Theory of high-temperature superconductivity

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A theory for high-temperature superconductivity is developed based on a hydrodynamic approximation to the many-body problem. Electrons confined to two-dimensional sheets exchange coupled two-dimensional plasmon and phonon modes. This leads to a strong electron-electron attraction. Bardeen-Cooper-Schrieffer theory is used to derive an expression for the transition temperature. The superconductivity comes about because of the existence of a low-frequency mode. Experimental consequences of theory are discussed.

I. INTRODUCTION

Recent experiments on high-temperature superconductors[1-6] reveal important information on both the structure and dynamics of such materials. A modified perovskite structure containing somewhat isolated planes of copper oxide is found. Band-structure calculations[7,8] indicate that these planes contain a significant number of free electrons. It also appears necessary to have multivalent ions, such as copper, in the crystal. The transition temperature is very sensitive to the stoichiometry and seems to be correlated with a mode-softening transition. In this paper a model based on the above observations is presented which offers a possible explanation for the high T_c. Because of the recent explosion of interest in this class of materials, it is difficult to cite all the relevant literature. The references merely represent a selection of some of the work related to points raised in this paper.

As we shall see, the theory will lean very heavily on the existence of a low-frequency mode in the system. The existence of this mode will permit us to calculate the transition temperature, to account for some of the observed experiments, and to make predictions for future experiments. In Sec. II the theory is developed and in Sec. III the results are discussed and the experimental consequences are explored.

II. THEORY

In the model I consider a set of two-dimensional electron-gas layers interacting with acoustic lattice vibrations. The layers are well separated from each other and to a first approximation may be treated as noninteracting. We therefore focus our attention on a single layer. The electron gas lies in the copper oxide plane ($z=0$) and is taken to be azimuthally isotropic. It will be assumed that the elastic properties in directions parallel and perpendicular to the plane are considerably different. This is consistent with the crystalline structure determined from x-ray scattering and with the existence of an observed structural phase transition. In directions parallel to the plane the modes are taken to be much softer than in a direction perpendicular to the plane. This leads to a decoupling of the respective modes and each mode may be studied separately. The modes propagating along the c axis are taken to be conventional acoustic phonons. We will primarily focus our attention here on those modes propagating perpendicular to the c axis. The approach is similar to that previously taken in studying surface excitations.[9]

Let M denote the mass of a complete unit cell of the crystal. In analyzing the charge distribution in the $z=0$ plane one must include the ionic charge, the free-electron charge, and the electronic charge that is bound to the ions. The free electron charge per unit area is N_e. The sum of the ionic charge and the bound electronic charge lying in a unit-cell projection on the plane $z=0$ is denoted by Ze. Note that Z need not be an integer. Let $\mathbf{u}(\mathbf{R},t)$ denote the two-dimensional displacement vector field, where $\mathbf{R}=\hat{\mathbf{i}}x+\hat{\mathbf{j}}y$.

In writing the equation of motion for the ions, the force is expressed as a sum of two contributions: the Coulomb force and the non-Coulomb force associated with chemical bonding or antibonding. It should be noted that band-structure calculations[7,8] show a significant occupancy of antibonding states. The non-Coulomb force is represented by a set of "bare" elastic constants. For the sake of simplicity, the ionic motion is taken here to also be azimuthally isotropic. This restriction may be readily lifted. The equation of motion for the displacement of the cell is

$$M\frac{\partial^2\mathbf{u}}{\partial t^2}=Ze\mathbf{E}_p+\mu_L\nabla_p^2\mathbf{u}+(\lambda_L+\mu_L)\nabla_p\nabla_p\cdot\mathbf{u}\,. \tag{1}$$

Here, λ_L and μ_L are the "bare" Lamé constants, $\mathbf{E}_p$ is the electric field projection parallel to the plane, and ∇_p is the gradient operator in the x-y plane. There is no *a priori* reason for the bare Lamé constants to be positive. The physically measured elastic constants include Coulombic corrections to the bare Lamé constants.

Let $\mathbf{v}(\mathbf{R},t)$ be the velocity field for the two-dimensional electron gas. The equation of motion is

$$m^*\frac{\partial\mathbf{v}}{\partial t}=-e\mathbf{E}_p-\nabla_p\mu\,, \tag{2}$$

where m^* is the effective mass of the electron and μ is the chemical potential. It will suffice to take μ to be the Fermi energy corresponding to the Fermi circle for N_e electrons per unit area, $\mu=\pi N_e\hbar^2/m^*$.

The continuity equation for the ionic motion is

$$\nabla_p \cdot \left[N_i \frac{\partial \mathbf{u}}{\partial t} \right] + \frac{\partial N_i}{\partial t} = 0 , \tag{3}$$

where N_i is the number of unit-cell projections on the $z=0$ plane per unit area. Similarly, the electron continuity equation is

$$\nabla_p \cdot (N_e \mathbf{v}) + \frac{\partial N_e}{\partial t} = 0 . \tag{4}$$

Finally, Gauss's law is

$$\nabla \cdot (\overleftrightarrow{\epsilon} \cdot \mathbf{E}) = 4\pi\delta(z)(ZeN_i - eN_e + \sigma_{ex}) , \tag{5}$$

where $\overleftrightarrow{\epsilon}$ is the dielectric tensor of the medium surrounding the plane. In this equation the full three-dimensional divergence is taken. A test charge density $\sigma_{ex}(\mathbf{R},t)$ has been included to facilitate the discussion of the electron-electron interaction later. It is convenient to express $\mathbf{E}$ in terms of the electrostatic potential $\phi(\mathbf{R},z,t)$: $\mathbf{E} = -\nabla\phi$. The test charge density is taken to be a plane wave,

$$\sigma_{ex} = \sigma_0 \exp[i(\mathbf{q}_p \cdot \mathbf{R} - \omega t)] .$$

Here, $\mathbf{q}_p$ is a two-dimensional wave vector parallel to the $z=0$ plane.

Let us now proceed to study the linear response of the system. Let

$$N_e = N_e^0 + n_e \exp[i(\mathbf{q}_p \cdot \mathbf{R} - \omega t)]$$

and

$$N_i = N_i^0 + n_i \exp[i(\mathbf{q}_p \cdot \mathbf{R} - \omega t)] .$$

The quantities $\mathbf{v}$ and $\mathbf{u}$ are assumed to have similar spatial and temporal behavior. The first-order perturbed equations are

$$M\omega^2 \mathbf{u} = iZe\mathbf{q}_p\phi + \mu_L q_p^2 \mathbf{u} + (\lambda_L + \mu_L)\mathbf{q}_p \mathbf{q}_p \cdot \mathbf{u} , \tag{6}$$

$$m^* \omega \mathbf{v} = -e\mathbf{q}_p\phi + \pi n_e \mathbf{q}_p \hbar^2/m^* , \tag{7}$$

$$N_i^0 \mathbf{q}_p \cdot \mathbf{u} = i n_i , \tag{8}$$

$$N_e^0 \mathbf{q}_p \cdot \mathbf{v} = \omega n_e . \tag{9}$$

The potential is

$$\phi = -E_0 |z| + \phi_0 \exp[i(\mathbf{q}_p \cdot \mathbf{R} - \omega t) - Q|z|] . \tag{10}$$

The dielectric tensor is taken to be of the azimuthally symmetric form

$$\overleftrightarrow{\epsilon} = \epsilon_p(\hat{\mathbf{i}}\hat{\mathbf{i}} + \hat{\mathbf{j}}\hat{\mathbf{j}}) + \epsilon_z \hat{\mathbf{k}}\hat{\mathbf{k}} .$$

The amplitudes ϕ_0 and E_0 in Eq. (10) are

$$\phi_0 = \frac{2\pi}{Q\epsilon_z}(Zen_i - en_e + \sigma_0) , \tag{11}$$

$$E_0 = \frac{2\pi}{\epsilon_z}(ZeN_i^0 - eN_e^0) . \tag{12}$$

The quantities Q and q_p are related by $q_p^2\epsilon_p = Q^2\epsilon_z$.

Forming the scalar products of Eqs. (6) and (7) and $\mathbf{q}_p$ and combining them with Eqs. (8) and (9) yields

$$(\omega^2 - q_p^2c^2)n_i = N_i^0 Zeq_p^2\phi_0/M , \tag{13}$$

and

$$(\omega^2 - \Lambda^2)n_e = -N_e^0 eq_p^2\phi_0/m^* , \tag{14}$$

where $c^2(\lambda_L + 2\mu_L)/M$ and $\Lambda^2 = \pi N_e(\hbar q_p/m^*)^2$. Although we use the suggestive notation c^2 in Eq. (13), we again emphasize that it may be either positive or negative. Equations (11), (13), and (14) may be solved simultaneously to give

$$\phi = 2\pi\sigma_0(\omega^2 - \Lambda^2)(\omega^2 - q_p^2c^2)/(q_p\epsilon\Delta) . \tag{15}$$

The denominator is given by

$$\Delta = (\omega^2 - \omega_s^2)(\omega^2 - q_p^2c^2 - \Omega^2) - \omega_d^2\Omega^2 .$$

Here, ω_s is the two-dimensional electron-gas plasmon frequency defined by the equation

$$\omega_s^2 = \omega_d^2 + \Lambda^2 , \tag{16}$$

where

$$\omega_d^2 = 2\pi N_e^0 e^2 q_p/(m^*\epsilon) . \tag{17}$$

The two-dimensional ionic plasmon frequency has been denoted by Ω, where

$$\Omega^2 = 2\pi N_i^0 (Ze)^2 q_p/(M\epsilon) . \tag{18}$$

The mean dielectric constant ϵ is defined as $\epsilon = (\epsilon_p\epsilon_z)^{1/2}$. The vanishing of the dispersion curves for the electronic and ionic plasmons at $q_p = 0$ is expected for a two-dimensional system.

The roots of the equation $\Delta = (\omega^2 - \omega_+^2)(\omega^2 - \omega_-^2) = 0$ define a set of coupled electronic-ionic two-dimensional plasmon modes. The resonant frequencies are given by

$$\omega_\pm^2 = \tfrac{1}{2}\{\omega_s^2 + q_p^2c^2 + \Omega^2 \pm [(\omega_s^2 + q_p^2c^2 + \Omega^2)^2 - 4\omega_s^2 q_p^2 c^2 - 4\Lambda^2\Omega^2]^{1/2}\} . \tag{19}$$

Note that the ω_- mode goes soft when

$$\omega_s^2 q_p^2 c^2 + \Lambda^2\Omega^2 = 0 . \tag{20}$$

When this occurs, a charge-density wave is set up and the system undergoes a structural phase transition.

In terms of Eq. (15) it is simple to write a formula for the Fourier transform of the interaction energy between two electrons

$$V = \frac{2\pi e^2}{q_p \epsilon_{\text{eff}}} , \tag{21}$$

where ϵ_{eff} is an effective dielectric function defined by

$$\epsilon_{\text{eff}}(q_p,\omega) = \epsilon \frac{(\omega^2 - \omega_+^2)(\omega^2 - \omega_-^2)}{(\omega^2 - \Lambda^2)(\omega^2 - q_p^2c^2)} . \tag{22}$$

The energy V includes the direct Coulomb repulsion as well as the exchange of coupled two-dimensional electron and ion plasma modes. This interaction energy is attractive at $\omega = 0$ if $0 > \omega_s^2 q_p^2 c^2 > -\Lambda^2\Omega^2$. It is this attractive interaction which is responsible for Cooper pairing and superconductivity. A necessary condition is that the combination of bare Lamé constants $\lambda_L + \mu_L$ be negative.

The interaction energy linking two electrons separated by a distance vector r is given by Eqs. (10) and (21) as

$$V(\mathbf{r}) = \sum_{q_p} \frac{2\pi e^2}{q_p \epsilon_{\text{eff}}(\mathbf{q}_p,\omega)} \exp(i\mathbf{q}_p \cdot \mathbf{R} - q_p |z|) . \quad (23)$$

It is useful to write this as a three-dimensional Fourier transform

$$V(\mathbf{r}) = \sum_{\mathbf{q}} V_3(\mathbf{q},\omega) \exp(i\mathbf{q}\cdot\mathbf{r}) . \quad (24)$$

A comparison of these two expressions gives

$$V_3(\mathbf{q},\omega) = \int_{-\infty}^{\infty} dz \frac{2\pi e^2}{q_p \epsilon_{\text{eff}}(\mathbf{q}_p,\omega)} \exp(-iq_z z - q_p |z|) . \quad (25)$$

so

$$V_3(\mathbf{q},\omega) = \frac{4\pi e^2}{q^2 \epsilon_{\text{eff}}(\mathbf{q}_p,\omega)} . \quad (26)$$

The interaction is seen to be highly anisotropic in q space.

As one creates vacancies or inserts ions into adjacent layers in the medium surrounding the copper oxide planes, it is possible for the electron density in the copper oxide plane to be altered. Oxygen is known to be a good acceptor of electrons, so oxygen defects are expected to be good electron donors. Since copper may exist in several oxidation states, it is able to receive these donated electrons. By varying the defect concentration in nearby layers, one may change the value of the sum $(\omega_s q_p c)^2 + (\Lambda\omega^2)$. This provides us with a "tuning" mechanism whereby the mode-softening transition may be approached.

Inserting Eq. (26) in the zero-temperature BCS gap equation gives

$$\Delta_0(\mathbf{k}) = -\tfrac{1}{2} \sum_{\mathbf{k}'} V_3(\mathbf{q},\omega) \Delta_0(\mathbf{k}') [(E'-\mu)^2 + \Delta_0^2(\mathbf{k}')]^{-1/2} . \quad (27)$$

where $\omega = (E'-E)/\hbar$ and $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. Let us simplify this equation by making two assumptions, both motivated by the physics. Band-structure calculations indicate that the electronic bands are rather flat along the direction in q space parallel to the c axis.[7,8] To a first approximation we may therefore write the electron energy as a two-dimensional parabolic band

$$E' = \frac{\hbar^2 k_p'^2}{2m^*} + \text{const} . \quad (28)$$

Experiment[10] reveals that the gap function is highly anisotropic. Therefore, let us look for a solution to Eq. (27) in which the gap function $\Delta(\mathbf{k})$ is a slowly varying function of k_z. Then Eq. (27) may be rewritten as

$$\Delta_0(\mathbf{k}_p,0) \approx -\tfrac{1}{2} \sum_{\mathbf{k}_p'} \frac{4\pi e^2 \Delta_0(\mathbf{k}_p',0)}{\epsilon_{\text{eff}}(q_p,\omega)[(E'-\mu)^2 + \Delta_0^2(\mathbf{k}_p',0)]^{1/2}} \times \int_{-\infty}^{\infty} \frac{dk_z'}{2\pi} \frac{1}{(\mathbf{k}_p' - \mathbf{k}_p)^2 + k_z'^2} , \quad (29)$$

where $\mathbf{q}_p = \mathbf{k}_p' - \mathbf{k}_p$. This, in turn, may be expressed as

$$\Delta_0(\mathbf{k}_p,0) = -\tfrac{1}{2} \sum_{\mathbf{k}_p'} \frac{2\pi e^2 \Delta_0(\mathbf{k}_p',0)}{q_p \epsilon(q_p,\omega)[(E'-\mu)^2 + \Delta_0^2(\mathbf{k}_p',0)]^{1/2}} . \quad (30)$$

The problem is therefore reduced to the solution of a two-dimensional gap equation with the interaction given by Eq. (21). The gap equation may be written as

$$\Delta_0(E) = -\frac{m^*}{4\pi\hbar^2} \int dE' \frac{U(E,E')\Delta_0(E')}{[(E'-\mu)^2 + \Delta_0^2(E')]^{1/2}} , \quad (31)$$

where U is the azimuthally averaged V,

$$U(E,E') = \frac{1}{2\pi} \int_0^{2\pi} d\phi V , \quad (32)$$

and $q^2 = 2m^*[E + E' - 2(EE')^{1/2}\cos\phi]/\hbar^2$.

Since the frequencies associated with ionic motion are low compared with electronic frequencies,

$$4[(\omega_s q_p c)^2 + (\Lambda\Omega)^2] \ll [\omega_s^2 + (q_p c)^2 + \Omega^2]^2 ,$$

and thus Eq. (19) also yields

$$\omega_-^2 \approx \frac{(\omega_s q_p c)^2 + (\Lambda\Omega)^2}{\omega_s^2 + (q_p c)^2 + \Omega^2} . \quad (33)$$

Evaluating $\omega_-(q_p)$ in the low-q_p limit shows it to be an acoustic-phonon mode with long-wavelength sound velocity

$$v_- = (aAc^2/2)^{1/2} , \quad (34)$$

where $a = \hbar^2\epsilon/(m^* e^2)$ is the effective Bohr radius and

$$A = \frac{2}{a} + \frac{\Omega^2}{q_p c^2} . \quad (35)$$

Since $c^2 < 0$, Eq. (34) implies that A is also negative.

An approximate formula for ω_- which is valid for q_p inside the Fermi circle is

$$\omega_-^2 \approx \frac{a}{2}(q_p c)^2 \frac{A + q_p}{1 + q_p a/2} , \quad (36)$$

where we have assumed that $\Omega^2 + (q_p c)^2 \ll \omega_d^2$. It is interesting to note that ω_-^2 vanishes for $A + q_p = 0$. We will see that this condition will play an important role in determining the strength of the electron-electron interaction.

The strength of the electron-electron interaction for both electrons on the Fermi circle ($E = \mu$) is determined from Eq. (32). Letting $\phi = 2\theta$ and taking $\omega = 0$ and $q_p = 2k_F \sin\theta$ yields the formula

$$U(\mu,\mu) = \frac{4e^2}{\epsilon} \int_0^{\pi/2} d\theta (A + 2k_F \sin\theta)^{-1} , \quad (37)$$

where k_F is the Fermi wave vector,

$$k_F = (2\pi N_e^0)^{1/2} . \quad (38)$$

In the situation where $A < -2k_F$ the integral in Eq. (37) yields

$$U(\mu,\mu) = -\frac{8e^2}{\epsilon(A^2 - 4k_F^2)^{1/2}} \tan^{-1}\left[\frac{2k_F - A}{(A^2 - 4k_F^2)^{1/2}}\right] . \quad (39)$$

As the oxygen-defect concentration is varied in these solids, one may imagine a situation in which A approaches

$-2k_F$ from below. Then,

$$U(\mu,\mu)\rightarrow \frac{-2\pi e^2}{\epsilon[-k_F(A+2k_F)]^{1/2}}. \tag{40}$$

$U(\mu,\mu)$ is thus seen to have an inverse-square-root divergence. Thus it is indeed possible for the interaction energy for two electrons on the Fermi circle (cylinder) to be very large. Before we are able to solve the gap equation, we must have some estimate of the range of ω values for which the interaction energy is negative. One expects this range to be small compared with typical electronic frequencies, so Eq. (21) may be approximated by

$$V\approx \frac{2\pi e^2}{\epsilon}\frac{1}{q_p+2/a}\frac{\omega^2-(q_pc)^2}{\omega^2-\omega_-^2}. \tag{41}$$

In general, we will have to obtain U numerically. This will be done in Sec. III. However, if we are willing to make two simplifying assumptions, an analytic formula may be obtained and an insight into the physics may be obtained. We begin by restricting our attention to the case in which $k_Fa/2\ll 1$; so, from Eq. (36),

$$V\approx \frac{\pi e^2 a}{\epsilon}\frac{\omega^2-(q_pc)^2}{\omega^2-a(q_pc)^2(A+q_p)/2}. \tag{42}$$

In performing, the angular average, U, we assume that the main contribution to the integral stems from values of q_p near $2k_F$. Then,

$$U(\mu,\mu+\omega)\approx \frac{2e^2a}{\epsilon}\times\int_0^{\pi/2}d\theta\frac{\omega^2-4(k_Fc)^2}{\omega^2-2a(k_Fc)^2(A+2k_F\sin\theta)}. \tag{43}$$

Evaluation of the integral gives

$$U(\mu,\mu+\omega)\approx -\frac{2\pi e^2}{\epsilon}\times\{-k_F[A+2k_F-\omega^2/(2ak_F^2c^2)]\}^{-1/2}. \tag{44}$$

The interaction U is attractive in the domain $-\omega_0<\omega<\omega_0$, where

$$\omega_0=[2ak_F^2c^2(A+2k_F)]^{1/2}. \tag{45}$$

The interaction energy possesses a square-root singularity at $\omega=\pm\omega_0$.

As $A\rightarrow -2k_F$ the strength of the interaction approaches $-\infty$, whereas the range in frequency space goes to zero. We may therefore try to represent U by a δ function. Noting that

$$\int_{-\omega_0}^{\omega_0}d\omega U(\mu,\mu+\omega)=-\frac{2\pi^2e^2}{\epsilon}(-2k_Fac^2)^{1/2}, \tag{46}$$

we obtain

$$U(\mu,\mu+\omega)\approx -\frac{2\pi^2e^2}{\epsilon}(-2ak_Fc^2)^{1/2}\delta(\omega). \tag{47}$$

This is expressible in terms of the long-wavelength speed of sound for motion perpendicular to the c axis. From Eq. (34), using the fact that $A\rightarrow -2k_F$,

$$U(\mu,\mu+\omega)\approx -\frac{2\pi^2e^2 2^{1/2}v_-}{\epsilon}\delta(\omega). \tag{48}$$

In solving the gap equation, Eq. (31), we note that, in those regions of energy space where $U>0$, Δ_0 will be small. To a first approximation the repulsive contribution may be neglected. We may expect the δ-function approximation to be valid when the range of U is small compared with the gap, i.e., $\hbar\omega_0\ll\Delta_0$. From Eqs. (34), (35), and (49) this implies

$$(ak_F)^2\ll\pi^2A/[8(A+2k_F)].$$

This equation will hold if $A\rightarrow -2k_F$.

The gap equation, Eq. (31), may now be trivially solved:

$$\Delta_0=\pi\hbar v_-/(a2^{1/2}). \tag{49}$$

The size of the gap is simply determined by the speed of sound of the low-frequency mode and the effective Bohr radius.

This temperature-dependent gap function is determined from the equation

$$\Delta=-\frac{m^*}{4\pi\hbar^2}\int dE'\frac{U(E,E')\Delta(E')}{[(E'-E)^2+\Delta^2(E')]^{1/2}}\times\tanh\left[\frac{[(E-E')^2+\Delta^2(E')]^{1/2}}{2k_BT}\right], \tag{50}$$

or as the nontrivial solution to the equation

$$\Delta=\frac{\pi\hbar v_-}{a2^{1/2}}\tanh\left(\frac{\Delta}{2k_BT}\right). \tag{51}$$

The critical temperature is defined by the condition that the above gap vanishes. Thus,

$$T_c=\frac{\pi\hbar v_-}{2k_Ba2^{1/2}}. \tag{52}$$

Note that the condition relating the critical temperature and the zero-temperature energy gap is

$$2\Delta_0=4k_BT_c. \tag{53}$$

An explicit solution for the temperature in terms of the gap follows from Eq. (51):

$$\frac{T}{T_c}=\frac{2\Delta}{\Delta_0\ln[(1+\Delta/\Delta_0)/(1-\Delta/\Delta_0)]}. \tag{54}$$

Using Eqs. (34), (35), and (52) and the relation $A\approx -2k_F$ and $k_Fa\ll 1$ allows us to obtain an expression for T_c:

$$T_c=\frac{\pi\hbar\Omega_F}{4k_B}, \tag{55}$$

where Ω_F is the two-dimensional ion plasma frequency evaluated at the electronic Fermi wave vector,

$$\Omega_F=\left[\frac{2\pi N_i^0(Ze)^2k_F}{M\epsilon}\right]^{1/2}. \tag{56}$$

III. RESULTS AND DISCUSSION

In Sec. II I have developed a theory for high-temperature superconducting oxides based on a hydrodynamic approximation to the many-body problem. A key consequence of this theory is the existence of coupled two-dimensional ionic and electronic plasmon modes. One of the coupled modes, ω_+, is basically electron-plasmon-like and is not of much interest in the present discussion, although its effect is included in our calculations. The low-frequency mode, ω_-, however, plays an important role in bringing about superconductivity.

In Fig. 1, I plot ω_+ as a function of the magnitude of the wave vector parallel to the conducting plane. It displays the characteristic square-root dispersion for small q_p expected for a two-dimensional plasmon. At higher wave vectors the curve becomes straighter due to the effect of the degeneracy pressure.

The numerical values of the parameters used in our calculations are presented in Table I and are appropriate to $La_{1.8}Sr_{0.2}CuO_4$. The value of the parameter M is obtained by computing the mass of the unit cell. The ionic areal density,[11] N_i^0, is the reciprocal of the unit-cell projection perpendicular to the c axis. The electronic areal density is obtained from experiment.[12] The value of the ionic charge, Z, is based on the standard valences for the ions in the CuO_2 plane. It should stressed again that Z determines how much ionic charge lies in the conducting plane. The effective mass of the electron is assumed to be the free-electron mass. The background dielectric constant, ϵ, is taken to be that for typical metal oxides.[13] Obviously, these numbers are not known exactly and must be regarded as just reasonable estimates at this point.

The key assumption in our theory involves the nature of the instability which leads to superconductivity. In formulating our model it was assumed that there are two competing mechanisms operating. One is the effect of the electrons occupying antibonding band states, which is assumed to act in a direction so as to destabilize the system. The other is the Coulomb effect, which tends to stabilize the system. If only the former effect were present, the crystal would undergo a structural phase transition. However, we believe that the two effects nearby balance each other and that the system is therefore soft. This is manifested by the existence of an anomalous acoustic phonon ω_-. This phenomenon occurs for a restricted class of materials and distinguishes the oxide superconductors from more conventional superconductors.

TABLE I. Parameters used in the calculation.

M	6.6×10^{-22} g
N_i^0	7.0×10^{14} cm^{-2}
N_e^0	2.0×10^{14} cm^{-2}
Z	-2
m^*	0.91×10^{-27} g
ϵ	4.0

In Fig. 2, I graph the behavior of ω_- as a function of q_p for several values of the parameter A of Eq. (35). One may think of this parameter as a measure of the stability of the system, in that the two contributions reflect the two competing mechanisms described above. We note three peculiar features of the dispersion curves. First, they are characterized by exceptionally low acoustic velocities. For example, using Eqs. (34) and (35) and the values of Table I gives, for the case where $A=-2k_F$, a velocity of 8.4×10^4 cm/s. Second, for some values of the stability parameter, A, the dispersion curves possess a maximum value and then bend over and fall with increasing q_p. Finally, if the condition $A=-2k_F$ is met, the dispersion curve returns to zero frequency at $q_p=2k_F$. In our calculation $2k_F=7.1\times10^7$ cm^{-1} and the effective Bohr radius, a, is 2.1×10^{-8} cm.

The above dispersion curves permit us to compute the interaction energy in Eq. (32), making use of the expres-

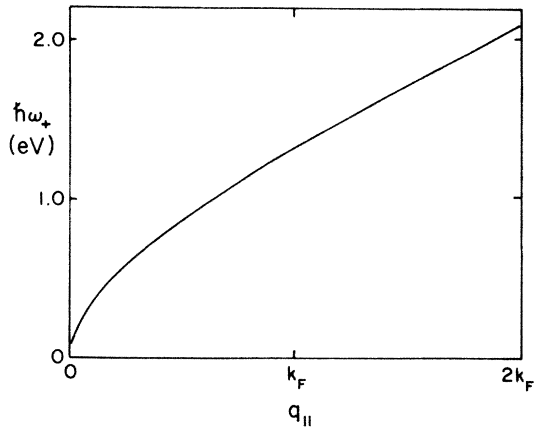

FIG. 1. Energy of the high-frequency mode as a function of the wave-vector projection parallel to the surface. The wave vector is expressed in units of the Femi wave vector k_F.

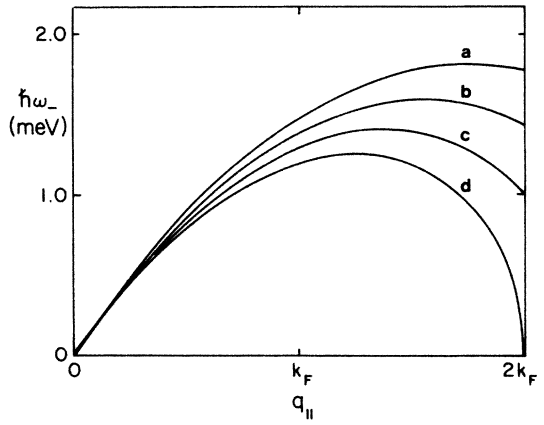

FIG. 2. Energy of the low-frequency mode as a function of the wave-vector projection parallel to the surface. The wave vector is expressed in units of the Fermi wave vector k_F. The curves are given for four values of the stability parameter A. The values of $A/(2k_F)$ in curves a, b, c, and d are -1.43, -1.27, -1.13, and -1.00, respectively.

sions in Eqs. (21) and (22). This interaction is presented as a function of the energy difference $\hbar\omega = E' - E$ in Fig. 3. For convenience, atomic units (1 atomic unit = 27.2 eV) are used here. The curve is generated for a value of A slightly less than $-2k_F$. We note the existence of an attractive band around $\omega = 0$ and the presence of a square-root divergence. This is to be expected based on our approximate formula, Eq. (44). The exact calculation is in good quantitative agreement with Eq. (44). Our calculations also have shown that as A approaches $-2k_F$, the band over which the attractive interaction exist narrows, in agreement with Eq. (45), while the strength of the interaction increases in such a way as have Eq. (46) obeyed. For ω values outside of the above attractive band, the interaction rapidly becomes repulsive.

In Fig. 4, I show how the strength of the interaction potential at $E' = E$ varies with the electron density, keeping all other parameters fixed. We see that the interaction grows to be very strong as the electron density is increased and diverges as the condition $A = -2k_F$ is reached. Again, U is expressed in atomic units in Fig. 4.

We may now calculate the superconducting transition temperature from Eq. (55). The ionic plasmon energy at the Fermi momentum is computed to be 4.9 meV, so the transition temperature is 44 K. This is in reasonable agreement with the observed value[14] of T_c of 36 K. Given the uncertainties in the parameters of the theory at this time, it is not reasonable to expect better accuracy.

An examination of Eqs. (55) and (56) shows the transition temperature to depend on only a few physical parameters: the ionic areal density, the planar cellular valence, the electron areal density, and the background dielectric constant. It does not depend on the effective mass of the electron. Also, since only the magnitude of the electronic charge enters, it makes no difference whether it is electrons or holes which are the mobile carriers.

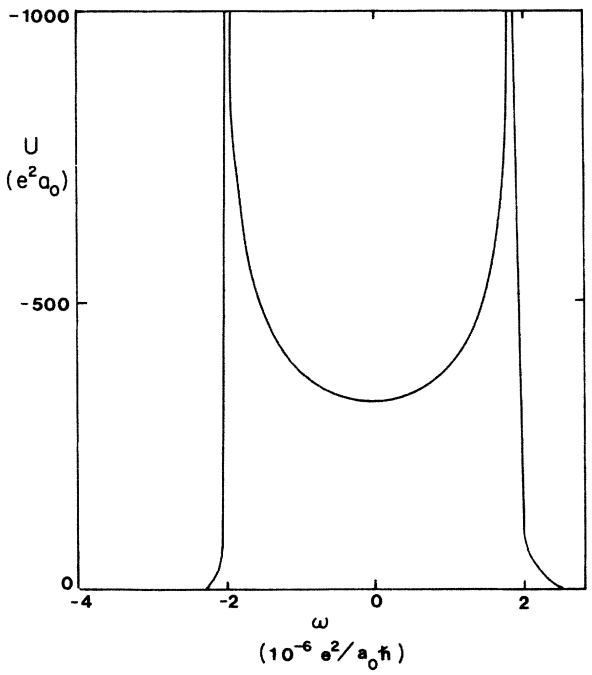

FIG. 3. Interaction strength U vs $\omega = (E' - E)/\hbar$ for an electron density $N_e^0 = 2\times10^{14}$ cm^{-2}. A value for A close to $-2k_F$ has been chosen. Atomic units are used.

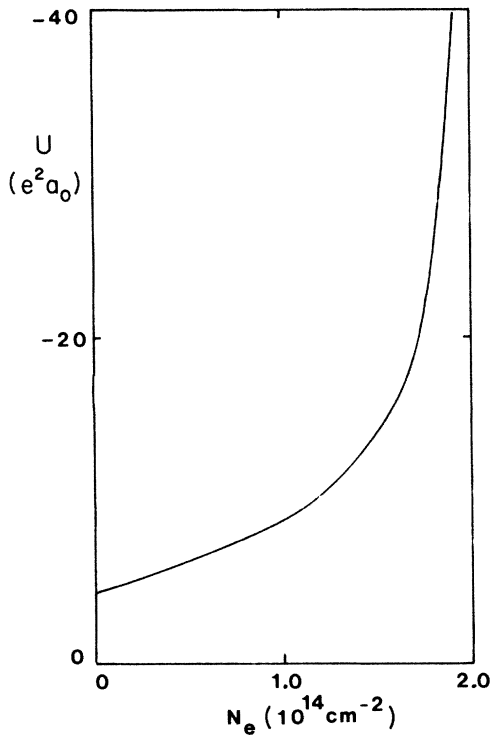

FIG. 4. Interaction strength U vs electron density N_e^0 for $E' = E$. Atomic units are used.

It is known that there are some superconductors, such as $YBa_2Cu_3O_7$, which possess several conducting layers per unit cell. While the theory developed here must be generalized to include such cases, a crude estimate of the effect can be obtained by assuming that the layers in a given unit cell are strongly coupled and thus may be thought of as constituting a single more dense layer. The net effect would be to increase the value of the parameter Z, which represents the net bound valence charge, while leaving the other parameters unchanged. The transition temperature is seen to be directly proportional to Z and thus one could possible account for the higher T_c values. In Fig. 5, I plot the behavior of the superconducting gap as a function of temperature below T_c, as given by Eq. (54). The ordinate is normalized to the zero-temperature gap, while the abscissa is normalized to the transition temperature. The curve approximately follows the same qualitative behavior as the BCS gap, although some quantitative differences exist. The main difference occurs in Eq. (53), where the value of $2\Delta_0$ is predicted to be $4k_BT_c$ instead[15] of the traditional $3.52k_BT_c$. This difference may be traced to our reduction of the three-dimensional gap equation to two dimensions, due to the highly anisotropic form of the interaction, and to our use of the δ-function approximation in Eq. (47). In addition, the conventional BCS gap equation involves the coupling in electrons to optic phonons. To a first approximation the dispersion of

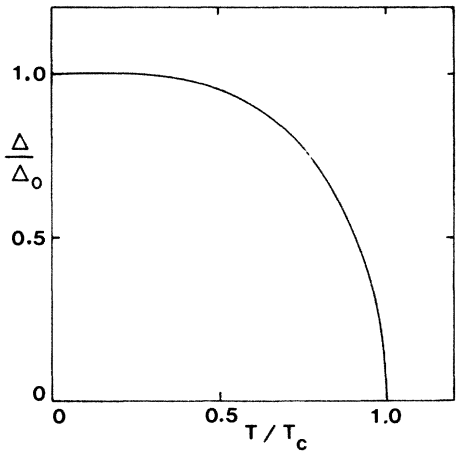

FIG. 5. Temperature-dependent gap function in units of the zero-temperature gap plotted as a function of the temperature expressed in units of the transition temperature.

these optic photons may be neglected with the result that the attractive electron-electron interaction exists for a set of electron states within some fixed band of energies about the Fermi surface. Inspection of Fig. 2 shows this not to be the case for the long-wavelength acoustic phonons studies in this paper. Thus the solution of the BCS gap equation is done slightly differently here to take this into account.

A central prediction of our theory is the existence of the low-frequency mode ω_-. Let us turn our attention to some of the experimental consequences posed by its existence. The anomalous dispersion relation could, in principle, be detected by cold-neutron scattering. A characteristic signature of the dispersion curve would be to have a low inelastic energy loss at $2k_F$. In Fig. 2 the maximum value of ω_- for the case in which $A=-2k_F$, expressed in thermal unit, is 14 K. The temperature of the neutron beam would have to be comparable to this to observe this effect.

One of the more puzzling features of the high-temperature superconductors is the behavior of the resistivity as a function of the temperature above T_c. As the temperature is lowered towards zero, the resistivity often appears to extrapolate linearly to zero until the critical temperature is reached.[16] Thereafter it falls precipitously to zero. Linear behavior of the resistivity in many metals occurs when the temperature exceeds the Debye temperature. In other words, the thermal energy must exceed characteristic acoustic-phonon energies. Since the characteristic temperature of the low-frequency mode in our problem is only 14 K, one may understand how the linear behavior of the resistivity is observed down to the transition temperature. A more quantitative description based on this theory will be presented in a future publication.

Experiments have revealed anomalies in the elastic constants and sound velocities in the high-temperature superconductors.[17] The measured sound velocities, however, are around a factor of 5 higher than those predicted in our theory. This may be due to several cases. First of all, the sound velocity along the c axis is not expected to be low. In a crystal with randomly oriented microcrystallites, pieces with fast characteristic velocities and pieces with slow characteristic velocities will occur in both series and in parallel combinations. The measured sound velocity is an appropriately averaged quantity. Second, it is quite possible that the superconducting microcrystallites comprise only some fraction of the sample. For observing zero resistivity it is only necessary for them to percolate into conducting paths. Similarly, to obtain a complete Meissner effect, it is only necessary for the planes to percolate into a union of closed surfaces (bubbles).

The present theory predicts the existence of an isotope effect. An isotope effect has recently been observed.[18] Since the ionic plasmon frequency depends on the mass of the unit cell we can estimate the size of the isotope effect to be expected. For 100% substitution ^{16}O by ^{18}O, we predict a shift in the ionic plasmon frequency, and hence the critical temperature, of 0.72 K. Experiment extrapolates to a shift of about 0.5 K. However, it should be pointed out that the temperature region over which the transition occurs is still larger than the isotope shift, so that there may yet be considerable uncertainty in the experimental results.

The specific heat of the system will be affected to some extent by the existence of the low-frequency mode. For temperatures corresponding to thermal energies above the typical maximum energy of the low-frequency mode, the specific heat assumes the approximate linear form $c=\text{const}\times(T-T^*)$. A more complete discussion of this effect will be discussed in a forthcoming publication.[19]

One of the issues not addressed in the present work is the relative stability of the superconducting transition compared with other possible transitions. A detailed discussion of this issue must be deferred to the future. The theory also omits the possible interplay of phonon and magnetic effects in determining the superconducting properties of the system. However, given the present theory and its experimental implications, I believe a reasonable case can be made for the Cooper pairing mechanism being phononlike in origin.

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[19]It will be shown that the specific heat is given approximately by $c=(k_Bk_F\eta)^2(T-T^*)/(3\hbar v_z)$, where k_B is Boltzmann's constant, $\eta=-A/(2k_F)$, and v_z is the sound velocity perpendicular to the conducting planes. The intercept temperature is given by $T^*=\hbar v-k_FJ/k_B$, where J is a number of order unity whose value depends on η and the product k_Fa. See J. I. Gersten (unpublished).