Plasmons in a spatially modulated quasi-one-dimensional quantum wire

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We consider a quasi-one-dimensional superlattice consisting of a quantum wire, the equilibrium carrier density of which is spatially modulated along its length. We apply a simple hydrodynamic model for the collective excitations of low-dimensional inhomogeneous systems to calculate the plasmon dispersion relation of the periodic heterostructure. As expected, the acoustic plasmon of the homogeneous quantum wire is folded into the first Brillouin zone due to the modulation and acquires optical branches. Gaps open at the zone boundary due to Bragg scattering, but unlike the two-dimensional and three-dimensional cases, no gap opens at the zone center for the modulated wire.

I. INTRODUCTION

Advances in the fabrication of mesoscopic semiconductor systems have produced devices where confinement plays a major role and whose physical properties, such as carrier densities, band gaps and widths, and even dimensionality, may be controlled. There are expectations of possibly producing very high speed transistors, photodetectors and lasers. On the other hand, theory predicts curious effects in one dimension, such as Peierls instability, Anderson localization, spin density excitations, etc. In quasi-one-dimensional (Q1D) quantum wires electrons move freely in one direction but their motion is confined, and therefore quantized, in the two other independent directions, originating electronic subbands. If only the lowest lying subband is occupied, a finite energy is required to excite the transverse degrees of freedom and a truly Q1D electron gas ensues. These systems have already been fabricated, for instance, by laterally modulating a quasi-two-dimensional electron gas. For experimental and theoretical reviews, see Refs. 1 and 2.

Another class of tunable systems which have attracted considerable attention are superlattices. In these, an artificial periodicity is imposed, reducing the Brillouin zones and resulting in the folding of the dispersion relations of all the elementary excitations, thus yielding tunable minigaps. Large wave-vector regions within the original Brillouin zone, which are inaccessible to some optical spectroscopies in homogeneous systems, may become accessible when folded into the reduced zone of a superlattice. By modulating the potential and, therefore, the carrier density of a low-dimensional electron gas, a Q2D or a Q1D superlattice[3] could be produced. Strongly modulated Q2D systems can be viewed as arrays of multiple quantum wires, weakly coupled among themselves through Coulomb and tunneling effects. They are the most frequently studied low-dimensional superlattices. In contrast, here we focus our attention on a quantum wire, the equilibrium density of which is periodically modulated along its length. Such Q1D superlattices could be fabricated by superposing two perpendicular electrode grids above a Q2D electron gas: a strong potential would be applied to the first to create the quantum wires and a weaker one to the second to modulate their density.

Among the various modes that form the elementary excitation spectra of periodically modulated Q1D wires, we are interested in the theoretical study of its plasmons. These collective charge excitations have attracted attention lately. For example, it has recently been proposed[4] that modulated Q1D systems might support current-driven plasma instabilities at much lower threshold drift velocities than in 3D systems. The plasmon dispersion relation for the unmodulated case is closely linked[5,6] to the dimensionality and depends on the width, but is rather insensitive to the geometry. It has been shown that, unlike the intersubband plasmon and the electronic eigenenergies, the intrasubband plasmon frequency is only marginally dependent on the wire shape. The plasmon dispersion relation of an unmodulated wire has been calculated within the random phase approximation (RPA) and within a hydrodynamic model. The latter is simpler and has proved to agree with more sophisticated treatments in the long-wavelength regime. In this paper, we employ a recent extension of the hydrodynamic model to inhomogeneous electron fluids[7] and apply it to the Q1D modulated case. A similar extension has been succesfully applied to calculate the linear and nonlinear optical response of metal surfaces having a smoothly varying electronic density profile.[8]

In the next section we present a hydrodynamic approach to the collective dynamics of our system, in

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Sec. III we present our results for the plasmon dispersion relation, and we present our conclusions in Sec. IV.

II. THEORY

Let us consider an inhomogeneous single quantum wire running along the Z direction. Assuming that the Q1D inhomogeneous electron gas has only one occupied electronic subband and that at temperature $T = 0$ can be treated as a strictly one-dimensional nonviscous fluid, its dynamics would be described by the 1D Navier Stokes equation,

$$\left(mn\frac{\partial}{\partial t}u\right) = -enE - \frac{\partial}{\partial z}P, \tag{1}$$

where e and n are the electronic charge and number density, m is the electron's effective mass, u is the average velocity field of the electronic fluid, E is the total macroscopic electric field (including the external field $E_{\rm ex}$ and the average of the Coulomb interparticle interaction), $P = n^2\partial(U/N)/\partial n$ is the hydrostatic pressure, assuming we have local equilibrium, and U/N the average internal energy per electron. We assume U/N is a local functional of the density and for simplicity, we neglect exchange and correlation contributions. Therefore, the Coulomb interaction is taken into account through the interaction with the self-consistent field E and U is given by the energy of a noninteracting fermion gas in one dimension,

$$U/N = \frac{1}{6}\gamma n^2, \tag{2}$$

where $\gamma = (\pi/2)^2\hbar^2/m$ is independent of the density profile n. Here, we have assumed implicitly that the spatial variations of the fields (density, electric potential, etc.) are small compared with the Fermi wavelength $2\pi/k_f$ and also that the frequencies ω of their temporal variations are below the interband thresholds.

Substituting Eq. (2) in (1), we obtain

$$en^{(0)}E^{(0)} = -\gamma(n^{(0)})^2\frac{\partial}{\partial z}n^{(0)}\ , \tag{3}$$

where $E^{(0)}$ is an effective static electric field required to maintain the equilibrium density profile $n^{(0)}(z)$. In the presence of an additional time-varying field $E(z,t)$, the density fluctuation $n^{(1)}(z,t) = n(z,t) - n^{(0)}(z)$ obeys to first order,

$$mn^{(0)}\partial_t u = -en^{(0)}E - en^{(1)}E^{(0)} - \gamma(n^{(0)})^2\frac{\partial}{\partial z}n^{(1)} - 2n^{(0)}n^{(1)}\frac{\partial}{\partial z}n^{(0)}\ . \tag{4}$$

Now we eliminate the first-order velocity field $u(z,t)$ through the first-order continuity equation $\partial n^{(0)}u/\partial z + \partial n^{(1)}/\partial t = 0$ and obtain

$$m\omega^2 n^{(1)}(z) = -e\frac{\partial}{\partial z}(n^{(0)}(z)E(z)) - \gamma\frac{\partial}{\partial z}\left((n^{(0)})^2(z)\frac{\partial}{\partial z}n^{(1)}(z)\right) - \frac{1}{2}\gamma\frac{\partial}{\partial z}\left(\delta n(z)\frac{\partial}{\partial z}(n^{(0)})^2(z)\right), \tag{5}$$

for a monochromatic oscillation of frequency ω.

To obtain the collective normal modes of this system, we eliminate the external field and we set the oscillating field $E(z)$ to the self-consistent field generated by the charge fluctuation $-en^{(1)}$. To deal with the singularity of the Coulomb interaction in a zero-width system, we follow Ref. 5, where a finite-width wire described by a profile function $N(x,y)$ is introduced. We assume that the density fluctuation in 3D is given by $n^{(1)}(\vec{r}) = n^{(1)}(z)N(x,y)$, so that the scalar potential $\varphi(\vec{r})$ of the wire is written as

$$\varphi(\vec{r}) = -e\int d^3r\frac{n^{(1)}(z')N(x',y')}{|\vec{r}-\vec{r}'|}. \tag{6}$$

We average this potential over the cross section of the wire to get the effective 1D potential,

$$\Phi(z) = \int dx\int dyN(x,y)\varphi(\vec{r}) = -e\int\frac{dq}{2\pi}n^{(1)}(q)\int dxdy\int dx'dy'N(x,y)N(x',y') \times\int_{-\infty}^{\infty}dz'\frac{e^{iqz'}}{|\vec{r}-\vec{r}'|}, \tag{7}$$

the Fourier transform of which may be written as

$$\Phi(q) = -en^{(1)}(q)v(q), \tag{8}$$

where

$$v(q) = 2\int d\vec{R}\int d\vec{R}'N(\vec{R})K_0(|q||\vec{R}-\vec{R}'|)\,N(\vec{R}'), \tag{9}$$

is an effective Q1D Coulomb potential, $\vec{R} = (x,y,0)$, and K_0 is the modified zeroth order Bessel function. Here, we have defined the Fourier transform according to $\mathcal{F}(z) = \int dq/(2\pi)\mathcal{F}(q)e^{iqz}$.

Now we go back to Eq. (5), we write $E(z)$ in terms of $\Phi(q)$, and we use Eq. (8) to get the homogeneous equation,

$$\int dq'\left[m\omega^2\delta(q-q') - \frac{1}{2\pi}e^2qn^{(0)}(q-q')q'v(q') - \frac{1}{2\pi}\gamma q(n^{(0)})^2(q-q')\frac{1}{2}(q+q')\right]n^{(1)}(q') = 0, \tag{10}$$

the nontrivial solutions of which describe the normal modes of the Q1D superlattice. Here, we denote by $(n^{(0)})^2(q)$ the Fourier transform of the square of the equilibrium density, which must not be confused with the square of the Fourier transform.

For a periodic superlattice, the Fourier transform of the equilibrium density has a discrete nature,

$$n^{(0)}(q) = \sum_K n_K^{(0)}\delta(q-K), \tag{11}$$

$$(n^{(0)})^2(q) = \sum_K (n^{(0)})^2_K\delta(q-K), \tag{12}$$

where K spans the reciprocal lattice. We look for normal modes of the form of Bloch waves,

$$n^{(1)}(z)=\sum_K n_K^{(1)}(k)e^{i(k+K)z}. \tag{13}$$

Therefore,

$$n^{(1)}(q)=2\pi\sum_K n_K^{(1)}(k)\delta(k+K-q), \tag{14}$$

and hence, Eq. (10) is finally written as a matrix equation,

$$\sum_{K'}\Big[m\omega_k^2\delta_{K,K'}-e^2(k+K)n_{K-K'}^{(0)}(k+K')v(k+K') -\frac{\gamma}{2}(k+K)(n^{(0)})^2_{K-K'}(2k+K+K')\Big]\,n_{K'}^{(1)}(k)=0, \tag{15}$$

the nontrivial solution of which defines the dispersion relation $\omega=\omega_k$ of the plasmons of the modulated Q1D wire.

To proceed, we have to specify the actual profiles of our system: $N(x,y)$ and $n^{(0)}(z)$. We assume parabolic confinement, and that along the Y direction it is much stronger than along the X direction. This implies that the excitation of motion along Y requires an energy much higher than that associated with the X confinement. Therefore, the Q1D system looks like a flat strip of a characteristic width, say a. With this choice,

$$N(\vec{R})=\frac{\sqrt{2}}{a}\,e^{-2\pi x^2/a^2}\,\delta(y), \tag{16}$$

yielding

$$v(q)=e^{q^2a^2/8\pi}K_0(q^2a^2/8\pi), \tag{17}$$

For the ground-state electronic density, we choose a simple sinusoidal modulation of period λ,

$$n^{(0)}(z)=n_a+\Delta\cos(gz), \tag{18}$$

with n_a the unmodulated electron density, Δ the modulation amplitude, and $g=\frac{2\pi}{\lambda}$ the first reciprocal lattice wave vector along the direction of the wire. Therefore, the Fourier transforms of $n^{(0)}(z)$ and of $(n^{(0)})^2(z)$ are

$$n^{(0)}(q)=2\pi\left[n_a\delta(q)+\frac{\Delta}{2}\delta(q+g)+\frac{\Delta}{2}\delta(q-g)\right], \tag{19}$$

$$(n^{(0)})^2(q)=2\pi\Big[\Big(n_a^2+\frac{\Delta^2}{2}\Big)\delta(q) +n_a\Delta[\delta(q+g)+\delta(q-g)] +\frac{\Delta^2}{4}[\delta(q+2g)+\delta(q-2g)]\Big]. \tag{20}$$

III. RESULTS

In this section, we calculate the plasmon dispersion relation obtained by diagonalizing the matrix in Eq. (15). We assume that the quantum wire is made of GaAs with effective mass $m=0.068m_e$, that its characteristic width is $a=400$ Å, its average electronic number density is $n_a=4\times10^5$ cm^{-1}, and that the modulation length is $\lambda=2000$ Å. All of these parameters are well within the accessible experimental range.[9,10]

The total number of locally occupied subbands can be calculated from the well known formula $n_0=\sum_{i\vec{k}}f(\epsilon_{i\vec{k}})$, with f the Fermi distribution and $\epsilon_{i\vec{k}}$ the electronic energy corresponding to wave vector $\vec{k}$ within band i. In Q1D at $T=0$, it gives

$$n_0=2\frac{\sqrt{2m}}{\pi\hbar}\sum_i(\epsilon_F-\epsilon_i)^{1/2}, \tag{21}$$

where ϵ_F is the Fermi energy and ϵ_i is the quantized energy associated to the harmonic confinement $\epsilon_i=i\hbar\omega_0$, with $i=1,2,3,\ldots$ up to the highest occupied subband, $\omega_0=\frac{2\pi\hbar}{ma^2}$, and we included a factor of 2 to account for spin. Equation (21) is solved self-consistently for the total number of occupied subbands and total Fermi energy.

With our choice of parameters, we can increase the density modulation of the wire up to $\Delta/n_a\approx0.4$, before we start filling the second subband. The Fermi energy is $\epsilon_F=6.63$ meV, the effective Fermi velocity of the fluid is $v_F=1.07\times10^7$ cm/s, and $\epsilon_1=4.4$ meV. Notice that we can write γ in terms of the Fermi velocity, as $\gamma=mv_F^2/n_0^2$. It has been shown by Mendoza and Schaich[5] that with this choice of γ, the plasmons of a homogeneous quantum wire calculated within the hydrodynamic model are in good agreement with the RPA calculation in both the low and high frequency limit. In this regard, Q1D systems are unique, since a single choice of γ reproduces both frequency limits.

In Fig. 1, we have plotted the dispersion relation $\omega(q)$ for a relatively small modulation $\Delta/n_a=0.1$ and a large modulation $\Delta/n_a=0.4$. We also display the dispersion relation $\omega_u(q)$ for the unmodulated wire, given by

$$\omega_u^2(q)=\frac{e^2n_a}{m^*}q^2v(a|q|)+\beta^2q^2. \tag{22}$$

We notice that $\omega(q)$ follows $\omega_u(q)$, except at the boundary of the Brillouin zone, where a gap develops. The size of the gap increases almost in linear proportion to the modulation Δ. We mention that the phase space where the gap falls is within the experimental range of values that could be experimentally explored with inelastic Raman light scattering.[11]

No gap is apparent in Fig. 1 neither at the center of the Brillouin zone nor at the crossing between the third and fourth bands. However, in Fig. 2, we amplify that crossing for the case $\Delta/n_a=0.4$ and observe that there is indeed a small gap. Its size scales roughly as Δ^3, which is the result we would expect using perturbation theory, i.e., the gap opens due to the modulation induced interaction between the unmodulated plasmon at $q=3g/2$ and the degenerate plasmon at $q=-3g/2$, going through the intermediate states $q=\pm g/2$.

Similarly, we could have expected a gap at the zone center due to the interaction between the unmodulated plasmons at $q=\pm g$ going through that at $q=0$. However, an analysis of Eq. (15) shows that the degeneration

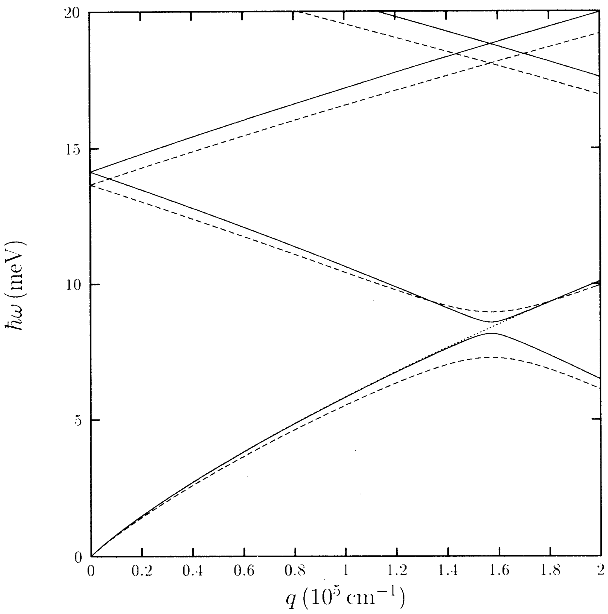

FIG. 1. Dispersion relation ω vs q for the plasmons of a modulated Q1D wire, with modulation amplitude $\Delta/n_a = 0.1$ (continuous), $\Delta/n_a = 0.4$ (dashed), and for the unmodulated wire $\Delta/n_a = 0.0$ (dotted). The other parameters are discussed in the text.

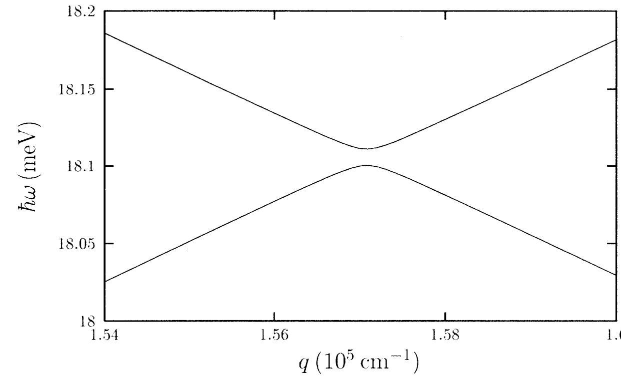

FIG. 2. Detail of the dispersion relation shown in Fig. 1, showing the gap that develops between the third and fourth bands at the zone boundary for the modulation $\Delta/n_a = 0.4$.

at the zone center is exact. The second term of this equation is zero when $k = 0$ and $K = 0$, due to the presence of the factor $k + K$. Therefore, the plasmon at $q = g$ is uncoupled to that at $q = 0$ and the term linear in the density modulation $n_g^{(0)}$ is uncapable of coupling the states at $q = \pm g$. On the other hand, the third term of Eq. (15) is also zero when $k = 0$, $K = -g$, and $K' = g$, due to the presence of the factor $2k + K + K'$. Therefore, the direct coupling among $q = \pm g$ through the term quadratic in the modulation is also absent. Then, there is no interaction among the plasmons at $q = \pm g$ and their degeneracy is not lifted. A gap would appear at the zone center if we add more Fourier components to the modulation. For example, a term proportional to $\cos(2gz)$ would induce a gap at $q = g$, in a similar way as the gap at $g/2$ displayed in Fig. 1 was induced by a term proportional to $\cos(gz)$. That gap would be zone folded into the center of the zone. However, the induced density would still have no Fourier components with a wave vector close to $k = 0$, except for $\omega \approx 0$. As a consequence, the usual strategy of superlattice-induced zone folding the Brillouin zone to make short-wavelength elementary excitations observable with long-wavelength probes is not applicable to the collective charge oscillations of a Q1D wire.

IV. CONCLUSIONS

We have developed a hydrodynamic model to calculate the plasmon spectra of a Q1D wire, the ground state of which has a smoothly varying density along its length. We applied our model to a periodic Q1D superlattice with a single sinusoidal modulation term and we obtained its corresponding band structure. As expected, a series of gaps open at the first Brillouin zone boundary, which may be probed using inelastic Raman scattering. Surprisingly, we found no gap at the zone center due to a vanishing coupling between degenerate states when Bloch's wave vector is zero. This null coupling has physical consequences even if a gap may be produced artificially by including additional modulating terms.

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