Gap Anisotropy and Critical Temperature of Anisotropic Superconductors

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We study the gap anisotropy and critical temperature of superconductors within Eliashberg theory. We consider a general anisotropy and spectral shape. In the attractive strong-coupling limit, we find a qualitatively new universal result: The gap becomes isotropic. This sets severe constraints on standard strong-coupling theories of high-T_c superconductors. In the weak-coupling limit, the gap is sensitive to anisotropy. We obtain exact results for the critical temperature both in the strong- and the weak-coupling limits. We propose a simple natural interpolation in the intermediate regime.

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In the classical theory of superconductivity, it is a fairly standard procedure[1] to assume that one deals with an isotropic superconductor. The usual justification is that one works in the dirty limit, where the scattering of the electrons by impurities is fast enough and leads to an effective averaging of the electronic properties over the Fermi surface. Most standard superconducting materials are indeed dirty enough to be in this limit. This situation is a convenient one because it is difficult to know quantitatively the anisotropic properties of a compound and how they affect specifically the superconductive properties. Nevertheless, starting with Markowitz and Kadanoff[2] and Clem,[3] and continuing with Carbotte and collaborators,[4] properties of anisotropic superconductors have been explored, mostly within the separable model and oriented toward weakly coupled superconductors.

In the new high-T_c compounds, anisotropy is expected to be important. Indeed, the layered Cu-based compounds have very anisotropic electronic properties.[5] Here we consider only semiclassical or classical theories of these superconductors, which we define as the theories where there are Cooper pairs of degenerate fermions due to an attractive interaction mediated by the exchange of any kind of bosons, these bosons being phonons for classical theories and not phonons for semiclassical ones. Provided that these bosons have an energy much smaller than the Fermi energy, these superconductors can be described within the framework of Eliashberg theory.[1] For high-T_c compounds it is reasonable to expect a fairly anisotropic attractive interaction. Many semiclassical theories do indeed predict very anisotropic interactions as does the spin-bag model,[6] for example. The electron-phonon interaction is also likely to be anisotropic, due, for example, to the expected screening anisotropy. However, in contrast to standard superconductors, it is unlikely that high-T_c compounds are in the dirty limit. Instead, they are rather clean,[7] basically because the high T_c makes the coherence length shorter than the mean free path. Therefore, effective averaging should not occur and the effect of anisotropy must be considered in these compounds.

In this paper we consider the gap anisotropy and the critical temperature for anisotropic superconductors as obtained from Eliashberg theory. We consider a general anisotropy and spectral shape. We solve this problem exactly in general terms both in the strongly attractive regime and in the weak-coupling limit. For the intermediate coupling region, we propose an interpolation formula. This is the generalization of a similar formula[8] for isotropic superconductors which has proved to be very successful both qualitatively and quantitatively. This set of results provides a satisfactory answer for the calculation of the critical temperature of anisotropic superconductors.

However, our most striking and interesting result is about the anisotropy of the gap. We find that, whatever the spectral or the angular dependence of the interaction, the gap becomes isotropic in the strong-attractive-coupling limit. This result turns out to be true not only at T_c, but also at any temperature below T_c. Physically this is related to the well-known fact that, in this regime, quasiparticle renormalization by the boson field tends to decrease T_c. In the strong-coupling limit, this competes with the natural increase of T_c when the strength of the attractive interaction is increased. For anisotropic superconductors, quasiparticle renormalization tends to dominate and its effect can only be curbed by taking an isotropic gap, that is, moving back to the isotropic situation where these two opposite effects essentially cancel. Therefore, we come to the universal conclusion that, as the attractive coupling strength increases, an anisotropic superconductor tends to self-average and its gap tends to become isotropic.

We believe that this result is of interest for high-T_c superconductors. Indeed, a classical interpretation requires a fairly strong attractive coupling[9] (say an average coupling constant of the order of magnitude of 3). Our result shows that this implies necessarily a rather weak gap anisotropy. There is, however, an obvious restriction to our result. If two different types of electrons are not coupled, there is clearly no reason for them to have the same gap. If these two types of electrons are only weakly coupled, the corresponding gaps can be rather different. This might apply, for example, to $YBa_2Cu_3O_7$ where the plane and chain electrons are possibly weakly coupled. But strong coupling within each type of electron implies a weakly anisotropic gap for each. Therefore, our result provides a stringent test of consistency for classical strong-coupling theories of high-T_c superconductors, since gap anisotropy might hopefully be measured, for example, by angle-resolved high-resolution photoemission[10] or temperature dependence of penetration depth in monocrystals.[11] A strong anisotropy would be very difficult to accommodate by these theories, and would clearly favor semiclassical theories. Conversely, a weakly anisotropic gap would eliminate many semiclassical theories and be fully consistent with classical ones. Therefore, gap anisotropy turns out to be a test on the mechanism of high-T_c superconductivity. Interestingly it is a qualitative test, in contrast with the comparison of experiment for standard ratios [$\Delta(0)/T_c$, for example] with their BCS weak-coupling values where uncertainty in experiment and interpretation always leaves some doubt.

Let us finally mention a possible indirect hint of weak gap anisotropy. Most high-T_c compounds have shown a fairly stable critical temperature, rather independent of the care in preparation, provided naturally that one ends up with a well-defined compound (since T_c is known to be very sensitive to the oxygen content). Since early methods of preparation are by necessity very rough, one would expect the impurity and defect content to have varied widely. For an anisotropic gap, the insensitivity of T_c to these conditions can only be understood by assuming either the dirty or the clean limit. We have seen that the short coherence length makes the dirty limit unlikely. On the other hand, it is hard to believe that, despite this short coherence length, all the materials including the probably very dirty early ones have been in the clean limit. A more likely explanation is that these compounds have a fairly isotropic gap which makes their T_c insensitive to impurity and defect content anyway.

Let us now give our results and sketch their derivation.[12] In Eliashberg theory[1] the interaction of an anisotropic superconductor is characterized by the generalization $\alpha^2F(\mathbf{k},\mathbf{k}',\omega)$ of the standard Eliashberg function, which gives physically the coupling strength for scattering a fermion from $\mathbf{k}$ to $\mathbf{k}'$ on the Fermi surface by emission of a boson of energy ω. The superconducting order is characterized by an anisotropic gap function $\Delta_n(\mathbf{k})$ defined for imaginary Matsubara frequencies $\omega_n=(2n+1)\pi T$. In this imaginary-frequency formalism, the interaction comes in through the spectral function:

$$\lambda_p(\mathbf{k},\mathbf{k}')=\int d\omega\, 2\omega\alpha^2F(\mathbf{k},\mathbf{k}',\omega)/(\omega^2+\omega_p^2)\,, \qquad (1)$$

where $\omega_p=2\pi pT$ is the boson Matsubara frequency. The gap function satisfies the following Eliashberg equations:

$$\begin{aligned}\Delta_n(\mathbf{k})Z_n(\mathbf{k})&=\pi T\sum_m\int d_2k'\lambda_{n-m}(\mathbf{k},\mathbf{k}')\Delta_m(\mathbf{k}')\\&\qquad\times[\omega_m^2+\Delta_m^2(\mathbf{k}')]^{-1/2}\,,\\ \omega_n[Z_n(\mathbf{k})-1]&=\pi T\sum_m\int d_2k'\lambda_{n-m}(\mathbf{k},\mathbf{k}')\omega_m\\&\qquad\times[\omega_m^2+\Delta_m^2(\mathbf{k}')]^{-1/2}\,.\end{aligned} \qquad (2)$$

Here the integration d_2k' over the Fermi surface is weighted by the fractional local density of states $[(2\pi)^3N_0v_{k'}]^{-1}$ and is normalized. $Z_n(\mathbf{k})$ is the normal quasiparticle renormalization factor. At T_c, $\Delta_n(\mathbf{k})$ goes to zero and Eqs. (2) are linearized into

$$f_n(\mathbf{k})\bar{\Delta}_n(\mathbf{k})=\sum_m\int d_2k'\lambda_{n-m}(\mathbf{k},\mathbf{k}')\bar{\Delta}_m(\mathbf{k}')\,, \qquad (3a)$$

$$f_n(\mathbf{k})=2n+1+\int d_2k'\left[\lambda_0(\mathbf{k},\mathbf{k}')+2\sum_1^n\lambda_p(\mathbf{k},\mathbf{k}')\right], \qquad (3b)$$

where $\bar{\Delta}_n(\mathbf{k})=\Delta_n(\mathbf{k})/|\omega_n|$ and the expression for $f_n(\mathbf{k})=|\omega_n|Z_n(\mathbf{k})/\pi T$, an even function of ω_n, is given for $\omega_n>0$. We have omitted the Coulomb pseudopotential μ^* but we will comment in time on its effect.

We consider first the strong-coupling limit where the (attractive) coupling strength and T_c grow indefinitely (naturally such a situation is unphysical and considered only for mathematical purposes; reasonably large λ are considered below). In this regime one can see from the argument below that T_c grows at most as $\lambda^{1/2}$, as for the isotropic case (λ is an average coupling strength). Then, for $T_c\sim\lambda^{1/2}$, λ_p has for $p\neq 0$ a finite limit for large λ while λ_0 grows indefinitely. Therefore the term $n=m$ dominates in Eq. (3a) and $f_n(\mathbf{k})\approx\lambda_0(\mathbf{k})$. We have defined $\lambda_0(\mathbf{k})=\int d_2k'\lambda_0(\mathbf{k},\mathbf{k}')$ (we can forget the $2n+1$ term in f_n since actually only the lowest values of $|\omega_n|$ matter in the strong-coupling limit). Therefore, we are left with

$$\bar{\Delta}_n(\mathbf{k})\int d_2k'\lambda_0(\mathbf{k},\mathbf{k}')-\int d_2k'\lambda_0(\mathbf{k},\mathbf{k}')\bar{\Delta}_n(\mathbf{k}')=0\,. \qquad (4)$$

The first term comes from quasiparticle renormalization and the second one from the pairing interaction. The operator acting on $\bar{\Delta}_n(\mathbf{k})$ in Eq. (4) is diagonally dominant and its eigenvalues are non-negative: The operator from the first term dominates over the second one. This is easily seen by summing Eq. (4) over $\mathbf{k}$ after multiplying by $\bar{\Delta}_n(\mathbf{k})$. One obtains

$$\int d_2k\, d_2k'\lambda_0(\mathbf{k},\mathbf{k}')[\bar{\Delta}_n(\mathbf{k})-\bar{\Delta}_n(\mathbf{k}')]^2=0\,, \qquad (5)$$

where we have used $\lambda_0(\mathbf{k},\mathbf{k}')=\lambda_0(\mathbf{k}',\mathbf{k})$ from microreversibility. Since λ_0 is positive, the left-hand side is always positive. Equations (4) and (5) can only be satisfied by taking $\bar{\Delta}_n(\mathbf{k})=\bar{\Delta}_n(\mathbf{k}')$ for any $\mathbf{k}$ and $\mathbf{k}'$. Therefore, the gap function (and the gap itself by analytic continuation) is forced to be isotropic in this strong-coupling limit. The only possible exception corresponds to a degenerate situation where two pieces S_1 and S_2 of the Fermi surface are not coupled so that $\lambda_0(\mathbf{k},\mathbf{k}')=0$ for all $\mathbf{k}\in S_1$, $\mathbf{k}'\in S_2$, as would be the case for two physically separated superconductors. In practice this means that, if we keep the coupling between S_1 and S_2 weak, whereas we let the coupling inside S_1 and S_2 grow indefinitely, the gaps of S_1 and S_2 will not become equal.

Our result is readily generalized for temperature below T_c, once it is realized that the $n=m$ terms will again dominate in Eq. (2) when the coupling strength grows indefinitely. Then Eq. (2) reduces to

$$\Delta_n(\mathbf{k})\int d_2k'\frac{\lambda_0(\mathbf{k},\mathbf{k}')}{[\omega_n^2+\Delta_n^2(\mathbf{k}')]^{1/2}} - \int d_2k'\frac{\lambda_0(\mathbf{k},\mathbf{k}')\Delta_n(\mathbf{k}')}{[\omega_n^2+\Delta_n^2(\mathbf{k}')]^{1/2}}=0\,. \qquad (6)$$

Multiplying by $\Delta_n(\mathbf{k})[\omega_n^2+\Delta_n^2(\mathbf{k})]^{-1/2}$ and summing over $\mathbf{k}$, we end up with an equation similar to Eq. (5) which shows again that $\Delta_n(\mathbf{k})=\Delta_n(\mathbf{k}')$. However, an apparent problem is that the number of relevant $n\neq m$ terms increases when the temperature is lowered and they can be neglected only by going to even higher coupling. But, actually, one can see that the $\omega_m\approx\omega_n$ terms have the same effect as the $\omega_m=\omega_n$ term in forcing $\Delta_n(\mathbf{k})=\Delta_n(\mathbf{k}')$. In fact, we can obtain our result at $T=0$ by an argument very similar to the one given above. Therefore, the gap is isotropic at any temperature.

Once we know that the gap is isotropic, the critical temperature is easily obtained. Equation (3) is a Hermitian eigenvalue problem.[1] We treat all the terms of Eq. (3) not included in Eq. (4) as a perturbation. The zeroth-order terms [Eq. (4)] give an eigenspace corresponding to isotropic $\bar{\Delta}_n(\mathbf{k})$, but the ω_n dependence is not given at this order. It is obtained by solving the eigenvalue problem [Eq. (3)] in this isotropic eigenspace. But this problem is the same as finding T_c in the strong-coupling limit for an isotropic superconductor. Therefore, T_c is given in this regime by the standard result[1] $T_c=0.182\langle\lambda\omega^2\rangle^{1/2}$, where $\langle\lambda\omega^2\rangle$ is for

$$\int d\omega\, d_2k\, d_2k' 2\omega\alpha^2F(\mathbf{k},\mathbf{k}',\omega)\,.$$

In other words, we have merely to use an average Eliashberg function corresponding to the isotropic gap. We note also that, if we include the repulsive Coulomb pseudopotential μ^*, this is necessarily a small term in the strong-attractive-coupling limit: We should include it in the first-order terms, not in zeroth order. Therefore, our conclusions are unchanged: The gap is isotropic, but the result for T_c is affected by μ^* in the usual way.

Finally, one must naturally wonder what our result means for an actual strong-coupling superconductor with an average coupling constant λ of, say, order 3. From perturbation theory one expects the anisotropy to be of order $1/\lambda$. To see this explicitly, it is agreeable to treat the strong-coupling situation in a slightly simplified way. It is known that,[13] in this regime, the terms $|\omega_n|=\pi T$ of $\Delta_n(\mathbf{k})$ (which are equal) are the dominant ones, as can be seen from Eq. (3). The other ones must be retained quantitatively for exact results, but are not important qualitatively. Keeping only these two terms $\bar{\Delta}_0(\mathbf{k})=\bar{\Delta}_{-1}(\mathbf{k})\equiv\bar{\Delta}(\mathbf{k})$, multiplying Eq. (3a) by $\bar{\Delta}(\mathbf{k})$ (assumed to be normalized), and summing over $\mathbf{k}$, one obtains

$$1+\tfrac{1}{2}\int\lambda_0(\mathbf{k},\mathbf{k}')[\bar{\Delta}(\mathbf{k})-\bar{\Delta}(\mathbf{k}')]^2 = \int\lambda_1(\mathbf{k},\mathbf{k}')\bar{\Delta}(\mathbf{k})\bar{\Delta}(\mathbf{k}')\,, \qquad (7)$$

where the integral is over all the variables. As a rough approximation, valid only for very large T, the right-hand side may be written as

$$[2/(2\pi T)^2]\int\omega\alpha^2F(\mathbf{k},\mathbf{k}',\omega)\bar{\Delta}(\mathbf{k})\bar{\Delta}(\mathbf{k}')\,.$$

T_c is the highest temperature for which Eq. (7) is satisfied. Therefore, we want to minimize the left-hand side which clearly leads to our result $\bar{\Delta}(\mathbf{k})\approx\bar{\Delta}(\mathbf{k}')$. We set $\bar{\Delta}(\mathbf{k})=1+\varepsilon d(\mathbf{k})$, where ε is expected to be small since λ_0 is large; $d(\mathbf{k})$ is of order unity and satisfies $\int d(\mathbf{k})=0$. Inserting into Eq. (7) and maximizing T with respect to ε, one obtains

$$\varepsilon=2\int\lambda_1(\mathbf{k},\mathbf{k}')d(\mathbf{k}')\Big/\int\lambda_0(\mathbf{k},\mathbf{k}')[d(\mathbf{k})-d(\mathbf{k}')]^2$$

to lowest order, where we can use in λ_1 the zeroth-order value of T_c obtained above. Since λ_1 is of order 1, we see that ε and the gap anisotropy is indeed of order $1/\lambda$ [$d(\mathbf{k})$ could be obtained directly from Eq. (3)]. Therefore, for $\lambda\sim3$, the gap anisotropy is indeed reasonably small.

Let us now turn to the weak-coupling limit. In this regime we make no assumption on the sign of the effective interaction. We solve the problem by iterating Eq. (3) in a way similar to the isotropic case.[8,14] The calculation is naturally complicated by the additional $\mathbf{k}$ dependence, but fortunately the singular behavior of the weak-coupling limit leads to a $\mathbf{k}$ dependence for the gap function $\Delta_n(\mathbf{k})$ independent of the frequency dependence. We find[12] that the $\mathbf{k}$ dependence of $\Delta_n(\mathbf{k})$ is given by the eigenvector $\delta(\mathbf{k})$ of $M(\mathbf{k},\mathbf{k}')=\lambda_0(\mathbf{k},\mathbf{k}')/[1+\lambda_0(\mathbf{k})]$ with largest eigenvalue β. Then the frequency-dependent part is handled in a way similar to the isotropic case. We obtain for T_c a result essentially identical formally to the isotropic case:[8,14]

$$T_c=(2/\pi)e^{C-1/2}\omega_{\log}\exp(-1/\beta-R)\,, \qquad (8)$$

where C is the Euler constant. This result is exact in the weak-coupling limit in the sense that the difference for $\ln T_c$ between the exact value and Eq. (8) vanishes when the coupling goes to zero. In Eq. (8), β plays the same role as the term $\lambda/(1+\lambda)$ in the isotropic situation and taking β as the largest eigenvalue amounts to making T_c as large as possible by taking full advantage of the anisotropy of the superconductor. In order to give the expressions for $\omega_{\log}$ and R in Eq. (8), we need only $\delta(\mathbf{k})$ and β to lowest order, that is the (normalized) eigenvector $\delta_0(\mathbf{k})$ of $\lambda_0(\mathbf{k},\mathbf{k}')$ with largest eigenvalue β_0; to first order, β itself is given by $(\beta-\beta_0)/\beta_0=\int d_2k\,\lambda_0(\mathbf{k})\delta_0^2(\mathbf{k})$. Then $\omega_{\log}$ is given by

$$\ln\omega_{\log}=(2/\beta_0)\int\delta_0(\mathbf{k})\delta_0(\mathbf{k}')\alpha^2F(\mathbf{k},\mathbf{k}',\omega)\ln\omega/\omega\,. \tag{9}$$

Finally, R, which is physically a measure of the intrinsic width of the spectrum, is

$$R=\int g(\mathbf{k},\omega_1)g(\mathbf{k},\omega_2)F(\ln(\omega_2/\omega_1))\,, \tag{10}$$

where $F(x)=\frac{1}{2}(x\coth x-1)$ and

$$g(\mathbf{k},\omega)=(1/\beta_0)\int d_2k'(2/\omega)\alpha^2F(\mathbf{k},\mathbf{k}',\omega)\delta_0(\mathbf{k}')$$

is a $\mathbf{k}$-dependent normalized spectral density. The dominant term for $\ln T_c$ is $-1/\beta_0$. When considered for a separable potential or a weakly anisotropic potential, this dominant term leads to previous results in the literature.[1-3] In the case of nonzero Coulomb pseudopotential $\mu^*(\mathbf{k},\mathbf{k}')$ and for this dominant term, β_0 becomes the largest (positive) eigenvalue of $\lambda_0(\mathbf{k},\mathbf{k}')-\mu^*(\mathbf{k},\mathbf{k}')$ and $\delta_0(\mathbf{k})$ is the corresponding eigenvector. The existence of a positive eigenvalue has already been studied[4] for an isotropic $\mu^*(\mathbf{k},\mathbf{k}')$ to investigate the existence of the superconducting state. In conclusion, we note that the weak-coupling regime is the one where strong gap anisotropy may be expected, since it may arise naturally in order to optimize T_c, mostly when there is a sizable repulsive contribution in the interaction. Semiclassical theories are likely to be in this regime. In particular, this may lead to nodes in the gap and unconventional pairing. Our weak-coupling result is of interest for all these theories.

We consider finally a very natural interpolation which allows us to bridge empirically between the weak- and the strong-coupling regimes. Such an approach has been quite successful for isotropic superconductors.[8] First, the fact that the $\mathbf{k}$ dependence of $\Delta_n(\mathbf{k})$ corresponds to the eigenvector of $M(\mathbf{k},\mathbf{k}')$ with largest eigenvalue applies in both regimes. This is indeed what we have found in weak coupling, and in strong coupling the largest eigenvalue of $M(\mathbf{k},\mathbf{k}')\approx\lambda_0(\mathbf{k},\mathbf{k}')/\lambda_0(\mathbf{k})$ is 1 for an isotropic $\delta(\mathbf{k})$, as easily seen. Then it is natural as an interpolation to take for any coupling constant the $\mathbf{k}$ dependence of the gap function as the eigenvector $\delta(\mathbf{k})$ of $M(\mathbf{k},\mathbf{k}')$ with largest eigenvalue β. Moreover, we have found that, in both extreme regimes, T_c is controlled by a single characteristic frequency. In the intermediate regime we can interpolate as in the isotropic case[8] between these two frequencies, which leads to

$$\int\delta(\mathbf{k})\delta(\mathbf{k}')\ln\left[1+\left(\frac{\omega}{aT}\right)^2\right]\frac{\alpha^2F(\mathbf{k},\mathbf{k}',\omega)}{\omega}=\frac{1+\bar{\lambda}}{1+\lambda}\,, \tag{11}$$

with $a=3.9$. We have set $\lambda=\int d_2k'\delta(\mathbf{k})\delta(\mathbf{k}')\lambda_0(\mathbf{k},\mathbf{k}')$ and $\bar{\lambda}=\int d_2k\,\delta^2(\mathbf{k})\lambda_0(\mathbf{k})$ [note that $\beta=\lambda/(1+\bar{\lambda})$]. The left-hand side of Eq. (11) is the natural generalization of the isotropic formula.[8] The right-hand side takes into account that the effective coupling strength for attraction and renormalization are different. It leads to the correct result on the weak-coupling side and goes to 1 in the strong-coupling limit. Our formula is not completely satisfactory on the weak-coupling side, since it misses the shape-dependent term R, as in the isotropic case. Nevertheless, from our experience with the isotropic case we believe that our formula should give T_c with a very reasonable accuracy.

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