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

Michael E. Flatté
Department of Physics, University of California, Santa Barbara, California 93106-9530
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I 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) and (210) directions in \(Y\)Ba\(_2\)Cu\(_3\)O\(_7\) would determine whether the gap is predominantly \(s\) wave or \(d\) wave. I 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 the phonon-mediated pairing that 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 antiferromagnetic fluctuations and is predominately \(d\) wave [3]. Theoretical work on high-\(T_c\) materials has produced theories too diverse and numerous to list. Since all these theories address the form of the gap function, accurate measurements of the gap would provide a strong test which each must pass.

The experiments that look for gap anisotropy provide limited information. With the exception of angle-resolved photoemission spectroscopy, which has poor energy resolution (\(\sim 10\) meV), either they provide some average of the gap magnitude over all or a large part of the (normal) Fermi surface or they identify nodes in the gap on the Fermi surface. Reflectivity [4], tunneling current [5], and ultrasonic attenuation [6] measurements, as well as a variety of other transport measurements, yield an average value of the gap magnitude. Nodes on the Fermi surface are identified by measuring the temperature dependence of such quantities as ultrasonic attenuation [7], specific heat [8], or magnetic relaxation rate [9]. Unfortunately, the exponential temperature dependence, which would rule out nodes, and the power-law dependence, which would indicate nodes, are difficult to distinguish. Even if the evidence for a node is convincing, its location is hard to determine.

I 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 an \(s\)-wave or a \(d\)-wave function. This method should also locate any nodes on the Fermi surface. Recognizing that gaps which are approximately \(s\) or \(d\) wave are special cases of an anisotropic gap, I also 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, now possible using inelastic neutron scattering [10,11].

Previous measurements and analyses of superconductivity's effect on phonon frequencies and lifetimes, called phonon renormalization, were either performed on nonlayered materials or examined zone-center phonons. This Letter will show that superconductivity's effect on phonons with crystal momentum greater than an inverse coherence length \(\xi^{-1}\) in quasi-two-dimensional materials is qualitatively different and especially useful. In layered high-\(T_c\) materials, phonon renormalization is well known in Raman phonons [12]. Since these are zone-center phonons, their renormalization measures an average of the gap.

Measurements of the gap's effect on phonons with finite crystal momentum are well known from inelastic neutron scattering measurements on niobium [13] and Nb\(_3\)Sn [14]. Because the Fermi surfaces of these materials are not quasi-two-dimensional, measurements on these materials similarly yield averages of the gap. Even though a small gap anisotropy was observed in niobium, it is not possible to map out the gap function in this material using the technique presented in this Letter. I will now present the theory of phonon anomalies due to superconductivity in a quasi-two-dimensional material.

The Fermi surface shape and the gap at the Fermi surface completely determine the minimum energy required for a phonon to decay into two Bogoliubov quasiparticles. The minimum-energy excitation is the creation of both quasiparticles on the Fermi surface. On an inversion-symmetric Fermi surface, the positions where the quasiparticles are created can be found by placing the phonon momentum vector \(q\) in the Brillouin zone so that its head and tail are on the Fermi surface (see Fig. 1). The quasiparticles are created at the head and the Fermi surface point opposite the tail. For zone-center phonons the head and tail of the vector are the same point, so quasiparticles can be created anywhere on the Fermi surface. However, for \(q > \xi^{-1}\) there are typically only two places on the Fermi surface where quasiparticles can be created (as shown in Fig. 1). This Letter exploits this difference.

The Fermi surface shape is described by a function \(k_F(\theta)\), 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 \(k_F(\theta)\), one can find the an-
angles $\phi$ and $\tilde{\phi}$ where $q$’s head and tail lie, from the equation

$$q = k_F(\phi) - k_F(\tilde{\phi}).$$

The placement of the phonon momentum, and thus $\phi$ and $\tilde{\phi}$, are usually twofold degenerate for a two-dimensional Fermi surface such as YBa$_2$Cu$_3$O$_7$. 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 $\pi$. YBa$_2$Cu$_3$O$_7$’s Fermi surface is inversion symmetric, and an inversion-symmetric gap magnitude conforms to current expectations [15]. I will discuss situations with nontrivial degeneracies below.

The minimum or threshold energy is the sum of the gap magnitude at the two points $k_F(\phi)$ and $k_F(\tilde{\phi})$ on the Fermi surface. These two points are uniquely determined by $q$ and the function $k_F(\theta)$, so the threshold energy, denoted $\Delta$, can be considered as a function of $q$ and a functional of $k_F$:

$$\Delta(q) = |\Delta(\phi)| + |\Delta(\tilde{\phi})|. \tag{2}$$

$\Delta(q)$ is the gap at the point on the Fermi surface where the head of $k_F(\phi)$ is. As will be discussed later, $\Delta$ depends on $q$ in markedly different ways if the gap is $d$-like instead of $s$-like. In the remainder of this Letter functional dependence on $k_F$ is understood.

The method to determine the shape of the surface defined by $\Delta(q)$ in energy-momentum space is identical to the method used to measure the average gap in Nb$_3$Sn. The new quasiparticle channel which opens at the threshold surface causes anomalous behavior in the lifetimes and frequencies of phonon branches which cross the threshold.

The transition from below to above the threshold is sharp. Consider for illustrative purposes a weak-coupling BCS model where other influences on the phonon lifetime are approximated by a constant lifetime $\tau_0$. Follow a phonon dispersion curve which crosses the threshold, beginning with $q_1$ such that $\hbar \omega(q_1) < \Delta(q_1)$ and concluding with $q_3$ such that $\hbar \omega(q_3) > \Delta(q_3)$. With $\tilde{q}$ fixed, $\Delta(q)$ defines a threshold line instead of a surface. [With $\tilde{q}$ fixed, $\Delta(q)$ defines a threshold line instead of a surface.] At $q_2$ the phonon frequency is on the threshold line: $\hbar \omega(q_2) = \Delta(q_2)$. The model predicts the lifetime is $\tau_0$ for $q_1 < q < q_2$. The lifetime at $q = q_2$ will be $[16] \tau' = \tau_0/[1 + \tau_0 \nu(q_2)]$, where $\nu > 0$. As $q$ increases beyond $q_2$, the lifetime will increase. This model captures the essence of the transition since calculations including strong electron-phonon coupling and Coulomb interactions [17] indicate that the lifetime retains large anomalous features at threshold.

Points on a threshold line can thus be identified by determining where in $(q, \omega)$ space phonon lifetimes drop precipitously. These points satisfy the equation

$$\hbar \omega(q) = |\Delta(\phi)| + |\Delta(\tilde{\phi})| = \Delta(q). \tag{3}$$

Equations (1) and (3) will be referred to as the kinematic equations. Each time a phonon dispersion curve crosses the threshold line, one can determine a point on the line. Since there is a finite number of dispersion curves, $\Delta(q)$ will be measurable at a few points. This does not determine $\Delta(\theta)$ completely, but suffices to distinguish predominately $s$-wave or $d$-wave superconductivity. In addition, a particular phonon can be located either above or below the threshold surface depending on its lifetime change due to temperature. This technique avoids possible complications from $q$- and $\omega$-dependent electron-phonon coupling. Although the Raman experiments and the niobium and Nb$_3$Sn experiments measured temperature shifts in phonons, a threshold surface like the one described here did not exist.

Figure 2 is a plot of the threshold line $\Delta(q)$ in the (100) direction for the Fermi surface [18] of YBa$_2$Cu$_3$O$_7$ (shown in Fig. 1). Plotted is the threshold line for a $d$-wave gap

$$\Delta(\theta) = \Delta_0 \cos[k_F(\theta) \sin \theta] - \cos[k_F(\theta) \sin \theta]. \tag{4}$$

where $2\Delta_0 = 38$ meV [19]. Also plotted is the threshold for $\Delta(\theta) = 19$ meV. The node in $\Delta(q)$ signifies the existence of nodes in the gap function, since the phonon momentum (shown as $q_m$ in Fig. 1) must connect two nodes on the Fermi surface. The diameter of the Fermi sea in the (100) direction exceeds the phonon Brillouin zone, resulting in a double-valued threshold near the zone boundary. When the threshold is double valued, both thresholds will yield anomalies since they originate from geometrically separate quasiparticle excitations.

Here I emphasize that the weak-coupling BCS model was used for illustrative purposes; this is not a weak-coupling effect. The single-pair creation process is not re-
required to be overwhelming, merely substantial. In a strong-coupling model the anomalies should occur at the same energies and momenta, and with the same magnitude. Their detailed structure may differ from the weak-coupling case, although that is not important for the gap-determination technique presented here.

Raman measurements of the temperature-dependent frequency and lifetime of the 41-meV $A_g$ phonon stimulated an experiment to detect shifts in that phonon branch in the (100) direction [11] using inelastic neutron scattering. These experiments show shifts at the zone center and middle, but not at the boundary. This favors the $d$-wave threshold in Fig. 2 over the $s$ wave.

The threshold differs greatly in other directions, such as (210) (Fig. 3). Vanishing temperature shifts for the above phonon branch with $q\parallel$[210] and close to the zone center would also support a $d$-wave gap. For more conclusive results, anomalies in other phonons due to Cu-O planar motion, such as the 14-meV $A_g$ phonon, should be explored.

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 $(q, \omega)$ space. At least one solution to the kinematic equations exists for each value of $\phi$ unless one has a pathological case. For each $\phi$ pick one solution and identify it with $\phi$. For each solution $\omega(q)$ and $\phi$ are known, so these quantities can now be considered functions of $\phi$. Define the Fourier coefficients of a function of $\phi$ as follows: $f(\phi) = \sum_n f_n \cos(n\phi) + \sum_n f_n \sin(n\phi)$. Equation (3), the energy equation, becomes the following set of coupled linear equations for the Fourier coefficients $|\Delta_{ln}|^2$ of the gap magnitude:

$$H \omega_{ln} = |\Delta_{ln}| + \sum_{jm} c_{lnjm} |\Delta_{jm}|,$$

where

$$c_{ln2m} = \frac{1}{\pi} \int_0^\pi d\phi \sin(m\phi) \cos(n\phi)$$

and the other $c_{lnjm}$ involve the other three combinations of trigonometric functions. Inversion of Eq. (5) determines the gap magnitude everywhere on the Fermi surface.

For a three-dimensional Fermi surface, such as in niobium or Nb$_3$Sn, this inversion procedure is no longer possible. For a momentum $q$, Eq. (2) has an infinite number of solutions for $\phi$ and $\phi$, which are now solid angles. In addition, the transition across the threshold for a three-dimensional system with an anisotropic gap is marked only by a discontinuity in the slope of the phonon lifetime. Thus a threshold surface in the sense of this Letter does not exist.

The coherence factor in the electromagnetic response function provides a minor complication. For a system with the gap of Eq. (4), this factor vanishes for a phonon parallel to (110) whose head and tail lie on the Fermi surface. The minimum-energy excitation does not contribute to this phonon’s self-energy. This complication occurs only in particular phonon directions. If this were observed it would provide information about the phase of the gap function.

So far I have presented the geometry of these anomalies without discussing the possibility of observing them. I emphasize that for the purposes of this Letter, the accurate magnitude of an anomaly is not needed so long as it is observable. Early experiments on niobium- and Nb$_3$Sn were hampered by the low $T_c$, which required low-energy phonons with large (percentage) linewidths. Certain high-$T_c$ materials do not have these problems.
The following table summarizes the experimental situation:

<table>
<thead>
<tr>
<th>Material</th>
<th>$\omega$ (meV)</th>
<th>$2\gamma$ (meV)</th>
<th>$\Delta(2\gamma)$ (meV)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Niobium</td>
<td>2.38</td>
<td>0.17</td>
<td>0.06 $\pm$ 0.01</td>
<td>[13]</td>
</tr>
<tr>
<td>$\text{La}<em>{1.85}\text{Sr}</em>{0.15}\text{CuO}_4$</td>
<td>6.2</td>
<td>0.25</td>
<td>...</td>
<td>[20]</td>
</tr>
<tr>
<td>$\text{YBa}_2\text{Cu}_3\text{O}_7$ (exp) $\Gamma$</td>
<td>41</td>
<td>2.6</td>
<td>0.7</td>
<td>[12]</td>
</tr>
<tr>
<td>$\text{YBa}_2\text{Cu}_3\text{O}_7$ (exp) $\Gamma$</td>
<td>14</td>
<td>0.95</td>
<td>0.36</td>
<td>[12]</td>
</tr>
<tr>
<td>$\text{YBa}_2\text{Cu}_3\text{O}_7$ (calc) $Y_1$</td>
<td>11</td>
<td>...</td>
<td>0.23</td>
<td>[21]</td>
</tr>
<tr>
<td>$\text{YBa}_2\text{Cu}_3\text{O}_7$ (calc) $\Sigma$</td>
<td>12</td>
<td>...</td>
<td>0.16</td>
<td>[21]</td>
</tr>
</tbody>
</table>

$2\gamma$ is the full width at half maximum of the phonon in the superconducting state and $\Delta(2\gamma)$ is the change in $2\gamma$ when $T > T_c$. The numbers for niobium and $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ are taken from inelastic neutron scattering experiments in which $2\gamma$ is resolution limited. The $\text{YBa}_2\text{Cu}_3\text{O}_7$ experimental numbers are taken from Raman scattering data (zone-center or $\Gamma$ phonons). These phonons are associated with copper-oxygen bond stretching and should couple strongly to the copper-oxygen planes. Experimentally the $2\gamma$'s for $\text{YBa}_2\text{Cu}_3\text{O}_7$ phonons are well above those in $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$, in both absolute and percentage terms. Similarly, their $\Delta(2\gamma)$'s are well above those in niobium. Therefore anomalies should be readily observable.

$\Delta(2\gamma)$ can also be estimated from frozen-phonon calculations. Unfortunately, these calculations are extremely difficult, and good results only exist in $\text{YBa}_2\text{Cu}_3\text{O}_7$ for zone-center, $S=(\pi/a,\pi/b,0)$, and $Y_1=(0,\pi/b,0)$ phonons [21]. Since $S$ and $Y_1$ are not nesting vectors, the width there should be representative of the width in the rest of the zone. The lowest-energy phonons at these points are the last two entries in the table. These phonons would be of the most interest because even for a weakly anisotropic gap all of this branch should narrow upon entering the superconducting state, while for a gap with nodes some phonons in this branch will not. The change in width calculated for these phonons is well within observational parameters; Chou at Brookhaven recently measured the linewidths of phonons in the same energy range down to 0.2 meV with accuracy $\pm$ 0.1 meV or better. These results also indicate that $\text{YBa}_2\text{Cu}_3\text{O}_7$ should have observable anomalies.

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(a) Present address: Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106-4030.