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BINDING ENERGIES OF EXCITONS IN QUANTUM WELL STRUCTURES

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Binding energies of excitons in quantum well structures have been studied by solving the time-dependent Schrödinger equation where the potential is made up by the confining quantum well potentials of arbitrary form and the Coulomb interaction between the electron and hole. The problem is solved without the usually assumed variational procedure and the separation ansatz for the confined electron and hole states. The wave functions for electrons and holes can be extracted from the exciton wave function and are used for the interpretation of the charge localization.

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1. Theory

Excitons in dimensional reduced structures have been intensively studied by various theoretical methods. In most approaches variational procedures have been included and a separation ansatz for the electron and hole wave functions has been used [1, 2]. The dependence of the exciton binding energy on band-band coupling and of band structure nonparabolicities has been thoroughly analyzed [3].

In this paper we present an approach which allows us to avoid the use of a large number of variational parameters as well as the separation ansatz for the z -dependence of the exciton wave function. The only fitting parameters are the effective masses of the electron and the hole. Heavy-hole (HH) and light-hole (LH) excitons are treated separately by solving two sets of 2D time dependent Schrödinger equations. In the first step, the coupling between HH and LH bands and the influence of band nonparabolicities are neglected. This procedure is justified because of our intention to study in first respect the dependence of the binding energies on different types of confinement potentials and the interplay with the Coulomb interaction in the localization of electrons and holes.

The advantage of the method is that we obtain directly the exciton binding energy from the solutions of Schrödinger equations with and without Coulomb interaction. Furthermore, the method allows us to study excitons of different type of localization (e.g., direct and indirect) in simple and highly sophisticated quasi-2D structures like single quantum wells (SQW), asymmetric double (ADQW) or multi quantum (MQW) wells of arbitrary shape of the potential without any modification of the theoretical assumptions for the model.

The problem is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m_e}\Delta_e - \frac{\hbar^2}{2m_h}\Delta_h + V_e + V_h + V_C, \quad (1)$$

where m_e and m_h are the effective masses of the electron and the hole. The potentials V_e and V_h are determined by the geometry of the structures and the band offsets of the different materials. V_C is the Coulomb interaction between the electron and the hole. Transforming the electron and hole coordinates into coordinates for the center of mass motion and the relative motion we obtain a Schrödinger equation where V_e and V_h depend only on the z -components z_e and z_h of the relative coordinate, respectively. The wave function reads $\Psi(r, z_e, z_h, \phi) = \exp(im\phi)\psi_m(r, z_e, z_h)$. Considering the cylindrical symmetry of the problem we make the ansatz

$$\psi_m(r, z_e, z_h) = \sum_{j=0}^{\infty} c_{m,j}(z_e, z_h) J_m\left(\frac{k_{m,j}r}{l}\right) \quad (2)$$

and obtain a set of coupled differential equations for the coefficients $c_{m,j}(z_e, z_h)$. $k_{m,j}$ are the zeros of the Bessel functions $J_m(y)$ and l is the expansion radius.

The energy spectrum is derived independently of the calculation of the electron and hole wave functions from the autocorrelation function

$$F(t) = \langle \Psi(t) | \Psi(0) \rangle = \sum_j |\langle j | \Psi \rangle(t_0)|^2 \exp\left[-\frac{i}{\hbar} E_j(t - t_0)\right] \quad (3)$$

and its Fourier transform

$$f(\omega) = \sum_j |\langle j | \Psi \rangle(t_0)|^2 \delta(\omega - E_j/\hbar). \quad (4)$$

j labels the different eigenvalues of the Hamiltonian H (Eq. (1)).

2. Results and discussion

We have calculated the binding energies for excitons in CdTe/CdMnTe quantum well structures consisting of wells formed by CdTe and barriers formed by CdMnTe. The barrier height can be changed by the variation of the Mn content. The valence band offset is chosen to be 33% of the total band offset.

Binding energies for different barrier heights have been calculated for direct excitons in SQWs (see Fig. 1) and for indirect excitons in an MQW structure where the electron and the hole are separated by a barrier of varying thickness (see Fig. 2). The dependence of binding energies on the well width is in good agreement with results calculated with the widely used formula of Leavitt and Little [4] despite the fact that neither fitting parameters nor a variational procedure have been applied. In the same manner the change of the binding energies of the excitons have been

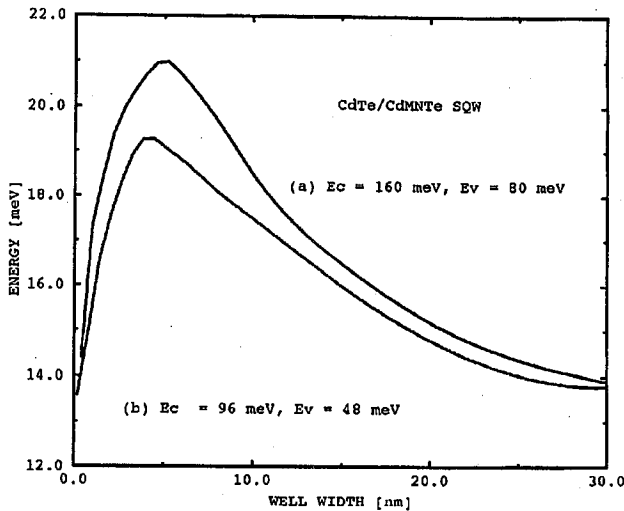


Fig. 1. Binding energy of the direct HH exciton in a CdTe/CdMnTe SQW in dependence on the well width for different band offsets.

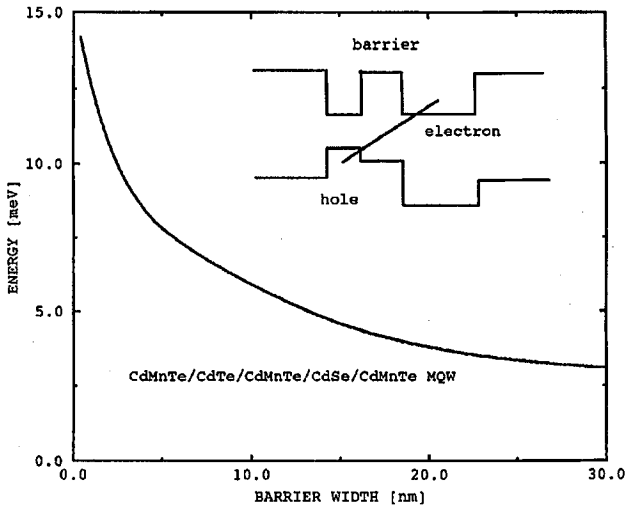


Fig. 2. Binding energy of the indirect HH exciton in a CdMnTe/CdTe/CdMnTe/CdSe/CdMnTe MQW in dependence on the thickness of the CdMnTe barrier between the CdTe and CdSe wells.

studied if the structure undergoes a type I – type II transition. The binding energy of the indirect exciton is diminished approximately by 10 meV in comparison to the direct one. Furthermore, it was found that the confined electron localizes the hole via Coulomb interaction even if the valence band well is very flat. However, there are some different results which may be connected with avoided separation ansatz

for the wave function. Recently, Glutsch et al. [5] have calculated the binding energy of excitons in *T*-shaped quantum wires without a separation ansatz and have reported a greater binding energy.

The classification of the states appearing in the structure follows the well-known scheme for the in-plane radial part and the *z*-dependent part of the wave function. The radial part $R(r)$ is a smooth function of r which is zero for $r = l$. The states are distinguished from each other by the nodes of their wave functions after extracting the wave functions $R(r)$, $\phi_e(z_e)$ and $\phi_h(z_h)$ from the exciton wave function $\Psi(r, z_e, z_h)$.

The method can be applied for QW potentials of any arbitrary *z*-dependence. Simple and complicated structures are calculated in the same framework. The results are directly comparable. Therefore, one can study not only QW structures of any sophisticated ordering of the layers of different type but also other types of variations of the potential in growth direction, which may appear as a result of smearing out of the doping profile in the sample by diffusion or inherent disorder effects of the ternary-binary interface.

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