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THE BINDING ENERGY OF THE SCREENED COULOMB CENTER IN A SEMICONDUCTOR QUANTUM WIRE

The formalism of the screened Coulomb center binding energy in the semiconductor quantum wire embedded in a barrier environment is calculated. With the account of strongly low dielectric properties of the barrier environment, both the analytical expression of the binding energy is derived for the first time and the numerical analysis of the latter depending on wire radius is provided.

Keywords: quantum wire, dielectric confinement, binding energy.

The energy spectrum and other physical characteristics of the Coulomb centers (impurities and excitons) in quasi-one-dimensional (Q1D) semiconductor quantum wires (QWr) surrounded by the low dielectric constant barrier environment are under intensive investigations. These nanosystems are favorable because in addition to size quantization effects, which make Coulomb center Q1D, image potentials due to the large contrast between dielectric constants of the semiconductor and dielectric barrier media (dielectric confinement (DC) effect) also play an important role [1- 5].

Quasi-free carriers may screen the Coulomb centers in QWr system, where the Q1D electron gas (Q1D EG) can be produced by intense optical illumination of undoped QWr sample or by modulating the doping material. As a result, Q1D EG may coexist with the photo excited excitons and screen, as in the quantum wells (QWs), Coulomb polarization fields of excitons and impurity centers. This phenomenon in the low-dimensional structures holds both by strong quasiparticle correlations and weak static screening of Coulomb interaction.As a result, the influence of screening produced by electrons in the Q1D structure is considerably weaker than in 3D or 2D semiconductor systems. In this paper, we investigate the screened exciton bound state energy properties of semiconductor QWr enhanced due to the DC effect by using both the Bessel equation and variational methods of calculations.

Let us consider an infinitely long semiconductor cylindrical QWr of radius R filled by semiconductor material with the dielectric constant ε_w and embedded in the dielectric barrier environment with the dielectric constant ε_b. A QWr contains a Q1D EG where the electrons are confined to move in a QWR and are free to move along the axis of the wire by means of linear density n_L . Moreover, a strong confinement regime is accepted in discussing the case, assuming that the quantum wire radius R is small compared with the Bohr radius a_0 in the semiconductor bulk samples ($a_0 >> R$).

For that case, large asymptotic distances between the interacting particles along the wire axis $|z|>>R$ are essential. As shown in [6], the tunability of the Coulomb interaction in the QWr due to the DC effect enhances and modifies the Q1D screening potential. As a result, in the intermediate distance range for a cylindrical wire $R<|z|\sim q_L^{-1}$, the interaction potential depends exponentially on the interparticle distance z

$$V_S^{Q1D}(z)=-\frac{e^2}{\varepsilon_w R}\frac{1}{q_L R}e^{-q_L|z|}\ , \tag{1}$$

where $q_L=\sqrt{q_S^2+q_d^2}$. The screening parameter q_S is defined in Ref. [7] and is expressed as:

$$q_S^{-2}=R^2\left[\frac{\pi^2}{32r_S}+\frac{K_1}{16}\sqrt{\pi x}+\frac{r_S x}{4}+\frac{K_2}{K_3}\frac{x}{4}\left[\frac{1}{r_S}+\frac{4}{K_3}\sqrt{\frac{x}{\pi}}\right]^{-1}\right]$$

where $x=k_BT/R_0$ and $R_0=\hbar^2/2m_wa_0^2$ is the bulk semiconductor effective Rydberg. Here $r_S=1/2a_0\,n_L$ is the interparticle 1D spacing of the free carriers in units of Bohr radius.

In Exp.(1) the screening parameter q_S is renormalized by small parameter $q_d=(1/R)\sqrt{2/(\varepsilon_r\ln\varepsilon_r)}$, the existence of which is caused by the DC effect. As follows, q_L can be considered the DC effect influenced effective screening parameter for discussing the case because of the strong dependence of the dielectric constants ratio ε_r.

Now we are interested in finding the screened excitonic bound states energy levels in the potential (1). For that we shall solve the Schrödinger wave equation:

$$-\frac{\hbar^2}{2m_w}\frac{d^2\psi}{dz^2}+V_S^{Q1D}(z)\psi=E\psi\ \cdot \tag{2}$$

Eq. (2) does not change under reflection $z\to -z$, therefore in accordance with the standard treatment of the 1D problem, the solutions $\psi(z)$ must possess both even and odd parity. We look for bound state solutions of wave equation (2) and thus introduce proper substitutions for that case: $E=-\hbar^2\chi^2/2m_w$, $y=\xi\exp(-q_L|z|)$, $\xi=\sqrt{8m_wE_R/q_L^2\hbar^2}$, $E_R=e^2/\varepsilon_wR\,q_LR$, $\nu=2\chi/q_L$ ($\chi>0$). Afterwards Eq.(2) takes the Bessel equation form:

$$\frac{d^2\psi}{dy^2}+\frac{1}{y}\frac{d\psi}{dy}+(1-\frac{\nu^2}{y^2})\psi=0\ \cdot \tag{3}$$

Because $\psi(x)$ must decrease as $z \to \infty$ ($y \to 0$), we have the solution of Eq.(3) in the standard form

$$\psi(x) = C\,J_\nu(x) = C\,J_\nu[\xi \exp(-q_L z)] \ . \tag{4}$$

The eigenvalues of the system at the origin $z \to 0$ are defined by the conditions of

$$\frac{d}{dz} J_\nu[\xi \exp(-q_L z)]\bigg|_{x=0} = 0 , \tag{5}$$

$$J_\nu[\xi \exp(-q_L z)]\big|_{x=0} = 0 . \tag{6}$$

for both the even and odd states respectively. Eqs. (5) and (6) give the screened exciton energy eigenvalues of the system for the given mean linear density n_L, permitted reduced temperature parameter and QWr radius R. In particular, from Eq.(5) we calculate the enhanced ground-state energy, namely, the screened exciton binding energy graphical dependence versus R and compare with the unscreened exciton counterpart.

For the purpose of giving a more comprehensive analytical description of the problem and for comparison as well, we develop the variational method for calculating both the binding energy and dimension of a quasi-one-dimensional exciton confined in a QWr inside a bulk dielectric media. Unlike the former technique this approach makes it possible to receive the analytical expressions for the screened exciton binding energy and 1D extent of wave function around exciton (exciton 1D mean length) in QWr.

The standard variational principle deals with the functional

$$E[\phi] = \int \phi^* [H_{kin} + V_S^{Q1D}]\, \phi dV , \tag{7}$$

where the average value over $|\psi(z)|^2$ of the screened potential $< V_S^{Q1D}(z) >$ should be used. According to the strong confinement regime, the normalized one parameter trial wave function of the exciton ground state is chosen as

$$\psi(z) = \sqrt{1/L}\sqrt{\lambda/2}\, \exp(-\lambda z/2), \tag{8}$$

where λ is the variational parameter, L is the wire length. After the necessary standard calculations, both the variational parameter and the screened exciton ground state binding energy are obtained in the form below:

$$\lambda = \left(\frac{2}{a_0 R^2}\right)^{1/3} \lambda_{q_L, R} , \tag{9}$$

$$E_b(q_L, R) = -\frac{e^2}{\varepsilon_w R}\frac{1}{q_L R}\left[\left[1 + q_L R\left(\frac{a_{ex}}{R}\right)\right]^{-1} - \frac{q_L R}{8}\frac{a_0}{a_{ex}}\frac{R}{a_{ex}}\right]. \quad (10)$$

In Exp.(9)

$$\lambda_{q_L,\,R} = \sqrt{1 + \left(\frac{q_L R}{3}\right)^3 \frac{a_0}{2R} + \sqrt{1 + 2\left(\frac{q_L R}{3}\right)^3 \frac{a_0}{2R}}} + \sqrt{1 + \left(\frac{q_L R}{3}\right)^3 \frac{a_0}{2R} - \sqrt{1 + 2\left(\frac{q_L R}{3}\right)^3 \frac{a_0}{2R}}}\,.$$

In order to display numerically the screened Coulomb properties we refer to the model with the PbSe based QWR embedded in the mesoporous silica SBA-15 barrier environment. Accordingly, the following material parameters are adopted: $m_w \approx 0.0355 m_0$ (m_0 is the free electron mass) and $\varepsilon_w \approx 23$, which leads to $a_0 \approx$ 34.45 nm and $R_0 \approx$ 0.91 meV parameter values. With the $\varepsilon_b = 2$ we have the dielectric constants ratio value ε_r = 11.5. For the numerical analysis of q_S^{-2} , the moderately high linear density $n_{L1} \approx 1.5.10^6$ cm^{-1} and the moderately low temperature $T \approx 26$ K values are taken into consideration. For that case, the DC effect responsible term $q_d R$ exceeds just 1.5 times the screening effect counterpart $q_S R$ in $q_L R$, indicating that these contributions are in the same order. In Fig. 1, we outline the graphical results of the screened exciton binding energy as a function of the "moderately" thick QWr radius R in accordance with Exps.(5) and (10). The received graphical lines are shown in comparison with the QWr unscreened potential graphical curves ($q_S \to 0$). The top two solid and solid-dashed bold lines correspond to the unscreened potential case both for the Bessel and variational equations (Eqs.3, 5), respectively. While the low standing two thin solid and solid-dashed lines corresponds to the screened potential case (Eq.(1)) for the foregoing equations, respectively. As it follows, in "moderately" thick QWr with the DC effect, the screened exciton binding energy is seen to exceed the bulk effective Bohr energy $R_0 \approx$ 0.91 meV by more than one order of magnitude. In Table 1 we present the binding energy $E_b(q_L, R)$ calculation results when QWr radius decreases from $R_1 \approx 10$nm to $R_2 \approx 5$nm. We can see the numerical results the screening from both the graph and table.

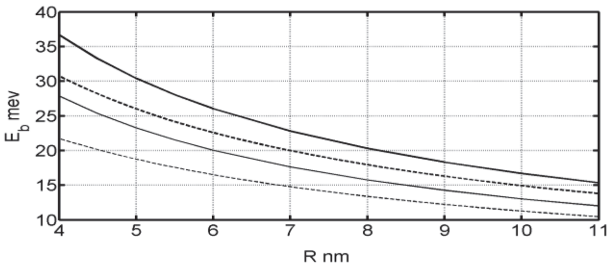

Fig. 1. The binding energy of the screened exciton as the function of QWr radius R for the fixed linear density ($n_L \approx 1.5.10^6$ cm^{-1}) and temperature ($T \approx 26$K)

Table 1

The numerical results of binding energy E_b for the QWr radius $R_{1(2)}$=10(5)nm with the fixed linear density ($n_L \approx 1.5.10^6$ cm^{-1}) and temperature ($T \approx 26K$)

method	Variational				Bessel equation			
$R_{1(2)}$=10(5)nm	E_{b1}	E_{b2}	E_{b2}/E_{b1}	E_{b2} - E_{b1}	E_{b1}	E_{b2}	E_{b2}/E_{b1}	E_{b2} - E_{b1}
Unscreened	14.9	23.3	1.56	8.4	16.7	33.4	2.0	16.7
Screened	11.3	18.8	1.66	7.5	13	23.3	1.8	10.3

The effect reduces distinctly DC effect enhanced exciton binding energy E_b and the latter is more effective for the small values of R in the permitted radius range. Nevertheless, the screened exciton E_b values are enhanced enough due to the DC effect that even for the "moderately" thick QWr radius value R=10nm will support a distinguished stability in the exciton pair. Note, that the Bessel equation wave function type calculations overestimate the E_b values in relation to the variational equation Coulomb type wave functions (corresponding graphical curves are enhanced more strongly), but, meanwhile, the E_b modifying rate is almost the same for both methods.

In summary, by using both the Bessel equation and variational methods a formalism for studying the screened exciton states in lead salt/mesoporous silica SBA 15 phase realistic semiconductor QWr system is developed theoretically. For the "moderately thick" QWr, the problem of the screened exciton binding energy E_b has been investigated both analytically and numerically. The strong enhancement of the binding energy E_b (~ $20 \div 30$ meW) in comparison with the unscreened bulk value (~ 0.9 meW) is received in the presence of the exponential-the types of potential, demonstrating that quantum and dielectric confinement overbalance together to the Q1D screening effect. The permissible intervals of Q1D screened exciton E_b in correlation with QWr radius is also established.

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ԷԿՐԱՆԱՎՈՐՎԱԾ ԿՈՒԼՈՆՅԱՆ ԿԵՆՏՐՈՆԻ ԿԱՊԻ ԷՆԵՐԳԻԱՆ ԿԻՍԱՀԱՂՈՐԴՉԱՅԻՆ ՔՎԱՆՏԱՅԻՆ ԼԱՐԵՐՈՒՄ

Հաշվարկված է արգելքային միջավայր ներառված կիսահաղորդչային քվանտային լարերում էկրանավորված կուլոնյան կենտրոնի կապի էներգիան: Դիէլեկտրական սահմանափակման երևույթի հաշվառումով առաջին անգամ ստացված է կուլոնյան կենտրոնի կապի էներգիայի արտահայտությունը: Կատարված է վերջինիս թվային վերլուծություն՝ կախված քվանտային լարի շառավղից:

Առանցքային բառեր. քվանտային լար, դիէլեկտրիկ սահմանափակում, կապի էներգիա:

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ЭНЕРГИЯ СВЯЗИ КУЛОНОВСКОГО ЦЕНТРА В ПОЛУПРОВОДНИКОВЫХ КВАНТОВЫХ НИТЯХ

Вычислена энергия связи экранированного кулоновского центра в полупроводниковых квантовых нитях, вкрапленных в барьерную среду. С учетом явления диэлектрического ограничения впервые получено выражение для энергии связи. Проведен численный анализ последней в зависимости от радиуса квантовой нити.

Ключевые слова: квантовая нить, диэлектрическое ограничение, энергия связи.