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# Acoustic plasmon exchange in multilayered systems: I. The effective interaction potential

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**Abstract.** Using a plasmon exchange model, analytic expressions for the effective interaction between charge carriers in a multilayered system containing one, two, three and four conducting layers per unit cell has been calculated. The interaction is mediated by one pseudo-optical plasmon band and  $L - 1$  proper narrow acoustic plasmon bands where  $L$  is the number of layers per cell. It is found that the pseudo-optical plasmon band has a proper optical (high energy) limit, equivalent to bulk plasmon modes, as well as an acoustic (low energy) limit. In the following paper we show that this interaction can lead to superconductivity in the high- $T_c$  superconductors.

## 1. Introduction

In recent years there has been considerable interest on superlattices because of their potential applications in solid state devices [1–3]. Two types of superlattices have been identified. A type-I superlattice is a periodic array of quasi-two dimensional electron gas [4], whereas a type-II superlattice is that with a basis (two conducting layers per unit cell) as can be found in such physical systems as InAs–GaSb. The physical properties of type-I superlattices have been studied by several authors [4–7]. The energy loss of a fast charged particle in a type-II superlattice has been studied by Gumbs [8] and its light scattering properties has been studied by Tzoar and Zhang [9]. With the advent of the high- $T_c$  superconductors a type-III superlattice having three conducting CuO layers per unit cell has been identified in the Th- and Bi-based cuprate superconductors [10, 11].

In this paper, we calculate the effective interaction between two charge carriers in a metallic multilayered system based on a two-dimensional plasmon exchange model. Using the RPA approximation we develop the intra-layer pairing interaction between two charge carriers as a result of intra- and inter-layer plasmon exchanges. We have achieved exact results for the infinite periodic systems with one and two layers per unit cell. We have also been able to calculate the approximate expressions for the effective interaction for the three- and four-layer periodic systems. Results obtained in this paper should be useful in studying the many-body effects on various electronic properties of various types of superlattices. For example, our theory can easily be used to calculate the plasmon contribution to other optical and scattering properties [12] of such superlattices.

These results were used in a first approach to the study of superconductivity in these Tl- and Bi-based compounds [13].

This paper is divided into several sections. Section 2 contains a description of the model that we have used to obtain the effective interaction between two charge carriers in a superlattice. We include the plasmon exchanges which may occur inside the same layer (intra-layer), or between the layers of the same unit cell (intra-cell), and also between the layers of different cells (inter-cell). In section 3 exact analytic expressions for the effective interaction are obtained for the infinite periodic system with one and two conducting layers per unit cell. Section 4 provides an approximate treatment of the inter-cell plasmon exchanges for infinite periodic samples with one-, two-, three- and four-layers per unit cell and is thus an extension of section 3. Our calculation gives analytic expressions for the effective interaction which is found to be mediated by one pseudo-optical plasmon band (bounded by a proper optical (high energy) as well as an acoustic (low energy) limit) and  $(L - 1)$  narrow acoustic bands. Conclusions are drawn in section 5.

## 2. The model

We assume that the metallic layers in the multilayered system can be considered as 2D electron gases (2DEGs) and that all these layers have the same density  $n_s$  of charge carriers (electrons or holes) in every layer. These charge carriers (henceforth to be designated as 'electrons') interact with each other within the same layer, as well as from layer to layer via an effective Coulomb interaction which will be treated, in this paper, in the framework of the random phase approximation (RPA). The locations of the various layers will be given by their ordinates  $z_r$  which will be specified below for various situations.

The Coulomb interaction between two electrons located in layers of ordinates  $z_0$  and  $z$  is given by

$$v(q, z - z_0) = v_0(q) e^{-q|z - z_0|} \quad (1)$$

where  $q$  represents a 2D wavevector parallel to the layers and where

$$v_0(q) = 2\pi e^2/q. \quad (2)$$

When both charge carriers are in the same layer,  $v$  reduces to  $v_0$ . Since the electrons constitute a many-body system, their Coulomb interaction can be replaced by a frequency dependent effective interaction

$$\begin{aligned} V(q, z - z_0, \omega) = & v(q, z - z_0) - \sum_{z_1} v(q, z - z_1) \Pi(q, \omega) v(q, z_1 - z_0) \\ & + \sum_{z_1, z_2} v(q, z - z_1) \Pi(q, \omega) v(q, z_1 - z_2) \Pi(q, \omega) v(q, z_2 - z_0) - \dots \end{aligned} \quad (3)$$

where  $\Pi(q, \omega)$  is the RPA irreducible polarization propagator in a 2DEG. In the plasmon region of the  $(q, \omega)$  plane, one has

$$\Pi(q, \omega) = -n_s q^2 / m \omega^2 \quad (4)$$

for small  $q$ . Note that in (4) higher order terms of relative order  $a_B q$  have been neglected ( $a_B$  being the Bohr radius). Using (1) let us write (3) in the form

$$V(q, z - z_0, \omega) = v_0(q) \sum_{s=0}^{\infty} C_s(q, z - z_0) [-v_0(q) \Pi(q, \omega)]^s \quad (5)$$

with the geometric factors  $C_s$  given by

$$C_s(q, z - z_0) = \sum_{z_1 \dots z_s} \prod_{r=0}^s e^{-|z_{r+1} - z_r|q} \quad (6)$$

with  $z_{s+1} \equiv z$ .

In this paper we calculate the interaction between electrons within the same layer which means that we only consider  $V(q, \omega) \equiv V(q, 0, \omega)$ . In the following sections, several different cases of layer distributions will be considered.

### 3. Periodic systems of layers

Let us consider the general system of an infinite crystal with a periodic distribution of layers of 2DEGs. This, in fact, is the actual situation met in several superconductors such as  $\text{Ti}_2\text{Ba}_2\text{Ca}_{L-1}\text{Cu}_L\text{O}_{2L+4}$  or  $\text{Bi}_2\text{Sr}_2\text{Ca}_{L-1}\text{Cu}_L\text{O}_{2L+4}$  where one has a periodic distribution of CuO layers. In this section we assume that the electrons of *all* the 2DEGs of the crystal contribute to potential (5). Such a treatment can be performed exactly and is straightforward for  $L = 1$  and  $L = 2$ , where  $L$  stands for the number of layers per unit cell.

#### 3.1. Single layer system ( $L = 1$ )

Here we consider a system with only one spacing  $c$  between the conducting layers and write  $z_r = n_r c$  ( $c$  is the lattice constant and  $n_r$  is an integer). The geometric factor  $C_s$  can be calculated in terms of the Fourier transform of

$$e^{-|\Delta z|q} = e^{-|\Delta n|cq} = 1/2\pi \int_{-\pi}^{\pi} d\kappa f(\kappa) e^{-i\Delta n\kappa} \quad (7)$$

which is

$$f(\kappa) = \sum_{\Delta n=-\infty}^{\infty} e^{-|\Delta n|cq} e^{i\Delta n\kappa} = \frac{\sinh cq}{\cosh cq - \cos \kappa}. \quad (8)$$

Introducing (7) in (6), we obtain

$$C_s(q, 0) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\kappa [f(\kappa)]^s$$

and (5) takes the form

$$V_1(q, \omega) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\kappa \frac{v_0 f(\kappa)}{1 + v_0 \Pi f(\kappa)} \quad (9)$$

or, using (2), (4) and (8),

$$V_1(q, \omega) = \frac{v_0}{\pi} \int_0^{\pi} d\kappa \frac{S_1}{A_1 - \cos \kappa} \quad (10)$$

with the following definitions

$$\begin{aligned} S_1 &= \sinh cq \\ A_1 &= \cosh cq - \beta^{-1} \sinh cq \end{aligned} \quad (11)$$

and

$$\beta = - (v_0 \Pi)^{-1} = m\omega^2 / 2\pi e^2 n_s q. \quad (12)$$

The subscript 1 in (9) and (10) means that the present system has an infinite number of equally separated single conducting layers. Note that (10) can be integrated exactly, giving

$$V_1(q, \omega) = v_0 S_1 (A_1^2 - 1)^{-1/2} [\Theta(A_1 - 1) - \Theta(-A_1 - 1)] \quad (13)$$

where  $\Theta$  represents the usual step function. However, in view of the subsequent analysis of the present paper, we will maintain the non-integrated form (10), which we rewrite in the 'standard form' as

$$V_1/v_0 = 1 + \frac{1}{\pi} \int_0^{\pi} d\kappa \frac{w(\kappa)}{\beta - \beta(\kappa)} \quad (14)$$

with

$$\beta(\kappa) \equiv f(\kappa) = (\sinh cq) / (\cosh cq - \cos \kappa) \quad (15)$$

and  $w(\kappa) = [f(\kappa)]^2$ .

The following property of  $f(\kappa)$

$$\frac{1}{\pi} \int_0^{\pi} d\kappa f(\kappa) = 1 \quad (16)$$

has been used in calculating (14). Here and below, expressions like (14) will be called the 'standard form' of  $V$ , with  $\beta = \beta(\kappa)$  giving the dispersion relation for the plasmon mode. Such a system was first considered by Das Sarma and Quinn [7] and they obtained a similar dispersion relation.

### 3.2. Double-layer system ( $L = 2$ )

We now consider a system composed of 2DEG's alternately spaced by the distances  $a$  and  $c - a$ , with  $a < c - a$ . Thus, two successive layers separated by the small distance  $a$  can be considered to be in a unit cell (double layer) which repeats itself with lattice constant  $c$ .

For this double-layer system the geometrical factor  $C_s$ , given by (6), is described in terms of three different factors. The first one is as before  $e^{-|\Delta x|cq}$  with its Fourier transform  $f(\kappa)$  given by (8). However, here this factor describes only the connection between two lower or two upper layers. The connection between a lower (upper) and

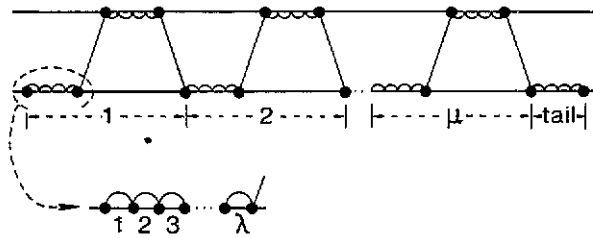


Figure 1. Diagrammatic representation of a term of  $E_2$  as given by (21).

an upper (lower) layer either within the same cell ( $\Delta n = 0$ ) or in two different cells ( $\Delta n \neq 0$ ) requires the new factors  $g_+(\kappa)[g_-(\kappa)]$  given by

$$g_{\pm}(\kappa) = \sum_{\Delta n=-\infty}^{\infty} e^{\nu_{\pm} q} e^{i\Delta n \kappa} \tag{17}$$

with

$$\nu_+ = \begin{cases} -\Delta n c - a & \text{for } \Delta n \geq 0 \\ \Delta n c + a & \text{for } \Delta n < 0 \end{cases}$$

$$\nu_- = \begin{cases} -\Delta n c + a & \text{for } \Delta n > 0 \\ \Delta n c - a & \text{for } \Delta n \leq 0 \end{cases}$$

which, when the summation is performed, becomes

$$g_{\pm}(\kappa) = [\sinh(c - a)q + e^{\pm i\kappa} \sinh aq] / (\cosh cq - \cos \kappa). \tag{18}$$

The corresponding interaction potential can be expressed as

$$V_2 = -\frac{1}{2\pi\Pi} \int_{-\pi}^{\pi} d\kappa E_2 \tag{19}$$

a form similar to (9) where the subscript 2 implies that we are considering an infinite number of cells each containing two 2DEGs.

To simplify the diagrammatic analysis of  $E_2$ , let us introduce

$$F = f(\kappa)/\beta \quad \text{and} \quad G_{\pm} = g_{\pm}(\kappa)/\beta. \tag{20}$$

Then,  $E_2$  appears as a sum over all possible products of  $F$  and  $G_{\pm}$  factors. Figure 1 shows a term of that sum in a reduced scheme representation where the lower (upper) horizontal line corresponds to the set of all lower (upper) 2DEGs. Since  $V_2$  is the interaction between two electrons in the same layer, the interaction line must start and end at the same layer (this corresponds to taking  $z = z_0$  as was done in deriving (9)). This also means that each diagram of  $E_2$  must have equal numbers of  $G_+$  and  $G_-$  factors, the lowest order term being  $F$ . Hence  $E_2$  takes the form

$$E_2 = \sum_{\mu} \left[ \left( \sum_{\lambda} F^{\lambda} \right) G_+ \left( \sum_{\lambda} F^{\lambda} \right) G_- \right]^{\mu} \sum_{\lambda} F^{\lambda} - 1 \tag{21}$$

with summations over  $\lambda$  and  $\mu$  running from 0 to  $\infty$ . Note the presence of a ‘tail’ factor

$\Sigma F^{\lambda}$  after the brackets, as shown in figure 1, and of a term  $-1$  which is required to cancel the spurious zeroth order term included in the summation in (21) (for  $\mu = 0$ ). Carrying out the summation in (21), we obtain

$$E_2 = [1 - F]/[(1 - F)^2 - G_+ G_-] - 1 \quad (22)$$

and, substituting (22) into (19), we can express  $V_2$  as

$$V_2(q, \omega) = \frac{V_0}{\pi} \int d\kappa \frac{S_2}{A_2 - \cos \kappa} \quad (23)$$

an expression similar to (10), where  $S_2$  and  $A_2$  are given by

$$S_2 = \sinh cq - (2/\beta) \sinh aq \sinh(c - a)q \quad (24)$$

$$A_2 = \cosh cq - (2/\beta) \sinh cq + (2/\beta^2) \sinh aq \sinh(c - a)q.$$

Equation (13), with the subscript 1 replaced by 2, is also applicable to  $V_2$ . In fact, we can check that all the above results for  $V_2$  reduce to those for  $V_1$ , if we let  $c = 2a$  (and then replace  $a$  by  $c$ ).

Note that by appropriate manipulation of (23), we can rewrite it in the 'standard' form as

$$\frac{V_2}{v_0} = 1 + \frac{1}{\pi} \sum_{\kappa=1}^2 \int_0^{\pi} d\kappa' \frac{w_{\kappa}(\kappa')}{\beta - \beta_{\kappa}(\kappa')} \quad (25)$$

### 3.3. Triple and quadruple layer systems ( $L = 3$ and $4$ )

At this point, it would be useful to develop similar expressions for  $V_3$  and  $V_4$ , the interaction potentials with three and four 2DEGs per unit cell.  $V_3$  and  $V_4$  can also be expressed in the form of (19) with  $E_2$  replaced by  $E_3$  and  $E_4$ , respectively. Calculation of  $E_3$  and  $E_4$  will involve not only factors  $F$  and  $G_{\pm}$  given in (20), but also two extra factors

$$H_{\pm} = h_{\pm}/\beta \quad \text{and} \quad K_{\pm} = k_{\pm}/\beta \quad (26)$$

corresponding to inter-layer interactions between the second and third neighbouring layers, respectively. Note that  $K_{\pm}$  is non-zero only for a four-layer system. As in (21), these factors are then needed to be renormalized by

$$\mathcal{H}_{\pm} = H_{\pm}/(1 - F) \quad \text{and} \quad \mathcal{K}_{\pm} = K_{\pm}/(1 - F)$$

where  $1/(1 - F)$  stands for the series  $\Sigma_{\lambda} F^{\lambda}$ . Exact calculations of these factors and hence of  $E_3$  and  $E_4$  are algebraically complicated and are not necessary for our purposes. Instead, in the next section we will derive the results after making an approximation.

## 4. Approximate effective interaction

The calculation of the approximate effective interaction is facilitated by the exact results of the effective interaction in an isolated cell containing one to four layers of 2DEGs. These results are given in Appendix A. Our approximation consists of simplifying the distances between layers belonging to different unit cells (inter-cell distances). We assume that the inter-layer distance  $a$  is small within all the cells, except for the one in

which the potential is being calculated. This means that the interaction factor  $g_{\pm}(\kappa)$  given by (17) can be simplified by replacing the exponents  $\nu_{\pm}$  by

$$\nu_{\pm} = \begin{cases} -|\Delta n|c & \text{for } \Delta n \neq 0 \\ -a & \text{for } \Delta n = 0 \end{cases}$$

whence we get  $g_{+}(\kappa) = g_{-}(\kappa) \equiv g(\kappa)$  as

$$g(\kappa) = \gamma - 1 + f(\kappa) \quad (27)$$

which replaces (18) and where  $\gamma = e^{ca}$ .

Similar simplifications can be made for factors  $h_{\pm}(\kappa)$  and  $k_{\pm}(\kappa)$  connecting layers which are second and third neighbours. It is straightforward to show that we will obtain

$$g(\kappa) = c_1(\kappa) \quad h(\kappa) = c_2(\kappa) \quad \text{and} \quad k(\kappa) = c_3(\kappa)$$

with

$$c_n(\kappa) = \gamma^n - 1 + f(\kappa) \quad (28)$$

and, of course,  $c_0(\kappa) \equiv f(\kappa)$ . Again subscripts + or - can be dropped in  $h(\kappa)$  and  $k(\kappa)$ . This is the essential point in our approximation and this enables us to utilize the formulation of Appendix A with the proviso that expressions (A1) and (A2) are to be replaced by

$$F(\kappa) = c_0(\kappa)/\beta \quad G(\kappa) = c_1(\kappa)/\beta \quad H(\kappa) = c_2(\kappa)/\beta \quad K(\kappa) = c_3(\kappa)/\beta. \quad (29)$$

One then arrives at the 'compact' expressions for the potentials  $V_L$  similar to (A3)–(A6) of Appendix A. Note that when the lattice constant  $c$  is large (i.e. when the inter-cell interaction is weak),  $f(\kappa)$  given by (8) tends to 1, and one recovers the expressions (A1) and (A2) of the isolated unit cell model. These potentials can also be given in their 'standard form' similar to (A7). The 'standard form' (A1) has, however, to be modified since the mode index  $\kappa$  now has  $L$  continua of values ranging from 0 to  $\pi$  giving rise to  $L$  plasmon bands, i.e. (A7) is modified to

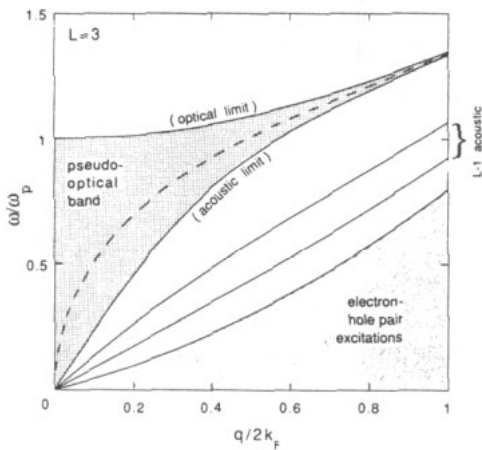
$$\frac{V_L}{v_0} = 1 + \frac{1}{\pi} \sum_{\kappa=1}^L \int_0^{\pi} d\kappa' \frac{w_{\kappa}(\kappa')}{\beta - \beta_{\kappa}(\kappa')} \quad (30)$$

where  $w_{\kappa}(\kappa')$  and  $\beta_{\kappa}(\kappa')$  can be expressed in terms of  $c_n(\kappa')$ , given in Appendix B, and where the first term, equal to one, comes from

$$\frac{1}{\pi} \int_0^{\pi} d\kappa' c_0(\kappa') = \frac{1}{\pi} \int_0^{\pi} d\kappa' f(\kappa') = 1.$$

As shown in figure 2,  $\kappa = 1$  in (30) corresponds to the pseudo-optical plasmon mode which has the dispersion relation of the bulk plasmon at the high energy limit  $\kappa' = 0$  and it gives an acoustic plasmon mode at the other limit  $\kappa' = \pi$ . For other values of  $\kappa$ , we have very narrow acoustic plasmon bands as indicated in figure 2. Finally, let us note that for  $L = 1$  the above approximate method is in fact exact (and in agreement with (14)–(16)), since there is no inter-layer distance  $a$  to cancel. For  $L = 2$ , the validity of the approximate method can be checked against the exact calculation performed in section 3—see (23) and (24). In most applications the difference between the results yielded by both methods will be found to be quite negligible (see our following paper).





**Figure 2.** Representation of the plasmon bands contributing to the effective interaction between the charge carriers. The upper band is the pseudo-optical band which has the proper optical mode at the upper limit and the acoustic mode at the lower limit. The other bands correspond to the  $L - 1$  narrow acoustic bands discussed in the text. For completeness the low frequency particle-hole continuum is also shown. The broken curve gives the plasmon mode for a single 2D electron gas.

## 5. Summary

In this paper we have calculated the effective interaction between two charge carriers located in the same layer of an infinite superlattice containing up to four metallic layers (2DEGs) per unit cell. The calculation is based on the plasmon exchange model of the RPA. Exact analytic expressions for the effective interactions have been obtained for the infinite periodic systems containing one and two metallic layers per unit cell. This calculation is then extended to obtain approximate analytic expressions for this effective interaction for  $L = 1, 2, 3$  and 4 layers per cell. The interaction is found to be mediated by one pseudo-optical plasmon band and  $L - 1$  acoustic bands. The pseudo-optical plasmon band is found to have an optical value ( $\omega \approx \text{constant}$ ) equivalent to the bulk plasmon mode in one limit and in the other limit it corresponds to the upper limit of the acoustic plasmons. The other  $L - 1$  narrow acoustic plasmon bands correspond to pure acoustic modes for small values of  $q$ . The results derived in this paper should have direct relevance to the many-body properties of the various types of superlattices identified in recent years, including the high- $T_c$  superconductors [14].

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## Appendix A

Here we present the effective interaction for the case of an isolated unit cell containing  $L$  2DEG layers with  $L = 1, 2, 3$  and 4. This corresponds to a model where only the intra-cell interactions are considered. For  $L = 1$  and 2, the calculations are similar to those of

section 3, except that they are simpler since all subscripts  $\pm$  can be dropped. Indeed one has

$$F = 1/\beta \quad \text{and} \quad G = \gamma/\beta \quad (\text{A1})$$

with  $\gamma = \exp(-aq)$ . The extension to the systems with  $L = 3$  and 4 is rather straightforward and the results will involve

$$H = \gamma^2/\beta \quad \text{and} \quad K = \gamma^3/\beta \quad (\text{A2})$$

The results can be expressed in the form of the following 'compact' expressions [13]

$$V_1(q, \omega) = v_0\beta/(\beta - 1) \quad (\text{A3})$$

$$V_2(q, \omega) = (v_0\beta/2)[(1 + \gamma)/(\beta - 1 - \gamma) + (1 - \gamma)/(\beta - 1 + \gamma)] \quad (\text{A4})$$

$$V_{3s}(q, \omega) = (v_0\beta/2)\{\beta(\beta - 1)/[(\beta - 1)^2 - \gamma^2(\beta - 1) - 2\gamma^2] + \beta/(\beta - 1 + \gamma^2) - 2\} \quad (\text{A5a})$$

$$V_{3m}(q, \omega) = v_0\beta(\beta - 1 + \gamma^2)/[(\beta - 1)^2 - \gamma^2(\beta - 1) - 2\gamma^2] \quad (\text{A5b})$$

$$V_{4s}(q, \omega) = (v_0\beta/2)\{\beta(\beta - 1 - \gamma)/[(\beta - 1)^2 - \gamma(1 + \gamma^2)(\beta - 1) - \gamma^2(1 + 2\gamma)] \\ + \text{idem}(\gamma \rightarrow -\gamma)\} \quad (\text{A6a})$$

$$V_{4m}(q, \omega) = (v_0\beta/2)\{(1 + \gamma)(\beta - 1 + \gamma^2)/[(\beta - 1)^2 - \gamma(1 + \gamma^2)(\beta - 1) - \gamma^2(1 + 2\gamma)] \\ + \text{idem}(\gamma \rightarrow -\gamma)\}. \quad (\text{A6b})$$

Note that these results are given in terms of only two parameters  $\beta$  and  $\gamma$ . For  $L = 3$  and 4, the potentials in the side and middle layers are specified by a second subscript ( $s$  and  $m$ , respectively).

A series of quick checks can be made regarding the validity of these expressions. The number of modes, given by the number of poles, is equal to  $L$ . The poles of  $V_{3s}$  and  $V_{3m}$  are identical, as well as those of  $V_{4s}$  and  $V_{4m}$ . For  $\gamma \rightarrow 0$ , the distance between the layers become infinity and one obtains  $V_L = V_1 = v_0\beta/(\beta - 1) = v_0/(1 + v_0\Pi)$  which is the potential for an isolated layer. For  $\gamma \rightarrow 1$ , the various layers of the unit cell collapse into a single layer and we have  $V_L = v_0\beta/(\beta - L) = v_0/(1 + Lv_0\Pi)$  which is again the potential for a single layer, with the electron density getting multiplied by  $L$ .

A last point to note is that for small  $q$  (i.e. for  $\gamma \rightarrow 1$ ), one pole tends to 1 and the other poles tend to be proportional to  $1 - \gamma \approx aq$ . This implies that one pole corresponds to a planar plasmon mode with the pseudo-optical dispersion relation  $\omega \propto q^{1/2}$  and the others represent  $(L - 1)$  acoustic plasmon modes with  $\omega \propto q$ .

The potentials  $V_L$  given by (A3)–(A6) can also be written in the 'standard form' as

$$\frac{V_L}{v_0} = 1 + \sum_{\kappa=1}^L \frac{w_\kappa}{\beta - \beta_\kappa} \quad (\text{A7})$$

where the  $w_\kappa$  and  $\beta_\kappa$  can be expressed in terms of  $c_n \equiv \gamma^n = \exp(-naq)$ , and they are given in Appendix B.

## Appendix B

Remembering that the  $w_\kappa(k')$  and  $\beta_\kappa(k')$  appearing in (30) can be expressed in terms of

the  $c_n$  given by (28), i.e. by

$$c_n(\kappa') = \gamma^n - 1 + f(\kappa') \quad (\text{B1})$$

we now give the expressions for  $w_\kappa$  and  $\beta_\kappa$ .

For  $V_1$ , one has

$$\beta_1 = c_0 \quad w_1 = c_0^2.$$

For  $V_2$ , one has

$$\beta_1 = c_0 + c_1 \quad \beta_2 = c_0 - c_1$$

and

$$w_1 = \beta_1^2/2 \quad w_2 = \beta_2^2/2.$$

For  $L = 3$  and  $4$ , we have to distinguish between the side (s) and the middle (m) layers.

For  $V_{3s}$ , one has

$$\beta_1 = c_0 + (c_2 + r)/2 \quad \beta_2 = c_0 + (c_2 - r)/2 \quad \beta_3 = c_0 - c_2$$

with

$$r = (8c_1^2 + c_2^2)^{1/2}$$

and

$$w_{1s} = \beta_1^2(\beta_1 - c_0)/2r \quad w_{2s} = -\beta_2^2(\beta_2 - c_0)/2r \quad w_{3s} = \beta_3^2/2.$$

For  $V_{3m}$ , the  $\beta_\kappa$ s are the same as for  $V_{3s}$  and one has

$$w_{1m} = \beta_1^2(\beta_1 - c_0 - c_2)/r \quad w_{2m} = -\beta_2^2(\beta_2 - c_0 - c_2)/r \quad w_{3s} = 0.$$

For  $V_{4s}$ , one has

$$\beta_1 = c_0 + (c_1 + c_3 + r_+)/2 \quad \beta_2 = c_0 + (c_1 + c_3 - r_+)/2$$

$$\beta_3 = c_0 - (c_1 + c_3 - r_-)/2 \quad \beta_4 = c_0 - (c_1 + c_3 + r_-)/2$$

with

$$r_\pm = \pm [(c_1 - c_3)^2 + 4(c_1 \pm c_2)^2]^{1/2}$$

and

$$w_{1s} = \beta_1^2(\beta_1 - c_0 - c_1)/2r_+ \quad w_{2s} = -\beta_2^2(\beta_2 - c_0 - c_1)/2r_+$$

$$w_{3s} = \beta_3^2(\beta_3 - c_0 + c_1)/2r_- \quad w_{4s} = -\beta_4^2(\beta_4 - c_0 + c_1)/2r_-.$$

For  $V_{4m}$ , the  $\beta_\kappa$ s are the same as for  $V_{4s}$  and one has

$$w_{1m} = \beta_1^2(\beta_1 - c_0 - c_3)/2r_+ \quad w_{2m} = -\beta_2^2(\beta_2 - c_0 - c_3)/2r_+$$

$$w_{3m} = \beta_3^2(\beta_3 - c_0 + c_3)/2r_- \quad w_{4m} = -\beta_4^2(\beta_4 - c_0 + c_3)/2r_-.$$

From these expressions it can be shown that

$$\sum_\kappa \frac{w_\kappa}{\beta_\kappa} = c_0 \quad (\text{B2})$$

giving

$$\sum_{\kappa} \frac{w_{\kappa}(\kappa')}{\beta_{\kappa}(\kappa')} = f(\kappa').$$

Using (16) one has

$$\frac{1}{\pi} \int_0^{\pi} d\kappa' \sum_{\kappa} \frac{w_{\kappa}(\kappa')}{\beta_{\kappa}(\kappa')} = 1 \quad (\text{B3})$$

In fact, these expressions are the sum rules due to the analytic properties of the RPA potentials, namely  $V_L(q, \omega)$  tends to zero for  $\omega \rightarrow 0$ , here within the plasmon region of the  $(q, \omega)$  plane where  $(2m\omega > q^2 + 2k_F q)$ .

Other useful expressions are

$$\sum_{\kappa} w_{\kappa} = \begin{cases} c_0^2 & \text{for } V_1 \\ c_0^2 + c_1^2 & \text{for } V_2 \\ c_0^2 + c_1^2 + c_2^2 & \text{for } V_{3s} \\ c_0^2 + 2c_1^2 & \text{for } V_{3m} \\ c_0^2 + c_1^2 + c_2^2 + c_3^2 & \text{for } V_{4s} \\ c_0^2 + 2c_1^2 + c_2^2 & \text{for } V_{4m}. \end{cases} \quad (\text{B4})$$

These comparatively simple expressions can be calculated directly from the above detailed expressions of  $\beta_{\kappa}$  and  $w_{\kappa}$ .

Note that for  $L = 3$  and  $L = 4$  we have to take the average over the side (s) and middle (m) layers, since the layers are always assumed to interact inside the unit cell. For  $L = 3$  one has

$$\sum_{\kappa} = \frac{2}{3} \sum_{\kappa(s)} + \frac{1}{3} \sum_{\kappa(m)}$$

and for  $L = 4$  one has

$$\sum_{\kappa} = \frac{1}{2} \sum_{\kappa(s)} + \frac{1}{2} \sum_{\kappa(m)}$$

We will thus write

$$\sum_{\kappa} w_{\kappa} = c_0^2 + (4/3)c_1^2 + (2/3)c_2^2$$

and

$$\sum_{\kappa} w_{\kappa} = c_0^2 + (3/2)c_1^2 + c_2^2 + (1/2)c_3^2$$

for  $L = 3$  and  $L = 4$ , respectively.

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