



## COLLECTIVE MODES OF A SUPERLATTICE - PLASMONS, LO PHONON-PLASMONS, AND MAGNETOPLASMONS

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The wavevector-frequency dependent dielectric constant is investigated for a superlattice structure. Attention here is focused on the collective modes of the GaAs-GaAlAs superlattice with doped (or modulated doped) quantum wells. For wells widely separated in space, such that Bloch wave function overlap between wells is negligible, a Bloch-like plasmon can propagate along the superlattice direction mediated entirely by Coulomb interaction alone. Interaction of these plasmons with optical phonons and with a magnetic field is investigated.

### 1. Introduction

Man-made superlattice structures with precise interfacial and dimensional control are now a reality as a result of the recent advancements made by molecular beam epitaxy (MBE).<sup>1</sup> Layered structures, GaAs-GaAlAs being the most extensively studied and best characterized system, can be grown with periodicities ranging from  $\sim 5\text{A}$  to hundreds of Angstroms. In this paper, we focus on the collective modes of the GaAs-GaAlAs superlattice and present a calculation of the wave vector-frequency dependent dielectric constant.

The idea of collective plasmon modes in a layered structure, most notably in the context of graphite and intercalated transition-metal dichalcogenides, has been studied by various workers in the field. The plasmon excitations of a thin metallic layer were first demonstrated theoretically by Ritchie<sup>2</sup> in 1957. Stern<sup>3</sup> derived the polarizability and plasmon dispersion relation of a two-dimensional electron gas in the self-consistent field approximation. Equiluz, et al.<sup>4</sup> have calculated the plasmon modes of the MOS inversion layer including the interaction with the photon field. A rather complete analysis of the electrodynamics of the quasi-two-dimensional gas is found in the work of Dahl and Sham.<sup>5</sup> In a multicomponent plasma, two plasmon branches are found; a high frequency optical branch and a low frequency acoustic branch (which is highly damped by electron-hole excitations).<sup>6</sup> For a layered electron gas Visscher and Falicov<sup>7</sup> have calculated the static dielectric constant. Within a hydrodynamic model, Fetter<sup>8</sup> has derived the equations describing the plasmon modes of an infinite array of two-dimensional sheets of electrons. Apostol<sup>9</sup> has done a similar analysis using an equation of motion (RPA) approach to derive the plasmon dispersion relation and Caille et

al.<sup>10</sup> have attempted to include phonons. In a similar spirit, Mele and Ritsko<sup>11</sup> investigated the frequency-wave vector dependent longitudinal dielectric constant for FeCl<sub>3</sub>-intercalated graphite.

In this paper, we use standard many-body techniques to calculate the plasmon dispersion relation for a GaAs-GaAlAs superlattice structure. Previous treatments based on equation of motion and hydrodynamic approaches allow one to derive the R.P.A. result but approximations beyond this are quite difficult. The approach we have taken for the superlattice is a generalization of that taken by Das Sarma and Madhukar<sup>12</sup> for the double heterojunction quantum-well structure which led to the prediction of an anomalous acoustic plasmon ( $\omega_{\text{q}}$ ) distinct from the electron-hole continuum.<sup>13</sup> We focus here on the plasmon modes of a superlattice structure leaving to a later paper an investigation of more subtle many-body effects (self-energy, exchange, depolarization, inter-subband excitations). In addition, we consider the effects of interaction with longitudinal optical phonons and with a magnetic field on the dispersion relation of the superlattice plasmon.

### 2. Theory and Results

In Fig. 1, we show the conduction and valence band profiles of a GaAs-GaAlAs superlattice. Here  $d$  is the distance between wells (the periodicity) and  $l$  is the well thickness. We focus on the case where  $l$  ( $\sim 50\text{A}$ ) is much smaller than  $d$ . Thus, the electron wave function is essentially confined to the quantum well and the normal Bloch wave function overlap is taken to be negligible. This will be relaxed in a later publication. In this situation, long-range Coulomb interaction is still operative between the wells and leads to plasmons propagating along the direction of the superlattice.<sup>8</sup>

Each well is considered to be equivalent and arranged on a periodic lattice. Each well

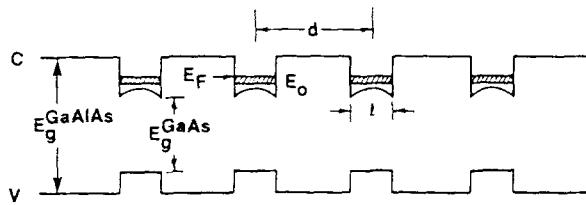


Figure 1.

A superlattice of GaAs-GaAlAs consisting of a periodic array of quantum wells with periodicity  $d$ . The modulation of the conduction and valence band by the superlattice potential is shown. Each well is doped (or modulated doped) with  $n$  electrons.  $l$  is the width of the well,  $E_0$  is the ground subband energy, and  $E_F$  is the Fermi level.

is either doped (or modulated doped) with electrons (or holes) to a density  $n$ . Results for alternating electron-hole wells (with equal masses) will also be given. For different masses ( $n_1, m_1, n_2, m_2, \dots$  superlattice) or different densities ( $n_1, n_2, n_1, n_2, \dots$ ), optical and acoustic-like branches are found.<sup>14</sup>

Consider a single quantum well doped with  $n$  electrons. It has a ground subband energy  $E_0$  (see Fig. 1) and Fermi-level  $E_F$ . Its motion is confined to the well but free-electron like perpendicular to the well (along the plane perpendicular to the superlattice direction) with dispersion relation

$$E_{q''} = E_0 + \frac{\hbar^2 q''^2}{2m^*} \quad (1)$$

where  $q''$  is the wave-vector parallel to the plane (i.e. perpendicular to the superlattice direction),  $m^*$  is the electron effective mass. In the two-dimensional limit, the plasmon dispersion relation  $\omega$  was first calculated by Stern<sup>3</sup> and shown to be proportional to  $q''^1$ . When one has  $n$  such 2-D quantum wells arranged on a periodic lattice, the simple 2-D plasmon dispersion relation will broaden into a band.

To determine the collective modes of a homogeneous electron gas, one sets the dielectric constant equal to zero. For a superlattice, for each quantum well, the subband wave function is given by  $\psi \sim e^{i\vec{q}'' \cdot \vec{r}} \phi_i(z)$  where  $\vec{r}$  is the wave vector within the plane,  $\phi_i(z)$  is the quantized wave function in the well and  $i$  is the subband index. In general, for such an inhomogeneous system, the dielectric constant is a fourth-rank tensor<sup>12</sup> with indices  $(ijlm)$ . For example, the Coulomb interaction expanded on the subband basis is

$$V_{ijlm}(z, z') = \iint dz dz' \frac{2\pi e^2}{\epsilon_0 q''} e^{-q''|z-z'|} \phi_i^*(z) \phi_j(z) \phi_l^*(z') \phi_m(z') \quad (2)$$

where  $ijlm$  label the different subbands and different wells. In this paper, we focus on the ground state properties and consider only

the ground subband ( $i = 0$ ). The diagonal approximation, which is valid for the Si inversion layer<sup>15</sup>, is also applied here; namely  $i = j$  and  $l = m$ . Within these approximations, the dielectric constant is a matrix on well index

$$\epsilon_{ij}(\vec{q}'', \omega) = \delta_{ij} - \frac{V_{0000}}{\epsilon_0 q''} \pi_{jj}^0(\vec{q}'', \omega) \quad (3)$$

where  $\pi_{jj}^0(\vec{q}'', \omega)$  is the bare polarization bubble. Since only the 0'th subband is considered, the indices  $i$  and  $j$  label here different wells. The collective excitations are given by the zeroes of the dielectric constant Eq. (3) which in this case (for  $n$  quantum wells on a periodic lattice) is a  $n \times n$  matrix and is given by setting the determinant of  $\epsilon_{ij}$  to zero. Following Das Sarma and Madhukar,<sup>12</sup> we consider the approximation where the wave function is highly localized within the well (delta-function like) and  $d$  is large so that Bloch overlap is negligible. It is appropriate to note that this approximation is not necessary and via Eq. (2) the complete internal structure of the quantum subband can be included. This approximation leads to a Coulomb interaction between planes.

$$V_{ij} = \frac{2\pi e^2}{\epsilon_0 q''} e^{-q''|z_i - z_j|} \quad (4)$$

where  $\epsilon_0$  is the static dielectric constant. Since each well is doped with  $n$  electrons ( $n$  is a 2-D density) and is equivalent to all others, the ground subband polarization  $\pi_{jj}^0$  in the high frequency regime is simply given by

$$\pi_{jj}^0(q'', \omega) = \frac{n}{m^*} \frac{q''^2}{\omega^2} \text{ for } \omega > q'' V_F \text{ and for all } j \quad (5)$$

where  $V_F$  is the Fermi velocity. The introduction of many-body effects (self-energy and vertex corrections) beyond the R.P.A. is given by appropriate modifications to the bare polarization bubble  $\pi^0$  (e.g., Hubbard-type corrections).

Within the above approximations and in the limit  $q''d \gg 1$ , we need consider only nearest well interactions. The Coulomb interactions between wells becomes

$$V_{i,i+1} = \frac{2\pi e^2}{\epsilon_0 q''} e^{-q''d} \quad (6)$$

The matrix for the dielectric constant Eq. (3) is now seen to be equivalent to the matrix for

the eigenenergies for the tight binding model (namely  $i - V_{ii} \rightarrow \epsilon_0 - \omega$  and  $-V_{i,i+1} \pi_{i+1,i+1}$  →

$t_{i,i+1}$ ). This can be diagonalized by going over to collective coordinates. The result obtained for the energy of the collective mode (plasmon) of the superlattice is

$$\omega = \omega_p^{2.0} (1 \pm 2e^{-q_{\perp}d} \cos q_{\perp}d)^{\frac{1}{2}} \quad (7)$$

where  $\omega_p^{2.0} = \left[ \frac{2\pi n e^2 q_{\perp}}{\epsilon_0 m^*} \right]^{\frac{1}{2}}$  is the single-well plasmon dispersion relation;  $q_{\perp}$  is along the superlattice direction and  $q_{\perp}$  perpendicular to the superlattice direction. The + sign is for electron-electron interaction; the - sign for electron-hole interaction.

For  $q_{\perp}d \ll 1$ , the more important physical limit, the interaction between all quantum wells becomes important and we must sum the Coulomb interaction over all wells. We obtain for the interplane Coulomb interaction

$$V = \frac{4\pi e^2}{\epsilon_0 q_{\perp}} \frac{e^{-q_{\perp}d} - e^{-2q_{\perp}d}}{1 - 2e^{-q_{\perp}d} \cos q_{\perp}d + e^{-2q_{\perp}d}} \quad (8)$$

for the case of electron-electron interaction. The determinant of  $V_{ij}$ , Eq. (3), equal to zero is easily solved. The result is equivalent to going beyond the nearest neighbor approximation in the tight binding model. The result for the collective oscillations is

$$\omega = \omega_p^{2.0} \left[ \frac{-2q_{\perp}d}{1 - e^{-2q_{\perp}d}} \right]^{\frac{1}{2}} \quad (9)$$

where quantities have been defined in Eq. (7). This result, with the concurrent delta-function approximation, is equivalent to that obtained by the authors mentioned previously (see ref. 8 and 9). If we relax the approximation stated by Eq. (4), namely delta-like wave functions, then the internal structure of the quantum well will be evident in  $V_{ij}$  and a modified plasmon dispersion will be obtained. However, qualitatively the results will be quite similar. We note the band type motion ( $\cos q_{\perp}d$ ) of the plasmon occurring along the superlattice direction. A plot of Eq. (9) is shown in Fig. 2 for  $q_{\perp}d$  taken to be 0.13. We see that the single quantum well plasmon has been transformed into a band along the superlattice as a result of long-range Coulomb interaction between wells. The solid line is for electron-electron interaction; the broken line for electron-hole. We note that for  $q_{\perp}d = 0$  and  $q_{\perp}d$  small,

$$\omega = \left[ \frac{4\pi n e^2}{\epsilon_0 m^* d} \right]^{\frac{1}{2}} \quad (10)$$

which is the bulk plasmon for a homogeneous system with 3-D density,  $n^{3.0} = n/d$ . For  $q_{\perp}d = \pi$  and  $q_{\perp}d$  small, an acoustic-like mode ( $\omega \propto q$ ) is found.

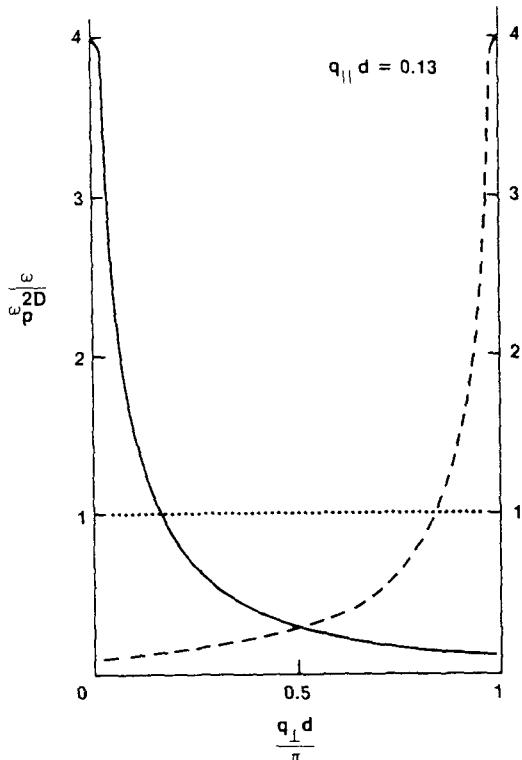


Figure 2.

Plot of the plasmon dispersion relation Eq. (9) as a function of  $q_{\perp}d$ . Here  $q_{\perp}d$  is taken to be 0.13. The broadening of the single sheet plasmon  $\omega_p^{2.0}$  (dotted line) into a band is evident. The bandwidth is determined by the properties of the superlattice as discussed in text. Solid line is for electron-electron interaction. Broken line is for electron-hole

$$\omega = \left[ \frac{\pi n e^2}{\epsilon_0 m^* d} \right]^{\frac{1}{2}} (q_{\perp}d) \quad (11)$$

As shown by Das Sarma and Madhukar<sup>12</sup>, there exists a critical periodicity distance  $d_c$  for which  $d$  must be larger than in order for eq. (11) to hold. In the high frequency regime,  $\omega$  must be greater than  $q_{\perp}V_F$ . This leads to a critical periodicity  $d_c$  equal to  $\frac{8a_0}{\hbar^2 \epsilon_0}$  for the validity of eq. (11). Here  $a_0 = \frac{m^* e^2}{\hbar^2 \epsilon_0}$  is the effective Bohr radius. Thus, in the regime in which eq. (11) holds, this is the generalization of the anomalous acoustic plasmon of Das Sarma and Madhukar<sup>12</sup> to the case of a superlattice. For  $q_{\perp}d$  large,  $\omega$  reduces to the two-dimensional plasmon,  $\omega_p^{2.0}$ , since in this limit, the quantum wells are isolated from each other.

The bandwidth is the difference between Eqs. (10) and (11) and for GaAs with  $n \approx 10^{12} \text{ cm}^{-2}$ ,  $\epsilon_0 = 12.35$ ,  $d \approx 200 \text{ \AA}$ ,  $m^* = 0.068 m_{el}$ ;

the bandwidth is about 30 meV which is a number comparable to intersubband energies and longitudinal optical phonon energies. We also note from Fig. 2 that for a large range of  $q_{\perp}d$  the plasmon relation is outside of the electron-hole continuum and thus should be a long lived excitation. We now include the effects of interaction with LO-phonon and magnetic field.

GaAs is a polar material with a longitudinal optical phonon with energy 36.8 meV. Depending on the value of the parameters occurring in Eq. (10), the plasmon bandwidth can be above or below this value. Consequently, the plasmon and LO phonon can interact. We take for  $\epsilon(\omega)$ , the dielectric constant for the GaAs well, which includes the LO phonon interaction, the same form as used by Pinczuk, et al.<sup>16</sup> for the single quantum well; namely,

$$\frac{1}{\epsilon(\omega)} = \frac{1}{\epsilon_{\infty}} \left( 1 + \left[ \frac{\alpha \omega_{LO}^2}{\omega^2 - \omega_{LO}^2} \right] \right) \quad (12)$$

where  $\alpha = 1 - \frac{\epsilon_{\infty}}{\epsilon_0}$  and  $\epsilon_{\infty} = 10.48$ ,  $\epsilon_0 = 12.35$ ,  $\omega_{LO}$  is the LO-phonon frequency; thus,  $\alpha = .151$ .

In the formalism presented above, we include electron-phonon interaction by replacing  $1/\epsilon_0$  by Eq. (12) in Eq. (4). The dielectric matrix is diagonalized as before and we obtain a collective plasmon-phonon mode with excitation energy,

$$\omega^2 = \omega_{LO}^2 + \omega_p^2 \pm \sqrt{\left( \omega_{LO}^2 - \omega_p^2 \right) + 4\alpha\omega_{LO}^2\omega_p^2} \quad (13)$$

where  $\omega_p$  is here the plasmon mode of the superlattice given by Eq. (9). In Fig. 3, we plot Eq. (13) for  $d \sim 100\text{\AA}$ ,  $n \sim 10^{12}\text{cm}^{-2}$ , which sets the top of the plasmon band at 41 meV which is higher than  $\omega_{LO}$ . The dotted line

is the bare plasmon and  $q_{\perp}d$  is 0.13. In Fig. 4, we take the top of the band to be 30 meV ( $\sim 200\text{\AA}$ ) which is lower than  $\omega_{LO}$ . The effect of the coupling between the plasmon and LO phonon is seen to be quite strong leading to coupled plasmon-LO phonon modes.

For the case of a magnetic field applied along the superlattice direction, we follow the analysis of Kobayashi, et al.<sup>17</sup> who considered the  $q_{\perp}d = 0$  limit. We extend their results to include finite  $q_{\perp}d$ . For simplicity, we ignore the LO phonon interaction. With a magnetic field applied along the superlattice, the electron's motion in the plane becomes quantized into a series of Landau orbits with energies  $(n + 1/2)\hbar\omega_c$ . The effect of this quantization leads to a polarization  $\pi^0(q_{\perp}, \omega)$  for a single well given by

$$\pi^0(q_{\perp}, \omega) = \frac{2}{\pi\ell^2} \sum_{\substack{n \\ m > -n}} f_n \frac{m\omega_c}{\omega^2 - (m\omega_c)^2} J_{n+m, n}(q_{\perp}) \quad (14)$$

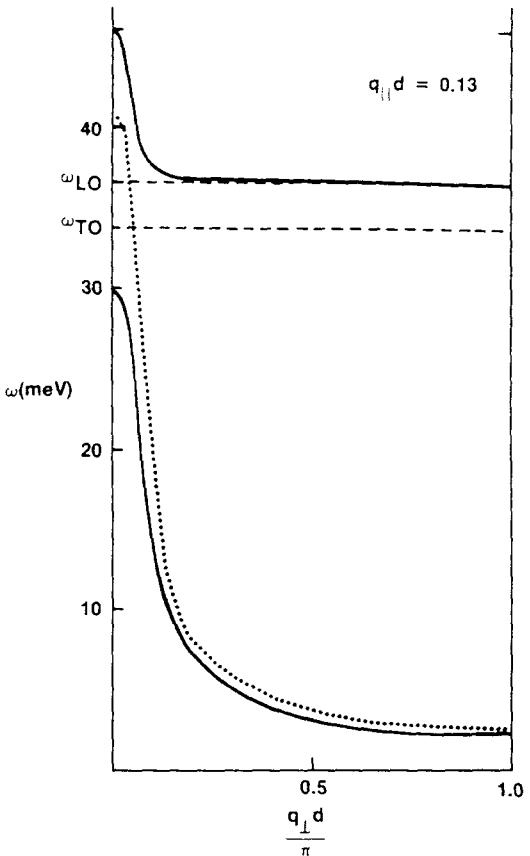


Figure 3.

Plot of the coupled plasmon-phonon mode energies as a function of  $q_{\perp}d$ . The dotted line is the bare plasmon mode. The top of the bare plasmon band was taken to be 41 meV and  $q_{\perp}d = 0.13$ .

where

$$J_{nn'}(q_{\perp}) = \int_{-\infty}^{+\infty} e^{iq_{\perp}x} \phi_n\left(\frac{x}{\ell}\right) \phi_{n'}\left(\frac{x}{\ell}\right) dx \quad (15)$$

and  $f_n$  is the Fermi distribution function,  $\ell^2 = \hbar/m^* \omega_c$  is the cyclotron orbit radius,  $\phi_n(x)$  is the Landau wave function, and  $\omega_c = \frac{eH}{m^* c}$  is the cyclotron energy. For  $q_{\perp}\ell \ll 1$ , we obtain for the coupled magneto-plasmon mode

$$\omega^2 = \omega_c^2 + (\omega_p^{2,D})^2 \left[ \frac{\frac{-2q_{\perp}d}{1-e}}{1 - (\pm 2^{-2}q_{\perp}d \cos q_{\perp}d) + e^{-2q_{\perp}d}} \right] \quad (16)$$

where  $\omega_p^{2,D}$  is defined after Eq. (7). This agrees with Kobayashi, et al. for  $q_{\perp}d = 0$ . There are also other Bernstein type modes occurring at  $\omega = n\omega_c$  ( $n = 2, 3, \dots$ ); however, as shown in Ref. 16 the coupling to these modes is very weak.

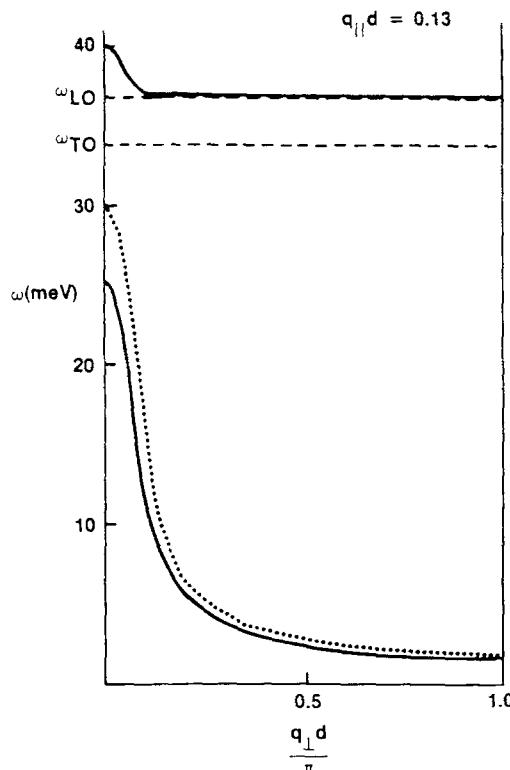


Figure 4.

Same as Figure 3, but here the top of the bare plasmon band was taken to be 30 meV.

In conclusion, we have studied the collective modes of a superlattice structure including electron-phonon and magnetic field interactions. In a future publication, we will consider the effects of a superlattice on the collective modes between quantum subbands (de-polarization and exciton effect), inclusion of subband wave functions, and the effect of finite Bloch overlap between wells. Here, we have shown that the plasmon-dispersion relation in a superlattice quantum well structure follows very simply from the determinant of the dielectric matrix. The simple 2-D plasmon dispersion relation is broadened into a band

along the superlattice direction. The width of this band is adjustable simply by choosing appropriate parameters. Interaction of these modes with LO phonons and magnetic field lead to interesting hybrid modes that may be observable by light scattering techniques. In order to get a finite  $q_{\parallel}$ , a grating might be applied to the superlattice surface. The GaAs-GaAlAs superlattice structure appears to be an ideal system to test out these ideas.

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