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The energy of excitons in parabolic quantum wells investigated by the effective variational Hamiltonian method

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Abstract. We calculate the energy of excitons in parabolic quantum wells using the effective variational Hamiltonian (EVH) method which allows us to find *all* energy levels of the exciton by searching for solutions within a very broad class of trial functions whose form is also subject to variation. We use the new method to find the exciton binding energy of 1s, 2s and 3s states of an exciton formed below the ground electron and hole subbands in parabolic quantum wells made of (Ga, Al)As and (Cd, Mn)Te. We calculate also the binding energies of excitons formed between excited quantum well levels. The calculations are performed for various values of an external magnetic field parallel to the growth axis of the heterostructure.

1. Introduction

In the present paper we shall analyse the effect of the presence of a confining potential on the states and the energy of excitons in III–V and II–VI semiconductor heterostructures. In structures available now it is possible to observe sharp exciton lines corresponding to optical transitions between excited states of the interacting electron–hole pair, such as e.g. 3s exciton states [1–3]. These transitions can be observed both for excitons formed by particles occupying the lowest quantum well (QW) subbands as well as for the excitons formed by particles in excited QW subbands. In quasi-two-dimensional heterostructures the problem of the interacting electron–hole pair is of a great importance because the positions and the intensities of excitonic lines are frequently used to determine the structure parameters [4]. Recent progress in fabrication of structures containing quantum wells of arbitrary shape, e.g., parabolic, half-parabolic or triangular [4–8], resulted in samples with quality sufficient for observation of a large number of excitonic transitions. This calls for the development of fast, accurate and reliable theoretical methods of determination of the energies of exciton states which can be easily applied for various QW structures.

The most common method of calculation of the energy of various exciton states is the variational method, with the Ritz method and the perturbation approach used less frequently. All methods have been extensively used in the context of excitons confined in rectangular QWs [4, 9–15]. The emphasis was on determination of the energy of the lowest state of the interacting electron–hole pair assuming either 2D or 3D character of its wave function. To describe the hole kinetic energy, either the effective-mass approximation with the full Luttinger Hamiltonian [13–15] or a simpler one-band dispersion [4, 9–12] was employed. When the interface-related effects, such as change of the effective mass or the dielectric constant across the interface, were taken into account [9, 10], a satisfactory agreement between the exciton energy calculated theoretically and that observed experimentally was achieved [4].

In the present work we introduce another method of calculation of the excitonic energy in the QW heterostructures, which may be applied to quantum wells with arbitrary shape of the confining potential. The method, the effective variational Hamiltonian (EVH) method, is a combination of the variational method and the Hartree approximation and it allows us to calculate *all* exciton energy levels. Generally, in the EVH method we simplify the initial problem of an interacting electron–hole–pair Hamiltonian by partially averaging over several independent variables using a suitably chosen trial function. The function is assumed to be in the form of a product of two functions ($\psi\phi$), of which at least one (say ϕ) is to be determined at later stages of the calculation. The expectation value of the Hamiltonian calculated with the use of such a trial function, $\psi\phi$, approximates from above the eigen-energy of the exciton. The two main advantages of the EVH method over the variational method that are (i) the EVH method gives the lowest energy for all exciton states for an entire given class of the trial functions and (ii) once the effective Hamiltonian is derived, we may calculate its excited states using the same numerical procedure. The methods based on effective Hamiltonians have been widely used in statistical physics [16]. The advantage of the use of the effective Hamiltonians for the problem of excitons was demonstrated by Wu [17], where the excitons in very shallow quantum wells were considered, and by Pollmann [18], who introduced a self-consistent perturbation method for partially averaged Hamiltonians.

In the present work we shall illustrate the EVH method by applying it to the problem of the exciton in parabolic QWs in the presence of an external magnetic field parallel to the heterostructure growth axis. The choice of the parabolic QW has several motivations: first, in contrast to the case of excitons in rectangular QWs, the problem of the excitons in parabolic QWs is less frequently discussed in the literature [5–8, 23]. Yang and Yang [23] calculated the exciton binding energy using the variational method and analysed the dependence of the exciton binding energy of the 1s exciton state on the external electric field. Experimental measurements of the exciton binding energies in parabolic QWs in (Ga, Al)As structures were performed by Miller *et al* [6], Gossard [5] and Cheong *et al* [8] and of those in (Cd, Mn)Te structure QWs by Wojtowicz *et al* [7]. Second, the parabolic confining potential allows us to define several dimensionless quantities which are suitable for parametrizing the exciton binding energies and eigenstates over a wide range of heterostructure parameters. Finally, in the case of parabolic QWs the eigenproblem of the effective Hamiltonian appearing in the EVH method can be partly solved analytically.

The plan of the paper is as follows. In the next two sections we shall formulate the effective variational Hamiltonian method for excitons in parabolic QWs. In section 4 we propose an improved version of the EVH method which is applicable to the determination of the exciton binding energy in wide parabolic quantum wells. In section 5 we compare the values of the 1s exciton energy obtained using the EVH method with the energy obtained using the variational method and the method based on Born–Oppenheimer approximation proposed by Leavitt and Little [19, 20]. In the last section we apply the EVH method to determine the exciton binding energy in two representative semiconductor systems.

2. Assumptions of the model

Consider a heterostructure which contains a single parabolic QW of type I (i.e., with the electron and hole confined in the same spatial region) in the z -direction. This is achieved by continuously varying the molar composition of, say, $\text{Al}_x\text{Ga}_{1-x}\text{As}$ or $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ along the growth axis with a suitable profile. Hereafter, we shall denote by e.g. $\text{Cd}_{1-y}\text{Mn}_y\text{Te}$ – $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ the parabolic QW which contains a molar fraction y of Mn atoms at its centre and a molar fraction x of Mn in its outermost barriers ($y < x$). Lowering of the symmetry

along the z -axis removes the degeneracy of the valence band of the material constituting the heterostructure. The electron–hole Coulomb coupling leads, then, to formation of two exciton systems, the first associated with the heavy holes (with total angular momentum $\vec{J} = 3/2$) and the second with light holes (with $\vec{J} = 1/2$). Experimentally, the energies of the heavy- and light-hole excitons are well separated. Therefore in the simplest approximation we shall ignore the coupling between heavy- and light-hole excitons. In other words, we shall consider only the diagonal part of the Luttinger Hamiltonian, as is often done in theoretical calculations of the exciton energy in rectangular QWs [4, 9–12, 19–22]. The effective masses of the light and the heavy holes are assumed to be anisotropic. Although such an approximation is in wide use, it was questioned by Eckenbeck and Altarelli [13]. Peyla *et al* [20] suggested, therefore, treating the four effective masses as adjustable parameters of the model. In our EVH method applied for parabolic QWs, we obtain the exciton binding energy as a function of several *dimensionless* parameters, each being a nonlinear combination of the effective masses, valence band offsets etc. Therefore, the rigorous definition of the effective-mass values is not of such importance as in the case of rectangular QWs and a simple rescaling is possible here.

The Hamiltonian of the interacting electron–hole pair in the parabolic confining potential is

$$\hat{H} = -\frac{\hbar^2}{2m_e} \left(\frac{\partial^2}{\partial x_e^2} + \frac{\partial^2}{\partial y_e^2} + \frac{\partial^2}{\partial z_e^2} \right) - \frac{\hbar^2}{2m_{\parallel}} \left(\frac{\partial^2}{\partial x_h^2} + \frac{\partial^2}{\partial y_h^2} \right) - \frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z_h^2} - \frac{e^2}{\kappa |\vec{r}_e - \vec{r}_h|} + V_e(z_e) + V_h(z_h). \quad (1)$$

In the equation above, m_e stands for the effective mass of the electron, m_{\parallel} is the effective mass of the hole in \vec{x} - or \vec{y} -directions, m_z is the effective mass of the hole in the \vec{z} -direction, κ is a dielectric constant (assumed to be constant throughout the structure) and the finite parabolic potentials are defined as

$$V_i = \begin{cases} k_i z_i^2 & \text{for } |z| \leq \frac{1}{2} L_w \\ U_i & \text{for } |z| > \frac{1}{2} L_w \end{cases} \quad (i = e, h) \quad (2)$$

where $k_e = 4U_e/L_w^2$ and $k_h = 4U_h/L_w^2$ are the curvatures of the parabolic potential acting on the electron and on the hole, respectively. U_e and U_h are the discontinuities of the band edges between the centre of the well and its outermost layers, while L_w is the QW well width.

In writing equation (1), we made use of the following approximations. First, we neglected the z -dependence of the effective masses of the carriers. For rectangular QWs several authors included the z -dependence of the masses in the kinetic energy terms assuming linear changes of the Luttinger parameters γ_1 and γ_2 with the concentration x of, say, Al in GaAs–Al $_x$ Ga $_{1-x}$ As QWs. The ensuing correction due to such z -dependence of the effective masses is small, and it can be taken into account by suitably averaging the electron and hole masses over the heterostructure. Possible ways of taking properly averaged effective masses are given in, e.g., references [9, 19, 22]. Secondly, we neglected also electrostatic effects arising at the interfaces due to the variation of the dielectric constant with z . We do not expect that these will introduce sizable corrections. Furthermore, in our calculation we shall approximate the finite QW potentials for the electrons and the holes by infinite potentials. That is, we shall replace finite parabolic potentials $V_i(z_i)$ ($i = e, h$) in equation (2) by infinite parabolic potentials $V_i = k_i z_i^2$. In contrast with the case for rectangular QWs [5], use of the infinite parabolic potential leads to only small changes of the energies of the electron and the hole confined in the QW provided that the corresponding energy levels are situated well below the finite-QW top. The reason for this is that even for the infinite parabolic potential the electron and the

hole penetrate the barrier to a considerable extent [25]. Formally, if for a given structure the dimensionless quantity $\Omega_i = 2m_i U_i (L_w/2)^2 / \hbar^2$ ($i = e, h$) is larger than approximately 3, then the difference between the ground-state energies of the finite and the infinite QWs is negligible [26]. Similarly, for $\Omega > 7$ a difference between the energies of the first excited states in the finite and the infinite parabolic QWs nearly vanishes. Note that for the real structures reported in references [5–8] the parameter Ω defined above is of the order of 20–60, so the approximation of the finite QW by the infinite parabolic QW is very good indeed.

3. Formulation of the effective variational method for excitons in parabolic quantum wells

For parabolic QWs reported in the literature [5–8, 23] the separation between the energy levels of the electron (or hole) confined by the QW is much larger than the excitonic Rydberg. Because of this fact it is reasonable to factor out in the exciton trial wave function the terms proportional to the wave functions of the electron (or the hole) in the one-dimensional parabolic well potential. Then, in the optical experiments only the exciton states with s-like symmetry are normally observed [11, 27] so in this work we limit consideration to these states only. For s-like exciton states we shall assume the excitonic wave function in the so-called separable form:

$$F_{m,n}(\vec{r}_e, \vec{r}_h) = \phi_e^m(z_e) \phi_h^n(z_h) f(|\vec{\rho}_e - \vec{\rho}_h|) \quad (3)$$

where $\phi_e^m(z_e)$ is the wave function of the m th state of the electron, $\phi_h^n(z_h)$ the wave function of the n th state of the hole in a parabolic QW, $\vec{\rho}_i = (x_i, y_i)$ ($i = e, h$), and the exact form of the function $f(\cdot)$ is to be determined later. The separable form of the trial exciton wave function means that the function $f(\cdot)$, which mixes the electron and hole states, depends neither on z_e nor z_h , so it depends on four coordinates only (x_e, y_e, x_h, y_h). Hereafter, the excitons formed by the electron in the m th state the hole in the n th state of the parabolic QW will be referred to as (m, n) excitons.

The form of $F(\vec{r}_e, \vec{r}_h)$ suggests that the exciton Hamiltonian (1) can be simplified by a transformation to the cylindrical coordinates. Let the external magnetic field \vec{B} be parallel to the z -axis of the system, so that the vector potential can be chosen as $\vec{A} = (B/2)(-y, x, 0)$. Performing the usual transformation of coordinates x_e, x_h and y_e, y_h to the centre-of-mass (X, Y) and to the relative-motion (x, y) variables, changing the energy unit to the effective Rydberg $\text{Ryd}^* = 2\mu_{\parallel} r_B^2 / \hbar^2$ and the length unit to the effective Bohr radius $r_B = \hbar^2 \kappa / (e^2 \mu_{\parallel})$, we obtain, neglecting the spin,

$$\hat{H} = \hat{H}_{\rho} + \hat{H}_B + \hat{H}_{z_e} + \hat{H}_{z_h} + \hat{H}_{Coul} \quad (4)$$

where

$$\begin{aligned} \hat{H}_{\rho} &= -\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho}\right) & \hat{H}_B &= \frac{1}{4} \gamma^2 \rho^2 & \hat{H}_{z_e} &= -\frac{\mu_{\parallel}}{m_e} \frac{\partial^2}{\partial z_e^2} + b_e z_e^2 \\ \hat{H}_{z_h} &= -\frac{\mu_{\parallel}}{m_z} \frac{\partial^2}{\partial z_h^2} + b_h z_h^2 & \hat{H}_{Coul} &= -\frac{2}{\sqrt{\rho^2 + (z_e - z_h)^2}} \end{aligned}$$

where $\mu_{\parallel}^{-1} = m_e^{-1} + m_h^{-1}$ and $\vec{\rho} = (x, y)$. The parameter $\gamma = (e\hbar B)/(c\mu_{\parallel} \text{Ryd}^*)$ is the reduced magnetic field, while $b_e = k_e r_B^2 \text{Ryd}^{-1}$, $b_h = k_h r_B^2 \text{Ryd}^{-1}$ are dimensionless curvatures of the parabolic QW for the electrons and the holes, respectively. In equation (4) we omitted the centre-of-mass motion in the QW plane since it does not couple to the relative-motion terms and the φ -dependent terms.

Let us now calculate the effective Hamiltonian for the lowest electron and hole states confined in the parabolic QW. The trial function of equation (3) is then given as

$$F_{0,0}(\vec{r}_e, \vec{r}_h) \equiv F_{0,0}(\rho, z_e, z_h) = \exp(-q_e z_e^2) \exp(-q_h z_h^2) f(\rho) \tag{5}$$

with $f(\rho)$ yet to be determined and with

$$q_e = \frac{1}{2} \sqrt{m_e b_e / \mu_{\parallel}} \quad q_h = \frac{1}{2} \sqrt{m_z b_h / \mu_{\parallel}}.$$

The expectation value of the energy of the system is

$$\begin{aligned} E[f^*(\rho), f(\rho)] &= \left(\int \exp(-q_e z_e^2 - q_h z_h^2) f^*(\rho) (\hat{H}_{\rho} + \hat{H}_{z_e} + \hat{H}_{z_h} + \hat{H}_B + \hat{H}_{Coul}) \right. \\ &\quad \times \exp(-q_e z_e^2 - q_h z_h^2) f(\rho) dz_e dz_h \rho d\rho \Big) \\ &\quad \times \left(\int \exp(-2q_e z_e^2 - 2q_h z_h^2) f^*(\rho) f(\rho) dz_e dz_h \rho d\rho \Big)^{-1}. \end{aligned} \tag{6}$$

In the equation above, the integrals involving \hat{H}_{ρ} , \hat{H}_{z_e} , \hat{H}_{z_h} and \hat{H}_B (cf., equation (4)) are straightforward. The double integral over the Coulomb potential can be obtained analytically in terms of the modified Bessel function $K_0(x)$ [24]. The function $f(\rho)$ which minimizes $E[f^*(\rho), f(\rho)]$ satisfies the eigen-equation

$$\begin{aligned} \hat{H}_{eff} f(\rho) &\equiv \left(-\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} - 2\sqrt{\frac{2q_a}{\pi}} \exp(q_a \rho^2) K_0(q_a \rho^2) + \frac{1}{4} \gamma^2 \rho^2 \right) f(\rho) \\ &= (E - E_e - E_h) f(\rho) \end{aligned} \tag{7}$$

where

$$q_a = \frac{q_e q_h}{q_e + q_h} = \frac{1}{2} \left(\frac{m_e m_z b_e b_h}{\mu_{\parallel} (m_e b_e + m_z b_h)} \right)^{1/2} \tag{8}$$

and

$$E_e = \sqrt{m_e b_e / \mu_{\parallel}} \quad E_h = \sqrt{m_z b_h / \mu_{\parallel}}$$

are energies of the levels of electrons and holes in the parabolic QW, respectively. The dimensionless quantity q_a defined by equation (8) plays an important scaling role in our theory. It is a nonlinear combination of the three effective masses and the dimensionless curvatures b_e and b_h of the electron and hole confining potentials. Note that the effective Hamiltonian in equation (7) (and so also its eigen-energies) depends on q_a and γ , but not directly on the electron or hole masses. Let us define the exciton binding energy E_B as $E_B = E - E_e - E_h$ in the absence of the magnetic field and $E_B = E - E_e - E_h - (2n + 1)\gamma$ for nonvanishing magnetic field. The Landau level index $n = 0, 1, \dots$ equals the number of zeros of the wave function $f(\rho)$ in the given quantum state. For the exciton wave function of the form of $F_{m,n}(\rho, z_e, z_h) = \phi_m(z_e) \phi_n(z_h) f(\rho)$ the intensity of the transition is proportional to the oscillator strength $O_{m,n}$ [11, 27]:

$$O_{m,n} \propto \left(\int dt \phi_m(t) \phi_n(t) |f(0)|^2 \right) / \left(\int |F_{m,n}(\rho, z_e, z_h)|^2 \rho d\rho dz_e dz_h \right). \tag{9}$$

From equation (9) it follows that for the excitons in a parabolic QW (i) the oscillator strength is nonzero for s-like symmetric electron-pair states only, where $f(0) \neq 0$, and (ii) that the oscillator strength $O_{m,n}$ vanishes for the excitons formed by the particles in the states possessing different parities, i.e. for $m = n \pm 1, n \pm 3, \dots$ etc.

Finally let us consider the general case of (m, n) excitons. The trial wave function is then

$$F_{m,n}(\rho, z_e, z_h) = h_m(\sqrt{q_e}z_e)h_n(\sqrt{q_h}z_h) \exp(-q_e z_e^2 - q_h z_h^2) f_{m,n}(\rho) \quad (10)$$

where $h_n(x)$ is the n th Hermite polynomial. Functions $F_{m,n}$ and $F_{m',n'}$ are orthogonal for $m \neq m', n \neq n'$ because of the orthogonality of Hermite polynomials of common arguments [25], so the eigen-energies of the effective Hamiltonian calculated for $F_{m,n}(\rho, z_e, z_h)$ approximate from above the energies of (m, n) excitons. Although, it is possible to derive analytical expressions for effective Hamiltonian corresponding to (m, n) excitons, they are too long to be presented here. Instead, in the last section we shall present the exciton binding energy calculated numerically for the case of the $(1, 1)$ exciton.

4. An improved EVH method for excitons in wide QWs

Let us briefly analyse the limiting cases for H_{eff} in equation (7). For large ρ or q_a (i.e., for narrow QW),

$$K_0(x) \simeq \sqrt{\pi/(2x)} \exp(-x)$$

so the term in equation (7) with the K_0 -function reduces to the Coulomb term $(-2/\rho)$ and \hat{H}_{eff} describes the hydrogen atom in two dimensions, with eigen-energies $E_B = 4/n^2$ Ryd, (n is a positive integer). For small q_a (i.e., for wide QW), $K_0(x) \propto \ln(x)$, so for $q_a \rightarrow 0$ the Coulomb potential term vanishes as $\sqrt{q_a} \ln(q_a)$ and \hat{H}_{eff} reduces to the Bessel equation rather than to the equation describing the three-dimensional hydrogen atom. Therefore, we may expect equation (7) to be a correct approximation of true exciton energies in the case of a narrow parabolic QW, while it is not suitable for excitons in wide quantum wells. To understand this fact better, let us consider an exciton in a wide parabolic QW, where the potential energy of the exciton due to the barriers of the quantum well is a small correction to the energy of the free exciton in three-dimensional space. In this case the wave function of the exciton in the QW is very close to the wave function of the exciton in bulk material. In contrast, in wide quantum wells a trial wave function of the exciton given in equation (3) is too weakly localized in the z_e - and z_h -directions, because its z_e -, and z_h -dependent parts decay with characteristic lengths of the order of $1/\sqrt{q_e}$, $1/\sqrt{q_h}$ (cf., equation (5)) rather than r_B . Therefore, in wide parabolic quantum wells the trial function of the exciton from equation (3) differs significantly from the true wave function of the exciton, which leads to large errors in the determination of the energy (and so also the binding energy) of the exciton in wide parabolic quantum wells.

To improve the separable-wave-function approximation for excitons in wide quantum wells, let us replace the function $F(\vec{r}_e, \vec{r}_h)$ from equation (3) by a function \mathcal{F} having the following properties:

- (i) for narrow QW the z_e -, and z_h -dependent parts of \mathcal{F} are close to the wave functions of the m th and n th states of the electron and the hole in the parabolic QW and
- (ii) for wide quantum wells the characteristic lengths of the z_e -, and z_h -dependent parts of \mathcal{F} are of the order of the exciton Bohr radius r_B .

For $(0, 0)$ excitons a trial function fulfilling the conditions above can be realized as follows:

$$\mathcal{F}_{0,0}(\rho, z_e, z_h) = \exp(-Q_e z_e^2) \exp(-Q_h z_h^2) f(\rho) \quad (11)$$

with Q_e and Q_h being adjustable parameters. Note that in this approximation the z_e - and z_h -parts of $\mathcal{F}_{0,0}$ are *not* eigenfunctions of the electron or hole states in the parabolic QW. Using a trial function of the exciton given by equation (11), we obtain the so-called improved

effective Hamiltonian:

$$\hat{H}_{eff}(Q_e, Q_h) = -\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} - 2\sqrt{\frac{2Q_a}{\pi}} \exp(Q_a \rho^2) K_0(Q_a \rho^2) + \frac{1}{4} \gamma^2 \rho^2 + \frac{\mu_{\parallel}}{m_e} Q_e + \frac{b_e}{4Q_e} + \frac{\mu_{\parallel}}{m_z} Q_h + \frac{b_h}{4Q_h} \quad (12)$$

where

$$Q_a = \frac{Q_e Q_h}{Q_e + Q_h}.$$

The last four terms in equation (12) describe the average values of the operators \hat{H}_{z_e} and \hat{H}_{z_h} over Gaussian-like trial functions. The minimum of the eigen-energy E of the improved effective Hamiltonian (12) in the Q_e - Q_h plane approximates from above the true energy of the exciton.

For narrow parabolic quantum wells, $b_e, b_h \rightarrow \infty$, so the last four terms of $\hat{H}_{eff}(Q_e, Q_h)$ in (12) dominate over the screened Coulomb potential. Therefore the minimum of the exciton energy occurs for

$$Q_e \simeq q_e = \frac{1}{2} \sqrt{m_e b_e / \mu_{\parallel}} \quad Q_h \simeq q_h = \frac{1}{2} \sqrt{m_z b_h / \mu_{\parallel}}$$

i.e., for the same values as in the case the effective Hamiltonian in equation (5). However, for wide quantum wells where $b_e, b_h \rightarrow 0$, both Q_e and Q_h (and so also Q_a) remain finite and the improved effective Hamiltonian (12) has a nonvanishing Coulomb potential term. The values of (Q_e, Q_h) corresponding to the minimum of the energy of the exciton determine the size of the exciton in the z_e - and z_h -directions, which is of the order of the exciton Bohr radius r_B even in very wide parabolic quantum wells.

A trial function of the (m, n) exciton in wide quantum wells is (cf., equation (10) and equation (11))

$$\mathcal{F}_{m,n}(\rho, z_e, z_h, Q_e, Q_h) = h_m(\sqrt{Q_e} z_e) h_n(\sqrt{Q_h} z_h) \exp(-Q_e z_e^2 - Q_h z_h^2) f_{m,n}(\rho) \quad (13)$$

where (Q_e, Q_h) are adjustable parameters and $h_m(x), h_n(x)$ are Hermite polynomials. If the functions $\mathcal{F}_{i,j}$ ($i = 0, \dots, m; j = 0, \dots, n$) are orthogonal, then the eigen-energies of the effective Hamiltonian calculated using $\mathcal{F}_{i,j}$ approximate from above the energies of the (i, j) exciton. However, we may not minimize the eigen-energies of (i, j) excitons in the Q_e - Q_h plane independently from eigen-energies of (i', j') excitons because the parameters (Q_e^i, Q_h^j) corresponding to the minimum of the eigen-energy of the (i, j) exciton depend on the (i, j) indices and on the quantum state of the ρ -dependent part of the exciton. Thus, for some (i_1, j_1) and (i_1, j_2) excitons (where $i_1, i_2 = 0, \dots, m; j_1, j_2 = 0, \dots, n$), functions \mathcal{F}_{i_1, j_1} and \mathcal{F}_{i_1, j_2} possessing the same parity may be not orthogonal, in view of the lack of orthogonality of Hermite polynomials of different arguments (cf., equation (13)). Similarly, 1s, 2s, ... functions of (i, j) excitons are not orthogonal, if the minimization of the exciton energy with respect to (Q_e^i, Q_h^j) is done independently for 1s, 2s, ... states.

To ensure the proper orthogonality of all states of the exciton within the improved EVH method, we propose the following approach. First, we calculate the effective Hamiltonian (12) for the 1s state of $(0, 0)$ excitons. Next, we find values (Q_e^0, Q_h^0) which minimize the eigen-energy of this Hamiltonian (i.e., the energy of the 1s state). Then in calculating the energies of 1s, 2s, 3s, ... states of (i, j) excitons ($i = 0, \dots, m; j = 0, \dots, n$) we use the parameters (Q_e^0, Q_h^0) . This procedure ensures both the proper behaviour of the exciton trial wave functions in the z_e -, z_h -directions and the orthogonality of the functions $\mathcal{F}_{i,j}$ for $i = 0, \dots, m; j = 0, \dots, n$, because the z_e - and z_h -dependent parts of $\mathcal{F}_{i,j}$

($i = 0, \dots, m; j = 0, \dots, n$) are Hermite polynomials with *common* values of (Q_e^0, Q_h^0). The procedure described above is used in section 6 to determine the energies of 2s excitons within the improved EVH method.

5. Comparison of results from the EVH and other methods of calculation

In the variational method proposed by Yang and Yang [23] the trial function of the 1s state of the (0, 0) exciton was chosen in the form

$$F_{var}(\rho, z_e, z_h) = \exp(-q_e z_e^2 - q_h z_h^2) \exp\left(-\frac{\rho}{\lambda}\right) \quad (14)$$

where q_e, q_h have their previous meanings and λ is the variational parameter. In the absence of the magnetic field the energy of the system is then

$$E = \min_{\{\lambda\}} \left[\frac{1}{\lambda^2} - \frac{8}{\lambda^2} \sqrt{\frac{2q_a}{\pi}} \int_0^\infty \rho \, d\rho \exp(q_a \rho^2) K_0(q_a \rho^2) \exp\left(-\frac{2\rho}{\lambda}\right) \right]. \quad (15)$$

In the method proposed by Leavitt and Little [19, 20] the wave function of the 1s state of the (0, 0) exciton is assumed to be

$$G(\vec{r}_e, \vec{r}_h) = \exp(-q_e z_e^2 - q_h z_h^2) g(\rho, |z_e - z_h|). \quad (16)$$

The exciton binding energy as calculated within the Born–Oppenheimer approximation for $B = 0$ is

$$E = \sqrt{\frac{2q_a}{\pi}} \int_{-\infty}^\infty dz \exp(-2q_a z^2) E^{2D}(|z|). \quad (17)$$

For 1s excitons the function $E^{2D}(|z|)$ was parametrized by Leavitt and Little [19], while for 2s, 3s and 4s excitons it was parametrized by Peyla *et al* [20].

In figure 1 we show the binding energy of the 1s state of (0, 0) excitons obtained using the EVH method, the improved EVH method (assuming equal masses and valence band offsets for the electrons and the holes), the variational method and the Leavitt and Little method. Note first that the binding energy calculated using the EVH method is *greater* than the binding energy found using the variational calculation. This confirms the expectation of the EVH method giving the best results within a given *class* of trial functions—e.g., the class of separable wave functions, equation (3). Secondly, for small values of q_a , which corresponds to wide quantum wells, the improved EVH method gives larger binding energy than the normal EVH method. For narrow wells (i.e. large q_a) the two methods lead to the same results, which agrees with the analysis from the previous section. Thirdly, the EVH method gives an upper estimate of the true value of the quantum state while the Leavitt and Little method estimates the energy of the quantum state from below. We see in figure 1 that the difference between the two results is rather small, so both methods approximate the true value of the exciton binding energy with high accuracy. The method proposed by Leavitt and Little is more convenient for calculating the energy of (0, 0) excitons in the absence of the magnetic field. This is because a simple parametrization of $E^{2D}(z)$ exists [19, 20]. In the case of the nonvanishing magnetic field the two methods are comparable as regards numerical effort, since in both of them one has to find eigenvalues of a one-dimensional differential equation.

6. (0, 0) and (1, 1) exciton energies in real structures

The eigen-energies and the eigenstates of \hat{H}_{eff} were calculated numerically using the shooting method [28]. In this method, we choose a trial value of the eigen-energy $E_B^{(1)}$ and solve

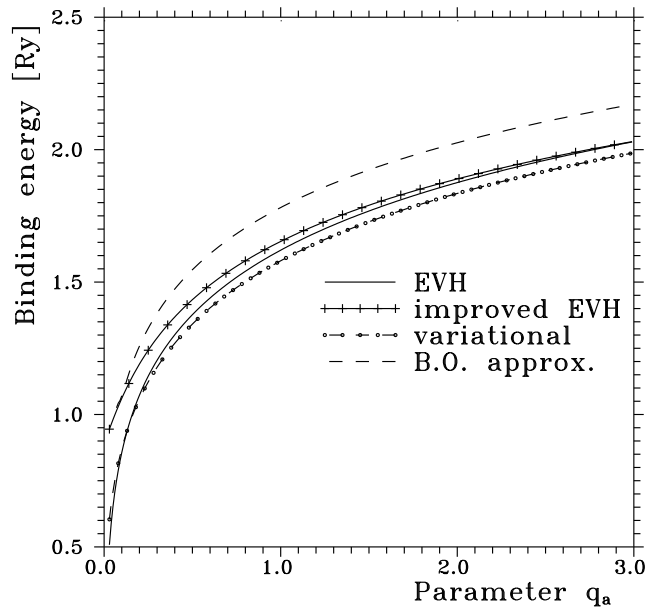


Figure 1. The binding energy of the 1s (0, 0) exciton calculated using the EVH approximation (solid line), the improved EVH approximation assuming equal masses and the valence band offsets for the electron and the hole (solid–crosses line), the usual variational method (dashed–points line) and the method proposed by Leavitt and Little (Born–Oppenheimer approximation).

the differential equation using the fourth-order Runge–Kutta method. For s-symmetric states of the Hamiltonian (4), the boundary conditions for the solutions of the differential equation are $f(0) = c$ ($c \neq 0$) and, in order to ensure the continuity of $f(\rho)$ at $\rho = 0$, $(df(\rho)/d\rho)|_{\rho=0} = 0$. For large ρ a square-integrated solution of equation (4) decays to zero, so by analysing the behaviour of $f(\rho)$ for large ρ we may easily recognize whether a trial value $E_B^{(1)}$ overestimates or underestimates the true value of E_B . Then, we choose a new value of the eigen-energy, $E_B^{(2)}$, and repeat the calculations. Using a bisection method we can bracket E_B with arbitrary accuracy. In our calculation we performed 16 iterations with trial values of $E_B^{(n)}$, which gives a relative accuracy in the determination of E_B of the order of 10^{-4} of the initial range of (E_B^{min}, E_B^{max}) . We found eigen-energies and eigenstates of the effective Hamiltonians for 1s, 2s, 3s and 4s states in this way.

In figure 2 we show E_B (in effective Rydberg units Ryd^*) versus q_a for 1s, 2s and 3s states of the (0, 0) exciton for $\gamma = 0$ and for $\gamma = 1.0$. All curves in figure 2 can be parametrized using a formula

$$E_B = \sum_{n=0}^3 a_n t^n \quad t = \ln(q_a) \tag{18}$$

where the a_n are coefficients of the fitting polynomial. The parametrizations of the exciton binding energy from equation (18) can be applied to the determination of the exciton binding energy for wide wells within the improved EVH method. Indeed, for a wide parabolic well the exciton binding energy can be obtained as (cf., equation (12))

$$E_B = \min_{\{Q_e, Q_h\}} \left\{ \sum_{n=0}^3 a_n t^n + \frac{\mu_{\parallel}}{m_e} Q_e + \frac{b_e}{4Q_e} + \frac{\mu_{\parallel}}{m_z} Q_h + \frac{b_h}{4Q_h} \right\} \quad t = \ln \left(\frac{Q_e Q_h}{Q_e + Q_h} \right) \tag{19}$$

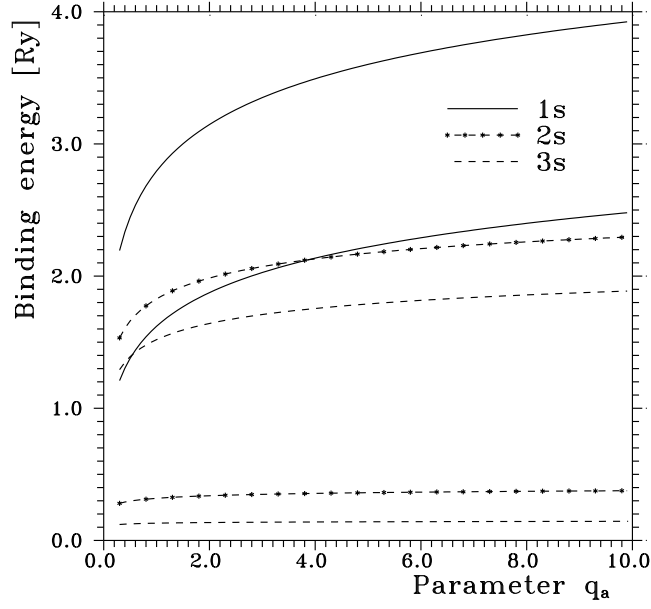


Figure 2. The dimensionless exciton binding energy for 1s, 2s and 3s (0, 0) exciton states. Solid lines from bottom to top: the 1s exciton energy for $\gamma = 0$ and $\gamma = 1$. Dashed-points lines from bottom to top: the 2s exciton energy for $\gamma = 0$ and $\gamma = 1$. Dashed lines from bottom to top: the 3s exciton energy for $\gamma = 0$ and $\gamma = 1$.

which is a rather simple numerical task. The method of calculation of the energy of excited states of the electron-hole pair within the improved EVH method was discussed in section 4.

Table 1. Material parameters for GaAs-Al_{0.3}Ga_{0.7}As and CdTe-Cd_{0.22}Mn_{0.78}Te.

Quantity	Symbol	CdTe-Cd _{0.22} Mn _{0.78} Te	GaAs-Al _{0.3} Ga _{0.7} As
Electron mass	m_e	$0.095m_0$ [7]	$0.0667m_0$ [8]
In-plane heavy-hole mass	m_{\parallel}^h	$0.5m_0$ [20]	$0.115m_0$ [20]
Heavy-hole mass along the growth direction	m_z^h	$0.65m_0$ [7]	$0.34m_0$ [20]
Dielectric constant	κ	10.6 [29]	12.15 [20]
Valence band offset	Q_v	0.4 [7]	0.35 [8]
Total QW depth	$U_e + U_h$	1260 meV [7]	380 meV [20]

As an example of the application of the numerical results of figure 2 we use them in the determination of the (0, 0) exciton binding energies of 1s and 2s heavy-hole excitons in GaAs-Al_{0.3}Ga_{0.7}As and CdTe-Cd_{0.22}Mn_{0.78}Te structures. The material parameters taken for the calculation of the binding exciton energy are listed in table 1. For these structures we plotted in figure 3 binding energies and transition energies for the 1s and 2s states of the heavy-hole exciton as a function of the quantum well width. Solid and points-solid lines show the values of the exciton binding energy for the 1s state of the exciton calculated using the EVH (solid lines) and improved EVH methods (points-solid lines). The dotted lines show the transition energies E_{1s-2s} for transitions between 1s and 2s states of the exciton in the EVH approximation. A triangle and squares represent experimental data from references [7, 8].

For the GaAs-Al_{0.3}Ga_{0.7}As parabolic quantum well of width $\approx 1000 \text{ \AA}$ reported on in

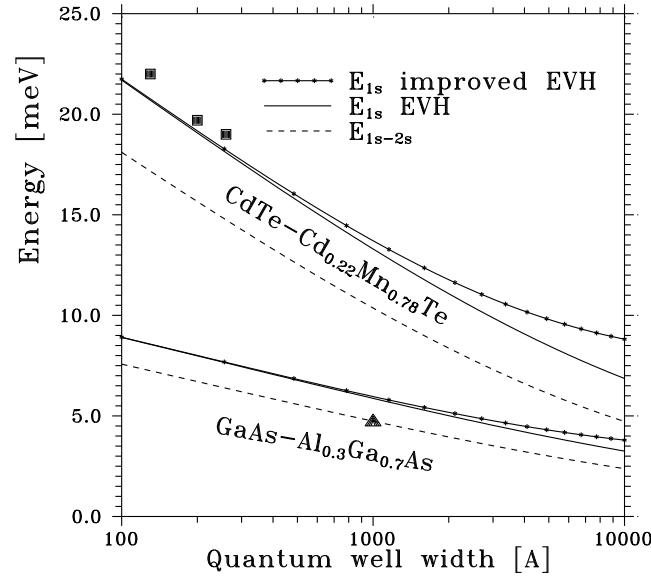


Figure 3. The exciton binding energy versus the finite parabolic QW width for the heavy-hole (0, 0) exciton in GaAs–Al_{0.3}Ga_{0.7}As and CdTe–Cd_{0.22}Mn_{0.78}Te heterostructures. The material parameters are taken from table 1. Solid lines: the EVH approximation. Solid–points lines: the improved EVH method. Dotted lines: the transition energy E_{1s-2s} for transitions between 1s and 2s states of the exciton. Triangle: the experimental value of the energy E_{1s-2s} , after reference [8]; squares: the experimental 1s-exciton binding energy, after reference [7].

reference [8] we found the transition energy E_{1s-2s} to be $E_{1s-2s} = 4.8$ meV, which is in very good agreement with experimental data. For the CdTe–Cd_{0.22}Mn_{0.78}Te structures analysed in reference [7] we compared our results with 1s-exciton binding energies of quantum wells with widths of 41, 62, 82 monolayers which corresponds to widths of 133 Å, 201 Å and 266 Å, respectively. For the heavy-hole mass we assumed $m_{\parallel}^h = 0.5m_0$ found experimentally in [20] for magnetoexcitons in CdTe/Cd(Zn)Te rectangular quantum wells. There is also a good agreement between our theory and experimental results. Small discrepancies between them arise, possibly, from uncertainties in the values of the effective masses, valence band offsets and dielectric constants for CdTe and Cd_{1-x}Mn_xTe compounds. From figure 3 we note that for parabolic quantum wells fabricated today and reported on in references [5–8], the binding energy of excitons calculated using the EVH method is very close to that found using the improved EVH method. The difference between the two methods is visible only for very wide quantum wells, where the exciton binding energy calculated using the improved EVH method is as much as 20% larger than the binding energy obtained using the EVH method.

Finally, in figure 4 we calculated the energy of (1, 1) excitons in GaAs–Al_{0.3}Ga_{0.7}As heterostructures. This energy was calculated for 1s states of heavy-hole excitons for $B = 0$, $B = 5$ T and $B = 15$ T. We assume the trial wave function of the (1, 1) exciton in the form

$$F_{1,1}(\rho, z_e, z_h) = z_e z_h \exp(-q_e z_e^2 - q_h z_h^2) f_{1,1}(\rho). \quad (20)$$

Note, that for (1, 1) heavy-hole excitons the binding energies are *smaller* than the binding energies for (0, 0) excitons. In the absence of the magnetic field the difference is of the order of 2 meV, i.e., of the order of 20%–25% of the exciton binding energy. For magnetic fields of $B = 15$ T the difference between the (0, 0) and (1, 1) exciton energies is of the order of 4 meV. The positions of the higher exciton peaks in parabolic quantum wells were used

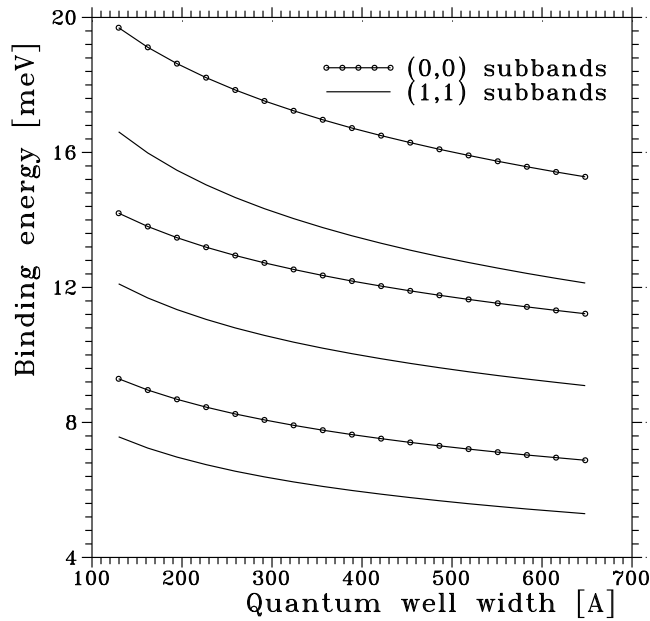


Figure 4. Comparison of the binding energies of the 1s heavy-hole exciton in GaAs–Al_{0.3}Ga_{0.7}As formed by particles in (0, 0) parabolic QW subbands (solid–points lines) and of that formed by particles in (1, 1) subbands (solid lines). The calculation is done for three values of the magnetic field: $B = 0$, $B = 5$ T, $B = 15$ T, respectively, from bottom to top.

in references [7, 8] in the determination of the valence band offsets in CdTe–Cd_{1–x}Mn_xTe and GaAs–Al_xGa_{1–x}As heterostructures. In both works the authors assumed that the binding energy of the exciton formed by particles from excited states of the parabolic QW equals the binding energy of the (0, 0) exciton. From figure 4 we see that such an approximation is not justified and the differences between the values for (0, 0) and (n, n) excitons ($n > 0$) have to be taken into account in precise determinations of the material parameters from the positions of the excitonic peaks in photoluminescence spectra of parabolic quantum wells.

Let us briefly summarize this paper. We proposed a new method of calculation of the binding energy of excitons confined in one-dimensional quantum well potentials. We applied this method in the determination of energy levels of the excitons in parabolic QWs. We compared the values of the exciton binding energies in real structures with experimental data and we found good agreement between them. The EVH method introduced in this paper allows for fast and accurate determination of the whole spectrum of exciton states in quasi-two-dimensional heterostructures. This feature of the EVH method looks very promising for future applications of this method for other confining potentials which occur in newly fabricated structures.

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