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Interband electroabsorption in CdSe nanoplatelets

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Abstract. In CdSe nanoplatelet, interband transitions in the presence of an axial electric field are considered. It is shown that at certain nanoplatelet thicknesses, the combined effect of polarization and confining potentials forms an effective parabolic potential in the axial direction. As a consequence, the influence of the electric field in this direction can be described within the framework of the one-dimensional mixed oscillator model. Analytical formulas for the energy spectrum and wave function are obtained, threshold frequencies are determined for different monolayer thicknesses.

Keywords: CdSe nanoplatelets, interband absorption, electric field

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1. Introduction

Semiconductor nanoplatelets (NPLs) are quasi-two-dimensional hybrid structures occupying an intermediate position between quantum dots and quantum wells [1–3]. From a geometric point of view, they are rectangular parallelepipeds, one side of which is significantly shorter than the other two. Despite the large dimensions of the two sides of the nanoplatelet, it is nevertheless necessary to take into account the dimensional quantization in these directions, as evidenced by the experimentally discovered dimensional quantization of the motion of the exciton center of mass in CdSe nanoplatelets [4]. The effect of size quantization in the direction of the small length of the nanoplate (the Oz axis) is significantly greater than in the plane perpendicular to this axis. Consequently, the energy spectrum of electrons and holes in the NPL has a pronounced subband character. Such a character of the energy band structure of the NPL leads to an extremely rich picture of optical transitions in such systems, both intraband and intersubband, and interband (see, for example, [5–10]). In work [5], the effects of the influence of electron-hole interaction on the character of interband and intraband absorption in CdSe NPL were studied taking into account the effects of polarization at the NPL-environment transition boundary in the axial direction. The influence of the axial electric field on the exciton absorption in CdSe NPL was discussed in [6] taking into account the presence of imaginary charges in the axial direction within the Takagahara model [11]. It should be noted that the axially symmetric potential restricting the particle motion in the Oz direction is formed from the confining potential of the size quantization $V^{||}{}_{\mathrm{conf}}(z)$ itself, as well as from the potentials of imaginary charges $V_{\mathrm{self}}(z)$:

$$V_{\mathrm{total}}(z) = V^{||}{}_{\mathrm{conf}}(z) + V_{\mathrm{self}}(z) \quad (1)$$

As a result, the particle performs quantum motion in the axial direction in the effective field formed from the above potentials. In the case where $V^{||}{}_{\mathrm{conf}}(z)$ is a rectangular well of finite depth,

and $V_{\text{self}}(z)$ is described by the Takagahara model [5,6], $V_{\text{total}}(z)$ has the profile shown in Fig. 1.

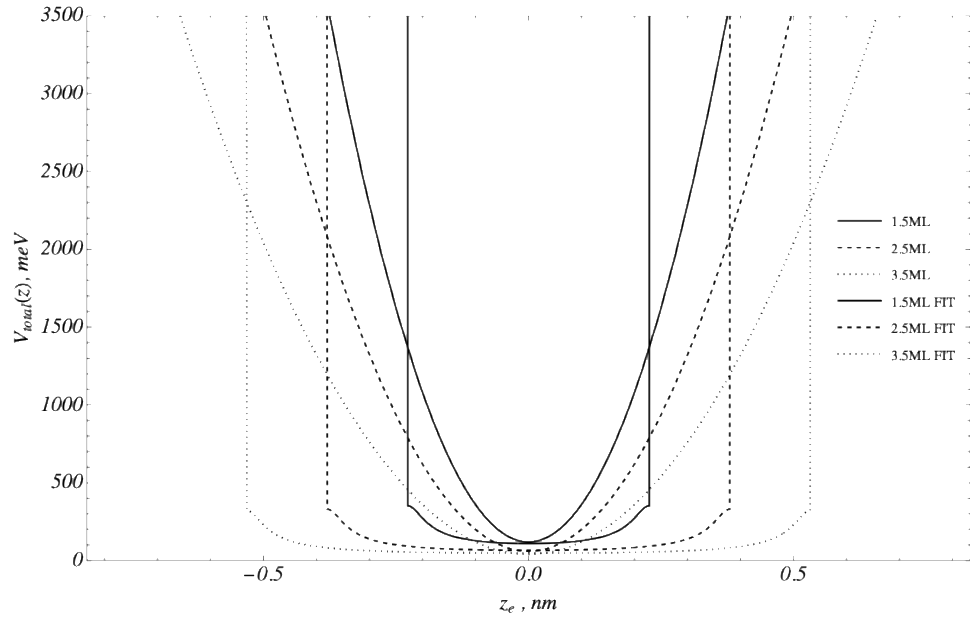

Figure 1. Dependence of the potential profile $V_{\text{total}}(z)$ on z_e.

The axial Schrödinger equation with $V_{\text{total}}(z)$ is not analytically solvable in the general case. However, by selecting the parameters of the NPL, the $V_{\text{total}}(z)$ profile can be approximated to a parabolic one, then for relatively low levels of electrons and holes in the NPL, we can assume:

$$V_{\text{total}}(z) = \frac{\mu\omega^2 z^2}{2}, \tag{2}$$

where $\omega -$ is the frequency of the parabolic potential, determined by comparing the exact and approximate curves $V_{\text{total}}(z)$. If we consider in the xOy plane, the confining potential $V^{\perp}{}_{\text{conf}}(x,y)$ within the framework of the model of infinitely deep rectangular walls:

$$V^{\perp}{}_{\text{conf}}(x,y) = \begin{cases} 0, M \in NPL \\ \infty, M \notin NPL \end{cases}, \tag{3}$$

then the single-particle Schrödinger equation will be exactly solvable, including in the presence of a uniform axial electric field $\vec{\mathcal{E}}$. The latter circumstance allows us to conduct a detailed analytical study of interband optical electroabsorption in CdSe NPL. This is the problem that this paper is devoted to.

2. Wave functions and energy spectrum

Consider a particle in a CdSe NPL, in the presence of a uniform electric field $\vec{\mathcal{E}}$ directed along the Oz axis. Taking into account the arguments expressed in the introduction regarding the confinement potentials in the Oz and xOy directions, as well as the influence of the polarization potential in the axial direction for a single-particle Hamiltonian, we can write:

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2\mu_\perp}\left(\frac{\partial^2}{\partial \mathrm{x}^2}+\frac{\partial^2}{\partial \mathrm{y}^2}\right)-\frac{\hbar^2}{2\mu_{||}}\left(\frac{\partial^2}{\partial \mathrm{z}^2}\right)+\mathrm{V}^{\perp}{}_{\mathrm{conf}}(\mathrm{x},\mathrm{y})+\mathrm{V}_{\mathrm{total}}(\mathrm{z})-\mathrm{e}\mathcal{E}\mathrm{z}, \quad (4)$$

where $\mu_{\perp(||)}$ is the effective mass of a particle (electron or hole) in the xOy plane (along the Oz axis). The Schrödinger equation $\widehat{\mathrm{H}}\psi = \mathrm{E}\psi$ is exactly solvable and the wave function $\psi(\mathrm{x},\mathrm{y},\mathrm{z})$ can be represented as a product of two functions $\psi_\perp(\mathrm{x},\mathrm{y})$ and $\psi_{||}(\mathrm{z})$:

$$\psi(\mathrm{x},\mathrm{y},\mathrm{z}) = \psi_\perp(\mathrm{x},\mathrm{y}) \times \psi_{||}(\mathrm{z}). \quad (5)$$

These functions satisfy the following equations:

$$-\frac{\hbar^2}{2\mu_\perp}\left(\frac{\partial^2}{\partial \mathrm{x}^2}+\frac{\partial^2}{\partial \mathrm{y}^2}\right)\psi_\perp + \mathrm{V}^{\perp}{}_{\mathrm{conf}}(\mathrm{x},\mathrm{y})\psi_\perp = \mathrm{E}_\perp\psi_\perp, \quad (6)$$

and

$$-\frac{\hbar^2}{2\mu_{||}}\left(\frac{\partial^2}{\partial \mathrm{z}^2}\right)\psi_{||} + \frac{\mu\omega^2\mathrm{z}^2}{2}\psi_{||} - \mathrm{e}\mathcal{E}\mathrm{z}\psi_{||} = \mathrm{E}_{||}\psi_{||}. \quad (7)$$

The solution to equation (6) is well known and has the following form [12]:

$$\psi_\perp(\mathrm{x},\mathrm{y}) = \sqrt{\frac{2}{\mathrm{L}_1}}\sqrt{\frac{2}{\mathrm{L}_2}}sin\left(\frac{\pi \mathrm{n}_1}{L_1}\mathrm{x}+\delta n_1\right)sin\left(\frac{\pi \mathrm{n}_2}{L_2}\mathrm{y}+\delta \mathrm{n}_2\right), \quad (8)$$

$$\mathrm{E}_\perp = \frac{\pi^2\hbar^2}{2\mu_\perp}\left(\left(\frac{\mathrm{n}_1}{\mathrm{L}_1}\right)^2+\left(\frac{\mathrm{n}_2}{\mathrm{L}_2}\right)^2\right), \quad (9)$$

where $\mathrm{n}_{1(2)}$ are the quantum numbers of the characterized energy levels in the Ox(Oy), direction, $\delta \mathrm{n}_{1(2)}$ are the initial phases of the quantum states ($\delta n_{1(2)} = 0$ for odd levels, and $\mathrm{n}_{1(2)} = \frac{\pi}{2}$ for even levels). Equation (7) describes the states of a particle of a mixed oscillator in the axial direction. For a particle with charge e, the wave functions and energy spectrum have the following form:

$$\psi_{||}(\mathrm{z}) = \mathrm{C}_{\mathrm{n}_3}\mathrm{e}^{-\frac{\left(\mathrm{z}-\frac{\mathrm{e}\mathcal{E}}{\mu_{||}\omega^2}\right)^2}{2\mathrm{a}_\omega^2}}\mathrm{H}_{\mathrm{n}_3}\left(\frac{\mathrm{z}-\frac{\mathrm{e}\mathcal{E}}{\mu_{||}\omega^2}}{\mathrm{a}_\omega}\right), \quad (10)$$

$$\mathrm{E}_{||} = \hbar\omega\left(\mathrm{n}_3+\frac{1}{2}\right)-\frac{\mathrm{e}^2\mathcal{E}^2}{2\mu_{||}\omega^2}, \quad (11)$$

where n_3 is the oscillator quantum number, $\mathrm{H}_{\mathrm{n}_3}$ is the Hermite polynomial, $\mathrm{a}_\omega = \sqrt{\frac{\hbar}{\mu\omega}}$ is the oscillator length. We note right away that the Stark splitting is proportional to the square of the electric field strength.

2. Interband electroabsorption

Based on the results obtained above, it is possible to calculate the interband absorption coefficient taking into account the influence of the external electric field. The specified coefficient is determined according to the formula [13]:

$$K(\Omega) = \mathrm{A}\sum_{\mathrm{n}_1{}^{\mathrm{e}},\mathrm{n}_2{}^{\mathrm{e}},\mathrm{n}_3{}^{\mathrm{e}}}\sum_{\mathrm{n}_1{}^{\mathrm{h}},\mathrm{n}_2{}^{\mathrm{h}},\mathrm{n}_3{}^{\mathrm{h}}}\left|\int \psi_{\mathrm{n}_1{}^{\mathrm{e}},\mathrm{n}_2{}^{\mathrm{e}},\mathrm{n}_3{}^{\mathrm{e}}}\psi_{\mathrm{n}_1{}^{\mathrm{h}},\mathrm{n}_2{}^{\mathrm{h}},\mathrm{n}_3{}^{\mathrm{h}}}\mathrm{dV}\right|^2\delta(\hbar\Omega-\mathrm{E}_{\mathrm{g}}-\mathrm{E}_{\mathrm{n}_1{}^{\mathrm{e}},\mathrm{n}_2{}^{\mathrm{e}},\mathrm{n}_3{}^{\mathrm{e}}}-\mathrm{E}_{\mathrm{n}_1{}^{\mathrm{h}},\mathrm{n}_2{}^{\mathrm{h}},\mathrm{n}_3{}^{\mathrm{h}}}), \quad (12)$$

where E_g is the band gap, $E_{n_1{}^e,n_2{}^e,n_3{}^e}$ is the electron energy, $E_{n_1{}^h,n_2{}^h,n_3{}^h}$ is the hole energy, A is the coefficient proportional to the matrix element constructed on the Bloch amplitudes of the valence band and conduction band, Ω is the frequency of the incident radiation, under the influence of which these transitions occur, and the δ function ensures the fulfillment of the law of conservation of energy during transitions.

Let us turn to the calculation of the integrals in (12). In the directions Ox and Oy we will have an integral of the following form:

$$\frac{2}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} sin\left(\frac{\pi n_e}{L}x+\delta n_e\right) sin\left(\frac{\pi n_h}{L}x+\delta n_h\right)dx=\begin{cases}1, & n_e=n_h\\ 0, & n_e\neq n_h\end{cases}. \tag{13}$$

From equation (13) the following selection rules are obtained:

$$\left.\begin{aligned} n_1 \equiv n_1{}^e = n_1{}^h\\ n_2 \equiv n_2{}^e = n_2{}^h\end{aligned}\right\}. \tag{14}$$

In the axial direction, the following integral is obtained:

$$I = C_{n_3{}^e}C_{n_3{}^h}\int_{-\infty}^{\infty} e^{-\frac{(z-\frac{e\mathcal{E}}{\mu_{||}\omega_e{}^2})^2}{2a_{\omega_e}^2}} H_{n_3{}^e}\left(\frac{z-\frac{e\mathcal{E}}{\mu_{||}\omega_e{}^2}}{a_{\omega_e}}\right)\times e^{-\frac{(z+\frac{e\mathcal{E}}{\mu_{||}\omega_h{}^2})^2}{2a_{\omega_h}^2}} H_{n_3{}^h}\left(\frac{z+\frac{e\mathcal{E}}{\mu_{||}\omega_h{}^2}}{a_{\omega_h}}\right)dz\,. \tag{15}$$

The integral (15) is calculated numerically and its values are nonzero for different combinations of $n_3{}^e$ and $n_3{}^h$. Thus, the imposition of the eclectic field in the axial direction removes the selection rules for interband transitions in the Oz direction.

From the argument of the $\delta-$function in (12) we find the threshold value Ω_0 of the interband absorption frequency:

$$\hbar\Omega_0 = E_g + \frac{\pi^2\hbar^2}{2\mu_\perp}\left(\frac{1}{L_1{}^2}+\frac{1}{L_2{}^2}\right)+\frac{\hbar}{2}(\omega_e+\omega_h)-\frac{e^2\mathcal{E}^2}{2}\left(\frac{1}{\mu_{||}{}^e\omega_e{}^2}+\frac{1}{\mu_{||}{}^h\omega_h{}^2}\right), \tag{16}$$

where $\frac{1}{\mu_\perp}=\frac{1}{\mu_\perp{}^e}+\frac{1}{\mu_\perp{}^h}$.

3. Numerical Calculations

In order to find the value Ω_0 of the interband absorption frequency, we will use the data shown in table 1. These parameters were estimated from calculations obtained using the density functional theory method [14,15]. Numerical values of $\hbar\omega_e$, $\hbar\omega_h$ for different NPL thicknesses are presented in the table 2.

n	m_{z_e}, m_0	m_{z_h}, m_0	E_g, eV	$\mu_\perp, (m_0)$
1.5	0.25	1.04	2.7	0.13
2.5	0.19	0.98	2.45	0.108
3.5	0.157	0.96	2.3	0.103
4.5	0.144	0.92	2.15	0.09

Table 1: $m_{z_e}, m_{z_h}, E_g, \mu_\perp$ parameters are shown for different NPL thicknesses (n).

n	$\hbar\omega_e$, eV	$\hbar\omega_h$, eV
1.5	3.82	1.79
2.5	3.35	1.36
3.5	2.78	1.05
4.5	2.18	0.72

Table 2: Numerical values of $\hbar\omega_e, \hbar\omega_h$ are shown for different NPL thicknesses (n).

Based on the abovementioned numerical values of $\hbar\omega_e, \hbar\omega_h$ and from formula (16), it is possible to determine the numerical value of the threshold frequencies of absorption at different thicknesses of the nanoplatelet. Table 3 shows the values of the threshold frequencies of absorption at different thicknesses of the nanoplatelet.

	n = 1.5	n = 2.5	n = 3.5	n = 4.5
$\hbar\Omega_0, eV$	5.50502	4.80502	4.21503	3.60003

Table 3: Numerical values of the threshold frequencies of absorption ($\hbar\Omega_0$) at different thicknesses of nanoplatelet (n).

From the given numerical values, it follows that with the growth of the number of monolayers the threshold frequency of the invitation decreases. This is a consequence of the weakening of the size quantization in the axial direction, as a result of which the interlevel distances decrease and the energy of the interband transitions also decreases.

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