Dielectric Mismatch at Finite Barrier Cubic Quantum Dots

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Abstract. We study the exciton states in the cubic quantum dots with finite potential barrier at the presence of dielectric mismatch. The dependence of electron and hole ground states as well as exciton binding energy and oscillator strength are found as a function of quantum dot size and dielectric constant of quantum dot and surrounding matrix. The developed theoretical approach has been applied to analyze the peculiarities of exciton spectra in CdTe quantum dots embedded in a variety of dielectric matrices.

1. Introduction

For the last two decades quantum dots (QDs), as well as other nanometer size structures have been attracting the increasing interest of experimental and theoretical researchers. From one side, such an interest is fueled by the possession by QD systems of unique physical properties that still require the thorough investigation and adequate explanation, and on the other hand by the perspectives of practical use of such materials, especially in the optoelectronic devices [1-4]. A variety of techniques was successfully developed to fabricate quantum dots: colloidal growth [5-7], molecular beam epitaxy [8], embedding into glass matrix by melting, quenching and subsequent nanocrystal growing [9]; twofold cleaved edge overgrowth technique [10] and some others. Great progress was also achieved in investigation of absorption and emission spectra of QDs and their behavior in electric and magnetic fields [11-14]. A number of studies have also been performed in order to explain the observed electronic and optical properties and theoretically model the physical processes in quantum dots [15-25].

Most of the existing theoretical investigations of excitons in QDs are based on some of the few simplifying approaches. Among them are:
1. An effective mass approach, which allows the use of theoretical techniques developed for the bulk semiconductor materials.
2. An infinite barrier potential approximation, in which particle and exciton wave functions are localized inside QD and vanish beyond its boundary.
3. Strong confinement approximation (SCA) that treats electron-hole interaction as a perturbation to their kinetic energy and permits the presentation of exciton wave functions as the product of electron and hole parts. SCA validity range is limited to the size of QDs less than exciton Bohr radius.

4. Assumption of the same dielectric constants for QD and surrounding matrix, that neglects creation of induced image charges at boundaries.

5. Assumption of spherical shape of QDs, which simplifies calculations and allows presentation of the solution in the analytical form.

In a number of papers researchers tried to consider more realistic models and get beyond the indicated simplifications, but overcoming even a few of them simultaneously is not an easy procedure. In Ref. [15], for example, the finite potential barriers for electrons and holes were introduced while studying cubic QDs in strong confinement regime with the same dielectric constants for QD and matrix. The authors of Ref. [16] went beyond SCA by using Ritz variational principle for investigating disc shape QD with no dielectric mismatch taken into account. The mismatch of dielectric constants between QD and surrounding matrix was accounted for in Ref. [17], where spherical and cubic shape QDs were considered in strong confinement regime and infinite barrier approximation.

It should be noted that the effective mass approximation (EMA) was questioned, taking into account the limited size of QD, and violation of the long range periodicity in it [18]. Evidently, it should be some small size limit for validity of EMA. By comparison of EMA results with data obtained through tight binding model and some other theoretical methods as well as with the experimental measurements, it was shown in Ref. [18,19], that EMA in the finite potential barrier model, can be applied to QDs as small as 15-20 Å. Partially it can be explained by the fact that exciton properties are obtained by averaging envelope functions and, therefore, are not so sensitive to small details of one-particle energy spectrum. There were also a few attempts to improve EMA by considering energy and position dependent electron and hole effective masses [20], or by introducing to QD effective masses much heavier than for bulk crystals that are anisotropic in case of large aspect ratio [21]. In this paper we consider a combined effect of finite barrier, dielectric mismatch, beyond the strong confinement approximation approach, and cubic shape on electronic and optical properties of QDs.

2. Theory
Let’s consider cubic shape QD of size $b$ with dielectric constant $\varepsilon_Q$ that is embedded in dielectric matrix with dielectric constant $\varepsilon_M$. In this paper we consider quantum dots that are large enough ($\geq 20$ Å) to assume the validity of effective mass approximation, as well as to assign the QD the same value of the dielectric constant as for the appropriate bulk material. Such an approach was questioned in Ref. [18,19], and authors have shown that the effect of the permittivity change due to the limited volume of QD, and formation of image charges on the size dependent properties of QD is not significant. Following Ref. [21], we also neglect the complex nature of the electron and hole energy spectrum (in the case of CdTe, for example, only dominating heavy holes contribution is taken into consideration) and employ the single band effective mass approach. The considered system is described by the electron-hole Hamiltonian

$$H = H_e(\vec{r}_e) + H_h(\vec{r}_h) + W(\vec{r}_e, \vec{r}_h)$$

$$= -\frac{\hbar^2}{2m_e} \nabla_e \left( \frac{1}{m_e(\vec{r}_e)} \nabla_e \right) + V_e(\vec{r}_e) - \frac{\hbar^2}{2m_h} \nabla_h \left( \frac{1}{m_h(\vec{r}_h)} \nabla_h \right) + V_h(\vec{r}_h) + W(\vec{r}_e, \vec{r}_h),$$

(1)
where \( \bar{r}_e, \bar{r}_h \); \( m_e(\bar{r}_e), m_h(\bar{r}_h) \); and \( V_e(\bar{r}_e), V_h(\bar{r}_h) \) are coordinates, coordinate-dependent effective masses and finite confinement potentials for electrons and holes, respectively:

\[
\begin{align*}
m_{e,h}(\bar{r}_{e,h}) &= \begin{cases} m_{Q,e,h}, & |x_{1,2,3}| \leq b/2, \ x_1 = x, \ x_2 = y, \ x_3 = z \\
m_{M,e,h}, & \text{otherwise} \end{cases}, \\
V_{e,h}(\bar{r}_{e,h}) &= \begin{cases} -V_{e,h}^0, & |x_{1,2,3}| \leq b/2 \\
0, & \text{otherwise} \end{cases}.
\end{align*}
\tag{2}
\]

In some works on excitons in QD electron-hole interaction potential \( W(\bar{r}_e, \bar{r}_h) \) was chosen in the Coulomb form [16, 22] which can be justified in the strong confinement approximation when dot size is considerably smaller than exciton Bohr radius: \( b \ll a_B \). When QD size becomes comparable with \( a_B \) (for CdTe, for example, \( a_B = 69 \, \text{Å} \)), the electrostatic interaction potential is affected by the image charges induced at the boundary of QD and surrounding matrix, which leads to the appearance of the self-polarization correction term \( W_S(\bar{r}_e, \bar{r}_h) \):

\[
W(\bar{r}_e, \bar{r}_h) \equiv W_e(\bar{r}_e, \bar{r}_h) + W_h(\bar{r}_e, \bar{r}_h) = -\frac{e^2}{\varepsilon_0 |\bar{r}_e - \bar{r}_h|} + W_S(\bar{r}_e, \bar{r}_h).
\tag{3}
\]

It should be mentioned that in the case of common dielectric mismatch, when matrix permittivity is considerably less than the one of QD, the electron-hole interaction in QD increases substantially compared to the bulk crystal [23].

The electron-hole interaction potential can be obtained from the Poisson equation with given boundary conditions. Such an analytical solution for cubic QD with infinite confinement potential was found in Ref. [17], but it appeared to be divergent with increase of QD to matrix permittivity ratio, so authors of [17] had to mend it with the addition of “correcting function”, which appears to have an approximately constant value for the set of parameters considered there. In addition, electrostatic potential found in [17] is divergent at QD interfaces, which creates a problem for performing integration in the case of finite potential barriers.

Another way to proceed with analysis would be to follow the challenging numerical calculations using, for example, finite difference method [24], but results achieved in such a way are limited to the specific material parameters.

In our current work we propose to approximate the potential term \( W_S(\bar{r}_e, \bar{r}_h) \) for the cubic QD by the composition of three potentials for mutually orthogonal quantum wells:

\[
W_S(\bar{r}_e, \bar{r}_h) = W_{S,xy}(\bar{r}_e, \bar{r}_h) + W_{S,yz}(\bar{r}_e, \bar{r}_h) + W_{S,xz}(\bar{r}_e, \bar{r}_h).
\tag{4}
\]

The analytical solution for single nanolayer (quantum well) located in X-Y plane and surrounded by the dielectric matrix was found in [23, 25] to have a form:
\[ W_{S_{xy}}(\vec{r}_e, \vec{r}_h) = \epsilon^2 \left( 1 - \frac{\epsilon_M}{\epsilon_Q} \right) \times \int_0^\infty \frac{dk J_0(k\rho)}{\epsilon M + \epsilon Q} e^{ik(z_e + z_h)} \left( (e^{2ikz_e} + e^{2ikz_h}) (-\epsilon_M + \epsilon_Q) + (e^{ik(b+2z_e+z_h)})(\epsilon_M + \epsilon_Q) \right), \]

\[ (5) \]

where \( \rho = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2} \); \( J_0 \) - Bessel function of the first kind. Potential \( W_{S}(\vec{r}_e, \vec{r}_h) \) appears due to the dielectric mismatch which leads to the presence of connected interface charges, so \( W_{S}(\vec{r}_e, \vec{r}_h) \approx 0 \), if \( \epsilon_Q \approx \epsilon_M \). Similar expressions can be written for two other planes by interchanging the appropriate coordinates.

There is no exact solution for the Schrödinger equation in the case of cubic QD and finite confinement potential, even for one-particle Hamiltonian, so we will employ the variational method. We start from finding the approximate solution of one-particle Schrödinger equation:

\[ \hat{H}_{e,h} \phi_{e,h}(\vec{r}_e, \vec{r}_h) = E_{e,h} \phi_{e,h}(\vec{r}_e, \vec{r}_h), \]

and then consider one-particle wave functions \( \phi_e(\vec{r}_e) \) and \( \phi_h(\vec{r}_h) \) as a basis for finding the connected electron-hole wave function \( \Psi(\vec{r}_e, \vec{r}_h) \).

Following Ritz variational procedure, the trial ground state one-particle (electron or hole indexes are dropped for brevity) wave function has been chosen in the form:

\[ \phi(\vec{r}) = \prod_{i=1}^3 \phi_i(x_i), \]

where for cubic crystal:

\[ \phi_i(x_i) = \begin{cases} C_1 \cos(\beta k_i), & |x_i| \leq b/2 \\ C_2 \exp(-\gamma |x_i|), & |x_i| > b/2 \end{cases}, \]

\[ (8) \]

\( \beta \) and \( \gamma \), \( (\gamma > 0) \) are variational parameters. The total one-particle function consists from QD and matrix parts contributing with the weight coefficients \( C_1 \) and \( C_2 \), respectively, that can be found from the conditions of normalization and continuation.

Using connection rules, i.e. continuity of the wave function and component of the velocity normal to the interface, we obtain the system of uniform equations. It can be shown that such a system has a nontrivial solution if variational parameters satisfy the condition:
Performing minimization of the energy of electron (hole) system we found the appropriate sets of variational parameters $\beta$ and $\gamma$, as well as constants $C_1$ and $C_2$. It should be mentioned that there is a difference between found parameters for electrons and holes in view of different effective masses and confinement potentials for them. At the same time, because of the cubic symmetry of the system, found variational parameters and constants have the same value for all of the directions of coordinate axes.

The ground state of bound electron-hole pair can be found from Schrödinger equation:

$$\hat{H}\Psi(\vec{r}_e, \vec{r}_h) = E\Psi(\vec{r}_e, \vec{r}_h),$$

(10)

We again apply Ritz variational theory to search for the approximate solution. The trial wave function has been chosen in the form:

$$\Psi(\vec{r}_e, \vec{r}_h) = \phi(\vec{r}_e) \phi(\vec{r}_h) \exp\{-\alpha |\vec{r}_e - \vec{r}_h|\},$$

(11)

where $\alpha$ – variational parameter, and electron-hole interaction is accounted by the exponential term. The exciton energy can be determined by minimizing the functional:

$$E(\alpha) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$  

(12)

Substituting an envelope function (11) into functional (12) and performing a minimization, we obtain the set of six- and seven-fold integrals that include Bessel functions. The multiplicity of such integration can be reduced at least by the order of two by taking into consideration the symmetry of the system, but even after such reduction the numerical minimization procedure still requires the challenging calculations, that are explained below.

For illustration and comparison purposes we will first consider the case of an infinite barrier that requires relatively simpler calculations. In order to simplify the computations, we introduce the “reduced” variables and constants, related to QD:

$$\bar{a} = \alpha \frac{b}{\pi}, \quad \bar{b} = \frac{b}{a_0}, \quad \bar{k} = \frac{kb}{\pi}, \quad \xi_{e,h} = \frac{\pi}{b} x_{e,h}, \quad \xi_\alpha = \xi_e - \xi_h,$$

$$a_0 = \frac{\varepsilon_0 \hbar^2}{\mu e^2}, \quad 1 = \frac{1}{\mu} \frac{1}{m_e} + \frac{1}{m_h}, \quad R_0 = \frac{e^2}{2 \varepsilon_0 a_0}.$$  

After straightforward, but tedious, calculations we obtain the exciton energy expressed as a function of renormalized variational parameter $\bar{\alpha}$:
\[ E(\tilde{\alpha}) = T_0 + T_1(\tilde{\alpha}) + T_2(\tilde{\alpha}) + P_e(\tilde{\alpha}) + P_p(\tilde{\alpha}), \]  

(13)

The first three terms in expression (13) give the expectation value of the kinetic energy of the particles:

\[ T_0 = \frac{3\pi^2\hbar^2}{2\mu b^2}, \quad T_1 = -\left(\frac{\pi}{b}\tilde{\alpha}\right)^2, \quad T_2 = \frac{\pi^2}{b^2}B_0^{-1}(\tilde{\alpha})K(\tilde{\alpha}), \]  

(14)

where:

\[ B_n(\tilde{\alpha}) = \int_0^{\infty} d\xi_1 \int_0^{\infty} d\xi_2 \int_0^{\infty} d\xi_3 f(\xi_1)f(\xi_2)f(\xi_3)t^n e^{-2\xi t}, \quad n = 0, -1, \]

\[ f(\xi_i) = 2(\pi - \xi_i)(2 + \cos 2\xi_i) + 3\sin 2\xi_i; \quad t = \sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}; \]

\[ K(\tilde{\alpha}) = \tilde{\alpha}B_0(\tilde{\alpha})\exp(-2\tilde{\alpha}\sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}) \times \sum_{(i,j,k)\neq (\alpha,\xi,\xi)} \frac{1}{512} L_{\gamma k}(\tilde{\alpha}), \]

and

\[ L_{\gamma k} = -f(\xi_1)f(\xi_2) \left[ 2\xi_1^2 + \left(\pi + \xi_1\right)(\xi_1^2 + \xi_3^2) \right] \cos(2\xi_3) + \left[ 2\xi_1^2 + (\pi - \xi_1)(\xi_1^2 + \xi_3^2) \sin(2\xi_3) - \right. \]

\[ -2\left[ 2\xi_1^2 - (\pi - 2\xi_1)(\xi_1^2 + \xi_3^2) + \xi_1(\pi - \xi_1)(\xi_1^2 + \xi_3^2) \sin(2\xi_3) \right]. \]

The electron-hole Coulomb interaction is accounted by the fourth term in expression (13). It can be shown that due to cubic symmetry, all three terms of the potential (4) contribute equally to the fifth term of the potential energy \( P_p(\alpha) \) that is related to the polarization effect. After some calculations we obtain:

\[ P_p(\tilde{\alpha}) = P_1(\tilde{\alpha}) + P_2(\tilde{\alpha}), \]  

(15)

\[ P_1(\tilde{\alpha}) = \frac{1}{512} \int d\xi_1 \int d\xi_2 \int d\xi_3 \int d\vec{k} f(\xi_1)f(\xi_2)f(\xi_3)J_0(\vec{k}\sqrt{\xi_1^2 + \xi_2^2})e^{-2\vec{k}t} \times \]

\[ \times \frac{2ch(\tilde{\kappa})}{\exp[2(\gamma + \pi\tilde{\kappa})]} - 1 \]

where:

\[ P_2(\tilde{\alpha}) = \frac{1}{64} \int d\xi_1 \int d\xi_2 \int d\vec{z}_3 \int d\vec{z}_4 \int d\vec{k} f(\xi_1)f(\xi_2)J_0(\vec{k}\sqrt{\xi_1^2 + \xi_2^2}) \times \]

\[ \times \frac{ch(\tilde{\kappa}(\vec{z}_3 + \vec{z}_4))}{sh(2\gamma + \pi\tilde{\kappa})}. \]
For the finite confinement potential, the calculations become more complex and are reviewed in the Appendix. The detailed analysis of exciton energy dependence upon the properties of the QD and surrounding dielectric matrix is performed in the next section.

3. Numerical results and discussion

The numerical calculations were performed for CdTe QD with the parameters: \( m_{eQ} = 0.11m_0; \) \( m_{hQ} = 0.35m_0; \) \( \varepsilon_Q = 10.9, \) where \( m_0 \) is the mass of free electron. In the experimental study [6] the QD was embedded in a variety of materials often with not precisely known electron and hole effective masses and magnitudes of the potential barrier, therefore in our calculations we consider a variety of values for the matrix confinement potentials as well as electron and hole effective masses (Fig.1-Fig.4). In order to study the properties of the system, we consider initially the electron and hole ground state energies (Fig.1), and later analyze the properties of exciton ground state.

As can be seen from Fig.1, electron and hole energies are decreasing functions of the QD size \( b. \) Because of the smaller electron effective mass, the corresponding energy dependence \( E(b) \) has a steeper slope than for a hole. Such behavior is observed for both: an infinite (lines 1 and 4) and finite (lines 2, 3, 5 and 6) confinement potentials. We have considered two cases with the effective mass of electrons in the matrix to be \( m_{eM} = 0.11m_0 \) (line 2) and \( m_{eM} = m_0 \) (line 3), and effective mass of the hole \( m_{hM} = 0.35m_0 \) (line 5) and \( m_{hM} = m_0 \) (line 6), and as we see, the increase in the effective mass leads to decrease in the ground state energy of particles. It can be seen from Fig.1, that there is a substantial difference between results obtained in the infinite confinement potential and finite barrier models for \( b < 100\,\text{Å} \) in the case of electrons, and \( b \leq 40\,\text{Å} \) for holes.

![Figure 1](image_url)

**Figure 1.** Electron (1,2,3) and hole (4,5,6) ground state energy versus QD size \( b. \) Dashed lines (1,4) represent an infinite confinement potential, solid lines (2,3,5,6) correspond to \( V_e^0 = 0.5\,\text{eV}, V_h^0 = 1.0\,\text{eV}; 2 - m_{eM} = 0.11m_0; 3 - m_{eM} = m_0; 5 - m_{hM} = 0.35m_0 \) and \( 6 - m_{hM} = m_0. \)
Figure 2 illustrates dependence of exciton binding energy $E_c = E - T_0$ upon cubic QD size $b$.

![Graph showing dependence of exciton binding energy on QD size](image)

**Figure 2.** Exciton binding energy as a function of QD size $b$ for various matrix dielectric constants:

1. $\varepsilon_M = 1$; 2. $\varepsilon_M = 4$; 3. $\varepsilon_M = 7$; 4. $\varepsilon_M = \varepsilon_0 = 10.9$.

Dashed lines represent an infinite confinement potential, solid lines correspond to $V_0 = 0.5 \, eV$, $V_h = 1.0 \, eV$.

It should be noted that for CdTe QD of size $b = 20 \, \text{Å}$, magnitude of exciton binding energy exceeds the one for the bulk crystal more than five times for the finite barriers and more than ten times in case of infinite confinement potential. Binding energy is a monotonically increasing function of the QD size $b$ and decreasing function of the matrix dielectric constant. At the absence of the dielectric mismatch (line 4 in Fig.2) the dependence of $E_c$ upon QD size and its dielectric properties qualitatively remains similar to the described above, but its magnitude has a lower value. For example, at $b = 20 \, \text{Å}$, $|E_c| \approx 20 \, \text{meV}$ which is only two times larger than the appropriate value for the bulk crystal. In other words, accounting for the dielectric mismatch leads to the increase in differences of exciton binding energy between QD and bulk crystal, which is similar to the results obtained for the quantum wells [23, 25].

The other important characteristic of the exciton state is the oscillator strength $f$, which can be expressed by formula [22]:

$$\frac{f}{f_{ex,1s}} = \frac{\pi a_0^3}{V} \left| \int d^3 r \Psi(\mathbf{r}, \mathbf{\hat{r}}) \right|^2 \frac{E_{ex,1s}}{E_c}, \quad (16)$$
where \( f_{ex,1s}, E_{ex,1s} \) — oscillator strength and \( 1s \) exciton binding energy for the bulk crystal of the volume \( V \); \( E_c \) — exciton binding energy for QD, \( \Psi(\vec{r},\vec{r}) = \Psi(\vec{r}_e,\vec{r}_h) \bigg|_{\vec{r}_e=\vec{r}_h} \) — exciton wave function for electron and hole located at the same point \( \vec{r} \).

Figure 3 illustrates the ratio of oscillator strengths for QD and bulk CdTe.

![Figure 3](image-url)  

**Figure 3.** Oscillator strength versus QD size for various QD dielectric constants  
1 — \( \varepsilon_d = 1 \); 2 — \( \varepsilon_d \approx \varepsilon_0 \).

Obtained according to formula (16) oscillator strength monotonically increases with decrease of QD size (Fig.3). At the absence of dielectric mismatch \( \frac{f}{f_{ex,1s}} = 10 \) for \( b = 55 \text{ Å} \). Consideration of the image boundary charges leads to increase in the oscillatory strength. For the same QD size \( b = 55 \text{ Å} \) and \( \varepsilon_d = 1 \) we obtain \( \frac{f}{f_{ex,1s}} = 13 \).

One of the explanations of the Stocks shift in exciton absorption and photoluminescence spectra is based on the introduction of the bright and dark exciton states [26]. The difference between the energy of those states equals to the exchange interaction energy between electron and hole. If only short-range interaction is taken into account, then QD exciton exchange energy is expressed by formula [22]:

\[
E_{e,exch} = E_{exch} \pi a_0^3 K_0 \, ,
\]  

where \( a_0 \) is Bohr radius.
where \( K_0 = \int d^3 r |\Psi(\vec{r}, \vec{r})|^2 \); \( E_{\text{exch}} \) – exchange energy for \( 1s \)- exciton in the bulk crystal. The dependence of the ratio of QD exchange energy to the one of bulk crystal upon QD size at few values of QD dielectric constant is presented by Figure 4.

![Figure 4](image-url)

**Figure 4.** Exchange energy as a function of QD size, magnitude of confinement potential and matrix dielectric constant: 1,1′ – \( \delta_d = 1 \); 2,2′ – \( \delta_d \approx \delta_q \); 3 – \( \epsilon_M = 4 \); 4 – \( \epsilon_M = 81 \) (H₂O);

dotted lines 1′, 2′ correspond to the infinite barrier, solid line 1-4 to the confinement potential \( V_e^0 = 0.5\text{eV}, \; V_h^0 = 1.0\text{eV} \).

As it can be seen from the Fig.4, there is a drastic change in the exchange energy as QD decreases in size, especially at small \( b \). Such behavior of \( E_{c,\text{exch}} \) was experimentally confirmed for CdTe in [6] and our theoretical results show a qualitative agreement with the experimental data of the cited reference.

If we assume for bulk CdTe crystal Stocks shift equal to 0.15 meV [6, 22], then for small-size QD we obtain the next results (Table 1).

| QD size (b), Å | \( E_{c,\text{exch}}(V_{0_e} = V_{0_h} = \infty) \) | \( E_c(V_{0_e} = 0.5\text{eV}, V_{0_h} = 1\text{eV}) \) | Stocks shift [6] |
|----------------|---------------------------------|---------------------------------|------------------|
| 30             | 21 meV                          | 10 meV                          | 170 meV          |
| 25             | 45 meV                          | 20 meV                          | 180 meV          |
| 20             | 75 meV                          | 35 meV                          | 200 meV          |
For comparison purpose the last column of this table contains the experimental results [6]. As we can see, the experimental observation of Stocks shift provides higher values of $E_{c,exch}$ than were obtained in our calculations. In addition, the analysis of the theoretical results shows that in the framework of the current model, $E_{c,exch}$ has only a weak dependence upon the matrix permittivity. In our opinion it can be caused by the fact, that current theory underestimates the probability of charge localization near the QD boundary. It decreases, in turn, the matrix influence on the exciton and leads to a smaller magnitude of exciton exchange energy as well as its weak dependence upon $\varepsilon_M$.

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Appendix

The calculations for finite confinement potential are similar to the infinite potential case but obtained functional $E(\alpha)$ has considerably more complicated form. The components of formula (8) are expressed now by the next formula:

$$T_0 = N^{-1}(\delta)[J_e(\delta) + J_h(\delta)], \quad T_1 = 3N^{-1}(\delta)\bar{m}\delta[I_e(\delta) - I_h(\delta)], \quad T_2 = -\bar{m}\delta,$$

$$P_e = -2N^{-1}(\delta)(1 - \bar{m}\delta)\Pi_3(\delta), \quad P_p = -3N^{-1}(\delta)\Pi_4(\delta),$$

where $\delta = a_0 \alpha$, $\eta_e = \eta_0$, $\bar{m} = \frac{\mu_0}{\mu_3}$, $m_e = m_{eQ}W_{eQ} + m_{eM}W_{eM}$, $m_h = m_{hQ}W_{hQ} + m_{hM}W_{hM}$; $W_{eQ}, W_{eM}, W_{hQ}, W_{hM}$ - probability of finding electron (hole) in quantum dot and matrix respectively; $N(\delta)$ - normalization coefficient that for finite confinement potential has a form:

$$N(\delta) = \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \prod_{i=1}^{3} F_i(\eta_i) \exp\left(-2\sqrt{\frac{\eta_1^2 + \eta_2^2 + \eta_3^2}{\delta}}\right).$$

where:
\[ F(\eta) = \begin{cases} I_1(\eta), & 0 \leq \eta \leq \tilde{b} \\ I_2(\eta), & \eta > \tilde{b} \end{cases}, \quad \tilde{b} = \frac{b}{a_0}, \quad I_i(\eta) = \sum_{n=1}^{6} K_n(\eta), \]

\[ K_1(\eta) = \int_{-\infty}^{b} d\xi \left[ \phi_2 \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h \left( \frac{1}{2} \left( \xi - \eta \right) \right) \right]^2, \]

\[ K_2(\eta) = \int_{b}^{\infty} d\xi \left[ \phi_2 \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h \left( \frac{1}{2} \left( \xi - \eta \right) \right) \right]^2, \]

\[ K_3(\eta) = \int_{-\infty}^{b} d\xi \left[ \phi_2 \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h \left( \frac{1}{2} \left( \xi - \eta \right) \right) \right]^2, \]

\[ I_2(\eta) = \int_{-\infty}^{\infty} d\xi \left[ \phi_2 \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h \left( \frac{1}{2} \left( \xi - \eta \right) \right) \right]^2. \]

It should be noticed that similar to the infinite quantum well [25], the kinetic energy in QD case is expressed through quadratic and linear variational parameters.

\[ J_{\mid b \rangle} = \int_0^{\infty} d\eta \int_0^{\infty} d\xi F_{0}^{h}(\eta) F_{2}^{b}(\xi) F_{3}(\eta) \exp(-2 \sqrt{\xi + \eta}), \]

where:

\[ F_{0}^{s}(\eta) = \begin{cases} I_1(\eta), & 0 \leq \eta \leq \tilde{b} \\ I_2(\eta), & \eta > \tilde{b} \end{cases}, \quad I_3(\eta) = \sum_{n=1}^{6} K_n(\eta), \]

\[ K_4(\eta) = \int_{-\infty}^{b} d\xi \phi_2^* \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h^2 \left( \frac{1}{2} \left( \xi - \eta \right) \right) \Phi_h(\eta, \xi), \]

\[ K_5(\eta) = \int_{b}^{\infty} d\xi \phi_2^* \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h^2 \left( \frac{1}{2} \left( \xi - \eta \right) \right) \Phi_h(\eta, \xi), \]

\[ K_6(\eta) = \int_{-\infty}^{b} d\xi \phi_2^* \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h^2 \left( \frac{1}{2} \left( \xi - \eta \right) \right) \Phi_h(\eta, \xi), \]

\[ I_4(\eta) = \int_{-\infty}^{\infty} d\xi \phi_2^* \left( \frac{1}{2} \left( \xi + \eta \right) \right) \phi_h^2 \left( \frac{1}{2} \left( \xi - \eta \right) \right) \Phi_h(\eta, \xi), \]

\[ \Phi_h(\eta, \xi) = \frac{\partial^2}{\partial \xi^2} \phi_h \left( \frac{1}{2} \left( \xi - \eta \right) \right). \]

The function \( F_{0}^{s}(\eta) \) can be calculated similar to \( F_{0}^{h}(\eta) \) by substituting all the quantities with the hole indexes with the ones with electron indexes.
The quantities $I_{e,h}(\delta)$, which also are contributing to kinetic energy of electron-hole system, can be determined by the formula

$$I_{e,h}(\delta) = \int_0^\infty d\eta \int_0^\infty d\eta' \int_0^\infty d\eta F_{e,h}^{\eta}(\eta) F_2(\eta') F_3(\eta') \frac{\exp\left(-2 \sqrt{\eta^2 + \eta'^2 + \eta'^2}\right)}{\sqrt{\eta^2 + \eta'^2 + \eta'^2}}.$$ 

Functions $F_{e,h}^{\eta}(\eta)$ are expressed in a similar way to $F_{e,h}^{0}(\eta)$ with:

$$\Phi_{e,h}(\eta, \eta') = \eta \frac{\partial}{\partial \eta} \phi_{e,h} \left(\frac{1}{2} (\eta' \pm \eta)\right).$$

The last two terms in the expression (8) are related to the potential energy. First one of them ($\Pi_3$) is connected to electron-hole Coulomb interaction and can be obtained with the help of the formula:

$$\Pi_3 = \int_0^\infty d\eta \int_0^\infty d\eta' \int_0^\infty d\eta \prod_{i=1}^3 F_i(\eta) \frac{\exp\left(-2 \sqrt{\eta^2 + \eta'^2 + \eta'^2}\right)}{\sqrt{\eta^2 + \eta'^2 + \eta'^2}}.$$ 

The interface polarization is taken into account by the term $\Pi_4$:

$$\Pi_4 = \int_0^\infty d\eta \int_0^\infty d\eta' \int_0^\infty d\eta \int_{-\infty}^\infty d\xi \int_{-\infty}^\infty dx \phi_e(\xi) \phi_h(x) \exp\left(-2 \sqrt{\eta^2 + \eta'^2 + (x - \xi)^2}\right) \times$$

$$\times J_0\left(\sqrt{\eta^2 + \eta'^2}\right) \left(\hat{\xi} - \hat{\xi}'\right) e^{\frac{\beta}{2} ch\left[\xi(\xi + \xi') - (\xi' - \xi)^2\right]} - \left(\hat{\xi} - \hat{\xi}'\right) e^{\frac{\beta}{2} ch\left[\xi(\xi + \xi')\right]} \right).$$

