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Quasistationary Electron States for CdTe/ZnTe/CdTe Open Spherical Quantum Dots

D. Stojanović* and R. Kostić

University of Belgrade, Institute of Physics, Center for Solid State Physics and New Materials

P.O. Box 68, 11080 Belgrade, Serbia

The energy spectra of an electron in open spherical quantum dot (QD) within the effective mass approximation (EMA) and rectangular potential model is presented. Energy structure of quantum dots is important because of their possible applications in electronic and optoelectronic devices. For proper description and interpretation of tunneling processes knowledge of resonant states of quantum dots is necessary. Energy values depend on parameter like size of system and spatial composition. The lifetimes of the quasistationary states are computed within the framework of the scattering S-matrix method. It is shown how core radius and barrier thickness for the CdTe/ZnTe/CdTe example influence electron states and their lifetimes.

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1. Introduction

Research on structures in the nanometers size regime has proven to be one of the most rapidly growing fields of modern science over the past two decades. This sector is investigated by solid state physicists, inorganic chemists, physical chemists, colloid chemists, material scientists, and recently even biological scientists, medics and engineers.

In QD as quasi zero-dimensional (0D) system there is complete discreetness of electron energy levels, bound state, completely unbound states or resonance states (temporally bound) [1]. If there is control of QD composition, the shape and dimension, the structure of QD energy levels and number of confined electrons are under control too [2]. These possibilities have made QD like systems to become unusually attractive objects for both fundamental physics research and device applications. These systems have potentials to use for high speed, high efficiency optoelectronics and photonic devices, quantum dot lasers, high density memory or biosensing and biolabeling [3–6].

In this paper we present results of calculations of open spherical QD that consists of the CdTe/ZnTe/CdTe heterostructure. We performed our calculations in very well known and widely used EMA approximation [7–10]. Parameters for the calculation in EMA are effective masses of materials in the structure and conduction and valence offsets between materials. Despite the fact that present paper presents simplified approach, results for this heterostructure are basically correct and very illustrative.

* corresponding author; e-mail: dusanka@ipb.ac.rs

2. Model

The single quantum dot we consider is barrier spherical heterosystem composed of CdTe core, ZnTe barrier with a Δ thickness (radius $r_1 - r_0$) surrounded by CdTe (see Fig. 1).

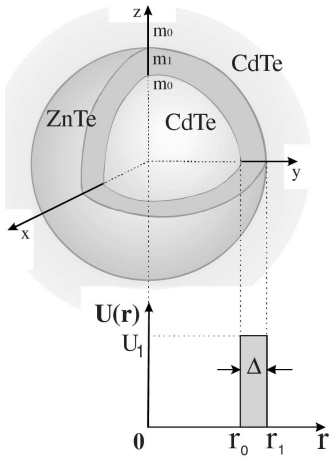

Fig. 1. Schematic of a spherical CdTe/ZnTe/CdTe heteronanocrystal structure, along with the corresponding radial energy diagram.

The dot center is center of our coordinates. Electrons and holes in such a system are characterized by their effective masses and potentials. Effective masses are:

$$m^*(r) = \begin{cases} m_0 & r < r_0, \quad r_1 < r < \infty \\ m_1 & r_0 \leq r \leq r_1 = r_0 + \Delta \end{cases} \tag{1}$$

In this case m_0^* are CdTe effective masses of electron and hole, and m_1^* are ZnTe effective masses.

Potentials are:

$$U(r) = \begin{cases} U_{0,2} = 0, & r < r_0, \quad r_1 < r < \infty \\ U_1 & r_0 \le r \le r_1 \end{cases} \tag{2}$$

Considering that electron spectra are mainly formed by the size quantization, the stationary Schrödinger equation for a single particle, in this case, may be expressed as:

$$\left(-\frac{\hbar^2}{2}\nabla\frac{1}{m^*(r)}\nabla + U(r)\right)\Psi(r) = E\,\Psi(r)\,. \tag{3}$$

For spherically symmetric potential $U(r)$ the separation of radial and angular coordinates leads to:

$$\Psi(r) = R_l(r)Y_{lm}(\theta,\varphi)\,, \tag{4}$$

where $R_l(r)$ is the radial wave function, $Y_{lm}(\theta,\varphi)$ is a spherical harmonic, $l = 0, 1, 2\ldots$; $m = 0, \pm1, \pm2, \ldots$.

$$R_{\mathrm{Kl}}(r) = \begin{cases} R_l^0(K_0r) = K_0A_l^0[h_l^-(K_0r) \\ \quad + h_l^+(K_0r)] & r \le r_0 \\ R_l^1(K_1r) = K_1A_l^1[h_l^-(K_1r) \\ \quad - S_l^1\ h_l^+(K_1r)] & r_0 \le r \le r_1 \\ R_l^2(K_2r) = K_2A_l^2[h_l^-(K_2r) \\ \quad - S_lh_l^+(K_2r)] & r_1 < r = \infty \end{cases}, \tag{5}$$

where:

$$K_i = \sqrt{\frac{2m_i^*}{\hbar^2}(U_i - E)} = \begin{cases} k, & i = 0, 2 \\ i\chi, & i = 1. \end{cases}$$

$h_l^{(\pm)}$ are Hankel spherical functions and S_l is scattering matrix. The coefficient $A_l^2 = 1/\sqrt{2\pi}$ is determined by the normalization condition for $R_{kl}(r)$, $\int_0^\infty R_{kl}^*(r)R_{kl}r^2\,\mathrm{d}r = \delta(k-k')$. The solution must satisfy continuity of the wave functions and the boundary conditions:

$$R_l^i(K_ir)\big|_{r=r_i} = R_l^{i+1}(K_{i+1}r)\big|_{r=r_i},$$

$$\frac{1}{m_i^*}\left.\frac{\mathrm{d}R_l^i(K_ir)}{\mathrm{d}r}\right|_{r=r_i} = \frac{1}{m_{i+1}^*}\left.\frac{\mathrm{d}R_l^{i+1}(K_{i+1}r)}{\mathrm{d}r}\right|_{r=r_i}, \quad i = 0, 1. \tag{6}$$

Equations (7) lead to a system of 4 linear equations with the 4 unknown coefficients (A_l^0, A_l^1, S_l^1 and S_l).

Expression for the scattering matrix S_l is:

$$S_l = \frac{\left(\alpha_l\frac{\mathrm{d}}{\mathrm{d}r_1} + \beta_l - \gamma_l\frac{\mathrm{d}}{\mathrm{d}r_1} - \lambda_l\right)h_l^-(kr_1)}{\left(\alpha_l\frac{\mathrm{d}}{\mathrm{d}r_1} + \beta_l - \gamma_l\frac{\mathrm{d}}{\mathrm{d}r_1} - \lambda_l\right)h_l^+(kr_1)},$$

where

$$\alpha_l = m_1\zeta_l h_l^-(i\chi r_1)h_l^+(i\chi r_0) - h_l^-(i\chi r_0)\big(h_l^+(i\chi r_1)\big)\,;$$

$$\beta_l = km_0^2\big(h_l^-(kr_0) + h_l^+(kr_0)\big) \times\left(\frac{\mathrm{d}h_l^-(i\chi r_0)}{\mathrm{d}r_0}\frac{\mathrm{d}h_l^+(i\chi r_1)}{\mathrm{d}r_1} - \frac{\mathrm{d}h_l^-(i\chi r_1)}{\mathrm{d}r_1}\frac{\mathrm{d}h_l^+(i\chi r_0)}{\mathrm{d}r_0}\right);$$

$$\gamma_l = km_0m_1\big(h_l^-(kr_0) + h_l^+(kr_0)\big) \times\left(h_l^+(i\chi r_1)\frac{\mathrm{d}h_l^-(i\chi r_0)}{\mathrm{d}r_0} - h_l^-(i\chi r_1)\frac{\mathrm{d}h_l^+(i\chi r_0)}{\mathrm{d}r_0}\right);$$

$$\lambda_l = m_0\zeta_l\left(h_l^-(i\chi r_0)\frac{\mathrm{d}h_l^+(i\chi r_1)}{\mathrm{d}r_1}\right) - \left(h_l^+(i\chi r_0)\frac{\mathrm{d}h_l^-(i\chi r_1)}{\mathrm{d}r_1}\right);$$

$$\zeta_l = km_1\frac{\mathrm{d}h_l^-(kr_0)}{\mathrm{d}r_0} + \frac{\mathrm{d}h_l^+(kr_0)}{\mathrm{d}r_0}\,.$$

In the case $l = 0$, $S_{l=0} = S_0$ [11, 12]:

$$S_0(k) = \mathrm{e}^{-2\,\mathrm{i}\,kr_1}\frac{g^- + \Delta m}{g^+ + \Delta m}\frac{\mathrm{e}^{-2\chi\Delta} + \frac{g^+ - \Delta m}{g^- + \Delta m}\xi_0(k)}{\mathrm{e}^{-2\chi\Delta} + \frac{g^- \Delta m}{g^+ + \Delta m}\xi_0(k)},$$

where:

$$\xi_0(k) = \frac{m_1kr_0\,\mathrm{ctg}\,(kr_0) + m_0r_0\chi + \Delta m}{m_1kr_0\,\mathrm{ctg}\,(kr_0) - m_0r_0\chi + \Delta m},$$

$$\Delta = r_1 - r_0\,, \quad \Delta m = m_0 - m_1$$

and

$$g^\pm = (m_0\chi \pm ikm_1)r_1\,.$$

For $l = 1$, $S_{l=1} = S_1$, $S_1(k) = \mathrm{e}^{-2\,\mathrm{i}\,kr_1}G_+(k)\times\frac{\mathrm{e}^{-2\chi\Delta} - G_-^*\,\xi_1(k)}{\mathrm{e}^{-2\chi\Delta} - G_-(k)\xi_1(k)}$,

$$G_\pm(k) = \Big\{2\Delta m(1 \pm ikr_1)(\chi r_1 \pm 1) + r_1^2\big[m_0\chi^2 + m_1k^2 \pm k\chi r_1(km_1 + i\chi m_0)\big]\Big\}\Big/\Big\{2\Delta m(1 - ikr_1)(\chi r_1 + 1) + r_1^2\big[m_0\chi^2 + k\chi r_1(km_1 - i\chi m_0)\big]\Big\},$$

$$\xi_1(k) = \frac{2\Delta m\eta_-(1 + \chi r_0) + r_0^2\big[m_0\chi^2\eta_- + m_1k^2(1 + \chi r_0)\big]}{2\Delta m\eta_-(1 - \chi r_0) + r_0^2\big[m_0\chi^2\eta_+ + m_1k^2(1 + \chi r_0)\big]}$$

$$\eta_\pm = 1 \pm kr_0\,\mathrm{ctg}\,(kr_0)\,.$$

Similar expressions, but more complicated, can be written for $S_2(k)$ and $\xi_2(k)$.

The real and the imaginary part of the S_l matrix poles give the resonance energy spectrum E_{nl} and the half-widths of the bands Γ_{nl} of electron and hole quasi-steady states in spherical QD; n is numerator of the solution. In this case S_l matrix poles are not found analytically. In solving this problem we use approximation that $\chi\Delta \gg 1$. In this case S_l matrix poles are $\xi_l(k)$ nulls. S can be expressed in form:

$$S(E) = \mathrm{e}^{2\,\mathrm{i}\,\varphi}\frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}\,.$$

Expression for life-time is $\tau_{n,l} = \hbar/\Gamma_{nl}$.

These calculations were performed for electrons, giving the electron energies E_{nl}^e, and half-widths of the bands Γ_{nl}^e, i.e. lifetimes $\tau_{n,l}^e$.

3. Results and discussion

The calculations of the electron spectra in the heterosystem under study were performed according to the model described in the previous section. Parameters of CdTe and ZnTe effective masses, lattice constants and conduction offset are transferred from literature [13] (see Table).

TABLE

Material parameters of the system: a — lattice constant, E_g — energy gap, U_e — conduction band offset potential (energetic scale is $U_e = 0$ eV in CdTe), m^* — effective mass, m_e — electron mass.

	a [Å]	E_g [eV]	U_e [eV]	m_e^*/m_e
ZnTe	6.1037	2.3	0.67	0.116
CdTe	6.481	1.49	0	0.0999

We investigated the influence of the barrier width Δ to electron quasistationary energies and lifetimes when a quantum well dimension r_0 is fixed. To illustrate this influence we present results of our calculations for dot of core radius $r_0 = 15a_{\mathrm{CdTe}} = 9.7215$ nm, Fig. 2. We present electron quasistationary energy spectra (Fig. 2a,b,c), and electron lifetimes (Fig. 2d,e,f) spectra for $l = 0, 1, 2$. All energies presented in Figs. 2 and 3 are in energetic scale assumed in Table. Varying barrier width do not change electron energy level significantly while the lifetime increases dramatically for all states. Electron lifetime is higher, i.e. half-width is small, for the lower energy states. Low energy and high lifetime is a sign that electron does not penetrate through the barrier.

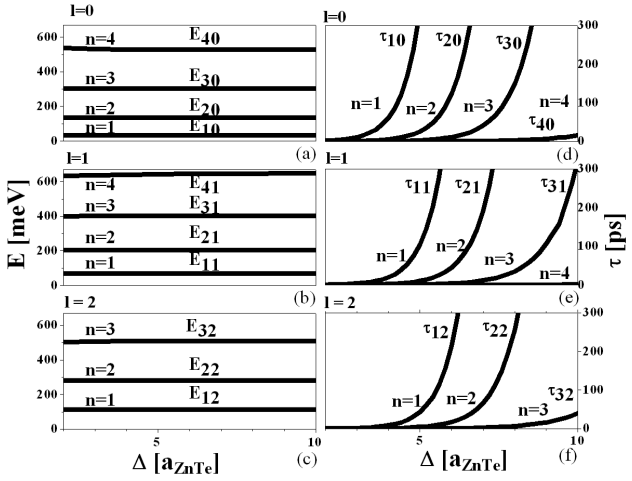

Fig. 2. Electron quasistationary energy and lifetimes dependences on ZnTe barrier thickness Δ for $l = 0, 1, 2$ in case $r_0 = 15a_{\mathrm{CdTe}}$.

Core radius variations change electron energy position significantly (Fig. 3a,b,c), as well as quasiparticle lifetimes (Fig. 3d,e,f). Increase of r_0 lowers electron energies and increases lifetimes. Barrier of the same height and width more efficiently prevents electron penetration through the barrier for larger r_0 i.e. larger core.

Resonance energies E_{nl} and half-widths Γ_{nl} (life-times τ_{nl}) are functions of core radius r_0 and barrier width Δ dimensions (Fig. 1) and material parameters m_0^* (electron effective mass in the core), m_1^* (electron effective

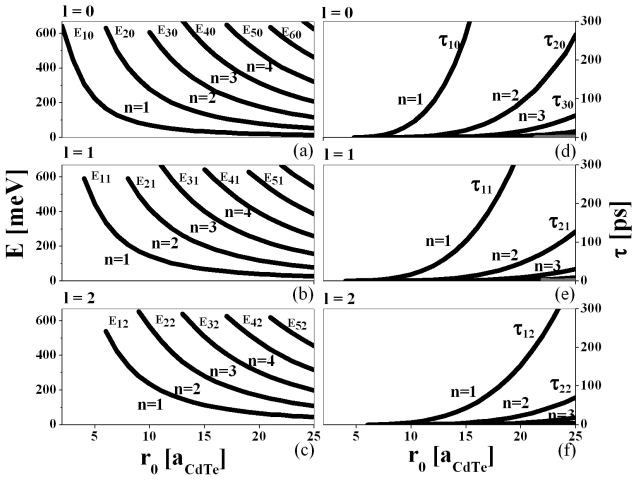

Fig. 3. Electron quasistationary energy and lifetimes dependences on CdTe core radius. ZnTe barrier thickness is $\Delta = 5a_{\mathrm{ZnTe}}$ for $l = 0, 1, 2$.

mass in the barrier) and U (potential offset between two materials). Influence of r_0, Δ and U is obvious. Increase of r_0 leads to decrease of resonance energies E_{nl} and half-widths Γ_{nl} (decrease of life-times τ_{nl}). While we are in regime $\chi\Delta \gg 1$, Δ does not influence the resonance energies E_{nl}, and increase of Δ leads to decrease of half-widths Γ_{nl} (increase of life-times τ_{nl}). Increase of barrier height U leads to decrease in resonance energies E_{nl} and half-widths Γ_{nl} (increase of life-times τ_{nl}).

Influence of material parameters m_0^*, m_1^* is not so obvious. We scaled over a wide region of m_0^* and m_1^* values and present resonance energies E_{nl} and life-times τ_{nl} dependence on m_1^* and m_1^*/m_0^* in Figs. 4 and 5. We focused on lowest energy state ($l = 0$, $n = 1$) to illustrate behavior of the system. Energies E_{nl} of the other states have the similar behavior.

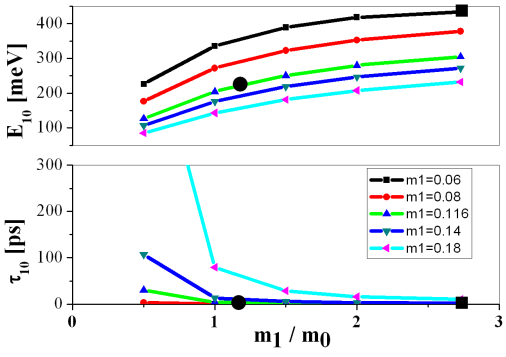

Fig. 4. Electron quasistationary energy and lifetime dependences on m_1^* and m_1^*/m_0^* for fixed parameters: $r_0 = 5a_{\mathrm{CdTe}} = 3.24$ nm, $\Delta = 5a_{\mathrm{ZnTe}} = 3.052$ nm, $U = 0.67$ eV. Results for CdTe/ZnTe/CdTe ($m_1^* = 0.0999$, $m_1^*/m_0^* = 0.116/0.0999 = 1.16$) are marked with (•), and results that correspond to InAs/GaAs/InAs ($m_1^* = 0.063$, $m_1^*/m_0^* = 0.063/0.023 = 2.73$) are marked with (■).

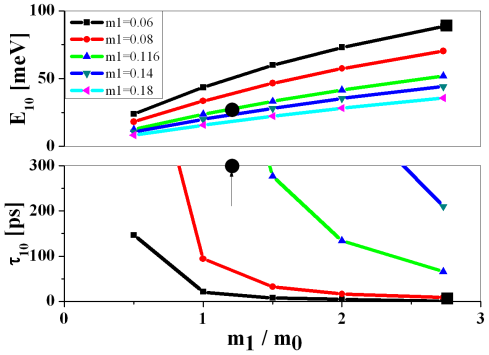

Fig. 5. Electron quasistationary energy and lifetime dependences on m_1 and m_1^*/m_0^* for fixed parameters: $r_0 = 17a_{\mathrm{CdTe}} = 11.02$ nm, $\Delta = 5a_{\mathrm{ZnTe}} = 3.052$ nm, $U = 0.67$ eV. Results for CdTe/ZnTe/CdTe ($m_1^* = 0.0999$, $m_1^*/m_0^* = 0.116/0.0999 = 1.16$) are marked with (•), and results that correspond to InAs/GaAs/InAs ($m_1^* = 0.063$, $m_1^*/m_0^* = 0.063/0.023 = 2.73$) are marked with (■).

Dependence of the energy spectrum of electrons in an open InAs/GaAs/InAs quantum dot on core size and barrier width was investigated and presented in detail [12]. Parameters for calculations were: $m_0^* = m_{\mathrm{InAs}}^* = 0.023$, $m_1^* = m_{\mathrm{GaAs}}^* = 0.067$, $U = 0.535$ eV, $m_1^*/m_0^* = 2.73$. The main difference between CdTe/ZnTe/CdTe and InAs/GaAs/InAs open quantum dot structure is in effective masses. We will discuss results for parameters close to InAs/GaAs/InAs.

We have chosen structure $r_0 = 5a_{\mathrm{CdTe}} = 3.24$ nm, $\Delta = 5a_{\mathrm{ZnTe}} = 3.052$ nm, $U = 0.67$ eV, and scaled over m_1^* and m_1^*/m_0^*. Results for this structure are presented in Fig. 4. For fixed m_1^* increase in m_1^*/m_0^* imply increase in resonance energies E_{10} and half-widths Γ_{10} (decrease of life-times τ_{10}).

For fixed m_1^* smaller m_1^*/m_0^* ratio i.e. larger m_0^* prevents electron to penetrate through the barrier. For fixed m_0^* it is better to have smaller m_1^*/m_0^* ratio i.e. smaller m_1^*. As m_1^* and m_1^*/m_0^* increase we slowly leave region where $\chi\Delta \gg 1$ condition is fulfilled. This is the case for InAs/GaAs/InAs like structure in this case. For InAs/GaAs/InAs effective mass parameters and $U = 0.67$ eV, this quantum dot is to small to be properly treated in this way. Problem should be treated more generally, that is beyond the scope of this work.

In case $r_0 = 17a_{\mathrm{CdTe}} = 11.02$ nm, $\Delta = 5a_{\mathrm{ZnTe}} = 3.052$ nm and $U = 0.67$ eV (see Fig. 5), energies and half-widths are smaller than in the first case. Chosen geometry is similar to the InAs/GaAs/InAs geometry in [12]. E_{10} and τ_{10} have the same trend as in the first case. This core dimension is large enough to prevent electron in this state to penetrate through the barrier.

4. Conclusions

To illustrate the influence of geometric parameters to resonance energies we combined CdTe and ZnTe and formed the spherical heterosystem CdTe/ZnTe/CdTe.

Both the energy levels and the lifetimes of the quasistationary states are found as functions of the geometric parameters of the system. The lifetime of an electron in such a system is very sensitive to the geometric characteristics. We present the analysis of the influence of effective masses in structure to energy levels and lifetimes.

Acknowledgments

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