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Acoustic plasmons in a coupled array of sheets and chains and their role in $YBa_2Cu_3O_7$

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There is considerable evidence that the electronic behavior of orthorhombic $YBa_2Cu_3O_7$ is dominated by energy bands associated with Cu-O sheets and chains. We discuss the long-wavelength plasmon modes expected in an array of parallel metallic sheets and chains, coupled by the Coulomb interaction and using the random-phase approximation. We show that in the *a-b* plane there is a low-energy acoustic plasmon mode in addition to the usual high-energy bulk plasmon. This new acoustic plasmon does not arise in an array of coupled layers or in an array of parallel chains. Depending as it does on electronic motion in the chains along the *b* axis, the frequency of the mode is highly anisotropic in the *a-b* plane.

It is well known that the orthorhombic structure of $YBa_2Cu_3O_7$ is composed of Cu-O sheets and Cu-O chains. Moreover, while the high-temperature superconductivity is thought to be associated with Cu-O sheets, there is strong evidence that the presence of the Cu-O chains plays a crucial role.[1] Finally, we note that electronic band-structure calculations[2] show the metallic charge densities are strongly concentrated on these Cu-O sheets and chains, with almost none in the regions near the Y and Ba positions. The Fermi surface apparently can be well described by the Cu(2)-O(2)-O(3) sheet-related bands [with two-dimensional (2D) character] and the Cu(1)-O(1)-O(4) chain-related bands [with one-dimensional (1D) character].

In the present paper, we examine the collective charge fluctuations (plasmons) of a system composed of a periodic array of alternating sheets and chains, as a simple model of the $YBa_2Cu_3O_7$ orthorhombic structure. The calculations are similar to the familiar ones for a periodic array of parallel conducting sheets (as in a semiconductor superlattice[3,4]) and an array of parallel chains (as in quasi-one-dimensional conductors[5,6]). Our main new result is that the coupled sheet-chain system always exhibits a low-energy acoustic plasmon (which we denote as ω_-) in addition to the usual high-energy bulk plasmon (which we denote as ω_+). This ω_- mode exists in the *a-b* plane since it arises from correlated electronic motion in the sheets and chains. More specifically, since it depends on coherent electronic motion in the chains, the ω_- mode can only occur with ordered Cu-O chains.[1] Since below about 300 K, the O(1) sites at $(0,\frac{1}{2},0)$ are occupied and the O(1) sites at $(\frac{1}{2},0,0)$ are empty, our sheet-chain model should be valid up to this temperature. On the other hand, the ω_- mode will not exist in the tetragonal phase[1] of $YBa_2Cu_3O_{7-\delta}$.

Our results are clearly relevant for the optical properties of the $YBa_2Cu_3O_7$ material since, in effect, we are calculating the longitudinal dielectric function $\epsilon(\mathbf{q},\omega)$. Observation of the low-frequency ω_- plasmons would confirm the basic correctness of our model and encourage a more detailed theoretical study. However, in the long-wavelength limit, the ω_- modes do not involve any net charge fluctuation and thus may be difficult to detect. Even more interesting is the role that the ω_- modes might play as a new source of an attractive interaction between electrons in the Cu-O sheets and hence high-temperature superconductivity.

The plasmon modes we predict are quite different from those invoked by other workers trying to explain the high transition temperature superconductivity in both $La_{2-x}Ba_xCuO_{4-y}$ and $YBa_2Cu_3O_{7-y}$ compounds. In our work, the ω_- plasmon arises as a general feature of a coupled array of sheets and chains, and thus is only relevant to the $YBa_2Cu_3O_7$ material. Previous studies by Ruvalds[7] as well as by Kresin[8] were, in contrast, largely concerned with the 2D-like plasmons of a single Cu-O sheet. Other workers[9] have suggested that soft (low-energy) plasmons might arise as a result of a charge-density wave (CDW) but with no specific reference to the chains.

In Fig. 1 we show a periodic array of two sheets and one plane of chains, such as one has in the Y-Ba-Cu-O com-

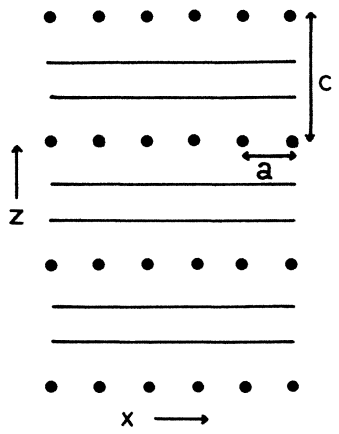

FIG. 1. The Cu-O sheets (lines) and Cu-O chains (filled circles) are shown for the Y-Ba-Cu-O compound (Ref. 1). The lattice distances shown are approximately $a = 3.8$ Å and $c = 11.7$ Å. The smallest distance between two Cu-O sheets is approximately 3.4 Å.

pound. We treat the sheets as a uniform 2D electron gas (in the x-y or a-b plane) and the chains as a uniform 1D electron gas (along the y or b axis). We shall refer to electrons, although in Y-Ba-Cu-O one is actually dealing with holes.[2] We ignore any band-structure effects within the chains and sheets, apart from different effective masses. Effectively, the electrons are assumed to be locked into their lowest transverse states (in the z direction for the sheets and in the x-z plane for the chains). We ignore the "puckering" of the Cu-O sheets.[1] The structure shown in Fig. 1 may be viewed as periodic in the z direction (with period c), with a *basis* of three elements (say, two Cu-O sheets and one plane of Cu-O chains). As discussed in other problems,[3-6,10] the form factors describing the localization to sheets and chains, as well as the geometry of the periodic array, can all be incorporated into a modified Coulomb potential. However, in the long-wavelength limit, one can use the continuum limit and work with the usual 3D Coulomb potential (as long as $qc \ll 1$, where c is a distance characteristic of the lattice of chains and sheets).

Working within the standard random-phase approximation (RPA), it is then straightforward to solve for the coupled response functions for our sheet-chain array. One finds that the dielectric function in the long-wavelength limit reduces to

$$\epsilon(\mathbf{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\left[\frac{1}{A_c}\chi_1^0(q_y,\omega) + \frac{2}{d_s}\chi_2^0(\mathbf{q}_\parallel,\omega)\right] , \quad (1)$$

where $\chi_d^0(\mathbf{q},\omega)$ represents the Lindhard function of d-dimensional uniform noninteracting electron gas. Here $A_c = ca$ is the area of the unit cell of the 2D chain lattice and $d_s = c$ is the spacing between the planes described in the preceding paragraph. Comparing (1) with the usual 3D bulk RPA expression

$$\epsilon(\mathbf{q},\omega) = 1 - v(\mathbf{q})\chi_3^0(\mathbf{q},\omega) , \quad (2)$$

we see that, as expected, the restriction of electronic motion to the chains and the two sheets has the effect of "contracting" the full 3D expression for the Lindhard function down to that given by (1). The same sort of "contraction" occurs in the case of two coupled mutually perpendicular arrays of chains in Hg chain compounds.[10]

Analytic expressions for χ_1^0 and χ_2^0 are given in the literature (Refs. 5 and 11, respectively) but we only need the long-wavelength limit ($q \ll k_F$). In particular, we use the well-known Tomonaga approximation for χ_1^0,

$$\chi_1^0(q_y,\omega) = N_1(\epsilon_{1F})[v_{1F}^2 q_y^2/(\omega^2 - v_{1F}^2 q_y^2)] . \quad (3)$$

Here the density of states at the Fermi surface is $N_1(\epsilon_{1F}) = 2/\pi v_{1F}$ and the 1D Fermi wave vector is given by $n_c \equiv (N_c/L) = 2k_{1F}/\pi$, where N_c is the number of electrons in a chain of length L. (Throughout this paper we set $\hbar = 1$.) The real part of χ_2^0 is easily found to be

$$\chi_2^0(\mathbf{q}_\parallel,\omega) = \begin{cases} N_2(\epsilon_{2F})\{[\omega/(\omega^2 - v_{2F}^2 q_\parallel^2)^{1/2}] - 1\}, & \omega > v_{2F}q_\parallel, \\ -N_2(\epsilon_{2F}), & \omega < v_{2F}q_\parallel, \end{cases} \quad (4)$$

where the density of states at the Fermi surface is $N_2(\epsilon_{2F}) = m_s/\pi$ and the 2D Fermi wave vector is given by $n_s \equiv (N_s/A_s) = k_{2F}^2/2\pi$. N_s is the number of electrons (of mass m_s) on a sheet of area A_s. We remark that (3) and (4) have the correct behavior in the limit of high and low frequencies. In much of the literature on periodic planar arrays, the simpler hydrodynamic approximation is often used in describing a noninteracting 2D electron gas, namely[3]

$$\chi_2^0(\mathbf{q}_\parallel,\omega) = N_2(\epsilon_{2F})[s^2 q_\parallel^2/(\omega^2 - s^2 q_\parallel^2)]$$
$$= \frac{n_s}{m_s}[q_\parallel^2/(\omega^2 - s^2 q_\parallel^2)] , \quad (5)$$

where $s^2 = v_{2F}^2/2$. This form has the advantage of having the same structure as $\chi_1^0(q_y,\omega)$ given in (3), and calculation shows that (5) and (4) give very similar results for the zeros of $\epsilon(\mathbf{q},\omega)$ in (1). However, we shall use the more correct long-wavelength expression (4).

In Fig. 2 we give a schematic plot of $\epsilon(\mathbf{q},\omega)$ as a function of the frequency ω, based on (3) and (4). For concreteness we assume $v_{1F}q_y < v_{2F}q_\parallel$. The collective modes corresponding to the zeros of ϵ are denoted by $\omega_\pm(\mathbf{q})$. The ω_- mode is bracketed by the poles of χ_1^0 and χ_2^0,

$$v_{1F}q_y < \omega_-(\mathbf{q}) < v_{2F}q_\parallel . \quad (6)$$

Analytically, one easily finds (with $\mathbf{q}$ in spherical coordinates)

$$\omega_+^2(\mathbf{q}) = (\omega_s^2 + \omega_c^2 \sin^2\phi)\sin^2\theta + O(q^2) , \quad (7)$$

$$\omega_-^2(\mathbf{q}) = v_{1F}^2 q^2\left[1 + \frac{N_1(\epsilon_{1F})}{N_2(\epsilon_{2F})}\frac{d_s}{2A_c}\right]\sin^2\theta\sin^2\phi . \quad (8)$$

Here we have introduced the effective bulk plasmon frequencies[3,5]

$$\omega_c^2 = \frac{4\pi e^2 \bar{n}_c}{m_c};\ \bar{n}_c \equiv \frac{n_c}{A_c},$$
$$\omega_s^2 = \frac{4\pi e^2 \bar{n}_s}{m_s};\ \bar{n}_s \equiv \frac{2n_s}{d_s} . \quad (9)$$

Clearly $\bar{n}_c$ ($\bar{n}_s$) is the effective bulk electron density in the chain (sheet) array. The second term in the square bracket in (8) can also be written as $\tilde{n}_c/2n_s$, where $\tilde{n}_c = n_c/a$ is the effective surface density of electrons in a sheet of chains.

We call attention to the following points.

(1) The fact that both ω_+ and ω_- are proportional to $\sin\theta$ arises because the electrons can only move in the x-y plane and hence only the $\mathbf{q}_\parallel$ component of $\mathbf{q}$ contributes.

(2) If we just had an array of sheets *or* an array of

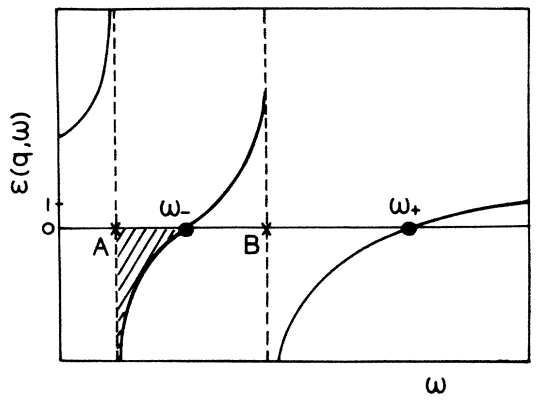

FIG. 2. A schematic drawing of the sheet-chain dielectric function $\epsilon(\mathbf{q},\omega)$ vs frequency ω, as given by (1) in conjunction with (3) and (4). A represents the pole of χ_1^0 at $v_{1F}q_y$ and B represents the pole of χ_2^0 at $v_{2F}q_\parallel$. The plasmon modes, denoted by $\omega_\pm(\mathbf{q})$, only involve charge motion in the x-y (or a-b) plane and hence disappear if $q_\parallel=0$. The hatched region corresponds to the frequencies which may be important for Cooper pairing.

chains, only the high-energy bulk plasmon ω_+ would exist in the a-b plane ($q_z=0$).

(3) While the dispersion relation of the low-frequency acoustic mode ω_- given by (8) depends on the specific forms used for χ_1^0 and χ_2^0, it is expected to arise in any coupled set of sheets and chains. Indeed, the physics involved in this acoustic mode is similar to that obtained in the RPA analysis of any *two* component system,[12,13] such as an electron-ion plasma.

(4) In the long-wavelength limit being considered here, there is no imaginary part to χ_1^0. Such damping does arise at larger values of q and it can be calculated from expressions given in the literature.[5,11] However, we emphasize that (1) is only valid for $qd_s \ll 1$.

(5) The region where $\epsilon(\mathbf{q},\omega)<0$ is especially important for the Bardeen-Cooper-Schrieffer (BCS) kind of superconductivity.[12,13] This occurs (see Fig. 2) in the region between $v_{1F}q_y$ and ω_-. A more detailed study valid at higher values of q would be necessary before one can assess the potential importance of these ω_- modes as a mechanism for Cooper pairing. However, (8) already suggests that the attractive region would be larger if we only had *one* Cu-O sheet to every plane of Cu-O chains (rather than two).

One may use the RPA equations of motion for the various response functions to evaluate the induced charge densities on the sheets ($\delta\rho_s$) and chains ($\delta\rho_c$). One finds that the ratio is given by

$$\frac{\delta\rho_c(\mathbf{q},\omega)}{\delta\rho_s(\mathbf{q},\omega)}=\frac{d_s}{2A_c}\frac{\chi_1^0(q_y,\omega)}{\chi_2^0(\mathbf{q}_\parallel,\omega)} . \tag{10}$$

This ratio gives considerable insight into the physics involved in the $\omega_\pm$ plasmon modes (see, also, Ref. 10). Using (7) in (10), we obtain the not unexpected result

$$\delta\rho_c(\mathbf{q},\omega_+)/\delta\rho_s(\mathbf{q},\omega_+)=(\omega_c^2/\omega_s^2)\sin^2\phi . \tag{11}$$

On the other hand, using (8) in (10) gives

$$\frac{\delta\rho_c(\mathbf{q},\omega_-)}{\delta\rho_s(\mathbf{q},\omega_-)}=-1 . \tag{12}$$

That is, the ω_- plasmon involves charge fluctuations in the sheets and chains which (in the long-wavelength limit) are completely out of phase with each other. Consequently, in this limit, the ω_- mode involves no net charge fluctuation and hence will *not* be excited by an electromagnetic wave.[14] Of course, this feature is ultimately the reason why the ω_- mode is acoustic, with its energy going to zero. The high-frequency plasmon ω_+ in (11) does involve a net charge fluctuation and will show up in the optical properties. The kind of analysis needed in optical studies when dealing with an anisotropic plasmon dispersion relation as in (7) is discussed in Refs. 5 and 15.

The possibility of a 1D CDW in these chains and its effect on enhancing the 2D superconductivity in the Cu-O sheets has been recently studied.[16] It would be interesting to examine the implications of the strong chain-sheet coupling we have considered in this paper on the formation of such 1D CDW's.

A more detailed derivation of (1) and its generalized form valid at arbitrary values of q will be presented elsewhere.[17] Similar models are applicable to semiconductor superlattices with a basis (i.e., alternating 2D layers with different electronic properties).

Note added in proof. (1) In the long wavelength limit, the imaginary part is

$$\mathrm{Im}\chi_2^0(\mathbf{q}_\parallel,\omega)=-N_2(c_{2F})\frac{\omega}{(v_{2F}^2q_\parallel^2-\omega^2)^{1/2}} ,$$

for $\omega<v_{2F}q_\parallel$ and zero for $\omega>v_{2F}q_\parallel$. Thus the closer $v_{1F}q_y$ is to $v_{2F}q_\parallel$, the more the ω_- mode will be damped. The ω_- mode would appear to be most effective for $q_x \gg q_y$. (2) The key requirement is that the Cu-O chains should be long enough to exhibit charge fluctuations characteristic of a 1D metal. In this regard, see M. W. C. Dharma-wardana [Phys. Lett. A **126**, 61 (1987)]. (3) A BCS order parameter induced by such a ω_- plasmon would be highly anisotropic in the a-b plane. However, in most properties, such anisotropic effects would be averaged over as a result of randomly oriented twin boundaries.

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