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Collective excitation spectra of one-dimensional electron systems

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We calculate, within the random-phase approximation, the elementary excitation spectrum of quasi-one-dimensional electron systems as occurring, for example, in semiconductor microstructures. Using multisubband models, we derive and discuss the dispersion relations for both intrasubband and intersubband excitations and consider the mode-coupling effect between them. We show that the depolarization shift correction for the intersubband excitation could be very large, increasing the intersubband collective mode energy substantially above the single-particle intersubband separation, and, thus explaining a puzzling recent far-infrared spectroscopic experimental observation.

Recently, there has been increasing theoretical[1-3] and experimental[4-6] interest in quasi-one-dimensional electron systems (1D ES's) based on semiconductor microstructures. In transport studies,[7,8] one finds interesting quantization of the ballistic conductance which is understood[9] on the basis of the opening or closing of 1D subbands (which are also called the "channels" as in the multichannel Landauer formula). The usual energy separations between these 1D subbands are of the order of a few meV so that far-infrared optical spectroscopy is one of the main experimental techniques[4,5] to study the electronic excitations in these 1D ES structures, either with or without an external magnetic field. In this Rapid Communication, we theoretically derive and discuss the plasma excitation spectrum of such 1D ES.

The usual practice in studying electronic properties of semiconductor systems of restricted dimensionality is to discuss two different kinds of elementary excitations: namely, the intrasubband and intersubband excitations. The intrasubband excitations involve electron dynamics only along the "free" direction (i.e., along the one-dimensional direction in our case), whereas the intersubband excitations are associated with quantum transitions between the electron subbands, thus necessarily involving dynamics along the directions of confinement. Clearly, this intuitively appealing separation of the elementary excitation spectrum into distinct intrasubband and intersubband modes is strictly valid only at long wavelengths ($q \rightarrow 0$) because at finite wave vectors the electric fields associated with the "longitudinal" and "transverse" motions couple and the distinction between intrasubband and intersubband excitations is no longer strictly valid. We calculate both intrasubband and intersubband plasma modes of 1D ES's and discuss the mode coupling between them. One of our important findings is that the 1D intersubband collective mode can be significantly higher in energy than the single-particle excitation at the subband separation. This is in agreement with the recent experimental results of Demel *et al.*[5] who studied the far-infrared response of such a system. In Ref. 5 it was found that the maximum absorption peak is located at a frequency about four times higher than the simple energy-level separation determined by the dc magnetotransport measurement. Based on our calculation we suggest that the observed absorption peak is the intersubband collective excitation which is depolarization shifted from the intersubband separation by a very large amount. This situation is different from the usual two-dimensional case where the typical depolarization shift is less than the subband separation.

Our model is of electrons confined in a zero-thickness (along the z direction) xy plane for the sake of simplicity. We shall use the same notation as in Ref. 10. The generalized dielectric function for a single 1D ES is given by[10]

$$\epsilon_{ijmn}(q,\omega)=\delta_{im}\delta_{jn}-v_{ijmn}(q)\Pi_{mn}(q,\omega)\,, \tag{1}$$

where i,j,m,n denote quantized 1D subbands because of y confinement (since we assume the z width to be zero, we are always in the lowest subband of the z motion). q is a wave vector in the x direction in which the motion is free. The function $\Pi_{mn}(q,\omega)$ is a generalized 1D irreducible polarizability function. The subband matrix element of the Coulomb interaction is given by

$$v_{ijmn}(q)=\int dy\int dy'\phi_i(y)\phi_j(y)v(q,y-y')\phi_m(y')\phi_n(y')\,, \tag{2a}$$

with

$$v(q,y-y')=\frac{2e^2}{\epsilon}\int_0^\infty\frac{\cos qx}{[x^2+(y-y')^2]^{1/2}}dx$$
$$=\frac{2e^2}{\epsilon}K_0(|q(y-y')|)\,. \tag{2b}$$

$\phi_i(y)$ is a confining wave function of the ith subband and $K_0(x)$ is a modified Bessel function of the second kind. ϵ is the background lattice dielectric constant.

The collective excitation spectrum is obtained by the condition of the vanishing of the determinant of the dielectric matrix given in Eq. (1):

$$\det|\epsilon_{ijmn}|=0\,. \tag{3}$$

If we restrict ourselves to a two-subband model in which only the lowest subband (denoted by 1) is occupied by electrons, Eq. (3) gives

$$(1-v_{1111}\Pi_{11})(1-v_{1212}\chi_{12})-v_{1112}^2\Pi_{11}\chi_{12}=0\,, \quad (4)$$

where $\chi_{12}=\Pi_{12}+\Pi_{21}$ is the intersubband polarizability. Within the random-phase approximation (RPA) one can use the noninteracting polarizability function ("bare bubble") for Π in Eq. (3).

These noninteracting 1D polarizability functions at zero temperature are easily calculated to be

$$\Pi_{11}(q,\omega)=\frac{m}{\pi q}\ln\left[\frac{\omega^2-(E_q-qv_F)^2}{\omega^2-(E_q+qv_F)^2}\right], \quad (5a)$$

$$\chi_{12}(q,\omega)=\frac{m}{\pi q}\ln\left[\frac{\omega^2-(E_{21}-qv_F+E_q)^2}{\omega^2-(E_{21}+qv_F+E_q)^2}\right], \quad (5b)$$

where the subband separation $E_{21}=E_2-E_1$, $E_q=q^2/2m$, and $v_F=k_F/m$ is the Fermi velocity (we use $\hbar=1$ in this paper). In the long-wavelength limit, i.e., when $q\rightarrow 0$,

$$\Pi_{11}(q,\omega)=\frac{N_s}{m}\frac{q^2}{\omega^2}+O(q^4)\,, \quad (5c)$$

$$\chi_{12}(q,\omega)=\frac{2E_{21}N_s}{\omega^2-E_{21}^2}+O(q)\,. \quad (5d)$$

Here N_s is the 1D density of electrons (i.e., number of electrons per unit length). Notice that the long-wavelength forms of polarizability given by Eqs. (5c) and (5d) are independent on the dimensionality of the system and have the same form as in Eqs. (5c) and (5d) for higher dimensions as well.

If we take the confining potential in the y direction to be of square-well form, then the quantizing wave function is

$$\psi(x,y,z)=(1/\sqrt{L})e^{ikx}\phi_n(y)[\delta(z)]^{1/2}\,, \quad (6a)$$

where

$$\phi_n(y)=\begin{cases}\left[\frac{2}{a}\right]^{1/2}\sin\frac{n\pi y}{a}\,, & 0\le y\le a\,,\\ 0\,, & \text{otherwise}\end{cases} \quad (6b)$$

with a denoting the width of the square well.

For a symmetric potential well, $v_{ijmn}(q)$ is strictly zero for arbitrary q if $(i+j+m+n)$ is an odd number.[11] In our case, v_{1112} is zero and, therefore, the mode-coupling term [the last term on the left-hand side of Eq. (4)] vanishes. Equation (4) in this situation becomes decoupled, with $1-V_{1111}\Pi_{11}=0$ determining the intrasubband one-dimensional plasma mode which has earlier been calculated by Das Sarma and Lai.[1] It was shown in Ref. 1 that this plasma mode dispersion depends strongly on the width a of the 1D ES. The other decoupled mode corresponds to the intersubband collective excitation

$$1-v_{1212}(q)\chi_{12}(q,\omega)=0\,. \quad (7)$$

We can solve Eq. (7) using Eqs. (2) and (5),

$$\omega^2=[A(qa)\omega_+^2-\omega_-^2]/[A(qa)-1]\,, \quad (8a)$$

where

$$A(qa)=\exp[q\pi/mv_{1212}(q)]\,, \quad (8b)$$

$$\omega_\pm=E_{21}\pm qv_F+q^2/2m\,. \quad (8c)$$

In the long-wavelength limit $q\rightarrow 0$, we can simplify (8) as

$$\omega^2=E_{21}^2+2E_{21}N_sv_{1212}(q)=E_{21}^2+W_p^2+O(q)\,, \quad (9)$$

where $W_p=[2E_{21}N_sv_{1212}(q\rightarrow 0)]^{1/2}$ is the so-called depolarization shift[12] which measures the energy difference between the intersubband single-particle and collective excitations. $v_{1212}(q\rightarrow 0)$ is about $1.2e^2/\epsilon$ for a square-well potential. Physically, this intersubband collective excitation corresponds to the collective motion of electrons in the transverse y direction.

In Fig. 1, we show the calculated dispersion of the intersubband collective excitation between the first and the second subbands and the corresponding intersubband single-particle excitation which is determined by the zeros of $\chi_{12}^{-1}(q,\omega)$ within the two-subband model. One can see that for $q=0$ the collective excitation frequency is about six times as high as that of the single-particle excitation. This is in qualitative agreement with the experimental result of Demel *et al.*[5] To characterize this large enhancement due to the electronic collective motion, we introduce a parameter.

$$\gamma_{12}(q)=\omega_{12}^c(q)/\omega_{12}^s(q) \quad (10)$$

as the ratio of the intersubband collective excitation and the single-particle excitation frequencies. $\gamma_{12}(q=0)$ is about 6.3 in our two-subband model. The parameters used in our calculation are chosen according to the experimental situation in Ref. 5 (sample A) except that N_s is scaled down for our calculation from the experimental *total* electron density by a factor

$$\frac{N_{s1}}{N_{s12}}=\frac{(E_{F1}-E_1)^{1/2}}{\sum_{n=1}^{12}(E_{F12}-E_n)^{1/2}}\,, \quad (11)$$

which takes into account the fact that the experimental sample[5] has twelve subbands occupied whereas in our model calculation only one subband is assumed to be populated. $E_n=n^2\pi^2/2ma^2$ is the energy bottom of the nth

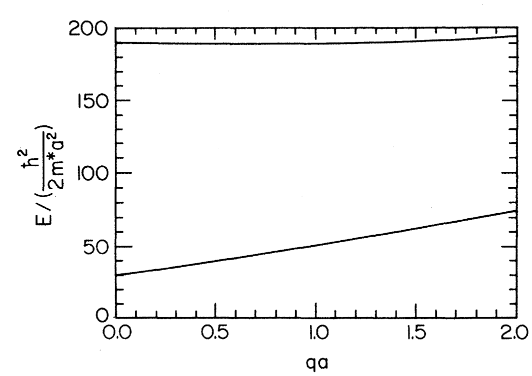

FIG. 1. The intersubband single-particle excitation (lower branch) and the intersubband collective excitation (higher branch) between subbands 1 and 2 as a function of qa in a two-subband model. (The parameters $a=390$ nm, $N_s=0.166\times10^6$ cm^{-1} are chosen according to Ref. 5).

subband and E_F is the Fermi energy. We further assume that the Fermi energy E_{F1} (E_{F12}) is at the bottom of the second (thirteenth) subband. Because the generalized dielectric matrix defined by Eq. (1) has a dimension $B^2 \times B^2$, where B is the number of subbands in the model, it is numerically impossible to calculate the elementary excitation spectrum for a thirteen-subband model using our method. Thus the semiquantitative comparison between theory and experiment as carried out here is the best one can do at this stage. In the rest of this paper, we extend our calculation of the elementary excitation spectrum to a three-subband model which exhibits some interesting features not found in the two-subband calculation described above. In particular, the mode coupling between the intrasubband and intersubband excitations shows up in the three-subband model. We also discuss the intersubband collective and single-particle excitations between second and third subbands. The agreement between theory and experiment improves in this three-subband calculation, lending further support to our model.

In the three-subband model, we assume that only the two lowest subbands are occupied. Using this condition and the symmetry of the potential well, Eq. (3) can be decoupled to two 4×4 determinants which can be further reduced to the following two equations after considerable algebra:

$$(1 - v_{1212}\chi_{12})(1 - v_{2323}\chi_{23}) - v_{2321}^2\chi_{12}\chi_{23} = 0\,, \qquad (12)$$

and

$$(1 - v_{1313}\chi_{13})[(1 - v_{1111}\Pi_{11})(1 - v_{2222}\Pi_{22}) - v_{1122}^2\Pi_{11}\Pi_{22}] - 2v_{1122}v_{1113}v_{2213}\Pi_{11}\Pi_{22}\chi_{13} - (1 - v_{1111}\Pi_{11})v_{2213}^2\Pi_{22}\chi_{13} - (1 - v_{2222}\Pi_{22})v_{1113}^2\Pi_{11}\chi_{13} = 0\,. \qquad (13)$$

Clearly Eq. (12) is the mode coupling between intersubband collective excitations of subbands 1 and 2 and that of subbands 2 and 3. Equation (13) is more complicated describing the coupling among the intersubband collective excitation of subbands 1 and 3 and the two intrasubband plasma excitations of subbands 1 and 2. We start with Eq. (12) which we believe includes the relevant physics needed to explain the experimental results of Demel *et al.*[5] First, we calculate the intersubband collective excitation $\omega_{23}^c(q)$ of subbands 2 and 3 which is determined by

$$1 - v_{2323}(q)\chi_{23}(q,\omega) = 0\,. \qquad (14)$$

In the three-subband model, γ_{23} ($q = 0$) is about 5.4, which is smaller than γ_{12} ($q = 0$) $= 6.3$ in our two-subband model and is closer to the experimental result[5] of $\gamma = 4.0$. In Fig. 2 we show the numerical solution $\Omega(q)$ of Eq. (12) as a function of qa. The uncoupled intersubband collective excitation modes ω_{23}^c and single-particle excitation ω_{23}^s are also plotted in the figure for comparison. After mode coupling, the collective excitation is about 1.3% above ω_{23}^c at $q = 0$. We can see that the correction due to

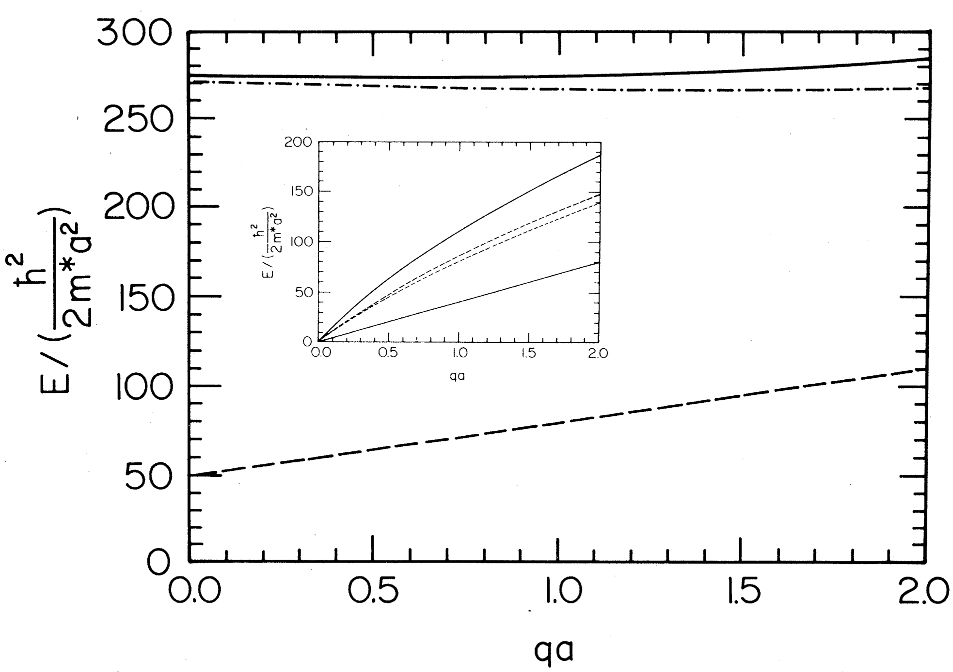

FIG. 2. The intersubband excitation between subbands 2 and 3 as a function of qa in a three-subband model ($a = 390$ nm, $N_s = 0.486 \times 10^6$ cm^{-1}). The solid line is for $\Omega(q)$, the solution of the coupled Eq. (12), whereas the dashed line and the dot-dashed lines are for the uncoupled single-particle and collective excitations, respectively. The coupling effect pushes the other branch of $\Omega(q)$ below the abscissa in the figure. Inset: The coupling between intrasubband plasma excitations as a function of qa in the same system. The solid lines are for the coupled modes and dashed lines are for the uncoupled individual plasma excitations of subbands 1 and 2, respectively.

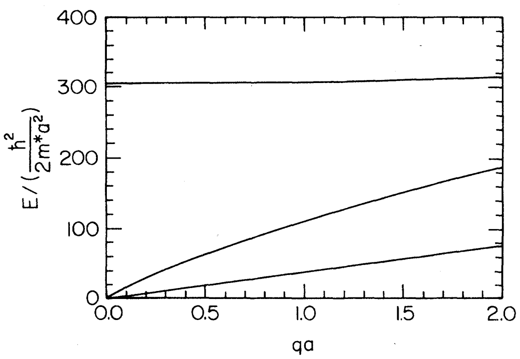

FIG. 3. The solution of Eq. (13) which describes the coupling between the intersubband collective excitation (13) and the intrasubband plasma excitations of subbands 1 and 2. The system is the same as in Fig. 2.

mode coupling is rather small here. The reason is that χ_{12} is much smaller than χ_{23} in the three-subband model as a result of our assumption that subbands 1 and 2 are occupied while subband 3 is empty.

In the inset of Fig. 2, we show the coupling between intrasubband plasma excitations of subbands 1 and 2:

$$(1-v_{1111}\Pi_{11})(1-v_{2222}\Pi_{22})-v_{1122}^2\Pi_{11}\Pi_{22}=0\,. \quad (15)$$

The uncoupled plasma modes ω_{11} and ω_{22} in each subband are also plotted for comparison. Finally, in Fig. 3 we plot the three branches of the solution of Eq. (13). Apparently, the highest branch corresponds to ω_{13} while the two lower branches correspond to the coupled intrasubband plasma excitations (cf. inset of Fig. 2).

Summarizing our results, we calculate the elementary excitation spectrum of a quasi-1D electron system within two-subband and three-subband models and using the RPA for the dielectric response. We find that the intersubband collective excitation energy can be significantly higher than the corresponding single-particle excitation energy for experimentally realizable parameter values.[5] Our calculation shows that the ratio of the two energies can be as high as 5–6.5 using the experimental parameters adopted from Ref. 5. This is in good qualitative and semiquantitative agreement with the experimental result.[5] We identify the experimentally observed infrared absorption peak to be the intersubband collective excitation mode. This identification is supported by the fact that the absorption peak was observed in Ref. 5 only when the light was polarized in the direction perpendicular to the 1D quantum wire but not when it was parallel. We urge more experimental study in samples with less subbands occupied (ideally only one or two) so that one can have a direct quantitative comparison between our theory and experiments.

We conclude by pointing out various approximations and limitations of our theory and their validity. We use the RPA rather uncritically, based mainly on the fact that we do not know how to go beyond the RPA ("the sum of the bubble diagrams") in a controlled approximation. The validity of the RPA in the 1D ES of interest here is unknown, but it is expected to be less valid than in higher dimensions. We are, however, encouraged by the excellent agreement[11] between the RPA theory and experiment on collective excitations in two-dimensional semiconductor quantum wells and superlattices, systems which are very closely related[4–6] to the 1D ES being studied here. Our use of a model confinement ("infinite square-well" potential) defined by Eq. (6) can be and should be improved in subsequent calculations in a more realistic self-consistent manner.[13] We do not expect this correction to be qualitatively significant though, because self-consistent calculations[13] show that our model confinement works well for 1D ES's with finite electron density.

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