Response functions of a superlattice with a basis: A model of oxide superconductors

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The new high-T_c oxide superconductors appear to be superlattice structures with a basis composed of metallic sheets as well as metallic chains. Using a simple free-electron-gas model for the sheets and chains, we obtain the dielectric function $\epsilon(\mathbf{q},\omega)$ of such a multilayer system within the random-phase approximation (RPA). We give results valid for arbitrary wave vector $\mathbf{q}$ appropriate to sheets and chains (as in the orthorhombic phase of Y-Ba-Cu-O) as well as for two different kinds of sheets (such as may be present in the Bi-Sr-Ca-Cu-O superconductors). The occurrence of acoustic plasmons is a general phenomenon in such superlattices, as shown by an alternative formulation based on the exact response functions for the individual sheets and chains, in which only the intersheet (chain) Coulomb interaction is treated in the RPA. These results generalize the long-wavelength expressions recently given in the literature. We also briefly discuss the analogous results for two arrays of mutually perpendicular chains, such as found in Hg chain compounds.

I. INTRODUCTION

In this paper, we give a general procedure for finding the charge-fluctuation response functions and associated collective modes in superlattice systems with a "basis" composed of metallic sheets and chains, coupled by the Coulomb interaction. We show that the random-phase-approximation (RPA) integral equation for the various response functions can be solved exactly if we limit ourselves to two-dimensional (2D) sheets (in which the electrons can only move in the x-y plane) and one-dimensional (1D) chains in which the electrons can only move along the chain direction (x or y). Our results are of interest in connection with a wide variety of condensed-matter systems but especially with the new oxide superconductors.

In Sec. II, we discuss such a superlattice system (periodic in the z direction) in which the basis is two metallic sheets (in the x-y plane) and a plane composed of chains (directed along the y axis). As argued in a recent paper,[1] the Cu-O network in the high-temperature superconductor ($\delta < 0.2$) $YBa_2Cu_3O_{7-\delta}$ can perhaps be modeled by such a periodic structure composed of sheets and chains. The interesting result was that such a coupled sheet-chain system generally leads to an acoustic plasmon, which might play a crucial role in Cooper pairing in the Y-Ba-Cu-O superconductors. Our present work generalizes the long-wavelength limit considered in Ref. 1 and gives the dielectric function $\epsilon(\mathbf{q},\omega)$ and response functions for arbitrary wave vector $\mathbf{q}$.

In Sec. III, we specialize the results of Sec. II by eliminating the chains. In this case, our general formulas reduce to those recently discussed[2,3] for a semiconductor type-II superlattice (in this case, the basis is composed of two different sheets). Our results involve a slight generalization in that we include the finite thickness of the sheets through form-factored Coulomb interactions. The newly discovered Bi-Sr-Ca-Cu-O high-temperature superconductors may be an example of a superlattice with a basis of two *different* kinds of metallic sheets (Bi-O and Cu-O sheets).

In Sec. IV, we discuss a set of two mutually perpendicular arrays of chains (usually referred to as the a and b chains) such as one finds in $Hg_{3-\delta}AsF_6$. Our present work extends the recent long-wavelength treatment[4] to arbitrary wave vectors. The general results we obtain and the conditions under which the two chain arrays decouple are similar to those found by Mohan.[5]

In Sec. V, we briefly discuss the generalization in which only the "inter-Coulomb" interaction is treated in the RPA. By inter-Coulomb, we mean that Coulomb interaction between electrons in different sheets or chains (or between sheets and chains). In contrast, the "intra-Coulomb" interaction between electrons in a *given* sheet is treated exactly.

Earlier references to the literature on these systems can be found in Refs. 1–5. This paper is mainly devoted to the technical details of how one solves the RPA integral equation in the various models. However, in Sec. VI, we briefly discuss the possible relevance of the acoustic plasmons which arise in such superlattices to high-temperature superconductivity.

II. SHEETS AND CHAINS: Y-Ba-Cu-O

The RPA integral equation for the inhomogeneous systems we are concerned with is given by (for further details, see the introduction of Ref. 4)

$$\chi_{ij}(\mathbf{r},\mathbf{r}',\omega)=\chi_i^0(\mathbf{r},\mathbf{r}',\omega)\delta_{ij}+\int d\mathbf{r}_1\int d\mathbf{r}_2\chi_{ii}^0(\mathbf{r},\mathbf{r}_1,\omega)v(\mathbf{r}_1-\mathbf{r}_2)\sum_{j'}\chi_{j'j}(\mathbf{r}_2,\mathbf{r}',\omega)\,. \tag{1}$$

Here $\chi_{ij}(\mathbf{r},\mathbf{r}',\omega)$ is the dynamic response function describing the correlation between the electronic density fluctuation $\delta\rho_i(\mathbf{r})$ in the ith sheet (or chain) and the electronic density $\delta\rho_j(\mathbf{r})$ in the jth sheet (or chain). $v(\mathbf{r}-\mathbf{r}')$ is the Coulomb interaction. We shall solve this by using Fourier transformation techniques and thus we will work with

$$\chi_{ij}(\mathbf{q},-\mathbf{q}')=\int d\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}}\int d\mathbf{r}'\, e^{-i\mathbf{q}'\cdot\mathbf{r}'}\chi_{ij}(\mathbf{r},\mathbf{r}')\,, \tag{2}$$

where, from now on, the frequency dependence will be left implicit. We treat the Coulomb interactions in a given sheet (or chain) as well as between different sheets (chains) on the same footing in (1). Thus, $\chi_i^0(\mathbf{r},\mathbf{r}')$ is the response function for noninteracting electrons in a sheet (or chain) of type i.

For our chain-sheet model of Y-Ba-Cu-O, we take our basis to be two metallic sheets (sheet a at $z=0$ and sheet b at $z=z_b$) and chains along the y axis (separated by a distance a in the x direction) in a plane at $z=z_c$. This basis will be repeated in the z direction with period c. Thus $i,j=a,b$, or c, where c represents one of the chains. We assume for simplicity that there is negligible charge transfer between the different sheets and chains. Moreover, we assume the electrons in the sheets can only move in the x-y plane and the electrons in the chains can only move in the y direction. That is, the electrons are in their lowest transverse states.

The charge fluctuation at $\mathbf{r}$ in a sheet of type a is given by [$\mathbf{r}_\parallel=(x,y)$]

$$\delta\rho_a(\mathbf{r})=\sum_{Z_s} w_s(z-Z_s)\delta\rho_{Z_s}(\mathbf{r}_\parallel)\,, \tag{3}$$

where $Z_s=mc$ (m an integer). Here $w_s(z)$ is a strongly peaked function which describes how localized the electrons are to a sheet [essentially $w_s(z)$ is related to the lowest transverse eigenstate in the z direction]. Similarly, the charge fluctuation at $\mathbf{r}$ in a sheet of type b is given by

$$\delta\rho_b(\mathbf{r})=\sum_{Z_s} w_s(z-Z_s-z_b)\delta\rho_{Z_s}(\mathbf{r}_\parallel)\,, \tag{4}$$

while for a fluctuation at $\mathbf{r}$ in a chain

$$\delta\rho_c(\mathbf{r})=\sum_{\mathbf{R}_c} w_c(\mathbf{r}_\perp-\mathbf{R}_c)\delta\rho_{\mathbf{R}_c}(y)\,. \tag{5}$$

Here $\mathbf{R}_c$ gives the position (in x-z plane) of the chain involved,

$$\mathbf{R}_c=(na,0,z_c+mc)\,, \tag{6}$$

where n,m are integers. These form a Bravais lattice. In (5), w_c describes the spatial extent of the lowest transverse eigenstate[4,5] in a chain centered at $\mathbf{R}_c$, with $\mathbf{r}_\perp$ standing for the x-z components perpendicular to the chain axis. It follows from the symmetry of this system that $\chi_{ij}(\mathbf{q},-\mathbf{q}')=0$ unless $\mathbf{q}'=\mathbf{q}+\mathbf{G}$, where $\mathbf{G}$ is a reciprocal-lattice vector in the (x,z) plane:

$$\mathbf{G}=(2\pi n_x/a,0,2\pi n_z/c);\quad n_x,n_z \text{ integers}\,. \tag{7}$$

Using the specific form given in (3), one can show that χ_{aa} has the following structure:

$$\chi_{aa}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})=\beta_s(q_z+G_z')\beta_s(q_z+G_z)\bar{\chi}_{aa}(\mathbf{q}+G_x',-\mathbf{q}-G_x)\,, \tag{8}$$

where the key point is that $\bar{\chi}_{aa}$ does not depend on the z components of $\mathbf{G}$ and $\mathbf{G}'$. Here the sheet "form factors" β_s are the Fourier transforms of $w_s(z)$. Similarly, one finds that

$$\chi_{cc}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})=\beta_c(\mathbf{q}_\perp+\mathbf{G}')\beta_c(\mathbf{q}_\perp+\mathbf{G})\bar{\chi}_{cc}(\mathbf{q})e^{-i(G_z-G_z')z_c}\,, \tag{9}$$

where $\mathbf{q}_\perp$ is the xz component of $\mathbf{q}$ and $\bar{\chi}_{cc}(\mathbf{q})$ is completely independent of $\mathbf{G}$ and $\mathbf{G}'$. Finally, we have

$$\begin{aligned}\chi_{ac}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})&=\beta_s(q_z+G_z')\beta_c(\mathbf{q}_\perp+\mathbf{G})\bar{\chi}_{ac}(\mathbf{q}+G_x')e^{-i(q_z+G_z)z_c}\,,\\ \chi_{bc}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})&=\beta_s(q_z+G_z')\beta_c(\mathbf{q}_\perp+\mathbf{G})\bar{\chi}_{bc}(\mathbf{q}+G_x')e^{-i(q_z+G_z)z_c}e^{i(q_z+G_z')z_b}\,.\end{aligned} \tag{10}$$

For the noninteracting response functions, only electrons in the same sheet or chain are correlated. One finds

$$\begin{aligned}\bar{\chi}_{aa}^0(\mathbf{q}+G_x',-\mathbf{q}-G_x)&=N_s\chi_{2a}^0(\mathbf{q}_\parallel)\,,\\ \bar{\chi}_{bb}^0(\mathbf{q}+G_x',-\mathbf{q}-G_x)&=N_s\chi_{2b}^0(\mathbf{q}_\parallel)\,,\\ \bar{\chi}_{cc}^0\mathbf{q}&=N_c\chi_1^0(q_y)\,,\end{aligned} \tag{11}$$

where $\chi_2^0(\mathbf{q}_\parallel,\omega)$ [$\chi_1^0(q_y,\omega)$] is the usual 2D (1D) Lindhard function. N_s is the number of sheets of type a (or type b) per unit volume and N_c is the total number of chains per unit volume. We also note explicitly that

$$\chi_{aa}^0(\mathbf{q}+G_x',-\mathbf{q}-\mathbf{G})=N_s\beta_s(q_z)\beta_s(q_z+G_z)\chi_{2a}^0(\mathbf{q}_\parallel,\omega)=\chi_{aa}^0(\mathbf{q},-\mathbf{q}-\mathbf{G})\,, \tag{12}$$

which will be needed later.

Fourier transforming (1), using the fact that $\chi(\mathbf{q},-\mathbf{q}')$ is zero unless $\mathbf{q}'=\mathbf{q}+\mathbf{G}$, gives

$$\chi_{ij}(\mathbf{q},-\mathbf{q}-\mathbf{G})=\chi_{ii}^0(\mathbf{q},-\mathbf{q}-\mathbf{G})\delta_{ij}+\sum_{\mathbf{G}'}\chi_{ii}^0(\mathbf{q},-\mathbf{q}-\mathbf{G}')v(\mathbf{q}+\mathbf{G}')\sum_{j'}\chi_{j'j}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})\,, \tag{13}$$

where $v(\mathbf{q})=4\pi e^2/q^2$. Thus we have

$$\chi_{cc}(\mathbf{q},-\mathbf{q}-\mathbf{G})=\chi^0_{cc}(\mathbf{q},-\mathbf{q}-\mathbf{G})+\sum_{\mathbf{G}'}\chi^0_{cc}(\mathbf{q},-\mathbf{q}-\mathbf{G}')v(\mathbf{q}+\mathbf{G}')$$
$$\times[\chi_{ac}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})+\chi_{bc}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})+\chi_{cc}(\mathbf{q}+\mathbf{G}',-\mathbf{q}-\mathbf{G})]\,. \quad (14)$$

Using (9) and (10), we find

$$\bar{\chi}_{cc}(\mathbf{q})=N_c\chi^0_1(q_y)+N_c\chi^0_1(q_y)\sum_{\mathbf{G}'}\beta_c(\mathbf{q}_\perp+\mathbf{G}')v(\mathbf{q}+\mathbf{G}')[\beta_s(q_z+G_z')\bar{\chi}_{ac}(\mathbf{q}+G_x')e^{-i(q_z+G_z')z_c}$$
$$+\beta_s(q_z+G_z')\bar{\chi}_{bc}(\mathbf{q}+G_x')e^{-i(q_z+G_z')(z_c-z_b)}$$
$$+\beta_c(\mathbf{q}_\perp+\mathbf{G}')\bar{\chi}_{cc}(\mathbf{q})]\,, \quad (15)$$

after canceling out $\beta_c(\mathbf{q}_\perp)\beta_c(\mathbf{q}_\perp+\mathbf{G})\exp(-iG_zz_c)$ from both sides. Proceeding similarly, one finds

$$\bar{\chi}_{ac}(\mathbf{q})=N_s\chi^0_{2a}(\mathbf{q}_\parallel)\sum_{\mathbf{G}'}\beta_s(q_z+G_z')v(\mathbf{q}+\mathbf{G}')[\beta_s(q_z+G_z')\bar{\chi}_{ac}(\mathbf{q}+G_x')+\beta_s(q_z+G_z')\bar{\chi}_{bc}(\mathbf{q}+G_x')e^{i(q_z+G_z')z_b}$$
$$+\beta_c(\mathbf{q}_\perp+\mathbf{G}')\bar{\chi}_{cc}(\mathbf{q})e^{i(q_z+G_z')z_c}]\,, \quad (16)$$

$$\bar{\chi}_{bc}(\mathbf{q})=N_s\chi^0_{2b}(\mathbf{q}_\parallel)\sum_{\mathbf{G}'}\beta_s(q_z+G_z')v(\mathbf{q}+\mathbf{G}')[\beta_s(q_z+G_z')\bar{\chi}_{ac}(\mathbf{q}+G_x')e^{-i(q_z+G_z')z_b}+\beta_s(q_z+G_z')\bar{\chi}_{bc}(\mathbf{q}+G_x')$$
$$+\beta_c(\mathbf{q}_\perp+\mathbf{G}')\bar{\chi}_{cc}(\mathbf{q})e^{i(q_z+G_z')(z_c-z_b)}]\,. \quad (17)$$

A major simplification of (15)–(17) results when one notes that

$$\chi_{ac}(\mathbf{q}+G_x',-\mathbf{q}-\mathbf{G})=\chi_{ac}(\mathbf{q},-\mathbf{q}-\mathbf{G})\,,$$
$$\chi_{bc}(\mathbf{q}+G_x',-\mathbf{q}-\mathbf{G})=\chi_{bc}(\mathbf{q},-\mathbf{q}-\mathbf{G})\,. \quad (18)$$

This can easily be seen using the RPA equation of motion for these quantities analogous to (14) for χ_{cc}, in conjunction with (12). It follows that

$$\bar{\chi}_{ac}(\mathbf{q}+Q_x')=\bar{\chi}_{ac}(\mathbf{q});\ \bar{\chi}_{bc}(\mathbf{q}+Q_x')=\bar{\chi}_{bc}(\mathbf{q})\,, \quad (19)$$

and thus (15)–(17) reduce to three coupled algebraic equations for $\bar{\chi}_{ac}$, $\bar{\chi}_{bc}$, and $\bar{\chi}_{cc}$, which are easily solved. We find

$$\bar{\chi}_{cc}(\mathbf{q})\epsilon_c=N_c\chi^0_1(q_y)+N_c\chi^0_1(q_y)[\bar{v}_{cs}(z_c)\bar{\chi}_{ac}(\mathbf{q})$$
$$+\bar{v}_{cs}(z_c-z_b)\bar{\chi}_{bc}(\mathbf{q})]\,,$$
$$\bar{\chi}_{ac}(\mathbf{q})\epsilon_a=N_s\chi^0_{2a}(\mathbf{q}_\parallel)[\bar{v}_{ss}(-z_b)\bar{\chi}_{bc}(\mathbf{q})+\bar{v}_{cs}(-z_c)\bar{\chi}_{cc}(\mathbf{q})]$$
$$\bar{\chi}_{bc}(\mathbf{q})\epsilon_b=N_s\chi^0_{2b}(\mathbf{q}_\parallel)[\bar{v}_{ss}(z_b)\bar{\chi}_{ac}(\mathbf{q})+\bar{v}_{cs}(z_b-z_c)\bar{\chi}_{cc}(\mathbf{q})]\,. \quad (20)$$

Here we have defined the following quantities:

$$\epsilon_c\equiv1-\tilde{v}_{cc}(\mathbf{q})N_c\chi^0_1(q_y)\,,$$
$$\epsilon_a\equiv1-\tilde{v}_{ss}(\mathbf{q})N_s\chi^0_{2a}(\mathbf{q}_\parallel)\,, \quad (21)$$
$$\epsilon_b\equiv1-\tilde{v}_{ss}(\mathbf{q})N_S\chi^0_{2b}(\mathbf{q}_\parallel)\,,$$

where the effective form-factored Coulomb potentials are

$$\tilde{v}_{cc}(\mathbf{q})\equiv\sum_{\mathbf{G}}|\beta_c(\mathbf{q}_\perp+\mathbf{G})|^2v(\mathbf{q}+\mathbf{G})\,,$$
$$\tilde{v}_{ss}(\mathbf{q})\equiv\sum_{\mathbf{G}}|\beta_s(q_z+G_z)|^2v(\mathbf{q}+\mathbf{G})\,,$$
$$\bar{v}_{cs}(\mathbf{q};z)\equiv\sum_{\mathbf{G}}\beta_c(\mathbf{q}_\perp+\mathbf{G})\beta_s(q_z+G_z)v(\mathbf{q}+\mathbf{G})e^{-i(q_z+G_z)z}\,, \quad (22)$$
$$\bar{v}_{ss}(\mathbf{q};z)\equiv\sum_{\mathbf{G}}|\beta_s(q_z+G_z)|^2v(\mathbf{q}+\mathbf{G})e^{-i(q_z+G_z)z}\,.$$

It is clear that $\epsilon_c(\mathbf{q},\omega)$ is the dielectric function of the chain array by itself, while $\epsilon_a(\mathbf{q},\omega)$ is the dielectric function of the system of coupled a sheets. We also note that all the effective potentials $\tilde{v}(\mathbf{q})$ and $\bar{v}(\mathbf{q})$ in (22) are periodic functions with respect to the reciprocal lattice vectors $\mathbf{G}$, i.e., $\tilde{v}(\mathbf{q}+\mathbf{G})=\tilde{v}(\mathbf{q})$, etc.

Solving the set of equations in (20) for the three response functions, we find they all involve the same denominator, namely the dielectric function of the coupled sheet-chain-sheet superlattice. This is given by [note $\bar{v}^*(z)=\bar{v}(-z)$]

$$\epsilon(\mathbf{q},\omega)=\epsilon_c[\epsilon_a\epsilon_b-N_s\chi^0_{2a}N_s\chi^0_{2b}|\bar{v}_{ss}(z_b)|^2]-\epsilon_bN_c\chi^0_1N_s\chi^0_{2a}|\bar{v}_{cs}(z_c)|^2$$
$$-\epsilon_aN_c\chi^0_1N_s\chi^0_{2b}|\bar{v}_{cs}(z_c-z_b)|^2-N_c\chi^0_1N_s\chi^0_{2a}N_s\chi^0_{2b}2\mathrm{Re}[\bar{v}_{cs}(z_c)\bar{v}_{ss}(-z_b)\bar{v}_{cs}(z_b-z_c)]\,. \quad (23)$$

The dispersion relation of the charge fluctuations is given by the zeros of $\epsilon(\mathbf{q},\omega)$. Using the periodicity of the effective potentials in (22), one may verify that $\epsilon(\mathbf{q}+G_z,\omega)=\epsilon(\mathbf{q},\omega)$ and thus the modes need only be considered for q_z in the first Brillouin zone ($-\pi/c<q_z<\pi/c$).

Several special limits of (23) are useful to consider. First of all, we note that if we remove the coupling between the a array, the b array, and the c array, the dielectric function reduces to $\epsilon=\epsilon_c\epsilon_b\epsilon_a$, as expected.

If we assume the electrons are well localized in the sheets and chains, we can set the form factors in (22) to unity as a first approximation. Then we have $\tilde{v}_{cc}=\tilde{v}_{ss}$ and $\bar{v}_{cs}=\bar{v}_{ss}$. In the long-wavelength limit (defined by

$q \ll G_{\min}$), we have the further simplification that all the effective potentials in (22) reduce to the bare Coulomb potential $v(\mathbf{q})$. In this case, (23) is given by

$$\epsilon(\mathbf{q},\omega) = 1 - v(\mathbf{q})(N_c\chi_1^0 + N_s\chi_{2a}^0 + N_s\chi_{2b}^0) . \tag{24}$$

This long-wavelength expression was the basis of our earlier paper[1] on this model. We recall that N_s is the total number of sheets N_s' divided by the volume. Since the volume $V = N_s'Ac$, where A is the area of one sheet, we have $N_s = 1/cA$. Similarly, N_c is the number of chains N_c' divided by the volume. Writing $V = N_c'LA_c$, where L is the length of a chain and $A_c = ca$, we have $N_c = 1/A_cL$.

We note that if we let the distance c between the sheet-chain-sheet "sandwiches" become very large, the zeros of ϵ will describe the resonances of these uncoupled units. Formally this limit is taken by treating the G_z summations in (22) as integrals. If we further restrict ourselves to the $q_\parallel \to 0$ limit, we need only keep the $G_x = 0$ term in the summations. Setting the form factors $\beta_c = \beta_s = 1$ [this corresponds to treating the chains (sheets) as strictly 1D (2D) systems], the effective potentials in (22) reduce to

$$\tilde{v}_{cc} = \tilde{v}_{ss} = \frac{2\pi e^2}{q_\parallel} c ,$$
$$\tilde{v}_{cs}(z) = \bar{v}_{ss}(z) = \frac{2\pi e^2}{q_\parallel} c e^{-iq_z z - q_\parallel |z|} . \tag{25}$$

One can use these results in (23) to find the dielectric function of a *single* sandwich. In the high momentum limit ($q_\parallel z_b$, $q_\parallel z_c \gg 1$), each sheet and plane of chains acts independently with

$$\epsilon_c(\mathbf{q},\omega) = 1 - \frac{2\pi e^2}{q_\parallel}\frac{\chi_1^0}{aL} ,$$
$$\epsilon_i(\mathbf{q}\omega) = 1 - \frac{2\pi e^2}{q_\parallel}\frac{\chi_{2i}^0}{A} \quad (i = a,b) , \tag{24'}$$

where $2\pi e^2/q_\parallel$ is recognized as the Fourier transform of the Coulomb potential in a 2D system. This result should be contrasted with the long-wavelength limit result in (24) for a coupled system of sandwiches, which is valid for $qc \ll 1$.

In using (23) for the plasmons in $Y_1Ba_2Cu_3O_{7-\delta}$ superconductors, an appropriate basis is that of two Cu-O sheets with a middle layer composed of Cu-O chains. To a good approximation, one can take $z_b = 2c/3$ and $z_c = c/3$, in which case $z_b - z_c = c/3$. Both Cu-O sheets are the same ($\chi_{2a}^0 = \chi_{2b}^0$), but we still expect three kinds of plasmons in this sheet-chain-sheet unit. In Ref. 1, we showed that in the long-wavelength limit described by Eqs. (24), one may have an acoustic plasmon (ω_-) as well as a bulk-type plasmon (ω_+). In the simple electron gas model for χ_1^0 and χ_2^0 that was used, it is clear that one must have $\omega_- < v_{2F}q_\parallel$. One may show that this requires

$$\left(\frac{q_x}{q_y}\right)^2 > \frac{v_{1F}^2}{v_{2F}^2}\left(1 + \frac{N_1(\varepsilon_{1F})}{N_2(\varepsilon_{2F})}\frac{1}{2a}\right) - 1 , \tag{26}$$

where N_1 (N_2) is the density of states at the Fermi surface of a 1D (2D) electron gas. The fact that q_x/q_y must be larger than a *critical* value shows once again that the existence of the $\omega_- \simeq v_{1F}q_y$ mode is associated with the screening effect of the Cu-O sheets on the charge fluctuations in the Cu-O chains along the y-axis.

III. SUPERLATTICE OF ALTERNATING SHEETS

While it is only a special case of (23), it is of interest to make a few specific remarks on a superlattice with two metallic sheets per unit cell. Formally, this corresponds to setting χ_1^0 to zero, which leaves us with two arrays of coupled sheets. The dielectric function of this system is given by [see first line of (23)]

$$\epsilon = \epsilon_a\epsilon_b - N_s\chi_{2a}^0 N_s\chi_{2b}^0 |\bar{v}_{ss}(d)|^2 , \tag{27}$$

where d is the distance between the a and b sheets. Solving (20) for the response functions gives

$$\chi_{aa}(\mathbf{q}) = \frac{N_s\chi_{2a}^0\epsilon_b}{\epsilon} ,$$
$$\bar{\chi}_{ba}(\mathbf{q}) = \frac{N_s\chi_{2b}^0\bar{v}_{ss}(\mathbf{q},d)N_s\chi_{2a}^0}{\epsilon} = \bar{\chi}_{ab}^*(\mathbf{q}) , \tag{28}$$
$$\bar{\chi}_{bb}(\mathbf{q}) = \frac{N_s\chi_{2b}^0\epsilon_a}{\epsilon} .$$

The effective potentials $\tilde{v}_{ss}$ and $\bar{v}_{ss}$ in (22) now only involve summations over $G_z = n_z 2\pi/c$.

Setting the form factors β_s to unity (i.e., the metallic sheets are infinitely thin 2D systems), one can write the potentials in terms of lattice sums

$$\tilde{v}_{ss}(\mathbf{q}) = 4\pi e^2 S(0) ,$$
$$\bar{v}_{ss}(\mathbf{q},d) = 4\pi e^2 S(d) , \tag{29}$$

where

$$S(z) \equiv \frac{c}{2q_\parallel}\sum_m e^{-iq_z(z+Z_m) - q_\parallel|z+Z_m|} . \tag{30}$$

In the limit $N_s \to \infty$, these sums can be carried out analytically to give[6]

$$\tilde{v}_{ss}(\mathbf{q}) = \frac{2\pi e^2}{q_\parallel} c\left(\frac{\sinh(q_\parallel c)}{\cosh(q_\parallel c) - \cos(q_z c)}\right) ,$$
$$\bar{v}_{ss}(\mathbf{q},d) = \frac{2\pi e^2}{q_\parallel} c\left(\frac{\sinh[q_\parallel(c-d)] + e^{-iq_z c}\sinh(q_\parallel d)}{\cosh(q_\parallel c) - \cos(q_z c)}\right) . \tag{31}$$

These results agree precisely with those recently given in the literature.[2,3] The special case of $d = c/2$ was originally discussed by Quinn and co-workers.[7] In this limit, (31) reduces to

$$|\bar{v}_{ss}(\mathbf{q},d)| = \frac{2\pi e^2}{q_\parallel} c\left(\frac{2\cos(q_z d)\sinh(q_\parallel d)}{\cosh(2q_\parallel d) - \cos(2q_z d)}\right) . \tag{32}$$

From the general structure of $\bar{v}_{ss}$ and $\tilde{v}_{ss}$ in (22), one sees that for $d = c/2$,

$$\tilde{v}(\mathbf{q}) = \tilde{v}_E(\mathbf{q}) + \tilde{v}_0(\mathbf{q}) ,$$
$$\bar{v}(\mathbf{q},d) = \tilde{v}_E(\mathbf{q}) - \tilde{v}_0(\mathbf{q}) , \tag{33}$$

where $\tilde{v}_E(\mathbf{q})$ is the part coming from the *even* terms in the G_z summations while $\tilde{v}_0(\mathbf{q})$ is from the *odd* terms. If all the layers have the *same* response functions ($\chi^0_{2a}=\chi^0_{2b}=\chi^0_2$), one can show that (27) reduces to

$$\epsilon(\mathbf{q},\omega)=(1-2\tilde{v}_E N_s\chi^0_2)(1-2\tilde{v}_0 N_s\chi^0_2)\,. \tag{34}$$

Calculating the full response function using

$$\chi(\mathbf{q},-\mathbf{q}-G_z)=\sum_{i,j}\chi_{ij}(\mathbf{q},-\mathbf{q}-G_z)\,, \tag{35}$$

one can show explicitly that it simplifies finally to the expected result, namely the response function of a superlattice with $2N_s$ sheets (per unit volume) with period d.

For further discussion of the collective-mode spectrum predicted by (27), we refer to the literature.[2,3,7,8] Under certain conditions, one has both acoustic and optical plasmon modes even for $q_z=0$. In the long-wavelength limit, we simply have[9]

$$\epsilon(\mathbf{q},\omega)=1-v(\mathbf{q})[N_s\chi^0_{2a}+N_s\chi^0_{2b}]\,. \tag{36}$$

In the opposite limit $cq_\parallel\gg 1$, the collective modes are those of two coupled parallel sheets separated by the distance d.[2]

We might remark that in the newly discovered Bi-Sr-Ca-Cu-O high-transition-temperature superconductors,[10] there is the possibility that one is dealing with a superlattice structure which involves two (or even three) different kinds of metallic layers.[11] It immediately follows from (36) that such a superlattice may give rise to acoustic plasmons,[2,3,7,8] as can be most easily seen by analogy to Fig. 2 of Ref. 1.

IV. COUPLED CHAIN SYSTEMS IN $Hg_{3-\delta}AsF_6$

In Hg chain compounds, one has a superlattice made up of two mutually perpendicular chain arrays of Hg ions. In a recent work,[4] the electronic response functions of this system were evaluated in the $q\to 0$ limit. In the present section, we generalize this analysis to arbitrary wave vectors.

As in Sec. II, it is convenient to introduce electronic response functions $\chi_{ij}(\mathbf{r},\mathbf{r}')$ which describe the correlation between a density fluctuation at $\mathbf{r}$ in a chain of type i (a or b) and a density fluctuation at $\mathbf{r}'$ in a chain of type j. We have

$$\delta\rho_a(\mathbf{r})=\sum_{\mathbf{R}_a}w_c(\mathbf{r}_\perp-\mathbf{R}_a)\delta\rho_{\mathbf{R}_a}(x)\,, \tag{37}$$

where the a chains are assumed to be along the x axis and $\mathbf{r}_\perp=(y,z)$. The positions (in y-z plane) of the a chains are denoted by $\mathbf{R}_c$ and form a triangular lattice, to a good first approximation. Similarly the density fluctuations in the b chains (along the y axis) are described by

$$\delta\rho_b(\mathbf{r})=\sum_{\mathbf{R}_b}w_c(\mathbf{r}_\perp-\mathbf{R}_b)\delta\rho_{\mathbf{R}_b}(y)\,. \tag{38}$$

The b-chain lattice is described by the Bravais lattice vectors $\mathbf{R}_b$ in the x-z plane and $\mathbf{r}_\perp=(x,z)$. Using (37) to calculate the Fourier transform of χ_{aa}, we find it has the following structure:

$$\chi_{aa}(\mathbf{q}+\mathbf{G}'_a,-\mathbf{q}-\mathbf{G}_a)=\beta(\mathbf{q}^a_\perp+\mathbf{G}'_a)\bar{\chi}_{aa}(\mathbf{q})\beta(\mathbf{q}^a_\perp+\mathbf{G}_a)\,. \tag{39}$$

Here the reciprocal-lattice vectors of the a sublattice are denoted by $\mathbf{G}_a$ (these are in the y-z plane). The key feature of (39) is that the dependence on $\mathbf{G}_a$ and $\mathbf{G}'_a$ is completely contained in the chain form factors. To remind us that only the yz component of $\mathbf{q}$ enters in the form factors of β, we use the notation $\mathbf{q}^a_\perp$. We recall that a general discussion of the symmetry properties of χ_{ij} was given in Ref. 4. Clearly, in our model, all band-structure effects in a *given* chain are ignored.

Proceeding in a similar manner, one finds

$$\chi_{bb}(\mathbf{q}+\mathbf{G}'_b,-\mathbf{q}-\mathbf{G}_b)=\beta(\mathbf{q}^b_\perp+\mathbf{G}'_b)\bar{\chi}_{bb}(\mathbf{q})\beta(\mathbf{q}^b_\perp+\mathbf{G}_b)e^{-i(G'_{bz}-G_{bz})D}\,, \tag{40}$$

where D is the closest distance between the a and b chains ($D=c_T/4\simeq 3.1$ Å in $Hg_{3-\delta}AsF_6$). The phase factors enter here because the b-chain sublattice is shifted upward (in z direction) from the a sublattice by the amount D. Finally, for the correlation function between chains of a different kind, calculation shows that

$$\chi_{ba}(\mathbf{q}+\mathbf{G}_b,-\mathbf{q}-\mathbf{G}_a)=\beta(\mathbf{q}^b_\perp+\mathbf{G}_b)\bar{\chi}_{ba}(\mathbf{q})\beta(\mathbf{q}^a_\perp+\mathbf{G}_a)e^{-iG_{bz}D}\,. \tag{41}$$

Using (39)–(41) in the RPA Eq. (13), we obtain

$$\begin{aligned}\bar{\chi}_{aa}(\mathbf{q})&=N_c\chi^0_1(q_x)+N_1\chi^0_1(q_x)\sum_{\mathbf{G}_a}\beta(\mathbf{q}^a_\perp+\mathbf{G}_a)v(\mathbf{q}+\mathbf{G}_a)[\beta(\mathbf{q}^a_\perp+\mathbf{G}_a)\bar{\chi}_{aa}(\mathbf{q})+\beta(\mathbf{q}^b_\perp+G_{az})\bar{\chi}_{ba}(\mathbf{q})e^{-iG_{az}D}]\\ \bar{\chi}_{ba}(\mathbf{q})&=N_c\chi^0_1(q_y)\sum_{\mathbf{G}_b}\beta(\mathbf{q}^b_\perp+\mathbf{G}_b)v(\mathbf{q}+\mathbf{G}_b)[\beta(\mathbf{q}^b_\perp+\mathbf{G}_b)\chi_{ba}(\mathbf{q})+\beta(\mathbf{q}^a_\perp+G_{bz})\bar{\chi}_{aa}(\mathbf{q})e^{iG_{bz}D}]\,.\end{aligned} \tag{42}$$

Solving these, we obtain

$$\bar{\chi}_{aa}(\mathbf{q},\omega)=\frac{N_c\chi^0_1(q_x)\epsilon_c(b)}{\epsilon(\mathbf{q},\omega)}\,,\quad \bar{\chi}_{ba}(\mathbf{q},\omega)=\frac{N_c\chi^0_1(q_y)\bar{v}_{ba}(\mathbf{q})N_c\chi^0_1(q_x)}{\epsilon(\mathbf{q},\omega)}\,, \tag{43}$$

where the dielectric function of the two coupled arrays is

$$\epsilon(\mathbf{q},\omega)=\epsilon_c(a)\epsilon_c(b)-\bar{v}_{ab}(\mathbf{q})\bar{v}_{ba}(\mathbf{q})N_c\chi^0_1(q_x)N_c\chi^0_1(q_y)\,, \tag{44}$$

with

$$\epsilon_c(a) \equiv 1 - N_c \chi_1^0(q_x) \tilde{v}_{aa}(\mathbf{q}) ,$$
$$\epsilon_c(b) \equiv 1 - N_c \chi_1^0(q_y) \tilde{v}_{bb}(\mathbf{q}) , \tag{45}$$

and the form-factored effective potentials

$$\tilde{v}_{aa}(\mathbf{q}) \equiv \sum_{\mathbf{G}_a} |\beta(\mathbf{q}_\perp^a + \mathbf{G}_a)|^2 v(\mathbf{q}+\mathbf{G}_a) ,$$
$$\tilde{v}_{bb}(\mathbf{q}) \equiv \sum_{\mathbf{G}_b} |\beta(\mathbf{q}_\perp^b + G_b)|^2 v(\mathbf{q}+\mathbf{G}_b) ,$$
$$\bar{v}_{ab}(\mathbf{q}) \equiv \sum_{\mathbf{G}_a} \beta(\mathbf{q}_\perp^a + \mathbf{G}_a)\beta(\mathbf{q}_\perp^b + G_{az}) v(\mathbf{q}+\mathbf{G}_a) e^{-iG_{az}D} , \tag{46}$$
$$\bar{v}_{ba}(\mathbf{q}) \equiv \sum_{\mathbf{G}_b} \beta(\mathbf{q}_\perp^b + \mathbf{G}_b)\beta(\mathbf{q}_\perp^a + G_{bz}) v(\mathbf{q}+\mathbf{G}_b) e^{-iG_{bz}D} .$$

The results in (43)–(46) give the exact RPA solution for the two coupled chain arrays.

As in earlier sections, the long-wavelength limit is easily recovered. In this limit, all the effective potentials in (46) reduce to the bare Coulomb potential $v(\mathbf{q})$ and (44) then simplifies to

$$\epsilon(\mathbf{q},\omega) = 1 - v(\mathbf{q})[N_c \chi_1^0(q_x) + N_c \chi_1^0(q_y)] . \tag{47}$$

This was the approximate form discussed in Ref. 4. As discussed there, one finds that (47) always leads to an acoustic plasmon in which the charge fluctuations in the a and b arrays are essentially out of phase with each other. We recall that $N_c = 1/A_c L$, where L is the length of a chain and A_c is the area of the unit cell of the a-chain sublattice.

Since the G_z components of the two arrays are identical, one immediately sees that

$$\tilde{v}_{ii}(\mathbf{q}+G_z) = \tilde{v}_{ii}(\mathbf{q}) ,$$
$$\bar{v}_{ab}(\mathbf{q}+G_z) = \bar{v}_{ab}(\mathbf{q}) e^{iG_z D} , \tag{48}$$
$$\bar{v}_{ba}(\mathbf{q}+G_z) = \bar{v}_{ba}(\mathbf{q}) e^{-iG_z D} .$$

Using these results, one may verify that $\epsilon(\mathbf{q}+G_z) = \epsilon(\mathbf{q})$ and hence we need only consider the plasmon modes $\omega(\mathbf{q})$ in the first Brillouin zone in the z direction ($-\pi/d < q_z < \pi/d$).

In contrast to Ref. 5, we do not find that the interarray response functions such as χ_{ba} in (41) vanish unless $G_{bx} = G_{ay} = 0$. As a result, the summations in $\bar{v}_{ab}$ and $\bar{v}_{ba}$ in (46) are not restricted to the G_z components. Apart from this difference, (44) is identical to that given by Mohan.[5] We note that if one considers a wave vector $\mathbf{q}$ close to some reciprocal-lattice vector $\mathbf{G}_a$ (with $G_{ay} \neq 0$), we have

$$\tilde{v}_{aa}(\mathbf{q}) = \tilde{v}_{aa}(\mathbf{q}-\mathbf{G}_a) ,$$
$$\bar{v}_{ab}(\mathbf{q}) = \bar{v}_{ab}(\mathbf{q}-\mathbf{G}_a) e^{iG_{az}D} , \tag{49}$$

while $\tilde{v}_{bb}(\mathbf{q})$ and $\bar{v}_{ba}(\mathbf{q})$ are very small. To the extent that we neglect the latter, we see that $\epsilon(\mathbf{q},\omega)$ in (44) reduces to $\epsilon_c(a)$ in (45). Thus, in agreement with Ref. 5, the plasmon modes would be that of the a array, essentially uncoupled from the b array. Similarly, if we take $\mathbf{q}$ to be close to $\mathbf{G}_b$ (with $G_{bx} \neq 0$), the response will be essentially that of the b array, uncoupled from the a array.

V. ALTERNATE FORMULATION IN TERMS OF EXACT RESPONSE FUNCTIONS FOR SHEETS AND CHAINS

All the calculations in this paper involve solving the RPA integral Eq. (1) for multilayered systems (superlattices) with a basis composed of metallic sheets and chains. The building blocks are the response functions χ_2^0 and χ_1^0 of noninteracting electrons in sheets and chains. Thus we have treated the intra-Coulomb interaction in sheets (chains) and the inter-Coulomb interaction between *different* sheets (chains) within the same RPA.

In real systems of interest, one is often dealing with sheets and chains in which correlation effects are very important. In particular, there is considerable experimental evidence that in the high-temperature oxide superconductors, the CuO sheets are not well described in terms of simple energy-band theory in that one must include strong on-site Coulomb repulsion as well as the Coulomb interaction between different sites.[12,13] In this section, we point out that it is straightforward to generalize the analysis in this paper so that *only* the inter-Coulomb interaction between different sheets and chains is treated in the RPA. In this case, our starting equation has the same structure as (1) but χ_1^0 is replaced by "exact" response functions χ_1 and χ_2 for *single* chains and sheets, while v is now limited to the inter-Coulomb part.[14]

We shall only discuss how the results of the sheet-chain-sheet model in Sec. II are modified. The new equations are easily seen to lead to (20) and (21) once again, with of course $\chi_1^0 \to \chi_1$ and $\chi_{2i}^0 \to \chi_{2i}$ ($i = a,b$). The effective Coulomb potentials $\bar{v}_{cs}$ and $\bar{v}_{ss}$ in (22) are already inter-Coulomb interactions between chains and sheets. The only changes are in the $\tilde{v}_{cc}$ and $\tilde{v}_{ss}$ in (21) and (22) since these must now be limited to the inter-Coulomb interaction.

The most convenient way of extracting out the intra-Coulomb interactions is to use expressions for $\tilde{v}_{cc}$ and $\tilde{v}_{ss}$ which explicitly involve summations over the different chains and sheets. Using (29) and (30), which are valid for the extreme limit of 2D metallic sheets [$\beta_s(q_z) = 1$], one has

$$\tilde{v}_{ss}^{\text{inter}}(\mathbf{q}) = \frac{2\pi e^2 c}{q_\parallel} \sum_{Z_m (\neq 0)} e^{-iq_z Z_m - q_\parallel |Z_m|} . \tag{50}$$

The term $Z_m = 0$ corresponds to intra-Coulomb interactions in a given sheet, namely

$$\tilde{v}_{ss}^{\text{intra}}(\mathbf{q}) = \frac{2\pi e^2 c}{q_\parallel} . \tag{51}$$

Similarly, the inter-Coulomb part of $\tilde{v}_{cc}$ is given by[15]

$$\tilde{v}_{cc}^{\text{inter}}(\mathbf{q}) = e^2 \sum_{\mathbf{R}_c (\neq 0)} e^{i\mathbf{q}_\perp \cdot \mathbf{R}_c} \times \int d\mathbf{r}_\perp K_0(q_y |\mathbf{r}_\perp + \mathbf{R}_c|) w_c(\mathbf{r}_\perp/\sqrt{2}) . \tag{52}$$

In the Gaussian approximation for the transverse electronic eigenstates, we have

$$w_c(\mathbf{r}_\perp) = \frac{1}{\pi r_0^2} e^{-r_\perp^2/r_0^2}, \tag{53}$$

where r_0 is the "radius" of the chain. Here $\mathbf{q}_\perp = (q_x, 0, q_z)$ and K_0 is the zeroth-order modified Bessel function. As discussed in more detail in Ref. 15, if we add the intrachain ($\mathbf{R}_c = \mathbf{0}$) contribution to (52), the resulting expression for $\tilde{v}_{cc}(\mathbf{q})$ is completely equivalent to the momentum-space expression given in (22) involving a sum over reciprocal-lattice vectors.

The advantage of this generalized formalism, which builds on the fully interacting response functions of the sheets and chains (χ_2 and χ_1), is that it allows one to concentrate on the *new* features which arise from the inter-Coulomb interaction. In particular, the basic message of Ref. 1 is that one expects acoustic plasmon modes in a superlattice structure whenever the basis is composed of subunits (sheets *or* chains) whose response functions have poles at *different* frequencies. Sheets and chains in YBaCuO and two different kinds of sheets in Bi-Sr-Ca-Cu-O thus may lead to similar kinds of acoustic plasmons. The key requirement is that the sheets and chains exhibit electronic charge fluctuations.

VI. CONCLUDING REMARKS

While it is not the main purpose of this paper, we wish to briefly discuss the role that the acoustic plasmons (which arise in superlattices with a basis) may have as a pairing mechanism in high-transition-temperature oxide superconductors.[1]

We first consider the Y-Ba-Cu-O superconductors which are described by the sheet-chain-sheet model of Sec. II. As we discussed here and in Ref. 1, the acoustic plasmon ω_- is clearly associated with the "Tomonaga phonon" of a noninteracting 1D electron gas, the intra-Coulomb interaction in the Cu-O chains being effectively canceled by the screening effect of the inter-Coulomb interaction with the Cu-O sheets. In a schematic sense, one expects that the effective interaction between electrons in a given Cu-O sheet will be given by $v(\mathbf{q})/\epsilon(\mathbf{q},\omega)$ and that as a result of the low-frequency chain mode $\omega_-(q_y)$, this effective interaction will be attractive. This attractive region will be most effective when $q_x \gg q_y$, since then it is well separated from the characteristic electronic frequencies of the Cu-O sheets and also the ω_- mode is only weakly damped.[1]

Our model is also especially interesting in connection with the 60-K superconducting phase of $Y_1Ba_2Cu_3O_{7-\delta}$ (with $\delta \gtrsim 0.3$)—sometimes called the ortho-II phase to distinguish it from the 90-K orthorhombic phase ($\delta \lesssim 0.2$). Apparently there is good evidence that in the 60-K phase, every other Cu-O chain is missing.[16–18] As can be seen from Eq. (8) in Ref. 1, the size of the frequency region associated with the acoustic plasmon in which $\epsilon(\mathbf{q},\omega)$ is negative (attractive) is proportional to density of the chains. This is certainly consistent[19] with the dramatic lowering of the transition temperature from 90 to 60 K.

While we assumed intraplane pairing in the Cu-O sheets in the above remarks, it is clear that the acoustic plasmon associated with the chains could also lead to interplane Cooper pairing.[20]

In our model, the role of the chains in YBaCuO superconductors is simply a source of charge fluctuations with a much lower frequency than that associated with the Cu-O sheets. Even with random oxygen vacancies and Cu(1) sites substitutions by other elements, as long as the middle layer associated with Cu-O chains exhibits a metalliclike behavior, one can expect our model dielectric function to be qualitatively correct.

In the case of the new Bi-Sr-Ca-Cu-O and Tl-Ba-Ca-Cu-O superconductors, it appears that the high-temperature phase may have three Cu-O sheets in the superlattice basis. It seems that there are no Cu-O chains but if either the BiO or the TlO sheets exhibit any metalliclike behavior, they would play the same role as chains and would give rise to low-energy acoustic plasmons.[21] If the plane of chains at z_c in Sec. II is replaced by a metallic sheet (labeled by c), the only change in (23) is $N_c\chi_1^0(q_y) \rightarrow N_s\chi_{2c}^0(\mathbf{q}_\parallel)$. Of course, in (22), the chain form factors $\beta_c(\mathbf{q}_\perp + \mathbf{G})$ are also replaced by $\beta_s(q_z + G_z)$ and the summations now only involve G_z components.

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