Image of the Energy Gap Anisotropy in the Vibrational Spectrum of a High Temperature Superconductor

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We present a new method of determining the anisotropy of the gap function in layered high-T_c superconductors. Careful inelastic neutron scattering measurements at low temperature of the phonon dispersion curves in the (100) direction in La_{1.85}Sr_{1.15}CuO_4 would determine whether the gap is predominately s-wave or d-wave. We also propose an experiment to determine the gap at each point on a quasi-two-dimensional Fermi surface.

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The anisotropy of the energy gap at the Fermi surface contains clues to the pairing mechanism operating in a superconductor. An s-wave gap\(^1\) successfully describes phonon-mediated pairing, which causes superconductivity in ordinary metals. A p-wave gap\(^2\) describes spin-flip-mediated pairing in helium-3. Current work suggests that the pairing in heavy fermion materials is mediated by anti-ferromagnetic fluctuations and is predominately d-wave\(^3\). Theoretical work on high-T\(_c\) materials has produced theories too diverse and numerous to list, even as classes, but all must address the form of the gap function. Therefore we expect that accurate measurements of the gap would provide a strong test which any theory of high-T\(_c\) materials must pass.

The experiments available to look for gap anisotropy provide limited information. These experiments can be divided into two classes: those which provide some average of the gap magnitude over all or a large part of the (normal) Fermi surface, and those which identify nodes in the gap on the Fermi surface.

Reflectivity\(^4\), tunneling current\(^5\), ultrasonic attenuation\(^6\) and thermal conductivity\(^7\) measurements, as well as a variety of other transport measurements, yield some average value of the gap magnitude. In addition to their fundamental limitation – providing an average over the gap – there are other difficulties characteristic of each technique, which are discussed in the above references. Identifying nodes on the Fermi surface is done by measuring the temperature dependence of quantities such as ultrasonic attenuation\(^8\), specific heat\(^9\), magnetic penetration depth\(^10\) or magnetic relaxation rate\(^11\). Unfortunately, the exponential temperature dependence, that would rule out nodes, and the power-law dependence, that would indicate nodes, are difficult to distinguish. And even if the evidence
for a node is convincing, its location is hard to determine because of the previously-mentioned averaging effects.

We present a new method of analyzing measurements of phonon dispersion curves which should determine whether the gap in a high-$T_c$ material is well described by a predominately s-wave or d-wave function. This method should also locate any nodes on the Fermi surface. In addition, recognizing that gaps which are approximately s, p, or d-wave are special cases of an anisotropic gap, we propose an experiment which can determine the gap magnitude everywhere on the Fermi surface. Both of these techniques require accurate measurements of phonon dispersion curves, which can now be made with inelastic neutron scattering\textsuperscript{12}.

The gap at the Fermi surface and the Fermi surface shape completely determine the minimum energy required for a phonon to decay into two Bogoliubov quasiparticles. For phonon wavelengths smaller than the coherence length, the minimum-energy excitation is the creation of both quasiparticles on the Fermi surface. The positions on the Fermi surface where the quasiparticles are created can be found by placing the phonon momentum vector in the Brillouin zone so that its head and tail are on the Fermi surface (see Figure 1). The quasiparticles are created at these points. The Fermi surface shape is described by a function $\vec{k}_F(\theta)$, which is the vector whose tail is at the center of the Brillouin zone, whose head lies on the Fermi surface, and whose angle to a fixed axis is $\theta$. Given the phonon momentum and the function $\vec{k}_F(\theta)$, one can find the angles $\phi$ and $\tilde{\phi}$ where $\vec{q}$'s head and tail lie. Therefore we have the following equation, which should be viewed as determining

\textsuperscript{3}
\( \phi \) and \( \tilde{\phi} \), given \( \vec{q} \) and the function \( \vec{k}_F(\theta) \):

\[
\vec{q} = \vec{k}_F(\phi) - \vec{k}_F(\tilde{\phi}).
\]  

(1)

The placement of the phonon momentum, and thus \( \phi \) and \( \tilde{\phi} \), are usually two-fold degenerate for a two-dimensional Fermi surface such as La\(_{2-x}\)Sr\(_x\)CuO\(_4\)’s. If the Fermi surface and the gap magnitude are inversion symmetric, this degeneracy is trivial and \( \phi \) can be considered defined only from 0 to \( \pi \). La\(_{2-x}\)Sr\(_x\)CuO\(_4\)’s Fermi surface is inversion-symmetric, and an inversion-symmetric gap magnitude conforms to current expectations\(^{13}\). We will discuss situations with non-trivial degeneracies at the end of this Letter.

The minimum, or threshold, energy is the sum of the gap magnitude at the two points \( \vec{k}_F(\phi) \) and \( \vec{k}_F(\tilde{\phi}) \) on the Fermi surface. These two points are uniquely determined by \( \vec{q} \) and the function \( \vec{k}_F(\theta) \), so the threshold energy, denoted \( \tilde{\Delta} \), can be considered as a function of \( \vec{q} \) and a functional of \( \vec{k}_F \). In the remainder of this Letter any dependence on \( \vec{k}_F \) will be considered implicit. This paragraph, therefore, can be summarized by the following equation:

\[
\tilde{\Delta}(\vec{q}) = |\Delta(\phi)| + |\Delta(\tilde{\phi})|
\]

(2)

where \( \Delta(\phi) \) is the gap at the point on the Fermi surface where the head of \( \vec{k}_F(\phi) \) is. As will be discussed later, \( \tilde{\Delta} \) depends on \( \vec{q} \) in markedly different ways if the gap is d-like instead of s-like.

We will now present a way to determine the shape of the surface defined by \( \tilde{\Delta}(\vec{q}) \) in energy-momentum space. Phonons with energies below the surface, which we will call the threshold surface, should in general live longer than those above it. However, a variety of
other influences on the phonon lifetimes blur this distinction. Fortunately, near and just above the threshold surface, the effect on the phonon lifetime due to the newly opened quasiparticle channel becomes strongly amplified. The lifetimes and frequencies of phonons are usually plotted as a function of momentum magnitude, $q$, with the direction $\hat{q}$ fixed. With $\hat{q}$ fixed, $\tilde{\Delta}(q)$ defines a threshold line instead of a surface. Our proposal to determine $\tilde{\Delta}(\vec{q})$ is to observe anomalous behavior in the lifetimes and frequencies of the phonon branches which cross the threshold line.

The transition from below to above the threshold line is sharp. Consider for illustrative purposes a weak-coupling BCS model where other influences on the phonon lifetime are approximated by a constant lifetime $\tau_o$. More realistic models will be discussed at the end of this Letter. We will follow a phonon dispersion curve which crosses the threshold line, beginning with a $q_1$ such that $\hbar\omega(q_1) < \tilde{\Delta}(q_1)$ and concluding with a $q_3$ such that $\hbar\omega(q_3) > \tilde{\Delta}(q_3)$. At the threshold momentum $q_2$, the phonon frequency is on the threshold line: $\hbar\omega(q_2) = \tilde{\Delta}(q_2)$. This model predicts the lifetime is $\tau_o$ for $q_1 < q < q_2$. The lifetime at $q = q_2$ will vanish. At and slightly above the threshold line, the lifetime will be proportional to $(q - q_2)^{1/2}$ and eventually will approach $\tau_o$ if $q_3$ is sufficiently larger than $q_2$.

This anomalous behavior suggests that points on the threshold surface can be identified by measuring the lifetimes of phonons and determining where in $\vec{q}, \omega$ space they drop precipitously. These points satisfy the equation

$$\hbar\omega(\vec{q}) = |\Delta(\phi)| + |\Delta(\tilde{\phi})| = \tilde{\Delta}(\vec{q}).$$  

Equations (1) and (3) will be referred to as the kinematic equations. Each time a phonon dispersion curve crosses the threshold surface, one can determine a point on the surface.
Since there are a finite number of dispersion curves, $\tilde{\Delta}(\vec{q})$ will be measurable at a few points. This does not determine the function $\Delta(\theta)$ completely, but suffices to distinguish predominately s-wave, p-wave, or d-wave superconductivity.

Figure 2 is a plot of the threshold line $\tilde{\Delta}(q)$ in the (100) direction for a modified tight-binding Fermi surface$^{14}$ (shown in Figure 1) with electron occupation 0.85. This is an approximation to the Fermi surface of La$_{1.85}$Sr$_{1.15}$CuO$_4$, which has the highest $T_c$ for La$_{2-x}$Sr$_x$CuO$_4$. Plotted is the threshold line for a d-wave gap

$$\Delta(\theta) = \Delta_o [\cos (k_F(\theta)\cos \theta) - \cos (k_F(\theta)\sin \theta)]$$  \hspace{1cm} (4)$$

and an s-wave gap $\Delta(\theta) = \Delta_o$. We draw the reader’s attention to the node in $\tilde{\Delta}(q)$ near the half-way point to the zone boundary. The only way to have a node in the threshold line is to have that phonon momentum connect two nodes on the Fermi surface (shown as $\vec{q}_n$ on Figure 1). So, this node in the threshold surface is a signature of nodes in the gap function.

The number of (100) phonon branches which cross the threshold in the d-wave case is approximately equal to the number of zone center phonons with energies less than twice the maximum gap. High-$T_c$ superconductors, therefore, are good materials to examine for this signature because of their large gap.

The gap function magnitude can be determined everywhere on the Fermi surface by performing a different experiment. For a particular phonon branch, the kinematic equations have solutions which form curves in $\vec{q}, \omega$ space. Assume that, given all these curves, at least one solution to the kinematic equations exists for each value of $\phi$. It requires
quite a pathological case for this not to be true. For each $\phi$ pick one solution and identify it with $\phi$. Knowing a solution to the kinematic equations means one knows the values of the quantities $\omega(\vec{q})$ and $\tilde{\phi}$. So these quantities can now be considered functions of $\phi$. Define the Fourier coefficients of a function of $\phi$ as follows: $f(\phi) = \sum_n f_1\cos(n\phi) + f_2\sin(n\phi)$. Equation (3), the energy equation, becomes the following set of coupled linear equations for the Fourier coefficients $|\Delta|_{in}$ of the gap magnitude:

$$\hbar \omega_{in} = |\Delta|_{in} + \sum_{jm} c_{injm} |\Delta|_{jm}$$

(5)

where

$$c_{1n2m} = \frac{1}{\pi} \int_0^{\pi} d\phi \sin(m\phi) \cos(n\tilde{\phi}(\phi))$$

(6)

and the other $c_{injm}$ involve the other three combinations of trigonometric functions. The inversion symmetry of the gap magnitude forces $|\Delta|_{in} = 0$ for $n$ odd. Matrix inversion of Equation (5) determines the $|\Delta|_{in}$, and thus the gap magnitude everywhere on the Fermi surface.

For a two-dimensional Fermi surface that is not inversion symmetric, or that is not convex, there are sometimes two or more non-trivial solutions to Equation (1) for $\vec{q}$. The kinematic equations no longer always uniquely determine $\phi$ and $\tilde{\phi}$ in terms of $\vec{q}$, therefore, the threshold energy $\tilde{\Delta}(\vec{q})$ becomes the minimum of $|\Delta(\phi)| + |\Delta(\tilde{\phi})|$ for all possible $\phi, \tilde{\phi}$ pairs. This newly defined threshold surface will still have structure if the gap is anisotropic. In particular, nodes in the gap function will be readily visible, with the threshold surface plunging to zero for a momentum connecting two nodes. The inversion procedure which culminates in Equation (5) remains unchanged if one is assured that any $\vec{q}, \omega$ solution to the kinematic equations which is used in the procedure only has a trivial degeneracy.
For a three-dimensional Fermi surface this inversion procedure is no longer possible. In this case for a momentum $\vec{q}$, Equation (2) has an infinite number of solutions for $\phi$ and $\tilde{\phi}$, which are now solid angles. A direct algorithm for evaluating $|\Delta(\theta)|$ using $\vec{k}_F(\theta)$ and the solutions to the kinematic equations is no longer possible because a fit of $|\Delta|_{in}$ now requires multiparameter root finding. However the concept of a threshold surface remains valid and the nodes of it still indicate a momentum which joins gap nodes on the Fermi surface.

Only a simple BCS model has been presented, but a calculation including strong electron-phonon coupling and Coulomb interactions\textsuperscript{15,16} indicates that the lifetime retains large anomalous features. In this calculation, the lifetime at $q = q_2$ does not reach zero and the discontinuity at this threshold momentum is smoothed. The rise of the phonon lifetime for $q > q_2$, however, is much faster than in the weak-coupling case. Because of these competing effects it is difficult to determine whether the transition from below to above the threshold surface would be easier or harder to observe in this more realistic model than in the weak-coupling model.

The coherence factor in the electromagnetic response function provides a minor complication. For a system with the d-wave gap of Equation (4), this factor vanishes for a phonon whose wavevector is parallel to the (110) direction and whose head and tail lie on the Fermi surface. For such a phonon, therefore, the minimum-energy excitation does not contribute to its self-energy. This phonon’s lifetime would still decrease upon crossing the threshold line, but would not be discontinuous at the threshold. We do not expect this behavior could be observed, considering current experimental capabilities. The solution to
this problem is simply to consider threshold lines in other directions, as done in Figure 2. Only particular phonon directions are affected, therefore this complication does not affect the inversion procedure described above for the gap magnitude.

Since an extremely sensitive probe of surface phonons exists in thermal energy inelastic helium scattering\textsuperscript{17}, we remark that similar arguments to those presented in this paper may lead to gap measurement techniques involving surface phonons.

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Figure 1. This is the Fermi surface for a one-band model with nearest-neighbor and next-nearest-neighbor hopping, taken from Ref. 14. The dispersion relation is

$$\epsilon(k, \theta) = -2t(\cos(k\cos\theta) + \cos(k\sin\theta)) - 4t'(\cos(k\cos\theta)\cos(k\sin\theta))$$

with $t = 430\text{meV}$ and $t' = -70\text{meV}$. The electron filling factor is 0.85. $\vec{q}_n$ connects two nodes on the Fermi surface if the gap is of this d-wave form.

Figure 2. This is a plot of the threshold line in the (100) direction for the Fermi surface depicted in Figure 1. The solid line is the line for the d-wave gap $\Delta(\theta) = \Delta_o [\cos(k_F(\theta)\cos\theta) - \cos(k_F(\theta)\sin\theta)]$ and the dashed line is for the isotropic $\Delta(\theta) = \Delta_o$ case.