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Binding Energy of the One-Sided Dielectrically Enhanced Screened Exciton in Semiconductor Quantum Well

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1. Introduction. Fundamental interest in quasi-two-dimensional (Q2D) electron gas (EG) properties in quantum wells (QW) is initiated both by fabrication advances and by request of optoelectronic technology. The properties of Q2D EG attract attention owing to excitons, which mostly are confined in QW with compressed wave functions. The results are the increased binding energy and enhanced contrast between the 1s exciton peak and continuum [1, 2].

In QW samples selective doping makes it possible that a Q2D electron channel can coexist with photo excited excitons, which results in the changes of the optical properties. The latter is caused by many-body effect such as a screening of the excitons by free carriers as a consequence of Coulomb mutual correlation [3-9]. The effect of excitons screening is twofold: decreasing the binding energy and altering the interband absorption spectra. In 2D structures the screening of excitons by free carriers is less effective than in 3D samples [3, 4] and the any exciton cannot be screened out at any 2D density.

Due to selective doping, the free carrier densities can govern the strength of interaction between the particles simultaneously with structural adjustment of the QW specific parameters such as the barrier height Δ, the QW width d and, particularly, a strong contrast of the neighboring media dielectric constants in heteroboundaries (dielectric confinement effect (DC)). The latter, as well known, turns up the exciton binding energy and oscillator strength essentially [3, 7, 10 -12].

A theoretical study of the screened Q2D Coulomb interaction with arbitrary dielectric constants of both the QW and barrier ($\varepsilon_w, \varepsilon_b$) have been started by Rytova in [3]. In particular, for the strong contrast between ε_w and ε_b values such as $\varepsilon_r = \varepsilon_w / \varepsilon_b \gg 1$ (the two-sided DC effect), a statically screened Q2D potential expression has been established in the form

$$V_S(\rho) = -\frac{2e^2}{\varepsilon_w d} K_0\left(\sqrt{\frac{2q_S}{d}}\rho\right) \tag{1}$$

for the moderate large in-plane distances $\varepsilon_r d/2 >> \rho >> d$ between the charges, where K_0 is the Bessel function of the second kind, q_S is the 2D screening parameter. Here screened potential strongly depend on the QW width and decay exponentially for large in-plane distances outside the circle with the radius of $\rho_0 = \sqrt{d/2q_S}$.

In Ref. [7] for the case of $\varepsilon_w \approx \varepsilon_{b1}$, $\varepsilon_w >> \varepsilon_{b2}$ (i.e. when the barrier media on each side of QW have the strongly different dielectric constants and the latter's mismatch is strong for just one heteroboundary only, while for the other one the DC effect is negligible (the one-sided DC effect)), the 2D Debye- Hückel - type analytical expression for the 2D screened potential

$$V_S(\rho) = -\frac{2e^2}{\varepsilon_w}\frac{(\exp(-\rho/\rho_0)}{\rho} \tag{2}$$

is obtained for the in-plane distances ρ such as $d << \rho \le \rho_0$ $\sqrt{\varepsilon_{w1}^{-1}[(e^2+1)/(e^2+1)]^2 - 1}$, where $\varepsilon_{w1} = \varepsilon_w / \varepsilon_{b1} \sim 1$, $e = 2.71..$ is the natural number.

As follows, both for the ***two-sided*** ($\varepsilon_w \gg \varepsilon_b = \varepsilon_{b1} = \varepsilon_{b2}$) [3] and ***one-sided*** ($\varepsilon_w \approx \varepsilon_{b1}$, $\varepsilon_w >> \varepsilon_{b2}$) [7] dielectric contrast affected cases, the DC effect leads to recovering of Q2D screening radius.

In the Refs.[13-15] the binding energy problem of screened Coulomb bound states in the semiconductor QW with screened Q2D potential after Exps.(1) has been explored. In particular, monotonic increase of the screened Coulomb center binding energy with decrease of both QW thickness and density / temperature ratio parameter is revealed.

The present work is devoted to the study of the screened exciton properties in one-sided dielectric contrast ($\varepsilon_w \approx \varepsilon_{b1}$, $\varepsilon_w >> \varepsilon_{b2}$) affected QW system. We present both the analytical and numerical study of the Q2D hidrogen-like (H-like) screened Coulomb centers binding energy problem, modeled by the screened potential after Exp. (2), namely for the 2D Debye -Hückel - type of limit.

2. Theoretical Background and Model. The H-like Coulomb bound states in QW system influenced both by quantum confinement and screening effects have been the subject of deep investigations in the past time. Experiments in this field based mainly on the III-V group semiconductors [16, 17], whereas the various calculation techniques all within the effective-mass approximation (EMA) such as the perturbation theory, the variational-perturbation method, the variational and numerical methods are performed theoretically (see, e.g. Refs. [29-41] in Ref.[13]). The discussed systems in this field are $GaAs/Al_xGa_{1-x}As$ and Si/SiO_2 QW structures by weak or negligible expressed DC effect.

At the same time, for the dielectrically heterogeneous ternary layer system with $\varepsilon_w \approx \varepsilon_{b1}$ and $\varepsilon_w >> \varepsilon_{b2}$ conditions the Coulomb interaction characterized by 2D Debye–Hückel type one-sided dielectrically enhanced potential (Exp.(2)) becomes larger due to the decreasing of the structure effective dielectric constant twice. As in the unscreened case [10], this would give rise to the screened exciton energy spectrum enhancement. The Exp.(2) is realized when the following the two conditions are simultaneously fulfilled: $qd << 1$ and $\rho_0^{-1} d << 1$, where q is the 2D electron wave vector. The first inequality corresponds to the strong confinement condition $\alpha_0 \gg d$ (α_0 is the electron Bohr radius in bulk sample), while the second matches to the relation $r_d >> d$, where r_d is the 3D Debye radius.

The 2D Debye–Hückel type potential has been widely applied in studies on H-like impurity binding energy [8], excitons oscillator strength [7] in QW systems, as well as on Dirac electrons spectra of the 2D H-like screened atoms, etc. (see, e.g. Ref.[18] and references therein).

In our discussed one-sided dielectric contrast affected case with 2D Debye–Hückel type enhanced potential the position of the screened exciton ground level one can determine with a great deal of accuracy if one utilizes a direct variational method. We are following to the strong confinement regime for that a distance between quantized energy levels is larger than an Coulomb $_{\text{interaction}}$ energy. Thus, a ground state wave function has a separable form such as $\phi = \phi(\rho, z) = \psi(\rho)\varphi(z)$, where $\psi(\rho)$ is an in-plane wave function and $\varphi(z)$ is an one-particle 1D Schrödinger-like equation EMA solution.

The model for the Q2D EG embedded in the QW is based on the nearly rectangular band alignment with band offset Δ_c. The Hamiltonian of Coulomb center in QW is $\hat{H} = H_{kin} + H_{eff} + V_S$, where $H_{eff} = V_{conf}(z) + V_{self-im}(z)$ - is the unperturbed part, V_S is the screened Coulomb potential, $V_{conf} = 0$ with $0 < z < d$ and $V_{conf} = \Delta_c$ with $z \le 0$, $z \ge d$. Here $V_{self-im}$ is the one-electron self-image interaction potential, which, as well as the size-quantized potential, modifies one-particle states, gives contribution to the band-gap renormalization and does not depend on the in-plane 2D distance between the charges. This contribution has the same order as the particle binding energy [10-14]. So, the self-image interaction changes the rectangular localizing potential weakly [4]. Thus, the Q2D screened potential $V_S(\rho)$ becomes weak, varies smoothly on the scale of k_F^{-1} ($k_F = \sqrt{2\pi n_s}$ is the 2D Fermi vector) and can be treated as the perturbation in subbands energy calculations. We discuss the states in the fundamental subband (size quantum limit (SQL)).

3. Analytical study of the Screened Exciton Binding Energy. The standard variational principle deals with the functional $E[\varphi] = \int \varphi^*[H]\,\varphi dV$. The binding energy E_b is obtaining by minimization of the $E[\varphi]$ by involving the screened potential after Exp. (3) and as the difference of the first subband energy E_1 and expectation energy E_{s1}.

According to the $a_0 \gg d$ condition, we choose the 1s exciton ground state normalized one parameter trial wave function in the form $\psi(\rho) = \sqrt{2/\pi}\,\lambda e^{-\lambda\rho}$ [9, 10, 12-15], where λ is the variational parameter. After needed calculations we have the E_b variational expression as

$$E_b = \frac{\hbar^2 \lambda^2 m_r}{2\mu_\perp} - \frac{\hbar^2 \lambda^2 m_r}{2\mu_\perp a_{0S}} \frac{8}{q_S + 2\lambda}, \qquad (3)$$

which gives the screened exciton binding energy in the final form

$$E_b = \frac{\hbar^2 m_r}{2\mu_\perp a_{scex}^2} \left[2 + (2 - q_S a_{scex}) \sqrt{1 + q_S a_{scex}} + \left(\frac{q_S a_{scex}}{2} \right)^2 \right] \left[\frac{\sqrt{1 + q_S a_{scex}} - 3}{\sqrt{1 + q_S a_{scex}} + 1} \right]. \qquad (4)$$

where $a_{sc\,ex} = a_{ex} / 2$, $a_{ex} = \varepsilon_w \hbar^2 / \mu_\perp e^2$, $\mu_\perp$ is the exciton effective mass.

As we can see from Exp. (4), in the zero-order approximation with respect to the small parameter q binding energy E_b does not explicitly depend on the QW width d. While, as will be show next, the dependence from d implicitly holds through validity criteria $\rho_0^{-1} d \ll 1$. As in the unscreened situation with DC enhanced case [10], here in-plane distances of the order of $a_{sc\,ex} = a_{ex} / 2$ are characteristic for the screened Coulomb problem. For that E_b takes the value 16 R_0 with $q_S \to 0$ instead of $4R_0$, where $R_0 \approx 0.34$ meV is the 3D exciton effective Rydberg.

In our model the Q2D charged (n- or p-type) channel contributes to the screening of the e-h pair. For that the Debye model 2D screening parameter q_S in the SQL limit is determined as [3, 9]

$$q_S = \frac{2}{a_{0e}} \left[1 - \exp\left(-\frac{\pi\hbar^2 n_S}{m_\perp k_B T}\right) \right], \qquad (5)$$

where $a_{0e} = \varepsilon_w \hbar^2 / m_\perp e^2$, $m_\perp$ is the electron effective mass.

After combining Exp. (5) with 2D screening radius expression $\rho_0 = \sqrt{d / 2q_S}$ both for the pure degenerate $(\pi\hbar^2 n_S / m_\perp k_B T >> 1)$ and pure non-degenerate $(\pi\hbar^2 n_S / m_\perp k_B T << 1)$ Q2D EG cases the Exp.(4) holding validity criteria would be established in the form

$$\begin{cases} a_{0e} >> 4d \dfrac{\pi n_S \hbar^2}{m_\perp k_B T} \\ a_{0e} >> 4d \end{cases}. \qquad (6)$$

With that, however, the n_S / T parameter's allowed ranges will be found numerically as well.

4. Numerical Calculation and Conclusions. As an illustration of offered model let now to carry out the Q2D screened exciton binding energy numerical calculations for InSb-based modulation-doped QW. In common these QW samples are grown on high dielectric constant-based substrates (large as InSb counterpart) such as $Al_xIn_{1-x}Sb$ and $Al_xGa_{1-x}As$ ternary materials [19].

InSb has the lightest effective mass $m_\perp = 0.014\ m_0$ and large dielectric constant $\varepsilon_w = 16.8$. By this reason free excitons are difficult to observe and do not appear as a decisive feature in bulk InSb samples due to the small exciton binding energy ($\sim 0.4 \div 0.5$ meV). As we will show next, in the model under discussion the screened Q2D exciton binding energy may substantially enhanced, which makes these systems an interesting nominee for excitonic device applications. The numerical data for the n_S/T parameter's permitted interval are shown in Table 1.

Table 1

The numerical data of n_S/T parameter's allowed interval for the QW fixed width values

d nm	1.5	3.0	5.0	10.0
n_S/T cm^{-2}/^{0}K	$10^6 \div 10^{12}$	$10^6 \div 4.10^8$	$10^6 \div 2.10^8$	$10^6 \div 10^8$

As follows, the density/temperature ratio parameter n_S/T allowed interval widening goes along with the decrease of the QW width d and this tendency keeps further tough as the QW becomes narrower. In particular, for the moderate thin QW case with d = 10nm and $n_S/T = 10^6 \div 10^8$ cm^{-2}/ ^{0}K the Q2D EG wholly behaves such as the nondegenerate gas. In turn, under d = 5nm QW width values the Q2D EG deviates from the pure nondegeneracy and demonstrates the fairly degenerate gas properties under strongly narrow QW cases (narrower than d ~ 20nm and $n_S/T > 1.5.10^9$ cm^{-2}/ ^{0}K).

Now let us display the Q2D screened exciton binding energy numerical calculations for the InSb-based QW system with 2D Debye – Hückel - type potential. In Fig.1 we plot the binding energy E_b dependence versus parameter n_S/T. Although E_b in our model approximation does not depend explicitly on QW width d , nevertheless, the correlation between the latter and n_S/T parameter specifically determines the validity criteria $\rho_0 >> d$ and, hence, the allowed ranges for the E_b as well. So, the latter implicitly depends from d in accordance with Table 1 results. On the graph the allowed ranges of n_S/T parameter for the fixed QW width d are marked by crosses.

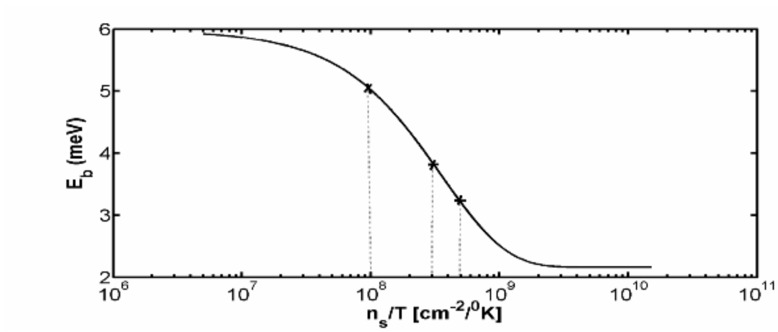

Fig. 1. The binding energy of the screened exciton E_b as the function of density / temperature ratio parameter n_S/T in the cases of QW width d=10nm ($10^6 \div 10^8$ cm^{-2}/ ^{0}K), d=5nm ($10^6 \div 2.10^8$ cm^{-2}/ ^{0}K), d=3nm ($10^6 \div 4.10^8$ cm^{-2}/ ^{0}K) and d=1.5nm ($10^6 \div 10^{12}$ cm^{-2}/ ^{0}K).

As follows from Fig.1, the screened exciton DC affected binding energy E_b is enhanced substantially in relation to bulk unscreened and DC absent result

($\sim 0.3 \div 0.4$ meV) for the n_S/T values less than 5.10^8 cm^{-2}/ ^{0}K and QW width values less than 5 nm. According to this, in the asymptotic n_S/T low limit range less than 4.10^6 cm^{-2}/ ^{0}K and for the aforementioned QW width values the unscreened DC enhanced $E_b \approx 16R_0$ result [9] is recovering.

In the transition region between moderate low (2.10^7 cm^{-2}/ ^{0}K) and high n_S/T values (4.10^8 cm^{-2}/ ^{0}K) for the nondegenerate Q2D EG case the screened binding energy E_b grows up sharply with decreasing of the indicated parameter and has enhanced more than twice for the QW width values less than 3nm. At n_S/T values larger than 10^9 cm^{-2}/ ^{0}K and QW width values less than $d = 2$ nm for the degenerate Q2D EG case E_b starts to saturate, but the remaining binding is still sizable (> 2 meV) and should permit for the observation of exciton-associated features in InSb-based QW's at low temperatures.

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Binding Energy of the One-Sided Dielectrically Enhanced Screened Exciton in Semiconductor Quantum Well

A formalism for the study of the two-dimensional screened exciton states in one-sided strong dielectric contrast affected ternary quantum well (QW) system modeled by the two-dimensional Debye-Hückel-type potential is presented. The numerical analysis depending on the specifics of InSb-based QW is provided. The appropriate density/temperature ratio parameter and QW width correlated ranges have been established for the variationally calculated two-dimensional screened exciton binding energy expression holds. The latter's strong enhancement (4÷6 meV) in relation to the unscreened exciton bulk value (0.3÷0.4meV) is received.

К. Г. Агаронян, Н. Б. Маргарян

Энергия связи экранированного экситона в полупроводниковой квантовой яме с односторонним диэлектрическим усилением

В модели двумерного дебай-хюккелевского потенциала взаимодействия в трехслойной квантовой яме представлен формализм для исследования экранированных экситонных состояний с учетом одностороннего сильного контраста диэлектрических постоянных. Проведены численные расчеты для структуры с квантовой ямой на базе InSb. Установлены соответствующие коррелированные промежутки для величин отношения двумерная плотность/температура и ширины квантовой ямы, при которых вычисленное вариационным методом выражение для энергии связи двумерного экранированного экситона имеет место. Получено строгое увеличение последней (4÷6 мэВ) по отношению к аналогичной величине (0.3÷0.4мэВ) для неэкранированного экситона в объемных образцах.

Կ. Հ. Ահարոնյան, Ն. Բ. Մարգարյան

Մեկկողմանի դիէլեկտրական ուժեղացմամբ էկրանավորված էքսիտոնի կապի էներգիան կիսահաղորդչային քվանտային փոսում

Երկչափ դեբայ-հյուկելյան բնույթի փոխազդեցության պոտենցիալի կիրառությամբ ներկայացված է եռաշերտ քվանտային փոսում երկչափ էկրանավորված էքսիտոնային վիճակների ուսումնասիրությունը՝ դիէլէկտրական հաստատունի մեկկողմանի կտրուկ թռիչքի հաշվառումով: Կատարված է թվային հաշվարկ՝ InSb-ի հենքով քվանտային քվազիերկչափ կառուցվածքի համար: Վեր են հանված երկչափ խտություն/ջերմաստիճան հարաբերության և քվանտային հորի լայնության արժեքների համապատասխան փոխկապակցված միջակայքերը, որոնց դեպքում երկչափ էկրանավորված էքսիտոնի՝ վարիացիոն սկզբունքով հաշված կապի էներգիայի արտահայտությունը տեղի ունի: Ստացված է վերջինիս մեծության էական աճ մինչև 4÷6 մէՎ՝ հոծ նմուշներում չէկրանավորված էքսիտոնի համապատասխան արժեքի (0.3÷0.4 մէՎ) նկատմամբ:

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