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Exciton energies as a function of electric field: Confined quantum Stark effect

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We have performed a variational calculation of the exciton binding energy as a function of electric field in a semiconducting quantum-well structure using a three-dimensional (3D) hydrogenic trial wave function and compared our results with earlier calculations in which a 2D hydrogenic trial wave function was used. Our results yield larger exciton binding energies for wide wells and strong electric fields. We find that the crossover between 2D and 3D behavior occurs at a critical well width which is of the order of the exciton Bohr radius in zero field and which decreases with increasing electric field.

In recent years there has been much interest in the effect of electric fields applied along the direction of carrier confinement in semiconducting quantum-well structures on the energy levels of the excitons confined to such quantum wells.[1–5] Miller *et al.*[1] have observed large shifts of the exciton peaks in the presence of strong electric fields in quantum-well structures. This effect has been called the quantum confined Stark effect (QCSE) and its use has been proposed in the fabrication of a hybrid optically bistable switch and in high speed optical modulation in a *p-i-p* diode structure.[2] The energy levels of excitons in electric fields have been calculated by Miller *et al.*[3] and by Wu and Nurmikko[4] taking the confinement of the exciton in the well and the presence of the electric field into account. This has been done by using the wave functions for free electrons and holes in the presence of the confining potential and electric field and using a two-dimensional (2D) hydrogenic wave function to describe the relative motion of the electron and hole in the exciton. However, Bastard *et al.*[6] have shown that in the presence of the electric field, a variational trial function where the relative motion has been taken into account through the use of a 3D hydrogenic wave function gives higher exciton binding energies than that obtained when the relative motion is taken into account by using a 2D hydrogenic wave function except in very narrow wells. For such narrow wells, they found that the exciton binding energy was the same using either trial wave function. In very narrow wells, however, there is not very much of a shift of the exciton binding energies except at very strong fields. Therefore, we have performed a similar variational calculation of the exciton energies except that we used the 3D hydrogenic wave function to describe the relative motion of the electron-hole pair in the exciton.

The Hamiltonian for an electron-hole pair confined in a quantum well in the presence of an electric field along the direction of the carrier confinement is the same as used by others.[3,4] Assuming carrier confinement in an infinite potential well, Miller *et al.*[3] and Wu and Nurmikko[4] used as a trial wave function in their variational calculations of the exciton energy, a 2D hydrogenic wave function of the form

$$\Psi(r) = Ae^{\beta_h z_h} e^{-\beta_e z_e} \cos(\pi z_e/L) \cos(\pi z_h/L) e^{-\alpha\rho} \qquad (1)$$

for $|z_e|$, $|z_h| < L/2$ and 0 elsewhere where z_e and z_h are the electron and hole coordinates along the direction of carrier confinement and ρ is the relative separation of the electron-hole pair in the plane of the well. Wu and Nurmikko's calculation[4] differed from that of Miller *et al.*[3] only in that they minimized the total exciton energy with respect to the three variational parameters α, β_e, and β_h simultaneously while Miller *et al.*[3] first minimized the energies of the free electron and hole in the electric field with respect to β_e and β_h and then minimized the relative energy of the bound electron-hole pair with respect to the variational parameter α. The use of the variational wave functions of the form $\xi_i(z_i) = e^{\beta_i z_i} \cos(\pi z_i/L)$ for the noninteracting electrons and holes has been shown to produce agreement with the exact results for dependence of the subband energies on the electric field by Miller *et al.*[3] and by Bastard *et al.*[7]

In our variational calculation of the exciton energies as a function of electric field, we used a 3D hydrogenic trial wave function of the form

$$\Psi(r) = Ae^{\beta_h z_h} e^{-\beta_e z_e} \cos(\pi z_e/L) \cos(\pi z_h/L) e^{-\alpha r}, \qquad (2)$$

where $r = [\rho^2 + (z_e - z_h)^2]^{1/2}$. The difference between the two trial functions comes only in the part of the function which takes into account the relative motion of the electron-hole pair in the exciton. In this case, the 2D hydrogenic wave function $e^{-\alpha\rho}$ is replaced by the 3D hydrogenic wave function $e^{-\alpha r}$. For wide wells, only the 3D hydrogenic trial function yields the correct limit for the binding energy of the exciton while the 2D hydrogenic trial function yields exciton binding energies which are much smaller than the bulk values. Since the shift in the exciton energy levels with electric field depends upon the

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potential drop due to the field across the well, for fixed electric fields, we would expect to have larger shifts in wider wells than in narrower wells as long as the width of the well is of the order or less than the average separation along the direction of confinement between the electron and hole in the well.

The variational calculation involves calculating the expectation value of the exciton Hamiltonian using the trial wave functions given in Eqs. (1) and (2). The expectation value of the exciton energy is then minimized with respect to the three variational parameters α, β_e, and β_h simultaneously to yield the minimum exciton energy for the particular trial wave function $E_{\rm min}$. The binding energy is given by

$$E_b = E_{e0} + E_{h0} - E_{\rm min}, \qquad (3)$$

where E_{e0} and E_{h0} are the energies of the free electron and hole in the same quantum well in the presence of the electric field F but in the absence of the attractive Coulomb interaction. Unlike the case using the 2D hydrogen trial wave function,[3,4] in the case of a 3D hydrogenic wave function, all the integrals occurring in the calculation of the expectation value of the exciton energy can be done analytically.

In Fig. 1, the difference in the exciton binding energy obtained using our quasi-3D variational wave function and that obtained using the quasi-2D variational wave function of Miller *et al.*[3] is shown as a function of the well width for four values of the applied field for the heavy hole exciton. The binding energy, well width, and electric field are given in terms of the natural excitonic units in which the energy is measured in exciton rydberg units $R_y = e^2/2a_B\kappa$, the well width in exciton Bohr radii $a_B = \kappa\hbar^2/\mu e^2$, and the electric field in units of $F_0 = e/\kappa a_B^2$. Using the values $m_e = 0.067m_0$ and $m_{hh} = 0.45m_0$ for the effective masses of the conduction electrons and heavy holes, respectively, and $\kappa = 12.5$, we find that for the heavy hole exciton, $R_y = 5.1$ meV, $a_B = 11.4$ nm, and $F_0 = 8.87 \times 10^5$ V/m. Our results show that while at zero well width, the results for the binding energy are the same for both variational wave functions, as the well width increases, the 2D variational wave function yields larger binding energies up to a critical well width which depends on the electric field. Above this critical well width, our 3D variational wave function yields the higher exciton binding energy. The well width at which the transition from 2D to 3D behavior occurs decreases as the electric field increases.

In Fig. 2, the difference in the exciton binding energy obtained using our quasi-3D variational wave function and that obtained using the quasi-2D variational wave function[3,4] is shown as a function of the electric field for several different wells for the heavy hole exciton. Except for the narrowest wells, our results show that the 3D variational wave function yields higher binding exciton binding energies than the 2D variational wave function. Also, the difference between the binding energies obtained using the two different variational wave functions increases with increasing electric field.

Finally, in Figs. 3–5, the variational parameters α, β_e, and β_h are shown as a function of the electric field for the heavy hole exciton for both our trial function and the quasi-2D trial function.[3,4] The variational parameter α decreases with the electric field but for the trial wave function of Miller *et al.*,[3] α decreases much more rapidly with electric field than for our trial function. This is one reason why our trial function leads to higher binding energies for excitons as the strength of the electric field increases. The difference between the values of α using the two trial wave functions becomes more apparent as the well width increases. As would be expected, β_e and β_h increase with the electric field. This is because the electric field tends to push the electron and the hole to

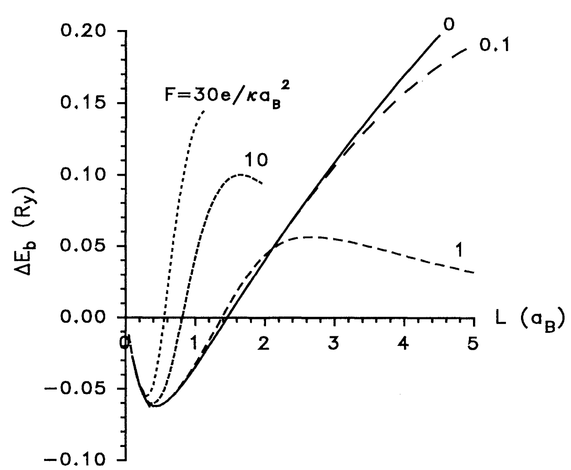

FIG. 1. The difference between the binding energy of the heavy hole exciton using our quasi-3D variational wave function and the quasi-2D variational wave function of Miller *et al.* (Ref. 3) is shown as a function of the well width for four values of the electric field. The binding energy is given in rydberg units while the electric field is given in units of $F_0 = e/\kappa a_B^2$.

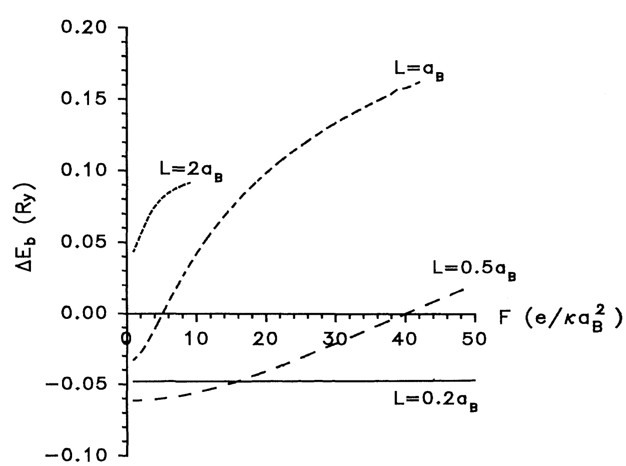

FIG. 2. The difference between the binding energy of the heavy hole exciton using our quasi-3D variational wave function and the quasi-2D variational wave function of Miller *et al.* (Ref. 3) is shown as a function of the electric field for several values of the well width.

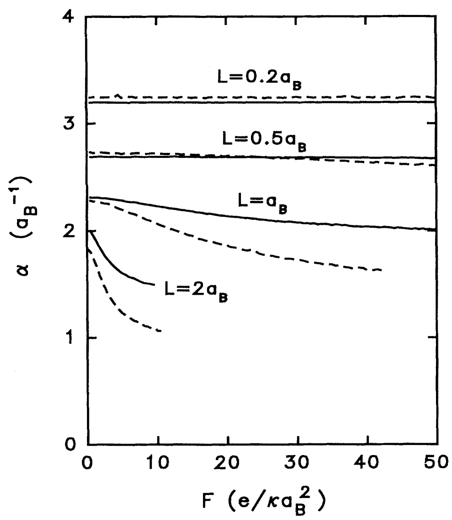

FIG. 3. The variational parameter α is shown as a function of the electric field for the heavy hole exciton for several values of the well width. The dashed curves represent the results of Miller *et al.* (Ref. 3) while the solid curves represent our results using the 3D hydrogenic trial function.

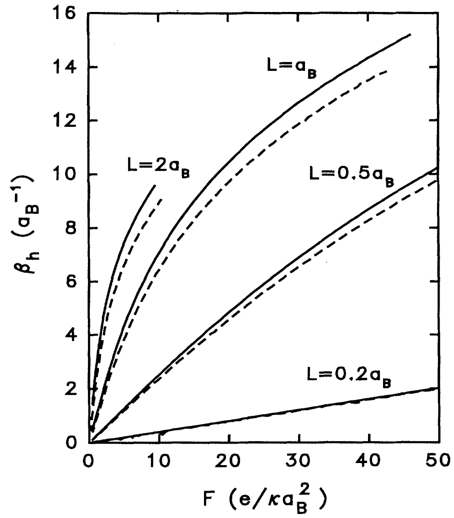

FIG. 5. The variational parameter β_h is shown as a function of the electric field for the heavy hole exciton for several values of the well width. The dashed curves represent the results of Miller *et al.* (Ref. 3) while the solid curves represent our results using the 3D hydrogenic trial function.

opposite sides of the well. Using our trial function, the values of parameters β_e and β_h are larger than those using the quasi-2D trial function[3,4] except for the narrowest wells.

In Fig. 6, the normalized oscillator strength is shown as a function of the electric field for the heavy exciton, again showing the comparison for both our trial function and the quasi-2D trial function.[3,4] The exciton oscillator strength is that defined by Matsuura and Kamizato,[9] which is proportional to the square of the wave function at zero separation,

$$f_{1s} = \frac{2}{L}|\epsilon \cdot \mathbf{p}_{cv}|^2 |\Psi(0)|^2 . \tag{4}$$

Here, f_{1s} is the oscillator strength, $\mathbf{p}_{cv}$ is the optical transition matrix element between the conduction and valence bands, and $|\Psi(0)|^2$ is defined as

$$|\Psi(0)|^2 = \left| \int_{-L/2}^{L/2} dz \xi_e(z) \xi_h(z) \right|^2 |\phi(0)|^2 .$$

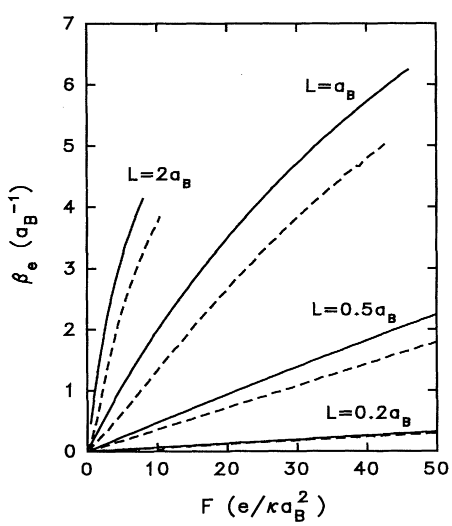

FIG. 4. The variational parameter β_e is shown as a function of the electric field for the heavy hole exciton for several values of the well width. The dashed curves represent the results of Miller *et al.* (Ref. 3) while the solid curves represent our results using the 3D hydrogenic trial function.

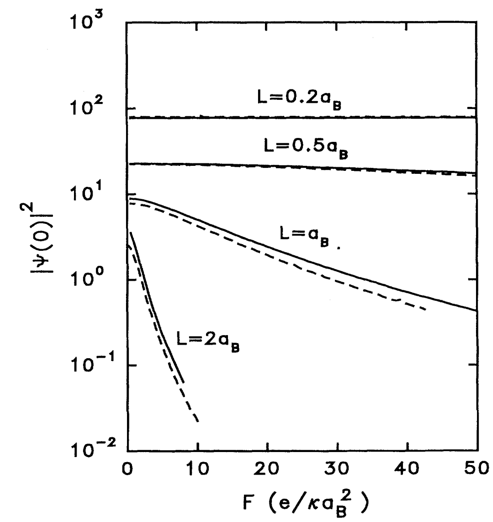

FIG. 6. The normalized oscillator strength for the excitons, $|\Psi(0)|^2$, for the heavy hole exciton is shown as a function of the electric field for several values of the well width. The dashed curves represent the results of Miller *et al.* (Ref. 3) while the solid curves represent our results using the 3D hydrogenic trial function.

Also, $\xi_e(z)$ and $\xi_h(z)$ are the confining parts of the wave functions for the electrons and holes, respectively, and $\phi(r)$ is the part of the wave function which describes the relative motion of the bound electron-hole pair. Using both trial functions, the oscillator strength decreases with increasing electric field. Here, again our calculations yield a larger oscillator strength than that obtained using the quasi-2D variational wave function.[3,4]

The fact that as the well width increases, the 2D variational wave function initially yields higher binding energies is in disagreement with the claim of Bastard *et al.*[6] that the 3D hydrogenic trial function is the best choice of variational wave functions for both thin wells and thick wells although the results using this trial function do not differ greatly from those obtained using the 2D hydrogenic trial function for narrow wells. Thus the results of our calculations indicate that the trial function used by Matsuura and Shinozuka,[8] which is a two variational parameter trial function in which there are different Bohr radii in the plane of the well and along the direction of carrier confinement, would yield better results for the exciton binding energy in the absence of the electric field than either the purely 2D or 3D hydrogenic trial functions. In fact, Matsuura and Kamizato[9] have performed a calculation of the exciton binding energy as a function of electric field using such an anisotropic hydrogeniclike trial function. However, they did not present any comparison of their results to those obtained by Miller *et al.*[3] so that it could not be determined whether the use of their anisotropic hydrogenic trial function gave better binding energies than those obtained by Miller *et al.*[3] We find that the crossover between 2D and 3D behavior for the exciton seems to occur when the well width is of the order of the exciton Bohr radius. This is what is usually expected although there does not seem to be any published work in which the comparison has been made between 2D and 3D behavior in the presence of the field. In addition, as the electric field increases, the use of the 3D hydrogenic trial function yields higher binding energies even for wells whose width is less than an exciton Bohr radius. Another interesting result of our calculation is that for wide wells, the binding energy goes to zero at finite electric fields. This would indicate that the exciton is no longer bound in these wells as the electric field increases beyond a certain threshold value which depends upon the width of the well. Although we have only shown the results of our calculations for the heavy hole exciton, we have obtained similar results for the light hole exciton.

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