

## Two Dimensional Coulomb Potential of Confined Excitons in Quantum Well Structures

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In this study, we have investigated an exciton confined in a single quantum well. For the first time, we have compared the different methods of approximating the effective two dimensional Coulomb potentials which had been previously reported in the literatures. The effect of different previously introduced trial wave functions on the exciton binding energy is also investigated. In order to have a consistent and stable calculation we have tried to find the true region of variations for free parameters of these trial wave functions. Effects of the barrier thickness and doping fraction are also investigated.

**Keywords:** Trial wave functions, Two dimensional Coulomb potentials, Exciton binding energy, Barrier thickness effect, Doping fraction effect.

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### 1. INTRODUCTION

A better understanding of the electrons and holes behavior in semiconductor materials leads to a deep insight into the physics of the problem. In the nanostructure systems these behaviors become more interesting and this is due to some special characteristics like quantum confinement effect. For example, the effect of quantum confinement effect on exciton behaviors have been also studied vastly during last years [1-2] and thus much experimental [3-4] and theoretical [5-7] works have been devoted to the quantitative understanding of the physical properties of a single quantum well structure especially in GaAs based ones.

During last decades, different excitonic properties of the nanostructures such as optical properties [8], magnetic properties [9], and density of states [10], exciton generation rate [11], exciton recombination [12], and transport properties [13] have been extensively studied. The theoretical studies of confined exciton in quantum well structures are usually done with exact diagonalization [14], self-consistent approach [15], Quantum Monte Carlo [16], and variational method [17-18]. Among these methods, variational technique is a pretty simple one which its computer implementation is not so difficult.

In this study we have used a variational method with some trial wave functions. Then the binding energy of an exciton confined in a GaAs<sub>(1-x)</sub>Al<sub>x</sub> / GaAs single quantum well (0 < x < 0.35) is calculated. We have also compared different approximation types of the effective two dimensional Coulomb potential of a confined exciton. Finally we have investigated the effect of different existing trial wavefunctions on the exciton binding energy. To find a reliable approach, we have varied their free parameters in different regions of variation and find the exciton binding energy. By comparing our results with previously obtained ones we have tried to find the right free parameters.

### 2. THEORY

An exciton confined in a single quantum well structure obeys the Hamiltonian of the Senger et al. [19]. In the cylindrical coordinate we have,

$$H = -\frac{\hbar^2}{2m_{e,h}} \frac{\partial^2}{\partial z_{e,h}^2} + V_{e,h}(z_{e,h}) + \frac{\hbar^2}{2\mu} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{e^2}{\epsilon_0 \sqrt{\rho^2 + (z_e - z_h)^2}} \quad (1)$$

where  $\frac{1}{\mu_{\pm}} = \frac{1}{m_e} + \frac{(\gamma_1 \pm \gamma_2)}{m_0}$  is the reduced mass corresponding to the heavy (+) and light hole (-),

$m_{h\pm}^z = \frac{m_0}{\gamma_1 \mp 2\gamma_2}$ ,  $m_h^{\pm} = \frac{m_0}{\gamma_1 + \gamma_2}$  are the heavy hole effective mass along the z direction and in the plane perpendicular to it [20],  $\rho = \rho_e - \rho_h$  is the relative coordinate and  $\gamma_1$  and  $\gamma_2$  are the Kohn-Luttinger band parameters which are the same as those of used in work of Senger et al. These parameters are taken from Ref [21].

The variables corresponding to different degrees of freedom are not analytically separable thus direct solution of the equation (1) is not simple. Therefore different approaches have been devised during last decades which include Fourier series expansion [22] and mapping onto an equation along a distinct direction.

The first way for separation of variables is to take the averaged two dimensional Coulomb potential as [23-24]:

$$V(\rho) = -\frac{e^2}{\kappa} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dz_e dz_h \frac{f_e^2(z_e) f_h^2(z_h)}{\sqrt{\rho^2 + (z_e - z_h)^2}} \quad (2)$$

Then the equation 1 can be separated along  $\rho$ ,  $z_e$  and  $z_h$  as:

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$$\left\{ -\frac{\hbar^2}{2\mu} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + V(\rho) - E_b \right\} \psi_{e-h}(\rho) = 0 \quad (3)$$

$$\left\{ -\frac{\hbar^2}{2m_{e,h}} \frac{\partial^2}{\partial z_{e,h}^2} + V_{e,h}(z_{e,h}) - E_{e,h} \right\} f_{e,h}(z_{e,h}) = 0 \quad (4)$$

Where  $f_{e,h}(z_{e,h})$  are some envelop functions,  $E_b$  is the exciton binding energy and  $E_{e,h}$  are the subband energies of the electrons and holes.

Introducing a form factor  $F(\rho)$  as follows is a second way to study the nature of an exciton confined in a quantum well [25]:

$$F(\rho) = \frac{1}{\pi} \int_{-\infty}^{\infty} du K_0(u) \int dz_e e^{iuz_e/\rho} |f_e(z_e)|^2 \int dz_h e^{iuz_h/\rho} |f_h(z_h)|^2 \quad (5)$$

Where  $K_0$  is the modified Bessel function. Now we have two dimensional Coulomb potential as:

$$V(\rho) = -\frac{e^2}{\kappa\rho} F(\rho) \quad (6)$$

Third way for separation of variable is the mapping of the three dimensional Coulomb potential onto an effective two dimensional Coulomb interaction along the  $\rho$  direction by introducing of a variational parameter  $\eta$ . In this approach the Coulomb potential term in equation (1) can be defined as [26]:

$$V(\rho) = \frac{e^2}{\epsilon_0 \sqrt{\rho^2 + (z_e - z_h)^2}} = \frac{e^2}{\epsilon_0} \frac{\eta}{\rho} \quad (7)$$

Then in the first order approximation  $\eta$  can be obtained from [26]:

$$\eta \left\langle \frac{1}{\rho} \right\rangle = \left\langle \frac{1}{\sqrt{\rho^2 + (z_e - z_h)^2}} \right\rangle \quad (8)$$

By having  $\eta$  the average of two dimensional Coulomb potential can be determined. In the fourth way the Coulomb potential can be approximated by [27]:

$$V(\rho) = \frac{e^2}{\epsilon_0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{f_e^2(z_e) f_h^2(z_h)}{\sqrt{\rho^2 + (z_e - z_h)^2}} dz_e dz_h = \frac{e^2}{\epsilon_0} \frac{1 - e^{-\gamma_x \rho}}{\rho} \quad (9)$$

Where  $\gamma_x^{-1}$  is a measure of the well width. In order to find the value of  $\gamma_x$  we have calculated the expectation value of the both sides of the equation (9):

$$\begin{aligned} \langle V(\rho) \rangle_\rho &= \frac{e^2}{\epsilon_0} \int_0^\infty \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{f_e^2(z_e) f_h^2(z_h)}{\sqrt{\rho^2 + (z_e - z_h)^2}} dz_e dz_h d\rho = \\ &= \frac{e^2}{\epsilon_0} \left\langle \frac{1 - e^{-\gamma_x \rho}}{\rho} \right\rangle_\rho \end{aligned} \quad (10)$$

Then we have changed the value of  $\gamma_x$  until this equation is satisfied.

This effective potential definition technique has been used previously for other excitonic systems like biexcitons in quantum wells [28]. This is because of some advantages, for example using equations (6), (7), or (9) instead of the real three dimensional Coulomb interaction given in equation (1) has the following bene-

fits. Firstly, it separates the Hamiltonian into some one dimensional Schrödinger equation and solution of one dimensional problems is less time consuming. Secondly, it leads to a more stable programming. Thirdly, a qualitative intuition of the two dimensional Coulomb interaction behavior related to an exciton confined in a quantum well will be revealed.

There are different methods in order to extract the variational parameters of the trial wave functions or to find the  $E_0$  by using equation (16). Differentiation with respect to the variational parameters and equating to zero is a way for this purpose. Plotting the energy as a function of the variational parameters in a multidimensional space [29] or using stochastic methods like Monte Carlo [30] and genetic algorithms [31] are other methods which may be used. In this work we have used Monte Carlo schema.

### 3. VARIATIONAL METHOD

Selecting an appropriate trial wave function with regard to the geometry and typical characteristics of the model system is the main step in the variational scheme. Although there are some attempts to compare different types of trial wave functions for a confined exciton in a quantum well [32-33] but there is not a comprehensive study in this area. In the literatures there are plenty of different types of these functions for a confined exciton in quantum wells. The most frequently used trial wave function has been used by Senger et al. [19]:

$$\begin{aligned} \psi(\vec{r}_e, \vec{r}_h) &= \\ &= f_e(z_e) f_h(z_h) e^{-\lambda \sqrt{\rho^2 + a^2(z_e - z_h)^2}} \times e^{-b^2 \rho^2} \end{aligned} \quad (12)$$

where  $\lambda$ ,  $a$  and  $b$  are the free parameters of this trial wave function and  $f_i(z_i=e,h)$  are the envelop functions which reads:

$$f_{e,h}(z_{e,h}) = \begin{cases} \cos(k_{e,h} z_{e,h}), & |z_{e,h}| < L/2 \\ A_{e,h} e^{-K_{e,h} |z_{e,h}|}, & |z_{e,h}| > L/2 \end{cases} \quad (13)$$

where  $e$  and  $h$  indicate the electron and hole.  $\lambda$ ,  $a$  and  $b$  are the free parameters of this trial wave function. Another form of the trial wave function has the following form [34-35]:

$$\psi(\vec{r}_e, \vec{r}_h) = f_e(z_e) f_h(z_h) e^{-\lambda \sqrt{\rho^2 + a(z_e - z_h)^2}} \quad (14)$$

The other form of the trial wave function reads [36-37]:

$$\psi_0(\rho) = e^{-\lambda \rho} \quad (15)$$

which contains no dependence on  $|z_e - z_h|$ . The variational parameter  $\lambda$  gives the exciton radius when the system energy is minimized [38].

Then the ground state energy can be found by the minimization of:

$$E_0 = \text{Min}_{a,b,\lambda} \langle \psi | H | \psi \rangle \quad (16)$$

Some other shapes of this trial wave function may be found in the Refs [39-41].

#### 4. RESULTS AND DISCUSSION

The exciton binding energy is written as  $E_b = E_g + E_e + E_h - E_{ex}$  where  $E_g$ ,  $E_e$  and  $E_h$  are energy gap and subband energies respectively.  $E_{ex}$  is defined as the energy eigenvalue of the Hamiltonian in equation (1). The subband energies may found by numerical solution of the equations (4) or by using these equations:

$$\begin{aligned} \left[ \frac{E_e}{V_e} \right]^{1/2} &= \cos \left[ \left[ \frac{m_e E_e}{2\hbar^2} \right]^{1/2} L \right], \\ \left[ \frac{E_h}{V_h} \right]^{1/2} &= \cos \left[ \left[ \frac{m_h E_h}{2\hbar^2} \right]^{1/2} L \right] \end{aligned} \quad (19)$$

These equations can be solved by bisection method [42]. Another way to find  $E_b$  is to solve equation (3) directly. If a perturbation like an electric field (e.g. along the growth direction) also apply on the system we are not able to use equations (19) for calculating  $E_e$  and  $E_h$ . In this case we have to perform other numerical methods such as finite difference schema. Here we have used equation (19) in order to find  $E_e$  and  $E_h$  as a function of the well width.

In order to include the effect of the effective mass mismatch in the well and barrier we have used the Ben-Daniel-Duke boundary condition [43]. The effective mass of the electron and hole in the well has also been obtained by the Vegard law [44].

We have used the material parameters as follows [45]. The total energy band gap difference  $\Delta E_g(x)$  between GaAs and  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  is  $\Delta E_g = 1.155x + 0.37x^2$  (eV). If we show the conduction and valance band offsets as of  $v_e^0$  and  $v_h^0$  respectively then we have  $v_e^0 = AE_g \times C$  and  $v_h^0 = AE_g \times (1 - C)$  where  $C$  a positive value.

Now we have used some trial wave functions and tried to find the exciton binding energy by means of the equation (3). We have firstly used the equations (7) and (8) in order to find  $\eta$  and then put it in the equation (3) to find the exciton binding energy. Variations of  $\eta$  and the exciton binding energy as a function of the well width have been shown in the Fig. 1 and 2 respectively. Fig. 1 shows a non-monotonic behavior for the two dimensional Coulomb interaction  $\eta$ . It reveals that the natures of the two dimensional Coulomb interaction along the  $\rho$  direction ( $\rho^2 = x^2 + y^2$ ) is not the same as for three dimensional Coulomb interaction along the  $r$  direction ( $r^2 = x^2 + y^2 + z^2$ ). We have calculated the exciton binding energy by using of the equations (12), (14), (15). The results have been shown in the fig (2). For comparison we have also plotted the exciton binding energy taken from the Ref [20-21]. As the figure shows if we use equation (15) or equation (14) as the trial wave function with  $a \in [0,1]$  &  $\lambda \in [0,10^8]$  the consistency between our calculated exciton binding energy and the results of the other groups have shown in the Ref [20-21] is not good. When we apply equation (14) with  $a \in [0,10^4]$  &  $\lambda \in [0,10^4]$  or equation (12) with  $a, b, \lambda \in [0,10^3]$  there is better agreement with the Refs [20-21]. In this calculation we have used smaller upper bound for the free parameters  $a$ ,  $b$ ,  $\lambda$ . If we choose two

or three of these parameters in a larger interval, e.g.  $a, b, \lambda \in [0,10^8]$ , this always leads to a zero trial wave function. In this case the probability of finding the electron and hole in all the space become zero.

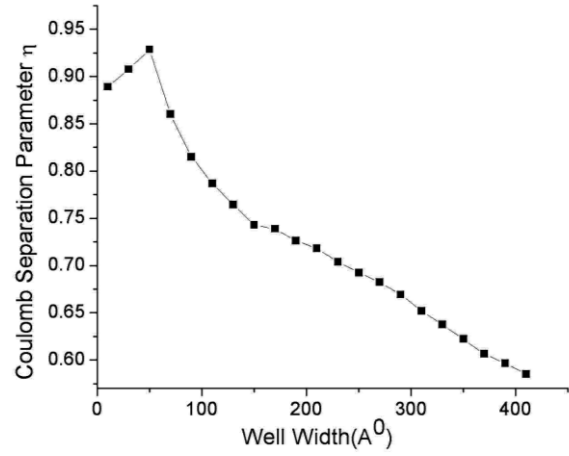


Fig. 1 – Variation of the Coulomb separation parameter  $\eta$  as a function of well width

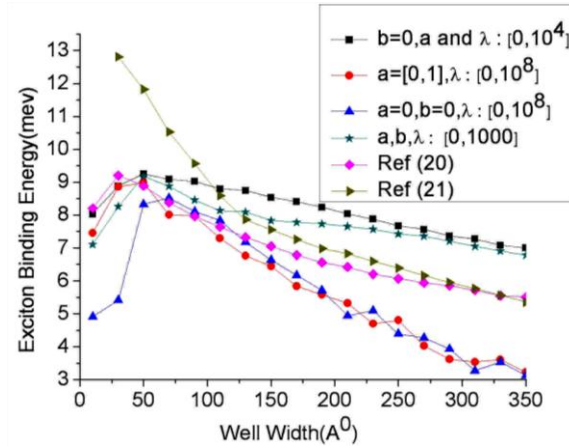


Fig. 2 – Variation of the exciton binding energy as a function of well width for different types of the trial wave functions, different intervals for the free parameters and the results of the Refs [20-21].

Magnetic field and effective mass dependence of  $\eta$  are also investigated previously [46-47] and here we have evaluated its variation versus the doping fraction  $x$ . The result is plotted in the Fig. 3. This plot shows that  $\eta$  has a monotonically increasing behavior. In order to calculate the exciton binding energy by equation (9), firstly we have to find the parameter  $\gamma_x$ . By using equation (10) we found this parameter. The result is presented in the Fig. 4. The same behavior was reported by the Ref [48]. The numerical difference is due to the fact that they have applied a dimension less Hamiltonian but we have used the complete Hamiltonian.

In order to compare the effect of the different methods of approximating the effective two dimensional Coulomb potential, the exciton binding energies obtained by equations (1), (7), (9) and the ones taken from Refs [20-21] are showed in the Fig. 5. We do not calculate exciton binding energy by the equation (6) because

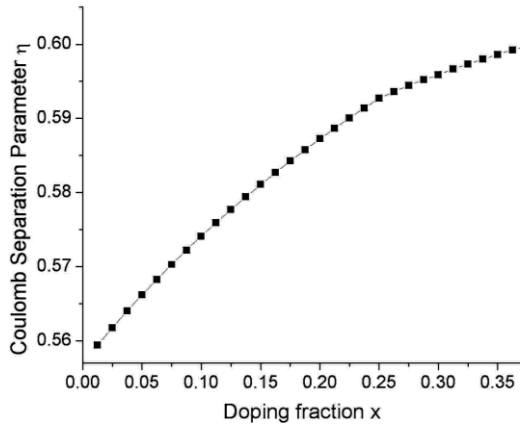


Fig. 3 – Variation of the Coulomb separation parameter  $\eta$  as a function of the doping fraction  $x$  up to 35 %

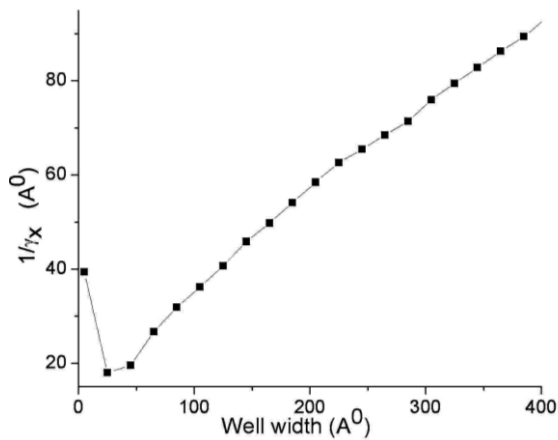


Fig. 4 – Variation of the trial wave functions free parameter ( $1/\gamma$ ) used in the equations 9 as a function of the well width

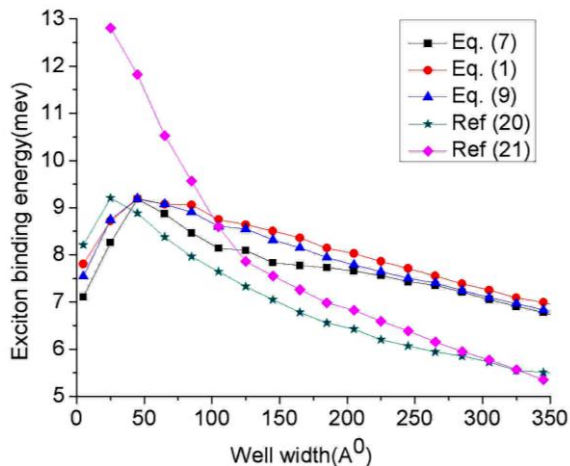


Fig. 5 – Variation of the exciton binding energy by means of the equations 1, 7, 9, and the results of the Ref [20-21] as a function of the well width

$F(\rho)$  plays the same role as  $\eta$  in the equation (7). But for comprehensiveness of the work we have presented its analytical form in the equation (6). As it can be seen the equation 7 is closer to the previously obtained results of Ref [20-21]. Although the difference of the three different methods of approximating the effective two

dimensional Coulomb potential is not too large but these methods of approximating have good advantages in the procedure of making the computational programs more efficient and faster.

In the Fig. 6 and 7 we have investigated the effect of the barrier thickness on the exciton binding energy and the parameter  $\eta$  respectively. In the Fig. 6 the effect of the barrier thickness on the exciton binding energy of a GaAs<sub>0.7</sub>Al<sub>0.3</sub>/GaAs quantum well is shown. This figure shows that when the barrier thickness increases the exciton binding energy decreases. Besides, the value of fluctuation (due to numerical inaccuracies) increases with increasing of the barrier thickness. This result is compared with the Ref [20-21]. The effect of the barrier thickness on the separation Coulomb parameter  $\eta$  is also investigated. The result which is presented in the Fig. 7 shows that when  $\eta$  decreases the barrier thickness increases and has a behavior approximately similar to exciton binding energy.

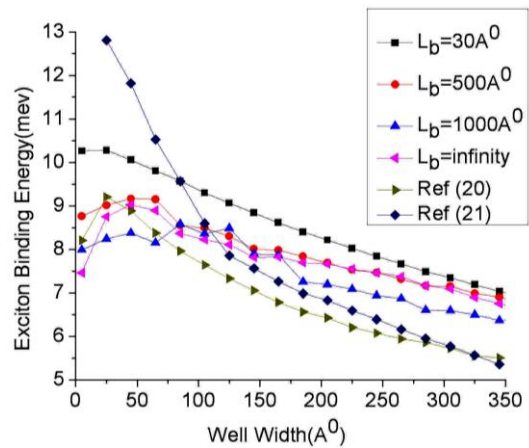


Fig. 6 – Variation of the exciton binding energy as a function of the well width for different values of the barrier thickness, 30 Å, 500 Å, 1000 Å, infinity, and the results of the Refs [20-21]

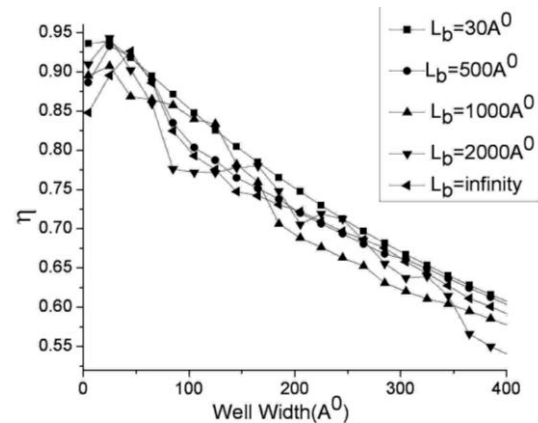


Fig. 7 – Variation of the the Coulomb separation parameter  $\eta$  as a function of the well width for different values of the barrier thickness, 30 Å, 500 Å, 1000 Å, 2000 Å and infinity

### 5. CONCLUSION

In this work, an exciton confined in a GaAs<sub>(1-x)</sub>Al<sub>x</sub>/GaAs single quantum well was revisited. The effect of the different methods of approximating the effective two dimensional Coulomb potential on the exciton

binding energy is investigated. It revealed that the natures of the two dimensional Coulomb interaction along the  $\rho$  direction ( $\rho^2 = x^2 + y^2$ ) was not the same as for three dimensional Coulomb interaction along the  $r$  direction ( $r^2 = x^2 + y^2 + z^2$ ). Different shapes of the trial wave function, number of free parameters, and interval of variation of these free parameters in these calculations were comprehensively studied. When we applied equation (14) with  $\alpha \in [0, 10^4]$  &  $\lambda \in [0, 10^4]$  or equation (12) with  $\alpha, b, \lambda \in [0, 10^3]$  there was better agreement with the Refs [20-21]. The effect of the barrier thickness on the exciton binding energy and the parameter  $\eta$

were investigated. Since we have used the Monte Carlo integration, there were some fluctuations in our results which we tried to reduce them by means of 15 times averaging.

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