Binding energy of the barbell exciton

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The exciton binding energy in asymmetric coupled double quantum wells is calculated. As the system is electrically tuned from type I to type II, the exciton binding energy decreases from that of a two-dimensional exciton to the binding energy of a spatially separated electron-hole pair, i.e., the *barbell exciton*. We compare our theoretical results with a recent experiment and find good agreement.

Theoretical models[1] have been constructed that predict high-temperature excitonic superconductivity ($T_c \geq 100$ K) in a two-dimensional (2D) system. These models require coupled gases of opposite charge, which are spatially separated. The superconducting state is one of a superfluid of excitonlike structures consisting of spatially separated electrons and holes. The two main issues involved in the creation of such an exciton gas are (1) to what extent are Coulomb correlations important and observable, and (2) how well can the recombination be suppressed in order to make the lifetime sufficiently long such that the carriers are able to thermalize with the lattice.

Experimentally such an exciton gas can be created in layered semiconductor systems by optical excitation of electron-hole pairs across the band gap. The main problem is the short lifetime of such excitons. In order to increase this lifetime one has to decrease the overlap between the electron and hole wave function. This can be realized by applying an electric field perpendicular to a quantum well. The electron and hole are pulled to opposite sides of the well and in so doing decrease the overlap. The barriers of the quantum well prevent field-ionization of the exciton. A further significant decrease of this overlap can be realized by inserting a barrier in the quantum well. Recent experiments[2,3] have demonstrated the practical feasibility of this idea.

In connection with Ref. 1 it is important to know the electron-hole correlation, and thus the exciton binding energy. It is this Coulomb interaction which is responsible for the pairing in the superconducting state. The calculation of this quantity in the asymmetric coupled quantum wells (ACQW) of Ref. 3 in the presence of an electric field is the aim of the present paper.

During the last decade[4-6] a number of calculations have been published on the exciton binding energy in single-quantum-well systems. Recently[7] also multiple-quantum-well structures and coupled double quantum wells[8,9] have been studied. Here we will investigate the effect on exciton binding energy when the exciton is electrically tuned from a 2D exciton to a spatially separated electron-hole pair, the *barbell exciton,* in the ACQW structure.

As an example we study the structure shown in the inset of Fig. 3 which consists of GaAs quantum wells and $Al_xGa_{1-x}As$ barriers. The approximations used in the present paper are as follows: (1) An effective mass approach. (2) Band nonparabolicity is neglected. (3) The dielectric constant in the GaAs and in the $Al_xGa_{1-x}As$ are taken to be the same and equal to $\epsilon = 12.5$. The effect of (3) on the binding energy is small because of (i) the small mismatch in ϵ between GaAs and $Al_xGa_{1-x}As$, and (ii) the small probability to find the electron and hole in the barrier. (4) Band mixing is neglected. Recent calculations[5] have shown that this may lead to an underestimation of the exciton binding energy by ~ 1 meV. This is within the accuracy of the experimental results. (5) Only the lowest electron and hole subbands are taken into account in calculating the exciton binding energy. This approximation is valid as long as the Coulomb mixing between the lowest-lying coupled well states is neglectable, which is the case for a thin barrier. For thick barriers this may be no longer the case over a certain electric field range and a more complicated calculation may be necessary.[8] (6) The electron-hole correlation is described by a two-parameter function. The parameters are determined by a variational calculation. This approach is able to recover the 3D results in the limit of very narrow quantum wells or for very wide quantum wells in the absence of an electric field. The recent calculations of Refs. 8 and 9 have *one* variational parameter and are not able to recover the 3D exciton results, and in this respect the present approach is more general.

The system under study is described by the Hamiltonian

$$H = H_{e,z} + H_{h,z} + \frac{1}{2\mu}(p_x^2 + p_y^2) - \frac{e^2}{\epsilon\sqrt{x^2+y^2+(z_e-z_h)^2}}\ , \tag{1}$$

where

$$H_{e,z} = \frac{p_{e,z}^2}{2m_e} + V_e(z_e) - eEz_e \tag{2a}$$

and

$$H_{h,z}=\frac{p_{h,z}^2}{2m_h}+V_h(z_h)+eEz_h \tag{2b}$$

are the Hamiltonians describing the z confinement of the electron and hole, respectively, with $e=|e|$ the elementary charge. x and y are the relative coordinates of the electron-hole pair in the 2D plane of the quantum well with conjugate momentum p_x and p_y and exciton reduced mass μ. The center-of-mass coordinates do not contribute to the energy in the limit of zero temperature. Under the assumption that the exciton binding energy is only a weak perturbation to the total energy, which is satisfied for not too narrow wells, we can first solve for the wave function in the z direction which gives us $\phi_e(z_e)$ and $\phi_h(z_h)$ with the corresponding energies $E_{e,z}$ and $E_{h,z}$. The 1D Schrödinger equations Eqs. (2a) and (2b) were solved numerically where the appropriate mass discontinuities at the semiconductor interfaces were included. Such a calculation is standard and can be done with arbitrary high accuracy.

The electron-hole correlation is then described by the two-parameter function $\exp[-(\rho^2+\alpha z^2)^{1/2}/\lambda]$, with $\rho=(x^2+y^2)^{1/2}$, $z=z_e-z_h$, and where λ is a measure of the extent of the exciton in the 2D plane of the quantum well. α gives the correlation between the electron and the hole in the z direction. For the problem under consideration α turns out to be small.

The total energy of the electron-hole pair is given by

$$E_{\text{total}}=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{3}$$

which is an upper bound to the exact result. The wave function is taken as

$$\Psi(z_e,z_h,\rho)=\phi_e(z_e)\phi_h(z_h)\exp[-(\rho^2+\alpha z^2)^{1/2}/\lambda]$$

which contains the two variational parameters α and λ. The exciton binding energy resulting from the Coulomb interaction is then given by

$$E_{\text{exciton}}=|E_{\text{total}}-E_{e,z}-E_{h,z}| \tag{4}$$

and is a lower bound on the magnitude of the exact binding energy.

The variational calculation was done for the $GaAs/Al_{0.31}Ga_{0.69}As$ asymmetric coupled quantum well (ACQW) structure of Ref. 10 which is shown in the inset of Fig. 3. We used the following parameters for (1) the electron a potential barrier of $V_e=301$ meV and a mass $m_e/m_o=0.0665$ in the GaAs and $m_e/m_o=0.0843$ in the $Al_xGa_{1-x}As$, and for (2) the hole a barrier of $V_h=200$ meV, a mass of $m_h/m_o=0.45$ in the quantum well and $m_h/m_o=0.466$ in the barrier. The heavy-hole exciton reduced mass was taken to be equal to $\mu/m_o=0.04$. The relation between the internal electric field (E) and the bias voltage (V_{bias}) for the system of Ref. 10 was $E=10.32[1.7-V_{\text{bias}}(\text{V})]$ kV/cm. In Fig. 1 the present theoretical results are compared with the experimental results of Golub *et al.*[10] The agreement is good in view of the experimental accuracy (a typical error bar on the experimental results is shown in Fig. 1) and the uncertainty in certain physical parameters like the widths of

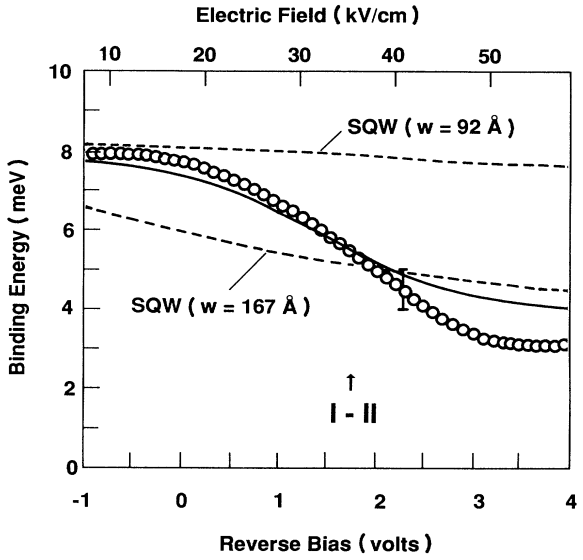
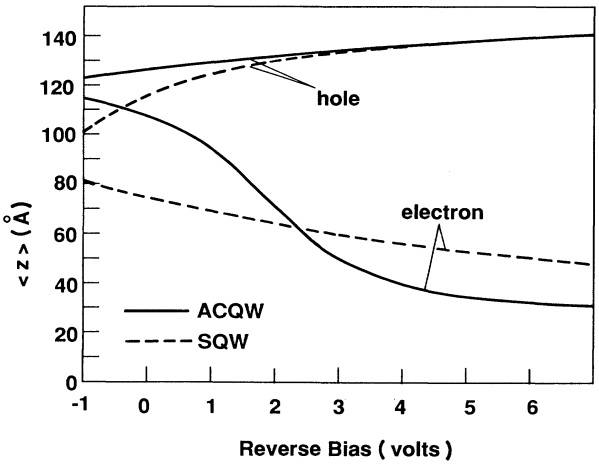
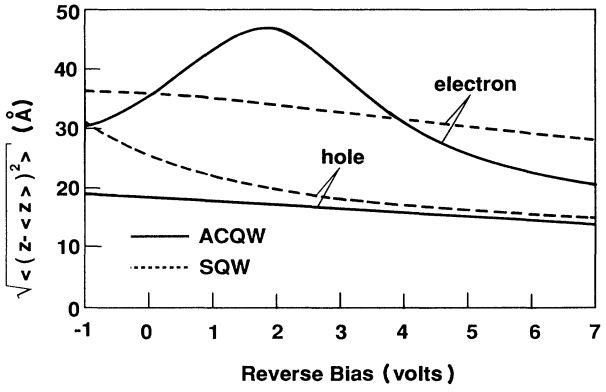


FIG. 1. The exciton binding energy as function of the reverse bias. The experimental results of Ref. 8 (circles) are compared with the theoretical results for asymmetric coupled quantum wells (solid curve) and for single quantum wells (dashed curves) of widths $w=92$ and 167 Å.

the quantum wells and barrier. For comparison we also show the exciton binding energy for an exciton in single quantum wells (SQW) of widths 92 and 167 Å. For small electric fields, the electron and hole are confined in the widest well and the exciton energy is practically equal to the energy of an exciton in a well of size 92 Å. The binding energy is slightly lower due to the fact that a small portion of the electron wave function is able to tunnel into the other well owing to the combined effects of the thin center barrier and small electron mass. With increasing electric field, the electron is shifted more and more to the left well. Concurrent with this transfer of wave function into the left well the separation between the electron and hole increases which leads to a decrease of the Coulomb energy. In the very high electric field limit the center barrier no longer plays a significant role and the exciton binding energy is given by the binding energy in a 167-Å-wide single quantum well. For intermediate-high electric fields the binding energy of the coupled quantum wells drops below the single quantum well because the barrier is effective in increasing the separation between the electron and the hole. This transition between small and large electric-field behavior becomes steeper with increasing barrier strength, hence decreasing interwell coupling. We found that the neglect of the mass discontinuity at the interfaces did not have any appreciable effect on the exciton binding energy.

In Fig. 2 the different single electron and hole properties are shown for the asymmetric coupled quantum wells and for the single quantum well without the center barrier. The hole properties are only slightly influenced by the electric field. In essence the hole is confined by the 92-Å-wide quantum well which explains why the averages $\langle z\rangle$ and $\langle(z-\langle z\rangle)^2\rangle^{1/2}$ are much less influenced





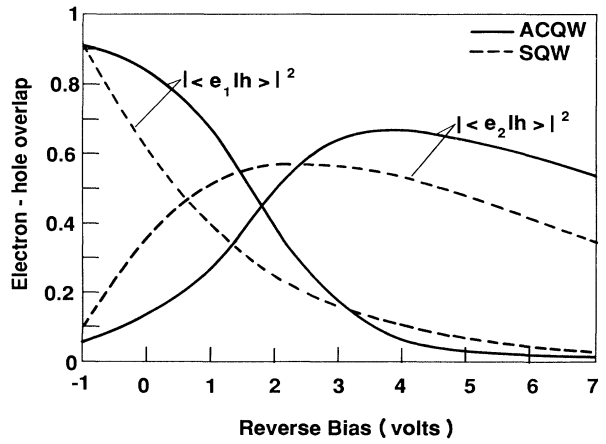


FIG. 2. The electron and hole average position (a), extent of the wave function (b), and overlap (c) for asymmetric coupled quantum wells (ACQW) and a single quantum well (SQW) of width $w=167$ Å.

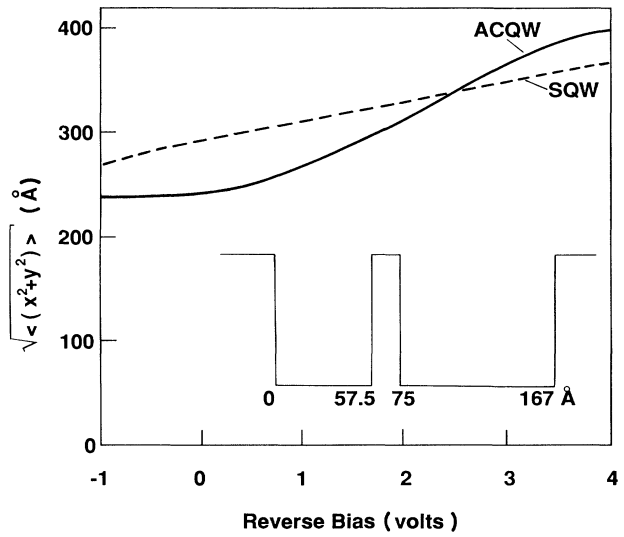


FIG. 3. The extent of the exciton wave function for asymmetric coupled quantum wells (ACQW) which is depicted in the inset, and for a single quantum well (SQW) of width $w=167$ Å.

by the electric field than the corresponding one in a single 167-Å quantum well. The electron in the asymmetric coupled quantum wells shows a switching behavior from the right well into the left well with increasing electric field. For an electron in a single 167-Å-wide quantum well a very gradual change of the averages is observed. The barrier has the effect of sharpening the transition from the low to the high electric-field behavior. This added degree of freedom may have applications in switching devices.

The extent of the exciton wave function along the free 2D plane of the quantum well is plotted in Fig. 3 as a function of the reverse bias. With increasing electric field the electron is pushed closer to the left barrier of the quantum well while the hole is shifted to the right barrier of the quantum well. As a consequence the exciton wave function is spread out more in the x,y directions and the barbell exciton consists of two spatial separated pancake-shaped functions. Note that the extent of the exciton grows larger as the binding energy grows smaller.

In conclusion we have calculated the exciton binding energy of an electron-hole pair in asymmetric coupled quantum wells. Near flat band the exciton is 2D-like while with increasing electric field a transition is observed to a barbell exciton composed of carriers confined to distinct GaAs quantum well layers and separated by an $Al_xGa_{1-x}As$ barrier. The spatially indirect exciton has a long lifetime[11] due to the small overlap of the electron-hole wave function. Its binding energy is nonzero and for the present system was a factor of 2 smaller than the binding energy of the 2D exciton.

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[1]Yu. E. Lozovik, Solid State Commun. **19**, 391 (1976); Zh. Eksp. Teor. Fiz. **71**, 738 (1976); [Sov. Phys. JETP **44**, 389 (1977)]; S. I. Shevchenko, Fiz. Nikh. Temp. **2**, 505 (1976) [Sov. J. Low Temp. Phys. **2**, 251 (1976)].

[2]Y. J. Chen, E. S. Koteles, B. S. Elman, and C. A. Armiento, Phys. Rev. B **36**, 4562 (1987); H. Q. Le, J. J. Zayhowski, and W. D. Goodhue, Appl. Phys. Lett. **50**, 158 (1987); S. R. Andrews, C. M. Murray, R. A. Davies, and T. M. Kerr, Phys. Rev. B **37**, 8198 (1988).

[3]J. E. Golub, P. F. Liao, Y. Prior, D. J. Eilenberger, J. P. Harbison, and L. T. Florez, Appl. Phys. Lett. **53**, 2584 (1988).

[4]G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **26**, 1974 (1982).

[5]R. L. Greene, K. K. Bajaj, and D. W. Phelps, Phys. Rev. B **29**, 1807 (1984).

[6]U. Ekenberg, and M. Altarelli, Superlatt. Microstruct. **3**, 199 (1987).

[7]G. D. Sanders and Y.-C. Chang, Phys. Rev. B **32**, 5517 (1985); **32**, 8027 (1985); G. Mo, and C. C. Sung, *ibid.* **38**, 1978 (1988).

[8]I. Galbraith, and G. Duggan, Phys. Rev. B **40**, 5515 (1989).

[9]J. Lee, M. O. Vassell, E. S. Koteles, and B. Elman, Phys. Rev. B **39**, 10 133 (1989).

[10]J. E. Golub, P. F. Liao, D. J. Eilenberger, J. P. Harbison, and L. T. Florez, Solid State Commun. **72**, 735 (1989).

[11]Lifetimes in excess of 200 nsec are reported in J. E. Golub, K. Kash, J. P. Harbison, and L. T. Florez, Phys. Rev. B **41**, 8564 (1990).