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Self-consistent approach for calculations of exciton binding energy in quantum wells

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Abstract

We introduce a computationally efficient approach to calculating characteristics of excitons in quantum wells. In this approach we derive a system of self-consistent equations describing the motion of an electron–hole pair. The motion in the growth direction of the quantum well in this approach is separated from the in-plane motion, but each of them occurs in modified potentials found self-consistently. The approach is applied to shallow quantum wells, for which we obtained an analytical expression for the exciton binding energy and the ground state eigenfunction. Our numerical results yield lower exciton binding energies in comparison to standard variational calculations, while require reduced computational effort.

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1. Introduction

Excitons play an important role in the band edge optical properties of low-dimensional semiconductor structures such as quantum wells, quantum wires, and quantum dots [1]. Quantum confinement of electrons and holes in such structures results in increased binding energy of

excitons, their oscillator strength, and a life-time. As a result, excitons, for instance, in quantum wells, are observed even at room temperatures, and play, therefore, a crucial role in various optoelectronic applications [2–4]. To be able to calculate effectively and accurately exciton binding energies in the quantum heterostructures is an important problem, and therefore, a great deal of attention has been paid to it during several decades [5–23]. However, this problem is rather complicated, and while significant progress has been achieved, new material systems and new type of

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applications require more flexible, accurate and effective methods.

Presently, the best results are usually obtained within the framework of the variational approach, where a certain form of the exciton wave function, depending on one or more variational parameters is being postulated. The exciton energy is then calculated by minimizing the respective energy functional with respect to the variational parameters. Unfortunately, even in the simplest (and, therefore, less accurate) realization of this approach it is not possible to express a value of the binding energy as a function of quantum well parameters. The best one can hope for is to obtain a set of complicated equations, which relate material parameters to several variational parameters. The latter are found numerically, and then used for numerical computation of the exciton energy. These difficulties result from the fact that variables in the Hamiltonian describing relative motion of the electron–hole pair cannot be separated: the presence of the quantum well potential breaks the translational invariance of the system, making it impossible to separate in-plane motion of the electrons and holes from the motion in the direction of confinement.

The standard variational approach is based upon a choice of a specific form of a trial function, which is usually chosen in the form of a product of three terms [5–7,9]. The first two are one-particle one-dimensional electron and hole wave functions for confined motion across the quantum well. The third term describes the relative motion of an electron and a hole due to Coulomb interaction. The accuracy of the results depends on the complexity of the third term of the trial function and the number of variational parameters. The more the parameters, the lower the binding energy, but, of course, the more extensive the calculations. There is ample literature dealing with accurate variational numerical calculations of exciton binding energy in quantum wells [5–19]. Most advanced of the calculations include the effects of Coulomb screening due to dielectric constant mismatch, as well as effective mass mismatch at heterojunctions and band degeneracy [9,10].

Another approach discussed in the literature [20–23] is based upon an expansion of the electron–hole envelope wave function in terms of the complete system of eigenfunctions of a one-particle Hamiltonian describing motion of electrons (holes) in the respective quantum well confining potentials. The coefficients of this expansion represent the wave functions of the in-plane motion. They satisfy an infinite set of differential equations, which are coupled because of mixing of different electron and hole sub-bands induced by Coulomb interaction. Such a system can be solved only numerically after an appropriate truncation of the basis. Another way is to solve the system in diagonal approximation and to treat the off-diagonal elements with the help of perturbation theory. The improvement of accuracy in this approach faces difficulties related to the unknown errors due to basis truncation.

Despite the significant achievement of the current approaches, they suffer from some principal limitations imposed by their very nature, and which cannot be, therefore, easily overcome. For instance, traditional variational approaches are limited by the need to deal with a variational function of a particular form, which tremendously restricts the functional space over which the minimum of the energy is being searched. This problem cannot be circumvented by an increase in the number of the variational parameters because of the difficulties solving optimization problems with three or more parameters. Besides, calculations presented in most papers are not self-consistent (some limited attempts to introduce self-consistency, which were made in the past [17,18] are discussed below in Section 2). At the same time self-consistence in calculations may become more important for material systems with wide band-gap materials. Thus, it is necessary to develop a method of calculating exciton binding energies, which would be more flexible and accurate than the existing methods, and which would allow to treat effects due to electron–hole interaction in a self-consistent way.

In this work we suggest such an approach, which is based upon application of the ideas of the self-consistent Hartree method to the excitons in quantum wells. The idea of this approach is that instead of imposing a particular functional dependence on the envelope wave function, we present it

as a special combination of some unknown functions, which depend on fewer than the total number variables. Applying the variational principle to this combination we derive a system of equations describing both the motion of electrons and holes in the direction of confinement, and the relative two-dimensional in-plane motion of the exciton. Effective potentials entering these equations have to be found self-consistently along with the wave functions.

This approach has a number of advantages compared to the previous methods. First of all, in its most general statement it must give better results for the exciton energy because we span a much larger functional space in the search for the minimum. Second, as it will be discussed below, this approach automatically gives a self-consistent description. Third, the approach can be naturally expanded to more complicated systems such as asymmetric quantum wells, and also allows incorporating external electric and magnetic fields, stress, and disordered potential acting on electrons and holes in QW because of inherent inhomogeneities of structure. All these effects, which modify the single particle part of the Hamiltonian, appear automatically in self-consistent equations for the variational functions. We show that for the case of strong confinement in QW the self-consistent approach with factorized form of the envelope wave function allows one to achieve a very good agreement with the results of the variational method for the most elaborate trial functions used in the literature before. The relative motion of the exciton in the in-plane directions is described in this treatment by the Coulomb potential averaged with the wave functions of electron's (hole's) motion in the direction of confinement. The latter, in turn, is characterized by an effective confining potential, which is obtained by combining the initial quantum well potential with the appropriately averaged Coulomb potential. Unlike the perturbative method [20], our approach takes into account the Coulomb mixing of the electron and hole sub-bands in a non-perturbative way, and is expected to give more accurate results even for the cases when such mixing is important.

In addition to carrying out self-consistent numerical calculations, we also provide detailed analysis of the first iteration of the self-consistent procedure. This analysis presents interest because it admits to a semi-analytical treatment, and it turns out that it gives rather accurate estimates for exciton binding energies at a fraction of the cost of full-fledged variational calculations. In addition, qualitative characteristics of the exciton effective potential, derived from this iteration, give a good understanding of a self-consistent effective potential. In particular, we show that this potential has two different regimes of behavior. For large distances the potential has three-dimensional Coulomb tails, while at very small distances it becomes logarithmic as it would be for the true Coulomb potential of a point charge in two dimensions. A crossover between these two regimes takes place around distance $r \sim d$, which is the average electron–hole separation in the quantum well in the z-direction. Understanding these basic properties of the potential allowed us to suggest a simple variational function, which yields to an analytical expression for exciton binding energy.

We apply our approach to a particular case of a shallow quantum well, which allows for obtaining some analytical results, which give important qualitative insight into the properties of more generic models as well. We use a δ-functional model to describe shallow quantum wells that allow us to obtain an explicit form of the effective Coulomb potential. We would like to stress here that δ-functional model itself is not an oversimplification, as it is often thought, but is a natural approximation for quantum wells, which have only one level inside. This model gives an accurate value of the energy level in such a well, and correctly describes the respective wave function in the barrier region. In some sense, the model of δ-functional QW is complimentary to the model of effective infinite quantum well [25], which is used to approximate finite QW with large widths, when the number of levels in a well is larger than one (see discussion in Section 3). For shallow quantum wells, the δ-functional model allows deriving a simple analytical formula for the exciton binding energy that depends only on one variational parameter. This formula gives results comparable to the best numerical results obtained

by the standard variational approach. On the other hand, the numerical iteration procedure within the framework of the self-consistent approach gives the binding energies, which are lower than energies obtained by variational method. Thus, we demonstrate that the method is both efficient and accurate; it can be applied to any quantum well with an average size of confinement smaller than the three-dimensional effective Bohr radius.

The paper is organized as follows. In Section 2 we discuss the model and derive the general self-consistent equations. In Section 3 we derive an analytical expression and discuss the different limits of the effective exciton potential. In this section we also derive the analytical expression for zero iteration of the exciton binding energy. Section 4 presents the comparison of the binding energies results for the self-consistent approach and the standard variational method. The last section presents the conclusions of our work. The auxiliary details of the calculations can be found in three appendices.

2. The model: 2D exciton in self-consistent field

We assume that both conduction and valence bands are non-degenerate, and that they both have an isotropic parabolic dispersion characterized by the masses m_e and m_h (the heavy hole mass), respectively. Throughout the paper we use effective atomic units (a.u.), which means that all distances are measured in units of the effective Bohr radius $a_B = \hbar^2 \varepsilon / \mu^* e^2$, energies in units of $\mu^* e^4 / \hbar^2 \varepsilon^2 \equiv 2\,\text{Ry}$, and masses in units of reduced electron–hole mass μ^*, where $1/\mu^* = 1/m_e^* + 1/m_h^*$. In this notation $m_{e,h} = m_{e,h}^* / \mu^*$, where $m_{e,h}^*$ are effective masses of an electron and a heavy hole. We assume that both the barrier and the well have close dielectric constants ε as well as dispersion laws. Thus, we neglect a dielectric constant difference and an effective mass mismatch. One of the goals of this paper is to compare our method with existing approaches. Therefore, we have made some of these simplifications deliberately. Important effects such as valence-band mixing, non-parabolicity of the conduction

band, dielectric constant and effective mass mismatches can be added to the model at later stages once the method is fully developed.

After the standard procedure of excluding the center-of-mass of the perpendicular motion in the plane of the layers, [5,6] the excitonic Hamiltonian is given by

$$\hat{H} = E_g + H_e + H_h + K_r + V_{\text{reh}},$$

$$H_e = -\frac{1}{2m_e}\frac{\partial^2}{\partial z_e^2} + V_1(z_e),$$

$$H_h = -\frac{1}{2m_h}\frac{\partial^2}{\partial z_h^2} + V_2(z_h),$$

$$K_r = -\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right],$$

$$V_{\text{reh}} = -\frac{1}{\sqrt{r^2 + (z_e - z_h)^2}}, \tag{1}$$

where E_g is a gap energy, z is the growth direction, r measures a relative electron–hole distance in the transverse direction $r = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2}$, and $V_{1,2}$ are the quantum well confining potential in z direction for the electron and the hole, respectively. We have already assumed that the ground state must be independent of an angle in the xy plane, and excluded the corresponding term from the kinetic energy of the relative motion, K_r.

A *variational principle* can be used in two different ways for calculation of approximate solutions for the Schrödinger equation with the Hamiltonian (1). The first approach is the *standard variational method*. It is well described in the literature [5–7,9,11–13,10,14–16]. According to this method, one needs to start from a variational principle for the functional $E[\Psi]$:

$$E[\Psi] = \int \Psi^* \hat{H} \Psi \, dV = \min \tag{2}$$

with the additional normalization condition

$$\int |\Psi|^2 \, dV = 1. \tag{3}$$

Then look for an approximate wave function within a class of functions of predetermined analytical coordinate dependence. These functions depend on several variational parameters, $\lambda_1, \lambda_2, \dots$.

Then the total energy

$$E = E(\lambda_1, \ldots, \lambda_n), \tag{4}$$

and numerical values of variational parameters can be obtained from minimization conditions

$$\frac{\partial E(\lambda_1, \ldots, \lambda_n)}{\partial \lambda_i} = 0, \quad i = 1, 2, \ldots, n. \tag{5}$$

The success of the method depends essentially on the choice of the trial function. It must be simple enough to lend itself easily to the calculations, but must vary in a sufficiently large domain for the energy obtained to be close to the exact one.

Another way to calculate the approximate solutions of Eq. (1) is to utilize the *self-consistent approach*. This approach also starts from the *variational principle*, Eqs. (2) and (3). However, instead of choosing a particular coordinate dependence of the trial function, we only assume a particular functional dependence on different coordinates for the entire wave function. Namely, we construct an approximate entire wave function $\Psi(z_e, z_h, r)$ with the help of the unknown functions $\psi_1, \psi_2, \ldots$, where each function ψ_k depends on a lesser number of variables than the entire wave function. Considering variations of these functions independently, from the variational principle, Eqs. (2) and (3), we obtain coupled integro-differential equations for ψ_k.

If localization in the quantum well is strong (the exciton "z-size" is smaller than its Bohr radius), then it is reasonable to suggest that the exact wave function for the ground state of Hamiltonian (1) is close to the simple product of functions of different coordinates

$$\Psi_{\text{exact}}(r, z_e, z_h) \longrightarrow \Psi_{\text{trial}}(r, z_e, z_h)$$
$$= \psi(r)\chi_e(z_e)\chi_h(z_h). \tag{6}$$

Assuming normalization of every function in this product, we substitute function Ψ in Eq. (2) by the trial function (6), vary each function in a product separately, and obtain the system of coupled integro-differential equations

$$\left[K_r + \overline{V}_r(r)\right]\psi(r) = E_X\psi(r), \tag{7}$$

$$\left[H_e + \overline{V}_e(z_e)\right]\chi_e(z_e) = E_e\chi_e(z_e), \tag{8}$$

$$\left[H_h + \overline{V}_h(z_h)\right]\chi_h(z_h) = E_h\chi_h(z_h), \tag{9}$$

where the following notations for effective potentials are introduced:

$$\overline{V}_r(r) = \langle \chi_e\chi_h | V_{\text{reh}} | \chi_e\chi_h \rangle, \tag{10}$$

$$\overline{V}_{e,h}(z_{e,h}) = \langle \psi\chi_{h,e} | V_{\text{reh}} | \psi\chi_{h,e} \rangle. \tag{11}$$

The angle brackets imply that the integration of the Coulomb potential with corresponding wave functions is carried out over two of three independent variables.

Solving system of equations (7)–(9) we obtain the best approximation for the entire wave function in the form of a product (6). The corresponding value of the total energy is given by Eq. (2) that can be rewritten in the form

$$E = \langle \Psi | \hat{H} | \Psi \rangle = E_e + E_h + E_X$$
$$- \langle \chi_e | \overline{V}_e | \chi_e \rangle - \langle \chi_h | \overline{V}_h | \chi_h \rangle. \tag{12}$$

The latter expression can be obtained by averaging each of Eqs. (7)–(9) and adding them together. The electrostatic term between the electron and the hole is counted three times in the summations, and so has to be subtracted twice to give Eq. (2). Thus the total energy is not just the sum of the exciton binding energy and the electron and the hole confining energies. The last two terms in Eq. (12) describe the renormalization of the total energy due to non-separability of the Hamiltonian.

In order to solve Eqs. (7)–(9) we apply the method of successive approximations. For strong localization inside the quantum well, the corrections to the single-particle energies due to effective Coulomb interaction potentials $\overline{V}_{e,h}(z_{e,h})$ in Eqs. (8) and (9) are small. Therefore, we begin by neglecting their contributions ($\overline{V}_{e,h}^{(0)} = 0$) and solve the equations

$$H_{e,h}\chi_{e,h}^{(0)}(z) = E_{e,h}^{(0)}\chi_{e,h}^{(0)}(z). \tag{13}$$

The obtained eigenfunctions are then substituted into Eq. (10) in order to get $\overline{V}_r^{(0)}(r)$, a zero approximation for $\overline{V}_r(r)$. This potential in turn should be substituted into Eq. (7). The resulting equation,

$$[K_r + \overline{V}_r^{(0)}(r)]\psi^{(0)}(r) = E_X^{(0)}\psi^{(0)}(r), \tag{14}$$

describes the formation of a two-dimensional exciton by an effective electron–hole interaction. The physical meaning of this effective interaction

is a quantum mechanical average of the Coulomb potential with confinement wave functions. The ground state eigenfunction computed from Eq. (7) can then be substituted into Eq. (11) to calculate a new approximation $\overline{V}_{e,h}^{(1)}(z_{e,h})$ for the effective potentials. This process can be continued until the potentials are self-consistent to a high order of accuracy, i.e., until the condition

$$\langle \psi | \overline{V}_r | \psi \rangle \approx \langle \chi_e | \overline{V}_e | \chi_e \rangle \approx \langle \chi_h | \overline{V}_h | \chi_h \rangle \tag{15}$$

is fulfilled. Eqs. (7)–(12) with condition (15) represent the complete system of equations for finding the minimum of the total energy for the Hamiltonian (1) if the trial function has a particular functional dependence (6).

The described procedure has several advantages in comparison with the standard variational method. First of all, at each step we solve one-dimensional differential equations.[1] Second, even if the resulting Eq. (7) for the exciton in the effective field cannot be solved analytically, the explicit form of the effective potential (10) gives some additional understanding of the form of the exciton eigenfunction, and hence improves the accuracy of calculations. Finally, the convergence of the successive iterations itself allows us to estimate to what degree a given functional dependence of the trial function is close to the exact wave function. The energy difference between the successive approximations shows how far the approximate energy is from the exact ground state energy. Certainly, we should expect a slow convergence for very broad and ultra-narrow quantum wells, where the entire wave function must be close to the wave function of the three-dimensional exciton. In this case, however, we can modify our self-consistent theory, rewriting Hamiltonian (1) in terms of the new independent variables: the three-dimensional radius R (which is determined by $R = \sqrt{r^2 + z^2}$), the angle θ (that links z and R coordinates: $z = R \cos \theta$) and the coordinate Z of center-of-mass in the z direction [$Z = (m_e z_e + m_h z_h)/M$]. Then we can apply the

variational principle for a trial function $\Psi_{\text{trial}}(R, \theta, Z) = \psi(R) f(\theta) g(Z)$, and obtain corresponding self-consistent equations for functions ψ, f, g. Detailed analysis of this issue is, however, out of the scope of this paper, in which we are focused mostly on standard type I quantum wells with their widths much smaller than the effective three-dimensional Bohr radius of the exciton. In the next section, we present the comparison of our self-consistent approach with the results of the standard variational method for the shallow quantum well. It is worth noting that the first iteration of our approach might be considered as an improved version of the standard variational method with a separable trial function (6), in which functions $\chi_{e,h}$ are the electron and the hole eigenfunctions without the interaction, and $\psi(r)$ is chosen in the form of a $1s$ function for a two-dimensional exciton.

We would like to note that some attempts to treat the Coulomb term in the Hamiltonian (1) in a self-consistent manner have been made in the past [8,17,18,21–24]. For example, in Refs. [17,18] an incomplete self-consistent procedure for single-particle wave functions was performed. Due to the more complicated form of the trial function $\Psi_{\text{trial}} = \psi(r, z_e - z_h) \chi_e(z_e) \chi_h(z_h)$ the authors in Refs. [17,18] treated the first term $\psi(r, z_e - z_h)$ in the product by the standard variational method, adjusting variational parameters. Then an attempt was made to look for self-consistent corrections to the electron and hole wave functions, $\chi_{e,h}$, with the help of equations similar to our Eqs. (8) and (9). In principle, it is possible to write the complete system of self-consistent equations for the trial function in the form $\psi(r, z_e - z_h) \chi_e(z_e) \chi_h(z_h)$. To do this, one needs to start again from the variational principle, Eqs. (2) and (3). Then by varying each function separately in the product one can get the complete system of the integro-differential equations similar to Eqs. (7)–(9). This system and the final expression for the total energy will have a more complicated form due to non-orthogonality of functions in the product for the entire trial function.

On the other hand, the first iteration of our method results in Eq. (14), which coincides with the zero approximation of the "truncated basis"

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[1] We assume that ground state energy for two-dimensional exciton in the central field is independent of angles. Therefore, resulting equation on the radial wave function is one-dimensional.

approach [21,23], when only the ground state confinement eigenfunctions are left. Our derivation of Eq. (7) shows, however, that it is more significant than merely a truncation of all but one term in the basis. The successive iterations of the Eqs. (7)–(9) take into account the Coulomb mixing of the electron and hole sub-bands in a non-perturbative way, and give more accurate results even for the cases when such mixing is important. Numerical calculations confirm that, indeed, Eq. (7) produces results, which are very close to those obtained by standard variational methods.

3. Effective potential for exciton in δ-functional shallow well and analytical expression for the exciton binding energy for first iteration

We define a shallow quantum well as such a well, in which only one bound state exists for both electrons and holes. In general, the energy spectrum of the quantum well with height U and finite length L is $E_n = \pi^2 x_n^2/(2mL^2)$, where x_n are the roots of the following transcendental equation:

$$x = n - 2/\pi \arcsin\left(\frac{\pi}{Lu_0} x\right), \quad n = 1, 2, \ldots, N$$
$$n - 1 \leqslant x_n \leqslant n. \tag{16}$$

Here we introduced a corresponding wave vector $u_0 = \sqrt{2mU}$ that characterizes potential height. The number of levels in the well is given by the condition

$$N = 1 + \left[\frac{u_0 L}{\pi}\right], \tag{17}$$

where $[\cdots]$ denotes the integer part of the number. The condition given by Eq. (17) can also be interpreted as a condition of a new level appearing when the potential grows in the well. For example, the second level appears when u_0 is equal to the wave vector of the ground state in the infinite well with the same length L: $u_0 = \pi/L$.

A transcendental form of Eq. (16) as well as a piecewise character of the eigenfunctions present additional obstacles for further calculations of the exciton binding energies. Therefore, different approximations of the finite quantum well are often

used. For a wide quantum well with several energy levels inside, the model of an infinite quantum well with a slightly larger effective length $L_{eff} = L/x_1$ is an appropriate one [25]. It gives the same ground energy and correct wave function behavior. However, for shallow quantum wells with one level inside, the use of this model is not justified. Indeed, for an infinite quantum well the ground state energy grows with the decrease of the well's width, while the ground state energy in the finite well has a different dependence, and tends to the finite limit U_0 when the width tends to zero: $E_1 \longrightarrow U - U^2 L^2 m/2$. Narrow quantum wells have a different analytical limit of the δ-functional potential [11],

$$V(z) = U - \alpha\delta(z), \tag{18}$$

where α is a δ-potential strength. If we define this parameter as

$$\alpha = UL_{eff} = \sqrt{\frac{2U}{m} - \frac{\pi^2 x_1^2}{m^2 L^2}}, \tag{19}$$

where L_{eff} is chosen to match the ground state energy of the finite well problem, then the well-width range of applicability of this approximation is extended up to the moment of the appearance of the second level in the finite quantum well. For typical parameters in AlGaAs/GaAs structures it corresponds to a well size $L \approx 40$ Å. Obviously, $L_{eff} \to L$ when L tends to zero. Fig. 1 shows typical energy dependence on well's width for the electron in the AlGaAs/GaAs quantum well for the finite quantum well and its approximations. Comparing the behavior of curves for the ground state of the finite width well and its δ-functional approximation with strength $\alpha = UL$, one can see that δ-functional curve stays always on the left. It means that the effective length parameter, determined by Eq. (19) should be smaller than the actual well width, which is opposite to the case of effective infinite quantum well width. In some sense, the model of δ-functional QW is complimentary to the model of effective infinite quantum well (EIQW) [25], which is used to approximate finite QW with large widths (and/or barrier heights), when the number of levels in a well is large. Indeed, the more discrete levels exist in the QW the better the EIQW model works, but if it fails and gives a wrong eigenstate dependence on L,
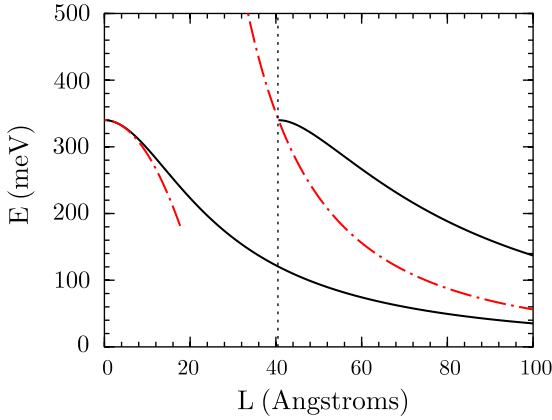
Fig. 1. The energy levels dependence on the well's width. The ground and the first excited levels (solid lines) are shown for the finite quantum well. Dot-dashed lines show the ground state level for the infinite well of the same width and δ-functional potential (18) with $\alpha = UL$. A vertical dashed line is the well's width at which the second level in the finite quantum well appears. It shows the range of applicability of the δ-functional potential with the effective strength $\alpha = UL_{\text{eff}}$. Parameters are taken for a conduction band electron in an $Al_{0.3}Ga_{0.7}As/GaAs$ quantum well (see below in a text).

when the well has only one level. On the other hand the δ-functional QW is not applicable for quantum wells with more than one level. The delta-functional approximation is applicable both to very narrow QW and to wells with a small band-gap offset [11], i.e., when the well width and/or the band offsets are very small so that the carrier wave functions are mostly in the barrier region. For the δ-functional potential it is more convenient to count energies from the barrier band edge rather than from the bottom of the well. In terms of the total Hamiltonian (1) it means that the energy band gap constant is the barrier's energy band gap: $E_g^{\text{bar}} = E_g^{\text{well}} + U_e + U_h$. The energy and wave function of a single localized state are well-known:

$$E_{e,h} = -\frac{\kappa_{e,h}^2}{2m_{e,h}},$$
$$\chi_{e,h}(z) = \sqrt{\kappa_{e,h}} \exp(-\kappa_{e,h}|z|). \qquad (20)$$

Parameters $\kappa_{e,h} = \alpha_{e,h} m_{e,h}$ determine the localization of wave functions of an electron and a hole, respectively. It is worth noting that even for a very shallow quantum well, the localization length ($\sim 1/\kappa$) might be much less than the effective Bohr

radius. In this case, we can expect a quasi-two dimensional behavior for the exciton, justifying the approximation for the mean field function in form (6). In the case of the AlGaAs/GaAs quantum wells, the electron (hole) localization length is smaller than Bohr's radius up to $L \approx 5\,\text{Å}$.

With the help of the wave functions (20), it is possible to obtain the analytical expression for the effective exciton potential $\overline{V}_r^{(0)}(r)$, which corresponds to the first iteration of the self-consistent procedure. The details of these calculations are given in Appendix A. The result is

$$\overline{V}_r^{(0)}(r; \kappa_e, \kappa_h) = -\frac{2\kappa_e\kappa_h}{\kappa_h^2 - \kappa_e^2}$$
$$\times [\kappa_h T(\kappa_e r) - \kappa_e T(\kappa_h r)], \qquad (21)$$

where the function $T(\kappa r)$ is a combination of zeroth-order Struve and Neuman functions [27]

$$T(\kappa r) = \frac{\pi}{2}[\mathbf{H}_0(2\kappa r) - Y_0(2\kappa r)]. \qquad (22)$$

The behavior of the potential (21) is shown in Fig. 2.

The behavior of the potential (21) has two regimes that are determined by the parameter

$$d = \sqrt{\frac{1}{2}\left(\frac{1}{\kappa_e^2} + \frac{1}{\kappa_h^2}\right)}. \qquad (23)$$

This parameter has the meaning of an average electron–hole separation in the z direction. For large distances, potential (21) has asymptotic behavior

$$V_{\text{asym}}(r) \approx -\frac{1}{\sqrt{r^2 + d^2}}, \quad r \gtrsim d. \qquad (24)$$

At small distances, the attraction becomes stronger. It has logarithmic behavior:[2]

$$V_{\text{sm}}(r) \approx \frac{1}{d}\left[\ln(r/d) - 1 + \gamma\right], \quad r \lesssim d, \qquad (25)$$

where $\gamma = 0.5772$.

Thus, the effective electron–hole interaction for the exciton in the quantum well starts from the

[2] For $\kappa_e \neq \kappa_h$ the series expansion of Eq. (25) gives $d = (\kappa_e^{-1} + \kappa_h^{-1})/2$, which is different from definition (23). However, the discrepancy between these two definitions is negligible for the whole range of $\kappa_{e,h}$ under the interest.
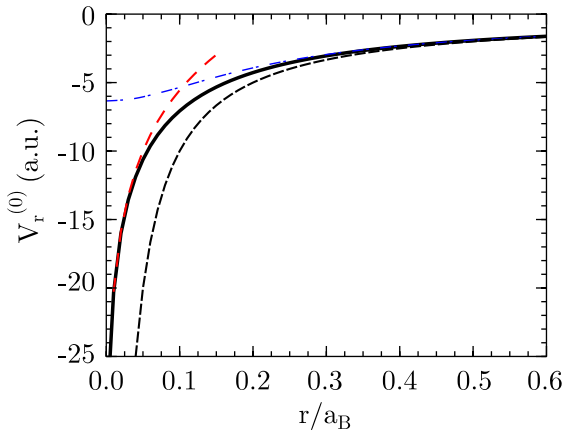
Fig. 2. An effective self-consistent potential $\overline{V}_r^{(0)}$ profile for a two-dimensional exciton. The solid thick line represents Eq. (21). The dashed-dotted line is the approximation $(r^2 + d^2)^{-1/2}$, the dashed line is the logarithmic regime Eq. (25) for small r, the dotted line represents $1/r$ behavior. All data are for $d/a_B = 0.16$ corresponding to $L = 20\,\text{Å}$ finite quantum well in AlGaAs/GaAs materials.

true logarithmic Coulomb potential of a point charge in two dimensions that smoothly transforms at distances $r \sim d$ to the screening potential (24) with three-dimensional Coulomb tails. For the strong confinement $d \ll 1$ we can approximate $V_{\text{eff}}(r)$ by Eq. (24) for all distances and take into account the logarithmic part on the next step as a perturbation.

It is interesting to note that potential (24) can be obtained without the self-consistent procedure from the following simple intuitive consideration. At the first step, let us neglect the electron–hole interaction in Hamiltonian (1). Then, we can solve the one-dimensional one-particle Schrödinger equations in the quantum well, and find the average square of the distance between the electron and the hole as

$$d^2 = \langle \chi_e(z_e)\chi_h(z_h) | (z_e - z_h)^2 | \chi_e(z_e)\chi_h(z_h) \rangle. \quad (26)$$

This yields the same result as Eq. (23). The next step in the approximation of the Hamiltonian (1) is to include the Coulomb attraction term, where $(z_e - z_h)^2$ is substituted by its average value $\langle (z_e - z_h)^2 \rangle$.

The Schrödinger equation for a radial wave function in the central field (21) does not have an analytical solution. However, the understanding of the role played by the parameter d helps to

substantially simplify calculations of the ground state energy. To obtain an approximate analytical expression for the exciton binding energy we will use the following procedure.

First of all, let us stress again that despite the fact that we consider a shallow quantum well with one single particle eigenvalue inside, the strong confinement persists up to very small widths. The parameter d is a good indicator of such confinement. For example, in Table 1 of the next section the data are presented for $Al_{0.3}Ga_{0.7}As/GaAs$ materials. We can see that for the well's width of $10\,\text{Å}$ this parameter is about one quarter of the three-dimensional Bohr radius and even smaller for larger quantum wells. For the case of strong confinement, $d \ll 1$, the effective potential (21) can be represented by Eq. (24) almost everywhere. Therefore, at the first step, it is reasonable to substitute the potential (21) by its asymptotic form (24) for all distances.

Although the Schrödinger equation with the potential (24) also does not have an analytical solution, we discovered that the ground state energy, obtained by the variational method for the single parameter trial function

$$\varphi_{\text{trial}} = \frac{2\exp(d/\lambda)}{\sqrt{\lambda(\lambda + 2d)}} \exp(-\sqrt{r^2 + d^2}/\lambda), \quad (27)$$

coincides with the exact one with excellent accuracy. To check this, we performed a precise numerical integration of the Schrödinger equation based on Pruefer transformation and a shooting method [26]. The difference in the ground state energies for the whole range of the parameter d was less than 0.01%, or $\sim 10^{-3}\,\text{meV}$! Such an agreement can be explained by the fact that trial function (27) has a correct analytical behavior for both small and large distances, r.

The expression for the ground state energy obtained for the trial function (27) is given by

$$E_X^{(0)}(\lambda)$$
$$= -\frac{2}{\lambda}\frac{1}{1 + 2d/\lambda}$$
$$+ \frac{1}{\lambda^2}\left[1 - \frac{(2d/\lambda)^2 E_1(2d/\lambda)\exp(2d/\lambda)}{1 + 2d/\lambda} \right], \quad (28)$$

Table 1
Effective parameters of single quantum well potentials, electron, hole and exciton binding energies (in a.u.) for different quantum well widths, L

L (Å)	L_{eff}^{e} (Å)	L_{eff}^{h} (Å)	d (a.u.)	$-E_{e}^{(0)}$	$-E_{h}^{(0)}$	$-E_{X}^{(1)}$	$-E_{X}^{(2)}$	$-E_{X}^{(3)}$	$-E_{X}^{\text{anal}}$	$-E_{X}^{\text{num}}$
10	9.15	8.89	0.257	5.11	1.37	1.0799	1.0975	1.1041	1.0948	1.1207
20	15.16	14.12	0.158	14.02	3.46	1.2617	1.2779	1.2843	1.2754	1.2878
30	18.63	16.88	0.130	21.18	4.95	1.3314	1.3467	1.3527	1.3443	1.3537
40	20.70	18.43	0.118	26.12	5.90	1.3655	1.3802	1.3855	1.3779	1.3862

Single particle electron and hole energies, $E_{e,h}^{(0)}$, are the initial step in the self-consistent field iterations (see Eq. (13)) when effective Coulomb terms $\overline{V}_{e,h}$ are omitted. These energies determine the strength parameters, $L_{\text{eff}}^{e,h}$, for corresponding δ-potentials and the average distance, d, between an electron and a hole (Eq. (23)). Energies $E_{X}^{(1),(2),(3)}$ are the exciton binding energies obtained by variational method with the trial functions given by Eqs. (32)–(34), respectively. The last two columns show the exciton binding energies obtained by the self-consistent approach. E_{X}^{anal} is the analytical expression of first iteration of the self-consistent approach $E_{X}^{\text{anal}} = E_{X}^{(0)} + E_{X}^{(1)}$ (see Eqs. (28) and (30)). E_{X}^{num} is the final result of the numerical iteration procedure for coupled self-consistent equations (7)–(9). The calculations are based on the following physical constants [25]: $m_{e}^{*} = 0.067m_{0}$, $m_{h}^{*} = 0.45m_{0}$, $U_{e} = 340\,\text{meV}$, $U_{h} = 70\,\text{meV}$, $\varepsilon = 13.8$. For these parameters the effective Bohr radius is $a_{B} = 125\,\text{Å}$ and the energy atomic unit is equal to 8.33 meV.
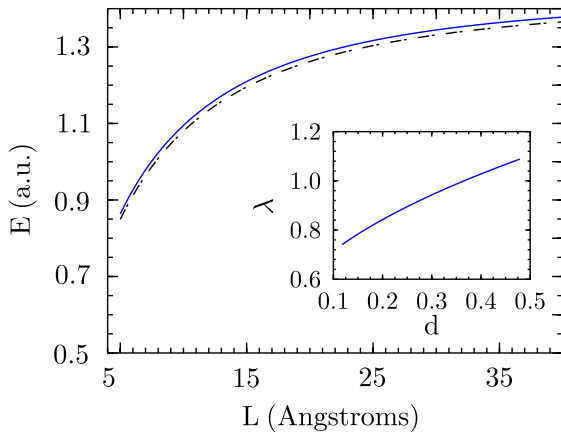

Fig. 3. The exciton binding energies in the shallow quantum well for different well widths L. The solid line represents the two-dimensional exciton ground state, Eqs. (28) and (30) in the effective potential. The dotted-dashed line is the exciton binding energy obtained with the help of the variational method with the trial function (32). The insert shows the dependence of the parameter λ on the average electron–hole separation d in Eq. (28). Both parameters are expressed in Bohr radius units and are presented for the same range of quantum well widths.

where $E_1(x)$ is the exponential integral [27]. The variational parameter λ changes from 1.1 to 0.74 when the average electron–hole distance d varies from 0.11 to 0.48. The latter corresponds to the

quantum well widths range from 40 to 5 Å for the AlGaAs/GaAs structures. The behavior of the parameter λ as a function of d is shown in the insert of Fig. 3. At small d it has the following form

$$\lambda \approx \frac{1}{2} + 4d + \frac{d^2}{\lambda^2}\left[4\ln\left(\frac{2d}{\lambda}\right) - 12\lambda + 4\gamma + 1\right].$$
(29)

At small distances the effective potential (21) differs from Eq. (24). The correction to the energy due to this difference can be taken into account with the help of perturbation theory:

$$E_X^{(1)} = \langle\varphi_{\text{trial}}|\Delta V|\varphi_{\text{trial}}\rangle$$
$$\approx \int_0^d \varphi_{\text{trial}}^2(r)\left[\frac{1}{d}\ln(r/d)\right]r\,dr$$
(30)
$$= -\frac{2d}{\lambda^2}\left[\frac{1}{2} - 0.557\frac{2d}{\lambda}\right.$$
$$\left. + 0.563\left(\frac{2d}{\lambda}\right)^2 + \cdots\right].$$
(31)

The last but one column (E_X^{anal}) of Table 1 in the next section represents the final sum $E_X^{sc} = E_X^{(0)} + E_X^{(1)}$ for the exciton binding energy obtained by the zero iteration of self-consistent approach.

4. Numerical results: comparison with standard variational approach

We performed a numerical iteration procedure described in Section 2 for self-consistent coupled equations (7)–(9). The results for the exciton binding energy are presented in the last column of Table 1. We found a fast convergence of the iterations in the range $L = 5$–$40\,\text{Å}$ of quantum well widths, where our model of shallow quantum well is applicable. Usually, it took 4–6 iterations to reach the accuracy 0.01% for the condition of Eq. (15). A fast convergence confirms that a separable form of function (6) is a reasonable choice for trial functions in QW with strong localization across the well.

To check the accuracy of our method we compared the results of the self-consistent approach with the results of the standard variational method for three different trial functions. These trial functions have the following forms:

$$\psi^{(1)}(z_{\text{e}}, z_{\text{h}}, r; \lambda) = \sqrt{\kappa_{\text{e}} \kappa_{\text{h}}} \exp(-\kappa_{\text{e}}|z_{\text{e}}| - \kappa_{\text{h}}|z_{\text{h}}|) \\ \times \exp(-r/\lambda), \tag{32}$$

$$\psi^{(2)}(z_{\text{e}}, z_{\text{h}}, r; \lambda, \beta) = \sqrt{\kappa_{\text{e}} \kappa_{\text{h}}} \exp(-\kappa_{\text{e}}|z_{\text{e}}| - \kappa_{\text{h}}|z_{\text{h}}|) \\ \times \exp(-\sqrt{r^2 + \beta^2}/\lambda), \tag{33}$$

$$\psi^{(3)}(z_{\text{e}}, z_{\text{h}}, r; \lambda, \beta) = \sqrt{\kappa_{\text{e}} \kappa_{\text{h}}} \exp(-\kappa_{\text{e}}|z_{\text{e}}| - \kappa_{\text{h}}|z_{\text{h}}|) \\ \times \exp(-\sqrt{r^2 + \beta^2 (z_{\text{e}} - z_{\text{h}})^2}/\lambda). \tag{34}$$

The first two functions are separable, while the third one is non-separable. The first wave function has one variational parameter λ, and two others have two variational parameters λ and β.

The details of variational calculations are given in Appendix B. Our results and their comparison with data obtained by the standard variational procedure are presented in Table 1. We can see that all, even the most elaborate variational calculations, yield higher binding energies, showing that our self-consistent approach is, in fact, more accurate.

We also found that already the first iteration of our approach gives lower binding energies than a variational method with separable trial functions (32),(33), while it yields energies slightly higher

than the non-separable trial function. However, subsequent iterations further decrease the self-consistent ground state energy, making it the lowest one.

We would also like to mention that analytical expressions (28)–(31) for exciton binding energy give results comparable with the values obtained by variational method with separable trial functions, while avoid a numerically difficult task of finding minima of several non-polynomial functions. The additional physical information about the effective potential allows one to find one of the variational parameters of function (33) without minimization.

5. Conclusions

We introduce a self-consistent approach for calculations of the exciton binding energy in a quantum well. For the case of strong confinement, the self-consistent Hamiltonian is separable and consists of three parts: one-dimensional Hamiltonians for electron and hole confined motions across the quantum well, and the Hamiltonian, which describes the motion of a two-dimensional exciton in the effective central field potential. This effective potential is a result of averaging over z coordinates of the Coulomb interaction and the quantum well potential. As a function of distance the effective potential has two different regimes of behavior which are determined by the average distance between electron and hole inside the quantum well, d. For small distances, $r \lesssim d$, the effective potential has a logarithmic form of a Coulomb potential of a point charge in two dimensions. At a distance $r \sim d$ this behavior crosses over to the three-dimensional Coulomb screened potential, $-1/\sqrt{r^2 + d^2}$.

Before carrying out numerical self-consistent solution, we analyzed in detail the first approximation of this approach. In this approximation the δ-functional model allows for obtaining analytical expressions, Eqs. (28) and (30), for the exciton binding energy. We found that binding energies calculated from these expressions are in an excellent agreement with much more elaborate standard variational calculations while requiring

computational time by orders of magnitude smaller than the later. The differences between the exciton binding energies in two approaches are generally smaller than 1%. For AlGaAs/GaAs structures it corresponds to differences smaller than 0.1 meV, i.e., smaller than corrections [9] due to non-parabolicity of the bulk conduction band or dielectric constant and effective mass mismatches.

While the simple first order semi-analytical calculation gives values of binding energy slightly greater than those obtained with the most elaborated trial function of the standard variational approach, the subsequent iterations of the self-consistent procedure brings the binding energy below the best results of the variational method. It is important to note that the numerical resources required for carrying out this procedure are comparable with those used in standard calculations. We can conclude, therefore, that the self-consistent approach is, indeed, superior to the standard variational methods and can be used to calculate exciton energies for a wide range of different nanostructures.

In derivation of our results we used three different approximations. They are: (i) the self-consistent approach itself, (ii) the use of the factorized form of the wave function, and (iii) the use of the delta-functional potential for a shallow quantum well. The self-consistent approach is broader than the standard variational method since we do not have to specify a particular functional dependence for a trial function. Instead, we just suggest that the trial function consists of some combination of unknown functions. The factorized form is the simplest form for such a combination but it is not required by our method. The method can be applied to other physical models where different types of trial functions would be more natural. For example, for a wide double quantum well, the better choice of the trial function of the ground state is a superposition of two factorized single-well functions. It will result in a system of coupled equations similar (but more complicated) to Eqs. (7)–(9). This approach can also be straight-forwardly expanded to include other effects, which were neglected in this paper. For instance, in order

to take into account the dielectric mismatch [9,14,10], we would need to correct the expression for the effective potentials, Eqs. (10) and (11), including effects of image charges into the respective integrals. The valence band degeneracy and anisotropy can be included by introducing a four component trial function, for which the self-consistent equations will have the similar form as Eqs. (7)–(9), but they should be understood as matrix equations.

Turning to the particular factorization used in our problem, it is obvious that the more strongly the exciton is localized in the z-direction (size of wave function in z-direction compared to the three-dimensional Bohr radius) the better our approximation works. If we consider the case of $Al_{0.3}Ga_{0.7}As$/GaAs quantum well, it means that our method will work for any quantum well with a width less than $100 \, \text{Å}$, but the best convergence will happen somewhere around 30–$50 \, \text{Å}$. Correspondingly, the factorized form of the trial function for the self-consistent method is applicable for any structure (e.g., asymmetric quantum well or quantum well in electric field), if a wave function localized in z-direction has such an extension. In a similar matter the self-consistent approach can be applied to the lower dimension systems such as quantum wires and quantum dots. Moreover, preliminary consideration showed that the problem of divergency of the exciton ground state in a one-dimensional Coulomb potential, which arises in other approaches to quantum wires, in this method does not appear at all.

The δ-functional potential is a good approximation if a one-dimensional quantum well has only one level (is shallow). For a typical case of $Al_{0.3}Ga_{0.7}As$/GaAs quantum well, it gives an applicability range of $L < 40 \, \text{Å}$. The approximation of the δ-functional potential gives simple single-particle wave functions that significantly simplify calculations of the effective potentials in Eqs. (10) and (11). If asymmetric quantum well or double quantum wells, or quantum well in electric field are shallow, the delta-functional approach will be applicable to such models. An asymmetric quantum well can be modelled by a quantum barrier and the δ-functional potential $(\delta(z) \rightarrow \delta(z)[1 + A\theta(z)]$, where θ is the step

function). An advantage of using the δ-functional potential is especially clear in the case of the quantum confined Stark effect for a shallow quantum well, where it allows one to obtain additional results related to the field-induced resonance widths for a single-particle as well as for the exciton quasi-bound states. These results will be published elsewhere.

Acknowledgements

Appendix A. Effective potential for 2D exciton

The effective field for quasi 2D exciton is given by the integral

$$V_{\text{eff}}(r) = -\int_{-\infty}^{\infty} \mathrm{d}z_e \int_{-\infty}^{\infty} \mathrm{d}z_h \frac{|\chi_e(z_e)|^2 |\chi_h(z_h)|^2}{\sqrt{r^2 + (z_e - z_h)^2}}.$$
(A.1)

For a shallow quantum well approximated by the δ-function potential it gives

$$
\begin{aligned}
V_{\text{eff}}(r) = &-\int_0^{\infty} \mathrm{d}z_1 \int_0^{\infty} \mathrm{d}z_2 \, e^{-2\kappa_1 z_1} \, e^{-2\kappa_2 z_2} \\
&\times \left[\frac{2\kappa_1 \kappa_2}{\sqrt{r^2 + (z_1 - z_2)^2}} + \frac{2\kappa_1 \kappa_2}{\sqrt{r^2 + (z_1 + z_2)^2}} \right] \\
= &\; V_1 + V_2.
\end{aligned}
$$
(A.2)

After making the coordinate transformation $\xi = z_1 - z_2$, $\eta = z_1 + z_2$ and taking into account that

$$
\begin{aligned}
\int_0^{\infty} \mathrm{d}z_1 &\int_0^{\infty} \mathrm{d}z_2 f(\xi, \eta) \\
&= \frac{1}{2} \int_0^{\infty} \mathrm{d}\eta \int_{-\eta}^{\eta} \mathrm{d}\xi f(\xi, \eta) \\
&= \frac{1}{2} \int_0^{\infty} \mathrm{d}\xi \int_{\xi}^{\infty} \mathrm{d}\eta \\
&\quad \times [f(-\xi, \eta) + f(\xi, \eta)],
\end{aligned}
$$
(A.3)

the first integration in these two integrated integrals becomes trivial and the second integration can be expressed through the function

$$
\begin{aligned}
T(\kappa r) &= \int_0^{\infty} \frac{\exp(-2\kappa t)\, \mathrm{d}t}{\sqrt{r^2 + t^2}} \\
&= \frac{\pi}{2} [\mathbf{H}_0(2\kappa r) - \mathbf{Y}_0(2\kappa r)],
\end{aligned}
$$
(A.4)

where $\mathbf{H}_0$ is the zeroth-order Struve function and $\mathbf{Y}_0$ is the zero-order Neumann or Bessel function of the second kind [27]. Then potentials V_1 and V_2 can be expressed as

$$V_{1,2} = -\frac{\kappa_1 \kappa_2}{\kappa_1 \pm \kappa_2} [T(\kappa_2 r) \pm T(\kappa_1 r)],$$
(A.5)

and the final result yields Eq. (21)

$$V_{\text{eff}}(r; \kappa_1, \kappa_2) = -\frac{2\kappa_1 \kappa_2}{\kappa_2^2 - \kappa_1^2} [\kappa_2 T(\kappa_1 r) - \kappa_1 T(\kappa_2 r)].$$
(A.6)

In the case when $\kappa_1 = \kappa_2 \equiv \kappa$ this expression is reduced to

$$V_{\text{eff}}(r; \kappa) = -\kappa [T(\kappa r) - \kappa T'(\kappa r)],$$
(A.7)

where

$$T'(\kappa r) = \frac{\partial T}{\partial \kappa} = 2r \left[\frac{\pi}{2} \mathbf{Y}_1(2\kappa r) - \frac{\pi}{2} \mathbf{H}_1(2\kappa r) + 1 \right].$$
(A.8)

Appendix B. Variational method for excitons in δ-function quantum wells

Following standard procedures, the envelope variational exciton wave function in a quantum well can be presented as a product of three terms,

$$\Psi(z_e, z_h, r; \lambda_i) = \chi_e(z_e)\chi_h(z_h)\phi(r, z_e, z_h; \lambda_i),$$
(B.1)

where λ_i is the set of variational parameters and ϕ is the variational wave function which minimizes the total energy of the Hamiltonian (1). Two other factors $\chi_{e,h}(z_{e,h})$ are simply normalized eigenfunctions of the one-particle electron or hole Hamiltonians of the quantum well:

$$E_{e,h}\chi_{e,h}(z_{e,h}) = \left[-\frac{1}{2m_{e,h}}\frac{\partial^2}{\partial z_{e,h}^2} - \alpha_{e,h}\delta(z_{e,h}) \right] \chi_{e,h}(z_{e,h}),$$

$$\chi_{e,h}(z_{e,h}) = \sqrt{\kappa_{e,h}} \exp(-\kappa_{e,h}|z_{e,h}|),$$

$$\kappa_{e,h} = m_{e,h}\alpha_{e,h}, \quad E_{e,h} = \kappa_{e,h}^2/2m_{e,h}. \tag{B.2}$$

To obtain more confident results we made calculations with three different trial functions ψ:

$$\psi^{(1)}(r; \lambda) = \exp(-r/\lambda), \tag{B.3}$$

$$\psi^{(2)}(r; \lambda, \beta) = \exp(-\sqrt{r^2 + \beta^2}/\lambda), \tag{B.4}$$

$$\psi^{(3)}(r, |z_e - z_h|; \lambda, \beta)$$

$$= \exp(-\sqrt{r^2 + \beta^2(z_e - z_h)^2}/\lambda). \tag{B.5}$$

The first two functions are independent of z coordinates, while the third one is non-separable with respect to z. The first wave function has one variational parameter λ, and two others have two variational parameters λ and β.

The total exciton energy is the minimum of the functional

$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \tag{B.6}$$

For the first two trial functions, which are independent of z, the functional (B.6) can be further simplified. In this case, the energy can be presented as

$$E = E_e + E_h + \overline{K}/N + \overline{V}/N, \tag{B.7}$$

where

$$N = \langle \Psi | \Psi \rangle \equiv \langle \psi(r) | \psi(r) \rangle, \tag{B.8}$$

$$\overline{K} = \langle \psi(r) | \hat{K}_r | \psi(r) \rangle \equiv \frac{1}{2} \int (\nabla \psi)^2 \, dA, \tag{B.9}$$

$$\overline{V} = -\left\langle \Psi \left| \frac{1}{\sqrt{r^2 + (z_e - z_h)^2}} \right| \Psi \right\rangle$$

$$\equiv \int \left(V_{eff}(r) |\psi(r)|^2 \right) dA. \tag{B.10}$$

Calculations for the trial function $\psi^{(2)}$ yield

$$N^{(2)} = \frac{\exp(-2\beta/\lambda)\lambda(\lambda + 2\beta)}{4},$$

$$\overline{K}^{(2)} = \frac{\exp(-2\beta/\lambda)}{8}\left[1 + \frac{2\beta}{\lambda}\right.$$

$$\left. - \left(\frac{2\beta}{\lambda}\right)^2 E_1(2\beta/\lambda)\exp(2\beta/\lambda)\right],$$

$$\overline{V}^{(2)} = -\frac{2\kappa_1\kappa_2}{\kappa_2^2 - \kappa_1^2}$$

$$\times [\kappa_2 V(\kappa_1, \lambda, \beta) - \kappa_1 V(\kappa_2, \lambda, \beta)], \tag{B.11}$$

where $E_1(x)$ is the exponential integral [27] and

$$V(\kappa, \lambda, \beta) = \int_0^{\pi/2} \cos(\phi) \, d\phi \int_0^\infty \exp(-2\kappa R \sin(\phi)$$

$$- 2\sqrt{R^2\cos^2(\phi) + \beta^2}/\lambda)R \, dR. \tag{B.12}$$

For the first trial function $\psi^{(1)}(r; \lambda) \equiv \psi^{(2)}(r; \lambda, 0)$ all integrals have analytical expressions:

$$N^{(1)} = \frac{\lambda^2}{4},$$

$$\overline{K}^{(1)} = \frac{1}{8},$$

$$V(\kappa, \lambda, 0) = \frac{\lambda^2}{4}\frac{1}{1 + \lambda^2\kappa^2}\left[\lambda\kappa - 1 + \frac{1}{\sqrt{1 + \lambda^2\kappa^2}}\right.$$

$$\left. \times \ln\left(\frac{1}{\lambda\kappa}\frac{\sqrt{1 + \lambda^2\kappa^2} + 1}{\sqrt{1 + \lambda^2\kappa^2} - \lambda\kappa}\right)\right]. \tag{B.13}$$

Integrals for the non-separable trial function $\psi^{(3)}$ can be numerically estimated following the procedure described in Refs. [13,1].

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