Excitons in spatially separated V-shaped quantum wells: Application to GaAs sawtooth-doping superlattices

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A variational calculation of the ground state of an exciton in spatially separated V-shaped quantum wells is presented. This is connected to the properties of excitons in sawtooth-doped superlattices. The binding energy, lateral extension, and vertical extension are calculated as functions of the superlattice period and δ-doping impurity concentration. In spite of the fact that electrons and holes are present in spatially separated regions, the binding energies are of magnitude similar to those found in compositional GaAs quantum wells.

Very recently, Schubert *et al.*[1,2] reported on the observation of quantum-confined excitonic interband transitions in absorption[1] and photoluminescence[2] measurements of GaAs sawtooth-doping superlattices.

Doping superlattices consist of alternating *n*-type and *p*-type doped layers of an epitaxially grown semiconductor (for a review see Ref. 3). A sawtooth-shaped band diagram is obtained if the thickness of the doped layer decreases, such that the dopants are localized on a scale length of a lattice constant (see Fig. 1).

In the case of the now familiar compositional superlattices, the band-edge modulation that gives rise to the periodic potential has its origin in the different band gaps of the components; these type of superlattices allow an unambiguous observation of quantum-confined interband transitions,[4] and excitons dominate the optical properties like absorption or luminescence spectra when the experiments are performed in the quantum-well configuration.[5-8]

Although the behavior of excitons in these compositional superlattices [for instance, GaAs/(Al,Ga)As] and quantum wells has frequently been studied by a number of techniques,[9-14] no quantitative predictions are yet available for sawtooth-doping superlattices. It is the purpose of this work to report on our variational calculations on the binding energy and spatial extension of excitons in GaAs sawtooth-doping superlattices in the limit of weak coupling among wells.

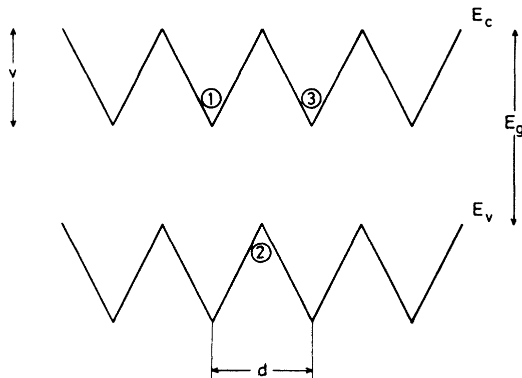

FIG. 1. Electronic band diagram of a sawtooth-doping superlattice. E_c (E_v) is the energy corresponding to the bottom (top) of the conduction (valence) band of GaAs, E_g is the bulk gap and V the band-edge modulation.

We assume that adjacent wells corresponding to the same band [for example, wells (1) and (3) in Fig. 1 for the conduction band] are sufficiently isolated by thick barriers so as to be independent,[15] but that the coupling between adjacent wells corresponding to different bands [(1) and (2) in Fig. 1] can be strong. This approximation is excellent for the study of the ground-state excitons reported in Ref. 1, but is not suitable for the description of the properties of excited state excitons. We will not attempt to calculate the properties of the excited excitons in this work.

In accordance with that simplifying assumption, the exciton state is composed of an electron in a V-shaped well bound to a hole in one of the adjacent V-shaped wells, separated by a distance $d/2$.

The z axis is taken to be parallel to the growth direction. The vertex of the V-shaped well associated with the electron is chosen as the origin of the z coordinate. The positions of the electron and hole are denoted by $\mathbf{r}_e$ and $\mathbf{r}_h$, respectively. Cylindrical relative coordinates ρ,ϕ,z are introduced as usual, for example, $\rho^2=(x_e-x_h)^2+(y_e-y_h)^2$.

The Hamiltonian of the relative motion of an exciton is then given by

$$H=H_e+H_h+H_\perp+H_{e\text{-}h} , \tag{1}$$

where

$$H_e=-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2}+eF|z_e| , \tag{2a}$$

$$H_h=-\frac{\hbar^2}{2m_\pm}\frac{\partial^2}{\partial z_h^2}+eF\left|z_h-\frac{d}{2}\right| , \tag{2b}$$

$$H_\perp=-\frac{\hbar^2}{2\mu_\pm}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right]+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right] , \tag{2c}$$

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$$H_{e\text{-}h}=-\frac{e^2}{\epsilon|\mathbf{r}_e-\mathbf{r}_h|} . \tag{2d}$$

In Eqs. (2a)–(2d) m_e is the isotropic electron effective mass, m_+ (m_-) the heavy- (light-) hole effective mass along the growth axis, μ_+ (μ_-) is the in-plane reduced mass associated with the heavy (light) hole, F is the built-in electric field in the superlattice, given by $F=2\pi eN^{2D}/\epsilon$ (N^{2D} is the two-dimensional concentration of impurities), and ϵ is the dielectric constant of bulk GaAs.

Heavy- and light-hole exciton Hamiltonians differ only by the definitions of $m_\pm$ and $\mu_\pm$ in terms of m_e and the valence-band Luttinger parameters[16]

$$\frac{1}{m_\pm}=\frac{1}{m_0}\left[\gamma_1\mp 2\gamma_2\right] , \tag{3}$$

$$\frac{1}{\mu_\pm}=\frac{1}{m_e}+\frac{\gamma_1\pm\gamma_2}{m_0} , \tag{4}$$

where m_0 is the free-electron mass and the plus (minus) sign correspond(s) to the heavy (light) hole.

As elliptically symmetric variational wave function we choose

$$\psi(\mathbf{r}_e,\mathbf{r}_h)=\frac{1}{\lambda}\left[\frac{2}{\pi}\right]^{1/2} f_e(z_e)f_h(z_h)e^{-\rho/\lambda} , \tag{5}$$

where $f_e(z_e)$ and $f_h(z_h)$ are the normalized ground-state wave functions of the V-shaped well without Coulomb interaction [exact solution of Eqs. (2a) and (2b), respectively]:

$$f_e(z_e)=\frac{1}{\sqrt{2\gamma_e}\mathrm{Ai}(-\beta_e\gamma_e)}\mathrm{Ai}(\beta_e(z_e-\gamma_e)) , \tag{6}$$

$$\beta_e=\left[\frac{2m_e eF}{\hbar^2}\right]^{1/3} , \quad \gamma_e=\frac{E_e}{eF} . \tag{7}$$

Here Ai(z) is the Airy function,[17] E_e is the energy of the first electron subband,[18] and λ is the variational parameter. For a given value of the electric field F (or equivalently, of the 2D-doping concentration N^{2D}), E_e and F are related by the equation[1]

$$E_e=|a_1'|\left[\frac{\hbar^2e^2F^2}{2m_e}\right]^{1/3} , \tag{8}$$

where $a_1'\cong 1.02$ is the first zero of the derivate of the Airy function.[17]

Similar equations to (6)–(8) hold for the heavy (light) hole, replacing m_e by m_+ (m_-), and z_e by $z_h-d/2$.

The rationality behind the one parameter trivial wave function (5) is as follows: the Coulombic term essentially binds the electron-hole reduced motion in the layer plane [as described by the exponential term in (5)], whereas the exciton motion along the grown axis is mostly dominated by the confining V-shaped wells at $z=0$ and $z=d/2$ [corresponding to the one-particle wave function $f_e(z_e)$ and $f_h(z_h)$].[19]

Once $f_e(z_e)$ and $f_h(z_h)$ are determined for a given value of F and d, the exciton binding energy is obtained through the minimization of

$$E(\lambda)=\frac{\hbar^2}{2\mu\lambda^2}+\frac{4}{\lambda^2}\int_0^\infty d\rho\,\rho e^{-2\rho/\lambda}V(\rho) , \tag{9}$$

where

$$V(\rho)=-\frac{e^2}{\epsilon}\int_{-\infty}^{\infty}dz_e\int_{-\infty}^{\infty}dz_h\frac{f_e^2(z_e)f_h^2(z_h)}{[\rho^2+(z_e-z_h)^2]^{1/2}} \tag{10}$$

is an average over z of the Coulomb interaction between hole and electron, and can be considered as an effective in-plane Coulomb interaction.

In addition to the binding energy, the expectation values $\langle\rho\rangle$ and $[\langle(z_e-z_h)^2\rangle]^{1/2}$ are relevant quantities which are useful to ascertain the accuracy of a trial wave function, as they provide some insight into its spatial extension.

These expectation values are readily obtained from $\psi(\mathbf{r}_e,\mathbf{r}_h)$, namely,

$$\langle\rho\rangle=\lambda , \tag{11}$$

$$[\langle(z_e-z_h)^2\rangle]^{1/2}=\left[\frac{d^2}{4}+\frac{8}{15}\left[1+\frac{3}{8|a_1'|^3}\right]\times(\gamma_e^2+\gamma_h^2)\right]^{1/2} . \tag{12}$$

The values of the physical parameters we use in the calculations are $m_e=0.0665m_0$, $\gamma_1=6.85$, $\gamma_2=2.1$, and $\epsilon=12.5$.[20] The equivalent three-dimensional effective Rydberg energy and Bohr radius with these in-plane parameters are 3.63 meV, 158.6 Å, 4.40 meV, and 130.8 Å for heavy-hole (hh) and light-hole (lh) excitations, respectively.

Because the band-edge modulation (V in Fig. 1) is given by

$$V=eF\frac{d}{2}=\frac{\pi e^2dN^{2D}}{\epsilon}$$

and the condition of weak coupling among the wells is fulfilled when $E_e,E_{hh},E_{lh}\ll V$ with E_e,E_{hh},E_{lh} independent of d [see Eq. (8)] it is clear that if d is too small the condition of weak coupling will be violated; we restrict ourselves to values of d where the above condition is fulfilled.

There is also a maximum value of d for the validity of our calculation approximately given by

$$E_g+E_e+E_{hh}\simeq eF\frac{d_{max}}{2}$$

because for $d>d_{max}$ the system will have a transition from a semiconductor to a semimetal configuration, as a consequence of the transfer of electrons from the valence band to the conduction band. We will not attempt here the study of excitons in the semimetallic configuration, where screening effects can be important. Notice that this is a real transition of the system not related with the weak-coupling approximation.

Now we turn to numerical results. In Fig. 2 the heavy-hole and light-hole ground-state exciton binding

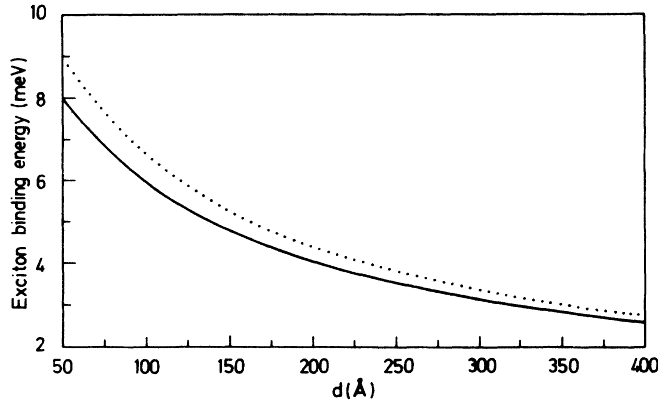

FIG. 2. Heavy- (solid line) and light- (dotted line) hole exciton binding energies as a function of d; impurity concentration $N^{2D}=1.25\times10^{13}$ cm^{-2}.

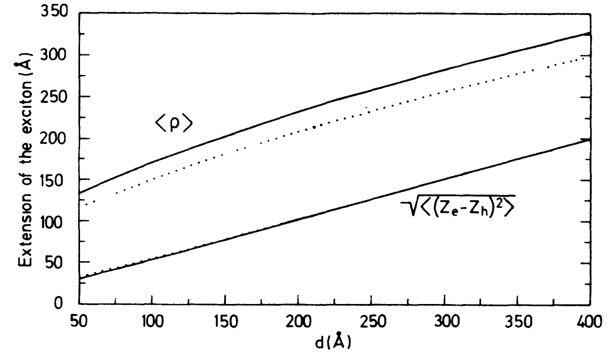

FIG. 3. Extension of heavy- (solid line) and light- (dotted line) hole excitons in the in-plane and z directions as a function of d; impurity concentration $N^{2D}=1.25\times10^{13}$ cm^{-2}.

energies are plotted as a function of d, the superlattice period; the concentration of impurities was taken equal to the value quoted in Ref. 1 ($N^{2D}=1.25\times10^{13}$ cm^{-2}).

As expected from physical grounds, the binding energy of hh and lh excitons decreases monotonically with increasing V-well separation: the effective in-plane Coulomb interaction given by Eq. (10) decreases when d increases. We note that the lh exciton binding energy is always larger than the hh exciton binding energy; this is a result of the larger in-plane mass of the lh exciton. The binding energies that we found are comparable to the binding energy in compositional GaAs quantum wells: for example, for $d=100$ Å, $E_b\simeq7$ meV, for the hh exciton.

We present in Fig. 3 the lateral extension of the exciton $\langle\rho\rangle$ [Eq. (11)] and the extension in the z direction $[\langle(z_e-z_h)^2\rangle]^{1/2}$, [Eq. (12)] as a function of d, for both hh and lh excitons.

The lateral extension of both excitons increases monotonically with increasing V-well separation; this again is a consequence of the weakening of the effective in-plane attraction; as mentioned above, the layer in-plane mass of the lh exciton gives a smaller lateral extension and as a consequence a larger binding energy than the hh exciton.

The inverse is true for the extensions in the z direction [according to Eq. (3), $m_+>m_-$] but in that case both extensions are very similar and approach asymptotically (as d increases) an effective 2D limit where the electron and hole are confined to move in different planes at a distance $d/2$;[21] this is a consequence of the strong confinement provided by the large built-in electric field ($F\simeq10^6$ V/cm).

With the purpose of investigating the dependence of these results on the value of the impurity concentration we present in Table I the binding energy and a parallel and perpendicular extension of the hh and lh hole excitons, for $d=150$ Å and two different values of N^{2D}.

As can be seen from Table I, the binding energy of both excitons is only weakly dependent on the impurity concentration (for a change of a factor 10 in N^{2D}, the corresponding change in the binding energy of the excitons is only about 4%); the slight increase in binding energy as N^{2D} decreases comes essentially from the change in the exciton extension in the growth direction.

Note the different behavior of the parallel and perpendicular extensions as the impurity concentration decreases: the first decreases while the second increases. The expansion in the growth direction is a natural consequence of the weaker confinement on the function $f_e(z_e)$ and $f_h(z_h)$; accordingly with that, the larger overlap between both functions in Eq. (10) gives a larger value of the effective in-plane Coulomb interaction and a shortening of the electron-hole average distance in the parallel direction.

In summary, we have calculated variationally the ground-state binding energy and spatial extension of hh and lh excitons in GaAs sawtooth-doping superlattices, within the approximation of weak coupling among the V-shaped wells.

We find that the binding energy decreases monotonically with increasing distance between wells with values of comparable magnitude to those obtained in the case of

TABLE I. Binding energy, lateral extension, and vertical extension of hh and lh excitons, for $d=150$ Å and two different values of N^{2D}.

N^{2D}	hh exciton			lh exciton		
	E_b	$\langle\rho\rangle$	$[\langle(z_e-z_h)^2\rangle]^{1/2}$	E_b	$\langle\rho\rangle$	$[\langle(z_e-z_h)^2\rangle]^{1/2}$
(10^{12} cm^{-2})	(meV)	(Å)	(Å)	(meV)	(Å)	(Å)
1.25	4.95	194.5	84.8	5.47	171.3	88.2
12.5	4.78	203.4	77.2	5.23	181.1	78.0

compositional superlattices.

While the in-plane extension of the exciton is given by the Coulombic attraction between hole and electron, the dimension in the grown direction is given essentially by the distance between the V-shaped wells.

It would be interesting, if possible, to measure directly the binding energy of the ground-state excitons in this system and compare it with the theoretical values obtained in this work.

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[18]The use of ground-state solutions $f_e(z_e)$ and $f_h(z_h)$ in Eq. (5) is well justified by the energy difference between the first excited- and ground-state well energies compared with typical exciton binding energies (~ 10 meV). For example, for $N^{2D} = 1.25 \times 10^{13}$ cm^{-2}, E_e (ground state) $\simeq 170$ meV, while E_e (first excited state) $\simeq 390$ meV.

[19]Also, it is possible to consider Eq. (5) as a generalization of the exact solution of (1) in the limit $d \to 0, F \to \infty$, in which case the Hamiltonian reduces to the two-dimensional hydrogen atom equation, with the Airy functions replaced by δ functions and $\lambda = a_0^*/2$ ($a_0^* = \epsilon\hbar^2/\mu e^2$).

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