Neutral-donor-bound collective excitations in the bulk and in quantum wells

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(Received 15 August 1994)

The bound states of plasmons, of phonons, and of coupled plasmon-phonon modes at neutral donors in bulk semiconductors and in semiconductor quantum-well systems are studied here. The binding is caused by the virtual excitation and deexcitation of the donor between its ground and first excited electronic states by the collective excitation which gives rise to an effective attraction between the collective excitation and the donor. The interaction of coupled plasmon-phonon excitations, which are important in compound semiconductor systems, with electrons and also the interaction of plasmons with electrons have been derived in the long-wavelength limit of the random-phase approximation. These interactions are used to derive expressions for the binding energies of these collective excitations to neutral donors. In the case of plasmons in bulk systems we find a strong dependence of the binding energy on carrier density. In quantum-well systems, the dependence of the binding energy of the coupled plasmon-phonon modes on the well width is found to be particularly rich. The present results are in generally good accord with available experimental data for quantum-well systems.

I. INTRODUCTION

The plasmon collective excitations of semiconductor quantum-well systems have attracted considerable attention. In recent Raman scattering experiments Gammon, Shannabrook, and Musser[1] have suggested that they have observed an unusual density-dependent state in $GaAs/Al_xGa_{1-x}As$ quantum-well systems. Using a macroscopic phenomenological approach they have suggested that these states involve plasmons bound to neutral donors and coupled to the longitudinal-optical (LO) phonons of this system. Nevertheless, neither a full quantum-mechanical formulation of this problem nor quantitative calculations have been done in order to identify these states microscopically.

We address this problem in both bulk and quantum-well systems. We propose that the physical mechanism giving rise to these bound states is similar to that involving bound states of LO phonons at neutral donors in bulk semiconductors. Such states have been observed for a number of donors,[2,3] and have been studied theoretically.[2,4,5] The physical mechanism involved is that the LO-phonon interacts with the shallow bound electron of the neutral donor and causes transitions between its ground state and its first excited state. Virtual excitation and deexcitation of these states gives rise to an attraction of the phonon to the donor and can give a dynamically bound phonon state there.

In the present work we give a full quantum-mechanical formulation of the bound states involving plasmons and coupled plasmon–LO-phonon modes in bulk and in quantum-well systems. The interactions between plasmons and carriers is less well understood than that of LO phonons with carriers. Here we obtain this interaction as well as that between coupled plasmon-phonon modes and carriers from the long-wavelength limit of the random-phase approximation. General results for the binding of these collective excitations at neutral donors are developed, and detailed results are given for both the bulk and quantum-well cases.

Among the interesting results that we obtain are that the binding energy of plasmons to donors in bulk systems has a strong dependence on carrier density, and that the binding energy of the coupled modes in quantum-well systems has a rich structure as a function of well width. The results for the overall magnitude of the binding, for their well width dependence, and for their carrier density dependence are in good overall agreement with the experimental results of Gammon, Shanabrook, and Musser.[1] This allows us to confirm that the states observed by these authors are indeed states of plasmon-phonon coupled modes which are bound dynamically at the neutral donors.

This paper is organized as follows. In Sec. II, we treat the binding of plasmons and coupled phonon-plasmon modes to neutral donors in the bulk. The corresponding results for quantum wells are derived in Sec. III. Finally, detailed results for quantum-well systems are given and are compared to experiment in Sec. IV.

II. THE BULK CASE

In this section, we will generalize the method of Ref. 4 to derive expressions for the binding energies of several collective excitations to neutral donors in the bulk. We begin with the derivation of the binding energy for a plasmon at a neutral donor. This derivation will serve as the basis of our generalization to the quantum-well case.

A. Plasmons

The interaction between bulk plasmons and free electrons is represented by a Hamiltonian of the form

$$H_{\rm int}=\sum_{\mathbf{K},\mathbf{q}}\gamma_{\rm pl}(q)a_{\mathbf{K}}^{+}a_{\mathbf{K}-\mathbf{q}}^{-}(b_{\mathbf{q}}^{-}+b_{-\mathbf{q}}^{+}) , \tag{2.1}$$

where $a_{\mathbf{K}}^{+(-)}$ and $b_{\mathbf{K}}^{+(-)}$ are the creation (annihilation) operators for the electrons and plasmons, $\mathbf{q}$ and $\mathbf{K}$ are three-dimensional wave vectors, and $\gamma_{\rm pl}(q)$ is the electron-plasmon coupling which we will derive below.

Because we are interested in the interaction between bulk plasmons and bound electrons, we convert Eq. (2.1) to the basis of the bound electron wave functions denoted by s and t [$\Psi_s(r)=\langle r|s\rangle=\langle r|a_s^{+}|0\rangle$]:

$$H_{\rm int}=\sum_{s,t,\mathbf{q}}\gamma_{\rm pl}(q)g_{st}(q)a_s^{+}a_t^{-}(b_{\mathbf{q}}^{-}+b_{-\mathbf{q}}^{+}) , \tag{2.2}$$

where $g_{st}(q)=\int d^3r\,\Psi_s^{*}(r)\exp^{-i\mathbf{q}\cdot\mathbf{r}}\Psi_t(r)$.

In the context of phonons, given an interaction of the form Eq. (2.2), Monecke *et al.*[4] have shown that a bound state can be formed, and they have derived an expression for the binding energy by using second-order degenerate Wigner-Brillouin perturbation theory and solving a set of coupled integral equations. The binding energy for a plasmon is[6(a)]

$$E_B=\frac{-2E_{st}}{E_{st}^2-(\hbar\omega_{\rm pl})^2}\int\frac{d^3K}{(2\pi)^3}|\gamma_{\rm pl}(K)|^2|g_{st}(K)|^2 , \tag{2.3}$$

where E_{st} is the energy difference between the s and t bound electron states, and $\omega_{\rm pl}$ is the plasmon frequency. Even though Eq. (2.3) has been derived in the context of plasmons, it is quite general and can apply to other excitations like phonons or coupled plasmon-phonon modes. To evaluate this expression for the plasmon case we must derive the electron-plasmon coupling.

The approach we employ to calculate $\gamma_{\rm pl}(q)$ is based on the methods of Lundqvist[6(b)] and DuBois.[7] We write the screened electron interaction as calculated in the long-wavelength limit of the random-phase approximation as the sum of the bare Coulomb interaction and a plasmon-mediated interaction, and then solve this equation for the one unknown, the electron-plasmon coupling strength. Our equation is illustrated in Fig. 1(a), where the term in the numerator on the left-hand side of the equation (and the first term on the right-hand side of the equation) is the bare Coulomb interaction, $v(q)=4\pi e^2/(\epsilon_0 q^2)$ where ϵ_0 is the low-frequency dielectric constant. The term in the denominator in Fig. 1(a) is the dielectric function, and the second term on the right-hand side is the product of the square of the electron-plasmon coupling and the plasmon propagator. We can write the equation in Fig. 1(a) as

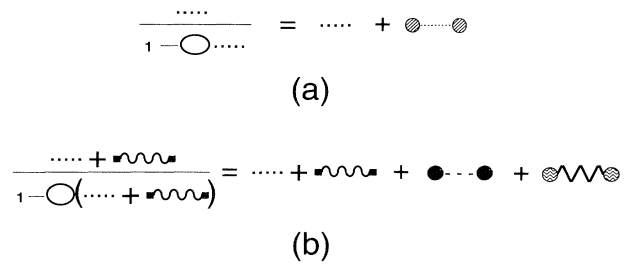

FIG. 1. Feynman diagrams representing (a) Eq. (2.4) and (b) Eq. (2.8). The dotted line is the bare Coulomb interaction, the ellipse is the electron polarization, the shaded circle is the electron-plasmon coupling, and the dashed line is the plasmon propagator. The filled square is the electron–LO-phonon coupling, the filled circle the electron-coupled mode (lower branch) coupling, the jaggedly shaded circle the electron-coupled mode (upper branch) coupling, the squiggly line the phonon propagator, the long dashed line the lower branch coupled mode propagator, and the jagged line the upper branch coupled mode propagator.

$$\frac{v(q)}{1-\pi(q,\omega)v(q)}=v(q)+|\gamma_{\rm pl}(q)|^2\frac{2\omega_{\rm pl}}{\hbar(\omega^2-\omega_{\rm pl}^2)} , \tag{2.4}$$

where $\pi(q,\omega)$ is the polarization operator, $\omega_{\rm pl}=\sqrt{4\pi ne^2/(m_e\epsilon_0)}$, n is the electron number density, and m_e is the effective mass of the electron. Here, we will neglect the dispersion of the plasmon frequency $\omega_{\rm pl}=\omega_{\rm pl}(q)$. Solving Eq. (2.4) for $\gamma_{\rm pl}(q)$, we find

$$\gamma_{\rm pl}(q)=\sqrt{v(q)\hbar\omega_{\rm pl}/2} , \tag{2.5}$$

where we have used the long-wavelength limit of the polarization operator, $\pi(q,\omega)\simeq nq^2/(m\omega^2)$. Equation (2.5) is equivalent to the result obtained by Lundqvist[6] by examining the structure of the density-fluctuation propagator near its poles. Note that in the long-wavelength limit the electron-plasmon coupling has the same q dependence as the Froehlich electron–LO-phonon coupling.

Knowing $\gamma_{\rm pl}(q)$ we can now evaluate Eq. (2.3) for the bound-state energy of a plasmon at a neutral donor in the bulk,

$$E_B=\frac{-2E_{\rm st}}{E_{st}^2-(\hbar\omega_{\rm pl})^2}\frac{56}{6561}\frac{e^2}{a_B}\hbar\omega_{\rm pl} , \tag{2.6}$$

where a_B is the Bohr radius of the hydrogenic donor electron. One of the salient features of this equation is that it has a strong dependence on the difference $E_{st}^2-(\hbar\omega_{\rm pl})^2$. By changing the electron number density, one can change not only the magnitude of the binding energy but also the sign. This is in contrast to the binding energy of a LO phonon bound to a neutral donor,

$$E_B=\frac{-2E_{st}}{E_{st}^2-(\hbar\omega_{\rm LO})^2}\frac{56}{6561}\frac{e^2}{a_B}\frac{\hbar(\omega_{\rm LO}^2-\omega_{\rm TO}^2)}{\omega_{\rm LO}} , \tag{2.7}$$

where such tuning is not as simple because the phonon frequency is not strongly electron density dependent. In Eq. (2.7), $\omega_{\rm LO}$ is the LO-phonon frequency, $\omega_{\rm TO}=\omega_{\rm LO}\sqrt{\epsilon_\infty/\epsilon_0}$ is the transverse-optical (TO)-phonon

frequency, and ϵ_∞ is the high-frequency dielectric constant. Note that the overall structure of Eqs. (2.6) and (2.7) is similar.

B. Coupled phonon-plasmon modes

In compound semiconductor systems, the plasmons and LO phonons couple to each other, and it is the coupled modes that become bound to the neutral donors. To calculate these binding energies, we can again use Eq. (2.3), but we must derive the coupled mode energies and the expressions for the coupling between the electrons and the coupled modes.

The strategy we use to calculate these quantities is similar to the technique used above for the case of the pure plasmon modes. We write the fully screened electron interaction (with the phonon mediated interaction included) as the sum of the bare Coulomb interaction, the bare phonon-mediated interaction, and the coupled-mode-mediated interactions, and then solve the resulting equation for the coupled mode energies and for the electron-coupled mode coupling. This equation is illustrated in Fig. 1(b) and can be written

$$\frac{v(q)+v_{\rm ph}(q)}{1-\pi(q,\omega)[v(q)+v_{\rm ph}(q)]} = v(q)+v_{\rm ph}(q)+|\gamma_+(q)|^2\frac{2\omega_+}{\hbar(\omega^2-\omega_+^2)} + |\gamma_-(q)|^2\frac{2\omega_-}{\hbar(\omega^2-\omega_-^2)} , \tag{2.8}$$

where $v_{\rm ph}(q)=\gamma_{\rm ph}^2(q)D(\omega)$ is the phonon-mediated electron interaction, $\gamma_{\rm ph}(q)$ is the Froehlich electron–LO-phonon coupling,

$$\gamma_{\rm ph}(q)=\left[\frac{2\pi e^2\hbar\omega_{\rm LO}}{q^2}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2} , \tag{2.9}$$

$D(\omega)=2\omega_{\rm LO}/\hbar/(\omega^2-\omega_{\rm LO}^2)$ is the phonon propagator, $\gamma_\pm(q_\parallel)$ are the electron-coupled mode couplings, and $\omega_\pm$ are the coupled mode frequencies. $v(q)$ and $\pi(q,\omega)$ have the same meanings as in Eq. (2.4). This equation can be rewritten as

$$|\gamma_+(q)|^2\frac{2\omega_+}{\hbar(\omega^2-\omega_+^2)}+|\gamma_-(q)|^2\frac{2\omega_-}{\hbar(\omega^2-\omega_-^2)} = \frac{[v(q)+v_{\rm ph}(q)]\pi(q,\omega)[v(q)+v_{\rm ph}(q)]}{1-\pi(q,\omega)(v(q)+v_{\rm ph}(q))} . \tag{2.10}$$

Equation (2.10) can now be solved to find $\omega_\pm$ and $\gamma_\pm(q)$. The energies of the coupled modes $\hbar\omega_\pm$ are found from the energies at which the right-hand side diverges. This gives

$$\omega_\pm=(\omega_{\rm LO}+\omega_{\rm pl})/2\pm\sqrt{(\omega_{\rm LO}+\omega_{\rm pl})^2-4\omega_{\rm pl}\omega_{\rm TO}}/2 . \tag{2.11}$$

Using this result, we arrive at

$$|\gamma_\pm(q)|^2=\pm\frac{v(q)\hbar\omega_{\rm pl}^2(\omega_\pm^2-\omega_{\rm TO}^2)^2}{2\omega_\pm(\omega_+^2-\omega_-^2)(\omega_\pm^2-\omega_{\rm LO}^2)} . \tag{2.12}$$

Therefore the binding energies of the coupled modes at neutral donors in the bulk are

$$E_B=\pm\frac{-2E_{st}}{E_{st}^2-(\hbar\omega_\pm)^2}\frac{56}{6561}\frac{e^2}{a_B}\frac{\hbar\omega_{\rm pl}^2(\omega_\pm^2-\omega_{\rm TO}^2)^2}{\omega_\pm(\omega_+^2-\omega_-^2)(\omega_\pm^2-\omega_{\rm LO}^2)} . \tag{2.13}$$

One can see that the binding energies for the coupled modes have much more structure than those of the pure modes. In particular the factor $\omega_-^2-\omega_{\rm LO}^2$ in the numerator has the potential to produce kinks in the electron-density-dependent curve since $\omega_-=\omega_-(n)$ passes through $\omega_{\rm TO}$.

III. THE QUANTUM-WELL CASE

We apply our methods to the quantum-well case in this section. We consider a quantum well such as the GaAs/Al_xGa_{1-x}As system in which the larger band gap of the Al_xGa_{1-x}As relative to GaAs causes the electrons to be quantized into subbands in the GaAs layer. We will consider the binding of quantum-well collective excitations via the virtual excitation and deexcitation of electrons between the states commonly referred to as the $1s$ and $2p_z$ states of shallow neutral donors in quantum wells. (z is taken to be the direction perpendicular to the quantum well.) This is the case of experimental interest in Ref. 1. We treat the electrons as hydrogenic, and assume that they are located in the center of the quantum well. The $1s$ state is the ground state of the donor, and is associated with the lowest-lying subband (denoted by the subscript 0) which has no node perpendicular to the quantum well. The $2p_z$ state has one node in the z direction, and its energy is just below that of the first excited subband (denoted by the subscript 1) in the quantum well. The association of the $1s$ ($2p_z$) state with the lowest (first excited) subband is illustrated in Fig. 2(a).

There are two types of plasma excitations in a quantum well. The acoustic plasmon has an electric field polarized parallel to the quantum well and, because there is no resulting restoring force on the plasma, its energy vanishes as $q\rightarrow 0$. This is illustrated in Fig. 2(b). Because the acoustic plasmons have no lower bound for their dispersion, well-defined bound states are less likely to occur with them. In addition, because their dispersion lies so close to the particle-hole continuum, acoustic plasmons easily decay. Therefore we will not consider them here. A second kind of plasmon whose dispersion contains a gap [see Fig. 2(b)] is known as the intersubband plasmon, because it involves transitions between two subbands. Its energy is slightly larger than the bare intersubband energy; this shift (the so-called depolarization shift) can be attributed to the polarization of the electron gas during the intersubband excitation. Because the dispersion of the intersubband plasmons has a lower bound, it can give rise to well-defined bound states. It is these plasmons with which we will be primarily concerned. To treat the LO phonons, we use a model of bulk GaAs phonons and

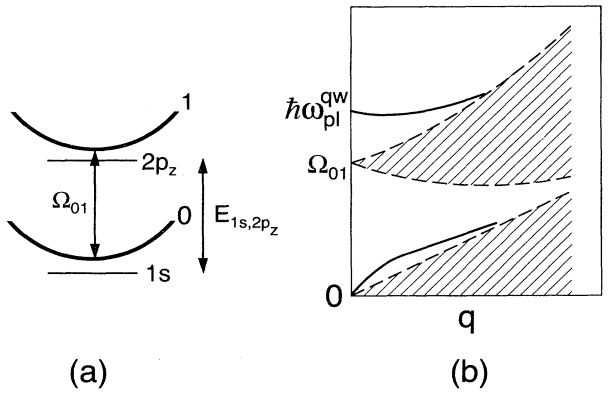

FIG. 2. (a) An illustration of the $1s$ and $2p_z$ donor states and their associations with lowest (0) and first subband (1). (b) The dispersion of the two types of plasmons occurring in a quantum well. The uppermost curve corresponds to the intersubband plasmon, the plasma excitation with which we will be primarily concerned. The shaded area is the electron-hole continuum.

neglect the effects of phonon confinement in the quantum well. It has been shown that this approach gives a good account of such quantities as electron-phonon-scattering rates in confined geometries.[8,9]

In order to derive an expression for the binding energy of phonons, plasmons, and coupled modes to a neutral donor in a quantum well, we follow a procedure similar to that used for the bulk case. We will take the potential barrier to be infinite and for the donor states we will use a separable variational wave function $\Psi_n(r)=\phi_n(z)\psi_n(\rho)$, where n indicates the shallow donor state (e.g., $1s$, $2p_z$, etc.). We will use $\psi_n(\rho)=\sqrt{2}\alpha_n/\sqrt{\pi}\exp[-\alpha_n\rho]$, where ρ is the two-dimensional vector parallel to the well. For $\phi_n(z)$, we use the envelope function of the corresponding subband. That is, for the donor state associated with the lowest (first excited) subband, we use $\phi_{1s}(z)=\zeta_0(z)$ $=\sqrt{2/L}\cos(\pi z/L)[\phi_{2p_z}(z)=\zeta_1(z)=\sqrt{2/L}\sin(2\pi z/L]$. Converting Eq. (2.1) to this basis, we find

$$H_{\rm int}=\sum_{m,n,\mathbf{q}_\parallel,q_z}\gamma(q_\parallel,q_z)f_{mn}(q_\parallel)f'_{mn}(q_z)\times a_m^+a_n^-(b_{\mathbf{q}}^-+b_{-\mathbf{q}}^+)\ , \tag{3.1}$$

where $\mathbf{q}_\parallel$ is the wave vector parallel to the quantum well, and $\mathbf{q}$ is the total wave vector. Here

$$f_{mn}(q_\parallel)=\int d^2\rho\,\Psi_m^*(\rho)\exp^{-i\mathbf{q}_\parallel\cdot\rho}\Psi_n(\rho) \tag{3.2}$$

and

$$f'_{mn}(q_z)=\int dz\,\phi_m^*(z)\exp^{-iq_zz}\phi_n(z)\ . \tag{3.3}$$

Applying the methods used above we arrive at an expression for the binding energy which is analogous to that for the bulk case:

$$E_B=\frac{-2E_{mn}}{E_{mn}^2-(\hbar\omega_{\rm exc})^2}\int\frac{d^2q_\parallel}{(2\pi)^2}|f_{mn}(q_\parallel)|^2|\gamma^{qw}(q_\parallel)|^2\ , \tag{3.4}$$

where E_{mn} is the energy difference between the m and n electronic states of the donor, $\omega_{\rm exc}$ is the energy of the collective excitation of interest, and $\gamma^{\rm qw}(q_\parallel)$ is the quantum-well electron-collective excitation coupling:

$$|\gamma^{\rm qw}(q_\parallel)|^2=\int\frac{dq_z}{2\pi}|f'_{mn}(q_z)|^2|\gamma(q_\parallel,q_z)|^2\ . \tag{3.5}$$

Since we are mainly interested in transitions between the ground state and the first excited state, we will associate m with the $1s$ state and n with the $2p_z$ state. Because the form factor $f'_{mn}(q_z)$ depends only upon subband wave functions, we will use the corresponding subband indices (0, 1, etc.) for it.

To evaluate the expression in Eq. (3.4), several quantities must be determined. We will begin with $f_{1s2p_z}(q_\parallel)$. The first step in determining $f_{1s2p_z}(q_\parallel)$ is to perform the integral in Eq. (3.2) to find

$$f_{1s2p_z}(q_\parallel)=\frac{4\alpha_{1s}\alpha_{2p_z}(\alpha_{1s}+\alpha_{2p_z})}{[(\alpha_{1s}+\alpha_{2p_z})^2+q_\parallel^2]^{3/2}}\ . \tag{3.6}$$

The calculation of α_{1s} and α_{2p_z} involves the variational solution of the following Hamiltonian:

$$H=-\frac{\hbar^2\nabla^2}{2m_e}-\frac{e^2}{\epsilon_0[\rho^2+(z-z_i)^2]^{1/2}}+V_{\rm conf}(z)\ , \tag{3.7}$$

where z_i is the location of the donor (which we take to be the center of the well), and $V_{\rm conf}(z)$ is the confinement potential:

$$V_{\rm conf}=\begin{cases}0, & z\le L/2\\ \infty, & z>L/2\ ,\end{cases} \tag{3.8}$$

where L is the width of the well. The resulting expressions must be minimized numerically to determine α_{1s} and α_{2p_z} for each value of the well width. We will leave the discussions of calculating $f'_{01}(q_z)$ until Sec. IV.

The variational approach used here gives reasonably good results for the donor bound wave functions and energies for well widths that are not too large. In experimental situations, however, E_{1s2p_z} depends on such additional effects as screening and the finite potential barriers involved. If we use the present variational approach, which neglects these influences, we find that E_{1s2p_z} is slightly larger than the bare intersubband energy $\Omega_{01}=3\pi^2\hbar^2/(2L^2m)$. In experiments however, the results vary. Perry *et al.*[10] found in their resonant Raman-scattering experiments that E_{1s2p_z} was larger than Ω_{01} by a few millielectron volts (meV). Gammon, Shanabrook, and Musser,[1] on the other hand, observed Ω_{01} larger than E_{1s2p_z} by the same margin. Here we are interested in demonstrating the physics in this bound-state system, and we will use the approximation $E_{1s2p_z}\simeq\Omega_{01}$. We now turn to calculating the couplings between the electrons and the various collective excitations.

A. Phonons

We first consider the case of the binding of phonons and use the expression (2.9) for the electron-phonon coupling. One can then insert $\gamma_{\rm ph}(q)$ into Eq. (3.5) to perform the integral over q_z:

$$|\gamma_{\rm ph}^{\rm qw}(q_\parallel)|^2=\frac{e^2\hbar\omega_{\rm LO}}{L^2}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\left[\pi L\left[\frac{1}{q_\parallel^2+(\pi/L)^2}+\frac{1}{q_\parallel^2+(3\pi/L)^2}\right]-2\pi q_\parallel(1+e^{-iq_\parallel L})\left[\frac{1}{[q_\parallel^2+(\pi/L)^2]^2}-\frac{2}{[q_\parallel^2+(3\pi/L)^2)(q_\parallel^2+(\pi/L)^2]}+\frac{1}{[q_\parallel^2+(3\pi/L)^2]^2}\right]\right], \tag{3.9}$$

where we have used the result

$$f'_{01}(q_z)=\frac{-4ie^{-iq_zL/2}q_zL(1+p)[1-(-1)^pe^{iq_zL}]}{\pi^2[(q_zL/\pi)^2-(p+2)^2][(q_zL/\pi)^2-p^2]}, \tag{3.10}$$

with $p=n-m=1$. Equation (3.9) defines a quantity, $\gamma_{\rm ph}^{\rm qw}(q_\parallel)$, the coupling between electrons confined to a quantum well and bulk phonons. We use $p=1$ because we are interested in transitions between donor states associated with the lowest subband (0) and the first excited subband (1). The remaining integral over $q_\parallel$ in Eq. (3.4) must be done numerically, which we will discuss in Sec. IV. We will find it useful to do this integral neglecting the $q_\parallel$ dependence of the coupling. In that case,

$$\gamma_{\rm ph}^{\rm qw}(q_\parallel=0)=\sqrt{\alpha_{11}\hbar\omega_{\rm LO}\Omega_{01}/(4n_{\rm 2D})(1-\epsilon_\infty/\epsilon_0)},$$

and for the binding energy of the phonon to the neutral donor one finds

$$E_B=\frac{-2E_{1s2p_z}}{E_{1s2p_z}^2-(\hbar\omega_{\rm LO})^2}\left[\frac{\alpha_{1s}\alpha_{2p_z}}{\alpha_{1s}+\alpha_{2p_z}}\right]^2\times\frac{\Omega_{01}\alpha_{11}}{2\pi n_{\rm 2D}\omega_{\rm LO}}\hbar(\omega_{\rm LO}^2-\omega_{\rm TO}^2), \tag{3.11}$$

where

$$\alpha_{11}=\frac{80}{27\pi^3}\frac{L^3n_{\rm 2D}}{a_B}\frac{\epsilon_0}{\epsilon_\infty}.$$

The expression in Eq. (3.11) is similar to the bulk expression Eq. (2.7) with the difference that the sign and magnitude of the phonon binding energy in a quantum well can be controlled by changing the well width. The well width dependence enters through α_{11}, α_{1s}, α_{2p_z}, and E_{1s2p_z}.

B. Plasmons

We now derive the formula for the coupling between quantum-well electrons and intersubband plasmons employing the method used in Sec. II, where we derived the coupling between electrons and plasmons in the bulk from the screened electron-electron interaction. Since intersubband plasmons involve electronic transitions between subbands, we will need the expression for the screened electron-electron interaction in quantum wells in which one electron is excited into the next higher subband. The long-wavelength limit of this quantity has been derived by Wendler and Pechstedt[11] using the random-phase approximation:

$$V_{11}(q_\parallel)=[\alpha_{11}-\mu_{11}q_\parallel-\gamma_{11}q_\parallel^2]\Omega_{01}/(2n_{\rm 2D})+O(q_\parallel^3), \tag{3.12}$$

where α_{11} is defined above, $\mu_{11}=128/(45\pi^2)L\alpha_{11}$, $\gamma_{11}=23/(45\pi^2)L^2\alpha_{11}$, and the subscript 11 denotes an intersubband excitation.[12] Those authors[11] have also derived the quantum-well expression for the polarization in the long-wavelength limit:

$$\pi_{11}(q_\parallel,\omega)=2n_{\rm 2D}\Omega_{01}/[(\hbar\omega)^2-\Omega_{01}^2], \tag{3.13}$$

Substituting these two expressions into the corresponding bulk terms of Eq. (2.4), one finds the energy of an intersubband plasmon,

$$\hbar\omega_{\rm pl}^{\rm qw}=\Omega_{01}(1+\alpha_{11})^{1/2}, \tag{3.14}$$

where α_{11} is the so-called depolarization shift of the intersubband transition energy for finite carrier densities, and the quantum-well electron-intersubband plasmon coupling

$$\gamma_{\rm pl}^{\rm qw}=\sqrt{V_{11}(q_\parallel=0)\alpha_{11}\Omega_{01}/(1+\alpha_{11})^{1/2}}. \tag{3.15}$$

In Eq. (3.14), we have neglected the dispersion of the intersubband plasmon. Calculating the binding energy using Eq. (3.15), we find

$$E_B=\frac{-2E_{1s2p_z}}{E_{1s2p_z}-(\hbar\omega_{\rm pl}^{\rm qw})^2}\left[\frac{\alpha_{1s}\alpha_{2p_z}}{\alpha_{1s}+\alpha_{2p_z}}\right]^2\frac{\Omega_{01}^3\alpha_{11}^2}{2\pi n_{\rm 2D}\hbar\omega_{\rm pl}^{\rm qw}}. \tag{3.16}$$

Comparing this to the bulk expression, we note that we may not be able to change the magnitude and sign of Eq. (3.16) as readily in that case. This is because now $\omega_{\rm pl}^{\rm qw}$ is only weakly dependent on the electron density and E_{1s2p_z} and $\omega_{\rm pl}^{\rm qw}$ have approximately the same well width dependence.

C. Coupled phonon-intersubband plasmons

In quantum wells composed of compound semiconductor materials, like the GaAs/$Al_xGa_{1-x}As$ system of interest here, the longitudinal phonons and intersubband plasmons couple to each other. To find the energies of these modes and their couplings to the carriers, we must solve Eq. (2.10) using the quantum-well equivalents of each of the terms. Doing so, we find the frequencies of the coupled modes,

$$(\omega_{\pm}^{qw})^2=[\omega_{LO}^2+(\omega_{pl}^{qw})^2]/2\pm\sqrt{[\omega_{LO}^2+(\omega_{pl}^{qw})^2]^2-4\Omega_{01}^2(\omega_{LO}^2+\alpha_{11}\omega_{TO}^2)/\hbar^2}/2\ , \tag{3.17}$$

and the coupling of the coupled modes with the electrons,

$$|\gamma_{\pm}^{qw}(q_{\parallel})|^2=\pm V_{11}(q_{\parallel}=0)\alpha_{11}\Omega_{01}^2\frac{[(\omega_{\pm}^{qw})^2-\omega_{TO}^2]^2}{\hbar\omega_{\pm}^{qw}[(\omega_{+}^{qw})^2-(\omega_{-}^{qw})^2][(\omega_{\pm}^{qw})^2-\omega_{LO}^2]}\ . \tag{3.18}$$

The corresponding binding energies at neutral donors are

$$E_B=\pm\frac{-2E_{1s2p_z}}{E_{1s2p_z}^2-(\hbar\omega_{\pm}^{qw})^2}\left[\frac{\alpha_{1s}\alpha_{2p_z}}{\alpha_{1s}+\alpha_{2p_z}}\right]^2\frac{\Omega_{01}^3\alpha_{11}^2}{2\pi n_{2D}}\frac{[(\omega_{\pm}^{qw})^2-\omega_{TO}^2]^2}{\hbar\omega_{\pm}^{qw}[(\omega_{+}^{qw})^2-(\omega_{-}^{qw})^2][(\omega_{\pm}^{qw})^2-\omega_{LO}^2]}\ . \tag{3.19}$$

The similarities found between the quantum-well and bulk expressions for the phonon and plasmon binding energies are also found for the coupled modes.

IV. RESULTS

In this section, we summarize our results for collective excitations bound to neutral donors in quantum wells, analyze the electron density and quantum-well-width dependence of the binding energies, and compare our results with experimental data. For the quantities m_e, a_B, ω_{LO}, ω_{TO}, ϵ_0, and ϵ_∞, we have used values characteristic of GaAs, the quantum-well material of Ref. 1. For the fixed carrier density case, we use $n_{2D}=1.5e11\ \mathrm{cm}^{-2}$.

The binding energies for the collective excitations that we have considered can be written, from Eqs. (3.11), (3.16), and (3.19),

$$E_B=\frac{-2E_{1s2p_z}}{E_{1s2p_z}^2-(\hbar\omega_{exc})^2}\left[\frac{\alpha_{1s}\alpha_{2p_z}}{\alpha_{1s}+\alpha_{2p_z}}\right]^2\frac{\Omega_{01}^3\alpha_{11}^2}{2\pi n_{2D}\hbar\omega_{exc}}\Lambda_{exc}\ , \tag{4.1}$$

where

$$\Lambda_{exc}=\begin{cases}\dfrac{\hbar^2(\omega_{LO}^2-\omega_{TO}^2)}{\Omega_{01}^2\alpha_{11}} & \text{for LO phonons with } \omega_{exc}=\omega_{LO}\\ 1 & \text{for intersubband plasmons with } \omega_{exc}=\omega_{pl}^{qw}\\ \pm\dfrac{[(\omega_{\pm}^{qw})^2-\omega_{TO}^2]^2}{[(\omega_{+}^{qw})^2-(\omega_{-}^{qw})^2][(\omega_{\pm}^{qw})^2-\omega_{LO}^2]} & \text{for coupled modes with } \omega_{exc}=\omega_{\pm}^{qw}\ .\end{cases} \tag{4.2}$$

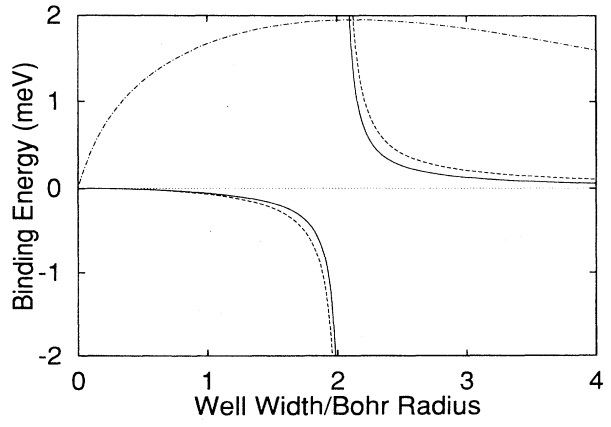

FIG. 3. The binding energies of phonons [Eq. (3.11), dashed line] and plasmons [Eq. (3.16), dot-dashed line] in quantum wells plotted vs the well width. The solid curve is explained in the text (Sec. IV).

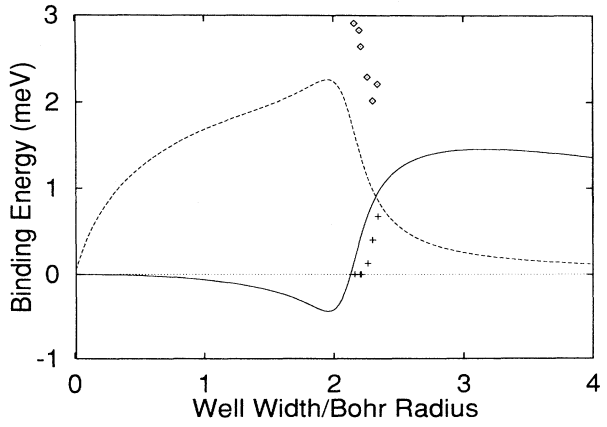

FIG. 4. The binding energy of the plasmonlike coupled mode (solid line) and the phononlike couple mode (dashed line) plotted vs the well width. Also included are experimental data from Ref. 1. The diamonds represent the binding energy of the phononlike mode, and the plus signs the plasmonlike modes.

In Fig. 3 we have plotted, as a function of well width and at a density $n_{20}=1.5\times10^{11}$ cm^{-2}, Eq. (3.11), the binding energy for LO phonons (dashed line), and Eq. (3.16), the binding energy for intersubband plasmons in a quantum well (dot-dashed line). For phonons, one observes that the binding energy diverges and changes sign near $\hbar\omega_{\rm LO}=E_{1s2p_z}$, but that otherwise the binding energies are on the order of at most a few meV. The binding energy for the intersubband plasmon, on the other hand, does not change sign in Fig. 3. This is because E_{1s2p_z} and $\omega_{\rm pl}^{\rm qw}$ have approximately the same well width dependence.

In Fig. 4, we have plotted the binding energies for the coupled intersubband plasmon-phonon modes. We can understand the general trends in this case by comparison with the case of phonons and plasmons shown in Fig. 3. One can see that the upper (or phononlike) branch of the coupled modes (dashed line) behaves like the intersubband plasmon for smaller well widths, and crosses over to behave like the LO-phonon curve for larger well widths. The opposite is true for the lower (or plasmonlike) branch of the coupled mode binding energy (solid line). Also plotted in Fig. 4 are the data[13] from Ref. 1. The diamonds correspond to the binding energies of phononlike modes, and the plus signs to the plasmonlike modes in the data. Note that the data are in rather good agreement with the results of our calculations for the limited values of well widths studied. Moreover, our results indicate that the structure of the binding energy as a function of the well width is much richer than the original experiments indicated.

In calculating Eqs. (3.11), (3.16), and (3.19), we neglected the $q_\parallel$ dependence of the coupling between the electron and the collective excitation being considered. In the case of the electron–LO-phonon coupling, the full $q_\parallel$ dependence is known [see Eq. (3.9)], and we have plotted the binding energy calculated using that expression in Fig. 3 (solid line). One can see that the $O(q_\parallel^0)$ curve is a good approximation to the full $q_\parallel$ dependence. We have assumed that this will be the case for the intersubband plasmon and the coupled intersubband plasmon and LO phonon, where the couplings with the carrier can be determined only to $O(q_\parallel^2)$, a condition imposed by the order in $q_\parallel$ to which $V_{11}(q_\parallel)$ [Eq. (3.12)] is known.

We can also derive the electron-density dependence of the binding energies. In Fig. 5, we have plotted the binding energy for the quantum-well coupled modes as a function of electron density for a given well width:[13] $L=2.21a_B$. The phononlike mode is the dashed curve, and the plasmonlike mode the solid curve. The corresponding data for the phononlike modes (diamonds) from Ref. 1 are also plotted. (We have not included the data for the plasmonlike modes because they were taken at a well width where the binding energy was zero within experimental resolution.) There is good overall agreement between our model and the data. The differences between the binding energy seen in the experiment and that in the present calculations probably result from effects like screening, finite barriers, and nonseparable wave functions.

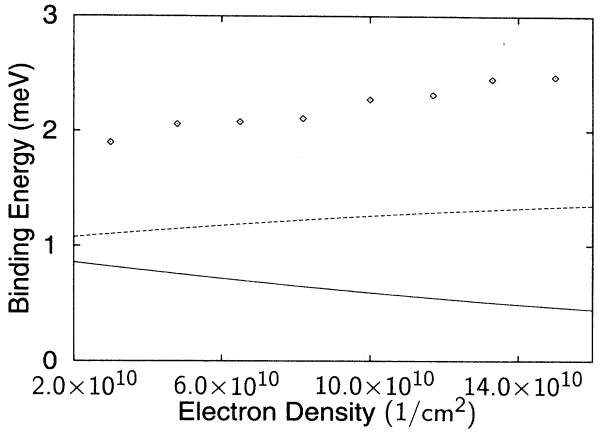

FIG. 5. The binding energy of the plasmonlike (solid line) and phononlike coupled mode (dashed line) as a function of the electron density. The experimental data of the phononlike mode (diamonds) from Ref. 1 are also shown.

V. CONCLUSIONS

We have obtained the binding of plasmons to neutral donors in the bulk, and found that their binding is strongly tunable with carrier density. We have given results for the binding of coupled plasmon-phonon modes, which are of importance in compound semiconductor systems, in both bulk systems and quantum wells. We have shown that the coupling of these excitations to neutral donors via the virtual excitation and deexcitation of the donor states gives binding energies on the order of a few meV. We argue that the binding of coupled phonon-plasmon modes at neutral donors accounts for recent experimental data on GaAs/$Al_xGa_{1-x}As$ quantum-well systems.

ACKNOWLEDGMENTS

Several fruitful discussions with Dr. D. Gammon and Dr. B.V. Shanabrook are gratefully acknowledged. This work was supported in part by a National Research Council Research Associateship and in part by the Office of Naval Research.

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[12]11 is actually a contraction for 0101. See Ref. 11.

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