Collective Modes in Layered Superconductors

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(Received 8 March 1990)

We calculate the collective-mode spectrum for a layered superconductor structure. We find that for wave vectors directed close to the direction of the superlattice axis, the plasmon mode remains *below* the superconducting gap edge (i.e., the Anderson-Higgs mechanism does not give rise to a massive collective mode as it does in the bulk three-dimensional system). We also find a clear signature of superconductivity in the form of a unique line splitting in the collective-mode spectrum as the plasmon crosses the superconducting gap. Experimental implications are discussed.

PACS numbers: 74.30.Gn, 71.45.Gm, 74.70.Jm

The discovery of high-T_c superconductors has inspired a tremendous amount of research on how the structure of these materials affects their properties.[1] These systems generally have a pronounced layered structure; the conducting layers of the system are so well separated that the tunneling between them is small. For example, a recent experiment[2] on the bismuth-based compounds yielded a ratio of 3×10^3 for the in-plane to interplane effective masses. In this work, we investigate how the layered structure affects the collective-mode spectrum of a superconductor. Since there is at present no consensus as to the mechanism of pairing in high-T_c materials, we will work in the BCS approximation, at $T=0$, using the s-wave pairing. Our model is thus a periodic multilayer superlattice in the z direction composed of superconducting layers in the x-y plane. This work is also directly relevant to artificially made superconducting superlattices.[3]

In what follows, we will show that if one ignores tunneling between layers in this type of superconductor, it necessarily follows that there are collective modes whose energy may be smaller than the gap, 2Δ. This result contrasts with the situation in an isotropic three-dimensional superconductor, for which the plasmon modes have energies on the order of the plasma frequency $\omega_p=(4\pi e^2\rho/m)^{1/2}$, where ρ is the electron density, so that the plasmon lies well above the gap (typically $\omega_p\sim$eV and $2\Delta\sim$meV). In fact, it is generally believed that there are no excitations whose energy is smaller than 2Δ for a clean, isotropic (s-wave) BCS superconductor.[4-7]

In addition, we find that the electromagnetic response of the layered superconductor has very unusual behavior when the wave vector is increased such that the collective-mode energy is pushed above the gap. Specifically, there is a line splitting in the absorptive part of the dielectric function just as the plasmon mode crosses the gap. This line splitting may be attributed to mixing by the Coulomb interaction of pair-breaking excitations and the collective sound mode associated with the long-range phase coherence of a superconductor. The effect is unique to this system: It requires the presence of a gap (and hence does not appear in normal superlattice systems), but does not occur in isotropic superconductors because of their screening properties. This line splitting allows one, in principle, to unambiguously determine the gap of this system directly from the collective-mode spectrum.

The question of whether one can observe excitations inside the gap in a superconductor has enjoyed a good deal of attention for many years.[4-7] The problem may be briefly stated as follows: In a neutral superfluid, one has a sound mode with velocity $v_0=v_F/\sqrt{3}$ in three dimensions, where v_F is the Fermi velocity. When one introduces the Coulomb interaction in a charged system, the mode is pushed out of the gap, to essentially the plasma frequency, by the Anderson-Higgs mechanism.[4] This behavior in fact arises from the detailed form of the Coulomb interaction in three dimensions $(4\pi e^2/q^2)$ at small q. In some sense, then, the fact that a mode does not appear in the gap for a superconductor is a question of detail rather than of physical necessity. Indeed, this observation led Belitz *et al.*[6] to investigate the possibility of finding modes in the gap for dirty superconductors, for which the disorder effectively changes the Coulomb interaction. They found, however, that the acoustic modes did not remain in the gap, even in the limit of very strong disorder. In contrast, for the superlattice, due to the layered structure the effective Coulomb interaction is softer,[8] and allows the sound mode to remain in the gap when $k_\parallel/k_z\ll1$, where $\hat{\mathbf{z}}$ is the direction along the superlattice and $k_\parallel$ is the wave vector along the layers.

To summarize the situations in which there are collective modes in the gap, one may draw a "phase diagram" in the $k_\parallel$-k_z plane (as done in Fig. 1). In this work, we ignore tunneling between planes, so the phase diagram is periodic in k_z, and we present data only for $0\le k_z a\le2\pi$, where a is the superlattice period. An interesting consequence of this periodicity is that the plasmon mode $\omega(\mathbf{k})$ can in principle enter and leave the gap several

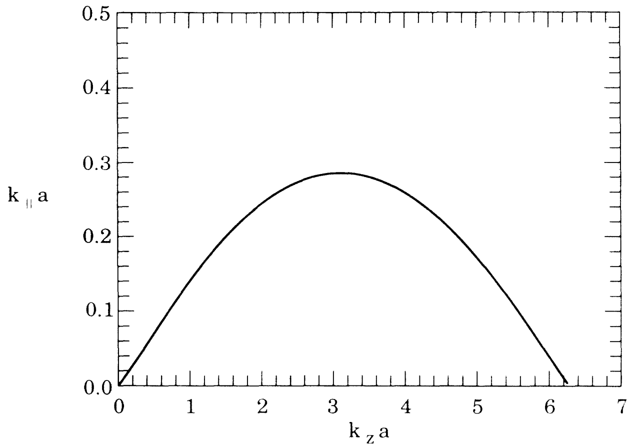

FIG. 1. Wave vectors for which the plasmon mode lies in the gap; the region below the curve indicates where the modes are present. The diagram is periodic in $k_z a$ with period 2π. Only data for $0 \le k_z a \le 2\pi$ are shown. Material parameters are the same as in Fig. 3.

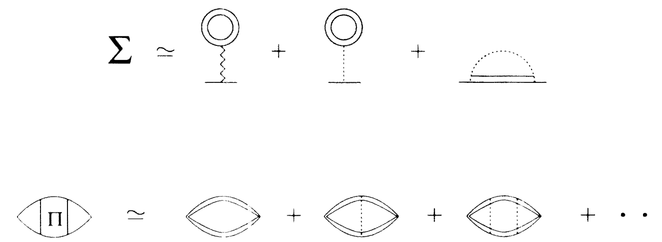

FIG. 2. Approximation used for the self-energy and the polarizability. Dotted line represents contact interaction, wiggly line represents Coulomb interaction, whereas the double lines indicate renormalized propagators.

times as a function of $|\mathbf{k}|$ for a fixed angle θ, if θ is small enough.

In this work, we study the density response function $\chi(\mathbf{k},\omega)$, which may be written in terms of an irreducible polarizability $\Pi(\mathbf{k},\omega)$:

$$\chi(\mathbf{k},\omega)=\Pi(\mathbf{k},\omega)/[1-\tilde{v}(\mathbf{k})\Pi(\mathbf{k},\omega)]\,, \tag{1}$$

where the effective interaction $\tilde{v}$ contains both the Coulomb interaction and an attractive short-range interaction $(-V_0)$ that produces superconductivity,

$$\tilde{v}(\mathbf{k})\equiv\sum_n e^{ik_z na}\int d^2r_{\|}\,v_{n0}(\mathbf{r}_{\|})e^{i\mathbf{k}_{\|}\cdot\mathbf{r}_{\|}}-V_0 = \frac{2\pi e^2}{\kappa k_{\|}}f(\mathbf{k})-V_0\,, \tag{2}$$

where $v_{n0}(\mathbf{r}_{\|})$ is the interaction between particles in layers n and 0, separated by a transverse vector $\mathbf{r}_{\|}$, κ is the appropriate lattice dielectric constant, and the form factor

$$f(\mathbf{k})=\sinh(k_{\|}a)/[\cosh(k_{\|}a)-\cos(k_z a)]$$

arises[8] from the layering.

Our calculation of the irreducible response function Π in Eq. (1) follows a gauge-invariant conserving approximation,[4-7,9] defined by the diagrams presented in Fig. 2. Poles of $\chi(\mathbf{k},\omega)$ give the collective modes of the system. Because we neglect interlayer electron-tunneling effects, the irreducible polarizability Π is manifestly diagonal in the layer index and becomes the corresponding two-dimensional polarizability, which can be calculated by summing the ladder diagrams. We find for $\Delta, k_{\|}^2/2m \ll E_F$ [note that E_F is the two-dimensional Fermi energy and $\Pi(\mathbf{k},\omega)\equiv\Pi(k_{\|},\omega)$ because of the absence of interlayer tunneling]

$$\Pi(k_{\|},\omega)=2C(k_{\|},\omega)[1-V_0C(k_{\|},\omega)]^{-1}\,, \tag{3}$$

where

$$C(k,\omega)=-iF_+(k,\omega)+\frac{V_0[\omega G(k,\omega)]^2}{1-iV_0F_-(k,\omega)}\,, \tag{4}$$

$$F_\pm(k,\omega)=-i\int\frac{d^2q}{(2\pi)^2}\frac{-E_{q+}E_{q-}-\Delta^2\pm\bar{\varepsilon}_{q+}\bar{\varepsilon}_{q-}}{4E_{q+}E_{q-}}\left\{\frac{1}{\omega-E_{q-}-E_{q+}+i\delta}-\frac{1}{\omega+E_{q+}+E_{q-}-i\delta}\right\}, \tag{5}$$

$$G=-i\int\frac{d^2q}{(2\pi)^2}\frac{\Delta}{4E_{q+}E_{q-}}\left\{\frac{1}{\omega-E_{q-}-E_{q+}+i\delta}-\frac{1}{\omega+E_{q+}+E_{q-}-i\delta}\right\}, \tag{6}$$

$q_\pm=|\mathbf{q}\pm\frac{1}{2}\mathbf{k}|$, $E_{q\pm}=(\Delta^2+\bar{\varepsilon}_{q\pm}^2)^{1/2}$, and $\bar{\varepsilon}_{q\pm}=q_\pm^2/2m-E_F$. The real parts of $F_\pm$ and G may be written down explicitly in terms of elliptic integrals; we can then numerically obtain the imaginary parts by performing Kramers-Kronig transforms on these. In this way, one obtains $\Pi(k,\omega)$ and $\chi(k,\omega)$ over a large range of values for $\mathbf{k}$ and ω. We have performed this calculation, and will report the details of these results elsewhere.[10] We first need to show that there can be collective modes with energy $\omega<2\Delta$ even when screening is included. Towards this end, we perform an expansion of Eqs. (3)-(6) in the parameter $v_Fk_{\|}/\Delta$. These expansions turn out to be well behaved so long as $\omega<2\Delta-v_Fk_{\|}$, thus allowing us to map out the values of $\mathbf{k}$ for which $\omega(\mathbf{k})$ is smaller than the gap. For $\omega\ll2\Delta$, we obtain after considerable algebra,

$$\Pi(k_{\|},\omega)\simeq-\frac{m}{\pi}\frac{v_F^2k_{\|}^2/2}{(mV_0/2\pi+1)v_F^2k_{\|}^2/2-\omega^2}\,. \tag{7}$$

There is a pole in the irreducible polarizability at

$\omega=(1/\sqrt{2})v_F(1+mV_0/2\pi)^{1/2}k_\parallel$; this is essentially the acoustic mode one finds for a neutral superfluid, and is the two-dimensional analog of Anderson's result.[4] To find the collective modes for the fully interacting system, we note that these occur when χ diverges, or from Eq. (1), when $\Pi(k_\parallel,\omega)=1/\tilde{v}(\mathbf{k})$. This immediately gives the result

$$\omega(\mathbf{k})\simeq\frac{v_F k_\parallel}{\sqrt{2}}\left[1+\frac{2me^2}{k_\parallel}f(\mathbf{k})-\frac{m}{2\pi}V_0\right]^{1/2}. \qquad (8)$$

For a weak contact potential, the last term may be ignored and Eq. (8) then gives us the acoustic-plasmon mode which necessarily lies in the gap for $k_\parallel \ll k_z$.

To completely map out the poles inside the gap, we evaluate Eqs. (5) and (6) in the small-$k_\parallel$ limit without assuming ω is small; the resulting expansion is well behaved for $\omega<2\Delta$. (The explicit expressions are quite lengthy, and are omitted for brevity.) In Fig. 3, we present $\omega(\mathbf{k})/\Delta$ as a function of k for several fixed angles $\theta=\arctan(k_\parallel/k_z)$. The parameters of the system are chosen to roughly model a high-T_c compound. Specifically, we have taken $a=10$ Å, $n_s=10^{14}$ cm^{-2} as the sheet density, effective in-plane mass $m^*=5m_0$, lattice dielectric constant $\kappa=4$, and for the order parameter, we use the BCS form $\Delta=1.76k_BT_c$, with $T_c=125$ K. We see that as θ increases, the plasmon mode is pushed out of the gap. To illustrate this explicitly, we have plotted several points for $\omega(k)\sim2\Delta$, as obtained by direct numerical integration of Eqs. (5) and (6); it is clear that the frequency of the plasmon mode is well behaved as the gap edge is crossed. For the above parameters, one finds that there are no subgap plasmon modes for $\theta>6°$.

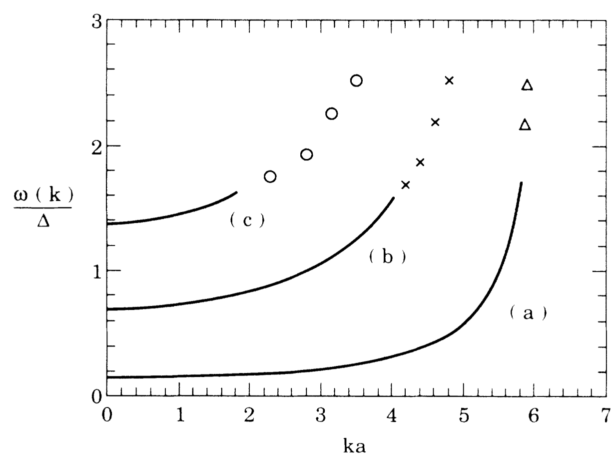

FIG. 3. Plasmon dispersion $\omega(\mathbf{k})/\Delta$. Solid lines are obtained using expansions in $v_Fk_\parallel/\Delta$ for, curve a, $\theta=0.01$, curve b, $\theta=0.05$, and curve c, $\theta=0.1$ rad. All other points are obtained by direct numerical integration of Eqs. (5) and (6); circles are for $\theta=0.1$, crosses for $\theta=0.05$, and triangles for $\theta=0.01$ rad. Material parameters are chosen such that $n_s=1.0\times10^{14}$ cm^{-2}, $m^*=5m_0$, $k=4$, and $T_c=125$ K.

We note also that because $\tilde{v}(\mathbf{k})$ is periodic in k_z, the plasmon frequency $\omega(\mathbf{k})$ for a given angle θ may in principle enter and leave the gap several times as a function of $|\mathbf{k}|$; we find, however, that the angles necessary to achieve this are quite small.

It is also interesting to observe how the density response function behaves as the wave vector is increased (at fixed angle) such that the plasmon mode exits the gap. In Fig. 4 we plot the absorptive part of the response function (Imχ) for $\theta=5.7°$ and three values of k, as a function of unitless frequency, ω/Δ. [These results were obtained by direct numerical integration of Eqs. (5) and (6). Details will be given elsewhere.[10]] For $ka<2.82$, there is still a sharply defined plasmon mode below 2Δ; as the wave vector is increased beyond this threshold, one gets mixing between the collective mode and the pair-breaking excitations above 2Δ. The line shape of this mixed mode takes on a double-peaked form; the lower of these two peaks is maximum at the gap edge 2Δ, while the upper peak position moves to higher frequencies with increasing k. For larger values of k, the lower-frequency peak has very little oscillator strength, and one can only distinguish the upper mode.

The origin of this line splitting is somewhat subtle, and requires a detailed examination of the density response function in the *absence* of Coulomb interactions, $\Pi(k_\parallel,\omega)$. One can show[10] that Π must have Van Hove singularity cusps at $\omega=2\Delta$ and $\omega=(4\Delta^2+v_F^2k_\parallel^2)^{1/2}$ due to the available phase space for pair-breaking excitations at a given ω and $k_\parallel$. These cusps can only be seen on a very fine scale in $\Pi(k_\parallel,\omega)$ because the oscillator strength of the plasmon mode overwhelms that of the pair-breaking excitations at small wave vectors. However, when one introduces the Coulomb interaction, the near vanishing denominator in Eq. (1) as the plasmon pole crosses the

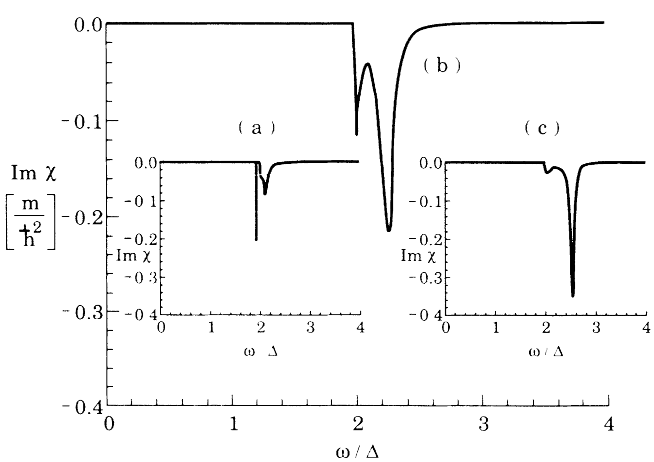

FIG. 4. Absorptive part of dielectric response as a function of unitless frequency, ω/Δ, in units of $m/\hbar^2$. Material parameters as in Fig. 3, $\theta=0.1$ rad, and (a) $ka=2.8$ (sharp line represents a δ function at the position of the plasmon pole), (b) $ka=3.15$, and (c) $ka=3.5$.

gap acts as a huge amplification factor for this structure in Π, allowing the unusual behavior seen in Fig. 4. *This structure is unique to layered superconductors:* One must have a gap in the spectrum to get the cusped behavior, but in isotropic superconductors, the Coulomb screening is so strong that the plasmon mode is pushed far above the gap edge, so that this structure does not occur.

Finally, we note that if one simply follows the position of the collective mode $\omega(\mathbf{k})$ as a function of $\mathbf{k}$, it is not immediately obvious whether one can tell when the gap edge has been crossed, because the width of the plasmon pole tends to be quite small even above the gap if $k_\parallel$ is small. However, the line splitting shown in Fig. 4 allows one to determine precisely when the collective mode has crossed the gap.

We believe that the plasmon modes described in this work should be observable in both light-scattering[11] and electromagnetic absorption[12] experiments. The latter situation contrasts with the case for plasmons in an isotropic three-dimensional system where light can only couple to transverse excitations, and plasmons are purely longitudinal excitations. In our case, the plasmons are only longitudinal in the sense that $\nabla n_s(\mathbf{r}_\parallel,t) \parallel \mathbf{k}_\parallel$, where $n_s(\mathbf{r}_\parallel,t)$ is the local density on a sheet. A light wave may be polarized such that the projections of the electric field and $\mathbf{k}$ vectors onto the layer planes are parallel, thus allowing them to couple to these modes. A direct observation of these plasmon modes via an inelastic-light-scattering experiment[11] should also be possible.

Does one expect to see these modes in a real high-T_c material? There are two major approximations going into our calculations whose applicability needs to be evaluated before these questions can be answered. The first is the assumption that one can ignore tunneling between layers in these systems; the highly anisotropic effective-mass ratio seen in these materials[2] suggests that this is a good approximation. We believe, however, that whatever the tunneling rate is between layers, this will set a lower limit on the frequencies of collective excitations of the system. Second, the treatment of the high-T_c materials as s-wave BCS superconductors cannot be justified at this point, because the pairing mechanism is still not known. If the pairing is such that there is an acoustic mode when one ignores the Coulomb interaction, it seems likely that the considerations in this work would lead one to conclude that, when long-range interactions are included, there will remain collective modes in the gap. The line splitting in the density response is a signature of having a superconducting gap and should exist (in a quantitatively modified form) in other models of pairing also.

We thank S. K. Yip, D. Belitz, R. E. Prange, H. D. Drew, K. Karraï, and Thi Pham for helpful discussions. This work was supported by the NSF, the U.S. ONR, and the U.S. ARO. Computer time was provided by the University of Maryland.

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