

Plasmons and high-temperature superconductivity

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Long-wavelength charge fluctuation models are constructed for 1:2:3 superconductors. These include planar plasmons ($\omega \sim \sqrt{q}$) plus numerous acoustical plasmons ($\omega \sim q$). We show that these modes do *not* cause pairing of electrons into a superconductor state. Our results rule out interlayer and intralayer pairing by long-wavelength charge fluctuations.

I. INTRODUCTION

The discovery of high-temperature superconductivity has renewed interest in this field.¹ Particularly exciting are the 1:2:3 materials such as $\text{YBa}_2\text{Cu}_3\text{O}_7$ which have transition temperatures near 95 K.^{2,3} There is much theoretical interest in the mechanisms which cause the superconductivity at high temperature. Numerous experiments indicate that the electrons are paired with an energy gap.⁴ The absence of an isotope effect⁵⁻⁷ suggests that the electron-phonon interaction is not causing the electrons to pair. Thus, the materials appear to behave like ordinary Bardeen-Cooper-Schrieffer (BCS)⁸⁻¹⁰ superconductors, but the pairing force may not be phonons.

There have been numerous suggestions of other pairing mechanisms. Many theories are built around spin fluctuations¹¹⁻¹³ while others depend upon charge fluctuations.¹⁴⁻²⁰ Here we provide a critical examination of the charge-fluctuation theories. At long wavelength the coupled chains and planes have numerous planar ($\omega \sim \sqrt{q}$) and acoustical ($\omega \sim q$) plasmon modes. We have carefully examined their role in pairing electrons, and have concluded that they do not cause pairing. The reason is quite simple: The Coulomb repulsion between electrons is quite strong, and is sufficient to overcome any attractive force from the plasmons. We conclude that *long-wavelength* charge fluctuations cannot cause superconductivity. Short-wavelength models such as those described in Refs. 19 and 20 are not included in our analysis, and are possible pairing mechanisms. We also cite calculations which conclude that the pairing is due neither to spin fluctuations²¹ nor to phonons.²² Thus, the theoretical picture is quite muddled.

It has also been suggested that electron pairing is enhanced when the two electrons are in different planes—we call this interlayer pairing.^{23,24} We have examined this possibility and have concluded that long-wavelength plasmons do not cause interlayer pairing. In doing this calculation, we also include the interlayer plasmons.

Our calculations are valid for long-wavelength excitations. We use existing band-structure calculations^{25,26} to construct simple analytical models of the electron energy

bands which cross the Fermi surface. These are used to compute the dielectric response in random-phase approximations (RPA).¹⁰ The bands in various chains and planes are coupled only through Coulomb interactions. We find more plasmon modes than others have reported,¹⁴⁻¹⁸ but they are insufficient to cause pairing. Our pairing calculations are done at two levels. One is a strong-coupling calculation where we solved the gap equations²⁷ at zero temperature for both interlayer and intralayer pairing. No solutions are found with a finite-energy gap. Then, we constructed analytical arguments using (a) weak-coupling theory, and (b) McMillan-type arguments.²⁸ Both of these approaches also indicate the lack of pairing from long-wavelength excitations.

In Sec. II we describe the theory of the dielectric response function $S_{\alpha\beta}(q, \omega)$. For an isotropic system $S = 1/\epsilon$ where $\epsilon(q, \omega)$ is the longitudinal dielectric function. For a layered system, α and β are indices which denote the planes. Poles in this function identify collective excitations which are the plasmons. Section III describes the pairing theory, and the unsuccessful attempts to find nonzero solutions to the gap equations.

II. DIELECTRIC RESPONSE

The 1:2:3 materials such as $\text{YBa}_2\text{Cu}_3\text{O}_7$ are planar. In this section we derived the dielectric response of a model system composed of two planes which have between them parallel chains of atoms. This system of planes and chains is meant to approximate the copper-oxide bonding system in a single unit of the z -axis unit cell. The three-dimensional crystal is obtained by stacking these two-dimensional units. We treat the Y^{3+} and Ba^{2+} ions as inert charged spheres. This idealized model provides an adequate description of the energy-band structure near the Fermi surface.²⁵ The chains and planes are separated sufficiently so that they are noninteracting except through Coulomb interactions.²⁵ Thus, we can find the dielectric response separately for each plane and chain. Afterwards we couple them through the Coulomb interaction.

A. Chains

Band-structure calculations suggest that two different one-dimensional energy bands cross the Fermi surface. Each band we represent by a simple $\cos(ka)$ dispersion relation

$$\epsilon_a(k) = C_a - B_a \cos \theta,$$

where $\theta = ka$. Values for the bandwidth B and band center C are given below. The RPA response function Π_1 is evaluated easily at zero temperature. The lattice constant a is along the chain while b is perpendicular to it.

$$\begin{aligned} \Pi_1(q, \omega) &= \frac{2}{ab} \int \frac{d\theta}{2\pi} (n_k - n_{k+q}) \\ &\quad \times [\omega + \epsilon(k) - \epsilon(k+q) + i\delta]^{-1}, \\ \text{Im}\Pi_1(q, \omega) &= [ab(\omega_x^2 - \omega^2)^{1/2}]^{-1} \text{ if } \omega_1 < \omega < \omega_2, \end{aligned}$$

where

$$\omega_x = 2B \sin(qa/2),$$

$$\omega_{2,1} = \sin(qa)[B^2 - (C - \mu)^2]^{1/2} \pm 2(C - \mu) \sin^2(qa/2),$$

and

$$\text{Re}\Pi_1(q, \omega) = -\frac{1}{\pi\Omega ab} \ln \left[\frac{(\Omega_1 + \Omega)(\Omega_2 - \Omega)}{(\Omega_1 - \Omega)(\Omega_2 + \Omega)} \right],$$

where

$$\Omega = (\omega_x^2 - \omega^2)^{1/2},$$

$$\Omega_{1,2} = (\omega_x^2 - \omega_{1,2}^2)^{1/2}.$$

Some band-structure calculations show two chain modes which cross the Fermi surface.²⁵ The σ -bonded band has a large bandwidth with $B = 1.0$ eV and $C = 0.7$ eV. The π band has a narrow width with $B = 0.25$ eV and $C = 0.1$ eV. Figure 1 shows $a^2\Pi_1(q, \omega)$ for the sum of the two bands as a function of ω for several values of qa . The real part is the dotted line and the imaginary part is the solid line. The imaginary part for each band has a finite width. The very narrow band at lower energy is from the π -bonded energy bands. The wider band is from the σ -bonded energy bands. $\text{Im}\Pi_1$ is nonzero over a finite range of frequencies, which does not extend to zero. For finite q there is a gap in the excitation spectrum at low frequencies. However, the Cu-O planes provide excitations which eliminate this gap.

The other interesting feature of these bands is their contribution to the plasma frequency. At large ω and small q we find for each band

$$\text{Re}\Pi_1(q, \omega) = \frac{2}{\pi} \frac{(qa)^2}{\omega^2 ab} [B^2 - (C - \mu)^2]^{1/2}. \quad (1)$$

The plane of parallel chains has a collective mode which is a two-dimensional plasmon with $\omega^2 \sim q$. This mode is a planar plasmon. It makes a strong peak in a plot of the spectral function $S(q, \omega) = \text{Im}(1/\epsilon)$. Since there are two separate chain bands, there is also an acoustic plasmon mode which has a linear dispersion $\omega \sim q$ at long wavelength. We call this the first acoustical plasmon. It can

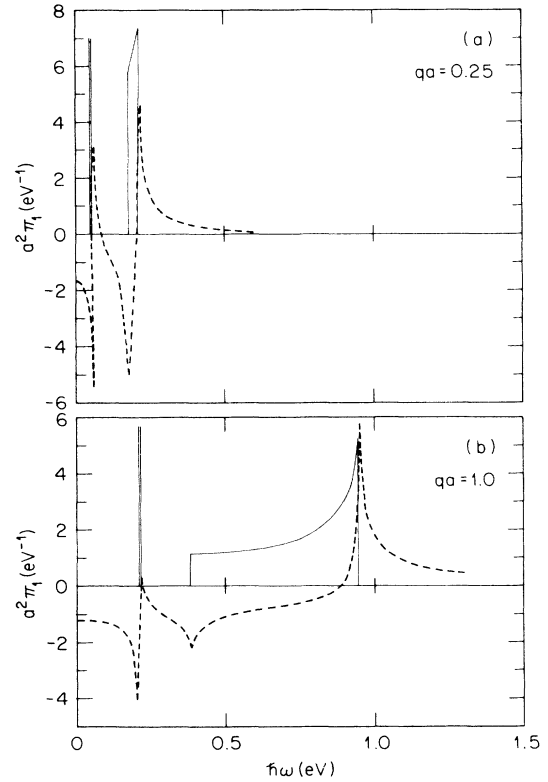


FIG. 1. The polarization response of the conduction electrons in a single chain. Solid line is the imaginary part of $a^2\Pi_1$ and the dashed line is the real part. (a) has $qa = 0.25$ and (b) has $qa = 1.0$. Horizontal axis is frequency in units of electron volts. Vertical axis has units of inverse electron volts.

be deduced from Fig. 1 by the fact that $\text{Re}\Pi_1$ crosses zero in the low-frequency region where $\text{Im}\Pi_1 = 0$. One can also see that its oscillator strength is small. This strength is proportional to $(\text{Re}\partial\Pi_1/\partial\omega)^{-1}$ at the pole, and the slope is obviously large in this region. The acoustic plasmon makes a negligible peak in $S(q, \omega)$. Its strength is about 1% or 2% of that of the planar plasmon. It is sufficiently weak that we choose to ignore it. Some band-structure calculations do not have the π -bonded chain band crossing the Fermi surface.²⁶ If we leave it out, the main result is that we lose the presence of this very weak acoustic plasmon. Thus, there is negligible difference in the plasmon model between a three- or four-band model.

B. Planes

Each of the planes has a σ -bonded band of wide width which crosses the Fermi surface. These bands are approximately half full. The Fermi surface is nearly a circle about the zone corner—which is designated as the S point.²⁵ In order to have a simple band dispersion which produces a hole Fermi surface which is circular, we employ the dispersion relation

$$\epsilon(k) = E_0 - \Delta k^2,$$

where $E_0 = 1.7$ eV. We assume that the unit cell is square and $a = b$. That is, we ignore the distortion associated with $a \neq b$. This simple form reproduces well the unoccupied band states, but is poor for the occupied electron states. The density of states in the band is a constant equal to $1/\Delta$. We estimate $\Delta \sim 4.8$ eV \AA^2 . The simple functional form for $\epsilon(k)$ makes it easy to calculate the polarizability correlation function for this band, which we call $\Pi_2(q, \omega)$.

$$\begin{aligned} \text{Im}\Pi_2(q, \omega) &= \frac{1}{4\pi\Delta^2q^2} \{ [4\Delta^2q^2k_F^2 - (\omega - \Delta q^2)^2]^{1/2} - [4\Delta^2q^2k_F^2 - (\omega + \Delta q^2)^2]^{1/2} \}, \\ \text{Re}\Pi_2(q, \omega) &= \frac{-1}{4\pi\Delta^2q^2} \{ 2\Delta q^2 + [(\omega - \Delta q^2)^2 - 4\Delta^2q^2k_F^2]^{1/2} - [(\omega + \Delta q^2)^2 - 4\Delta^2q^2k_F^2]^{1/2} \}. \end{aligned} \quad (2)$$

The square-root terms are only included when their argument is positive. Besides Δ , the other important parameter is the Fermi wave vector which we estimate²⁵ to be $k_F \sim 0.7\pi/a$. At high frequency and at low wave vector the contribution to the planar plasmon is

$$\text{Re}\Pi_2(q, \omega) \sim \frac{\Delta}{\pi} \frac{k_F^2 q^2}{\omega^2}. \quad (3)$$

Figure 2 shows plots of $a^2\Pi_2$ in units of $(1/\text{eV})$ as a function of ω for several values of qa . The solid line is the imaginary part, while the dashed line is the real part. The behavior is very similar to the electron gas in three dimensions, where $\text{Im}\Pi_2$ is linear in ω for small frequencies.

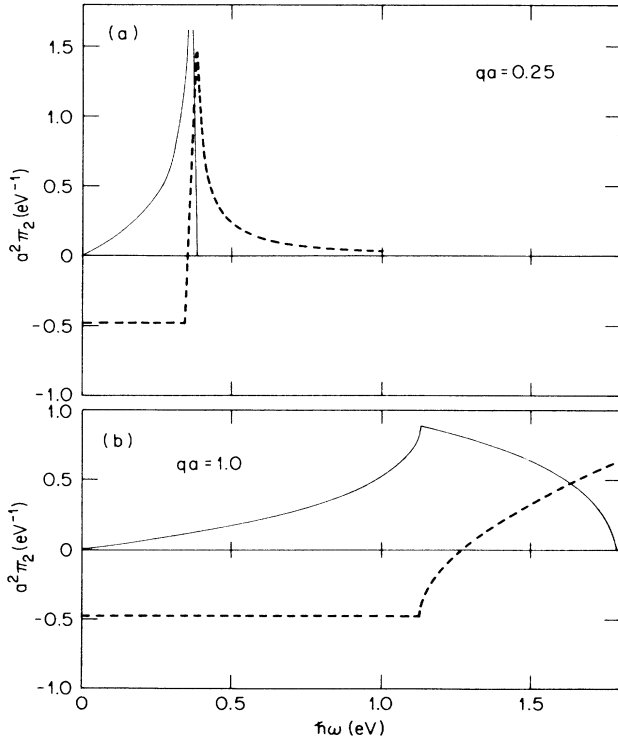


FIG. 2. The polarization response of the conduction electrons in a single plane. Solid line is the imaginary part of $a^2\Pi_2$ and the dashed line is the real part. (a) has $qa = 0.25$ and (b) has $qa = 1.0$. Horizontal axis is frequency in units of electron volts. Vertical axis has units of inverse electron volts.

C. Coupling between planes and chains

We assume that the chains and planes are sufficiently separated and that their only interaction is through the Coulomb potential. The two-dimensional transform of the three-dimensional Coulomb interaction produces an interaction between planes of the form $\exp(-q|z|)$:

$$\begin{aligned} \frac{1}{r} &= \int \frac{d^2q}{(2\pi)^2} v_q e^{i\mathbf{q} \cdot \boldsymbol{\rho} - q|z|}, \\ v_q &= 2\pi e^2/q\epsilon_0, \end{aligned}$$

where ϵ_0 is the background dielectric constant. We are unsure whether this important parameter should have a low value $\epsilon_0 \sim 2$ (electronic) or a high value $\epsilon_0 \sim 10$ (including phonons).

Use the indices 2,1,3 in order to denote the top plane, the plane of chains, and the lower plane. The c -axis separation between planes and chains is $d = 4.15$ \AA . Denote $S_{\alpha\beta}$ as the quantity which is equivalent to $1/\epsilon(q, \omega)$ between planes α and β . The expansion for the density-density correlation function produces the matrix equation

$$S_{\alpha\beta} = e^{-q|z_\alpha - z_\beta|} + v_q \sum_\gamma \Pi_\gamma(q, \omega) e^{-q|z_\alpha - z_\gamma|} S_{\gamma\beta}(q, \omega).$$

These equations are easily solved. The solutions can be presented in compact form by defining some quantities:

$$\begin{aligned} \chi_\alpha &\equiv v_q \Pi_\alpha, \quad \theta = qd, \\ V^{(\pm)} &= 1 - \chi_2(1 \pm e^{-2\theta}), \\ D &= V^{(+)} - \chi_1 V^{(-)}, \end{aligned} \quad (4)$$

then

$$\begin{aligned} S_{11} &= V^{(-)}/D, \quad S_{12} = e^{-\theta}/D, \\ S_{22} &= [1 - (1 - e^{-2\theta})(\chi_1 + \chi_2 e^{-2\theta}/V^{(-)})]/D, \\ S_{23} &= e^{-2\theta}/V^{(-)}D, \\ S_{21} &= e^{-\theta}[\chi_1 + e^{-\theta}(1 - \chi_1)]/D. \end{aligned}$$

Later we will discuss the coupling between the two planes in detail. When coupling two identical objects, one is always interested in the symmetric and antisymmetric components. Thus, between the two planes we have

$$S_+ = \frac{1}{2} (S_{22} + S_{23}) = [1 + e^{-2\theta} - \chi_1(1 - e^{-2\theta})]/2D, \quad (5)$$

$$S_- = \frac{1}{2} (S_{22} - S_{23}) = \frac{1}{2} (1 - e^{-2\theta})/V^{(-)}.$$

D. Plasmons

The symmetric interaction S_+ has the denominator D in Eq. (4). It has two collective plasmon modes from the interaction between chains and planes. D is evaluated in the limit of large frequency and for $a=b$

$$\lim_{\omega \rightarrow \infty} D = 1 - \frac{\omega_{2+}^2}{\omega^2} - \frac{\omega_{1q}^2}{\omega^2} \left(1 - \frac{\omega_{2-}^2}{\omega^2} \right),$$

$$\omega_{1q}^2 = g_1 q \cos^2 \theta_x,$$

$$g_1 = 4e^2 \sum_a [B_a^2 - (C_a - \mu)^2]^{1/2} / \epsilon_0,$$

$$\omega_{2\pm}^2 = \omega_{2q}^2 (1 \pm e^{-2\theta}),$$

$$\omega_{2q}^2 = g_2 q, \quad g_2 = 2e^2 \Delta k_f^2 / \epsilon_0.$$

We estimate $g_1 = 30 \text{ eV}^2 \text{ \AA}$ and $g_2 = 23 \text{ eV}^2 \text{ \AA}$. The equation $D=0$ has two solutions

$$\omega^2 = \frac{1}{2} (\omega_{2+}^2 + \omega_{1q}^2) \pm \frac{1}{2} [(\omega_{2+}^2 + \omega_{1q}^2)^2 - 4\omega_{1q}^2 \omega_{2-}^2]^{1/2}. \quad (6)$$

The $+$ mode is a planar plasmon with a dispersion $\omega \sim \sqrt{q}$. It is denoted $\omega_p(q)$. The $-$ mode has a long-wavelength dispersion of $\omega \sim v_{a2} q$. We call it the second acoustical plasmon ω_{a2} . We estimate its velocity as

$$v_{a2} = \left| \frac{2dg_1 g_2 \cos^2 \theta}{g_1 \cos^2 \theta + 2g_2} \right|^{1/2} \sim 8.7 \text{ eV \AA} = 1.3 \times 10^8 \text{ cm/s},$$

where the numerical estimate for v_{a2} is for $\cos \theta = 1$. Both ω_p and ω_{a2} depend upon the angle θ that the q vector makes in the xy plane. These two modes were previously described by Griffin.¹⁸

The antisymmetric coupling S_- has the denominator $V^{(-)}$ in Eq. (5). Setting $V^{(-)}$ to zero in the plasmon limit produces another mode which is called the third acoustical plasmon $\omega_{a3} = \omega_{2-}$. Its velocity at long wavelength is

$$v_{a3} = (2dg_2)^{1/2} \sim 14 \text{ eV \AA} = 2.1 \times 10^8 \text{ cm/s}.$$

This mode does not couple to the chains, so it does not depend upon the angle θ of the wave vector in the plane. It is isotropic in two dimensions in the approximation that the unit cell is square and $a=b$.

We have used the Fermi surface model which has four bands crossing the chemical potential. Two one-dimensional bands are from the chains, and two two-dimensional bands are from the planes. Each band produces a plasmon mode. The Coulomb interaction couples these modes. The result at long wavelength is one planar plasmon with $\omega \sim \sqrt{q}$ and three acoustical plasmons with $\omega \sim q$. One acoustical plasmon mode comes from the beating of the two one-dimensional bands. It has such a small oscillator strength that we have chosen to ignore it. The other two acoustical plasmon modes have much stronger oscillator strengths.

In Sec. III we will investigate whether any of these plasmons can serve as an intermediate boson which can pair electrons in a theory of superconductivity. In this pairing calculation, we shall use the "plasmon pole" approximation. Here one assumes that the coupling func-

tions $S_{\pm}(q, \omega)$ have a frequency dependence given by simple poles at the various plasma frequencies. The residues M_j^2 for the modes ω_j are important quantities. In particular, we approximate

$$v_q S_+ = v_{c+} + M_p^2 2\omega_p / (\omega^2 - \omega_p^2) + M_{a2}^2 2\omega_{a2} / (\omega^2 - \omega_{a2}^2),$$

$$v_q S_- = v_{c-} + M_{a3}^2 2\omega_{a3} / (\omega^2 - \omega_{a3}^2), \quad (7)$$

where

$$v_{c\pm} = \frac{1}{2} v_q (1 \pm e^{-2\theta}),$$

$$M_p^2 = v_q \omega_p [\omega_p^2 (1 + e^{-2\theta}) - \omega_{1q}^2 (1 - e^{-2\theta})] / 4T,$$

$$M_{a2}^2 = v_q \omega_{a2} [\omega_{1q}^2 (1 - e^{-2\theta}) - \omega_{a2}^2 (1 + e^{-2\theta})] / 4T, \quad (8)$$

$$M_{a3}^2 = v_q \omega_{a3} (1 - e^{-2\theta}) / 4,$$

$$T = [(\omega_{2+}^2 + \omega_{1q}^2)^2 - 4\omega_{2-}^2 \omega_{1q}^2]^{1/2}.$$

Figure 3 shows a graph of these three modes and their coupling constant as a function of q . At long wavelength the coupling constant of the planar plasmon goes as $M_p^2 \sim 1/\sqrt{q}$ which diverges at the origin. The coupling constant for acoustical plasmons goes as $\sim q$. The results shown in this figure are calculated from the plasmon-pole equations (7) and (8). A more accurate way to find the matrix elements is to calculate the complete screening function $S_{\alpha\beta}(q, \omega)$ and to numerically find the strength of its poles. The resulting curve is quite similar, except that all matrix elements have their intensity reduced at large q . Furthermore, the entire intensity of the $a2$ mode is significantly reduced by Landau damping.

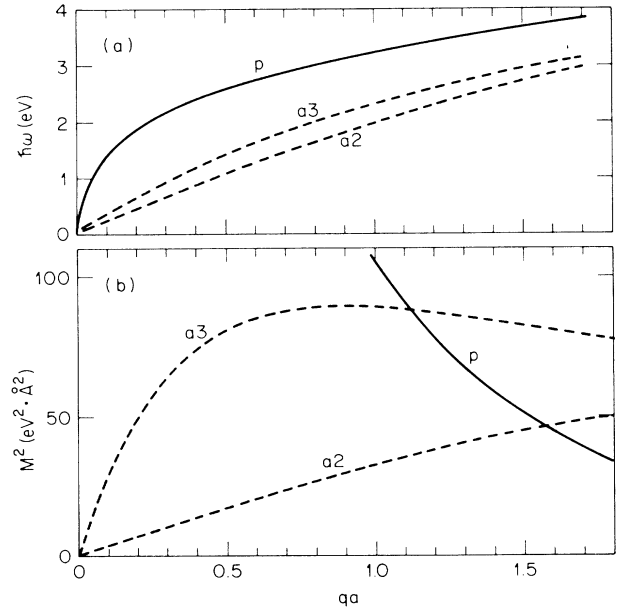


FIG. 3. Dielectric response in the plasmon pole approximation. (a) shows the dispersion of the planar plasmon (labeled p) and two acoustical plasmons. (b) shows the value of the matrix element as a function of q . The matrix element for the planar plasmon diverges as $1/\sqrt{q}$ at small q . Inclusion of Landau damping significantly reduces the matrix element $a2$.

E. Landau damping

Plasmon lifetime is an important consideration in pairing theory. One of the most important mechanisms for causing the decay of the charge density excitations is having them create electron-hole pairs. This process is called Landau damping. Electron-hole pair excitations may be created in either the chains or planes. However, the chains have a gap in the excitation spectra at low frequency. Long-wavelength excitations can only have Landau damping from the pairs in the planes. Pairs are created whenever $\text{Im}\Pi(q, \omega)$ is nonzero. Equation (1) shows that this occurs when

$$4\Delta^2 k_F^2 q^2 > (\omega - \Delta q^2)^2.$$

At long wavelength this expression reduces to $qv_L > \omega$ where

$$v_L = 2\Delta k_F \sim 5.5 \text{ eV } \text{\AA} = 8.4 \times 10^7 \text{ cm/s}.$$

The region of Landau damping is bounded by a line with a slope v_L . The numerical value of v_L is less than the velocity of the third acoustical plasmon, and we conclude it is undamped. The planar plasmon ω_p is also undamped. The second acoustical plasmon has a velocity that depends upon the angle θ that the wave vector makes in the xy plane. The velocity vanishes in the y direction. The mode is undamped for $|\cos\theta|=1$, and is damped when $\cos\theta=0$. So the mode is damped for plasmons headed in the y direction and is not damped for plasmons headed in the x direction. The first acoustical plasmon does have Landau damping, which is another reason it can be neglected.

III. PAIRING THEORY

In Sec. II we derived the excitation spectra for charge-density fluctuations in a system of three layers: two parallel planes, with another plane of chains midway between them. The parameters are chosen to model the 1:2:3 superconductors. Here we include these excitations in a strong-coupling theory of superconductivity. Our goal is to determine whether they can provide the intermediate boson which pairs electrons into the superconducting state. Our conclusion is that they do not cause pairing.

A. Gap equations

Our calculations utilize the strong-coupling theory of superconductivity. We introduce functions which describe the correlation between electrons of wave vector k , spin σ , and band index l

$$G_{ll'}(k, \tau - \tau') = -\langle T_{\tau} c_{kl\sigma}(\tau) c_{kl\sigma}^{\dagger}(\tau') \rangle, \quad (9)$$

$$F_{ll'}(k, \tau - \tau') = \langle T_{\tau} c_{-kl}(\tau) c_{kl}(\tau') \rangle.$$

They are used to define self-energy functions in the super-

conducting state

$$\Sigma_{ll'}(k, i\kappa) = -\int \frac{d^2q}{(2\pi)^2} v_q \frac{1}{\beta} \sum_{i,q} S_{ll'}(\mathbf{q}, iq) \times G_{ll'}(\mathbf{k} + \mathbf{q}, i\kappa + iq), \quad (10)$$

$$W_{ll'}(k, i\kappa) = -\int \frac{d^2q}{(2\pi)^2} v_q \frac{1}{\beta} \sum_{i,q} S_{ll'}(\mathbf{q}, iq) \times F_{ll'}(\mathbf{k} + \mathbf{q}, i\kappa + iq).$$

Phonon contributions are omitted, since the goal is to examine whether electron-based charge-density fluctuations can cause superconductivity. The quantities $S_{ll'}$ are the interlayer screening functions which were derived in Sec. II. The standard gap equations are extended to include the coupling between different planes:

$$\begin{aligned} (i\kappa - \xi_l)G_{ll'}(i\kappa) + \Sigma_{lm}(i\kappa)G_{ml'}(i\kappa) \\ + W_{ml}(i\kappa)F_{lm}^{\dagger}(i\kappa) = \delta_{ll'}, \\ (i\kappa + \xi_l)F_{ll'}^{\dagger}(i\kappa) + \Sigma_{ml}^{\dagger}(-i\kappa)F_{ml'}^{\dagger}(i\kappa) \\ + W_{lm}^{\dagger}(i\kappa)G_{ml'}(i\kappa) = 0, \end{aligned} \quad (11)$$

where one sums over the index m . In three dimensions, the standard strong-coupling theory for electron-phonon interactions utilizes the fact that the self-energy $\Sigma(i\kappa)$ is an antisymmetric function of the imaginary frequency $i\kappa$. That approximation is not obviously valid when applied to plasmon excitations. The issue here is of energy scales. An important ingredient in providing that Σ is antisymmetric is the fact that the phonon energies are all much smaller than the Fermi energy of the electron system. However, plasma excitations have an energy scale which is the same as that of the Fermi energy. That is, the complex gap function $\Delta(\omega)$ depends upon frequency. Experiments show that the magnitude of Δ is small—on the order to 10 meV. However, the issue here is the range of energies ω over which $\Delta(\omega)$ has finite values. This range is large if the pairing is due to plasma excitations. Over that large range Σ may no longer be antisymmetric. The self-energy Σ can be divided into a symmetric and antisymmetric components. The symmetric part just renormalizes the kinetic-energy term ξ . We shall assume that this renormalization does not change between the normal and superconducting states. Thus, we only consider the antisymmetric parts of this self-energy. Then the renormalization coefficient Z is defined in the usual way as $i\kappa - \Sigma_{ll'} = i\kappa Z_{ll'}$.

For a single band the gap equations are well known. Let $z = i\kappa Z$,

$$G = \frac{z + \xi}{z^2 - E^2}, \quad F = \frac{-W}{z^2 - E^2}, \quad E^2 = \xi^2 + |W|^2. \quad (12)$$

Next consider the case of two bands. It was suggested that pairing might be easier between electrons in different planes, since then the Coulomb repulsion is reduced.^{23,24} This case is considered. The two bands are one in each plane, and they have identical dispersion. They are labeled 2 and 3. At first it appears obvious that $G_{22} = G_{33}$ and $F_{22} = F_{33}$. The relative phase between U_{23} and U_{32} is

less obvious, where U is G , F , W , or Z . The correct choice for singlet pairing is $U_{23} = U_{32}$. Other possible choices of phase are related to possible triplet pairings²³ which we shall not consider. These solutions are most simply expressed by defining $U_{\pm} = (U_{22} \pm U_{23})/2$:

$$G_{\pm} = \frac{z_{\pm} + \xi}{z_{\pm}^2 - \xi^2 - |W_{\pm}|^2}, \quad F_{\pm} = \frac{-W_{\pm}}{z_{\pm}^2 - \xi^2 - |W_{\pm}|^2}. \quad (13)$$

These functions are used to evaluate the symmetric and antisymmetric self-energies. For example, the results for W_{\pm} are

$$W_{+} = - \int \frac{d^2q}{(2\pi)^2} v_q \frac{1}{\beta} \sum_{i,q} (F_{+} S_{+} + F_{-} S_{-}), \quad (14)$$

$$W_{-} = - \int \frac{d^2q}{(2\pi)^2} v_q \frac{1}{\beta} \sum_{i,q} (F_{+} S_{-} + F_{-} S_{+}).$$

The screening functions S_{\pm} were derived in Sec. II. Similar equations define Σ_{\pm} with F replaced by G . These set of equations provide a self-consistent definition of the correlations functions F_{\pm} which are only nonzero in the superconducting state. They form the basis for the remainder of our discussion.

B. Weak-coupling solutions

The above set of equations have been solved numerically at zero temperature using the screening functions derived in Sec. II. No solution was found which had a nonzero value of the energy gap $\Delta(\omega) \equiv W/Z$. We conclude that these plasmon excitations cannot cause pairing for a superconducting state. Since our conclusion is negative—no solution is found—it is always open to the criticism that there is a solution which we missed. Therefore, we have constructed other arguments which also indicate the lack of pairing. The first of these arguments is presented here.

The key to the entire discussion is the lack of screening on the direct Coulomb interaction. This repulsive term becomes large and cancels any attractive force from the various plasmons.

The weak-coupling solutions are meant to provide a model similar to the original one of BCS. Here we call $Z=1$ and the gap function $W=\Delta$ is a constant. This model works well in the limit of weak coupling.

The first case we consider is simple. There is a single band and a single plasmon. We use the form of the gap equations in Eq. (11). For the screening function we use

$$S(q, \omega) = 1 + \omega_p^2 / (\omega^2 - \omega_p^2). \quad (15)$$

Evaluating the Matsubara summation at zero temperature gives

$$\frac{1}{\beta} \sum_{i,q} S(q, iq) F(p+q, i\kappa+iq) = \Delta/2(E + \omega_p).$$

The gap equation for a single plasmon band becomes

$$\Delta = - \frac{\Delta}{2} \int \frac{d^2q}{(2\pi)^2} \frac{v_q}{E + \omega_p}. \quad (16)$$

The integral is a positive number since every factor in it is positive. Therefore, it is impossible to satisfy this equation since a positive number cannot be equal to a negative one. Thus, a single band of electrons cannot become superconducting through the interaction with a single plasmon mode. Note that this argument does not depend upon the dimensionality of the band nor the plasmon. The result applies also to three dimensions. Of course, it is well known there, since plasmon oscillations do not make aluminum into a high-temperature superconductor.

The same derivation can be made more rigorous with regard to the treatment of the dielectric function. Using the sign convention that $\text{Im}(1/\epsilon) < 0$ then an exact representation for $1/\epsilon(q, z) = S(q, z)$ is

$$S(q, z) = 1 - \frac{1}{2} [I(z) + I(-z)],$$

where

$$I(z) = - \frac{2}{\pi} \int_0^{\infty} d\omega \text{Im} \left[\frac{1}{\epsilon(q, \omega)} \right] \left[\frac{1}{\omega + z} \right].$$

Then, the equation for the gap function at zero temperature in the weak-coupling approximation is

$$\Delta = - \frac{\Delta}{2} \int \frac{d^2q}{(2\pi)^2} v_q \frac{1 - I(E)}{E}. \quad (17)$$

Since $I(0) > I(E)$ it is easy to prove the inequality

$$1 - I(E) > 1 - I(0) = 1/\epsilon(q, 0) > 0.$$

We have again that the integral in Eq. (17) is positive since everything in its integrand is positive. The gap function cannot be satisfied. The weak-coupling argument is valid for any kind of screening model.

The above argument suggests that there can never be superconductivity, even when mediated by phonons. Since this conclusion is wrong, the question is, how is the above argument changed by phonons? For the weak-coupling model, phonons permit the static dielectric function $S(q, 0)$ to be negative at large values of q . The integral in Eq. (17) can be negative because the integrand has negative regions, which permits the equation to be satisfied. This argument is discussed in detail in the Appendix.

We cheerfully admit that the above arguments are inconsistent. We began by constructing a dielectric function which was valid at long wavelengths, and then ended by using it to describe behavior at short wavelengths. However, our real conclusion is that superconductivity is not caused by the behavior of long-wavelength excitations. If it happens, it is due to excitations of short wavelength. This point is important since most proposed models of high-temperature superconductivity, from charge-density fluctuations, have been based on long-wavelength behavior. Our analysis shows that none of these long-wavelength models can cause superconductivity. Our model is not valid at large q for several reasons. Thus, we cannot prove or disprove models of superconductivity based upon excitations of short wavelength. In order to have a dielectric function which is valid at short wavelengths, we would have to construct it according to the method used in Ref. 29.

The next example of plasmon coupling is the two-band

model of Eq. (13). These equations encompass two important conjectures for the cause of high-temperature superconductivity. One is that the paired electrons are in different planes.^{23,24} Pairing is enhanced because the Coulomb repulsion is less. The second conjecture is that interlayer plasmons are important for causing the pairing. Our calculations suggest that neither of these conjectures are correct.

The frequency summations in Eq. (14) are evaluated in

$$H_+(\Delta) = \int \frac{d^2q}{(2\pi)^2} v_q \frac{[\omega_1^2(1 - e^{-2\theta}) + (\omega_p\omega_{a2} + E\omega_p + E\omega_{a2})(1 + e^{-2\theta})]}{2(E + \omega_p)(E + \omega_{a2})(\omega_p + \omega_{a2})},$$

$$H_-(\Delta) = \int \frac{d^2q}{(2\pi)^2} v_q \frac{1 - e^{-2\theta}}{2(E + \omega_{a3})},$$

where Δ means either Δ_{\pm} which is part of $E(\Delta)$. The set of equations has a solution only if

$$0 = 1 + H_+(\Delta_+) + H_+(\Delta_-) + H_+(\Delta_+)H_+(\Delta_-) - H_-(\Delta_+)H_-(\Delta_-).$$

However, it is easy to show that no solution is possible because of the identity

$$H_+(\Delta) > H_-(\Delta) > 0.$$

Earlier we derived Eq. (16) for a single band of electrons interacting with a single plasmon. The present analysis is the equivalent derivation for two planes and three plasmons. There is no pairing possible in the weak-coupling limit. Thus, we have shown that (i) interlayer pairing does not enhance superconductivity, and (ii) interlayer plasmons do not enhance superconductivity.

We have considered a variety of other models related to plasmons. For example, we have examined the other ordering of planes such as 1-2-3-1. We have removed the chains and considered the symmetric and antisymmetric modes which result by coupling two planes. None of these cases produces pairing of electrons. In each case, the arguments are quite similar to those detailed above. We have also done calculations where we avoided the plasmon-pole approximation. We separated out the pair and pole terms in the loss function, and use the pair part to partially screen the direction Coulomb interaction at large values of q . This complicated analysis also does not produce pairing. Each case has the same feature that the repulsive Coulomb interaction is large and overwhelms any attractive force from the plasmons.

C. Strong-coupling results

The strong-coupling gap equations in (13) and (14) can be solved numerically for plasmon-induced pairing mechanism by following the standard procedures used in solving the pairing state induced by electron-phonon coupling. The existence of a superconducting-ground state is indicated by a solution with $F \neq 0$ and $W \neq 0$ from the gap equations. Generally speaking, whether a system can

the weak-coupling approximation, and at zero temperature. This assumes that $Z=1$, $\Delta_{\pm} = \text{const}$, and $\kappa=0$. Then we find

$$\Delta_+ = -\Delta_+H_+(\Delta_+) - \Delta_-H_-(\Delta_-),$$

$$\Delta_- = -\Delta_+H_-(\Delta_+) - \Delta_-H_+(\Delta_-),$$
(18)

where

have a superconducting ground state depends on the relative strengths of two competing interactions. The electron-boson interaction provides the attractive mechanism for electrons to form superconducting pairs, while the repulsive interaction between electrons tends to suppress pairing and push the system into the normal state with $F=0$, $W=0$.

In calculating phonon-induced superconductivity, the repulsive interaction is taken to be the statically screened Coulomb interaction. The phonon frequencies are usually much smaller than the electron-plasmon frequency or the Fermi energy, so the effect of high-frequency excitations such as plasmons can be approximately included as reducing the bare Coulomb interaction into a screened one. In the static limit, the screened Coulomb interaction is always repulsive.

When investigating possible superconductivity induced by the plasmon mechanism, the two competing interactions are bare Coulomb interaction and electron-plasmon coupling, respectively. Each needs to be treated more carefully. We can separate the two interactions using the screening matrix S defined in Eq. (7), where, on the right side, the first term stands for the bare Coulomb interaction and the second term is the electron-plasmon coupling term which provides the attractive interaction for possible pairing between electrons. The latter is to be solved self-consistently from the matrix equation. The integral Eq. (10) for the gap function can be solved with the kernel S given above. The Green's functions G and F are expressed in terms of Σ and W from Eq. (13). Following standard procedures of carrying out the Matsubara summation and integrating out the ξ_{k+q} variables in G and F , Eqs. (13) are reduced into coupled one-dimensional integral equations. These equations are then solved by numerical integration. Despite varying over a wide range the related material parameters such as electron effective mass, background dielectric constant ϵ_0 , electron density, and interlayer distance, the solution always gives $W=0$. Therefore, the numerical solution from the strong-coupling theory leads to the conclusion that plasmons do not pair electrons into a superconducting state.

To make sure that our numerical results do not miss any possible solution with a finite-gap function, we ana-

lyzed the strong-coupling equations in detail. First, to ensure the numerical accuracy of our computation, we calculated the electron-phonon-induced superconductivity for a typical strong-coupling system (Pb) and found very good agreement with the result from existing literature.²⁷ To further extract physics from the numerical solution, we also performed calculations in which the direct Coulomb interaction v_c was reduced by an arbitrary numerical factor while the electron-plasmon coupling was kept to have the same strength as in a real physical system. When the Coulomb interaction is suppressed sufficiently by this artificial step, a nonzero gap function starts to emerge from the numerical solution. The amplitude of the gap function increases as the Coulomb interaction is further reduced. This observation indicates that the electron-plasmon interaction has the right tendency of forming superconductivity paired states. However, for a real physical system, both the bare Coulomb interaction and the electron-plasmon interaction originate from the electron-electron interaction. The strengths of the two competing parts of the electron-electron interaction are correlated to each other and cannot be varied arbitrarily by choosing material parameters of the system. The net effect of the electron-electron interaction is always repulsive and does not cause pairing, as demonstrated through the negative conclusion from our calculations performed for realistic systems.

D. Demonstration through empirical formula

The last argument we present to support the above conclusion is to use the following empirical formula for determining the superconducting-transition temperature:²⁸

$$k_B T_c \approx \omega_D \exp \left(- \frac{1 + \lambda}{\lambda - \mu^*} \right), \quad (19)$$

where ω_D is the upper cutoff energy of the intermediate boson, λ is the electron-boson coupling parameter,

$$\lambda = 2 \int_0^{\omega_D} \frac{\alpha^2 F(u)}{u} du, \quad (20)$$

with $\alpha^2 F(\omega)$ being the McMillan function for the appropriate interaction in consideration. The modified Coulomb interaction

$$\mu^* = \frac{\mu}{1 + \mu \ln(E_F/\omega_D)}, \quad (21)$$

is related to the averaged Coulomb repulsion μ . For electron-phonon interaction, μ^* is significantly reduced from μ because the electron Fermi energy E_F is much larger than the phonon Debye energy ω_D . A finite T_c exist for system with λ sufficiently larger than μ^* , as is the case of phonon-mediated superconducting systems. Recently, a similar argument has been applied to electron-plasma interaction in the context of explaining high- T_c superconductivity.¹⁴ However, in discussing the electron-plasmon mechanism, the parameters λ , μ , E_F , and ω_D are not independent to each other. It is incorrect to choose each parameter on the favorable side within the possible region, and to then fit them into the T_c formula Eq. (19).

On the contrary, when all the parameters are specified for a realistic system, Eq. (19) actually indicates that the plasmon mediated pairing would be completely suppressed by the Coulomb interaction.

As an illustration, we consider a system with a single two-dimensional electron gas layer,

$$\mu = \int \frac{dk}{(2\pi)^2} \frac{V_q}{\hbar v_F}, \quad (22)$$

and

$$\alpha^2 F(\nu) = \int \frac{dk}{(2\pi)^2} \frac{M_q^2}{\hbar v_F} \delta(\nu - \omega_q). \quad (23)$$

In both equations the wave-vector integrals are over the closed circular Fermi loop. In the second equation, M_q is the electron-plasmon matrix element and ω_q is the plasmon frequency. To consider the most favorable situation for superconductivity, we ignore the effect of Landau damping in reducing the electron-plasmon coupling parameter λ , and evaluate the matrix element M_q in the plasmon-pole approximation. Applying the f -sum rule for screening function leads to the identity

$$M_q^2 = V_q \frac{\omega_q}{2}. \quad (24)$$

Combining Eqs. (20)-(25) immediately gives the following simple relation between the two interaction parameters

$$\lambda = \mu. \quad (25)$$

It is also easy to verify that the plasmon cutoff frequency $\omega_D(\omega_q, q = 2k_F)$ for an electron gas is always larger than E_F for realistic choices of material parameters. So the modified Coulomb interaction μ^* is not reduced from μ by using Eq. (21). With all these considerations, it is quite clear that Eq. (19) does not yield a finite-transition temperature for electron-plasmon coupling in a single plane. Similar arguments have been applied to interlayer pairing between two planes, where we obtain the same conclusion.

IV. DISCUSSION

We have concluded that long-wavelength plasmons cannot cause electron pairing in high-temperature superconductors. That negative conclusion applies to both interlayer and intralayer s -wave pairing. We again emphasize that our calculations are only valid at long wavelengths. An accurate calculation at short wavelengths might come to an opposite conclusion. However, a short-wavelength calculation requires a full band-structure calculation for the response function $S(q, q', \omega)$, which is beyond our capability at this time.

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APPENDIX

In order to illustrate the role of phonons, consider the following simple but standard model for a metal with one longitudinal acoustical phonon. At long wavelengths one can write for the total dielectric function from electrons and phonons

$$S(q,z) = \frac{1 + \Lambda(q,z)}{1 - v_q P(q,z) [1 + \Lambda(q,z)]},$$

where $P(q,z)$ is the electron polarization operator in the RPA, while $\Lambda(q,z)$ is the ratio of the phonon mediated interaction divided by v_q . Writing the electron-ion interaction as $V_{ei}(q) = v_q C(q)$, where $C(q)$ is the influence of

the pseudopotential, we have

$$\Lambda(q,z) = -\frac{\omega_i^2 C(q)^2}{\omega_i^2 - z^2},$$

where ω_i is the ion plasma frequency. Thus, the static dielectric function ($z=0$) is

$$S(q,0) = \frac{\omega_i^2 [1 - C(q)^2]}{\epsilon(q) \omega(q)^2},$$

$$\omega(q)^2 = \omega_i^2 \left[1 - C(q)^2 \left(1 - \frac{1}{\epsilon(q)} \right) \right],$$

where $\epsilon(q)$ is the static dielectric function in RPA, and $\omega(q)$ are the phonons modes in the metal. $S(q,0)$ can be negative if $C(q)^2 > 1$. This can happen at large values of q without violating the obvious constraint that $\omega(q)^2 > 0$. Phonons permit the total dielectric function to be negative at large values of q , which then permits superconductivity in the weak-coupling model.

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- ¹J. G. Bednorz and K. A. Müller, *Z. Phys. B* **64**, 189 (1986).
²M. K. Wu, J. R. Ashburn, C. J. Torng, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, Y. Q. Wang, and C. W. Chu, *Phys. Rev. Lett.* **58**, 908 (1987).
³Z. Zhongxian *et al.*, *Kexue Tongbao* **32**, 661 (1987).
⁴P. J. M. van Bentum, L. E. C. van de Leemput, L. W. M. Schreurs, P. A. A. Teunissen, and H. van Kempen, *Phys. Rev. B* **36**, 843 (1987).
⁵L. C. Bourne, M. F. Crommie, A. Zettl, H.-C. zur Loye, S. W. Keller, K. L. Leary, A. M. Stacy, K. J. Chang, M. L. Cohen, and D. E. Morris, *Phys. Rev. Lett.* **58**, 2337 (1987).
⁶B. Batlogg, R. J. Cava, A. Jayaraman, R. B. van Dover, G. A. Kourouklis, S. Sunshine, D. W. Murphy, L. W. Rupp, H. S. Chen, A. White, K. T. Short, A. M. Mjjsce, and E. A. Rietman, *Phys. Rev. Lett.* **58**, 2333 (1987).
⁷K. J. Leary, H.-C. zur Loye, S. W. Keller, T. A. Faltens, W. K. Ham, J. N. Michaels, and A. M. Stacy, *Phys. Rev. Lett.* **59**, 1236 (1987).
⁸J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).
⁹*High Temperature Superconductivity*, edited by V. L. Ginzburg and D. A. Kirzhnits (Consultants Bureau, New York, 1982).
¹⁰G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
¹¹P. W. Anderson, *Science* **235**, 1196 (1987).
¹²V. J. Emery, *Phys. Rev. Lett.* **59**, 2794 (1987).
¹³R. H. Parmenter, *Phys. Rev. Lett.* **59**, 923 (1987).
¹⁴J. Ruvalds, *Phys. Rev. B* **35**, 8869 (1987).
¹⁵Z. Tešanović, *Phys. Rev. B* **36**, 2364 (1987).
¹⁶J. Ashkenazi, C. G. Kuper, and R. Tyk, *Solid State Commun.* **63**, 1145 (1987).
¹⁷J. I. Gersten, *Phys. Rev. B* **37**, 1616 (1988).
¹⁸A. Griffin (unpublished).
¹⁹C. M. Varma, S. Schmitt-Rink, and E. Abrahams, *Solid State Commun.* **62**, 681 (1987).
²⁰J. Hirsch, S. Tang, E. Loh, and D. Scalapino, *Phys. Rev. Lett.* **60**, 1668 (1988).
²¹S. H. Liu (unpublished).
²²L. Mattheiss and D. Hamann, *Physica B* **148**, 271 (1987).
²³M. Inoue, T. Takemori, K. Ohtaka, R. Yoshizaki, and T. Sakudo, *Solid State Commun.* **63**, 201 (1987); *J. Phys. Soc. Jpn.* **56**, 3622 (1987).
²⁴C.-F. Chen, D.-L. Yin, and R. S. Han, *Solid State Commun.* **63**, 411 (1987).
²⁵J. Yu, S. Massida, A. J. Freeman, and D. D. Koelling, *Phys. Lett.* **122**, 203 (1987).
²⁶L. F. Mattheiss, *Solid State Commun.* **63**, 395 (1987).
²⁷W. Shaw and J. C. Swihart, *Phys. Rev. Lett.* **20**, 1000 (1968).
²⁸W. L. McMillian, *Phys. Rev.* **167**, 331 (1968).
²⁹W. Hanke and L. J. Sham, *Phys. Rev. B* **12**, 4501 (1975).