Screened Coulomb bound states in a finite confining potential semiconductor quantum well

K H Aharonyan

Physics Department, State Engineering University of Armenia, 105 Teryan Street, Yerevan 375009, Armenia

Abstract. The model to investigate the screened Coulomb interaction in realistic EuS/PbS/EuS finite confining potential quantum well is theoretically developed. A strong contrast of existing material parameters across the well interfaces and typical band-nonnparabolicity effect of lead salt semiconductor are taken into account while a variational approach has been used. In presence of inhomogeneous dielectric polarization a quasi two-dimensional screened Coulomb form factor analysis is carried out by using random phase approximation. Initial deviations from the inhomogeneous polarization absent case are established and in particular quantum well width dependent screened logarithical-type interaction potential is obtained. A screened binding energy has been investigated and an explicit logarithical-type expression is used for the first time. Depending on the realistic nanostructure specifics a monotonic decrease of the enhanced binding energy is received when in-plane carrier density/temperature ratio parameter increases.

1. Introduction

A great deal of attention to a quasi-two-dimensional (Q2D) electron gas (EG) in a variety of semiconductor nanosystems (quantum wells (QW), double heterojunction structures (DHS), superlattices) is caused both by fabrication advances and purely scientific interest as well as by realization of these structures for the optoelectronic needs [1]. Carriers in a Q2D EG, that could be generated optically by intense illumination or by modulation doping, are confined within an active semiconductor layer with compressed wave functions (quantum confinement (QC)) and characterized by continuously varying carrier density probability distribution in the QW growth direction [2,3]. In these structures the advanced selective doping makes possible to investigate a charged electron (hole) system rather than by a neutral electron-hole plasma, as in the 3D samples [4]. The filling of the QW by free charge carriers results to the changes of the Q2D optical properties [5-8], which are caused by many-body effects such as a screening of the carriers Coulomb interaction. The way that the free carriers screen the bare Coulomb potential depends on the dimensionality of the system. In 3D bulk samples the screened potential decays exponentially in a real space and effectively becomes a short-range potential.

Conversely, in pure 2D system the real–space statically screened potential in long-wavelength limit is

\[ V_s(\rho) = -\left(\frac{e^2}{\varepsilon_w}\right)\left[\rho^{-1} - q_S \int_0^\infty dq J_0(q\rho)(q + q_S)\right]. \]  

(1)
In Eq. (1) $J_0(x)$ is the Bessel function, $\rho(x,y)$ is the in-plane 2D distance between the charges, $\varepsilon_w$ is the QW material static dielectric constant, $q_5$ is the 2D screening parameter [5] and $q$ is the 2D in-plane wave vector. The screened potential falls off in accordance with 2D pure Coulomb law at intermediate distances and then decays by power law at large distances [9-11]. There is no screening length in 2D system. Thus, the 2D screening effects decrease because the free carriers can only screen the Coulomb field between any two charges of the 2D system, whereas the part of the field extending outside the confinement region remains unscreened. So the field lines that abandon the system are not directly affected by those charges. Note, that the screening parameter dependence from the free carrier density is different in 2D and 3D cases [2,10]. The screening parameter is saturated for small temperature or large carrier density $n_5$ in a 2D EG (due to the constant density of states), while being continued to increase with volume density $n_v$ in a 3D EG. As a result of the 2D screening saturation a Coulomb center cannot be screened out at any 2D carrier density.

The realistic QW has a nonzero width $d$ and usually holds finite confining barrier potential height. A theoretical study of screened Q2D Coulomb interaction with arbitrary dielectric constants of the QW and barrier ($\varepsilon_w, \varepsilon_b$) have been started in the works of Ritova (Refs. 9, 10) by using diagram technique and Thomas-Fermi approximation (TFA), respectively. In Ref. 10 the author discussed the all possible relations between $\varepsilon_w$ and $\varepsilon_b$ ($\varepsilon_w \neq \varepsilon_b, \varepsilon_w - \varepsilon_b$). In particular, for the strong contrast relation case such as $\varepsilon_r = \varepsilon_w / \varepsilon_b >> 1$ (dielectric confinement (DC)), the statically screened Q2D potential has been established for the distances $\rho >> d$ (the long-wavelength limit) in the form

$$V_s(\rho) = -(2e^2 / \varepsilon_w d) K_0( \sqrt{2q_5 / d\rho} ),$$

(2)

where $K_0$ is the modified Bessel function of the second kind. Eq. (2) both qualitatively and quantitatively differs from the widely discussed pure 2D potential function (1). The latter corresponds to the weak or negligible DC and is independent from the QW width. Screened potential strongly depends on the QW width and exponentially decays for large in-plane distances outside the circle with the radius of $\rho_0 = (d / 2q_5)^{1/2}$. Hence, DC leads to the recovering of Q2D screening length. On the other hand, because of asymptotic behavior of $K_0(x)$ function for intermediate in-plane distances $d < \rho < \rho_0$, the Q2D potential function (2) becomes pure logarithmically spatially dependent and increases when QW width decreases. Thus, in this case the hydrogen-like properties of the Coulomb Q2D screened centers would be strongly enhanced compared with the systems where the DC is insufficient. This is confirmed by recent results which have been reported with logarithmical potential in EuS/PbS/EuS QW, where an effective enhancement of Coulomb unscreened bound states is revealed due to the DC [12, 13]. The purpose of present work is the study of screened Coulomb hydrogen-like bound states in the realistic EuS/PbS/EuS QW system. This is done in view of the finite height of the potential barrier and with strong material parameter contrast in the QW heteroboundaries (MPCH), namely the dielectric constants and effective mass.

2. Theoretical framework and model

Bound states of the screened Coulomb center influenced by spatial QW confinement have been the subject of intense investigations in the past time. The experiments in this field are based on the III-V group semiconductors [4, 14-16]. From standpoint of the theoretical interest the various calculation techniques within the effective-mass approximation (EMA) are performed. The binding energy studies
for both infinite and finite confining potential QW models are carried out by perturbation theory [17, 18], numerical resolution [19] and variational procedure [2, 3, 21-25]. In this field the most studied systems are GaAs/Al\(_{1-x}\)Ga\(_x\)As, Si/SiO\(_2\) DHS structures concerning to the cases of the screened impurities [2, 3, 20, 22] and excitons [17-19, 21, 23-25] by use of the random phase approximation (RPA) and TFA. All this binding energy issues refer to the situation, when the dielectric constants difference between QW and barrier (\(\varepsilon_w\), \(\varepsilon_b\)) is small or neglected. For the case of \(\varepsilon_w \gg \varepsilon_b\) the interaction turns out to be significantly larger [10] and the hydrogen-like center binding energy would greatly enhanced with decreasing of well width [26, 27]. Due to the large \(\varepsilon_w\) of the material that especially would take place in the lead salt based QW’s [12, 13]. Narrow-direct gap lead salt solid semiconductor solutions are very well lattice-matched materials with the europium salts (0.5 %) and can be epitaxially grown with the high quality in a controlled way. They possess a multivalley band structure with nearly mirror valence (v) and conduction (c) strong nonparabolic bands (NPB). There is no heavy hole band in the NaCl structure. Electrons and holes have small and almost the same effective masses \(m_w\). Due to the large dielectric constant the bound states in the bulk sample have tiny binding energies. In the europium salts (as a wide gap barrier material) the Bohr radius is smaller than the lattice parameter (for EuS material it is estimated to be about 0.25 nm with dielectric constant \(\varepsilon_b = 5\) and effective mass \(m_b = m_0\) [12]). Therefore in EuS/PbS/EuS DHS screened hydrogen-like bound states could enhance strongly with the DC. Firstly, it would concern to the binding energy in the long wave limit. The model for the Q2D EG embedded in a QW is based on the nearly rectangular band alignment with the finite c-band offset \(\Delta_c\). The Hamiltonian of Coulomb center in QW is

\[
\hat{H} = H_{kin} + H_{eff} + V_S, \tag{3}
\]

where \(H_{eff} = V_{fin}(z) + V_{self-im}(z)\) - is the unperturbed part and \(V_S\) is the screened Coulomb potential. \(V_{fin} = 0\) when \(0 < z < d\) and \(V_{fin} = \Delta_c\) when \(z \leq 0, z \geq d\), \(V_{self-im}\) is the one-electron self-image interaction potential, which, as well as the size-quantized potential, modifies one-particle states. This contribution has the same order as the quasiparticle binding energy [12, 13]. Since EuS/PbS/EuS QW system band offsets \(\Delta_c = 1.2\) eV (0.15 eV) [12]) are much larger than the ground state binding energies. In this case the self-image interaction changes the rectangular localizing potential into the smoothly shaped potential. Then a confinement feature does not change distinctly when the perturbing potential varies smoothly on the scale of \(k_f^{-1}\) (\(k_f = \sqrt{2\pi n_s}\) is the 2D Fermi vector) and is so weak, that can be treated in a first-order perturbation theory [2]. In doped QW’s the presence of both free carriers and charged impurities induces band bending [3]. We restrict ourselves to the n-type QW with the electrons occupying only states in the first \(\varepsilon_0^0\) subband (electric size quantum limit (SQL)). Within the accepted approximation the band bending could be treated perturbatively for thin QW’s which leaves eigenfunctions unchanged but shifts \(\varepsilon_0^0\). In present paper we are interested in this eigenfunctions and consider the finite rectangular symmetrical model. Our study involve two steps: 1. calculation of the screened Coulomb potential using RPA in presence of the MPCH, 2. carrying out the Coulomb impurity binding energy’s variational calculation in EuS/PbS/EuS QW with the nondegenerate Q2D EG.
3. The Screened Potential and the Binding Energy

Following to the strong confinement regime \( a_0 \gg d \), the distance between quantized energy levels is larger than interaction energy. Thus the appropriate ground state wave function has a separable form such as \( \phi = \phi(\rho, z) = \psi(\rho) \varphi(z) \). Here \( \psi(\rho) \) is an in-plane wave function and \( \varphi(z) \) is an one-particle 1D Schrödinger-like equation EMA solution along z axis. Because of strong confinement regime, such as in Refs. [12, 13], a long wave limit is used here. For the latter case there are effective wave vectors \( q < d^{-1} \) measured from the L point, wave function spatial change is determined by \( d \). In the variational calculations the functional \( E[\phi] = \int \phi^* [H_{kin} + H_{eff} + V_S] \phi dV \) is elaborated. So we have to determine the average value of the screened potential \( V_S \) over \( (\varphi(z))^2 \), which we will deal using RPA method. For the latter the Fourier expanded screened Coulomb interaction potential \( V_S(q, z) \) is related to the bare potential Fourier component \( V(q, z) \) as \( V_S(q, z) = V(q, z) / \varepsilon^{Q2D}_{\text{finite}}(q) \). Here \( \varepsilon^{Q2D}_{\text{finite}}(q) \) is the Q2D EG dielectric function and has the form [28]

\[
\varepsilon^{Q2D}_{\text{finite}}(\omega, q) = 1 - \frac{2 \pi^2}{|S q|} \cdot \gamma \cdot F_z(q).
\] (4)

In Eq. (4) \( \gamma \) is the irreducible polarizability of 2D EG, \( F_z(q) \) is the Coulomb form factor which takes into account the deviation from the pure two-dimensionality, \( S \) is the interface area. As follows from Eq. (4), only the wave vector dependent dielectric function of the Q2D EG and averages of bare potential \( V(q, z) \) over \( (\varphi(z))^2 \) are required. We have calculated the quantities \( \varepsilon^{Q2D}_{\text{finite}}(q) \) and \( <V_S(q)> \) in the recent works [13, 28]. In this case the lowest eigenfunction \( \varphi(z) \) used for the square-well potential is

\[
\varphi_w = N \cos(k_w z), \quad \varphi_0 = B \exp(-k_w z) \quad \text{with} \quad k_w = \sqrt{2m_w e_c^e / \hbar^2}, \quad k_\lambda = \sqrt{2m_{\lambda} (\Delta - e_c^e) / \hbar^2},
\] (5)

where \( N = (2/d)^{1/2} N_{F_{\lambda}}^{-1} \), \( N_{F_k} = 1 + (2 f / \sqrt{g} d) \), \( f = 1 + \alpha n_i (k_b / k_w)^2 \), \( g = 1 + (\alpha n_i k_b / k_w)^2 \), \( B = N / \sqrt{g} \). The subband energies have the form of the dispersion equation

\[
tg (k_w d / 2) = \alpha n_i k \lambda / k_w,
\]

where \( \alpha = (m_i / m_b) \), \( m_w = m_i n_i \), \( m_i \) is the longitudinal effective mass, \( n_i = \sqrt{1 + \left( 2 \hbar k_w^2 \right)^2 / m_i^0 E_g^w} \) is the NPB term. To take into account the latter we have used “energy-dependent effective mass” approach [29, 13].

In Ref. 28 using the self-consistent field approach or RPA in presence of the MPCH we revealed the Coulomb form factor implicit expression in the long - wavelength limit \( q < d^{-1} \). With the inequality \( k_w > k \) (\( k^{-1}, k_w^{-1} \) are the typical spatial changes of the potential energy’s Fourier-component and wave function in z direction, respectively) it gives the condition \( k_w d \sim 1 \) and form factor takes \( F_z(q) = 2/\left[ q d + (2/\varepsilon_i) \right] \) form. With this and for the static limit of irreducible polarization \( \gamma \) [22], the Eq. (4) finally goes to the expression

\[
\varepsilon^{Q2D}_{\text{finite}}(q) = 1 + \frac{2 q_S}{q (q d + (2/\varepsilon_i))}.
\] (7)

Recently [13], we have evaluated the averaged bare image potential-mediated interaction energy operator matrix element \( <\alpha|V(q)|\alpha> \). And according to Ref. [28] we get the Q2D form factor
expressing a deviation from the two-dimensionality with the MPCH for the finite confining barrier potential as \( F_C(q) = \{4N^2/(kq + 2\varepsilon_r^{-1})\}[(2k_b + q)\gamma + (d/4) + (\alpha_n, k_b)/2k_w^2] \). Now if combining Eq. (7) with the \( F_C(q) \) for the screened potential averaged value we have

\[
<V_S(q)> = \frac{4\pi \varepsilon^2}{\varepsilon_w} \frac{1}{q [1 + (2q_0/q)(q - d/\varepsilon_w)]} \frac{4N^2}{q d + 2\varepsilon_r^{-1}} \left( \frac{g^{-1}}{2k_b + q} + \frac{d}{4} + \frac{\alpha_n, k_b}{2k_w^2} \right).
\]  

(8)

Eq. (8) for the 2D vectors \( q \ll 2k_b \) is identical to the analogous result of Ref. 10 received by usage of TFA and this is quite expected because in long-wavelength limit the RPA and TFA coincide. In that case Eq. (8) goes to the following form

\[
<V_S(q)> = -(4\pi \varepsilon^2/\varepsilon_w) [q + (2/\varepsilon_w, d)] + (2q_0/d)]^{-1}.
\]  

(9)

In view of the long wave ( \( q d \ll 1 \) ) and the DC \( (\varepsilon_r^{-1} \ll 1) \) conditions there are two distinct 2D wave vector ranges, such as \( k_b d > k_w d > 1 > k d \gg 2\varepsilon_r^{-1} \) and \( k_b d > k_w d > 1 > 2\varepsilon_r^{-1} \gg kd \), hence Eq. (8), (9) possesses the following analytical features:

(i) For the moderate small wave vectors with \( k_b d > k_w d > 1 > k d \gg 2\varepsilon_r^{-1} \):

\[
<V_S(q)> = -(4\pi \varepsilon^2/\varepsilon_w) [q + (2/\varepsilon_w, d)]^{-1}.
\]  

(10)

(ii) For the small enough wave vectors with \( k_b d > k_w d > 1 >> 2\varepsilon_r^{-1} \gg kd \):

\[
<V_S(q)> = -(4\pi \varepsilon^2/\varepsilon_w)(q + \varepsilon_2 q_0)^{-1}.
\]  

(11)

Note, that when neglecting the linear term in denominator of Eq. (9), the condition \( 2q_0 d >> \varepsilon_r^{-2} \) have been used. Only in the case of moderate long wave related wave vectors Eq. (10) leads to the potential function from Eq. (2). Using \( K_0(x) \) Bessel function properties for the screened potential it can be written

\[
V_S(\rho) = \begin{cases} 
-\left(2\varepsilon^2/\varepsilon_w\right)\frac{1}{\sqrt{\rho_0/2\rho}} \exp\left(-\rho/\rho_0\right), & \rho > \rho_0, \quad a) \\\n-\left(2\varepsilon^2/\varepsilon_w\right)\left[\ln\left(\sqrt{\rho_0/2\rho} + \gamma\right)\right], & \rho_0 > \rho >> d, \quad b) 
\end{cases}
\]  

(12)

According to the Eq. (12a) the screening potential exponentially decays outside the circle with the radius \( \rho_0 = (d/2q_0)^{1/2} \) and a strong DC effect leads to the recovering of Q2D screening length [10]. At the same time, as shown in Eq. (12b), for the intermediate in-plane distances such as \( d < \rho < \rho_0 \) due to the DC Q2D screened potential function becomes logarithmically spatially dependent, deviates particularly from the pure 2D as well as 3D forms, and increases with decreasing of the \( d \). The latter enhancement of screened potential is quite natural, because the DC overbalances in relation of screening effect. In Eq. (11) the revealed new features of the screened potential with DC are the followings: a) a screened potential’s Fourier-image (therefore real–space statically screened potential) is more enhanced because instead of large QW dielectric constant it only depends on the barrier small analogous, b) the appropriate real–space statically screened potential with \( <V_S(q)> \) repeats the spatial dependence (1) only at very long wave related wave vectors, c) from Eq. (11) follows, that the screening length at very long wave related wave vectors depends from the dielectric contrast between the QW and barrier.

In this paper we are interested in the screened potential from Eq. (12b). For the ground 1s bound state level we choose normalized one parameter trial wave function in the form \( \psi(\rho) = \sqrt{2/\pi} (\lambda e^{-\rho}) \).
and minimize the functional versus the variational parameter $\lambda$. The binding energy $E_b^S$ is obtained as the difference of the first subband energy $\epsilon_i^0$ and expectation energy $E_i$. For the 2D kinetic energy operator’s matrix element from [13] $K(\lambda) = \hbar^2 \lambda^2 m_r^2 / 2m_1$, where $m_r = \alpha_e n_i, \gamma_r$ is the effective mass renormalization term with $\gamma = [2(1 + (k_b / k_w)^2) + g_{k_d}d / \alpha n_i] / (2f + g_{k_d}d)$.

The screened interaction energy operator matrix element with Eq. (12b) is

$$V_S(\lambda) = -(2e^2 / \epsilon_w d) \int \left[ \ln \left( \rho / 2 \rho_0 \right) + \gamma \right] |\psi(\rho)|^2 d\rho,$$

(13)

Finally, for the Coulomb center ground state screened binding energy in finite confining QW we have

$$E_b^S(d) = -(e^2 / \epsilon_w d) \left[ \ln \left( 16n_i / a_0 q_S m_{r\Lambda} \right) - 3 \right],$$

(14)

$m_{r\Lambda} = m_r - 4n_i \Lambda (d / a_0), \ \Lambda = k_b d (2 - g) / (k_w d)^2 (2f + g_{k_d}d)$. As follows, with decreasing of the QW width the screened binding energy mainly grows in terms of $E_b^S \sim d^{-1}$, which differs from the corresponding dependence $E_b \sim d^{-2} \ln d$ for the unscreened case with the DC effect [12,13].

Note that the dependence of $E_b^S(d)$ is much more complex, because the quantities $n_e$ and $m_{r\Lambda}$ weakly depend on QW width. The relevance of the Eq. (14) firstly depends on the feasibility of the condition $d << \rho < \rho_0$ and for that from an extra condition an under logarithm term holds. The latter is related to the abovementioned condition $2q_S d >> \epsilon_r^{-2}$. If combining both conditions we get $d^{-1} >> q_S >> \epsilon_r^{-2} d^{-1}$, which determines allowed interval for the key parameter $n_S / T$. In this work we pay an attention to the case of nondegenerate EG. For that the high temperatures and low densities are required and strong condition $m_w k_B T / \pi n_S h^2 >> 1$ is held. For this case the screening parameter expression in SQL $q_S = (2 / a_0) [1 - \exp(-\pi h^2 n_S / m_w k_B T)]$ [5] goes to $q_S = 4\pi n_S e^2 / \epsilon_w k_B T$ and eventually with the allowed interval condition leads to the relation as

$$\epsilon_w k_B / 8\pi e^2 d >> n_S / T >> \epsilon_w k_B / 8\pi e^2 d \epsilon_r^{-2}.$$

(15)

Now let’s carry out the Q2D screened binding energy on-center donor numerical calculations for EuS/PbS/EuS realistic DHS to illustrate the offered theoretical model.

Table 1. The numerical results of one-particle parameters in EuS/PbS/EuS SQW for c-band offset.

| $d$ (nm) | $k_+^s d$ | $k_-^s d$ | $f_\epsilon$ | $g_\epsilon$ | $n_e$ | $m_{r\Lambda}$ |
|----------|------------|------------|--------------|--------------|------|--------------|
| 1.5      | 1.83       | 8.21       | 6.82         | 2.68         | 2.74 | 0.96         |
| 5        | 2.17       | 29.13      | 26.41        | 4.61         | 1.35 | 0.98         |

In Table 1 numerical results of the one-particle electron state parameters are given (with the parameter ratios $\epsilon_r=34, \alpha_r = 0.105$) for the strongly nonparabolic c-band offset case (1.2eV). The model is solved for PbS QW grown with [111] orientation, where the four valleys are split into the one longitudinal and three equivalent oblique ones [29]. For PbS sample they are characterized by longitudinal (along [111]) and transversal (normal to [111]) band edge effective masses respectively: $m_+^* = 0.105 m_0, \ m_-^* = 0.08 m_0$ ($m_0$ is the free electron mass). For bulk PbS sample a static dielectric
constant value is $\varepsilon_w = 170$ with impurity Bohr radius $a_0 \approx 102.5 \text{nm}$. At this moment let’s display on-center donor binding energy numerical result (Eq. (14)) in presence of nondegenerate EG.

**Fig. 1.** The binding energy of the screened donor impurity as a function of the ratio $n_s / T$ in EuS / PbS / EuS DHS. The top (low) curve corresponds to the QW width 1.5 nm (5 nm) calculation result.

In Fig. (1) the binding energy dependence versus $n_s / T$ parameter is plotted for the QW width values $d = 1.5 \text{ nm}$ and $d = 5 \text{ nm}$, respectively. The top (low) curve in the graph corresponds to the $d = 1.5 \text{ nm}$ (5 nm) calculation result. As follows from the graph the enhanced screened binding energy logarithmic dependence for the nondegenerate EG extends approximately two decades with the ratio of $n_s / T$ (Eq. (15)). Except that the characteristic curve decreases almost linearly with increasing of $n_s / T$. As shown in Fig. 1, an influence of DC on the screening in the EuS/PbS/EuS QW is appreciably for thin enough QW’s in accordance with Eq. (14).

8. **Conclusions**

The theoretical study of screened Coulomb interaction in realistic EuS/PbS/EuS finite confining potential QW is carried out in the presence of QW and barrier material parameter’s strong contrast across the heteroboundaries. A characteristic band-nonparabolicity effect of the lead salt semiconductor material is taken into account. In the presence of inhomogeneous dielectric polarization of the QW system Q2D screened Coulomb form factor is evaluated using a random phase approximation. The enhanced 2D Coulomb-type (Eq. (11)) and logarithmic-type (Eq. (12 b)) screened Q2D potentials are revealed for the first time. A screened binding energy problem has been investigated variationally and an analytical logarithmic-type result is used for the first time. Depending of realistic EuS/PbS/EuS QW specifics, the numerical analysis is provided. A very strong enhancement of the binding energy $E_b^S (d)$ in relation to tiny unscreened bulk value (~ 0.1 meV) is received especially for the small QW widths. As follows, the screened binding energy decreases monotonically with increasing of parameter
\(n_s/T\) for the nondegenerate Q2D electron gas. The results indicate to the favorable conditions for detecting of screened Coulomb bound states in EuS/PbS/EuS finite confining potential QW system.

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