t}_n & 0 \\
\bar{\xi}_1 & \Delta_2 & -\bar{t}_1 & -\bar{\Delta}_1 & 0 & -\bar{t}_n \\
\xi_1 & \bar{\Delta}_1 & \tilde{t}_n & 0 & 0 & -\tilde{t}_n \\
-\bar{\xi}_1 & 0 & 0 & -\bar{\tilde{t}}_n & 0 & -\bar{\tilde{t}}_n \\
-\xi_3 & 0 & 0 & 0 & 0 & -\xi_3
\end{pmatrix}
\]

where one easily completes the matrix knowing that \( M^t = M^* \) and the energies and gaps written below (taking the lattice parameters \( a = b = c = 1 \))

\[
\xi_1 = -\epsilon_{||}(\cos k_x + \cos k_y) + 2\epsilon_d \cos k_x \cos k_y - \mu \\
\xi_3 = -\epsilon_n(\cos k_x + \cos k_y) - \mu \\
\tilde{t}_1 = -\epsilon_{\perp} e^{ik_x d} \\
\tilde{t}_n = -\epsilon_{n} e^{ik_{z} d'}
\]

with \( \epsilon_{\alpha} = \delta t_{\alpha} + J_{\alpha} \chi_{\alpha} \) for the various energies and \( \mu \) is the chemical potential which depends on \( \delta \). With these expressions one can reproduce the FS of \( YBCO \) while the FS of \( BSCCO \) is well represented if one neglects the next-nearest interactions, \( \epsilon_d = 0 \), and the hopping between bilayers, \( \epsilon_n = \delta t_n = 0 \). The FS of figure 2 is obtained upon adjusting the various parameters \( t_{\alpha} \) and \( J_{\alpha} \) in order to reproduce experimental data on optimally doped \( YBCO \) (i.e. for \( \delta \sim 0.25 \)) [24], that is (in eV), \( t_{||} \sim 0.4, \ t_d \sim 0.1, \ t_{\perp} \sim 0.05 \) and \( \tilde{t}_n \sim 0.0045 \). (We determine these values from \( t_n = \Gamma^2(a/d')^2 \), and \( t_{\perp} = \Gamma^2(a/d)^2 \), using \( \Gamma = 1/5, \ d'/a = 3, \ d/a = 1 \) while \( t_d \) comes from [24]). As it has been pointed out in case of \( BSCCO \) [16] the hopping term between layers is taken in the form \( \tilde{t}_{\perp} \sim (\cos k_x - \cos k_y)^2 \).

The gaps in \( M \) are given by

\[
\Delta_1 = \Delta_{||}(\cos k_x - \cos k_y) + 2\Delta_d \sin k_x \sin k_y \\
\Delta_{12} = \Delta_{\perp} e^{ik_x d}
\]
so that the pairing along the lattice axes is of $d_{x^2-y^2}$ type and, along the diagonals, of $d_{xy}$ type.

One can diagonalise the Hamiltonian (18) which gives the quasiparticle energies

$$E_{1,2} = \pm [(\xi_1 - \tilde{t}_\perp)^2 + (\Delta_1 - \Delta_{12})^2]^{1/2}$$

$$E_{3,4} = \pm [(\xi_1 + \tilde{t}_\perp)^2 + (\Delta_1 + \Delta_{12})^2 + \xi_3^2 + 4\tilde{t}_n^2 + S^{1/2}]^{1/2}$$

$$E_{5,6} = \pm [(\xi_1 + \tilde{t}_\perp)^2 + (\Delta_1 + \Delta_{12})^2 + \xi_3^2 + 4\tilde{t}_n^2 - S^{1/2}]^{1/2}$$  \(21\)

with

$$S = [(\xi_1 + \tilde{t}_\perp)^2 + (\Delta_1 + \Delta_{12})^2 - \xi_3^2]^{1/2} + 8\tilde{t}_n^2[(\xi_1 + \tilde{t}_\perp)^2 + (\Delta_1 + \Delta_{12})^2 + 2\xi_3(\xi_3 + \xi_1 + \tilde{t}_\perp)]$$  \(22\)

This yields the following free energy

$$F_\Delta = -2T \sum_r \sum_k \ln[2 \cosh(E_r(k)/2T)] + \frac{3N}{8} \left( \frac{\Delta_\parallel^2}{J_\parallel} + 2 \frac{\Delta_d^2}{J_d} + \frac{\Delta_\perp^2}{J_\perp} \right)$$  \(23\)

One then minimises (23) which gives the various OP. Here we restrict ourself to the above forms, see (20), for the OP, i.e. the degrees of freedom are $\Delta_\parallel$, $\Delta_d$ and $\Delta_\perp$ which are real. There are three critical temperatures respectively proportional to $J_\parallel$, $J_d$ and $J_\perp$; with the values that give figure 2, $J_\parallel$ dominates. In analogy with our previous OP, see (1), we set

$$\left\{ \begin{array}{l}
\Delta_\parallel = \Delta_0 \cos(2\alpha) \\
\Delta_d = \Delta_0 \sin(2\alpha)
\end{array} \right.$$  \(24\)

Clearly the value $\alpha \pmod{\pi/2} = 0$ (i.e. nodal lines at $45^\circ$ with respect to the lattice axes) will minimise the free energy since $J_\parallel >> J_d$ (this can be verified e.g. upon expanding the free energy in the small-$\Delta$ limit). The additional coupling $J_d$ creates a metastable state in which the OP has nodal lines along the lattice axes, separated from the lowest energy state by an energy barrier of order $J_\parallel$.

From (21) one easily verifies that the mixing of $\Delta_1$ and $\Delta_{12}$ leads to two nodal angles obtained by setting $\Delta_1 \pm \Delta_{12} = 0$ and denoted by $\alpha = \pm \alpha_0$. Considering the effects of the thermal fluctuations on the layered system studied in the previous section one gets an OP whose orientations fluctuate from one layer to another between the values $\alpha = \pm \alpha_0$. This will have dramatic consequences discussed in the following.
3.2 Density of States and conductance

In order to compute the DOS for this system one must have the eigenvectors of the matrix $M$. Indeed, denoting by $\mathbf{U}$ the unitary matrix which diagonalizes $M$, the DOS in the $s$-th layer is given by

$$\rho_s(E) = 2 \sum_{k,l} |U_{s,l}|^2 \delta(E - E_l(k))$$

(25)

where $l$ indexes the eigenvalues and $E$ is the energy measured relatively to the Fermi energy. In the absence of inter-bilayer coupling the $E_l(k)$ yield "nodal" contributions for the DOS in layers 1 and 2 and "normal" contributions for layer 3. A nodal contribution is obtained whenever both the $\xi$ and the $\Delta$ terms vanish in the quasiparticle spectrum; in that case the DOS varies linearly with $E$ for small $E$. If only a $\xi$ term vanishes, layer 3 which has $\Delta = 0$ yields a finite contribution for vanishing $E$. Including the inter-bilayer coupling will admix these two types of contributions such that by summing over $k$ in any given layer one may obtain a linear combination of "nodal" and "normal" DOS [28]. (As noted above the nodal and normal contributions arise from distinct ranges of integration in $k$ space).

With our model it is straightforward to compute $\mathbf{U}$ and we only quote the result for the DOS in layer 1:

$$\rho_1(E) = aE + b$$

(26)

where $b$ is proportional to the normal state DOS in layer 3, $\rho_N$, and

$$b = \rho_N \left( \frac{t_n w}{E_3} \right)^2$$

(27)

and

$$w(\mathbf{k}_0) = 2 \xi_1 + \tilde{t}_{\perp} - \left( (\xi_1 + \tilde{t}_{\perp})^2 + (\Delta_1 + \Delta_{12})^2 \right)^{1/2} \Delta_1 + \Delta_{12}$$

(28)

with $\mathbf{k}_0$ such that $\xi_3(\mathbf{k}_0) = 0$. The offset at the Fermi energy is also present in a DOS determined from an s-wave OP [28] while the linear in $E$ dependence is due to the d-wave symmetry.

In single-crystal $YBCO$, the DOS has been determined from the specific heat [18] which is dominated by a $T$-term at low temperature whose prefactor yields $\rho_1(E_F)/\rho_N \sim 1/5$. This is in close agreement with what we get for $(t_n w/E_3)^2$ using $t_n = 4.5 \times 10^{-3}$ eV and $\Delta_{YBCO} = 15meV$ [10]. On the other hand we get for $BSCCO$ $\rho_1(E_F)/\rho_N \sim 10^{-8}$ using $t_n = 4 \times 10^{-6}$ eV and $\Delta_{BSCCO} = 20meV$.

Furthermore the DOS (28) yields a tunneling spectrum along the c axis shown in figure 3 at zero temperature from

$$G(V) \sim \frac{d}{dV} \int_0^{eV} dE \rho_0(E) \rho_1(E - eV)$$

(29)
where $\rho_0$ is the DOS of a conventional superconductor. The predicted spectrum closely resembles what is found in experiments on the tunneling between YBCO and Pb \[10, 11\]. Above the critical temperature of Pb the finite offset at zero voltage that is measured is given in our analysis by the hopping energy $t_n$ (see \[27\)). Below this critical temperature, the offset induces the divergence at $\Delta_{Pb} = 1.38$ (see figure 3). Furthermore there is possibly a linear regime in these experimental data coming from the d-wave symmetry of the OP of YBCO. Finally one expects a slope change at $eV = \Delta_{Pb} + \Delta_{YBCO}$. (In figure 3 we use $\Delta_{YBCO} = 20meV$ which is lower than above since we now take the value given by conductance measurements \[10, 11\].) On the other hand no offset seems to be observed in experiments on BSCCO \[29\].

### 3.3 density of states and penetration depth in the c-direction

For a 2D d-wave superconductor one finds that the DOS depends linearly on $E$ for small $E$ (see e.g. \[30\] for a complete result). Indeed,

$$\rho(E) \propto \int \int kdkd\theta \ \delta(E - \sqrt{\xi_k^2 + \Delta_k^2}) \quad (30)$$

where $\Delta_k = \Delta_0(T)\cos(2\theta)$. We now compute the contribution to $\rho$ near $\theta = \frac{\pi}{4} (mod \frac{\pi}{2})$. Setting $\theta = \frac{\pi}{4} - \theta', \ x = \xi, \ y = 2\Delta_0\theta', \ r = \sqrt{x^2 + y^2}$ and $\psi = \tan^{-1}(y/x)$ we obtain

$$\rho(E) \propto \int \int rdrd\psi \ \delta(E - r) \quad (31)$$

Thus the linear behaviour is due to the nodal structure of $\Delta_k$ which lead us to address the question of the effect of the thermal fluctuations on the DOS and consequently on the penetration depth.

As discussed in the previous section, for bilayers, the contribution at $\theta = \frac{\pi}{4}$ (mod $\frac{\pi}{2}$) evolves into two modes at $\theta = \frac{\pi}{4} \pm \alpha_0$ (mod $\frac{\pi}{2}$). At $T = 0$ the inter-bilayer hopping term $t_n$ couples the bilayers and selects the $+\alpha_0$ or $-\alpha_0$ solution to form a coherent state. For $T > t_n$ however the bilayers are decoupled. The system in effect behaves in a 2D fashion. As a result, the contribution to the DOS along c coming from a particular orientation of the nodal line – say $\theta = \frac{\pi}{4} - \alpha_0$ – is given by

$$\rho_c(E, z) \propto \int d\psi \int_{\epsilon(z)} rdr \ \delta(E - r) \quad (32)$$

with $\epsilon(z) = 0$ or $\Delta_0\alpha_0$ so that

$$\rho_c(E, z) \propto E \quad \text{for} \quad E > \epsilon$$
$$\rho_c(E, z) = 0 \quad \text{for} \quad E < \epsilon \quad (33)$$
The average DOS is thus given by \( \rho_c(E) = \langle \rho_c(E, z) \rangle \), where \( \langle .. \rangle \) denotes averaging over the \( \epsilon \) distribution function. Since the nodal lines may take on two positions the system is equivalent to an Ising problem. The energy barrier between the two equilibrium positions in a bilayer is of the order of \( \Delta_0 \alpha_0 \), (and can be estimated to \( \sim 40K \) using realistic values for \( \Delta_0 \sim 25meV \) and for \( \alpha_0 \sim 10^\circ \).

The energy barrier in the vertical direction is of the order of \( t_n \). We note that for \( T \geq \Delta_0 \alpha_0 \) contributions to the DOS are not dominated by the nodal lines anymore, and gapped parts in k space must be included. In that limit the Ising analogy ceases to be valid. In the Ising regime \( (T < \Delta_0 \alpha_0) \) however we may write

\[
P(\epsilon(z)) = \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{\epsilon^2}{2\sigma^2}}
\]

where the variance \( \sigma \propto \frac{1}{L} \) (the susceptibility divided by the linear size along the c axis). Thus

\[
\rho_c(E) = \frac{E}{\sqrt{2\pi \sigma^2}} \int_0^E e^{-\frac{\epsilon^2}{2\sigma^2}} d\epsilon
\]

If the susceptibility is large enough, as is the case for a quasi 2D system and/or if \( L \) is small enough as is the case for thin films, one may have a situation where \( E \propto T \) and \( \sigma \gg T \) so that

\[
\rho_c(E) \propto E^2
\]

This situation may correspond to high \( T_c \) films and to the bismuth, mercury, and thallium compounds which behave as fairly 2D systems. On the other hand for large \( L \) and/or small \( \chi \) as is the case for single crystals and/or more isotropic compounds such as YBCO one recovers

\[
\rho_c(E) \propto E
\]

Inasmuch as in the thermal fluctuation dominated regime the penetration depth is given by

\[
\lambda_c^{-2}(T) = \lambda_c^{-2}(0)[1 - 2 \int -\frac{\partial f}{\partial E} \frac{\rho_c(E)}{\rho_N(0)} dE]
\]

where \( f(E) = \frac{1}{\exp(\beta E) + 1} \) and \( \rho_N(0) \) is the normal state DOS at the fermi energy, one sees that thermal fluctuations may genuinely yield

\[
\Delta \lambda_c^{-2} \propto T^2
\]

even in the absence of disorder([31]).

Experimentally it seems indeed that for the 2D-like materials a \( T^2 \) law is obtained for the c-axis penetration depth. For \( YBCO \) the situation is still not settled. Mao et al. recently reported findings of a linear \( T \) dependence for a \( YBCO \) single
crystal [4] whereas the UBC group seems to find a more quadratic dependence [13]. Moreover experiments on YBCO powders also see a $T^2$ dependence that is shown to be intrinsic [20]. As was pointed out in [20] the measured $\lambda_\parallel$ combines $\lambda_{ab}$ and $\lambda_c$ which is much larger. So even if the present model would give a linear behaviour for $\Delta\lambda_{ab}$, one could find $\Delta\lambda_\parallel \propto T^2$ in case of a quadratic $\Delta\lambda_c$.

4 conclusion

In this paper we consider superconductors consisting of layers with a d-wave OP that varies in momentum space according to

$$\Delta_k = \Delta_0(T) \cos[2(\theta - \alpha)]$$

(40)

($\tan \theta = \frac{k_y}{k_x}$) where $\alpha$ gives the nodal lines orientation. As for the phase of the OP, $\alpha$ may fluctuate in space. We consider an $\alpha$ that is homogeneous in the layers but can thermally fluctuate in the c-direction. We show how the value of $\alpha$ is fixed with respect to crystallographic axes when a reasonable band structure is taken into account (this leads to anisotropies of the Fermi surface). We use an extended t-J Hamiltonian with CuO$_2$ bilayers separated by a charge reservoir, yielding a FS for YBCO in fair agreement with that mapped out by ARPES measurements. This leads to various possible pairings of the type of (40) with different $\alpha$. Using the key idea of this paper of combining the inexpensive spatial fluctuations of $\alpha$ with the fact that the OP can choose between several orientations, we show that the thermal fluctuations of $\alpha$ change the $T$ dependence of $\Delta\lambda_c$ from linear to quadratic. Our model predicts this quadratic behaviour for thin films and quasi-2D systems where it is usually attributed to the disorder (see [32] for a review). We also show how the presence of the reservoir layers is revealed by conductance and specific heat measurements.

Here we did not consider the orthorhombicity that distinguishes YBCO, from e.g. BSCCO, that is, asymmetric d-wave amplitudes in the $a$ and $b$ directions. Then one gets a mixture of $d_{x^2-y^2}$ and $s_{x^2+y^2}$ (called extended s-wave) symmetries. If the s-wave component is small one still has node lines. In twined samples there will be domains of different orientation of these lines, an issue that we leave for a later publication.

Finally let us consider the case of a pure extended s-wave OP sometimes invoked for BSCCO. It has nodes and one can easily show that they yields a linear behaviour of the DOS near the Fermi energy. Since there are thermal fluctuations in the orientation of the OP as well (see section 2), one can conclude that the above results for the penetration depth persist.
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Appendix

In the following we give a summary of the derivation of the LG-equations for a general OP in the vicinity of $T_c$. As in section 2 we first derive the equations in a layer and then consider the LD-model. The OP is defined by

$$\Delta(r, r') = T V(r - r') \sum_\omega F^\dagger_\omega(r, r')$$

(41)

where $V$ is the attractive two-body interaction of the weak-coupling theory and $\omega = \pi T(2n + 1)$. We start from the Gor'kov equation of motion for the normal and anomalous Green functions (in the absence of a magnetic field)

$$\left\{ \begin{array}{ll}
(i\omega - \xi_k)G^\omega(k, k') + \sum_q \Delta^\omega(q, k') F^\dagger_\omega(q, k) &= \delta^2(k - k') \\
(i\omega + \xi_k) F^\dagger_\omega(k, k') + \sum_q \Delta^\ast(k, q) G^\omega(q, k') &= 0
\end{array} \right.$$  

(42)

where we omit the spin variable to simplify. The energy is described by $\xi(k) = \epsilon(k) - \mu$ with $\epsilon(k) = (k_x^2 + k_y^2)/(2m)$. As usual one introduces the Green function of the electron in the normal state

$$G^0_\omega(k, k') = \frac{\delta^2(k - k')}{i\omega - \xi_k}$$

(43)

and one expands in power of $\Delta$. One gets

$$\Delta^\ast(k_1, k_2) = T \sum_\omega \sum_{k,k'} \delta^2(k_1 + k_2 - k - k') V(k - k_1) \left\{ \frac{\Delta^\ast(k, k')}{(i\omega - \xi_k)(-i\omega - \xi_{k'})} - \sum_{q,q'} \frac{\Delta^\ast(k, q) \Delta(q, q') \Delta^\ast(q, k')}{(-i\omega - \xi_k)(i\omega - \xi_q)(-i\omega - \xi_{q'})(i\omega - \xi_{k'})} \right\}$$

(44)

We shall write $\Delta(k_1, k_2) = \Delta(k_1 - k_2, k_1 + k_2)$ which is the notation of section 2.

Then we make the substitution in various quantities

$$\xi_{k+q} = \xi_k + |q| \hat{v} \cdot \hat{k} + \frac{q^2}{2m} \quad \text{with} \quad \hat{k} = \frac{k}{|k|}, \quad |v| = \frac{|k|}{m}$$

(45)
and we expand in powers of $q$ (we set $D_k = i\omega - \xi_k$)
\[
\frac{1}{i\omega - \xi_{k+q}} \approx \frac{1}{D_k} \left\{ 1 + \frac{|v|}{D_k}q\hat{k} + \frac{|v|^2}{D_k^2}(q\hat{k})^2 + \frac{q^2}{2mD_k} + \frac{|v|^3}{D_k^3}(q\hat{k})^3 + \frac{|v|}{D_k^2} \frac{q^2}{m}(q\hat{k}) + \frac{|v|^4}{D_k^4}(q\hat{k})^4 + \frac{3|v|^2}{D_k^2} \frac{q^2}{2m}(q\hat{k})^2 + \frac{q^4}{4m^2D_k^2} \right\}
\]

In the following we shall keep only the dominant terms without loss of generality. This becomes valid when $\omega^2 << \mu^2$ which leads to substitute factors $v_F = (\mu/2m)^{1/2}$ for $|v|$. Furthermore one substitutes the integration $m \int d\xi \int d\theta$ for $\sum_k$ to which the terms with an even power of $\hat{k} = (\cos \theta, \sin \theta)$ won’t contribute. Thus we only keep in (46) three terms, the order 0 in $q$ and the first term written above at the order 2 and at the order 4.

Then the particular forms of the OP and the pairing potential, see (1), (2) and below (4), are to be introduced. Upon taking the Fourier transform with respect to the center-of-mass coordinate $q$, which gives gradients $\nabla_R$ of $\Delta$, one gets (5).

In case of layered systems the gap equations can be derived as above, with the energy (8). In the expansion of (43) we keep at each order in $(q, q_z)$ the dominant terms in the limits $|\omega| \sim T_c << \mu \sim v_F^2$ and $K << T_c$ at finite $K^2/(T_c v_F^2)$, that is,
\[
\frac{1}{i\omega - \xi_{k+q}} \approx \frac{1}{D_k} \left\{ 1 + \frac{|v|^2}{D_k^2}(q\hat{k})^2 + \frac{K^2}{D_k} [1 - \cos(dq_z)] \right. \\
+ \frac{|v|^4}{D_k^4}(q\hat{k})^4 + \frac{6v_F^2 K^2}{D_k^4} (q\hat{k})^2 [1 - \cos(dq_z)] \\
+ \frac{3K^4}{16D_k^2} \left[ \frac{15}{2} - 13 \cos(dq_z) + 8 \cos(2dq_z) - 3 \cos(3dq_z) + \frac{1}{2} \cos(4dq_z) \right] \right\}
\]

As before we also anticipated upon supressing terms that disapear after an integration over $(|k|, k_z)$. One substitutes (17) in (44) to get the gap equations and finally the free energy densities (6) and (9).
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Figure caption

Figure 1:

The hopping and exchange energies on a bilayer structure (1-2) separated by charge reservoir (3). The summation in the Hamiltonian (15) is restricted to nearest and next nearest neighbors within a layer (right figure) and to nearest neighbors in adjacent layers (left figure).

Figure 2:

The Fermi surface of $YBCO_7$ for a single bilayer in the $\Gamma XY$ quadrant. The solid (resp. dashed) line corresponds to a dispersion relation of the form $\xi_1+$ (resp. - $)$ $\tilde{t}_\perp$ (see eqn (18)). The degeneracy of the two branches at $\frac{\Pi}{2}$, $\frac{\Pi}{2}$ is lifted by $\tilde{t}_n$.

Figure 3:

Zero temperature tunneling conductance along the $c$ direction for a $YBCO/Pb$ junction. The DOS for $YBCO$ near the Fermi energy is given by eqn (21). The conductance diverges at the $Pb$ gap taken to be 1.38 meV.
Figure 1:
Figure 3: