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# Surface plasmons studied by the method of recurrence relations

H K Sy
Department of Physics, National University of Singapore, Kent Ridge, Singapore 0511

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**Abstract.** We study the plasma oscillations in a finite number of layers of a 2DEG. It is shown that by matching electromagnetic boundary conditions and solving the recurrence relations for the coefficients of the electric potential in different regions, a general equation can be obtained for the frequencies of all the plasmons under different types of surface discontinuity. Numerical results are shown for six layers with non-identical surface charge layers.

## 1. Introduction

The problem of surface plasmons occurring in a semiconductor superlattice system consisting of layers of two-dimensional electron gas (2DEG) has been investigated by many authors theoretically. Different types of surface discontinuity (mismatch) have also been considered. Giuliani and Quinn [1] and Jain and Allen [2–4] have studied the surface plasmons when there is a change in the dielectric constants at the interface. Sy and Chua [5] have investigated the case when the surface layer has a different charge density, with no dielectric change. And many authors [6–9] have considered the situation in which there are changes in both charge densities and dielectric constants. On the other hand, Bloss [10] has also considered the surface modes when a superlattice is in contact with a semi-infinite doped overlayer.

For a semi-infinite superlattice, the most straightforward theoretical approach is to consider the electric potential (or the equivalent transverse and longitudinal electric fields) in each region, and to apply the electrodynamic boundary conditions. The *ansatz* [1] of a decaying mode is then used to obtain an equation for the surface mode. This approach has been used, for example, in [1, 9] for a type-I system consisting of one kind of layers of 2DEG; in [8, 11, 12] for type-II superlattices, with two kinds of 2DEG layers in alternation; and also in [10].

For finite systems, the usual method is to start with the density correlation function in RPA or equivalently the density perturbation in each layer. The coupled equations for these quantities, or their Fourier transforms, are then solved numerically [2, 3, 5–7, 13]. For finite systems with a single surface layer [5], or finite systems with two identical surface layers [3, 5, 14], an explicit determinant equation whose zeros give the frequencies for all the modes can be derived. For more complicated types of surface or defect [6] discontinuity, and in particular for a finite system with non-identical surface layers, a simple determinant equation cannot be derived using this approach.

In this paper we will use the method of electric potentials for a finite system. By using the electromagnetic boundary conditions in the non-retarded limit, we obtain recurrence relations for the coefficients of the potential in each region. By solving the recurrence relations we obtain an equation for the frequencies, for all the plasmon modes, for an arbitrary number of layers of 2DEG and with quite general discontinuities. Some previous results in the literature are shown as special cases. Finally, as an application of our present approach, numerical results are obtained for a six-layer system, with two surface layers of different charge densities.

## 2. Recurrence relations for plasmon problems

We begin with the model of [15]. The system in figure 1 is made up of $(N+1)$ 2DEG layers at $z = ja$, $j = 0, \ldots, N$. All layers have charge density $n$ per unit area, except that layer $z = 0$ has $n_0$ and layer $z = Na$ has $n_{00}$. The region between the layers has dielectric constant $\epsilon$ and the regions outside have dielectric constant $\epsilon_0$ and $\epsilon_{00}$.

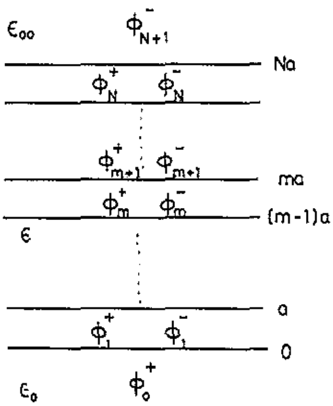


**Figure 1.** A semiconductor superlattice model of $N + 1$ layers of 2DEG.

This model describes the behaviour of a GaAs/($Al_xGa_{1-x}$)As superlattice between two media of dielectric constants $\epsilon_0$ and $\epsilon_{00}$. The doped GaAs layers are chosen to be very thin. The relatively thick $Al_xGa_{1-x}$As (of thickness $a$) act as large potential barriers, so that the charge carriers move only in the GaAs layer as a two-dimensional electron gas. Tunnelling is neglected and the electrons in different layers interact only by electromagnetic force.

We will work in the non-retarded limit. This is valid provided that our wave vector $k$ is larger than $\omega_p$ (plasmon frequency)/$c$. This is valid for the typical $k$ discussed in this problem, except for when $k < 10^3\ \mathrm{cm}^{-1}$. An extension to the calculation to include magnetic fields can be carried out, similar to those reported in many previous works [16], but this will not be attempted here.

We will only consider disturbance of the form $\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)}$, where $\boldsymbol{k}$ and $\boldsymbol{x}$ are in the plane of the 2DEG. Then in the source-free dielectric regions, the electric potential can be written as

$$\begin{gathered}\phi = \phi_m^+ \mathrm{e}^{k[z-(m-1)a]} + \phi_m^- \mathrm{i}^{-k[z-(m-1)a]} \\ (m-1)a < z < ma \qquad m = 1, \ldots, N.\end{gathered} \tag{1}$$

We will suppress all the dependence on $k$ and $\omega$.

Using the electromagnetic boundary conditions in the non-retarded limit for $E_\parallel$ and $D_\perp$ at $z = ma$, we have

$$\begin{gathered}\phi_{m+1}^+ + \phi_{m+1}^- = \phi_m^+ \mathrm{e}^{ka} + \phi_m^- \mathrm{e}^{-ka} \\ \left[\phi_{m+1}^- - \phi_{m+1}^+\right] - \left[\phi_m^- \mathrm{e}^{-ka} - \phi_m^+ \mathrm{e}^{ka}\right] = (2v\Pi/\epsilon)\left(\phi_m^+ \mathrm{e}^{ka} + \phi_m^- \mathrm{e}^{-ka}\right)\end{gathered} \tag{2}$$

where $v = 2\pi e^2/k$ is the 2D transform of the Coulomb potential, and $\Pi$ is the 2D polarizability, obtained in the long-wavelength limit as [14]

$$\Pi(k,\omega) = (m/\pi\hbar^2)\left\{\omega/kv_F/\left[(\omega/kv_F)^2 - 1\right]^{1/2} - 1\right\} \tag{3}$$

where $v_F = \hbar(2\pi n)^{1/2}/m$ and $k \ll (2\pi n)^{1/2}$.

The first boundary condition in (2) merely states the continuity of the transverse components of $\boldsymbol{E}$. The second boundary condition is called the 'additional boundary' condition in the literature [16]. Its relatively simple form originates from the infinitesimal thickness of the GaAs layers. For a more complicated structure (e.g. with finite GaAs layers), this second boundary condition has to be modified (see [17] and articles in [16]).

Equation (2) can be written as

$$\phi^+_{m+1} = A\phi^+_m + B\phi^-_m \qquad \phi^-_{m+1} = B'\phi^+_m + A'\phi^-_m \qquad m = 1, \ldots, N-1 \tag{4}$$

where $A = (1-F)e^{ka}$, $B = -Fe^{-ka}$, $A' = (1+F)e^{-ka}$, $B' = Fe^{ka}$ and $F = v\Pi/\epsilon$. By eliminating $\phi^-_m$, we obtain the following linear recurrence relation of second order:

$$\phi^+_{n+2} - 2b\phi^+_{n+1} + \phi^+_n = 0 \qquad n = 0, \ldots, N-2 \tag{5}$$

where $b = \cosh ka - F\sinh ka$.

Recurrence relations (5) and hence (4) can be solved using standard methods in terms of $\phi^+_1$, $\phi^-_1$:

$$\left.\begin{aligned} \phi^+_{m+1} &= (1/\sin\theta)\left[(A\sin m\theta - \sin(m-1)\theta)\phi^+_1 + B\sin m\theta\phi^-_1\right] \\ \phi^-_{m+1} &= (1/\sin\theta)\left[B'\sin m\theta\phi^+_1 + (A'\sin m\theta - \sin(m-1)\theta)\phi^-_1\right] \end{aligned}\right\} \qquad m = 1, \ldots, N-1 \tag{6}$$

where $\cos\theta \equiv b$ when $|b| \leqslant 1$. When $|b| > 1$, $\cosh\lambda \equiv |b|$, and $\sin m\theta$ is replaced by $(b/|b|)\sinh m\lambda$.

The recurrence relations of the form (4) have recently been studied for single-electron wave functions in a semiconductor superlattice [18] in the envelope-function approximation. By applying Bloch's condition in (5), we obtain the equation $\cos q_z a = b$ for the bulk plasmon modes.

## 3. Surface and extended modes for a general finite system

To study a finite system with two surfaces (interfaces), we need to match $\phi^+_1$, $\phi^-_1$ and $\phi^+_N$, $\phi^-_N$ with the potentials outside the superlattice. For this paper will take the regions outside to be source-free with dielectric constants $\epsilon_0 (z < 0)$ and $\epsilon_{00} (z > Na)$. The charge layers at $z = 0$ and $Na$ have density $n_0$ and $n_{00}$, respectively.

The potentials outside the superlattice can be written as

$$\begin{aligned} \phi &= \phi^+_0 e^{kz} \qquad z < 0 \\ &= \phi^-_{N+1} e^{-k(z-Na)} \qquad z > Na. \end{aligned} \tag{7}$$

The boundary conditions at $z = 0$ give

$$\phi^+_1 + \phi^-_1 = \phi^+_0 \qquad \epsilon(\phi^-_1 - \phi^+_1) + \epsilon_0\phi^+_0 = 2v\Pi_0\phi^+_0 \tag{8}$$

and boundary conditions at $z = Na$ give

$$\phi^+_N e^{ka} + \phi^-_N e^{-ka} = \phi^-_{N+1} \qquad \epsilon_{00}\phi^-_{N+1} - \epsilon\left[\phi^-_N e^{-ka} - \phi^+_N e^{ka}\right] = 2v\Pi_{00}\phi^-_{N+1} \tag{9}$$

where $\Pi_0$ and $\Pi_{00}$ are the polarizabilities at the two surface layers, obtained in (3) with $n_0$ and $n_{00}$, respectively.

Eliminating $\phi_0^+$ from (8) we have

$$\phi_1^-/\phi_1^+ = \eta_0 \equiv (\epsilon_0^- + \epsilon F_0)/(\epsilon_1^+ - \epsilon F_0). \tag{10}$$

Similarly, eliminating $\phi_{N+1}^-$ from (9):

$$(\phi_N^+/\phi_N^-)e^{2ka} = \eta_{00} \equiv (\epsilon_{00}^- + \epsilon F_{00})/(\epsilon_{00}^+ - \epsilon F_{00}) \tag{11}$$

where $F_0 = v\Pi_0/\epsilon$, $F_{00} = v\Pi_{00}/\epsilon$

$$\epsilon_0^\pm = (\epsilon \pm \epsilon_0)/2 \qquad \epsilon_{00}^\pm = (\epsilon \pm \epsilon_{00})/2. \tag{12}$$

Using equations (10) and (11), together with the recurrence relation solutions (6), we have

$$\eta_0\eta_{00}\left[(1+F)e^{-3ka}\sin(N-1)\theta - e^{-2ka}\sin(N-2)\theta\right] + Fe^{-ka}(\eta_0+\eta_{00})\sin(N-1)\theta$$
$$-(1-F)e^{ka}\sin(N-1)\theta + \sin(N-2)\theta = 0. \tag{13}$$

Equation (13) gives the solution for the frequencies of all the plasmon modes in a finite system of $N+1$ 2DEG layers with two interfaces. The two interfaces are characterized by $\eta_0$ and $\eta_{00}$.

Some special cases can be easily obtained.

(I) An $(N+1)$ finite system with no discontinuity, $n_0 = n_{00} = n$, $\epsilon_0 = \epsilon_{00} = \epsilon$ and $\eta_0 = \eta_{00} = F/(1-F)$. Equation (13) reduces to

$$(1-F)e^{ka}\sin(N+1)\theta - \sin(N\theta) = 0.$$

(II) A finite system with only a dielectric discontinuity [1,3], $n_0 = n_{00} = n$ and $\epsilon_0 = \epsilon_{00} \neq \epsilon$. Then $\eta_0 = \eta_{00} = (\epsilon_0^- + \epsilon F)/(\epsilon_0^+ - \epsilon F)$ in equation (13).

(III) A finite system with only a surface density change [5], $n_0 = n_{00} \neq n$, $\epsilon_0 = \epsilon_{00} = \epsilon$. Then $\eta_0 = \eta_{00} = F_0/(1-F_0)$.

(IV) A finite system with both a dielectric and a charge discontinuity [6–9], $n_0 = n_{00} \neq n$, $\epsilon_0 = \epsilon_{00} \neq \epsilon$. Then $\eta_0 = \eta_{00} = (\epsilon_0^- + \epsilon F_0)/(\epsilon_0^+ - \epsilon F_0)$.

(V) A semi-infinite system with both a dielectric and a charge discontinuity [6–9]. This can be obtained from equation (11) with $\eta_0 = F/(1-F)$ and using $\sinh(N\theta)/\sinh(N-1)\theta) \to \pm e^{\gamma a}$ in the limit $N \to \alpha$. By writing $e^{\gamma a} = b + (b^2-1)^{1/2}$ on obtains the equation for the surface plasmons as [6–9]

$$\pm(b^2-1)^{1/2}\sin(ka) + b\cosh(ka) + \alpha_{\mathrm{eff}}(b - \cosh(ka))e^{ka} = 1 \tag{14}$$

where $\alpha_{\mathrm{eff}} = (\epsilon_{00} + \epsilon F_{00})/(\epsilon_{00}^+ - \epsilon F_{00})e^{-2ka}$.

(VI) The model of Bloss [10]. When the region $z > Na$ has a uniform charge density, we need to replace $\epsilon_{00}$ by a frequency-dependent dielectric constant $\epsilon_{00}(\omega) = \epsilon_{00}(1-\omega_p^2/\omega^2)$.

## 4. Numerical results and discussion for non-identical surface layers

Numerical results have been achieved using (13) for the special cases mentioned in section 3, and they all agree with earlier results. Here, as an application of our present approach, we consider primarily the case in which $\eta_0 \neq \eta_{00}$, as this case has not been studied in the literature.

We will use the parameters for the GaAs/AlAs system in air, and $\epsilon_0 = \epsilon_{00} = 1$, $\epsilon = 10$ and $m = 0.068\ m_e$. The other parameters needed are $a = 1000$ Å, $n = 10^{12}$ cm$^{-2}$ and $N = 5$, so that the total number of layers is six. We will, however, allow the two surface charge densities $n_0$ and $n_{00}$ to vary.

The experimental study of plasmons in semiconductor superlattices is usually carried out using inelastic light scattering [19] or Raman scattering [20]. While the observation of the extended discrete modes in the bulk band is well established, the observation of the Giuliani–Quinn surface modes [1], with $n_0 = n_{00} = n$ and $\epsilon_0 = \epsilon_{00} \neq \epsilon$, remains elusive. One main reason for this difficulty is the depletion of the surface layers, so that the actual surface densities $n_0$ and $n_{00}$ become much less than that in the underlying layers. An investigation of the plasmons in a finite system with varying surface densities $n_0$ and $n_{00}$ is thus of current relevance.

In figure 2, we have shown our results for $n_0 = 0.8\ n$ and $n_{00} = 1.2\ n$. The bulk boundaries are also shown as broken curves. As expected, there are six modes. Modes a and b rise above the bulk band after certain finite values of $k$. We will call these nominally the surface modes as the amplitudes are localized at the respective surfaces. In the limit $N \rightarrow \infty$, these modes become the pure surface modes, with amplitude decaying exponentially away from the surfaces [9].

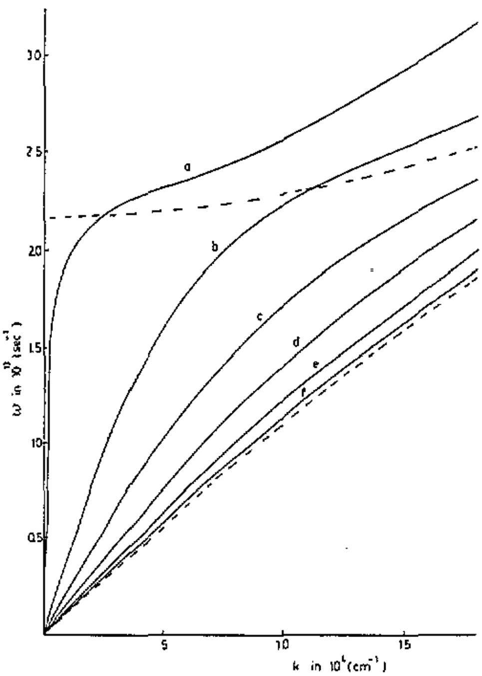


**Figure 2.** The plasmon dispersion relation for six layers with $n_0 = 0.8\ n$ and $n_{00} = 1.2\ n$.

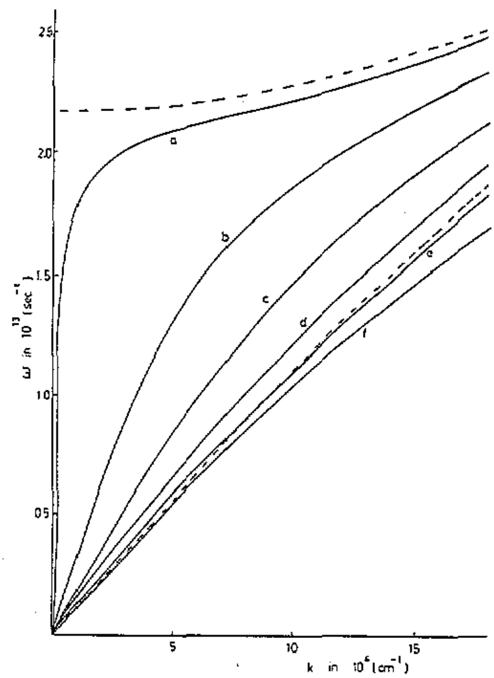


**Figure 3.** A finite system of six layers with $n_0 = 0.4\ n$ and $n_{00} = 0.5\ n$.

In figure 3, we have shown similar results for $n_0 = 0.4\ n$ and $n_{00} = 0.5\ n$. In this case, the two lowest modes, e and f, become the surface plasmon modes below the bulk modes. Note that in the special case II of section 3 [1, 3], $n_0 = n_{00} = n$ surface modes below the bulk are not possible for GaAs/AlAs in air, $\epsilon > \epsilon_0$. In our more general model, this is possible because $n_0$ and $n_{00}$ are chosen to be less than $n$. In both figures 2 and 3, the surface modes become the plasmon modes for a single 2DEG for large $k$.

For comparison, in figure 4 we have shown the results for identical surface layers, with $n_0 = n_{00} = 0.8\ n$. In this situation, coupling between the two surface modes is strong for small $k$, and gives rise to symmetric and antisymmetric combinations. For large $k$, the coupling is weak, and the surface modes are degenerate.

The fabrication of GaAs/AlAs superlattices with selective surface doping should not present too much difficulty. Because of the depletion of surface charges, the effective

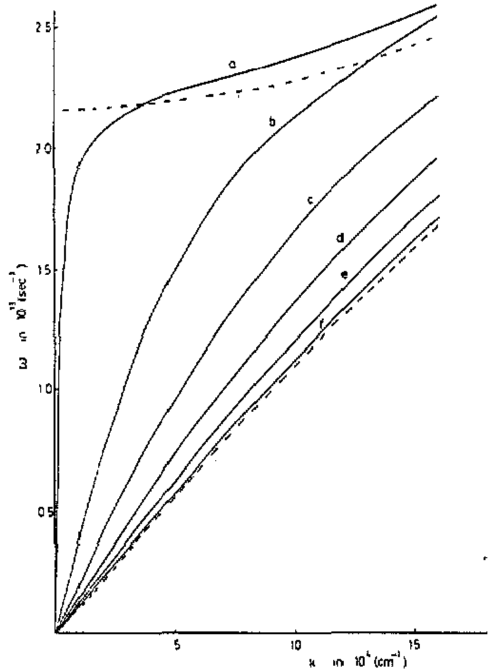


**Figure 4.** A finite system with identical surface layers $n_0 = n_{00} = 0.8\ n$.

surface densities will not be the original doping concentrations. It is hoped that our results will stimulate more experimental work on the observation of surface plasmons.

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