The gap maximum of anisotropic superconductors

R. Combescot

Laboratoire de Physique Statistique de l’Ecole Normale Supérieure, associé au CNRS et aux Universités Paris 6 et Paris 7,
24 rue Lhomond, 75005 Paris, France

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The last few years have seen a very important progress in the identification of the order parameter in some high $T_c$ superconducting compounds. Indeed there are now quite firm experimental evidences that, in $YBa_2Cu_3O_7$ (YBCO), it changes sign and that there are nodes in the gap \[3\]. More recently a linear dependence of the penetration depth has been observed in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) \[4\], and phase sensitive experiments have also given a positive answer \[5\]. There is also clear indication from Raman scattering experiments \[6\] of nodes in the gap in Hg compounds. Finally a spontaneous half magnetic flux quantum has been observed quite recently \[7\] in $Tl_2Ba_2CuO_{6+\delta}$ giving evidence for a change of sign of the order parameter. These features of the order parameter are a clear indication that there is some important repulsive contribution in the pairing interaction. The most obvious origin for such a contribution is Coulomb repulsion.

Yet this answer does not provide a complete physical picture for this repulsive component. Indeed \[8\] this repulsion can appear in a direct way, or it can also be the microscopic origin of low energy antiferromagnetic fluctuations, with pairing mostly due to exchange of these fluctuations between electrons. A qualitative difference between these two mechanisms is the characteristic energy of the pairing interaction. If we are dealing with direct Coulomb repulsion, the typical energy entering the interaction is of order of Coulomb interaction itself, that is typically a few eV. Since the critical temperature and the gap are quite small compared to this energy, the pairing interaction can be considered as instantaneous. This implies that pairing can be very well described by weak coupling BCS theory. On the other hand if pairing is due to the exchange of spin fluctuations, our characteristic energy is of the order of a spin fluctuation frequency, which is a few tenths of eV at most. In this case the critical temperature and the gap are no longer small compared to this energy, and the pairing interaction can not be considered as instantaneous. This means in particular that pairing has to be described by a strong coupling generalization of BCS theory \[9\]. Therefore we can obtain an indication on the kind of repulsive interaction we are dealing with by checking, as well as we can, if the superconductor is satisfactorily described by weak coupling theory or if there is a need for strong coupling effects.

As it is well known the consequences of weak coupling theory are much more restrictive than those of strong coupling. Therefore in this paper we will consider some consequence of weak coupling theory and see if it can be made to agree with experiments. Specifically we will deal with the zero temperature gap to critical temperature ratio. Naturally it is well known that, for isotropic pairing, this ratio is given by the famous BCS value $1.76$. However in this paper we will consider the much more general case of anisotropic weak coupling BCS theory for which no such a simple result exists. Actually, as we already mentioned, we can have nodes in the order parameter and in this case there is, strictly speaking, no gap at all for the whole excitation spectrum. On the other hand for a fixed value of the wavevector $\mathbf{k}$ of the excitation, we have a gap $|\Delta_{\mathbf{k}}|$ for the excitation energy where $\Delta_{\mathbf{k}}$ is the order parameter. We are interested in the maximum $\Delta_M$ of this gap over the Fermi surface, and its ratio $\Delta_M / T_c$ to the critical temperature.

Our reason for investigating this ratio is that we have some good experimental data for it. Surprisingly this is not so much for YBCO, the most investigated high $T_c$ superconductor, where the data are not very clear although $2 \Delta_M / T_c$ seems to range from 6 to 8 in most measurements. The clearest data are perhaps found in BSSCO where tunneling experiments perpendicular to the c axis \[10\] give a fairly sharp peak around 30 meV leading to $2 \Delta_M / T_c \approx 7.5$. The sharpness of the peak makes unlikely a shift to higher energy due to broadening. Angular dependent tunneling experiments in the a-b plane \[11\] give even a gap maximum reaching 40 meV. One may still worry that tunneling sees only a surface feature. However Raman scattering clearly samples the bulk, and it gives \[12\] a maximum around 550 cm$^{-1}$, which seems to confirm $2 \Delta_M / T_c \approx 7.5$. Although the data are broad which makes the interpretation less secure. Taken together these experiments are suggestive of a fairly high ratio. Raman data in Hg-1212 give similar...
results\cite{1}. Facing these experimental data, it is of interest to investigate if they can be explained by taking into account the anisotropy of the gap within weak coupling theory. This is the purpose of the present paper.

In weak coupling theory the order parameter $\Delta_k$ is obtained by solving the gap equation:

$$\Delta_k = \int d_2k' V_{k,k'} \Delta_{k'} 2\pi T \sum_{m=0}^{\omega_c/2\pi T} \left( \omega_m^2 + |\Delta_{k'}|^2 \right)^{-1/2}$$  \hspace{1cm} (1)

Here the integration $d_2k'$ over the Fermi surface is weighted by the local density of states $\left( \frac{(2\pi)^3 v_{k'}}{m} \right)^{-1}$. The summation over the Matsubara frequencies $\omega_m = (2m + 1)\pi T$ is limited to a cut-off $\omega_c$ large compared to the maximum $\Delta_M$ of $|\Delta_k|$ (and therefore to $T_c$). We make no assumption on the effective interaction $V_{k,k'}$ so the situation we consider is completely general. We note also that a multiband model can be considered as a particular case of gap anisotropy so this kind of situation is included in our study.

At the critical temperature $T_c$, this equation becomes linear. We call $\Delta_{0,k}$ the normalized eigenvector of $V_{k,k'}$ corresponding to the largest eigenvalue $\lambda_0$. It gives the shape of the gap at $T_c$. Making use of $2\pi T_c \Sigma 1/|\omega_m| = \ln \left( \frac{1.13 \omega_c}{T_c} \right) = 1/\lambda_0$, (valid in the weak coupling limit of large $\omega_c / T_c$), we have:

$$\Delta_{0,k} = \ln(1.13 \frac{\omega_c}{T_c}) \int d_2k' V_{k,k'} \Delta_{0,k'}$$  \hspace{1cm} (2)

Below $T_c$, $\Delta_k$ is obtained from Eq.(1). Now an essential feature of this equation is that the sum over Matsubara frequencies is dominated by the terms $\omega_m >> \Delta_M$. This is seen by rewriting it as:

$$\Delta_k = \ln(1.13 \frac{\omega_c}{T_c}) \int d_2k' V_{k,k'} \Delta_{k'} + \int d_2k' V_{k,k'} \Delta_{k'} \left[ 2\pi T \sum_{m=0}^{\omega_c/2\pi T} \left( \omega_m^2 + |\Delta_{k'}|^2 \right)^{-1/2} - \sum_{m=0}^{\omega_c/2\pi T_c} |m + 1/2|^2 \right]$$  \hspace{1cm} (3)

In the second term of the right-hand side we can let $\omega_c$ go to infinity because the result is convergent. Since in weak coupling $\ln(1.13 \omega_c / T_c)$ is large, we see that the first term dominates over the second one. Therefore to lowest order the shape of the gap below $T_c$ is still given by $\Delta_{0,k}$. However the size of the gap is fixed by the second term which is non linear. We can obtain a still exact equation for this size by multiplying Eq.(3) by $\Delta_{0,k}$ and integrating over $k$ (which takes into account the local density of states), leading to:

$$\int d_2k \Delta_{0,k} \Delta(k) [\pi T \sum_{m=0}^{\omega_c/2\pi T} \left( \omega_m^2 + |\Delta_{k'}|^2 \right)^{-1/2} - \sum_{m=0}^{\omega_c/2\pi T_c} |2m + 1|^2] = 0$$  \hspace{1cm} (4)

where we have made use of Eq.(2) to eliminate the interaction (using the fact that it is hermitian). Since this equation does not contain large terms anymore, we can replace $\Delta_{0,k}$ by $\Delta_k$ to lowest order. This equation can also be rewritten as:

$$\ln(\frac{T_c}{\Delta_M}) \int d_2k |\Delta_k|^2 = \int d_2k |\Delta_k|^2 2\pi T \sum_{m=0}^{\infty} \left[ |\omega_m|^{-1} - \left( \omega_m^2 + |\Delta_k|^2 \right)^{-1/2} \right]$$  \hspace{1cm} (5)

In particular we obtain at $T = 0$:

$$\ln\left( \frac{\Delta_M}{1.76 T_c} \right) = -\frac{\int d_2k \delta^2(k) \ln(\delta(k))}{\int d_2k \delta^2(k)}$$  \hspace{1cm} (6)

where we have introduced $\delta(k) = |\Delta_k| / \Delta_M$ which is the absolute value of the gap normalized to its maximum value. This equation has already been essentially obtained by Pokrovskii\cite{13}. Provided that we know the shape $\delta(k)$ of the gap, it gives us the maximum of the zero temperature gap $\Delta_M$ compared to the standard BCS value $1.76 T_c$. We see that the result is not sensitive to the detailed structure of the gap since the logarithm is a smooth function.

The above result has been obtained within weak coupling theory where the parameter $\omega_c / T_c$ is large. If we want to improve on this result, we have to consider that $\omega_c / T_c$ is not large anymore which implies to go to strong coupling theory anyway. There is no way to improve consistently on this result within weak coupling theory. Nevertheless we
might worry that the above result is a poor approximation because the dominant term is only logarithmically large. Fortunately the general situation is much better. This can be seen by rewriting the exact Eq.(3) at \( T = 0 \) as:

\[
\Delta_k = \ln(1.13 \frac{\omega_c}{T_c}) \int d^2k' V_{k,k'} \Delta_{k'} + \int d^2k' V_{k,k'} \Delta_{k'} \ln(\frac{1.76 T_c}{|\Delta_k|})
\]

(7)

and projecting it on the complete set of normalized eigenvectors \( \Delta_{m,k} \) of \( V_{k,k'} \). If the corresponding eigenvalues are \( \lambda_m \), this gives:

\[
\left( \frac{1}{\lambda_m} - \frac{1}{\lambda_0} \right) \int d^2k \Delta_{m,k} \Delta_k = \int d^2k \Delta_{m,k} \Delta_k \ln(\frac{1.76 T_c}{|\Delta_k|})
\]

(8)

where we can think of evaluating the right-hand side to lowest order by replacing \( \Delta_k \) by \( \Delta_{0,k} \). From this equation, the components \( a_m = \int \Delta_{m,k} \Delta_k \) of the gap on the eigenvectors with \( m \neq 0 \) are small because the eigenvalues \( \lambda_m \) are small (this is the weak coupling limit). In addition the subdominant order parameters \( \Delta_m \) will correspond in the general case to critical temperatures much smaller than \( T_c \), which implies \( \lambda_m \ll \lambda_0 \) for \( m \neq 0 \) (a specific example of this can be found in the recent work of Palumbo et al.\[4\] where, within a given channel, \( \lambda_1 \approx 0.1 \lambda_0 \) is found for all the channels). This implies that \( a_m \) is reduced by a factor \( \lambda_m / \lambda_0 \) with respect to a naive evaluation (in the case of a separable potential one has exactly \( \lambda_m = 0 \) and all the \( a_m \)'s are exactly zero). The opposite case of \( \lambda_m \approx \lambda_0 \) corresponds to an accidental situation and is most likely to be found for \( \Delta_{m,k} \) and \( \Delta_{0,k} \) belonging to different irreducible representations. This should give a smeared second transition below \( T_c \) which has not been seen up to now in high \( T_c \) superconductors (except for very recent experiments\[14\] on the penetration depth in YBCO which seems to indicate the need of a multiband description; we will come back to this below). Next we see that in the right-hand side of Eq.(8) the logarithm will have a rather small absolute value in most of the range of integration, and it will change sign. Moreover in the cases we are interested in, \( \Delta_k \) also changes sign, and so does \( \Delta_{m,k} \) in the general case. Therefore we have plenty of reasons for destructive interference which will make the right-hand side small in general. The conclusion is that taking \( \Delta_k \) proportional to \( \Delta_{0,k} \) is a quite good approximation. Moreover replacing in Eq.(4) \( \Delta_{0,k} \) by \( \Delta_k \) should not change much the result when their shape is similar. Hence this should give a very good evaluation for the maximum \( \Delta_M \) of the gap, which is not sensitive anyway to the detailed structure of \( \Delta_k \) as we have seen.

In order to calculate \( \Delta_M \) from Eq.(6) we only need to know the weight function \( N(\delta) \) for the reduced gap values \( \delta \). We introduce the integrated weight \( x \) by \( dx = N(\delta) \, d\delta \). In Eq.(6) we can assume by a change of variables that \( 0 \leq x \leq 1 \). This gives:

\[
\ln(\frac{\Delta_M}{1.76 T_c}) = -\int_0^1 dx \frac{\delta^2(x) \ln(\delta(x))}{\int_0^1 dx \delta^2(x)}
\]

(9)

where \( \delta(x) \) is a growing function of \( x \) with \( 0 \leq \delta \leq 1 \). In the case of two dimensional superconductors, which are a very good approximation for all the known high \( T_c \) superconductors, \( x \) is merely the curvilinear abscissa along the Fermi line weighted by the local density of states. We can check Eq.(9) in a variety of cases. For a constant gap, \( \delta = 1 \) and we have naturally the BCS result \( \Delta_M / T_c = 1.76 \) (with \( 1.76 = \pi / e^{\gamma} \) where \( \gamma \) is the Euler constant). For the \( A \) phase of superfluid \( ^3He \), \( \Delta_M / T_c = 1.76 \, \delta^{\beta/6} / 2 \approx 2.029 \) (here \( \delta(x) = |x(2-x)|^{1/2} \)). For \( d \)-wave, \( \delta(x) = \sin(\pi x/2) \) after change of variable and \( \Delta_M / T_c = 1.76 \, 2e^{-1/2} \approx 2.139 \). For the simple model introduced by Xu et al.\[14\], with a variable slope at the node, \( \delta(x) = x/\alpha \) for \( 0 \leq x \leq \alpha \) and \( \delta(x) = 1 \) for \( \alpha \leq x \leq 1 \). We find \( \Delta_M / T_c = 1.76 \exp(\alpha / (9 - 6\alpha)) \) which agrees with their result \( \Delta_M / T_c = 1.994 \) for \( \mu = 4 / (\pi \alpha) = 2 \); for \( \mu = 2.7 \) we find \( \Delta_M / T_c = 1.904 \) in agreement with them; finally for the upper limit \( \alpha = 1 \) this gives the highest possible value for this model \( \Delta_M / T_c = 2.462 \). We note that this ratio is not so large, even for this model which does not look very physical in this limit (at least for a single band). It is then interesting to generalize this model into \( \delta(x) = x^n \) which gives a very wide gap opening for large \( n \). This leads to \( \Delta_M / T_c = 1.76 \exp(n / (2n + 1)) \), which gives 2.631 for \( n = 2 \) and saturates at \( \Delta_M / T_c = 1.76 \exp(1 / 2) \approx 2.908 \) for \( n \to \infty \). These few examples show that it is quite hard to increase \( \Delta_M / T_c \) even by going to pretty unphysical models.

In order to explore more fully this question it is convenient to use \( y = \delta^2(x) \) as a new variable and \( X(y) = 1 - x \) as a new function. The graph \( X(y) \) is trivially related to the graph \( \delta^2(x) \) and it decreases from \( (y = 0, X = 1) \) to \( (y = 0, X = 1) \) (even when \( \delta(x) \) is discontinuous, which occurs for example when the gap is constant). We can then rewrite Eq.(9) into:

\[
\frac{\Delta_M}{1.76 T_c} = -\int_0^1 dy \frac{X^2(y) \ln(X(y))}{\int_0^1 dy X^2(y)}
\]

(10)
This expression Eq.(10) makes it obvious that, for fixed area \( \int dy X(y) = \int dx \delta^2(x) \), the maximum \( \Delta_M / T_c \) is obtained by squeezing as much as possible the weight of \( X(y) \) at low \( y \) in order to take advantage of the divergence of \( \ln(y) \) for \( y \to 0 \). At the same time one sees that this is not very efficient in order to obtain high \( \Delta_M / T_c \) since the divergence of \( \ln(y) \) is weak. This squeezing is optimally reached by taking a constant gap almost everywhere : 
\[
\delta(x) = \delta_m \text{ for } 0 < x < 1, \text{ with } \delta(0) = 0 \text{ and } \delta(1) = 1, \text{ equivalent to } X(y) = 1 \text{ for } 0 \leq y < \delta_m^2 \text{ and } X(y) = 0 \text{ for } \delta_m^2 < x \leq 1.
\]
This conclusion can also be found from Eq.(6) by a convexity argument , as done by Anderson and Morel [7]. The corresponding maximum value of the gap is \( \Delta_M / T_c = 1.76 / \delta_m \). This shows that, by letting \( \delta_m \to 0 \), we can obtain in principle \( \Delta_M / T_c \) as high as we like. However this optimal model is quite unphysical since the gap maximum has zero weight, and is therefore irrelevant ( it will not be seen in any experiment ). The real physical gap maximum in this model is \( \Delta_M \delta_m \), not \( \Delta_M \), and we find the BCS value for the gap to \( T_c \) ratio, which is expected since the gap is constant.

We can consider a slightly more reasonable model by giving a weight \( 1 - x_0 \) to the gap maximum. In order to obtain the optimal \( \Delta_M / T_c \) we take the rest of the gap at a constant value \( \delta_m \). Explicitly this leads us to the simple model \( \delta(x) = \delta_m \) for \( 0 < x < x_0 \), and \( \delta(x) = 1 \) for \( x_0 < x \leq 1 \). We could try to go continuously from \( \delta_m \) to \( 1 \), in order to obtain a better \( \Delta_M / T_c \). However it is quite clear that, if we want that the maximum gets a significant weight, the improvement will be very small. The above model gives \( \ln r = - x_0 \delta_m^2 \ln(\delta_m) / (x_0 \delta_m^2 + 1 - x_0) \) with \( r = \Delta_M / 1.76 T_c \). We can again in principle obtain \( \delta_m \) as high as we like by letting \( \delta_m \to 0 \) and \( 1 - x_0 \) go to zero. More generally, independently of a specific model, it is obvious from Eq.(10) that, in order to obtain a large \( \Delta_M / T_c \), we need qualitatively a gap maximum with a small weight and small gap with a large weight. However the contours of constant \( r \) of our optimal model are plotted in Fig.1 in the \( (\delta_m, x_0) \) plane and they make quite clear quantitatively the difficulty which is met when one tries to obtain at the same time a large \( \Delta_M / T_c \) and a sizeable weight \( 1 - x_0 \) for the maximum. For fixed \( r \), the maximum possible weight \( (1 - x_0)_{max} \) is given by \( (1 - x_0)_{max} = 1 / (1 + 2er^2\ln(r)) \) with a corresponding value \( 1 / (r\sqrt{e}) \) for \( \delta_m \). While \( 2 \Delta_M / T_c = 5 \) gives a maximum weight 0.2 with \( \delta_m = 0.42 \), the average experimental value \( 2 \Delta_M / T_c = 7 \) leads to a maximum weight of 0.06 . This is not compatible with the experimental data, such as tunneling or Raman scattering which give a gap maximum with a fairly sizeable weight. Also the rest of the gap would be at 0.3 the gap maximum value which is rather low. We note that, although the above model is already not compatible with experiments, it does not even have nodes in the gap. The following model for the gap distribution \( \delta(x) = (x / x_0) \delta_m \) for \( 0 < x < x_0 \), and \( \delta(x) = 1 \) for \( x_0 < x \leq 1 \), is similar to the preceding one, but it is somewhat more realistic since it allows for nodes in the gap. It leads to \( \ln r = x_0 \delta_m^2 (1/3 - \ln(\delta_m)) / (x_0 \delta_m^2 + 3(1 - x_0)) \). As expected it gives somewhat worst results for \( \Delta_M / T_c \).

Let us summarize the situation. We expect a physically reasonable one-band model to produce a fairly regular gap function, similar for example to the standard d-wave order parameter. All the various specific examples of this kind that we have considered above gave \( 2 \Delta_M / T_c \) scattered between 4 and 4.5 . Values near 5 correspond already to rather unphysical situations. Hence weak coupling is far off the experimental result. Since \( \Delta_M / T_c \) depends on broad features of the gap distribution and not on details, as we have discussed, this result is generic not accidental. The failure to find higher values than, say, 5 within weak coupling theory is not due to a lack of inspiration in finding the proper order parameter. It is a systematic deep limitation of weak coupling theory itself.

From Eq.(10) the only way to increase \( \Delta_M / T_c \) within weak coupling is to lower the average value of the gap, while keeping at the same time a sizeable weight near the gap maximum to obtain agreement with tunneling and Raman data. This goes in the direction of a somewhat discontinuous order parameter which does not look like a simple one-band model, although one might argue that the spin fluctuation model with strongly peaked interactions at wavevector \( (\pm \pi, \pm \pi) \) could produce such a result. We believe that a rather natural realization of such a strange gap structure is merely a two-band model (which is included in our study ), with one band corresponding to the maximum gap value and the other one to the small value. Nevertheless we have seen that even our optimized model cannot reproduce at the same time the fairly large \( \Delta_M / T_c \) observed experimentally together with a reasonable weight for this gap maximum. We come to the conclusion that simple weak coupling theory is not compatible with experiment.

What are the ways out ? The most obvious one is to question experiments. As we have seen, this is not an easy way since independent experiments are in reasonable agreement. However one may wonder if tunneling or Raman experiments do not miss a part of the Fermi surface. In this case the weight of the gap maximum might be less than it seems, releasing a part of the theoretical constraint. The most natural situation where this would occur is a two-band...
model, where the band with the gap maximum would be seen but not so much the other one. On the theoretical side one may object that the weak coupling equation Eq.(1) that we have used does not include the possibility of a density of states varying strongly perpendicularly to the Fermi surface, as could be produced by nearby Van Hove quasi-singularities. However we know [18] that in the isotropic case we have quite generally \(2 \Delta_M / T_c \leq 4\) even for such a varying density of states, so that the prospects in this direction are not good. Therefore, if we stop short of rejecting BCS theory altogether, the most likely explanation for the high experimental value of \(\Delta_M / T_c\) is that weak coupling theory does not apply because strong coupling effects are important. Indeed their existence is supported independently by various experiments and they are known to increase in a quite sizeable way this ratio. However strong coupling effects with isotropic pairing would have a hard time explaining \(2 \Delta_M / T_c = 7\), since this would require [19] a quite high coupling constant (at least 5). A possibility is to have strong coupling effects in a multiband model. On the other hand self-consistent calculations for simple d-wave pairing within the 2D Hubbard model have given results [20] as high as \(2 \Delta_M / T_c \approx 10\). Hence it seems that the large experimental \(\Delta_M / T_c\) can be accounted for by strong coupling together with anisotropy, whereas it is incompatible with weak coupling theory. This comes as a strong support in favor of a spin fluctuation mechanism in the debate about the nature of the repulsive pairing interaction that we considered in the introduction.

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FIG. 1. Fig. 1 Contours of constant \(r = \Delta_M / 1.76 T_c\) in the \(\delta_m - x_0\) plane for the model \(\delta(x) = \delta_m\) for \(0 < x < x_0\), and \(\delta(x) = 1\) for \(x_0 < x \leq 1\). The values of \(r\) are 1.1, 1.2, 1.3, 1.5, 1.7, 2, and 2.5 as indicated near the curves.
