Space-asymmetry-induced plasmon mode mixing and anticrossing in coupled bilayer structures

C.-M. Hu, C. Schüller, and D. Heitmann
Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstraße 11, 20355 Hamburg, Germany

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We show that the space symmetry of bilayer systems, coupled by both tunneling and Coulomb interaction, has fundamental influences on the collective charge-density excitations. In the general case of two-subband occupation, three modes with one intersubband and two (optical and acoustic, respectively) intrasubband plasmons are calculated. By breaking the space symmetry, these modes are found to be mixed, giving rise to an anticrossing behavior between the intersubband and optical intrasubband plasmons. For the asymmetric case, the acoustic intrasubband plasmon is not Landau damped in the long-wavelength limit.

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It has been well known that tunneling coupled bilayer systems create remarkable new quantum effects and many-body phenomena, due to the interplay of tunneling and Coulomb coupling.[1] Less emphasized is the influence of its space symmetry. Quite a number of experimental[2–6] and theoretical[7–11] letters have been devoted to symmetric bilayer systems. Only recently, based on the study of the ballistic transport in a single-particle picture, bilayer systems with controllable space symmetry have been proposed to make either a quantum transistor[12] for spintronics[13] or quantum gates[14] for quantum computing. Here we study the influence of the space symmetry on the many-body phenomena of a bilayer system by analyzing its plasmon modes. It permits a clear insight into the collective charge excitations in quantum confined structures where the subband structure under different space symmetries plays an important role.

It is well known that the collective excitations in multilayered and multisubband electronic systems can be coupled.[15,16] A most direct evidence was given already quite some time ago by Oelting *et al.*[17] who observed a pronounced anticrossing of the in-plane plasmon and the intersubband resonance in Si (100) metal-oxide-semiconductor systems. Shortly after, Jain and Das Sarma[18] predicted mode-coupling effects existing in an asymmetric single quantum well based on a GaAs-AlGaAs heterostructure. This interesting idea of mode mixing in a single quantum well is, however, up to now, experimentally not confirmed, possibly because of the unusual sample structure required.

In this paper we show that the tunneling-coupled bilayer system provides an ideal system to study the influence of space symmetry on collective excitations. The space symmetry of this system can be easily tuned using a front gate. Besides, the system can be viewed as a quasi-two-dimensional electron system (2DES) with "digitalized" subband information, so that we can describe the subband wave functions and the Coulomb interaction as 2D vectors and a matrix, respectively. This allows us to develop a transparent formalism for the charge-density excitations under variable space symmetry, which is otherwise sophisticated and tedious for a quasi 2DES. Analytical results for coupled plasmon modes are obtained for bilayer systems with arbitrary space symmetry. For symmetric bilayer systems, our results are consistent with that obtained recently.[19,20] We apply random-phase approximation (RPA) that is known to be reliable for systems with high densities, where the exchange interaction is small.[4,15,16,18,19,21] We note that interesting effects on plasmon modes caused by the exchange interaction have been studied in the low-density regime.[4,20] However, in this paper, we focus on the important influences of the space symmetry on the many-body effects in bilayer systems that has so far been neglected. For our purpose, the limiting RPA formalism would be sufficient since we are interested in the space asymmetry induced mode mixing and anticrossing behavior, which we find to be significant in bilayer systems with high densities.

The response of a quasi-2DES to longitudinal electric fields of arbitrary wave vector q and frequency ω, is given by the equations[18,21]

$$\delta_{ij,kl} - V_{ij,kl} D_{ij} = 0, \tag{1}$$

$$V_{ij,kl} = \frac{2\pi e^2}{\varepsilon q} \langle \xi_i(z)\xi_j(z) | e^{-q|z-z'|} | \xi_k(z')\xi_l(z') \rangle, \tag{2}$$

$$D_{ij} = 2 \lim_{\alpha\to 0} \sum_k \frac{f[E_j(k+q)] - f[E_i(k)]}{E_j(k+q) - E_i(k) - \hbar(\omega + i\alpha)}, \tag{3}$$

where $V_{ij,kl}$ is the Fourier transform of the Coulomb interaction, $\xi_i(z)$ is the wave function for the ith subband due to the quantum confinement along the z axis, and ε is the background static dielectric constant. D_{ij} is the polarizability function for the $i \to j$ transition in the absence of Coulomb interactions, $E_i(k) = E_i(0) + \hbar^2 k^2/2m^*$ is the single-particle energy in the ith subband, and $f(E)$ is the Fermi-Dirac occupation probability.

We consider a tunneling coupled bilayer system with arbitrary space symmetry in the z direction. With no loss of generality, we assume that the intralayer intersubband energy as well as the height of the tunneling barrier are much larger than the energy separation Δ of the lowest tunneling coupled symmetric- (+) and antisymmetriclike (−) states. Then the subband wave function ξ_i and Coulomb interaction $V(q)$ can be written in the layer-index space as[12]

$$\xi_+ = \begin{pmatrix} \sin\frac{\delta}{2} \\ \cos\frac{\delta}{2} \end{pmatrix},$$

$$\xi_- = \begin{pmatrix} \cos\frac{\delta}{2} \\ -\sin\frac{\delta}{2} \end{pmatrix}, \tag{4}$$

and

$$V(q) = \frac{2\pi e^2}{\varepsilon q} \begin{pmatrix} 1 & e^{-qd} \\ e^{-qd} & 1 \end{pmatrix}, \tag{5}$$

respectively. Here d is the interlayer distance and $\sin\delta = \Delta_{SAS}/\Delta$ reflects the space symmetry of the bilayer system along the z axis. For a symmetric bilayer system, Δ is equal to the tunneling gap Δ_{SAS} so that $\delta = \pi/2$. Using Eqs. (4) and (5), we can write Eq. (1) in the form

$$\begin{vmatrix} 1-V_A D_{++} & -V_{AA} D_{++} & V_{AR} D_{++} & V_{AR} D_{++} \\ -V_{AA} D_{--} & 1-V_A D_{--} & -V_{AR} D_{--} & -V_{AR} D_{--} \\ V_{AR} D_{+-} & -V_{AR} D_{+-} & 1-V_R D_{+-} & -V_R D_{+-} \\ V_{AR} D_{-+} & -V_{AR} D_{-+} & -V_R D_{-+} & 1-V_R D_{-+} \end{vmatrix} = 0, \tag{6}$$

where the Coulomb matrix elements are given by

$$V_A = \frac{2\pi e^2}{\varepsilon q}\left[1 - \frac{1}{2}(1-e^{-qd})\sin^2\delta\right],$$

$$V_R = \frac{2\pi e^2}{\varepsilon q}\left[\frac{1}{2}(1-e^{-qd})\sin^2\delta\right],$$

$$V_{AA} = \frac{2\pi e^2}{\varepsilon q}\left[e^{-qd} + \frac{1}{2}(1-e^{-qd})\sin^2\delta\right],$$

$$V_{AR} = \frac{2\pi e^2}{\varepsilon q}\left[\frac{1}{2}(1-e^{-qd})\sin\delta\cos\delta\right]. \tag{7}$$

The upper left 2×2 block in Eq. (6) describes the two coupled intrasubband plasmons. They lead to the optical and acoustic plasmon modes in a quasi-2DES if two subbands are occupied.[15,16,18] The lower right 2×2 block describes the intersubband plasmon. Here, the identical Coulomb matrix elements V_R, in both diagonal and off-diagonal terms, reflect a hidden symmetry for the charge excitation along the z axis. It allows only one intersubband plasmon mode even when both subbands are occupied. Mathematically, Eq. (6) can be reduced to

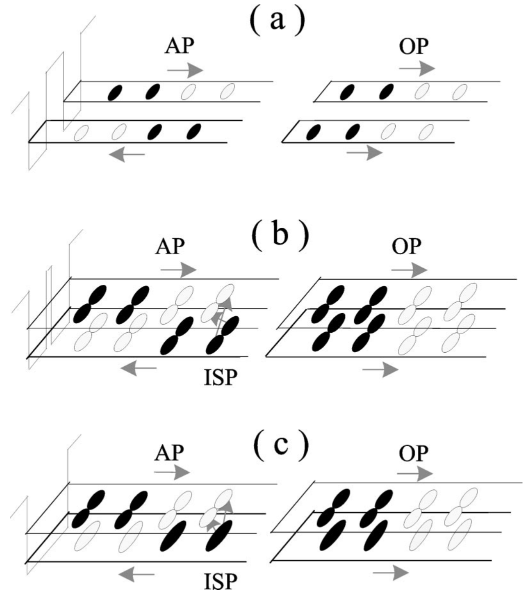

FIG. 1. Schematic collective charge oscillations (arrows) in (a) a two-quantum well system, (b) a bilayer structure, and (c) a single quantum well with two populated subbands. The dark (light) regions indicate the accumulation (depletion) of charges.

$$\begin{vmatrix} 1-V_A D_{++} & -V_{AA} D_{++} & V_{AR} D_{++} \\ -V_{AA} D_{--} & 1-V_A D_{--} & -V_{AR} D_{--} \\ V_{AR} D_R & -V_{AR} D_R & 1-V_R D_R \end{vmatrix} = 0, \tag{8}$$

where $D_R = D_{+-} + D_{-+}$ describes the noninteracting intersubband polarizability function. Equation (8) gives three mixed modes in a bilayer system with arbitrary space symmetry.

Before we start calculating these modes, we will first discuss a picture of charge oscillations in a bilayer system using different approaches. A tunneling coupled bilayer system can be formed using two quantum wells with a decreasing barrier in between. As shown in Fig. 1(a), the charges localized in the two quantum wells can oscillate in-plane, in- and out-of-phase due to Coulomb interactions, giving rise to the two-layer optical (OP) and acoustic plasmon (AP), respectively.[15,16,22] By decreasing the barrier, tunneling splits the single level in each quantum well and forms the symmetric and antisymmetric levels that are delocalized over both wells [Fig. 1(b)]. The interlayer charge-transfer process is now much faster than the collective intralayer charge oscillation, so that a two-layer acoustic plasmon can no longer be built up. However, as shown in Fig. 1(b), the charges that populate the symmetric and antisymmetric levels can oscillate in-plane and out-of-phase, due to Coulomb interactions, which gives rise to the intrasubband optical and acoustic plasmon, respectively. In addition, the collective charge oscillation along the z axis gives rise to an intersubband plasmon (ISP). These modes can also be visualized using a single quantum well [Fig. 1(c)] with two subbands populated, and has been well discussed by Jain and Das Sarma[18] However, we shall see later, that introducing a barrier in the center of a quantum well has a significant effect on the in-plane out-of-phase charge oscillation, which causes a mode softening of the intrasubband AP mode.

Now let us study these modes by looking at different limits. In the symmetric limit, $\delta=\pi/2$, we have from Eq. (7), $V_{AR}=0$ so that the intra- and intersubband plasmons are decoupled. Let us consider the leading terms of the polarizability function[18,21] in the long-wavelength limit $(q\rightarrow 0)$ with $D_{++}=n_+q^2/m^*\omega^2$, $D_{--}=n_-q^2/m^*\omega^2$, and $D_R=2(n_+-n_-)\Delta^2/(\omega^2-\Delta^2)$, where $n_\pm$ are the electron densities of the $\pm$ states and m^* is the electron effective mass. Equation (8) can be solved analytically and we get the dispersion of the intrasubband OP and the ISP modes with $\omega_{OP}^2=2\pi e^2(n_++n_-)q/\varepsilon m^*$ and $\omega_{ISP}^2=\Delta_{SAS}^2+\pi(n_+-n_-)q_{TF}d(1-qd/2)\Delta_{SAS}/m^*$. Here $q_{TF}=2m^*e^2/\varepsilon$ is the Thomas-Fermi wavelength (we take $\hbar=1$ in our paper). The intrasubband AP mode is Landau damped. In this symmetric case our results are identical to the recent calculations in Ref. 19. Please note that in the $q\rightarrow 0$ limit, the ω_{ISP} mode can be interpreted as the intersubband resonance, which is shifted with respect to the single-particle energy Δ_{SAS} by the depolarization effect,[23] i.e., the second term in ω_{ISP}. It has been investigated experimentally in Refs. 3 and 4 on symmetric bilayer systems.

Interesting physics occurs if we consider an asymmetric situation. To make the case simple, let us start by assuming that only one subband is occupied so that the Fermi energy $E_F=\pi N_s/m^*<\Delta=\Delta_{SAS}/\sin\delta$ and $n_+=N_s, n_-=0$. Equation (8) can again be solved analytically and we get

$$\omega_\pm^2=\frac{1}{2}(\omega_{OP}^2+\omega_{ISP}^2)\pm\frac{1}{2}\sqrt{(\omega_{OP}^2-\omega_{ISP}^2)^2+4\frac{V_{AR}^2}{V_AV_R}\omega_{OP}^2(\omega_{ISP}^2-\Delta^2)} \tag{9}$$

with $\omega_{OP}^2=2\pi e^2N_sq/\varepsilon m^*$ and $\omega_{ISP}^2=\Delta^2+2N_sV_R\Delta+Cq^2$ describing the intra- and intersubband plasmon, respectively. Here the parameter C that is not shown for brevity is determined by expanding D_R to the q^2 term. Equation (9) describes the anticrossing behavior of the ω_{OP} and ω_{ISP} modes. In the long-wavelength limit, the resonant condition is defined by $\omega_{OP}(q_0)=\omega_{ISP}$ with

$$q_0\approx\pi\frac{N_s}{q_{TF}}\left(\frac{\Delta_{SAS}}{E_F\sin\delta}\right)^2\left(1+\frac{q_{TF}dE_F\sin^2\delta}{\Delta_{SAS}}\right). \tag{10}$$

The splitting ω_G between the $\omega_\pm$ modes at the resonant point is given by

$$\omega_G^2\approx\frac{1}{8}q_0q_{TF}d^2\Delta_{SAS}E_F\sin\delta\cos^2\delta, \tag{11}$$

which is significant in high-density systems with large Fermi energies. We should remark that it is also in the high-density regime that RPA is known to be more reliable.

For the general case with neither restricting to the one-subband occupation nor to the long-wavelength limit, we calculate the collective excitation spectra of a coupled bilayer system by solving Eq. (8). The results are depicted in Fig. 2 with the shaded regions indicating the single-particle continua. The mode dispersions in the symmetric case are shown in Fig. 2(a). Here only the ISP and OP modes are found outside the Landau damping region. The AP mode compared with that in a single quantum well with two subbands populated, is softened and Landau damped. The reason can be understood by comparing the different charge distribution of the lowest subband shown in Figs. 1(b) and 1(c). The introducing of a barrier in the center of a quantum well brings a node to the wave function of the lowest subband, so that the charge distributions of the two subbands gets similar. To build up an AP mode between two charge components with the same effective mass, the Coulomb interaction within and between the two components (in our case V_A and V_{AA}, respectively) must be different. A good example studied is the

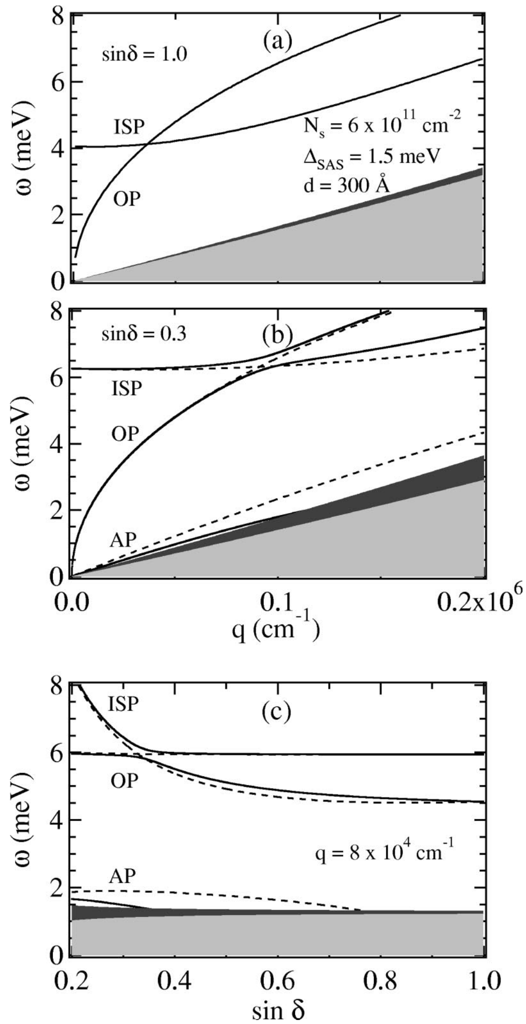

FIG. 2. Plasmon dispersions for a bilayer system with interlayer distance $d=300$ Å, electron density $N_s=6\times10^{11}$ cm^{-2}, and a tunneling gap $\Delta_{SAS}=1.5$ meV in (a) a symmetric case with $\sin\delta=1$ and (b) asymmetric case with $\sin\delta=0.3$. (c) Plasmon energies plotted as a function of $\sin\delta$ at a fixed wave vector $q=8\times10^4$ cm^{-1}. Dashed lines represent plasmon energies in the absence of coupling between inter- and intrasubband modes ($V_{AR}=0$). Shaded regions indicate the single-particle continua of the two populated subbands.

system with electrons localized in two quantum wells separated by a barrier.[15,16,22] By increasing the barrier thickness d, the interlayer Coulomb interaction becomes weaker compared with the intralayer Coulomb interaction so that the AP mode gains energy and moves out of the single-particle continuum. In the two-level populated tunneling-coupled bilayer system, we find that by changing the space symmetry, the charge distribution on the two levels changes, so that the ratio of V_{AA}/V_A can be tuned, which modifies the group velocity of the AP mode. In the asymmetric bilayer system, the AP mode is not Landau damped in the long-wavelength limit.

In Fig. 2(b), we plot the result calculated for a tunneling-coupled bilayer system with broken space symmetry (e.g., by applying a front gate voltage). Here not only the OP and ISP modes are mixed, but they are both mixed with the AP mode that appears now outside of the Landau damping region at long wavelengths. By setting the matrix element $V_{AR}=0$ (i.e., assuming that the inter- and intrasubband plasmons are decoupled), the AP mode recovers a linear dispersion (shown by a dashed line) that is typical for an acoustic plasmon. We predict that such a space-symmetry dependent resonant interaction between the OP and ISP modes, as well as the unique group velocity change of the AP mode in bilayer systems, can be observed by both Raman and FIR spectroscopy. In the Raman experiment, an asymmetric bilayer with a fixed value of $\sin\delta$ can be used. The resonant condition can be achieved by changing q. In the FIR experiment, a bilayer system can be fabricated with both a gate and a grating coupler. Then $q=2\pi/a$ is fixed by the grating-coupler period a. However, the resonant condition can still be reached by changing the gate voltage so that $\sin\delta$ is tuned.[12] In Fig. 2(c), results are shown for a fixed q by varying the space symmetry.

In summary, we study the space symmetry influence on the charge-density excitation spectrum of bilayer systems. Mode-mixing effects are found if the space symmetry is broken. Analytical results for an anticrossing behavior, due to resonant interaction of the intra- and intersubband plasmons, are obtained. Sample structure and experimental conditions to observe such mode-mixing behavior are suggested. The method developed here offers interesting new possibilities to bring insight into other phenomena influenced by space symmetry, for example, in spin-polarized systems.

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