

# Plasmons in asymmetric double quantum well structures

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Received 2 July 2002

Published online 19 December 2002 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2002

**Abstract.** We investigate the effects of spatial asymmetry, tunneling coupling, and exchange-correlation correction on the plasmon modes in asymmetric double quantum well (DQW) structures in a time-dependent local-density approximation. Special attention is paid to the properties of the  $\omega_-$  mode which is always damped in symmetric DQW systems. In addition, the results on the spectral weight of the excitations are also presented. In general, all the modes carry finite spectral weights and should be observable in resonant inelastic light scattering experiments for the specified values of the parameters.

**PACS.** 71.15.-m Methods of electronic structure calculations – 73.20.Mf Collective excitations (including excitons, polarons, plasmons and other charge-density excitations) – 73.21.-b Electron states and collective excitations in multilayers, quantum wells, mesoscopic, and nanoscale systems

As an important and elementary question in solid-state physics, many-body interactions have been continuously investigated for several decades. Two-component low-dimensional electron systems such as double quantum well (DQW) and double quantum wire structures provide ideal platforms in these studies because the interwell or interwire Coulomb interaction can counterbalance the kinetic energy of the electrons, allowing many-body effects to be dominant. In fact, collective excitations in DQW structures have attracted extensive interest over the last two decades ever since the existence of an undamped acoustic plasmon mode was predicted [1]. As has been pointed out, this acoustic mode is strongly influenced by tunneling as well as local field effects and the properties of it may serve as a sensitively experimental tool in studying many-body effects. Consequently, the prediction of its existence in DQW structures stimulates intensively theoretical [2–10] and experimental [11–13] investigations in this field. This acoustic mode, together with the optical mode, has been observed [13] recently in semiconductor double quantum well systems *via* inelastic light scattering spectroscopy which is a powerful and versatile tool for probing elementary excitations in low-dimensional semiconductor structures. However, most of the investigations [1,3–5,7–9,11–13] up to now focus on plasmons in symmetric systems and the effects of spatial asymmetry have been rarely concerned, which is rather surprising considering the extensive studies in this field.

In a recent paper [10], we studied the effects of tunneling coupling on the plasmon modes in asymmetric DQW (ADQW) structures in the random-phase approx-

imation (RPA). In this paper, we go beyond the simple RPA by including the exchange-correlation effects and consider the more realistic and experimentally relevant issue of the plasmon dispersions in ADQW structures in the time-dependent local-density approximation (TDLDA) [14]. The purpose is to conduct a systematically theoretical investigation in the effects of spatial asymmetry on plasmons in DQW structures. We also calculate the spectral weight of the excitations which is a direct measure of the spectral intensity in resonant inelastic light scattering experiments.

Our ADQW structure consists of two GaAs well layers (with widths  $W_1$  and  $W_2$ , respectively) separated by an undoped AlGaAs barrier layer (with a width of  $b$ ) and adjoining to two partly doped AlGaAs layers. Each of these two partly doped layer is composed of an undoped spacer layer (with a width of  $s_1$  or  $s_2$ ) and a uniformly doped layer (with a doped concentration of  $N_D$ ). Considering the depletion effect, we suppose that the donors in the doped layers are partly ionized. The depletion lengths  $d_1$  and  $d_2$  are determined self-consistently. Throughout this paper we adopt the local-density-functional theory to solve the Poisson's equation and the one-electron Schrödinger-like equation self-consistently for obtaining the subband energies and wave functions [14].

In the TDLDA, The dispersion relations of the plasmon modes are determined by [14,15]

$$\det \{ \delta_{ln'} \delta_{l'n} - [U_{ll',nn'}(\mathbf{q}) + V_{ll',nn'}^{xc}] \Pi_{nn'}(\mathbf{q}, \omega) \} = 0, \quad (1)$$

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where

$$U_{ll',nn'}(\mathbf{q}) = \iint dz dz' \xi_l(z) \xi_{l'}(z) \frac{e^2}{2\epsilon_r \epsilon_0 q} e^{-q|z-z'|} \xi_n(z') \xi_{n'}(z'), \quad (2)$$

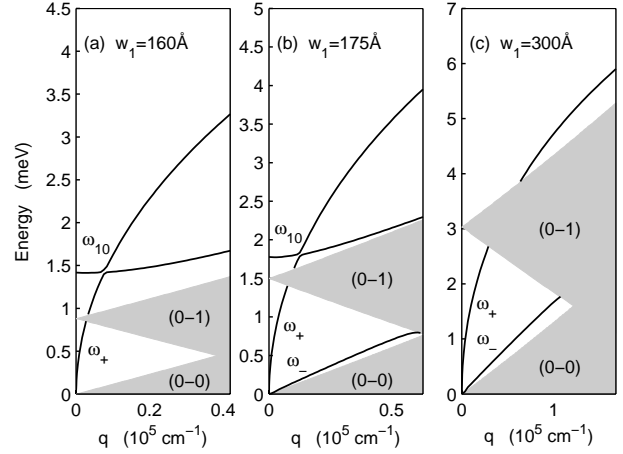
$$V_{ll',nn'}^{xc} = \int dz \xi_l(z) \xi_{l'}(z) \frac{\partial V_{xc}[n(z)]}{\partial n(z)} \xi_n(z) \xi_{n'}(z), \quad (3)$$

$$\Pi_{nn'}(\mathbf{q}, \omega) = 2 \sum_{\mathbf{k}} \frac{f_n(\mathbf{k}) - f_{n'}(\mathbf{k} + \mathbf{q})}{\hbar(\omega + i\eta) + E_n(\mathbf{k}) - E_{n'}(\mathbf{k} + \mathbf{q})}. \quad (4)$$

Here  $\epsilon_r$  is the relative dielectric constant of the host semiconductor,  $\epsilon_0$  is the dielectric constant of free space,  $V^{xc}$  is the exchange-correlation potential,  $n(z)$  is the  $z$ -dependent electron density,  $f_n(\mathbf{k})$  is the occupation factor of state  $|n, \mathbf{k}\rangle$ ,  $E_n(\mathbf{k})$  is the energy of  $|n, \mathbf{k}\rangle$ , and  $\eta$  is a phenomenological parameter taking care of scattering by impurities. The spectral weight or the dynamical structure factor  $S(\mathbf{q}, q_z, \omega)$  due to the charge-density excitations is given [2, 7, 16] by the imaginary part of the dynamical polarizability (density-density correlation function), where  $q_z$  is the probe wave vector normal to the layers of the electron gas.

It is well known that in symmetric DQW (SDQW) structures, the plasmon modes can be separated into two sets, namely the even parity modes and the odd parity modes. In the two-subband model, the even and odd parity modes correspond to the intra- and intersubband modes, respectively [6]. It has been pointed out that the equation determining the intrasubband modes is quadratic and should have two solutions  $\omega_{\pm}$ . However, one of these two intrasubband modes  $\omega_{-}$  always lies in the single-particle continua and is highly damped. Therefore, only the so-called “optical” intrasubband mode  $\omega_{+}$  shows up. In the zero-tunneling case, the intersubband mode  $\omega_{10}$  displays a linear dispersion at long wavelengths and has been called the “acoustic” mode. When tunneling is appreciable, this mode develops a long-wavelength gap [4, 6–8]. In ADQW structures, however, the situation becomes quite different. Due to the asymmetric nature of the wave functions, equation (1) cannot be separated into sub-equations, which means that all the modes are coupled together. We will show that the dispersion relations and the damping properties of the plasmon modes are drastically influenced by spatial asymmetry. Furthermore, because of the coupling between  $\omega_{+}$  and  $\omega_{10}$ , these two modes cannot cross to each other. Instead, a phenomenon called “anti-crossing” appears.

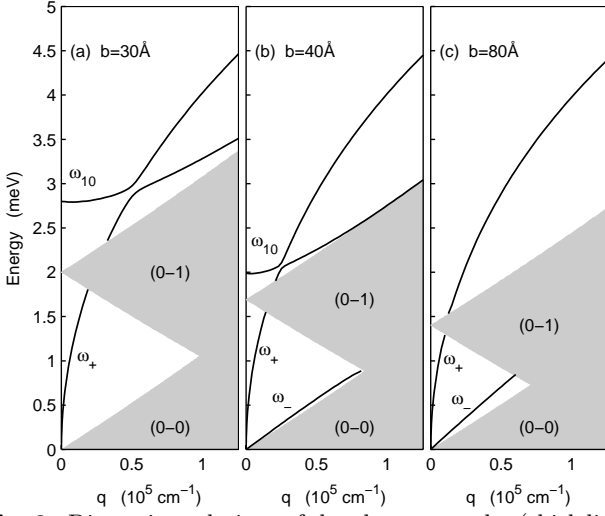
In our calculations, we assume  $s_1 = s_2 = 50 \text{ \AA}$ ,  $N_D = 5.0 \times 10^{17} \text{ cm}^{-3}$ ,  $\epsilon_r = 12.87$  and  $\eta = 0.1 \text{ meV}$ . The effective mass of the electrons in the well (barrier) layer is chosen to be  $m_0^* = 0.067m_e$  ( $m_b^* = 0.087m_e$ ) where  $m_e$  is the bare electron mass. The discontinuity between the electronic conduction band in the well layer and barrier layer is taken as 180 meV. To show the effects of the extent of spatial asymmetry on the charge-density excitations, we calculate the dispersion relations



**Fig. 1.** Dispersion relations of the plasmon modes as a function of wave vector for different widths of the first well while the width of the second is fixed to 150 Å in the ADQW structures with  $b = 40 \text{ \AA}$ , and  $n_{2D} = 3.0 \times 10^{11} \text{ cm}^{-2}$ . The shaded regions indicate the single-particle continua.

of the plasmon modes when  $W_2$  is fixed while the value of  $W_1$  is changed gradually. The results are shown in Figure 1, where  $W_2 = 150 \text{ \AA}$ ,  $b = 40 \text{ \AA}$ , and  $n_{2D} = 3.0 \times 10^{11} \text{ cm}^{-2}$  are assumed in the calculations. Here  $n_{2D}$  is the two-dimensional electronic density of the quantum well system. The shaded areas indicate the single-particle continua. It is seen that when the system deviates from spatial symmetry slightly [see panel (a)], the  $\omega_{-}$  mode still lies in the (0–0) single-particle continuum. As increasing the value of  $W_1$ , *i.e.*, increasing spatial asymmetry of the system, the  $\omega_{-}$  mode gradually moves out of the (0–0) continuum, as can be seen from panels (b) and (c). It is also noted that the dispersion relation and damping property of the  $\omega_{10}$  mode are substantially influenced by spatial asymmetry. We know that in SDQW structures,  $\omega_{10}$  always lies above the (0–1) single-particle continuum in the long-wavelength limit at ordinary electronic densities ( $n_{2D} > 1.0 \times 10^{11} \text{ cm}^{-2}$ ). In the asymmetric case, however, it is seen that  $\omega_{10}$  draws close to the (0–1) continuum gradually and finally becomes completely damped with the increase of spatial asymmetry. Our numerical results predict that at certain conditions (see panel (b)) the two intrasubband modes  $\omega_{\pm}$  and the intersubband mode  $\omega_{10}$  can coexist, which should be observable in experiments. In addition, the anti-crossing phenomenon can be also seen, as shown in panels (a) and (b).

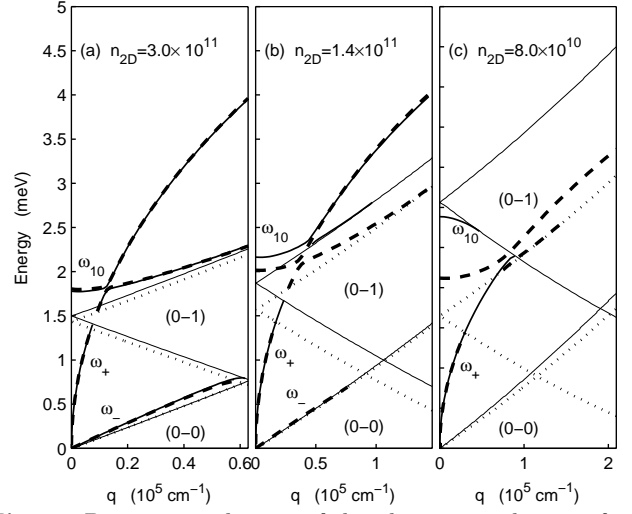
In Figure 2 we display the dispersion relations of the plasmon modes in TDLDA as a function of wave vector for different interwell barrier widths in the ADQW structures with  $W_1 = 175 \text{ \AA}$ ,  $W_2 = 150 \text{ \AA}$ , and  $n_{2D} = 2.0 \times 10^{11} \text{ cm}^{-2}$ . It is found that with the increase of the width of the interwell barrier, the  $\omega_{-}$  mode shifts out of the (0–0) single-particle continuum and becomes undamped while  $\omega_{10}$  gradually draws close to the (0–1) continuum and eventually becomes damped. When the barrier width is about 40 Å, these three modes coexist. An interesting phenomenon that accompanies the behaviors of the plasmon modes is the similarity of Figure 2 to



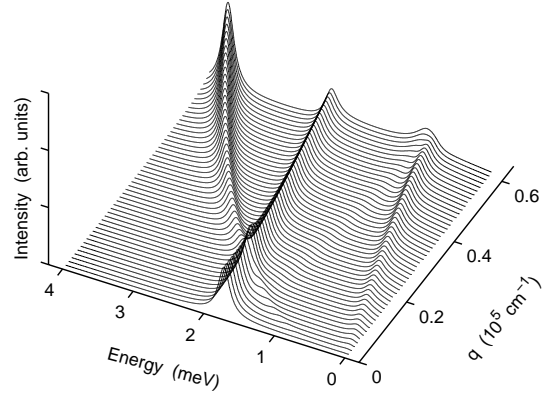
**Fig. 2.** Dispersion relations of the plasmon modes (thick lines) as a function of wave vector for different widths of the interwell barrier in the ADQW structures with  $W_1 = 175 \text{ \AA}$ ,  $W_2 = 150 \text{ \AA}$ , and  $n_{2D} = 2.0 \times 10^{11} \text{ cm}^{-2}$ . The gray areas indicate the single-particle continua.

Figure 1, where we vary the width of the first well (while we fix the width of the second) or the width of the interwell barrier, respectively. This similarity comes from the fact that with the increase of the barrier width, the electrons are more confined to the two wells and consequently, the deviation of the system from spatial symmetry becomes large.

In Figure 3, the calculated plasmon dispersions (thick lines) are shown for different electron densities in the ADQW structures with  $W_1 = 175 \text{ \AA}$ ,  $W_2 = 150 \text{ \AA}$ , and  $b = 40 \text{ \AA}$ . The solid and dashed curves indicate the TDLDA and RPA results, respectively. The thin solid lines and thin dotted lines correspond to the boundaries of the single-particle continua in the TDLDA and RPA, respectively. It is evident that the dispersion relations and damping properties of  $\omega_+$  and  $\omega_-$  differ little in these two approximations at all electronic densities. However, the exchange-correlation effects on the subband energies and the behaviors of the intersubband mode  $\omega_{10}$  depend substantially on the electronic density. When the electronic density is as high as  $3.0 \times 10^{11} \text{ cm}^{-2}$ , the TDLDA results deviate from the RPA results slightly. With the decrease of the electronic density, however, their difference increases monotonously. As continuously decreasing the electron density, the exchange-correlation effects become remarkably important. In the RPA,  $\omega_{10}$  lies above the (0-1) single-particle continuum at all electronic densities because the excitonic correction is zero while the depolarization shift is positive. In the TDLDA, however, the excitonic correction partially cancels the depolarization shift. As a result,  $\omega_{10}$  lies more closer to the (0-1) continuum than that in the RPA case. For the densities around  $8.14 \times 10^{10} \text{ cm}^{-2}$ , the energy of  $\omega_{10}$  coincides with the corresponding quasiparticle energy difference as the excitonic correction cancels the depolarization shift completely. As a result,  $\omega_{10}$  lies entirely inside the (0-1) continuum and is highly Landau damped. When decreasing



**Fig. 3.** Dispersion relations of the plasmon modes as a function of wave vector for different electron densities as shown in the ADQW structures with  $W_1 = 175 \text{ \AA}$ ,  $W_2 = 150 \text{ \AA}$ , and  $b = 40 \text{ \AA}$ . The solid and dashed lines correspond to the results in the TDLDA and RPA, respectively. The boundaries of the single-particle continua are also shown (thin lines).



**Fig. 4.** Spectral weight of the excitations for different wave vectors in an ADQW structure with  $W_1 = 175 \text{ \AA}$ ,  $W_2 = 150 \text{ \AA}$ ,  $b = 40 \text{ \AA}$ , and  $n_{2D} = 3.0 \times 10^{11} \text{ cm}^{-2}$ .

the electron density even further, the excitonic correction becomes larger in magnitude than the depolarization shift, thus, we obtain the interesting result that  $\omega_{10}$  lies below the (0-1) Landau continuum, as shown in panel (c).

Finally, it is useful to make some remarks upon the experimental aspects of the collective excitations in ADQW structures. The current work finds an important result that for sufficiently large extent of spatial asymmetry, the originally damped mode  $\omega_-$  becomes undamped and coexists with the intrasubband “optical” mode  $\omega_+$  and the intersubband mode  $\omega_{10}$ . To explore the possibility of observing these phenomena associated with the effects of spatial asymmetry in the inelastic light scattering experiment, we calculate the spectral weight for the collective modes in the ADQW structures. As an example, we plot in Figure 4 the spectral weight for the modes in an ADQW structure with  $W_1 = 175 \text{ \AA}$ ,  $W_2 = 150 \text{ \AA}$ ,  $b = 40 \text{ \AA}$ , and  $n_{2D} = 3.0 \times 10^{11} \text{ cm}^{-2}$  for different wave vectors and fixed  $q_z = 4.2 \times 10^5 \text{ cm}^{-1}$ . The most important message here

is that all the three modes in general carry finite spectral weights. Experimentally,  $\omega_+$  and  $\omega_{10}$  have been observed in SDQW structures. Consequently, we believe that  $\omega_-$  should also be observable in the inelastic light scattering experiment at low temperatures because its spectral weight is comparable to those of the other two modes.

In summary, we have investigated the effects of spatial asymmetry on plasmon modes in DQW structures in detail. We find that spatial asymmetry possesses essential effects on the plasmon modes. As increasing the width difference of the two wells or the width of the barrier gradually,  $\omega_-$  moves out of the single-particle continua while  $\omega_{10}$  draws close to the (0–1) single-particle continuum and becomes damped. At certain conditions these two modes as well as the always existing intrasubband mode  $\omega_+$  can coexist together. We show that with the decrease of the electronic density, the exchange-correlation effects become remarkably important. We also provide the numerical results on the spectral weights for the excitations. In general, all the three modes carry finite spectral weight and should be observable in the inelastic light scattering spectroscopy.

This work was supported by the National Science Foundation of China.

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