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Dielectric properties of electron gases in a quantum well wire: inter-subband modes

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Abstract. A self-consistent energy-functional perturbation theory is presented for electron gases confined in a quantum well wire. An analytical expression of the dynamical dielectric function is obtained both for the intra-subband and the inter-subband modes. Different from the quasi-one-dimensional wire, the inter-subband transition in this system can be taken into consideration. Plasmon excitations of inter-subband modes are discussed.

1. Introduction

The development of molecular-beam epitaxy as a technique for the growth of high-quality semiconductor crystals has given a new dimension to the study of the properties of narrow-channel microstructures in experiment. Quantum well wire (QWW) with cross sections as small as $20 \times 10\ \text{nm}^{-2}$ has been fabricated (Petroff *et al* 1982). Theoretical attention in recent literature has focused on plasmon excitations in quasi-one-dimensional (Q1D) quantum well wire (Das Sarma and Lai 1985) and transport properties of electron gases in Q1D systems (Arora 1981, Lee 1984, Peeters *et al* 1986, Peeters 1988, Chui 1986). The crossover of dimensionality from 1D to 3D as the wire radius increases has been studied (Bryant 1984). A special kind of QWW with electrons confined in a cylindrical potential well of inside radius a_1 and outside radius a_2 ($a_2 > a_1$) has also been proposed (Chen 1987, Zhu 1988). The propagating modes guided by a cylindrical quantum well (CQW) and optical absorption spectrum due to the inter-subband transition have been investigated (Huang *et al* 1988, Huang 1990). More recent works (Que and Kirezenow 1988, 1989, Cui 1989) on QWW include the studies of plasmon excitations in a multiwire superlattice with weak tunnelling between wires. These narrow-channel semiconductor microstructrures have been claimed to provide exciting new technological possibilities since the impurity content and distribution in these Q1D semiconductor structures can be selectively controlled and can produce enhanced mobility which may even exceed the very high mobility values achieved in modulation doped 2D GaAs–AlGaAs heterojunction electron transistors. In order to study the propagating waves or other optical properties of electron gases in a QWW, it is necessary to investigate the dielectric function for this system. Although the dielectric properties for electron gases in a QWW have already been studied for intra-subband modes, to the best of our knowledge, the inter-subband modes have not yet been studied.

Using the self-consistent energy-functional perturbation theory developed for the CQW system, we study the dielectric properties of electron gases confined in a QWW. In

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contrast to the Q1D system, in our calculations the inter-subband transition between different subbands can be taken into consideration. The plasmon excitation of inter-subband modes in a QWW is discussed. In section 2, we solve the eigenvalue problem of the electronic state in a QWW with a finite potential depth. In section 3, we obtain the dielectric response function of the electron gases. Some numerical results and discussions are presented in section 4.

2. Evaluation of subband energies

In a typical QWW system, electrons are confined in a cylindrical potential well of GaAs surrounded by an AlGaAs barrier with a potential well of radius a. Electrons are free to move along the axis direction. The motion in the plane perpendicular to the axis is quantised and a sequence of electric subbands is formed. The energy spectrum is $\varepsilon = \varepsilon_\nu + \hbar^2 k_z^2/2m^*$. It is similar to that of electrons confined to a quasi-2D layer with quantised motion perpendicular to the plane. Whereas the bottom of the νth subband is determined by both the radial and the angular quantum numbers $\varepsilon_\nu = \varepsilon(m, n)$, which would display remarkable features different from those for a quasi-2D system. Since the dielectric properties of the electron gas are strongly dependent on the subband energies and wavefunctions of electronic state, in this section, we solve the eigenvalue problem in a QWW with a finite potential depth.

In cylindrical coordinates, the potential of a QWW takes the simple form

$$V(r) = \begin{cases} 0 & r < a \\ V_0 & r > a. \end{cases} \tag{1}$$

For this potential the Schrödinger equation is easily solved, giving the radial part of the wavefunction both interior and exterior to the QWW

$$\xi(r) = \frac{1}{\Omega} \begin{cases} J_m(kr) & r < a \\ AK_m(\kappa r) & r > a. \end{cases} \tag{2}$$

Where J_m is the Bessel function of mth order, $m = 0, \pm 1, \pm 2, \ldots$, K_m is the modified Bessel function and Ω is a normalisation factor. The eigenvalues are

$$\varepsilon_\nu = \hbar^2 k_{mn}^2/2m^*. \tag{3}$$

The constant A, k_{mn} and κ_{mn} are determined by the boundary conditions at $r = a$, and the equation

$$k_{mn} + \kappa_{mn} = 2m^* V_0/\hbar^2. \tag{4}$$

For the lowest two eigenstates ($m = 0$ and $m = 1$), the boundary conditions give the following relations

$$(ka)J_1(ka)/J_0(ka) = (\kappa a)K_1(\kappa a)/K_0(\kappa a) \tag{5a}$$

$$(ka)J_0(ka)/J_1(ka) = -(\kappa a)K_0(\kappa a)/K_1(\kappa a). \tag{5b}$$

Equations (4)) and (5*a*) give the ground state eigenvalue and equations (4) and (5*b*) give the first excited state eigenvalue. For a finite potential V_0, the eigenvalues can be solved numerically. In figure 1, we calculate the eigenvalue ka as a function of the potential depth V_0 with a fixed QWW radius a. It can be seen that as V_0 increases, both the eigenvalue of the ground state ($m = 0$) and the first excited state ($m = 1$) increase and

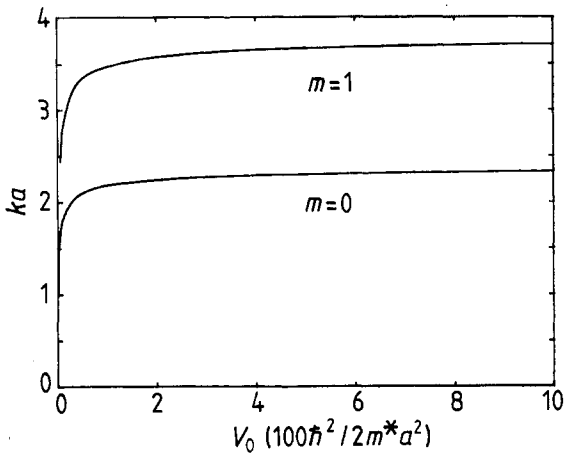

Figure 1. Eigenvalue of ka for the ground state ($m = 0$) and the first excited state ($m = 1$) in a quantum well wire as a function of the potential depth V_0 (in units of $100\hbar^2/2m^*a^2$). ka decreases to zero as the potential goes to zero for the $m = 0$ mode, while for the $m = 1$ mode ka decreases to a finite value as V_0 is close to a critical value. When V_0 is smaller than this critical value the first excited state does not exist.

go to the first zero-points of the Bessel function J_0 and J_1, respectively. Numerical calculations also show that the first excited state becomes weakly-bounded when the potential V_0 is very small (or equivalently, for a fixed V_0, the radius a is very small) which gives a critical radius r_c. Below this radius, the first excited state does not exist, there is only the ground state bounded in the QWW, and the system would behave in a 1D fashion. The critical radius will be discussed later.

There is no known way to solve equations (4) and (5) analytically, but for two limiting cases the results can be obtained more explicitly.

(i) $V_0 \gg \hbar^2 k_{mn}^2/2m^*$. In this case the condition $J_m(ka) = 0$ applies approximately and the zeros of J_m give the energy eigenvalues

$$\varepsilon_{mn} = \frac{\hbar^2 x_{mn}^2}{2m^* a^2}. \tag{6}$$

Where x_{mn} is the nth zero of the mth order Bessel function. The corresponding eigenfunctions are

$$\xi(r) = \begin{cases} J_m(x_{mn}(r/a)) & r < a \\ 0 & r > a. \end{cases} \tag{7}$$

(ii) QWW with a very small radius. In this case the subband energies are pushed up towards the top of the potential well, and the infinite potential approximation is no longer valid. For small radius wires, the value of k_{mn} can be obtained by expanding J_m and K_m about the origin. The small argument expansions for the first two J_m and K_m are given by

$$J_0(x) = 1 - (x/2)^2 \qquad J_1(x) = x/2 \tag{8a}$$

$$K_0(x) = -\ln\frac{x}{2} \qquad K_1(x) = \frac{1}{x}. \tag{8b}$$

We use these to investigate the ground as well as the first excited electronic states.

Applying the boundary conditions at $r = a$ for $m = 0$ mode, we get

$$ka = \left[\frac{2}{\frac{1}{2} - \ln(\kappa a/2)}\right]^{1/2}. \tag{9}$$

From equations (4) and (9), we can see that there is always a bound state for any values of V_0 and quantum wire radius a.

For the first excited state, we find that, as the potential V_0 or equivalently the radius a becomes smaller, the eigenstate becomes weakly-bounded ($\varepsilon_1 \rightarrow V_0$) and finally vanishes as the potential is close to zero. As estimated from the small argument expansion, the critical condition is given by

$$V_0 a^2 > 2\hbar^2/m^*. \tag{10}$$

For a fixed value of V_0, we obtain a critical radius r_c, $r_c = (2\hbar^2/m^* V_0)^{1/2}$, below r_c the first excited state no longer exists. The critical radius is demonstrated numerically in the calculations of the eigenvalue for $m = 1$ in figure 1. Calculations are carried out for a fixed value of radius a. For potential V_0 (in units of $\hbar^2/2m^*a^2$) smaller than 6 the $m = 1$ state is very close to V_0, and the $m = 1$ state vanishes as V_0 becomes smaller than 5, which is consistent with the theoretical estimate discussed above, i.e. that the first excited state does not exist when the potential V_0 is smaller than 4.

3. Dynamic response theory

Let us establish the dynamic response theory of an electron gas in a QWW in the absence of an external magnetic field. The effective-mass Hamiltonian describing an electron in the presence of the effective potential $V(r)$ can be written as

$$H = -(\hbar^2/2m^*)[\partial^2/\partial z^2 + \partial^2/\partial r^2 + (1/r\,\partial/\partial r) + (1/r^2\,\partial^2/\partial\varphi^2) + V(r)]. \tag{11}$$

Here (r, φ, z) are cylindrical coordinates. The electron wave functions are given by

$$|\nu\rangle = |m, n, k\rangle = \exp(ik_z z + im\varphi)\xi_{mn}(r) \tag{12}$$

where ξ_{mn} is the eigenfunction for motion in the effective potential $V(r)$ of the QWW.

An external perturbation of the form

$$\varphi^{\text{ext}}(r, \varphi, z; t) = \varphi^{\text{ext}}(q, \Delta m, \omega; r)\exp(i\omega t - iqz - i\Delta m\varphi) \tag{13}$$

will induce a perturbed electron density, which in turn induces perturbed Hartree and exchange-correlation potentials. The total perturbation

$$\varphi = \varphi^{\text{ext}} + \varphi^{\text{H}} + \varphi^{\text{xc}} \tag{14}$$

is also of the form of (13). Following the Ehrenrich–Cohen self-consistent-field prescription (Ehrenreich and Cohen 1959), the linear-response approximation leads to the induced electron density

$$\delta n = \sum_{\nu\nu'} \frac{f_0(\varepsilon_{\nu'}) - f_0(\varepsilon_\nu)}{\varepsilon_{\nu'} - \varepsilon_\nu - \hbar\omega} \langle\nu|H_1|\nu'\rangle\langle\nu'|\delta(x' - x)\,|\nu\rangle \tag{15}$$

where $H_1 = -e\varphi$. In the limit that only the lowest subband is occupied (electron quantum limit) the Fermi–Dirac distribution function at zero temperature will be

$$f_0(\varepsilon_\nu) = \delta_{m0}\delta_{n1}. \tag{16}$$

If we only consider the angular subband transitions, after some algebraic deduction equation (15) becomes

$$\delta n(q, \Delta m, \omega, r) = \Pi_{\Delta m}(q, \omega)\,\langle 0|H_1|\Delta m\rangle\,\xi_0(r)\xi_{\Delta m}(r) \tag{17}$$

with $\Pi_{\Delta m}$ the irreducible polarisation insertion given by

$$\text{Re}\,\Pi_{\Delta m}(q, \omega) = (m^*/\pi\hbar^2 q)\ln|(\omega^2 - \omega_-^2)/(\omega^2 - \omega_+^2)| \tag{18a}$$

and

$$\omega_{\pm} = \frac{\hbar q}{m^*} |q_f \pm [(q/2) + (m^*/\hbar^2 q)\varepsilon_{\Delta m}]|. \tag{18b}$$

The imaginary part of $\Pi_{\Delta m}$ is not zero only for ω with $\omega_- < \omega < \omega_+$,

$$\text{Im}\, \Pi_{\Delta m}(\mathrm{q}, \omega) = -(\mathrm{e}^2 \mathrm{m}^*/\pi\hbar^2 \mathrm{q}^3) \tag{19}$$

where q_f is the Fermi wavevector, and $\langle \Delta m | H_1 | 0 \rangle$ is defined as

$$\langle \Delta m | H_1 | 0 \rangle = \int \xi_0(r) \xi_{\Delta m}(r)(-e\varphi)\, \mathrm{d}r. \tag{20}$$

The perturbed Hartree potential can be obtained from the Poisson's equation

$$\varphi^{\mathrm{H}} = -\frac{e}{\varepsilon_s} \int G_{\Delta m}(r, r')\, \delta n(q, \delta m, \omega, r')\, \mathrm{d}r' \tag{21}$$

and the Green's function

$$G_{\Delta m}(r, r') = 4\pi K_{\Delta m}(qr_>) I_{\Delta m}(qr'_<). \tag{22}$$

The matrix elements for Hartree potential between the initial state and the final state are

$$\langle \Delta m | (-e\varphi^H) | 0 \rangle = \frac{e^2}{\varepsilon_s} \int\int G_{\Delta m}(r, r') \delta n(q, \Delta m, \omega, r') \xi_0(r) \xi_{\Delta m}(r)\, \mathrm{d}r\, \mathrm{d}r' \tag{23}$$

and all other elements are zero. With the introduction of the parameters M_m and $\eta_{\Delta m}$,

$$\eta_{\Delta m}(q, \omega) = (e^2/\varepsilon_s)\Pi_{\Delta m}(q, \omega) M_{\Delta m}(q). \tag{24a}$$

$$M_{\Delta m}(q) = \int\int K_{\Delta m}(qr_>) I_{\Delta m}(qr'_<) \xi_0(r) \xi_{\Delta m}(r) \xi_0(r') \xi_{\Delta m}(r')\, \mathrm{d}r\, \mathrm{d}r' \tag{24b}$$

equation (23) can be expressed as

$$\langle \Delta m | (-e\varphi^{\mathrm{H}}) | 0 \rangle = \eta_{\Delta m}(q, \omega) \langle \Delta m | (-e\varphi) | 0 \rangle. \tag{25}$$

The dielectric response function is defined as

$$\varepsilon = \langle \varphi^{\mathrm{ext}} \rangle / \langle \varphi \rangle. \tag{26}$$

From the expressions above

$$\varepsilon_{\Delta m}(q, \omega) = 1 - \eta_{\Delta m}(q, \omega). \tag{27}$$

If the QWW has an infinite potential depth, the eigen energies and the wavefunctions of the electronic state needed for the calculations are given by

$$\varepsilon_0 = \hbar^2 x_{01}^2 / 2m^* a^2 \qquad \varepsilon_1 = \hbar^2 x_{11}^2 / 2m^* a^2 \tag{28}$$

$$\xi_0 = J_0(x_{10}(r/a)) \qquad \xi_1 = J_1(x_{11}(r/a)). \tag{29}$$

4. Results and discussion

In the case of intra-subband transition, $\Delta m = 0$ and $\varepsilon_{\Delta m} = 0$. The result of (18) is simply the Kramers–Heisenberg electronic polarisability for the 1D electron gases within the

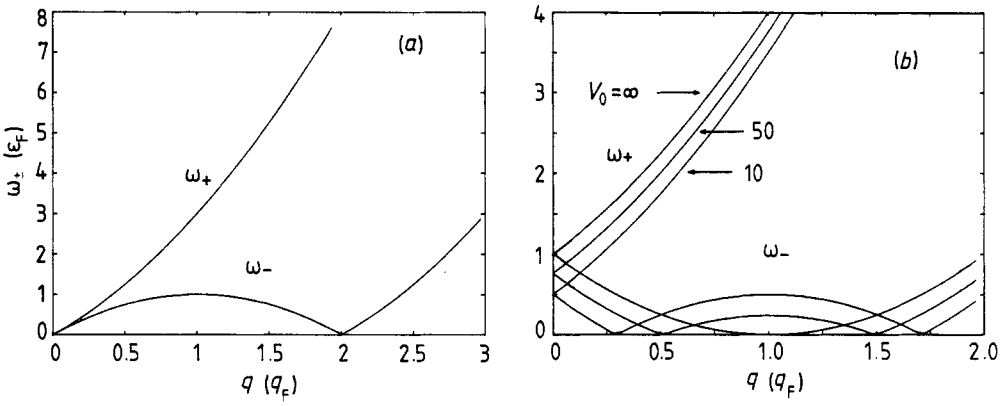

Figure 2. The poles of the inverse of the dielectric function, $\omega_\pm$ (in units of the Fermi energy), as a function of wavevector q (in units of the Fermi wavevector) for a quantum well wire with only the first subband occupied. (*a*) Intra-subband mode, $\varepsilon_{\Delta m} = 0$. In the long wavelength limit, $\omega_\pm \to 0$ as $q \to 0$. (*b*) Inter-subband modes with three different values of the potential depth $V_0 = 10$, 50, and ∞. As V_0 decreases the curve becomes lower in energy with a shape similar to that of the intra-subband mode. The potential V_0 is in units of $\hbar^2/2m^*a^2$.

self-consistent-field method (Friesen and Bergersen 1980). The inter-subband transition can be studied when $\Delta m \neq 0$. The Fermi wavevector in this system is given by

$$N_s = (1/\pi a)[q_F a + 2(q_F^2 a^2 - x_{1,1}^2)^{1/2} + \cdots + 2(q_F^2 a^2 - x_{n,m}^2)^{1/2}] \qquad (30)$$

with $x_{n,m} < q_F a$. The coefficient 2 is due to the degeneracy of the angular momentum if $m \neq 0$. Equation (30) can be solved self-consistently for a given number density of electrons per unit length N_s. The condition that there is only the lowest subband occupied is usually of special interests for discussion. The crossover of dimensionality occurs when more than one-subband is occupied. This corresponds to a larger number density of electrons, or equivalently, a larger radius of the wire.

The inverse of the dielectric function $1/\varepsilon_{\Delta m}(q, \omega)$ has poles at $\omega_\pm$ given by (18*b*). In the long wavelength limit, for intra-subband modes $\varepsilon_{\Delta m} = 0$, so $\omega_\pm \to 0$ as $q \to 0$, while $\hbar\omega_\pm = \varepsilon_{\Delta m}$ for inter-subband modes as $q = 0$. This result is similar to that in an array of Q1D quantum wire structures with the interaction between the wires being taken into consideration as discussed by Williams and Bloch (1974). The poles of the inverse of the dielectric function, $\omega_\pm$, are plotted for both intra-subband and inter-subband modes in figure 2(*a*) and 2(*b*), respectively. The numerical calculations are carried out for a QWW structure with only the first subband occupied, and $N_s = 10^6$ cm^{-1}. For the inter-subband mode, it is worth noting some interesting characteristics as shown in figure 2(*b*). As the potential V_0 decreases, the subband energy difference between $m = 0$ and $m = 1$ becomes smaller, and the $\omega_\pm$ curves (in units of $100\hbar^2/2m^*a^2$) as a function of q become lower in energy. In the limiting case where the first excited state is weakly-bounded, the curve is similar to that of the intra-subband mode.

The exchange-correlation potential φ^{xc} is taken to be a local function of the density by following the treatment of Kohn and Sham (Kohn and Sham 1965, Sham and Kohn 1966), i.e., φ^{xc} is given by taking a functional derivative of the exchange-correlation part of the ground-state energy with respect to the number density of electrons. The functional form of the ground-state energy is replaced by a product of the density and

the exchange-correlation energy per electron of a uniform electron gas with density δn. In this approximation, φ^{xc} becomes the exchange-correlation part of the chemical potential of the uniform electron gas. We only consider the effect of this part qualitatively in this paper.

Most of the important properties of electron gases, which responds to an external electric field, will be reflected by the dynamical dielectric function. Excitations of the electron gas are determined by the longitudinal dielectric function. The light absorption due to the electron excitations is relevant to the real part of the conductivity which is described by the Kubo formula, and proportional to the imaginary part of the inverse longitudinal dielectric function. The condition for the collective excitation (plasmon) of the system is that the self-sustaining oscillations in the electron density occur. As is well known, the dispersion relation of the collective modes is given by $\varepsilon_{\Delta m}(q, \omega) = 0$, from equation (27)

$$\eta_{\Delta m}(q, \omega) = 1. \tag{31}$$

The plasmon modes are free from damping since Im $\varepsilon = 0$ in this frequency region. For a long wavelength limit, the intra-subband transition gives the phonon-like plasmon excitation with $\omega_p \rightarrow 0$ as $q = 0$. And the inter-subband transition gives the photon-like modes with $\omega_p \neq 0$ as $q = 0$.

When the propagating modes in a QWW waveguide are investigated, for example, as an application to the laser device with a QWW structure, it is necessary to know the dielectric properties of the electron gas in this system, since the response of the electron gas to an external electric field will affect the propagating mode. The frequency of the guided wave must be chosen so as to be out of the non-zero region of the imaginary part of the dielectric function to avoid the absorption by the electron gases.

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