Plasmon modes in a system composed of Cu-O layers and chains

Shiow-Fon Tsay
Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 300 43, Republic of China
*and Department of Physics, National Sun Yat-sen University, Kaohsiung, Taiwan 804 24, Republic of China**

Shou-Yih Wang
Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 300 43, Republic of China

T. J. Watson Yang
Electrophysics Department, National Chiao-Tung University, Hsinchu, Taiwan 300 50, Republic of China
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Based on a free-electron model of both the quasi-two-dimensional CuO_2 layers and the quasi-one-dimensional Cu-O chains in high-T_c Y-Ba-Cu-O superconductors, we have calculated in this simplified system various Coulombic electron-electron interacting potentials $V(\mathbf{q})$, dielectric functions, dispersion relations, and various plasmon modes, including in particular the acoustic plasmons. The main contribution of the chains is to stabilize, isolate, and generate more acoustic plasmons ω_- which provide a pairing mechanism for high-T_c superconductivity.

I. INTRODUCTION

Ever since the discovery of high-T_c superconductors, various approaches to an understanding of possible unconventional superconductivity have been intensively pursued. Many models for the superconductivity mechanism have been proposed.[1-5] Most of these authors considered their mechanism on the basis of a Hubbard model within only one single CuO_2 layer. Others preferred the so-called generalized BCS theory, based on a number of experimental data.[6-9] This latter theory is an extension of the traditional BCS superconductivity, in the sense that the role of mediating phonons there may be played by one or more boson-type mediators in forming carrier pairs like the Cooper pair of electrons. One acceptable mediator would be the plasmons of electrons because collective excitations of the electrons with light effective mass m^* would yield higher T_c than excitations of ions with much heavier ion mass M. The elevation of T_c by a factor M/m^* would be due to the enhancement of the plasmon-mediated electron-pairing parameter λ.[10] The plasma frequency ω_p is much higher than the Debye frequency Θ_D for the conventional phonon-mediated case. If the BCS result $T_c \sim 0.7\Theta\exp[-(1+\lambda)/(\lambda-\mu^*)]$ were to be used for comparison, this fact would increase T_c via the effective characteristic temperature Θ, which could be related to an average frequency $\langle\omega\rangle$ in the plasmon-mediated case. On the other hand, higher Θ would increase the modified Coulomb repulsion μ^* through the relation $\mu^*=\mu/[1+\mu\ln(E_F/k_B\Theta)]$. Furthermore, higher boson frequencies would reduce the electron-pairing parameter λ (Ref. 10) due to the relation $\lambda=2\int d\omega\,\alpha^2F(\omega)/\omega$. This would again lower T_c. In view of the disadvantages of boson frequencies that may be too high, intermediate-energy, acoustic types of plasmons, would be most favorable in promoting a high T_c. Based on experimental evidence,[11-14] Emery[15] pointed out that in high-T_c superconducting mechanism—unlike the phonon-mediated case—the electron-electron pairing force is nonretarded. This again pointed to the acoustic plasmons as the most suitable mediator for the pairing mechanism compared with other types of plasmons. The reason lies in the linear dispersion relation of the acoustic plasmon, which allows low enough frequencies for the formation of pairs. The concomitant longer screening time is expected to serve a similar function as that of the retarded phonons in traditional BCS theory.

Acoustic plasmons in Y-Ba-Cu-O superconductors have been studied by Griffin[16] as arising from the usual three-dimensional (3D) Coulomb potential interaction among free electrons in the system. He later studied the same problem using a two-dimensional (2D) Coulomb potential.[16] Kresin *et al.*[17] worked out the dispersion relations of an electron-gas model in equally spaced layer system for high-T_c copper oxides. For a system containing all equally spaced CuO_2 layers, Nakamura and Tagawa[18] reported, among other things, the striking result that only a system with 2,5,8, . . . layers can support acoustic plasmons for the superconductivity. As to the role of chains, Lee and Mendoza[19] have shown theoretically that excitations called "slender acoustic plasmons" could provide a possible superconducting mechanism in a small, long structure. Park, Tsuei, and Tu[20] presented evidence that the Cu-O chains are metallic. However, results of electron-energy band structure indicate that the energy band due to Cu-O chains is almost empty.[21] Clearly, the carrier concentration in the chains is much lower than that in the CuO_2 layers. As a consequence, the associated acoustic plasmons must be damped out more rapidly. Therefore superconductivity via the acoustic-plasmon mechanism is more likely to occur in CuO_2 layers than in

the Cu-O chains. With recent experimental data, Bauhofer *et al.*[22] emphasized that the chains could act as a coupling between adjacent superconducting CuO_2-Y-CuO_2 blocks. Based on an independent observation, our previous work,[23] in which long-range Coulombic interactions among the ions were studied, also supports this reexamination of the role of the Cu-O chains. Thus the important question to ask on the theoretical side is what role the chains are expected to play when interactions between the chains and layers are taken into consideration. In this article, we present a detailed study of Coulomb interactions between electrons in a system containing only CuO_2 layers and Cu-O chains with unequal separations among them to simulate a simplified, though more realistic model of $YBa_2Cu_3O_{7-\delta}$ superconductors, which is depicted in Fig. 1.

In Sec. II, using a simple free-electron-gas model for the system of coupled layers and chains, we obtain interacting potentials of the system within the random-phase approximation (RPA). Various electron-electron Coulomb interactions, viz., intralayer, nearest-neighbor interlayer, intrachain, nearest-neighbor interchain, and layer-chain interactions, are all taken into account, but no charge transfer among these components is considered. In Sec. III, we obtain a matrix form of the dielectric function for the system composed of various layers and chains and discuss relevant plasmon mode in the long-wavelength domain. In Sec. IV, we analyze the dielectric functions of the layers and chains in the system and consider the plasmons. The dielectric functions, dispersion relations, and plasmon modes of the thin-film system containing various layers and chains and the system containing an infinite number of layers and chains are fully discussed in Secs. V and VI, respectively. Finally, some numerical results with discussions and conclusions are given in Sec. VII.

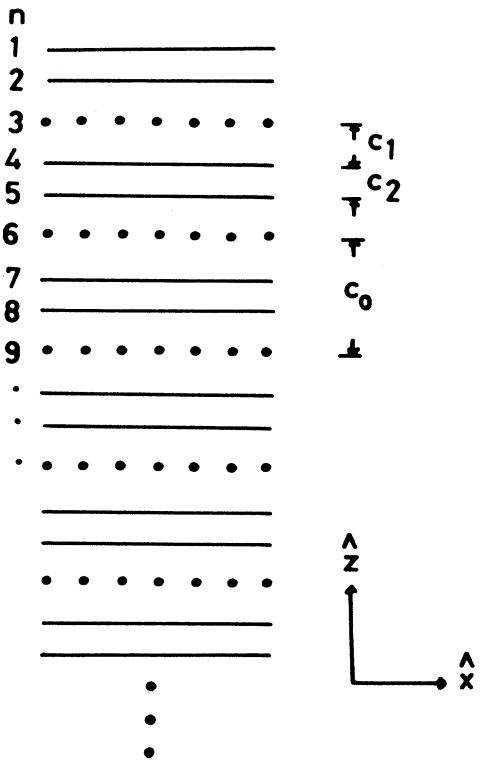

FIG. 1. A simplified model of $YBa_2Cu_3O_7$. The CuO_2 layers are represented by lines and the Cu-O chains by dots.

II. INTERACTION POTENTIALS $V(\mathbf{q})$

As shown in Fig. 1, this model consists of many layers, each with as large a surface area as that of an actual sample and each containing a quasi-two-dimensional electron gas. These layers, which are to simulate the copper oxide layers, are all placed parallel to the x-y plane. The N chains in an x-y plane, represented by N dots (Fig. 1), all lie along the y axis, equally spaced with separation a. Each chain contains a quasi-one-dimensional electron gas. Let the distance between two nearest-neighbor layers be c_2; that between a chain and a nearest-neighbor layer, c_1. The origin is chosen to be at the center of one particular chain. By symmetry, we assume the number of electrons per unit area in all layers to be the same and, furthermore, there is negligible charge transfer between any two of the components (layer or chain). For simplicity, we further assume, for the z-directionally periodic system, free-electron-type wave functions $\phi_{\mathbf{K}}^{(L)}(\boldsymbol{\rho}, z-mc_0)$ and $\phi_{\mathbf{k}}^{(c)}(x,y,z-mc_0)$, respectively, for the layers and the chains. These functions are periodical in the z direction, with periodicity $c_0=2c_1+c_2$, and m is an integer. For the N chains in any $(z=mc_0)$ plane, we have (taking $m=0$ for simplicity)

$$\phi_{\mathbf{k}}^{(c)}(x,y,z)=\frac{1}{\sqrt{L}}e^{ik_2y}\varphi_{k_1}(x)\eta(z) , \tag{1}$$

$$\varphi_{k_1}(x)=\frac{1}{\sqrt{N}}\sum_{j=0,\pm1,\ldots}^{(N-1)/2}\zeta(x-ja)e^{ik_1ja} , \tag{2}$$

where $\mathbf{k}=k_1\hat{\mathbf{i}}+k_2\hat{\mathbf{j}}$ is the electron wave vector for the chains in the x-y plane, L is the length of a chain, and j is an integer indicating the jth chain. The orthonormality conditions on $\varphi_{k_1}(x)$ impose the relation

$$\int_{-\infty}^{\infty}\zeta^*(x-j_1a)\zeta(x-j_2a)dx=\delta_{j_1j_2} . \tag{3}$$

For any single layer, taking for simplicity either one of the two layers in the zeroth ($m=0$) unit cell,

$$\phi_{\mathbf{K}}^{(L)}(\boldsymbol{\rho},z)=\frac{1}{\sqrt{A}}e^{i\mathbf{K}\cdot\boldsymbol{\rho}}\xi(z\pm c_1) , \tag{4}$$

where $\boldsymbol{\rho}=x\hat{\mathbf{i}}+y\hat{\mathbf{j}}$, with A the layer area and $\mathbf{K}$ the electron wave vector in the x-y plane of the layer. Since the overlapping charge-density distribution among different layers and different chains shows negligible amount in $YBa_2Cu_3O_7$,[24] we employ the following rather localized electron wave functions:

$$|\xi(z-mc_1)|^2=\delta(z-mc_1) , \tag{5}$$

$$|\zeta(x-ja)|^2=\delta(x-ja) , \tag{6}$$

$$|\eta(z)|^2=\delta(z) . \tag{7}$$

Thus we assume each layer to be strictly quasi-two-dimensional with essentially no overlap of wave functions between adjacent layers, and each chain to be strictly quasi-one-dimensional again with no overlapping. This approximation is very convenient for most of our analytical deductions, and the essential physics is not lost. The noninteracting single-particle energies in a layer and a chain are, respectively,

$$E_{\mathbf{K}}^{(L)}=\frac{\hbar^2}{2m_L^*}(K_1^2+K_2^2)+E_{0L}\ ,$$
$$E_{\mathbf{k}}^{(c)}=\frac{\hbar^2 k_2^2}{2m_c^*}+E_{0C}\ , \tag{8}$$

where E_{0L} is the z-directional quantization energy in the layer, and E_{0C} is the quantization energy in the chain along the x and z directions. For convenience, we set E_{0L} to zero, which implies that

$$E_F=\frac{\hbar^2 K_F^2}{2m_L^*}\ ,$$
$$E_{0C}=E_F-\frac{\hbar^2}{2m_c^*}k_{2F}^2\ , \tag{9}$$

where K_F is the magnitude of two-dimensional Fermi wave vector in a layer, and k_{2F} is the y component of the Fermi wave vector in a chain.

The Hamiltonian of the system can be written as

$$H=H_0+H_{\text{int}}\ , \tag{10a}$$

where

$$H_0=\sum_{\mathbf{K},L}E_{\mathbf{K},L}C_{\mathbf{K},L}^{\dagger}C_{\mathbf{K},L}+\sum_{k,j}E_{k,j}C_{k,j}^{\dagger}C_{k,j}\ , \tag{10b}$$

in which $E_{\mathbf{K},L}$ is the $E_{\mathbf{K}}^{(L)}$ of the Lth layer, while $E_{k,j}$ is the $\mathbf{E}_k^{(c)}$ of the jth chain. The interaction part of the Hamiltonian is

$$H_{\text{int}}=\tfrac{1}{2}\sum V_{\alpha\beta\nu\delta}C_{\alpha}^{\dagger}C_{\beta}^{\dagger}C_{\nu}C_{\delta}\ , \tag{11}$$

$$V_{\alpha\beta\nu\delta}=\int\phi_{\alpha}^*(\vec{r}_1)\phi_{\beta}^*(\vec{r}_2)V(\vec{r}_1-\vec{r}_2)\times\phi_{\nu}(\vec{r}_2)\phi_{\delta}(\vec{r}_1)d^3r_1\,d^3r_2\ , \tag{12}$$

where $V(\vec{r}_1-\vec{r}_2)$ is the Coulomb-potential energy; the summation is taken over all the indices α, β, ν, and δ; ϕ_{α}, ϕ_{β}, ϕ_{ν}, and ϕ_{δ} are electron wave functions in either chains or layer, which are given by Eqs. (1) and (4). We neglect the second-nearest-neighbor Coulomb interactions. Equation (12) consists of four parts: (i) intralayer interaction V_L;[18,25] (ii) intrachain interaction and interchain interaction between any two nearest-neighbor chains, V_C; (iii) interaction between two nearest-neighbor layers with separation c_2, $V_{LL'}$;[25] and (iv) interaction V_{LC} between chains and the nearest layer with separation c_1. They are readily calculated as

$$V_L=\frac{2\pi e^2}{Aq}\ , \tag{13}$$

$$V_C=\frac{2e^2}{NL}[2K_0(|q_2a|)\cos(q_1a)-\mathcal{C}_i(q_2a_{0C})]\ , \tag{14}$$

$$V_{LL'}=\frac{2\pi e^2}{Aq}e^{-qc_2}\ , \tag{15}$$

$$V_{LC}=\frac{2e^2}{A}\int_{-\infty}^{\infty}e^{iq_1u}K_0(q_2(u^2+c_1^2)^{1/2})du=\frac{2\pi e^2}{Aq}e^{-qc_1}\ , \tag{16}$$

where the cosine integral $\mathcal{C}_i(q_2a_{0C})$ is

$$\mathcal{C}_i(x)=-\int_x^{\infty}\frac{\cos z}{z}dz\ .$$

In Eqs. (13)–(16), $\mathbf{q}=q_1\hat{\mathrm{i}}+q_2\hat{\mathrm{j}}$, K_0 is the modified zeroth-order Bessel function. The first term of V_C in Eq. (14) is the nearest-neighbor interchain interaction, while the second term is the intrachain interaction.[26] Because of the Pauli exclusion principle, the closest separation between two interacting electrons in the intrachain case is assumed to be no smaller than a_{0C}, where a_{0C} can be an effective Bohr radius in the chain.[27] Comparison of (15) and (16) suggests that V_{LC}, the interaction between a layer and its nearest chains, can be considered as the interaction between a free-electron-gas layer and a hypothetical layer composed of the N chains. We only retain the nearest-neighbor interaction among the layers and/or chains. The Coulomb interaction V for the overall system can be expressed in matrix form, in which the matrix elements are the Coulomb interactions among various components (layer or chains) of the system, viz.,

$$\underline{V}(\mathbf{q})=\begin{pmatrix}
\ddots & & & & & & & \\
V_{LC} & V_C & V_{LC} & & & & & \\
 & V_{LC} & V_L & V_{LL'} & & & \underline{0} & \\
 & & V_{LL'} & V_L & V_{LC} & & & \\
 & & & V_{LC} & V_C & V_{LC} & & \\
 & & & & V_{LC} & V_L & V_{LL'} & \\
 & \underline{0} & & & & V_{LL'} & V_L & V_{LC} \\
 & & & & & & \ddots & \ddots
\end{pmatrix}\ . \tag{17}$$

This is a tridiagonal matrix (with a bandwidth of 3), all other off-diagonal elements being zero.

III. MATRIX FORM OF DIELECTRIC FUNCTIONS

The charge-density fluctuation ρ^{ind}, which is induced by an external charge density ρ^{ext}, has been given in linear-response theory[28] as

$$\rho_\alpha^{\text{ind}}(\mathbf{q},\omega)=\sum_\nu \sum_\mu K_{\alpha\mu}(\mathbf{q},\omega)V_{\mu\nu}(\mathbf{q})\rho_\nu^{\text{ext}}(\mathbf{q},\omega) , \tag{18}$$

where $K_{\mu\nu}(\mathbf{q},\omega)$ is the Fourier transform of a retarded density-density response function between the electron density ρ_μ in the μth layer (or chain) and the electron density ρ_ν in the νth layer (or chain). It is defined as

$$K_{\mu\nu}(\mathbf{q},\omega)=\lim_{\eta\to 0}\left[\frac{i}{\hbar}V\int_{-\infty}^{0}dt'\,e^{-i\omega t'+\eta t'}\langle[\rho_\mu^\dagger(\mathbf{q},t'),\rho_\nu(\mathbf{q},0)]\rangle\right] . \tag{19}$$

Equation (18) can be written in a matrix form:[18]

$$\vec{\rho}^{\,\text{ind}}(\mathbf{q},\omega)=\underline{K}(\mathbf{q},\omega)\underline{V}(\mathbf{q})\vec{\rho}^{\,\text{ext}}(\mathbf{q},\omega) . \tag{20}$$

Since the dielectric response function $\epsilon(\mathbf{q},\omega)$ is generally defined by

$$\epsilon(\mathbf{q},\omega)=\frac{\rho^{\text{ext}}}{\rho^{\text{ind}}+\rho^{\text{ext}}} , \tag{21}$$

of which the corresponding matrix form is

$$\underline{\epsilon}^{-1}(\mathbf{q},\omega)=\underline{I}+\underline{K}(\mathbf{q},\omega)\underline{V}(\mathbf{q}) , \tag{22}$$

where $\underline{\epsilon}^{-1}(\mathbf{q},\omega)$ is the inverse of the dielectric-response matrix $\underline{\epsilon}(\mathbf{q},\omega)$ and $\underline{I}$ is a unit matrix. In the random-phase approximation (RPA), the dielectric response matrix $\underline{\epsilon}(\mathbf{q},\omega)$ is reduced to a simpler form:[29]

$$\underline{\epsilon}(\mathbf{q},\omega)=\underline{I}-\underline{P}(\mathbf{q},\omega)\underline{V}(\mathbf{q}) , \tag{23}$$

where $\underline{P}(\mathbf{q},\omega)$ is the polarization matrix of the whole system. Since all the layers have the same polarization $P_1(\mathbf{q},\omega)$, $\underline{P}(\mathbf{q},\omega)$ is a diagonal matrix composed alternately of the two component polarizations $P_1(\mathbf{q},\omega)$ and $P_0(\mathbf{q},\omega)$, where $P_0(\mathbf{q},\omega)$ is the polarization of chains. Substituting Eq. (17) into Eq. (23), we find the tridiagonal dielectric response matrix:

$$\underline{\epsilon}(\mathbf{q},\omega)=\begin{bmatrix}
\cdot & \cdot & \cdot & & & & & & \\
E & A & B & & & & & & \\
 & B & A & E & & & \underline{0} & & \\
 & & D & C & D & & & & \\
 & & & E & A & B & & & \\
 & & & & B & A & E & & \\
 & & \underline{0} & & & D & C & D & \\
 & & & & & & E & A & B \\
 & & & & & & & B & A & E \\
 & & & & & & & & \cdot & \cdot & \cdot
\end{bmatrix} , \tag{24}$$

where $A\equiv 1-P_1V_L=\epsilon_L$ is the single-layer dielectric function; $B\equiv -P_1V_{LL'}=(\epsilon_L-1)e^{-qc_2}$; $C\equiv 1-P_0V_C=\epsilon_C$ is the multi-chain dielectric function;

$$D\equiv -P_0V_{LC}=(V_L/V_C)(\epsilon_C-1)e^{-qc_1} ;$$

$$E\equiv -P_1V_{LC}=(\epsilon_L-1)e^{-qc_1} .$$

In order to find collective excitations of the system, we solve for the dispersion relation[30] by requiring that

$$\det\underline{\epsilon}(\mathbf{q},\omega)\equiv F(\mathbf{q},\omega)=0 , \tag{25}$$

that is, $F_r(\mathbf{q},\omega)\equiv \text{Re}F(\mathbf{q},\omega)=0$, and $F_i(\mathbf{q},\omega)\equiv \text{Im}F(\mathbf{q},\omega)=0$. We note that

$$\epsilon_L(\mathbf{q},\omega)\equiv\epsilon_{Lr}(\mathbf{q},\omega)+i\epsilon_{Li}(\mathbf{q},\omega) , \tag{26}$$

and

$$\epsilon_C(q_2,\omega)\equiv\epsilon_{Cr}(q_2,\omega)+i\epsilon_{Ci}(q_2,\omega) . \tag{27}$$

IV. ANALYSIS OF THE LAYERS AND CHAINS

We use dimensionless variables $x=q/K_F$, $x_2=q_2/K_F$, and $y=\hbar\omega/E_F$, where E_F is the Fermi energy of the system, and K_F is the magnitude of Fermi wave vector of a layer. The two-dimensional K_F should be related to the surface charge-carrier density n_s of a layer via the relation

$$K_F=(2\pi n_s)^{1/2} . \tag{28}$$

A. Intralayer and interlayer dielectric functions

The imaginary part of the intralayer dielectric function of a single layer does not equal zero in the region $x^2-2x<y<x^2+2x$. This has been given by several authors.[18,31] In the long-wavelength (small q or small x) domain, ϵ_{Li} for a single layer is equal to zero when $y\geq x^2+2x$ [i.e.,

$$0\leq q\leq -K_F+(K_F^2+2m_L^*\omega/\hbar)^{1/2}] .$$

The real part of ϵ_L has been given by Ref. 18:

$$\epsilon_{Lr}=1+\frac{1}{x^3K_Fa_{0L}}\{2x^2+[(x^2-y)^2-4x^2]^{1/2} -[(x^2+y)^2-4x^2]^{1/2}\} , \tag{29}$$

where $a_{0L}=\hbar^2/m_L^*e^2$. In the long-wavelength limit, ϵ_{Lr} becomes

$$\epsilon_{Lr}\simeq 1-\frac{4}{K_Fa_{0L}}\frac{x}{y^2} . \tag{30}$$

This gives the well-known dispersion relation $y=[(4/K_F a_{0L})x]^{1/2}$, i.e., $\omega_1=[(2\pi e^2 n_s/m_L^*)q]^{1/2}$, which was first derived by Stern.[31]

The long-wavelength result Eq. (30) and the resulting dispersion relation can be regarded as describing a system containing only one single CuO_2 layer. For a system containing only two coupled layers with separation c_2, $F(\mathbf{q},\omega)$ can be reduced to A^2-B^2. The collective excitations occur at $A^2-B^2=(A-B)(A+B)=0$. In the long-wavelength domain, $y \geq x^2+2x$, the system has two branches of plasmon modes outside the electron-hole excitation region. One branch, the ω_+ mode, has a $q^{1/2}$-type dispersion relation which comes from the $A+B=0$ factor. The other mode ω_- yields a linear dispersion relation in q if $qc_2<1$, which is an acoustic-plasmon mode, coming from the $A-B=0$ factor. Explicitly, these plasmon modes are

$$\omega_+: \; y \simeq \left[\frac{8}{K_F a_{0L}}x\right]^{1/2}, \qquad \omega_-: \; y \simeq (4c_2/a_{0L})^{1/2}x \; . \tag{31}$$

B. Multichain dielectric function

The real part of dielectric function of a system of multiple chains can be shown, within RPA,

$$\epsilon_{Cr}=1+\frac{2}{\pi a_{0C} q_2}[2K_0(|q_2 a|)\cos(q_1 a)-\mathcal{C}_i(q_2 a_{0C})] \times \ln\left|\left\{\left[\frac{\omega}{q_2}\right]^2-\left[\frac{\hbar}{m_C^*}\left[k_{2F}+\frac{q_2}{2}\right]\right]^2\right\}\Big/\left\{\left[\frac{\omega}{q_2}\right]^2-\left[\frac{\hbar}{m_C^*}\left[k_{2F}-\frac{q_2}{2}\right]\right]^2\right\}\right| , \tag{32}$$

where $a_{0C}=\hbar^2/m_C^* e^2$. In the long-wavelength domain, ϵ_{Ci} equals zero when

$$y > \frac{m_L^*}{m_C^*}\left[x_2^2+2\left[\frac{K_{2F}}{K_F}\right]x_2\right] ,$$

i.e., $0<q_2<-k_{2F}+(k_{2F}^2+2m_C^*\omega/\hbar)^{1/2}$. The long- ($y$-component) wavelength (small x_2) form of ϵ_{Cr} obtained by expanding the right-hand side of Eq. (32) in orders of the small quantity $2(m_L^*/m_C^*)(k_{2F}/K_F)(x_2/y)$ is

$$\epsilon_{Cr}=1-\frac{16}{\pi a_{0C} k_{2F}}[2K_0(x_2 K_F a)\cos(x_1 K_F a)-\mathcal{C}_i(x_2 K_F a_{0C})]\left[\frac{k_{2F}}{K_F}\right]\left[\frac{m_L^*}{m_C^*}\right]^2\left[\frac{x_2}{y}\right]^2+\cdots , \tag{33}$$

in which $K_0(x)\simeq-\gamma-\ln(x/2)+\cdots$, $\mathcal{C}_i(x)\simeq\gamma+\ln x+\cdots$ for $x\ll 1$, where γ is Euler's constant. When $x_2 K_F a \ll 1$, and $x_1 K_F a \ll 1$, with the relation $\lim_{x_2\to 0}(x_2^2 \ln x_2)=-x_2^2/2$, Eq. (33) can be expressed as

$$\epsilon_{Cr}\simeq 1-[\alpha_1-\alpha_2(k_F a x_1)^2](x_2/y)^2+\cdots , \tag{34}$$

where

$$\alpha_1=\frac{16}{\pi a_{0C} K_F}\left[2\ln 2-3[\gamma+\ln(x_2 K_F a)]+\ln\left[\frac{a_{0C}}{a}\right]\right]\left[\frac{k_{2F}}{K_F}\right]\left[\frac{m_L^*}{m_C^*}\right]^2 ,$$

$$\alpha_2=\frac{16}{\pi a_{0C} K_F}[\ln 2-\gamma-\ln(x_2 K_F a)]\left[\frac{k_{2F}}{K_F}\right]\left[\frac{m_L^*}{m_C^*}\right]^2 ,$$

and α_1 and α_2 are positive constants.

The dispersion relation in the long-wavelength limit gives an acoustic mode $\omega_0 \propto q_2$, as can be clearly seen from Eq. (34). The phase velocity $v=\omega/q_2$ is related to the chain separation a. The result is similar to that of Refs. 32 and 33. We must emphasize that the acoustic-plasmon mode also appears in a quasi-one-dimensional single chain,[3,26] which is obtained by letting $a\to\infty$ in Eq. (32).

V. DIELECTRIC FUNCTIONS, DISPERSION RELATIONS, AND PLASMON MODES OF THE MANY-LAYER SYSTEM

We consider the systems which contain a finite number of layers and chains with two neighboring layers as the top boundary, as depicted in Fig. 1. In this paper, we do not investigate the surface plasmons of layered electron gas, such as the Giuliani-Quinn surface plasmon, which have been studied by Quinn and co-workers.[34,35] Let the dielectric function of the n layers (the plane of N chains also called a layer) be $\underline{\epsilon}^{(n)}(\mathbf{q},\omega)$. The determinants of the dielectric matrix $\det\underline{\epsilon}^{(n)}(\mathbf{q},\omega)\equiv F_n(\mathbf{q},\omega)$ for various systems of a finite number of layers are listed below, respectively:

$$
\begin{aligned}
&F_1(\mathbf{q},\omega)=A\ ,\\
&F_2(\mathbf{q},\omega)=A^2-B^2\ ,\\
&F_3(\mathbf{q},\omega)=(A^2-B^2)C-ADE\ ,\\
&F_4(\mathbf{q},\omega)=(A^2-B^2)(AC-DE)-A^2DE\ ,\\
&F_5(\mathbf{q},\omega)=(A^2-B^2)[(A^2-B^2)C-2ADE]\ ,\\
&F_6(\mathbf{q},\omega)=(A^2-B^2)[(A^2-B^2)C^2-3ACDE+D^2E^2]\\
&\qquad\qquad +A^2D^2E^2\ ,\\
&F_7(\mathbf{q},\omega)=(A^2-B^2)(AC-DE)[(A^2-B^2)C-3ADE]\\
&\qquad\qquad +A^3D^2E^2\ ,\\
&F_8(\mathbf{q},\omega)=(A^2-B^2)[(A^2-B^2)^2C^2-4(A^2-B^2)ACDE\\
&\qquad\qquad +4A^2D^2E^2-B^2D^2E^2]\ ,\ \ldots\ ,
\end{aligned}
\tag{35}
$$

where $F_1(\mathbf{q},\omega)$ represents the dielectric function of a system of only one single layer. We note that each $F_{3j-1}(\mathbf{q},\omega)$ with positive integers j contains the A^2-B^2 factor from recursion relations. As is seen clearly from Eq. (35), a system with $n=2,5,8,\ldots$ layers gives acoustic-plasmon modes. It is due to the $(A\text{-}B)$ factor from the coupling of the aforementioned two neighboring layers.

We next solve the dispersion relations from Eqs. (35) in the long-wavelength domain as defined by $y>2x+x^2$, and $y>(m_L^*/m_C^*)[x_2^2+2(k_{2F}/K_F)x_2]$. As stated above, $\epsilon_{Ci}(\mathbf{q},\omega)=\epsilon_{Li}(\mathbf{q},\omega)=0$ in this region. The determinants $F_n(\mathbf{q},\omega)$ are then set equal to zero. The D and E factors appearing in Eq. (35) can be readily calculated in this region as

$$
\begin{aligned}
D&=-V_{LC}P_0\\
&\simeq -e^{-qc_1}\frac{16}{aa_{0C}K_Fk_{2F}}\left[\frac{m_L^*}{m_C^*}\right]^2\left[\frac{k_{2F}}{K_F}\right]^2\frac{1}{x}\left[\frac{x_2^2}{y^2}\right]\ ,\\
E&=-V_{LC}P_1\simeq -e^{-qc_1}\left[\frac{4x}{a_{0L}K_Fy^2}\right]\ .
\end{aligned}
\tag{36}
$$

Because $4(m_L^*/m_C^*)^2(k_{2F}/K_F)^2(x_2^2/y^2)<1$, and $2x/y<1$, the contribution of D and E in Eq. (35) becomes weak when $x>1$ or $y>1$ in comparison to other terms such as A,C, or A^2-B^2. Consequently, Eq. (35) can be approximated as the following, when $x>1$ or $y>1$:

$$
\begin{aligned}
&F_1=A\ ,\\
&F_2=A^2-B^2\ ,\\
&F_3\simeq(A^2-B^2)C\ ,\\
&F_4\simeq(A^2-B^2)AC\ ,\\
&F_5\simeq(A^2-B^2)^2C\ ,\\
&F_6\simeq(A^2-B^2)^2C^2\ ,\\
&F_7\simeq(A^2-B^2)^2AC^2\ ,\\
&F_8\simeq(A^2-B^2)^3C^2\ .
\end{aligned}
\tag{37}
$$

Thus we can see that the plasmon modes clearly consist of ω_+ $(A+B=0)$, ω_- $(A-B=0)$, ω_1 $(A=0)$, and ω_0 $(C=0)$ modes. For qc_1 and qc_2 large, the exponential factors of Coulomb interaction of $V_{LL'}$ and V_{LC}, Eqs. (15) and (16), approach zero. Then each of the factors B, D, and E is small. As a consequence, the coupling between the coupled double layer and the chains vanishes. The system would appear as if the chains and the layers are isolated from each other. The ω_+ and ω_- modes of coupled double layers should approach the same ω_1 mode as that of a single layer.

VI. THE DISPERSION RELATIONS OF A SYSTEM CONTAINING AN INFINITE NUMBER OF LAYERS

We consider a system that is formed by the combination of two layers and a chain layer of N chains as a unit cell, with the two neighboring layers as the top boundary, Fig. 1. The dispersion relations of such a system with an infinite number of layers are solved in the Appendix. From the recurrence relations Eqs. (A2) and (A3b), we clearly see that the determinant of the dielectric function, $\det\underline{\epsilon}(q,\omega)=P_{m,j}$, has the factor (A^2-B^2), if $n=2,5,8,\ldots,3(m-1)+2$, with m a positive integer. This result is the same as that of Eq. (35). The zeros of the determinant of dielectric function $P_{m,j}$ of the system (see the Appendix) are given by the relation

$$
(A^2-B^2)C-2DE[A+B\cos\Theta]=0\ , \tag{38}
$$

where $\Theta=l\pi/(m-1)$, $l=0,1,\ldots,m-1$. These zeros have the following properties: (i) The zeros are nearly equally spaced on the Θ domain for the system with a large number of layers. (ii) The distribution of plasmon frequencies over Θ is quasicontinuous for an infinite number of layers. The plasmon branches form a band with band edges $\Theta=0$, and $\Theta=\pi$.

For $\Theta=0$, Eq. (38) is reduced to

$$
(A+B)[(A-B)C-2DE]=0\ , \tag{39}
$$

and for $\Theta=\pi$,

$$
(A-B)[(A+B)C-2DE]=0\ . \tag{40}
$$

Therefore, the acoustic plasmon ω_- mode, due to $A-B=0$, always exists in the system of an infinite number of layers. The location of the band edges are independent of the layer number n.

VII. NUMERICAL RESULTS AND CONCLUSIONS

The Fermi wave vector of the electrons in a two-dimensional layer is $K_F=(2\pi n_s)^{1/2}$, where n_s is the layer carrier concentration, whereas that of one-dimensional chain is $k_{2F}=\pi n_c/2$, in which n_c is the linear carrier concentration. Because experimentally available data are on the average carrier concentration, there is no direct way to obtain n_s and n_c separately. We employ the following averaging treatment by setting $n_s=nc_2$ and $n_c=na(c_0-2c_2)$, where n is the average carrier density. This is more realistic than the usual approach,[36,37] which

adopted equal separation among the layers and chains. Since the plasma frequency ω_p is available from experiment, we obtain the effective carrier mass m_L^* in a layer via the well-known plasma-frequency expression $\omega_P^2 = 4\pi ne^2/m_L^*$, with known n. Using the m_L^* and the relation $E_F = \hbar^2 K_F^2/2m_L^*$, we find the Fermi energy E_F of the system. In order to find the effective mass m_C^* for carriers in the chains, we apply the relation between the effective mass and the Sommerfeld constant $\gamma = C_{el}/T$;[36] C_{el} is the heat capacity due to electrons, and T is the temperature. This allows us the following relation:

$$\frac{m_C^*}{m_L^*} = \frac{\gamma_{1D}}{\gamma_{2D}} 2\pi na \frac{(C_0 - 2C_2)^2}{C_2} , \tag{41}$$

where γ_{1D} and γ_{2D} are Sommerfeld constants in 1D and 2D, respectively. If we assume that $\gamma_{1D} = \gamma_{2D}$ for the moment and omit a possible difference between the mass ratios m_C^*/m_L^* obtained from the heat capacity and that from plasma frequency, we have the value for m_C^* given below.

The experimental data for the lattice of $YBa_2Cu_3O_7$ are taken as $a = 3.8179$ Å, $b = 3.8828$ Å, $c_0 = 11.6807$ Å, $c_1 = 4.1291$ Å,[38] and $\omega_p = 2.6$ eV.[39] When $n = 7 \times 10^{21}$ cm^{-3}, we obtain $E_F \cong 0.40$ eV, $k_{2F} = 2.03 \times 10^{+7}$ cm^{-1}, $K_F \cong 3.87 \times 10^7$ cm^{-1}, $m_L^* = 1.43 m_0$, and $m_C^*/m_L^* = 4.33$ ($m_C^* = 6.20 m_0$), where m_0 is the rest mass of an electron. The four plasmon modes ω_1, ω_+, ω_-, and ω_0 for $q_1 = 0$, which correspond to single-layer, double coupled layers, and multichains, respectively, are depicted in Fig. 2. The region of electron-hole excitation of chain lies almost inside and below that of the electron-hole excitation of layers. The long-wavelength domain for the system of layers and chains given by $\epsilon_{Li} = 0$, and $\epsilon_{Ci} = 0$, can be expressed by $y \geq x^2 + 2x$, which is the domain above the upper boundary of the hatched region in the figure. The dispersion relations of the system must lie above the boundary of electron-hole excitation of the layer, below which any plasmon oscillations would be rapidly damped out. In the inset of Fig. 2, we show these modes in their long-wavelength limit. We denote the long-wavelength limit as only the small part (small x) of the long-wavelength domain, which has been defined as $y \geq x^2 + 2x$. The ω_- and ω_0 modes behave truly as an acoustic mode (near straight line). The ω_0 follows very closely the ω_- mode for $x_2 \leq 0.1$, but goes into the layers' electron-hole excitation region at $x_2 \simeq 1.4$. We note further in the inset that the ω_0 starts from values higher than those of ω_- and crosses ω_- at $q_2 \approx 0.1 k_F$. At the crossing, the energy (frequency) and wavelength of the collective motions ω_0 and ω_- have to be the same. This is for the case in which interactions between layers and chains are taken to be zero. In the cases with such interactions, due to the much smaller polarization P_0 of the chains relative to that of the layers, the collective oscillation ω_0 would be made to vanish slightly away from the crossing point. This helps explain why the modified ω_0 in an actual system starts from $q_2/k_F \geq 0.2$ (see Figs. 3 and 5). In this sense, we say the chains have the function of maintaining (or stabilizing) the acoustic mode ω_- of the doubly coupled layers. The dispersion curves of a many-layer system (for example, $n = 7$) are shown in Fig. 3. The $n = 7$ system contains two layers of multichains, two sets of coupled double layers, and a single layer. The dispersion relation consists of seven branches. Comparison of this with Fig. 2 indicates that these branches arise from the individual or unmodified modes ω_0, ω_+, ω_-, and ω_1 under the restriction from the composition of the system. For example, the existence of a modified ω_1 branch depends on whether or not the composition of the system contains a single layer. But for $q_2 > K_F$, those plasmon branches gradually approach the ω_+, ω_-, ω_1, and ω_0 modes, as shown Fig. 3. Since in this case the coupling factors D and E are rather small, the interaction between the coupled double layer and the multichains will become weakened and decoupled to some extent. In this way, the multichains may provide isolation between the two doubly coupled layers above and below the multichains; thus, aside from ω_1 and ω_0, only the modified ω_+ and ω_- modes of doubly coupled layers are seen in the figure. As q_2/K_F becomes so large as to be near 3.00 (i.e., in the very short-wavelength region), the Coulomb interactions V_{LL}, and V_{LC} [see Eqs. (15) and (16)] tend to be complete-

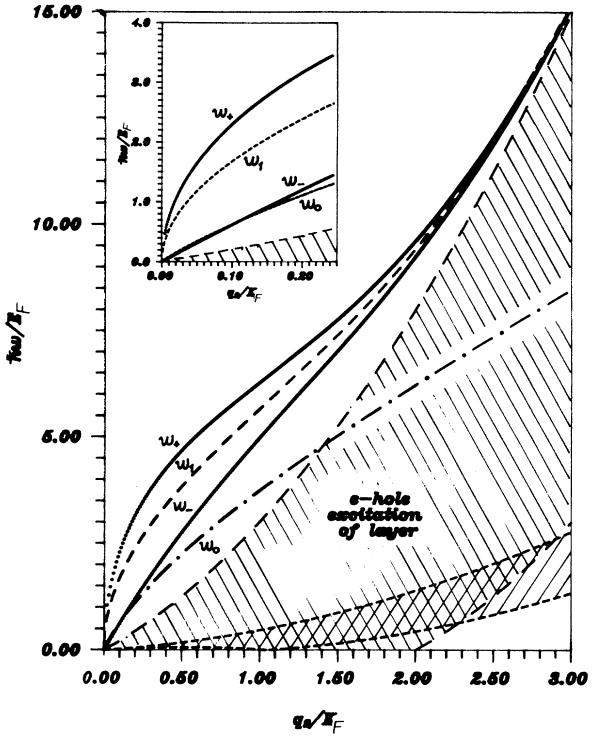

FIG. 2. The dispersion relations of the plasmons for the doubly coupled layers, ω_+ (upper solid line) and ω_- (lower solid line); single layer, ω_1 (dashed line); and the multichains, ω_0 (dot-dashed line) for $q_1 = 0$. The hatched portions are the electron-hole excitation continuum of the layer (upper) and that of the multichains (lower). Inset: Enlargement of the long-wavelength-limit region of Fig. 2. The ω_- mode and ω_0 mode cross at $x_2 \simeq 0.1$.

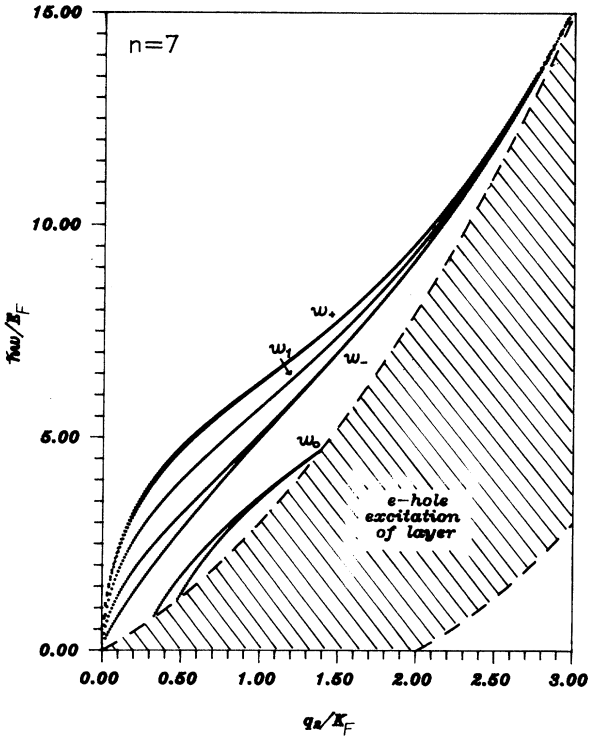

FIG. 3. The dispersion relations of the $n=7$ system with $q_1=0$.

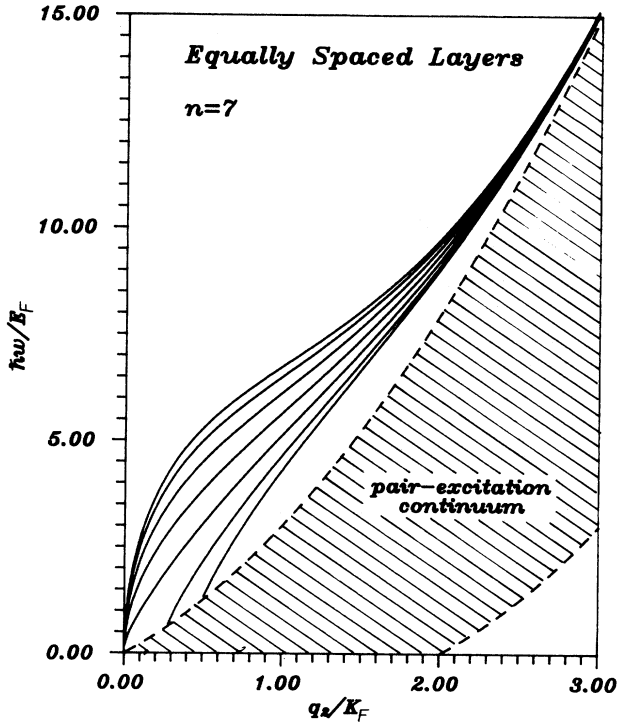

FIG. 4. The dispersion relations of the system which contains only seven equally spaced layers, showing the difference with chains (Fig. 3) and without chains.

ly turned off. In this case, all the components (layers and chains) are to be decoupled and what remains is only the single-layer plasmons ω_1, as shown in Fig. 3, where the plasmon ω_0 from the multichains has been damped out much earlier and quickly. If there were no chains, the dispersion relation would be very different. Following Ref. 18, the dispersion relations of the system with seven equally spaced largers are plotted in Fig. 4. These branches appear approximately equally spaced, as they all go together to ω_1 in the short-wavelength region, where, as just mentioned, all components are decoupled and only ω_1 remains.

For the system consisting of an infinite number of layers, the dispersion relations form three bands. Figure 5 shows the band distribution from Eq. (38). The band edges of the highest-energy band are $(A+B)C-2DE=0$ $(\Theta=\pi)$, and $A+B=0$ $(\Theta=0)$. A second band lies between $(A-B)C-2DE=0$ $(\Theta=0)$, and $A-B=0$ $(\Theta=\pi)$. But the lowest dispersion band of the chains does not begin at $q_2=0$ and, therefore, is not acoustic as the individual (unmodified) curves of Fig. 2. Thus the contribution from the chains to the high-T_c superconductivity is definitely not as important as the ω_- modes of the doubly coupled layers. The $\hbar\omega/E_F$ relative to the Θ value for $q_2=0.5k_F$ is shown in the inset of Fig. 5. It is obvious that the upper band is very narrow. While the lowest band of multichains enters the electron-hole excitation at $\Theta\leq\pi/4$, the upper two bands of these plasmons are gradually narrowed and approach the ω_+ and ω_- modes, respectively. Therefore, the

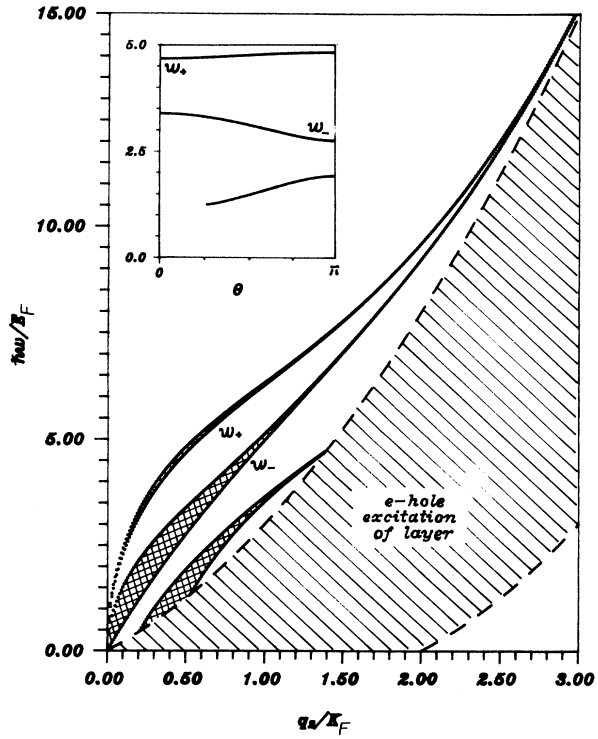

FIG. 5. The dispersion relations of the $n\rightarrow\infty$ system, forming three bands (cross-hatched). Inset: The bandwidth at $q_2=0.5K_F$ [the solutions of Eq. (38)]. The ordinate is the same as that of the main figure.

acoustic-plasmon mode ω_- due to $A-B=0$, always exists in the system containing an infinite number of layers. This result does not depend on the base of system or, in other words, the number of layers, n. If the system contain no chains but only equally spaced layers, acoustic modes ω_- exist only when the number of layers n is of the form $3(m-1)+2$, with $m=1,2,3,\ldots$. This accounts for the role of chains in generating more acoustic modes ω_- of the doubly coupled layers.

We next study the effect of the effective mass of the chain. If the effective mass of the chain were to equal to the effective mass of layer ($m_C^*/m_L^*=1$), the three frequency bands would lie close to one another as shown in Fig. 6. But even in this case, the acoustic plasmon ω_- still exists as the lower band edge for small x_2. On the other hand, if the effective mass of chains were much larger than the effective mass of layer, the plasmon band due to multichains would be damped out too quickly to appear. The dispersion curves for $m_C^*/m_L^*=8.67$ ($\gamma_{1D}=2\gamma_{2D}$) are shown in Fig. 7. It is clear that the energy bandwidth becomes very narrow. This can be understood in the following way: If the effective mass m_C^* is very heavy, the collective motion of chains can not occur easily and can not follow the collective motion of doubly coupled layers. Then the collective motion of the system is just that of the isolated coupled doubly layers.

To summarize, a basic formulation of a system containing only CuO_2 layers and Cu-O chains has been worked out. Dielectric functions and plasmon dispersion relations of various systems are presented and discussed, with emphasis on the role played by the chains and on the system containing infinitely many layers and chains. Special features of the effects arising from the multichains can be conveniently described according to the mass ratio m_C^*/m_L^* which in fact determines the plasmon energy-band structure. If $\gamma_{1D}=\gamma_{2D}$ is taken in Eq. (41), which means $m_C^*/m_L^*=4.33$, the acoustic plasmons ω_- of the doubly coupled layers would be stabilized in the small-q_2 region ($q_2/K_F<0.2$), where the chains' acoustic plasmon ω_0 does not appear. In the intermediate range of q_2 ($0.5\le q_2/K_F<1.5$), where ω_0 modes are available, the chains tend to isolate the two neighboring doubly coupled layers resulting in the gradually pronounced development of ω_+ and ω_- with increasing q_2. For large q_2 ($x_2\ge 1.50$), in which range the chains' ω_0 have been damped out, the doubly coupled layer modes ω_+ and ω_- approach the ω_1 of a single layer due to the decoupling of all the interactions among layers and chains via the factors $\exp(-qc_1)$, $\exp(-qc_2)$, etc., at large q. If we choose $m_C^*/m_L^*\gg 1$, the heavy mass m_c^* in addition to the small polarization of chains would make the ω_0 modes damp out rapidly, and the system would behave like a group of isolated doubly coupled layers. If $m_C^*/m_L^*=1$, which is rather inconsistent with the electronic band-structure results,[24] the dispersion curves become overlapped. For the $n\to\infty$ system, the dispersion curves form three narrowing bands and the chains provide possible generation of more acoustic modes ω_- of doubly coupled layer.

In short, the chains in general have the functions of stabilizing, isolating, and generating more acoustic modes

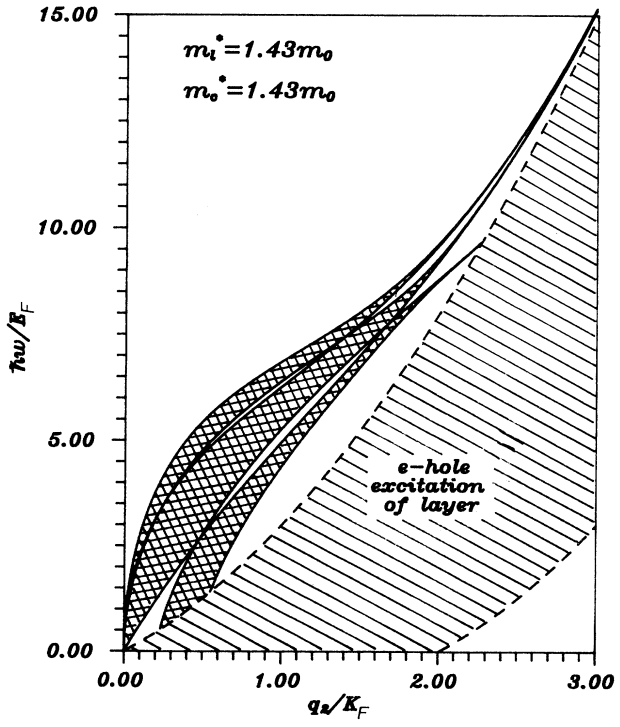

FIG. 6. The dispersion relations of the $n\to\infty$ system with $m_L^*=m_C^*=1.43m_0$, showing three plasmon bands.

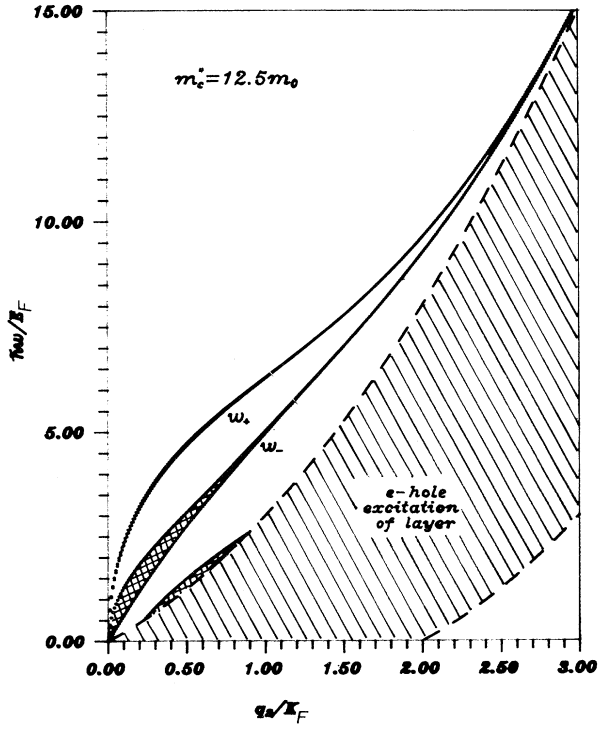

FIG. 7. The dispersion relations of the $n\to\infty$ system with $m_C^*=12.5m_0$, showing the narrowing of the bands.

ω_-, and it is these ω_- modes of doubly coupled layers that might provide a pairing mechanism for high-T_c superconductivity, because, based on our results (Fig. 5, e.g.), the nonacoustic behavior of the dispersion relations of the chains is unlikely to provide the essential superconductivity mechanism.

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APPENDIX: FORMAL DERIVATION FOR THE DISPERSION RELATIONS

The base cell of the system with infinite number of layers can contain either one, or two layers, or multichains. When the base cell is composed of three layers, the system becomes an infinite, perfectly periodic one. The layer index is $n=3(m-1)+j$, with $j=1,2,3$, where m denotes the mth cell (block) and j represents the jth layer of the base (lowest) cell (block). To solve the dispersion relations, we first calculate the determinant of the tridiagonal dielectric-function matrix $\underline{\epsilon}(q,\omega)$. Which we now set $\det\underline{\epsilon}(\mathbf{q},\omega)\equiv P_{m,j}$ for convenience. Then we have

$$P_{m,j}=\begin{vmatrix} A & B & & & & & & & \\ B & A & E & & & & & & \\ & D & C & D & & & \underline{0} & & \\ & & E & A & B & & & & \\ & & & B & A & E & & & \\ & & & & D & C & D & & \\ & & & & & E & \ddots & & \\ & & & & & & & D & \\ & & & & & & E & A & B \\ & & \underline{0} & & & & & B & A & E \\ & & & & & & & & D & C \end{vmatrix} . \tag{A1}$$

Here we are mainly interested in the limiting case $n\rightarrow\infty$ for a bulk sample. After some algebraic manipulation, we find the following recurrence relation for $P_{m+1,j}$, $P_{m,j}$, and $P_{m-1,j}$:

$$P_{m+1,j}+[2ADE-C(A^2-B^2)]P_{m,j} +B^2D^2E^2P_{m-1,j}=0 , \tag{A2}$$

and $P_{1,j}$ and $P_{2,j}$ are determined by the base (lower boundary) of sample. If the base is a single layer ($j=1$),

$$\begin{aligned} P_{1,1}&=A , \\ P_{2,1}&=(A^2-B^2)(AC-DE)-A^2DE . \end{aligned} \tag{A3a}$$

If the base is a coupled double layers ($j=2$),

$$\begin{aligned} P_{1,2}&=A^2-B^2 , \\ P_{2,2}&=(A^2-B^2)[(A^2-B^2)C-2ADE] . \end{aligned} \tag{A3b}$$

Finally, if the base contains two layers and N-chains ($j=3$), we have

$$\begin{aligned} P_{1,3}&=(A^2-B^2)C-ADE , \\ P_{2,3}&=(A^2-B^2)[(A^2-B^2)C^2-3ACDE+D^2E^2] \\ &\quad +A^2D^2E^2 . \end{aligned} \tag{A3c}$$

To solve, Eq. (A2) can be recast as

$$\begin{bmatrix} P_{m+1,j} \\ P_{m,j} \end{bmatrix} = \begin{bmatrix} C(A^2-B^2)-2ADE & -B^2D^2E^2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} P_{m,j} \\ P_{m-1,j} \end{bmatrix} . \tag{A4}$$

By iteration, $P_{m,j}$ can be expressed in $P_{1,j}$ and $P_{2,j}$:

$$\begin{bmatrix} P_{m,j} \\ P_{m-1,j} \end{bmatrix} = \underline{A}^{m-2} \begin{bmatrix} P_{2,j} \\ P_{1,j} \end{bmatrix} , \tag{A5}$$

where

$$\underline{A}= \begin{bmatrix} C(A^2-B^2)-2ADE & -B^2D^2E^2 \\ 1 & 0 \end{bmatrix} . \tag{A6}$$

To calculate the integer powers of $\underline{A}$, we diagonalize $\underline{A}$, so that

$$\underline{A}\underline{e}_i=\lambda_i\underline{e}_i .$$

The eigenvalues of $\underline{A}$ are

$$\begin{aligned} \lambda_{1,2}&=\tfrac{1}{2}[(A^2-B^2)C-2ADE] \\ &\quad \pm\tfrac{1}{2}\{[(A^2-B^2)C-2ADE]^2-4B^2D^2E^2\}^{1/2} . \end{aligned} \tag{A7}$$

The eigenvectors are

$$\underline{e}_1=\begin{bmatrix} \xi_1 \\ \eta_1 \end{bmatrix} = \frac{1}{(\lambda_1^2+1)^{1/2}} \begin{bmatrix} \lambda_1 \\ 1 \end{bmatrix} ,$$

$$\underline{e}_2=\begin{bmatrix} \xi_2 \\ \eta_2 \end{bmatrix} = \frac{1}{(\lambda_2^2+1)^{1/2}} \begin{bmatrix} \lambda_2 \\ 1 \end{bmatrix} .$$

Then

$$\underline{A}^{m-2}=\underline{S}\underline{D}^{m-2}\underline{S}^{-1} ,$$

where

$$\underline{S}= \begin{bmatrix} \xi_1 & \xi_2 \\ \eta_1 & \eta_2 \end{bmatrix}$$

and

$$\underline{D}^{m-2}= \begin{bmatrix} \lambda_1^{m-2} & 0 \\ 0 & \lambda_2^{m-2} \end{bmatrix} .$$

We finally obtain

$$P_{m,j}=\frac{P_{2,j}}{\lambda_1-\lambda_2}(\lambda_1^{m-1}-\lambda_2^{m-1}) - \frac{P_{1,j}}{\lambda_1-\lambda_2}(\lambda_2\lambda_1^{m-1}-\lambda_1\lambda_2^{m-1}) . \quad \text{(A8)}$$

In the following, we discuss various cases of λ_1 and λ_2 of Eq. (A7), be they complex or real.

Case 1: λ_1 and λ_2 of Eq. (A7) are, in general, complex if

$$[(A^2-B^2)C-2ADE]^2 \lesssim 4B^2D^2E^2 . \quad \text{(A9)}$$

In this case, $\lambda_1=\lambda_2^*$. To exploit this feature, we write

$$\lambda_1=\alpha+i\beta=re^{i\phi} , \quad \lambda_2=\alpha-i\beta=re^{-i\phi} , \quad \text{(A10)}$$

where

$$\alpha=\tfrac{1}{2}[(A^2-B^2)C-2ADE] , \quad \beta=(B^2D^2E^2-\alpha^2)^{1/2} , \quad r=(\alpha^2-\beta^2)^{1/2}=BDE , \quad \phi=\arctan\frac{\beta}{\alpha} . \quad \text{(A11)}$$

with the new variables, we obtain from Eq. (A8)

$$P_{m,j}=\frac{r^{m-2}}{\sin\phi}\{P_{2,j}\sin[(m-1)\phi] - rP_{1,j}\sin[(m-2)\phi]\} \quad \text{(A12)}$$

where ϕ from Eq. (A11), lies between 0 and π. We rewrite Eq. (A12) in the form

$$P_{m,j}=P\sin[(m-1)\phi+\psi] \quad \text{(A13)}$$

where

$$P^2=\left[\frac{r^{m-2}}{\sin\phi}\right]^2(r^2P_{1,j}^2+P_{2,j}^2-2rP_{1,j}P_{2,j}\cos\phi) , \quad \tan\psi=\frac{rP_{1,j}\sin\phi}{P_{2,j}-rP_{1,j}\cos\phi} .$$

The lth root ϕ_l of $P_{m,j}$ satisfies

$$(m-1)\phi_l+\psi_l=\pm l\pi , \quad \text{(A14)}$$

where $l=0,1,2,\ldots,m-1$. The solutions becomes particularly simple for large m, when ψ can be neglected, and we obtain

$$\phi_l=\pm\frac{l\pi}{m-1} . \quad \text{(A15)}$$

From the above analysis, the zeros of $P_{m,j}$ for large m are

$$(A^2-B^2)C=2DE\left[A+B\cos\left[\frac{l\pi}{m-1}\right]\right] .$$

Case 2: λ_1 and λ_2 are real, we can set

$$\lambda_1=\alpha+\beta'=re^{\phi'} , \quad \lambda_2=\alpha-\beta'=re^{-\phi'} , \quad \text{(A16)}$$

where $\beta'=i\beta$, $r=(\alpha^2-\beta'^2)^{1/2}$ and $\phi'=i\phi$, Eqs. (A12) and (A13) can be replaced by

$$P_{m,j}=\frac{r^{m-2}}{\sinh\phi'}\{P_{2,j}\sinh[(m-1)\phi'] - rP_{1,j}\sinh[(m-2)\phi']\} =P'\sinh[(m-1)\phi'+\psi'] , \quad \text{(A17)}$$

where $\psi'=i\psi$. Because the value of the hyperbolic sine function lies between $-\infty$ and ∞, the zeros of $P_{m,j}$ should satisfy

$$(m-1)\phi'+\psi'=0 . \quad \text{(A18)}$$

Substituting $\psi'=i\psi$ and Eq. (A18) into Eq. (A13) yields

$$\tanh[(m-1)\phi']=-\frac{rP_{1,j}\sinh\phi'}{P_{2,j}-rP_{1,j}\cosh\phi'} =\frac{\beta'P_{1,j}}{\alpha P_{1,j}-P_{2,j}} . \quad \text{(A19)}$$

From Eq. (A19), we can get a numerical solution which is dependent of the layer index n.

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