Plasmon theory of high-T_c superconductivity

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We present here a plasmon theory of high-T_c superconductivity. Some specific features of our theory are that the effect of layered or superlattice structure is fully taken into account and that plasma oscillations and the screened effective interaction between two charged carriers is studied on the basis of a tight-binding model. With an analysis of the gap equation and employing Gaussian functions for the various relevant atomic orbitals, we have evaluated numerically the superconducting critical temperatures of the La-, Bi-, and Tl-based oxides with very encouraging results.

I. INTRODUCTION

With the discovery of the high-T_c superconductors La-Sr-Cu-O,[1] Y-Ba-Cu-O,[2] Bi-Sr-Ca-Cu-O,[3] and Tl-Ba-Ca-Cu-O,[4] extensive experimental and theoretical studies have been made to bring to light the origin of high-T_c superconductivity in these oxides. It has generally been recognized that one may need a mechanism other than the phonon-mediated attraction, which is probably too weak to account for the observed high values of the critical temperature.[5] The most distinct evidence disfavoring the phonon mechanism is perhaps the small size of the isotope effect.[6]

Despite the failure of the phonon mechanism and of the conventional theory of superconductivity,[7] experimental results of flux quantization[8] and the Josephson effect[9] indicate that the carrier unit of supercurrent in these oxides has twice the electronic charge, implying Cooper pairing as a basic ingredient of the phenomenon. Besides, apart from strong anisotropy, experiments agree unanimously on a BCS-like behavior. People are naturally interested in mechanisms built on attractive interactions induced by charge[10–13] or spin[14] fluctuations. However, observation of phase coherence between high-T_c and conventional superconductors[15] and of the nuclear spin relaxation of Cu and ^{17}O (Ref. 16) confirm that the pairing has s-wave symmetry. Spin fluctuations would thus work destructively rather than constructively on the pairs. The remaining problem is then to clarify the concrete nature of the charge fluctuations underlying high-T_c superconductivity.

As an outstanding feature, all known oxide superconductors invariably exhibit layered superlattice-like structures. This is particularly striking in Bi- and Tl-based compounds. Either of them has a number of phases which differ in T_c in accordance with the size of the supercell or with the number of CuO_2 planes in a single period along the c axis. For example, the compound $Bi_2Sr_2CuO_6$ only has one Cu-O_2 layer per unit cell and a comparatively low T_c of about 6–22 K, while the double-layered compound $Bi_2Sr_2CaCu_2O_8$ has a much higher T_c of 84 K and the three-layered compound $Bi_2Sr_2Ca_2Cu_3O_{10}$ has a T_c as high as 104 K. The strong anisotropy also results from such a peculiar structure. Electronic band-structure calculations[17–20] show that the planes composed of CuO chains in $YBa_2Cu_3O_{7-\delta}$ and the $(BiO)_2$ [$(TlO)_2$] bilayers in Bi-based (Tl-based) materials (defined as M planes) provide, along with the CuO_2 planes, conduction bands intercepting the Fermi level. Therefore, it is natural to model a ceramic superconductor as a superlattice of two-dimensional (2D) conductive sheets with N CuO_2 planes and M of the M planes per supercell. The numbers N, M, and $L=N+M$ take the values listed in Table I.

What we wish to propose here is a new version of the plasmon theory[21] of high-T_c superconductivity. To our knowledge, previous studies[11] were largely concerned with the 2D collective excitation of a single Cu-O_2 sheet. Obviously, in a single, two-dimensional charged system, there is no possibility for the Coulomb interaction between a pair of carriers to be overscreened through virtual excitations of charge-density fluctuations in the same plane. But, in a superlattice of charged planes, it is possible to give rise to an attractive interaction through virtual excitations of plasmon modes in neighbor planes. A number of authors[12] have incorporated this idea with the plasmon mechanism. However, all previous discussions[11–13] of the plasmon mechanism employed free-electron (hole) models, probably due to the fact that reasonable calculations, like the random-phase approximation (RPA), are tractable only in this case. Such models are, in fact, not quite adequate; in view of the poor conductivity of the ceramic oxides in their normal state, the carriers are tightly bound rather than free. Difficulties are encountered in the study of plasma oscillations in tight-binding systems because the Coulomb vertex in momentum space ceases to be a function of the momentum transfer between two interacting particles alone. Nevertheless, in our studies[22] of superlattices, we have developed a plasmon theory for a one-dimensional tight-binding system which allows hops between nearest-neighbor quantum wells. The nature of the theory is to restore the property of the Coulomb vertex as a function of the momentum transfer alone by means of a specific renormalization procedure. It is possible to use the RPA or even go beyond it by summing over appropriate bubble

TABLE I. The numbers of CuO layers and of M layers of oxide superconductors. Here M denotes the planes composed of CuO chains or Bi-O and Tl-O bilayers in Y-, Bi-, and Tl-based oxides, respectively.

	N	M	$L=N+M$
$(La,Sr)_2CuO_{4-y}$	1	0	1
$YBa_2Cu_3O_{7-\delta}$	2	1	3
$Bi_2Sr_2Ca_{N-1}Cu_NO_{2N+4}$	1	1	2
	2	1	3
	3	1	4
$Tl_2Ba_2Ca_{N-1}Cu_NO_{2N+4}$	1	1	2
	2	1	3
	3	1	4

diagrams formed with renormalized vertices and propagators. The technique is readily extended to two and three dimensions.[23] We consider, therefore, the high-T_c superconductors as superlattices consisting of tightly bound conducting planes.

In Sec. II, we formulate a plasmon theory for the case of a superlattice consisting of tightly bound conducting planes. In Sec. III the effective interaction between two carriers in the same plane is derived and Sec. IV presents numerical estimates of the superconducting transition temperature T_c along with some discussion.

II. PLASMON THEORY OF A SUPERLATTICE OF CONDUCTING PLANES WITH TIGHT-BINDING CARRIERS

We write the wave function of a carrier localized near a site $\mathbf{R}_i$ in a 2D square lattice of constant a as

$$\phi_l(\mathbf{r}-\mathbf{R}_i)\xi_l(z-Z_l) , \tag{1}$$

where the integer l labels the conduction planes with coordinate Z_l along the c axis. For the sake of simplicity, we shall ignore charge transfer between the planes, i.e., we shall treat $\xi_l(z)$ as a localized function (or a δ function) and then neglect wave-function overlap in the z direction, although it is not necessary to do so. The carriers in each plane constitute a quasi-2D system with single-particle Bloch functions.

$$\psi_{\mathbf{k}l}(\mathbf{r},z)=S^{-1/2}A_{\mathbf{k}l}\sum_i \phi_l(\mathbf{r}-\mathbf{R}_i,z-Z_l)\exp(i\mathbf{k}\cdot\mathbf{R}_i) , \tag{2}$$

where S is the area of the planes and $A_{\mathbf{k}l}$ is the normalization constant given by

$$A_{\mathbf{k}l}^{-2}=1+S^{-1}\sum_{i(\mathrm{NN})}\exp(i\mathbf{k}\cdot\mathbf{R}_i)\int dz\int d^2r\,\phi_l^*(\mathbf{r},z-Z_l)\phi_l(\mathbf{r}-\mathbf{R}_l,z-Z_l)$$

$$=1+S^{-1}\sum_{i(\mathrm{NN})}\exp(i\mathbf{k}\cdot\mathbf{R}_i)\int d^2r\,\phi_l^*(r)\phi_l(\mathbf{r}-\mathbf{R}_i) . \tag{3}$$

The Hamiltonian of the system can be written as

$$\hat{H}=\hat{H}_0+\hat{H}_{\mathrm{int}} ,$$

$$\hat{H}_0=\sum_{\mathbf{k},l,\sigma}\varepsilon_{\mathbf{k}l}\hat{C}^\dagger_{\mathbf{k}l\sigma}\hat{C}_{\mathbf{k}l\sigma}\equiv\sum_{\mathbf{k},l}\hat{h}(\mathbf{k},l) ,$$

$$\hat{H}_{\mathrm{int}}=\tfrac{1}{2}\sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma,\sigma',\\ l_1,l_2,l_3,l_4}} V_{l_1l_2l_3l_4}(\mathbf{k},\mathbf{k}',\mathbf{q}) \times\hat{C}^\dagger_{\mathbf{k}+\mathbf{q},l,\sigma}\hat{C}^\dagger_{\mathbf{k}'-\mathbf{q}l_2\sigma'}\hat{C}_{\mathbf{k}'l_4\sigma'}\hat{C}_{\mathbf{k}l_3\sigma} . \tag{4}$$

In the approximation, including only the overlap between nearest-neighboring (NN) wave functions, the relevant conduction band is defined by

$$\varepsilon_{\mathbf{k}l}=A_{\mathbf{k}l}^2\{\varepsilon_{0l}-2J_l[\cos(k_xa)+\cos(k_ya)]\} \tag{5}$$

with ε_{0l} the on-site single-particle energy and J_l the hopping integral between nearest-neighbor sites:

$$\varepsilon_{0l}=S^{-1}\int dz\int d^2r\,\phi_l^*(\mathbf{r},z-Z_l)h(\mathbf{r},z)\phi_l(\mathbf{r},z-Z_l) , \tag{6}$$

$$J_l=-S^{-1}\int dz\int d^2r\,\phi_l^*(\mathbf{r},z-Z_l) \times h(\mathbf{r},z)\phi_l(\mathbf{r}-a\mathbf{i},z-Z_l) , \tag{7}$$

where $h(\mathbf{r},z)$ is the Fourier transform of $h(\mathbf{k},z)$. For the large enough lattice constant, we can write $A_{\mathbf{k}l}=1$ and then Eq. (5) reduces to the well-known form of the tight-binding band energy. The essential point of the theory is the observation that, in the same approximation, the matrix element of the Coulomb potential $V(\mathbf{r}-\mathbf{r}',z-z')$,

$$V_{l_1l_2l_3l_4}(\mathbf{k},\mathbf{k}',\mathbf{q})=\int dz\int dz'\int d^2r\int d^2r'\,\psi^*_{\mathbf{k}+\mathbf{q}l_1}(\mathbf{r},z)\psi^*_{\mathbf{k}'-\mathbf{q}l_2}(\mathbf{r}',z')V(\mathbf{r}-\mathbf{r}',z-z')\psi_{\mathbf{k}'l_4}(\mathbf{r}',z')\psi_{\mathbf{k}l_3}(\mathbf{r},z) \tag{8}$$

can be factorized to take the form

$$V_{l_1 l_2 l_3 l_4}(\mathbf{k},\mathbf{k}',\mathbf{q}) = A_{\mathbf{k}+\mathbf{q}l_1} A_{\mathbf{k}'-\mathbf{q}l_2} A_{\mathbf{k}l_1} A_{\mathbf{k}'l_1} \times \hat{T}^T(\mathbf{k}) \hat{V}_{l_1 l_2}(\mathbf{q}) \hat{T}(\mathbf{k}') \delta_{l_1 l_2} \delta_{l_2 l_4} , \quad (9)$$

where $\hat{T}^T(\mathbf{k})$ is a row matrix (the superscript T means a transpose)

$$\hat{T}^T(\mathbf{k}) = (1, \cos(k_x a), \sin(k_x a), \cos(k_y a), \sin(k_y a)) \quad (10)$$

and $\hat{V}_{ll'}(\mathbf{q})$ is a 5×5 matrix, which can be factorized further into

$$\hat{V}_{ll'}(\mathbf{q}) = \hat{p}_l(\mathbf{q}) V_{ll'}(\mathbf{q}) \hat{p}_{l'}^T(-\mathbf{q}) . \quad (11)$$

In Eq. (11), $\hat{p}_l^T(\mathbf{q}) = \{p_{li}(\mathbf{q})\}$, $i = 1, 2, 3, 4$, and 5, is again a row matrix with elements

$$p_{li}(\mathbf{q}) = \int d^2 r \phi_l^*(\mathbf{r}) \varphi_{li}(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) , \quad (12)$$

where

$$\varphi_{l1} = \phi_l(\mathbf{r}) ,$$
$$\varphi_{l2} = \phi_l(\mathbf{r}-\mathbf{X}) + \phi_l(\mathbf{r}+\mathbf{X}) ,$$
$$\varphi_{l3} = i[\phi_l(\mathbf{r}-\mathbf{X}) - \phi_l(\mathbf{r}+\mathbf{X})] ,$$
$$\varphi_{l4} = \phi_l(\mathbf{r}-\mathbf{Y}) + \phi_l(\mathbf{r}+\mathbf{Y}) ,$$
$$\varphi_{l5} = i[\phi_l(\mathbf{r}-\mathbf{Y}) - \phi_l(\mathbf{r}+\mathbf{Y})] ,$$

$\mathbf{X}$ and $\mathbf{Y}$ being the lattice vectors $(a,0)$ and $(0,a)$, respectively. The quantity $V_{ll'}(\mathbf{q})$ is given by

$$V_{ll'}(\mathbf{q}) = 2\pi e^2/(\epsilon_\infty q) \exp(-q|Z_l - Z_{l'}|) , \quad (13)$$

where ϵ_∞ is the high-frequency dielectric constant. It is now possible to combine the single-particle propagator

$$G_l(\mathbf{k},\omega) = [\omega - \varepsilon_{\mathbf{k}l} + i0^+ \mathrm{sgn}(\omega)]^{-1} \quad (14)$$

and the $\hat{T}^T$ matrix to define a new propagator $\hat{G}_l(\mathbf{k},\omega)$, which is a row matrix

$$\hat{G}_l^T(\mathbf{k},\omega) = A_{\mathbf{k}l} G_l(\mathbf{k},\omega) \hat{T}^T(\mathbf{k}) . \quad (15)$$

We are left with a simplified Coulomb vertex $\hat{V}_{ll'}(\mathbf{q})$, which is a function of the momentum transfer $\mathbf{q}$ only. The price paid is that both the propagator and the vertex become matrix quantities. Nevertheless, it is obvious then, that the standard Feynman-Dyson technique of many-particle theory can be readily followed, for example, in the RPA, to study the nature of screened interactions between a pair of charges. We note that the theory is not limited to the RPA. In principle, it is possible to go beyond the RPA by including higher-order polarization parts. But, for the sake of simplicity, we stay, in the following, within the RPA and shall leave more refined calculations to future publications.

III. THE EFFECTIVE INTERACTION

Consider a superlattice system with L conductive atomic layers within a supercell along the c axis. A double label (n,l) denotes the lth layer within the nth supercell. The effective interaction between a pair of carriers in the (n,l) and (n',l') layers, separately, can be obtained by summing over bubble diagrams (Fig. 1):

$$\hat{U}_{nl,n'l'}(\mathbf{q},\omega) = \hat{V}_{nl,n'l'}(\mathbf{q}) + \sum_{n''l''n'''l'''} \hat{V}_{nl,n''l''}(\mathbf{q}) \hat{\Pi}_{n''l''n'''l'''}(\mathbf{q},\omega) \times \hat{U}_{n'''l'''n'l'}(\mathbf{q},\omega) \quad (16)$$

with the density correlation function $\hat{\Pi}$ defined by

$$\hat{\Pi}_{nl,n'l'}(\mathbf{q},\omega) = \sum_{\mathbf{k},\mathbf{k}'} \hat{T}(\mathbf{k}) A_{\mathbf{k}l} A_{\mathbf{k}+\mathbf{q}l} A_{\mathbf{k}'l'} A_{\mathbf{k}'-\mathbf{q}l'} \times \hat{T}^T(\mathbf{k}') P_{nl,n'l'}(\mathbf{k},\mathbf{k}';\mathbf{q},\omega) , \quad (17)$$

where $P_{nl,n'l'}(\mathbf{k},\mathbf{k}';\mathbf{q},\omega)$ is defined as the hatched part in Fig. 1. Specifically, in the RPA, it can be shown that a single index fixes the density correlation part which has to be evaluated by numerical integration:

$$\hat{\Pi}_{nl,n'l'}(\mathbf{q},\omega) = \hat{\Pi}_l^0(\mathbf{q},\omega) \delta_{nn'} \delta_{ll'} , \quad (18)$$

$$\hat{\Pi}_l^0(\mathbf{q},\omega) = \sum_{\mathbf{k}} \hat{T}(\mathbf{k}) A_{\mathbf{k}l}^2 A_{\mathbf{k}-\mathbf{q}l}^2 [f(\varepsilon_{\mathbf{k}l}) - f(\varepsilon_{\mathbf{k}-\mathbf{q}l})] \times (\varepsilon_{\mathbf{k}l} - \varepsilon_{\mathbf{k}-\mathbf{q}l} + \hbar\omega + i0^+)^{-1} \hat{T}^T(\mathbf{k}-\mathbf{q}) . \quad (19)$$

After Fourier transformation with respect to $n-n'$,

$$\hat{U}_{ll'}(\mathbf{q},\omega,k_z) = N^{-1} \sum_{n,n'} \exp\left[ik_z \left[(n'-n)c + \sum_{i=1}^{l'} c_i - \sum_{i=1}^{l} c_i\right]\right] \hat{U}_{nl,n'l'}(\mathbf{q},\omega) , \quad (20)$$

where k_z is the wave vector, c is the lattice constant along the c axis, and c_i is the distance between the (n,i) and $(n,i+1)$ layers, we arrive at the following equation in the RPA:

$$\hat{U}_{ll'}(\mathbf{q},\omega,k_z) = \hat{V}_{ll'}(\mathbf{q},k_z) + \sum_{l''} \hat{V}_{ll''}(\mathbf{q},k_z) \times \hat{\Pi}_{l''}^0(\mathbf{q},\omega) \hat{U}_{l''l'}(\mathbf{q},\omega,k_z) . \quad (21)$$

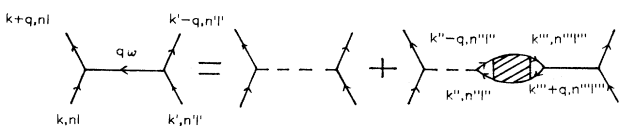

FIG. 1. Renormalized matrix Dyson equation of a superlattice of planes with tight-binding conduction carriers. The hatched part is denoted as $P_{n''l'',n'''l'''}(\mathbf{k},\mathbf{k}';\mathbf{q},\omega)$.

A relation similar to Eq. (11) holds for the effective (i.e., screened) interaction $\hat{U}_{ll'}(\mathbf{q},\omega,k_z)$,

$$\hat{U}_{ll'}(\mathbf{q},\omega;k_z)=\hat{p}_l(\mathbf{q})U_{ll'}(\mathbf{q},\omega;k_z)\hat{p}_{l'}^T(-\mathbf{q}) , \tag{22}$$

where $U_{ll'}(\mathbf{q},\omega;k_z)$ satisfies

$$U_{ll'}(\mathbf{q},\omega;k_z)=V_{ll'}(\mathbf{q},k_z)+\sum_{l''}V_{ll''}(\mathbf{q},k_z)\Pi^0_{l''}(\mathbf{q},\omega)U_{l''l'}(\mathbf{q},\omega;k_z) . \tag{23}$$

In the above equation,

$$V_{ll'}(\mathbf{q},k_z)=2\pi e^2/(\epsilon_\infty q)\sinh(qc)/[\cosh(qc)-\cos(k_z c)]D_{ll'}(q,k_z) \tag{24}$$

with

$$D_{ll}=1 ,$$

$$D_{ll'}=\{\sinh(qc-qc')\exp(ik_z c')+\sinh(qc')\exp[-ik_z(c-c')]\}/\sinh(qc) ,$$

$$D_{l'l}=D^*_{ll'} \quad (l'>l) , \tag{25}$$

$$c'=\sum_{i=l+1}^{l'}c_i , \tag{26}$$

and

$$\Pi^0_l(\mathbf{q},\omega)=\hat{p}_l^T(-\mathbf{q})\hat{\Pi}^0_l(\mathbf{q},\omega)\hat{p}_l(\mathbf{q}) . \tag{27}$$

The plasmon spectrum is then defined by the following dispersion equation:

$$\det|\delta_{ll'}-V_{ll'}(\mathbf{q},k_z)\Pi^0_{l'}(\mathbf{q},\omega,k_z)|=0 . \tag{28}$$

We now discuss various special cases.

A. Case A: $L=N=1, M=0$

In the simplest case $L=N=1$, $M=0$, i.e., in the case of $La_{2-x}Sr_xCuO_4$ oxides (in this case the label l is always equal to 1 and we shall omit it), the effective interaction is

$$U(\mathbf{q},\omega;k_z)=\frac{V(q,c)}{\Delta(\mathbf{q},\omega;c)-\cos(k_z c)} , \tag{29}$$

where

$$V(q,c)=2\pi e^2\sinh(qc)(\epsilon_\infty q)^{-1} \tag{30}$$

and

$$\Delta(\mathbf{q},\omega;c)=\cosh(qc)-\Pi^0(\mathbf{q},\omega)V(q,c) , \tag{31}$$

$$\Pi^0(\mathbf{q},\omega)=\sum_{\mathbf{k}}A^2_{\mathbf{k}}A^2_{\mathbf{k}-\mathbf{q}}[\hat{T}^T(\mathbf{k})\hat{p}(-\mathbf{q})]\times\frac{f(\epsilon_{\mathbf{k}})-f(\epsilon_{\mathbf{k}-\mathbf{q}})}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}}+\hbar\omega+i0^+}[\hat{T}^T(\mathbf{k}-\mathbf{q})\hat{p}(\mathbf{q})] . \tag{32}$$

The plasmon dispersion $\omega_p=\omega_p(\mathbf{q},k_z)$ is defined by

$$\Delta(\mathbf{q},\omega;c)-\cos(k_z c)=0 . \tag{33}$$

The solution in the case of free particles is well known. In the tight-binding case, plasmon modes exist for $\omega\geq\omega_m$, where

$$\omega_m=4J[|\sin(q_x a/2)|+|\sin(q_y a/2)|] \tag{34}$$

is the maximum excitation energy of an electron-hole pair in layer l. In Eq. (34) we have assumed that $(A_{\mathbf{kl}}-1)^n$ is vanishingly small for $n\geq 2$, which is usually satisfied for the tight-binding case. For $\omega\geq\omega_m$, we have the following analytic dispersion relation:

$$\omega_p^2(q,k_z)=2\pi e^2\epsilon_\infty^{-1}q\sinh(qc)\frac{a_1}{\cosh(qc)-\cos(k_z c)} , \tag{35}$$

where

$$a_1=-2S^{-1}\sum_{\mathbf{k}}f(\epsilon_{\mathbf{k}})\epsilon_{\mathbf{k}} . \tag{36}$$

A detailed investigation of the dispersion relation indicates that the interlayer Coulomb interaction modifies the simple two-dimensional plasmon spectrum significantly. In the layered structure, the whole spectrum is restricted to lie between a highest branch $\omega_H=\omega_p(k_z c=0)$ $[\Delta(\mathbf{q},\omega;c)=+1]$ and a lowest branch $\omega_L=\omega_p(k_z c=\pi)$ $[\Delta(\mathbf{q},\omega;c)=-1]$, which correspond, respectively, to the in-phase and out-of-phase oscillations of charges in adjacent planes. We note that the branch ω_H has a three-dimensional behavior, i.e., $\omega_H\sim$const even for $q=0$. On the other hand, the branch ω_L has an acoustic character, i.e., $\omega_L\sim q$ in the long-wavelength limit. We call a spectrum with characteristics like this an optical-like plasmon band. An illustration of the spectrum for the case of $(LaSr)_2CuO_4$ is given in Fig. 2 at typical carrier concentration. From Eq. (5), it is easily seen that the shape of the Fermi surface is determined by

$$\cos(k_x a)+\cos(k_y a)=f(n) .$$

Note that, for $f=0$, the Fermi surface reduces to the lines $\pm k_x\pm k_y=\pi/a$ and then that the vector $Q=(\pm\pi/a,\pm\pi/a)$ nests perfectly in the Fermi surface. The system is unstable under charge-density waves with this wave vector and an energy gap should exist around

the Fermi level if proper electron correlations are considered. We thus define the carrier concentration n as the number of holes per lattice site, for example, resulting from the substitution of La by Sr in La-based oxides. The function f is determined by the condition that the number of occupied states n_e should be $1-n$. In the concrete, f is 0.00, 0.15, 0.30, and 0.45 for $n=0.000$, 0.151, 0.261, and 0.354, respectively, for La-based oxides. In Fig. 2(b) we see that the plasmon bands are similar for little carrier concentration (i.e., $n \leq 0.35$) as expected.

We now consider the effective interaction between a pair of charges in the same plane which is given, for $\omega \geq \omega_m$, by

$$U(\mathbf{q},\omega)=V(q,c)[\Delta^2(\mathbf{q},\omega;c)-1]^{-1/2}\mathrm{sgn}[\Delta(\mathbf{q},\omega;c)] . \tag{37}$$

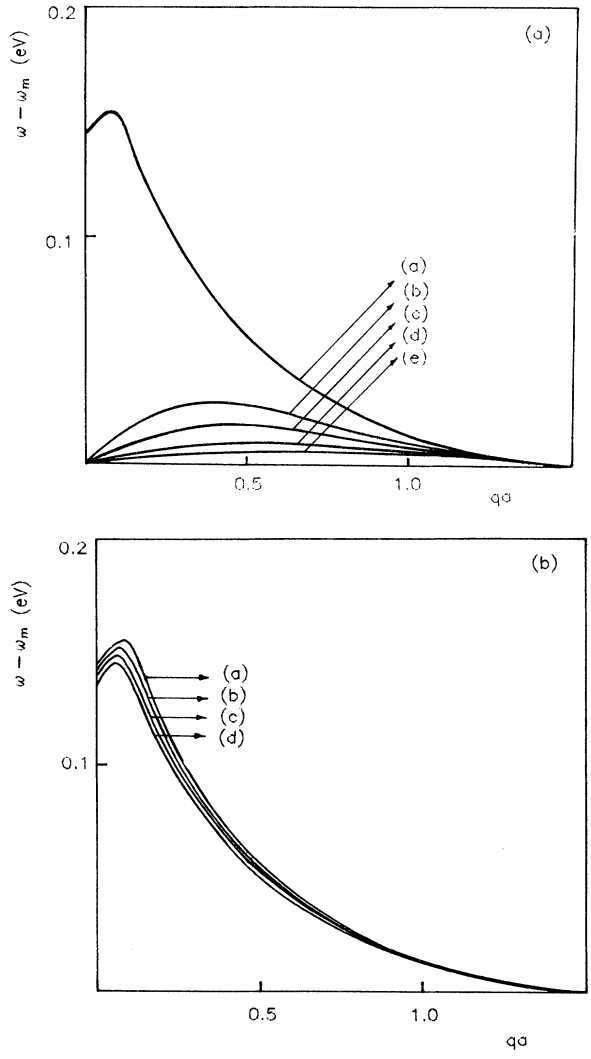

FIG. 2. Plasmon spectra of the $(La,Sr)_2CuO_4$ superconductor, $\omega-\omega_m$ vs q for (a) the carrier's density $n=0$ and curves (a)–(e) corresponding to phase $k_zc=0$, $\pi/3$, $\pi/2$, $2\pi/3$, and π, and (b) phase $k_zc=0$ and curves (a)–(d) corresponding to the carrier density $n=0.000$, 0.151, 0.261, and 0.354.

In Fig. 3 we show $U(\mathbf{q},\omega)$ schematically as a function of ω. Corresponding to the plasmon branches, we have two frequency ranges separated by a finite gap. Between the frequencies ω_m and ω_L, the effective interaction is an attraction, which is crucial for pairing of charges in the same CuO_2 plane. For frequencies $\omega>\omega_H$, the interaction is repulsive. Analysis shows that the attraction arises predominantly through exchange of momentum and energy via virtually excited plasmons in neighboring planes. We remark in passing that the effective interaction between two charges in different planes is always repulsive, for instance, between two charges in adjacent planes, we have

$$U_{(\mathrm{NN})}(\mathbf{q},\omega) = V(q,c)\{|\Delta(\mathbf{q},\omega;c)|[\Delta^2(\mathbf{q},\omega;c)-1]^{-1/2}-1\} .$$

B. Case B: $L=N+1$ ($N\geq 1$), $M=1$

The $L=N+1$ ($N\geq 1$) case can be handled along the same line. We shall assign subscripts C and M to signify quantities pertaining to CuO_2 and M layers, respectively. Let d_C and d_M be the respective lattice spacing between adjacent CuO_2 layers and between an M layer and its adjacent CuO_2 layer, then the lattice constant along the c axis is

$$c(n)=2d_M+(N-1)d_C .$$

From the matrix equations (21) and (22) we obtain the effective interaction of a pair of charges in a CuO_2 plane

$$U(\mathbf{q},\omega;k_z)=\frac{a(\mathbf{q},\omega;c)}{\Delta(\mathbf{q},\omega;c)-\cos(k_zc)} , \tag{38}$$

where

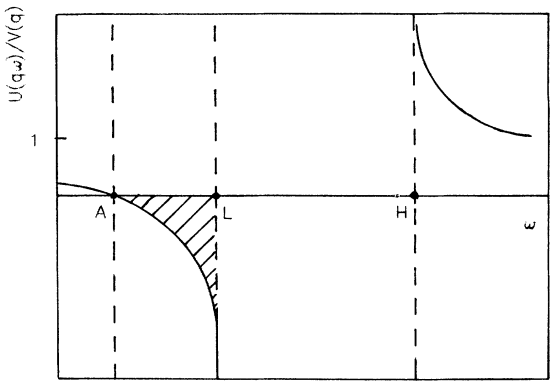

FIG. 3. Schematic plot of the effective interaction $U(\mathbf{q},\omega)$ vs frequency ω. A, L, and H signify ω_m, $\omega_p(k_zc=\pi)$, and $\omega_p(k_zc=0)$, respectively. The hatched region corresponds to the frequency range which is crucial for Cooper pairing.

$$a(\mathbf{q},\omega;c)=V(q,c)-2\Pi_M^0(q,\omega)V(q,d_M)V(q,c-d_M)$$
$$+\sum_{m=1}^{N}\sum_{\substack{0\le n_1<n_2<\cdots<n_m\\(n_1+\cdots+n_m=N-1)}}\{V(q,n_1d_C)\cdots V(q,n_md_C)V(q,(n_1+\cdots+n_m)d_C)[-2\Pi_C^0(\mathbf{q},\omega)]^m$$
$$+V(q,c-d_M)V(q,c-d_M-n_1d_C)V(q,n_2d_C)\cdots V(q,n_md_C)$$
$$\times V(q,(n_1+\cdots+n_m)d_C)(-2)^{m+1}[\Pi_C^0(\mathbf{q},\omega)]^m\Pi_M^0(\mathbf{q},\omega)\}\ , \tag{39}$$

$$\Delta(\mathbf{q},\omega;c)=\cosh(qc)-N\Pi_C^0(\mathbf{q},\omega)V(q,c)-\Pi_M^0(\mathbf{q},\omega)V(q,c)$$
$$+\sum_{m=1}^{N}\sum_{\substack{0\le n_1<n_2<\cdots<n_m\\(n_1+\cdots+n_m=N-1)}}V(q,n_1d_C)\cdots V(q,n_md_C)V(q,(n_1+\cdots+n_m)d_C)(-2)^m[\Pi_C^0(\mathbf{q},\omega)]^{m+1}$$
$$+\sum_{m=1}^{N}\sum_{\substack{0\le n_1<n_2<\cdots<n_m\\(n_1+\cdots+n_m=N)}}V(q,d_M+(N-n_1)d_C)V(q,n_2d_C)\cdots V(q,n_md_C)V(q,(n_1+\cdots+n_m)d_C)$$
$$\times(-2)^m[\Pi_C^0(\mathbf{q},\omega)]^m\Pi_M^0(\mathbf{q},\omega)\ . \tag{40}$$

The plasmon dispersion $\omega_p=\omega_p(\mathbf{q},k_z)$ and the corresponding damping $\gamma(\mathbf{q},k_z)$ are defined by

$$\mathrm{Re}\Delta(\mathbf{q},\omega;c)-\cos(k_zc)=0\ , \tag{41}$$

$$\gamma(\mathbf{q},k_z)=\frac{\mathrm{Im}\Delta(\mathbf{q},\omega;c)}{\partial\,\mathrm{Re}\Delta(\mathbf{q},\omega,c)/\partial\omega}\bigg|_{\omega=\omega_p(\mathbf{q},k_z)}\ . \tag{42}$$

Equations (38)–(42) are quite complicated. Analysis shows that the general result is the existence of $N+1$ plasmon bands, one optical-like plasmon band lying above ω_{mc} ($\omega_p>\omega_{mc}$) as in the $L=1$ case and N acoustic bands lying between ω_{mM} and ω_{mC} ($\omega_{mN}<\omega_p<\omega_{mC}$). Each acoustic band is restricted to lie between a highest branch ω_H^i ($k_zc=0$ or π) and a lowest branch ω_L^i ($k_zc=\pi$ or 0), $i=1,2,\ldots,N$. They all have acoustic behavior, i.e., $\omega_p\sim q$ in the long-wavelength limit. The numerical results for Bi-based oxides ($N=1$) is shown in Figs. 4 and 5.

In particular, for the $N=M=1$ case, there exist two plasmon bands. One is an optical-like band and another is an acoustic band. The modes of the optical-like band are all undamped due to $\omega_p>\omega_{mC}$. On the other hand, maybe $\mathrm{Im}\Delta(\mathbf{q},\omega,c)$ is nonzero for $\omega<\omega_{mC}$. So, the modes of acoustic band are damped except for $k_zc=\pi$. This is similar to that obtained for the free case of the 1:2:3 materials by Mahan.[24] In the small-q limit, γ of the acoustic band is found to be linear in q, and

$$\gamma(\mathbf{q},k_z)/\omega_p(\mathbf{q},k_z)=\frac{\omega_p(\mathbf{q},k_z)\cos^2(k_zc/2)}{2\omega_{mC}\Pi_M^0(\mathbf{q},\omega_p)\{\cosh(qc/2)/\mathrm{Re}[\Pi_C^0(\mathbf{q},\omega=0)]-V(q,c/2)\}}\ .$$

For $\omega_{mM}\ll\omega_p\ll\omega_{mC}$, γ is vanishingly small. One also sees that the quality of the modes of the acoustic band are quite good ($\gamma/\omega\le 5\%$, which we estimate at little n) for Bi-based oxides ($N=1$) although $\omega_{mM}\ll\omega_{mC}$ is not satisfied.

The effective interaction between two carriers in the same CuO_2 layer for $\omega_{mM}<\omega<\omega_{mC}$ is given by

$$\mathrm{Re}U(\mathbf{q},\omega)=[(\eta+\delta^2-\tau^2-1)/(2\eta^2\delta^2)]^{1/2}$$
$$\times[\delta\alpha+(\eta+\tau^2-\delta^2+1)\beta/(2\tau)]\ ,$$

where

$$\eta^2=(\delta^2-\tau^2-1)^2+(2\delta^2\tau^2)^2 \tag{43}$$

and δ and τ, and α and β are the real and imaginary parts of Δ, Eq. (40), and a, Eq. (39), respectively,

$$\Delta=\delta+i\tau\ ,$$
$$a=\alpha+i\beta\ .$$

A net attraction results within the frequency range $[\omega_{mM},\omega_L]$, where ω_L is the frequency of the mode which corresponds to an out-of-phase oscillation of charges on the M layer with respect to the neighboring CuO_2 plane. Analysis also shows that the attraction arises predominantly through virtual excitations of plasmons in neighboring planes. The larger is N, the smaller is the frequency of the lowest acoustic plasmon ω_L and a stronger effective attraction for BCS superconductivity.

We have, therefore, the following picture: Pairing of carriers in the same conductive plane occurs owing to attractive interaction resulting from exchange of virtual plasmons in neighboring layers.

IV. THE SUPERCONDUCTING TRANSITION TEMPERATURE

An analysis similar to Ref. 13 can now be performed. Beginning with the gap equation in the Gor'kov approximation (at $T=T_c$)

$$F^{\dagger}(\mathbf{p},i\omega_n)=-\beta^{-1}\sum_{\mathbf{q}\omega_{n'}}\frac{U(\mathbf{q},-\mathbf{q};\mathbf{p}-\mathbf{q},i\omega_n-i\omega_{n'})}{\omega_n^2+\varepsilon_p^2}\times F^{\dagger}(\mathbf{q},i\omega_{n'}) \tag{44}$$

with $\omega_n=(2n+1)\pi T_c$ and $\omega_{n'}=2n'\pi T_c$, and F the anomalous Matsubara function, one deduces

$$T_c=1.134\omega_L\exp[-(1+\langle F\rangle^2)/(\langle F^2\rangle-\mu)]\ , \tag{45}$$

where

$$\langle F^n\rangle=\int_{-\omega_L}^{\omega_L}d\Omega(2|\Omega|)^{-1}F^n(\Omega) \tag{46}$$

and $F(\Omega)$ is defined by the ansatz[25]

$$K_{00}(\Omega,\Omega')=[\mu+F(\Omega)+F(\Omega')]\Theta(\omega_L-|\Omega|)\times\Theta(\omega_L-|\Omega'|)\ , \tag{47}$$

$$K_{00}(0,0)=\mu\ . \tag{48}$$

In Eqs. (45) and (46), $K_{00}=K_{n=n'=0}$ and

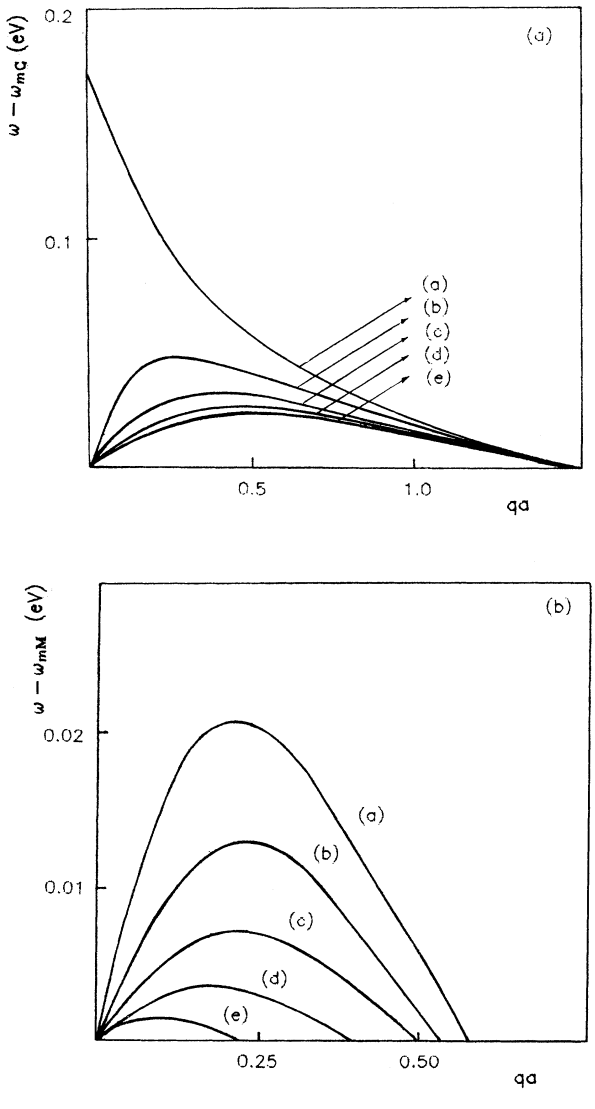

FIG. 4. Plasmon spectra of $Bi_2Sr_2CuO_6$. (a) The optical-like band $\omega-\omega_{mC}$ and (b) the acoustic band $\omega-\omega_{mM}$, at carrier density $n=0.000$ and electronic density on the Bi-O bilayer $n_e=0.300$. Curves (a)–(e) correspond to $k_zc=0$, $\pi/3$, $\pi/2$, $2\pi/3$, and π.

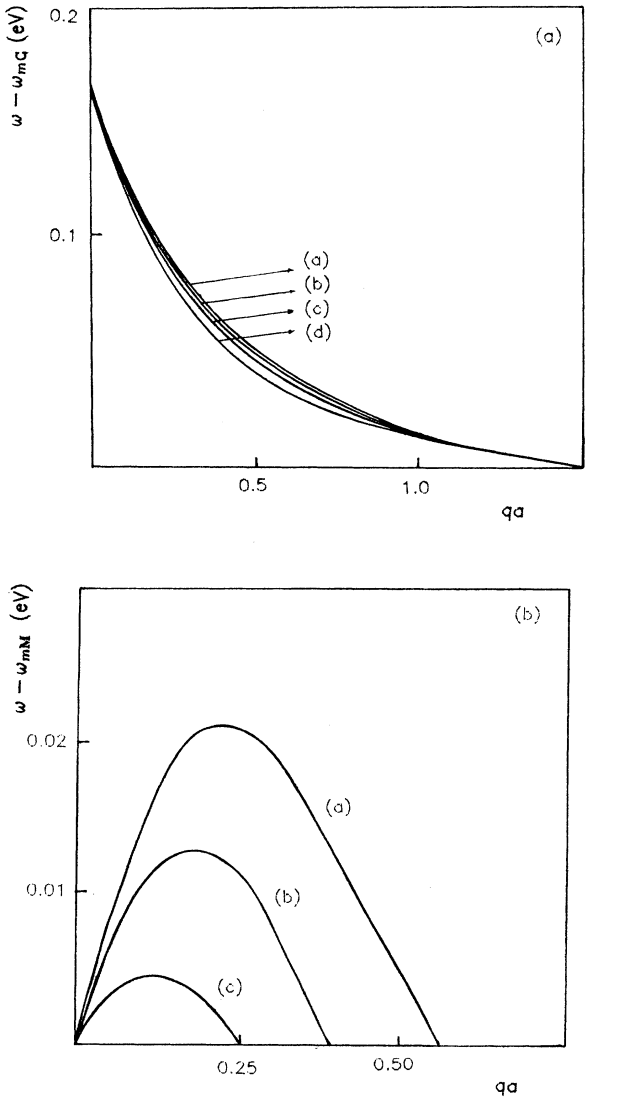

FIG. 5. Plasmon spectra of $Bi_2Sr_2CuO_6$. (a) The optical-like band $\omega-\omega_{mC}$ at carrier densities $n=0.000$, 0.151, 0.261, and 0.354 for curves (a)–(d), respectively, and electronic density on the Bi-O bilayer $n_e=0.300$ and (b) the acoustic band $\omega-\omega_{mM}$ at carrier density $n=0.000$ and electronic densities on the Bi-O bilayer $n_e=0.30$, 0.25, and 0.20 for curves (a)–(c), respectively. All the curves are for $k_zc=0$.

$$K_{nn'}(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})=\int \frac{d\Theta_{\mathbf{p}}d\Theta_{\mathbf{p}'}4\cos(n\Theta_{\mathbf{p}})\cos(n'\Theta_{\mathbf{p}'})K(\mathbf{p},\mathbf{p}')}{[(\varepsilon_{\mathbf{p}'}-\varepsilon_0+\varepsilon_F)^2\cos^2(2\Theta_{\mathbf{p}'})+16J^2\sin^2(2\Theta_{\mathbf{p}'})]^{1/2}(1+\delta_{n'0})} \tag{49}$$

with $K(\mathbf{p},\mathbf{p}')$ a kernel defined by

$$K(\mathbf{p},\mathbf{p}')=\frac{[\hat{T}^T(\mathbf{p}')\hat{p}(\mathbf{p}-\mathbf{p}')]^2}{A_{\mathbf{p}}^{-2}A_{-\mathbf{p}}^{-2}} \times\int d\Omega\frac{2}{\pi}\frac{(|\varepsilon_{\mathbf{p}}|+|\varepsilon_{\mathbf{p}'}|)U(\mathbf{p}-\mathbf{p}',i\Omega)}{\Omega^2+(|\varepsilon_{\mathbf{p}}|+|\varepsilon_{\mathbf{p}'}|)^2} \tag{50}$$

and

$$\Theta_{\mathbf{p}}=\tan^{-1}[\tan(p_y a/2)/\tan(p_x a/2)]\ . \tag{51}$$

Since there exists experimental evidence[15,16] favoring s-wave pairing, only the K_{00} component is effective in the reduction from (44) to (45).

According to Takada,[25] due to the specific behavior of the dispersion relations of different plasmon modes, the dominant contribution to $\langle F^n\rangle$ comes from interaction via excitation of intraplanar plasmons. Thus, we can approximately treat $\langle F^n\rangle$ as a pure 2D quantity. Meanwhile, we write $\mu=\mu_0-\lambda$, where μ_0 is of pure 2D nature and λ originates from interplanar coupling. In view of the fact[26] that purely 2D systems are unlikely to be superconducting and the complete nesting of the Fermi surface occurs in the half-filled case, $\langle F^2\rangle-\mu_0$ must be a negative quantity of vanishingly small magnitude, so that (45) becomes

$$T_c=1.134\omega_L\exp(-\lambda^{-1})\ . \tag{52}$$

This is true for arbitrary L and N (or M). We find $\lambda(L)$ given by

$$\lambda(L)=\{1-A(L)/[B^2(L)-1]^{1/2}\}/2\ . \tag{53}$$

In the $L=N=1$, $M=0$ case,

$$A=A(1)=-\Pi_C^0V(q=0,c)\ ,\qquad B=B(1)=1-\Pi_C^0V(q=0,c)\ , \tag{54}$$

and in the $L=2$ ($N=M=1$) case,

$$A=A(2)=-\Pi_c^0V(q=0,c)+2\Pi_C^0\Pi_M^0V(q=0,c/2)\ ,$$
$$B=B(2) \tag{55}$$
$$=1-(\Pi_C^0+\Pi_M^0)V(q=0,c)+2\Pi_C^0\Pi_M^0V(q=0,c/2)\ ,$$

where

$$\Pi_l^0=\Pi_l^0(q=0,0)=-2S^{-1}\sum_{\mathbf{k}}\delta(\varepsilon_{\mathbf{k}l}-\varepsilon_F) \tag{56}$$

is related to the overlap integral and the density of states of the carriers. Expressions for A and B become more and more complicated for larger L and/or N, and will be omitted for brevity.

In order to obtain an estimation of the superconducting transition temperatures, we proceed to perform numerical calculations. We first need input data. Since the structure of CuO_2 planes and the Cu-O_2 conduction bands resulting from band calculations are essentially identical in all types of ceramic superconductors, we take the same set of parameters for the CuO_2 planes in all oxides. We also overlook the differences in M layers in different phases of each kind of oxides. The adopted parameters are shown in Table II.

Next, we chose the Cu $3d_{x^2-y^2}$–O $2p_{xy}$ hybridized wave function localized within the vicinity of a lattice site in a CuO_2 layer as

$$\phi_l(\mathbf{r}-\mathbf{R}_i,z)=\sum_{i'}[f_{ii'}^d\phi_d(\mathbf{r}-\mathbf{R}_{i'},z-Z_l) -f_{ii'}^p\phi_p(\mathbf{r}-\mathbf{R}_{i'},z-Z_l)] \tag{57}$$

with $f_{u'}^d, f_{ii'}^p\geq 0$, ϕ_d the atomic Cu $3d_{x^2-y^2}$ wave function and ϕ_p a linear combination of atomic O $2p_{xy}$ wave function.

$$\phi_p(\mathbf{r}-\mathbf{R}_i,z)=[\phi_{p_x}(\mathbf{r}-\mathbf{R}_i+\mathbf{X}/2,z)-\phi_{p_x}(\mathbf{r}-\mathbf{R}_i-\mathbf{X}/2,z)]/2+[\phi_{p_y}(\mathbf{r}-\mathbf{R}_i+\mathbf{Y}/2,z)-\phi_{p_y}(\mathbf{r}-\mathbf{R}_i-\mathbf{Y}/2,z)]/2\ . \tag{58}$$

TABLE II. Parameters adopted for the La-, Bi-, and Tl-based superconductors: $8J_C$ is the Cu $3d$–O $2p$ bandwidth, $8J_M$ is the Bi (Tl) $6p$–O $2p$ bandwidth, d_C and d_M are the respective lattice spacings between adjacent Cu-O_2 layers and between an M layer and its adjacent Cu-O_2 layer, and ε_∞ is the high-frequency dielectric constant.

	$8J_C$ (eV)	$8J_M$ (eV)	d_C (Å)	d_M (Å)	a (Å)	ε_∞
La oxide	3.6 (Ref. 17)		6.6 (Ref. 27)		3.8 (Ref. 27)	20 (Ref. 30)
Bi oxides	3.6 (Ref. 17)	2.4 (Ref. 19)	3.7 (Ref. 28)	6.0 (Ref. 28)	3.8 (Ref. 27)	15
Tl oxides	3.6 (Ref. 17)	1.6 (Ref. 20)	3.2 (Ref. 29)	5.8 (Ref. 29)	3.8 (Ref. 27)	15

Gaussian fits to Slater wave functions ϕ_d and ϕ_p are used. We neglect the small overlap integrals between the ϕ_{p_x} and ϕ_{p_y} orbitals, but retain only the large overlap integral between the ϕ_d orbital and the neighboring ϕ_{p_x} or ϕ_{p_y} orbital. The coefficients $f_{ii'}^{d}$ and $f_{ii'}^{p}$ are considered to be vanishingly small when i and i' are not nearest neighbors. The relative phases of the wave functions are shown in Fig. 6. The Bi-O and Tl-O $6p_{xy}$-$2p_{xy}$ wave functions are constructed in a like manner.

We have studied $\langle F \rangle$, $\langle F^2 \rangle$, μ_0, and λ numerically in the RPA. In the half-filled case, singular behavior associated with the nesting of the Fermi surface causes $\langle F^2 \rangle$ and μ_0 to take maximum values and λ a minimum. With increasing filling factor, $\langle F^2 \rangle$ and μ_0 drop rapidly, whereas λ increases slowly. The resulting λ and T_c are shown as functions of carrier concentration in Fig. 7.

We have suggested a plasmon theory of a superlattice consisting of 2D tight-binding conducting planes. Due to the attraction resulting from exchange of virtual plasmons in neighboring planes, paring of carriers in the same conducting plane occurs, leading to superconductivity. Within the RPA, we have calculated the superconducting transition temperature with encouraging results.

We would like to make the following remarks.

(1) The value of λ stays between 0.1 and 0.2 in all cases. But since it appears in the exponential in Eq. (52), a small variation in λ may cause large changes in the value of T_c. This is the reason for large differences in T_c for different phases in each series of oxides.

(2) The value of ω_L is about 1.4 eV at little n for La-based oxides, and is larger for $N=1$, Bi-, Tl-based oxides, which is smaller than that obtained by fits to the Drude model [$\sim$2.4 eV (Ref. 32) for $LaCuO_4$], but larger than that measured by muon spin resonance [$\sim$0.9 eV (Ref. 33) for $LaCuO_4$]. ω_L decreases with increasing of carrier concentration n.

(3) The $6p_{xy}$ (Bi,Tl)$-2p_{xy}$(O) bands play an important

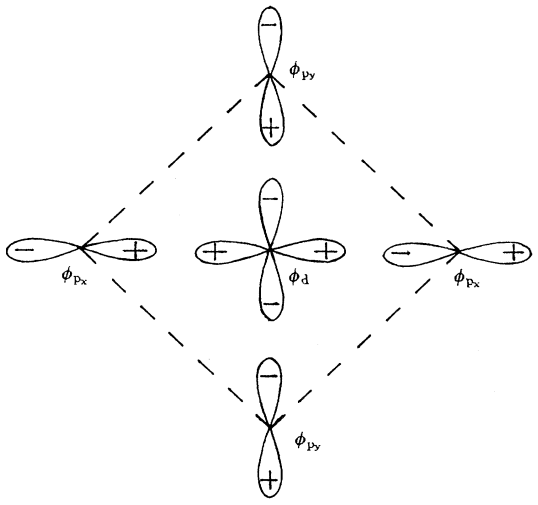

FIG. 6. Relative phases of the atomic wave functions.

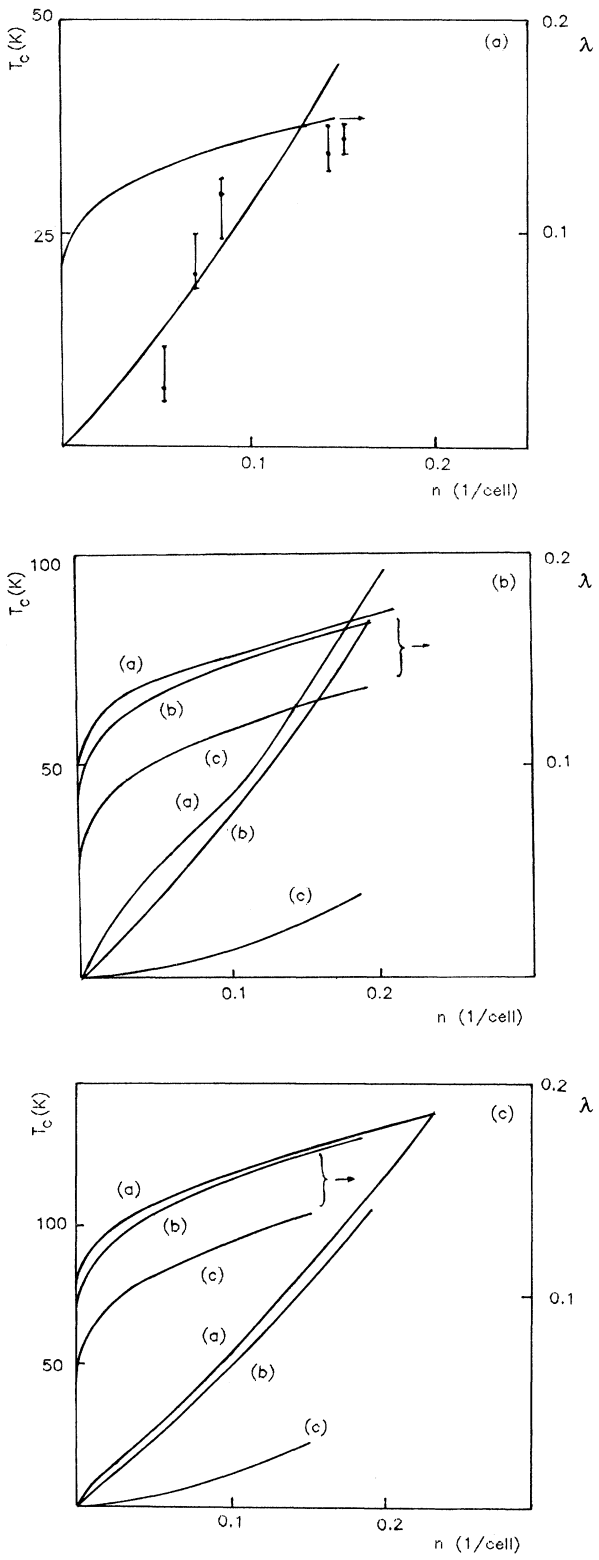

FIG. 7. Dependence of superconductivity transition temperature T_c and pairing strength λ on carrier concentration for (a) $(La,Sr)_2CuO_4$, (b) Bi-based oxides, and (c) Tl-based oxides. In (a), the crosses represent experimental results (Ref. 31). In (b) and (c), curves (a), (b), and (c) correspond, respectively, to $(L,M,N)=(4,1,3)$, $(3,1,2)$, and $(2,1,1)$.

role in raising T_c. We find higher T_c with narrower bandwidth.

(4) For each specific kind of material, T_c and λ increase with an increasing number of CuO_2 planes N, but become saturated for $N \geq 3$.

(5) The result in the $L=1$ case [Fig. 7(a)] is very encouraging. Figures 7(b) and 7(c) show that we obtain, for the Bi and Tl oxides, T_c values of the right orders of magnitude.

(6) Apart from the n dependence through λ, Eqs. (52) and (35) roughly imply a proportionality between T_c and $n^{1/2}$. This is in accordance with observation.[34]

(7) The theory needs only slight modifications to be applicable to the yttrium compound. It can also be refined by working, for example, in the generalized RPA (Refs. 35 and 36) (GRPA) to include more many-body effects. Work along these directions is in progress.[37]

Finally, we would like to draw attention to a basic problem in the theory of high-T_c superconductivity. The high T_c naturally requires a pairing interaction mediated by excitations with high characteristic frequency ω_L. On the other hand, the oxides have Fermi levels ε_F much lower than in metals, alloys, and metallic compounds. Thus, ω_L is comparable with ε_F instead of $\omega_L \ll \varepsilon_F$ as in conventional superconductors. This would make the whole Fermi sphere unstable against pairing, leading to contradiction with the apparent experimental confirmation[38] of the validity of a BCS and Fermi-liquid description. Despite this dilemma, we have followed, particularly in Sec. IV, the traditional BCS formulation. We believe a possible way out of this dilemma is to adopt a real-space pairing formalism along the general line of the old theory of Schafroth[39] and of the recent formulation by Lee[40] and by Micnas *et al.*[41]

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