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Quantum size effects on the plasma dispersion in quasi-two-dimensional electron systems

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A generalized many-body dielectric theory is developed for studying the collective excitation spectrum in quasi-two-dimensional electron systems in semiconductor inversion and accumulation layers and in semiconductor heterostructures and superlattices. In particular, the coupling between the intrasubband and intersubband collective modes (plasmons) is explicitly retained in the theory. This mode-coupling effect modifies the plasma dispersion relation in these systems and the theory explains the hitherto unexplained phenomenon of a plasmon mass increase at higher wave numbers observed in silicon inversion layers. In a superlattice this mode-coupling effect produces a leading-order modification of the plasma dispersion relation in contrast to other mode-coupling-type phenomena (which are usually higher-order processes away from resonance) giving rise to an improved agreement between the theory and light-scattering experimental results.

In this Communication I present results of a theoretical calculation of the collective excitation spectrum in quasi-two-dimensional electronic systems both for the single layer heterostructure and the multilayer superlattice situations. The theory explicitly includes the coupling between the two-dimensional intrasubband and the resonant intersubband collective modes ("plasmons"). This mode-coupling effect (which is nonzero for finite values of wave vector q parallel to the two-dimensional layer) has been ignored in earlier theories[1–5] for the collective excitation spectrum in two-dimensional systems because it was considered to be a "higher-order" effect. In this paper results are presented which show that this mode-coupling effect "reduces" the two-dimensional plasma frequency at high values of q from its classical value. This explains the unexpected (and so far "unexplained") plasmon mass enhancement observed at high wave vectors in silicon electron inversion layers.[6] In a multilayer type-I superlattice the coupling between the intrasubband and the intersubband[5] collective modes is shown to modify the two-dimensional plasma dispersion in the *leading order* in q. This is a novel type of mode-coupling phenomena which are usually higher-order effects. The theory also explains the slight disagreement between the experimentally measured[7,8] plasma dispersion in a semiconductor superlattice and earlier theoretical calculations,[3,4] as a manifestation of this mode-coupling effect.

The generalized dielectric function for a single two-dimensional electron layer (appropriate for a single heterojunction or for a metal-insulator-semiconductor structure[6]) is given by

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

where i,j,m,n denote subbands[9] for quantized motion along the direction perpendicular to the layer and δ_{im} is the Kronecker δ function. The function $\Pi_{mn}(\vec{q},i\omega)$ is the generalized polarizability function.[10]

In Eq. (1), v_{ijmn}, the matrix element of the Coulomb interaction (including any image effect[9] arising from the dielectric mismatch at the interface) is given by

$$v_{ijmn}(\vec{q})=\int dz\int dz'\zeta_i(z)\zeta_j(z)v_q(z,z')\zeta_m(z')\zeta_n(z') \ , \tag{2}$$

where $v_q(z,z')$ is the two-dimensional Fourier transform (in the x-y plane) of the three-dimensional Coulomb interaction including any image term, and $\zeta_i(z)$ is the quantized wave function[9] for the ith subband. In the above equations $\vec{q}$ is the (conserved) two-dimensional wave vector in the plane of the layer whereas $i\omega$ is the standard[10] Matsubara frequency.

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

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

If B subbands are kept in the problem then Eq. (3) defines a $B^2\times B^2$ determinantal equation in the most general situation. Restricting oneself to a two-subband model ($B=2$) in which only the lowest subband (denoted by 1) is occupied by electrons, Eq. (3) gives

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

where $\chi_{12}=\Pi_{12}+\Pi_{21}$ is the intersubband polarizability giving the resonant transitions between levels 1 and 2 and Π_{11} is the two-dimensional polarizability[11] function. The dependence on $\vec{q}$ and ω has not been explicitly shown in Eq. (4) for the sake of brevity. The last term in Eq. (4) couples the intra- and the intersubband plasmon terms which are individually given by $1-v_{1111}\Pi_{11}=0$ for the intrasubband two-dimensional plasmon[11] and by $1-v_{1212}\chi_{12}=0$ for the intersubband[12] plasmon. Using random-phase approximation[13] for the polarizability, one has[11,12] in the limit of small q

$$\Pi_{11}(q,\omega)\simeq\left(\frac{N_s}{m}\right)\left(\frac{q^2}{\omega^2}\right)$$

and

$$\chi_{12}(q,\omega)\simeq 2N_sE_{21}/(\omega^2-E_{21}^2) \ , \tag{5}$$

where $E_{21}=E_2-E_1$ is the subband energy separation and N_s is the electron density per unit area.

Using Eqs. (2) and (5) in Eq. (4) one gets the following coupled collective modes for the two-subband model:

$$\omega_{\pm}^2=\tfrac{1}{2}\{(E_{21}^2+W_p^2)+\omega_p^2\pm[(E_{21}^2+W_p^2-\omega_p^2)^2+4C^2q^2]^{1/2}\} \ , \tag{6}$$

where $\omega_p=(2\pi N_s e^2 q/\kappa m)^{1/2}$ is the two-dimensional plasma frequency first calculated[11] by Stern (κ is the average lattice dielectric constant) and

$$W_p=[2N_s E_{21} v_{1212}(q\to 0)]^{1/2}$$

is the so-called depolarization shift.[12,14] The constant C in Eq. (6) is given by

$$C=\{2N_s^2 E_{21}[v_{1112}(q\to 0)]^2/m\}^{1/2} \ . \tag{7}$$

Introducing $\omega_i^2=Cq$ in Eq. (6), the coupled modes become

$$\omega_\pm^2=\frac{1}{2}\{(\omega_{21}^2+\omega_p^2)\pm[(\omega_{21}^2-\omega_p^2)^2+4\omega_i^4]^{1/2}\} \ , \tag{8}$$

where $\omega_{21}=(E_{21}^2+W_p^2)^{1/2}$ is the depolarization shifted[12,14] intersubband transition frequency ("the intersubband plasmon" mode).

Experimental conditions for Ref. 6 were such that $\omega_{21} \gg \omega_p$ and then Eq. (8) gives two collective modes

$$\omega_+\simeq\omega_{21}\left[1+\frac{\omega_i^4}{2\omega_{21}^4}\right]$$

and (9)

$$\omega_-\simeq\omega_p\left[1-\frac{\omega_i^4}{2\omega_{21}^2\omega_p^2}\right] \ .$$

The two-dimensional plasmonlike mode ω_- has a lower frequency than the classical plasma frequency[11] ω_p and if one writes $\omega_-^2=2\pi N_s e^2 q/\kappa m(q)$ following Ref. 6, the plasmon mass $m(q)$ is given by

$$m(q)\simeq m\left[1+\frac{V_{1112}}{2\pi e^2 E_{21}}N_s q\right] \ , \tag{10}$$

where $V_{1112}=[v_{1112}(q\to 0)]^2$. Equation (10) suggests that the plasmon mass depends on the wave number q and the electron density N_s through the combination $N_s q$ since V_{1112} and E_{21} are only weak functions of electron density (and are independent of q). This is the experimental observation of Ref. 6. It should be emphasized that dispersion[11,15] and many-body[15] corrections to the plasma frequency always increase value lowering the plasmon mass whereas the experimental observation is the opposite. Also, the q values in the experimental[6,16] situation are such that higher-order dispersion corrections to the plasma frequency are negligible. The only other possible explanation for the plasmon mass increase is band nonparabolicity (which is very small for silicon electron inversion layer) which, however, should show no q dependence. Thus Eq. (10) is the only possible qualitative and quantitative explanation for the experimental observation[6,16] of a plasmon mass increase in silicon inversion layers at high q and N_s.

For a superlattice there are important modifications[3–5] of the theory outlined above. Tselis, Gonzales de la Cruz, and Quinn as well as Bloss have recently considered[5] the problem of intra- and intersubband collective modes in a superlattice where the individual layers have finite thicknesses. Our treatment of the superlattice collective-mode problem is equivalent to that of Ref. 5 except that the coupling between the intra- and intersubband collective modes is explicitly retained in our theory.

Generalizing the above analysis appropriate for a single layer problem to the type-I superlattice (e.g., GaAs-As-$Al_xGa_{1-x}As$ system[7,8]) situation, one gets the following equation for the coupled collective modes of an infinite periodic superlattice:

$$\tilde\omega_\pm^2=\frac{1}{2}\{\tilde\omega_{21}^2+\tilde\omega_p^2\pm[(\tilde\omega_{21}^2-\tilde\omega_p^2)^2+4\tilde\omega_i^4]^{1/2}\} \ , \tag{11}$$

where

$$\begin{aligned}\tilde\omega_{21}&=(E_{21}^2+2N_s f_{12}E_{21})^{1/2} \ ,\\ \tilde\omega_p&=(N_s f_{11}/m)^{1/2}q \ ,\\ \omega_i&=[N_s q(2E_{21}f_i\tilde f_i/m)^{1/2}]^{1/2} \ .\end{aligned} \tag{12}$$

In Eq. (12), f_{11}, f_{12}, f_i, and $\tilde f_i$ are form factors whose explicit forms are not shown in this paper. It should be pointed out that Eq. (11) for the superlattice is formally equivalent to Eq. (8) for a single layer problem. The decoupled modes, $\tilde\omega_{21}$, the intersubband[5] mode, and $\tilde\omega_p$, the intrasubband[3] mode in Eqs. (11) and (12), are identical to the ones obtained[5] recently by Tselis *et al.* The new feature of Eq. (11) is the interaction term $4\tilde\omega_i^4$ which couples the intra- and intersubband plasmons.

In the long-wavelength limit the form factors of Eq. (12) can be explicitly obtained, and in the experimentally interesting[7,8] limit of qa, $qb \ll 1$, with $a>2b$ (where a and b are, respectively, the superlattice period and the thickness of individual layers), one gets in the leading order

$$\tilde\omega_+\simeq\tilde\omega_{21}[1-O(q^2a^2)] \tag{13}$$

and

$$\tilde\omega_-\simeq\tilde\omega_p(1-\delta) \ , \tag{14}$$

where

$$\tilde\omega_p\simeq\{2\pi N_s e^2 a/[\kappa m(1-\cos k_z a)]\}^{1/2}q$$

is the decoupled, long-wavelength two-dimensional plasma frequency[3,4] for a type-I superlattice with k_z as the wave number in the superlattice direction. The constant δ is a small number ($\delta\simeq 0.1$) which depends on the form factors.

Equation (13) gives the intersubband plasmon mode

$$\tilde\omega_{21}\simeq(E_{21}^2+4\pi N_s e^2 E_{21}L_{12}/\kappa)^{1/2} \ ,$$

with

$$L_{12}=2\int_0^b dz\left[\int_0^z dz'\zeta_1(z')\zeta_2(z')\right]^2 \ ,$$

which has been first[5] obtained by Tselis *et al.* and Bloss. It is clear that the intersubband plasmon is unaffected in the leading order by mode-coupling effects since the correction in Eq. (13) goes as $O(q^2)$. On the other hand, Eq. (14) suggests that the two-dimensional intrasubband plasmon frequency $\tilde\omega_p$ is affected in *the leading order* by the mode-coupling effect since $\tilde\omega_-$ has a different phase velocity compared with $\tilde\omega_p$. As has been emphasized before this is a novel mode-coupling phenomenon since away from resonance (the situation being discussed) coupling of collective modes is usually a higher-order effect [as, for example, in Eq. (13)]. The intrasubband plasmon in a superlattice, the $\tilde\omega_-$ mode, is thus affected by the coupling in a significant fashion even for small q since the correction δ in Eq. (14) occurs in the *same* order as the leading decoupled term $\tilde\omega_p$. Thus the theoretical slope of the $\tilde\omega_-(q)$ curve against q is reduced by $100\delta\%$ compared with the $\tilde\omega_p(q)$ curve. An alternate way of stating the result is that the effective mass entering the plasma frequency in Eq. (14) is increased from m to $m(1+2\delta)$ due to intersubband transitions. This is a 10–15% increase in the effective mass due to hybridization. Actual use of the experimental parameters (appropriate for a modulation doped GaAs-Al_xGa_{1-x}As multilayer superlattice) corresponding to Ref. 7 gives $\delta \simeq 0.07$, reducing the slope of the theoretical curve by 7% and bringing the theoretical results in excellent agreement with all the experimental data points of Ref. 7. This last aspect is particularly significant since the comparison[7,8] of the experimental data with the decoupled plasmon frequency $\tilde{\omega}_p$ puts all the data points below the theoretical curve. Thus the experimental[7,8] results are explicitly showing the effects of mode coupling in a semiconductor superlattice.

In conclusion, coupling between the intra- and intersubband plasmons has been explicitly retained in the calculation for the collective-mode spectrum of quasi-two-dimensional electron systems both in the single layer case and in the multilayer superlattice situation. Mode coupling affects the intrasubband plasmons in a significant fashion providing an explanation for the hitherto unexplained observation[6,16] of a plasmon mass increase in silicon inversion layer. For a type-I superlattice, mode coupling gives rise to the novel phenomenon of a leading-order modification of the intrasubband plasmon frequency even in the nonresonant (i.e., $\tilde{\omega}_{21} \neq \tilde{\omega}_p$) situation. Thus the slope of the superlattice plasmon[7,8] curve against q is slightly reduced bringing experiment[7,8] and theory in excellent agreement with each other. The approximations used in the theory are the effective-mass approximation, the random-phase approximation, and the neglect of wave-function overlap from different layers in a superlattice—all of which are expected to be reasonable assumptions for actual systems of interest. Details of the theory will be published elsewhere.

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