Brief Reports

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Plasmon dispersion relation of a quasi-one-dimensional electron gas

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The plasmon dispersion relation of a quantum wire is derived by solving Maxwell's equations for an anisotropic dielectric waveguide including retardation effects. In the long-wavelength limit, and for the extreme quantum limit, the group velocity of the one-dimensional electron gas is found to be finite and given by the Fermi velocity.

There has been increasing interest in one-dimensional electron systems (1DES's) since quantum-wire structures have been fabricated with GaAs surrounded by $Al_xGa_{1-x}As$ by Petroff *et al.*[1] From a fundamental viewpoint, 1DES's are important since they constitute one of the simplest many-body systems of interacting fermions with properties basically different from three-dimensional particle systems. For this reason, a number of theoretical papers have attempted to describe the dielectric response and the collective excitations of 1DES's (Refs. 2–4) in relation to the electronic properties of quasi-1D metal or linear chains of organic conductors.[5] The emergence of low-dimensional artificial semiconductor structures has stimulated further work in this direction. In a recent experiment Demel and co-workers[6,7] have investigated the far-infrared (FIR) response of a multiple 1D semiconductor structure at low-temperature measurements and interpreted the FIR resonances as caused by the lateral quantization of the 2D plasmon modes. Meanwhile, a theoretical model of screening effects and elementary excitations in artificial 1DES's has been provided by Das Sarma and Lai,[8] who calculated the dielectric functions $\epsilon(q,\omega)$ for single quantum wires and 1D superlattices within the Bohm-Pines random-phase approximation (RPA). These authors obtained the plasmon dispersion relation by solving the standard equation $\epsilon(q,\omega)=0$. As a consequence of this model, however, the plasmon group velocity diverges logarithmically with the wave vector $q\rightarrow 0$[9] as well as with the radius of the quantum wire $r_0\rightarrow 0$. In this Brief Report, we derive the plasmon dispersion relation by considering the collective excitation as an induced electromagnetic wave which obeys Maxwell's equations and satisfies continuity conditions at the boundary between the confined structure and the surrounding materials.[10]

Generally, 1DES's are laterally and electrostatically confined at the interface of a modulation-doped structure. For the sake of simplicity, the physical system investigated here is a GaAs quantum wire of cylinder geometry embedded inside an $Al_xGa_{1-x}As$ material for which the 1DES eigenstates are given by a simple 2D harmonic oscillator:[11]

$$H_0=-\frac{\hbar^2\nabla^2}{2m^*}+\tfrac{1}{2}m^*(x^2+y^2)\Omega^2 . \tag{1}$$

Here m^* is the effective mass, Ω is the oscillator characteristic frequency, and ∇^2 is the three-dimensional Laplace operator. The eigenfunctions are given by

$$\phi_{nmk_z}(\mathbf{r})=\frac{1}{\sqrt{L}}\psi_n(x)\psi_m(y)e^{-ik_z z} . \tag{2}$$

In the self-consistent-field approximation,[2] the self-consistent-field dielectric function ϵ_{SCF} for GaAs is given by

$$\frac{\epsilon_{SCF}}{\epsilon}=1-\frac{\langle\nu'|V_s|\nu\rangle}{\langle\nu'|V|\nu\rangle} , \tag{3}$$

where ν is a collective label for the (n,m,k_z) indices, ϵ is the GaAs dielectric constant, and V_s is the self-consistent potential. Starting from the single-particle Liouville equation, we get the potential induced by a test charge,

$$V_s=\int d\mathbf{r}'\frac{K_0(q|\mathbf{r}-\mathbf{r}'|)}{2\pi}\frac{e^2}{\epsilon_0\epsilon L}\times\sum_{\nu,\nu'}\langle\nu'|\rho_1|\nu\rangle\phi_\nu^*(\mathbf{r}')\phi_{\nu'}(\mathbf{r}') , \tag{4}$$

where $K_0(x)$ is the zeroth-order modified Bessel function of the second kind with argument x; q is the z component of the wave vector for the Fourier component of the potential, ρ_1 is the operator describing the perturbation of the density matrix, and ϵ_0 is the dielectric constant in the vacuum.

At 0 K, if we assume the extreme quantum limit (EQL), i.e., all the electrons occupy the ground state, the 1D dielectric function is given by

$$\frac{\epsilon_{\rm SCF}}{\epsilon}=1-\frac{e^2}{2\pi\epsilon_0\epsilon}\langle K_0\rangle F(q,\omega)\ , \tag{5}$$

where

$$F(q,\omega)=\sum_{k,s}\frac{f_0(E_{k+q})-f_0(E_k)}{E_{k+q}-E_k-\hbar\omega}=\frac{m^*}{\pi\hbar^2 q}\ln\left|\frac{\left(k_F-\frac{q}{2}\right)^2-\left(\frac{m^*\omega}{\hbar q}\right)^2}{\left(k_F+\frac{q}{2}\right)^2-\left(\frac{m^*\omega}{\hbar q}\right)^2}\right| \tag{6}$$

with the Fermi wave vector k_F. The form factor

$$\langle K_0\rangle=\tfrac{1}{2}\int_0^\infty dt\frac{e^{-q^2 t}}{t+1/2\eta}\ , \tag{7}$$

with $\eta=m^*\Omega/\hbar$, is obtained after some tedious algebraic and integral manipulations.[11] At 0 K, these results are justified if $\hbar^2k_F^2/2m^*<\hbar\Omega$. For high temperatures and a large radius of the quantum wire, higher energy levels need to be considered.[12] But this condition, which also involves broadening effects, is beyond the scope of this Brief Report.

In order to derive the dispersion relation of a plasmon wave, we consider the GaAs quantum wire as a cylindrical dielectric waveguide embedded inside $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ material with a dielectric constant ϵ'. For a wave traveling along the z direction, the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ must satisfy the Maxwell equations[13]

$$\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}\ , \tag{8a}$$

$$\nabla\times\mathbf{H}=\frac{\partial\mathbf{D}}{\partial t}+\mathbf{J}\ , \tag{8b}$$

with $\mathbf{B}=\mu_0\mathbf{H}$ and $\mathbf{D}=\epsilon_0\epsilon\mathbf{E}$ for GaAs ($D=\epsilon_0\epsilon'\mathbf{E}$ for $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$). Here we assume that an induced current flows along the z direction with unit vector $\hat{\mathbf{z}}$; the current density is given by $\mathbf{J}=\epsilon_0\chi(\partial E_z/\partial t)\hat{\mathbf{z}}$ inside the waveguide, where χ is the polarization coefficient. Therefore, for GaAs the dielectric function $\overleftrightarrow{\epsilon}$ becomes a tensor,

$$\overleftrightarrow{\epsilon}=\begin{bmatrix}\epsilon & 0 & 0\\ 0 & \epsilon & 0\\ 0 & 0 & \epsilon_z\end{bmatrix}\ , \tag{9}$$

where

$$\epsilon_z=\epsilon+\chi\ ,$$

and we can redefine $\mathbf{D}'=\overleftrightarrow{\epsilon}\cdot\mathbf{E}$.

In the region outside the waveguide, the current density $\mathbf{J}$ is identically zero. Hence we can solve Eq. (8) separately in the inside and outside regions.

Inside the core, we assume the following form for the $\mathbf{E}$ field:

$$\mathbf{E}=\begin{bmatrix}E_{r0}J_1(\alpha r)\\ E_{\phi 0}J_1(\alpha r)\\ E_{z0}J_0(\alpha r)\end{bmatrix}e^{i\omega t-iqz}\ , \tag{10}$$

where J_n is the Bessel function of the first kind, q and α are the z and radial components of the wave vector for the $\mathbf{E}$ field, respectively, and E_{r0}, $E_{\phi 0}$, and E_{z0} are the magnitudes of the radial, angular ϕ, and z components of the field. From the Maxwell equations, we obtain the displacement current

$$\mathbf{D}'=\frac{1}{\omega^2\mu_0}\nabla\times(\nabla\times\mathbf{E})\ , \tag{11}$$

and from the constitutive relation $\mathbf{D}'=\overleftrightarrow{\epsilon}\cdot\mathbf{E}$, we derive the matrix equation

$$\begin{bmatrix}\omega^2\mu_0\epsilon_0\epsilon-q^2 & 0 & -iq\alpha\\ 0 & \omega^2\mu_0\epsilon_0\epsilon-(q^2+\alpha^2) & 0\\ iq\alpha & 0 & \omega^2\mu_0\epsilon_0\epsilon_z-\alpha^2\end{bmatrix}\begin{bmatrix}E_{r0}\\ E_{\phi 0}\\ E_{z0}\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}\ . \tag{12}$$

In order to obtain nontrivial solutions, the determinant of the matrix on the left-hand side must vanish, which yields the dispersion relations for longitudinal waves,

$$\omega^2=\frac{\alpha^2\epsilon+q^2\epsilon_z}{\mu_0\epsilon_0\epsilon\epsilon_z}\ , \tag{13}$$

and that for transverse waves, $\omega^2=(\alpha^2+q^2)/\mu_0\epsilon_0\epsilon$. For plasmon oscillations, only the longitudinal waves are relevant. The solutions of the electromagnetic fields are found to be

$$\mathbf{E}=E_0\begin{bmatrix}J_1(\alpha r)\\ 0\\ -i\frac{\epsilon\alpha}{\epsilon_z q}J_0(\alpha r)\end{bmatrix}e^{i\omega t-iqz}\ , \tag{14}$$

$$\mathbf{H}=E_0\begin{bmatrix}0\\ \frac{\epsilon\epsilon_0\omega}{q}J_1(\alpha r)\\ 0\end{bmatrix}e^{i\omega t-iqz}\ , \tag{15}$$

where E_0 is a constant.

Outside the 1DES, the wave is evanescent and must decay with the distance r away from the wire. We thus can choose the modified Bessel functions of the second kind, $K_0(\beta r)$ and $K_1(\beta r)$, where β is the radial decay constant. The solution is found to be

$$\mathbf{E}=E_0'\begin{bmatrix} K_1(\beta r) \\ 0 \\ i\frac{\beta}{q}K_0(\beta r)\end{bmatrix} e^{i\omega t-iqz} , \tag{16}$$

$$\mathbf{H}=E_0'\begin{bmatrix} 0 \\ \frac{\epsilon'\epsilon_0\omega}{q}K_1(\beta r) \\ 0\end{bmatrix} e^{i\omega t-iqz} , \tag{17}$$

with $\omega^2=(q^2-\beta^2)/\mu_0\epsilon_0\epsilon'$, and E_0' is a constant.

At the wire boundary $r=r_0$, the normal component of $\mathbf{D}$, the tangential component of $\mathbf{E}$ and $\mathbf{H}$ must be continuous. For nontrivial solutions of E_0 and E_0', we obtain the dispersion relation

$$\frac{\alpha J_0(\alpha r_0)}{\epsilon_z J_1(\alpha r_0)}+\frac{\beta K_0(\beta r_0)}{\epsilon' K_1(\beta r_0)}=0 . \tag{18}$$

When the current density $J=0$, this dispersion relation results in the solution of the classical dielectric waveguide.[13] Notice that Eqs. (13) and (17) describe retardation effects which are consequently included in Eq. (18).

The longitudinal plasmon modes are obtained by solving Eqs. (5) and (18) with $\epsilon_{\text{SCF}}=\epsilon_z$. Figure 1 shows a comparison between the dispersion relation derived from the relation $\epsilon_{\text{SCF}}=0$ and our results for two different confinement conditions. For our model, we have chosen $m^*=0.067m_e$, $\epsilon=13.2$ for the inside material, and $\epsilon'=12.51$ for the surrounding material. The results are, however, not very sensitive to the difference between ϵ and ϵ', so that the waveguide approximation seems to be justified. From Fig. 1 we can see as $q\to 0$ the two curves are somewhat different, but start to converge as $q\to\infty$. This is due to the constraints imposed by the Maxwell equations and the dispersion relation (18). At small radius r_0 and long wavelength, the modified Bessel functions of the second kind, K_0 and K_1, and the Bessel functions J_0 and J_1 are all positive. Therefore in order to obtain a solution from Eq. (18), the dielectric function ϵ_z must be negative. The longer the wavelength, the larger the absolute value of ϵ_z and, consequently, the larger the deviation from the $\epsilon_{\text{SCF}}=0$ solution. For large q, the ratio between the modified Bessel functions approaches unity while the ratio between J_0 and J_1 is of the same order. So the two curves begin to converge and Eq. (18) reduces to the standard self-consistent-field result $\epsilon_{\text{SCF}}=0$. In fact, as we can see from Fig. 1(b), the two curves are almost identical as the radius of the wire increases. Numerically, we always find the solutions of Eq. (18) in pairs, but we have eliminated the solution corresponding to single-particle excitation (i.e., the production of an electron-hole pair),[14] which is irrelevant and unphysical in this case. Another feature of our model is the existence of multiple solutions to Eq. (18) because of the multivalued Bessel functions J_0 and J_1. This result is inherent to the cylindrical geometry assumed in our model. The higher-order solutions correspond, however, to unusually large carrier concentrations and are irrelevant for the EQL condition considered here.

The slope of the plasmon dispersion curve gives the wave group velocity, which is an important characterization of the quantum wire. As we indicated earlier, the $\epsilon_{\text{SCF}}=0$ derivation provides a group velocity v_g which diverges logarithmically as $q\to 0$.[8] In our case, however,

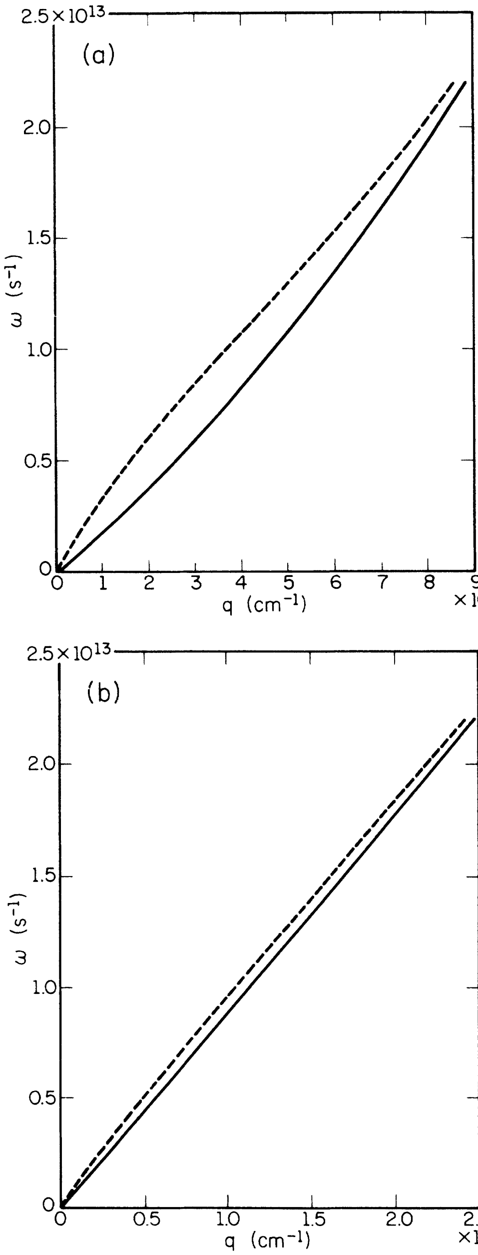

FIG. 1. Calculated plasmon dispersion relation of a quantum wire. The solid line describes our numerical result, while the dashed line results from $\epsilon_{\text{SCF}}=0$. (a) The radius r_0 is 70.7 Å and the Fermi wave vector k_F is 1.0×10^6 cm^{-1}. (b) r_0 is 353 Å and k_F is 5.0×10^6 cm^{-1}.

the dispersion relation [Eq. (18)] is satisfied for the negative pole of χ in the long-wavelength limit; therefore we find $v_g = \hbar(k_F+q)/m^*$ as $q \rightarrow 0$, i.e., the Fermi velocity.[15] Strictly speaking, this result is only valid at $T=0$ K; any broadening effect in the polarization will result in an r_0-dependent cutoff frequency for plasmon modes.

In summary, we derived the plasmon dispersion relation of one-dimensional electron gas embedded in a host material assuming the collective oscillations are confined in a cylindrical dielectric waveguide. This approximation does not seem to limit the validity of the model to more realistic configurations since the III-V compound semiconductors of interest the results are not very sensitive to the difference between the dielectric constants of the guiding region and the surrounding material. At $T=0$ K and in the long-wavelength limit, our waveguide model provides a finite group velocity, given by the Fermi velocity.

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