Transition between quasi 2 and 3D behaviour of the binding energy of screened excitons in semiconducting quantum well structures.

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We have calculated the binding energy of screened excitons in a semiconducting quantum well structure as a function of screening parameter and the width of the quantum well using variational wave functions to obtain upper bounds for the energy. The binding energy decreases with increasing values of the screening parameter and with increasing well width. However, as long as the well width is narrow enough so the electrons and holes occupy their lowest-energy subbands, the exciton remains bound even for large values of the screening parameter whenever the electron gas remains nondegenerate.

Keywords: Binding energy of screened excitons; low-dimensional structures; semiconductors

Calculamos la energía de amarre de excitones apantallados en un pozo cuántico semiconductor como función del parámetro de apantallamiento y el ancho del pozo usando funciones de onda variacionales para obtener cotas máximas de la energía. La energía de amarre decrece al aumentar los valores del parámetro de apantallamiento y el ancho del pozo. Sin embargo, cuando el ancho del pozo sea suficientemente pequeño para que los electrones y huecos ocupen las sub-bandas de mínima energía, el excitón permanece ligado aun para valores grandes del parámetro de apantallamiento, siempre que el gas de electrones permanezca degenerado.

Descriptores: Energía de amarre de excitones apantallados; estructuras de baja dimensionalidad; semiconductores.

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1. Introduction

With the development of the techniques of crystal growth such as molecular beam epitaxy (MBE) and metallo-organic chemical vapor deposition (MOCVD), there has been a growing interest in the behavior of excitons in semiconducting quantum well systems in which the electrons and holes are confined to move [1-7]. Dingle *et al.* [4] were the first to observe enhanced excitonic effects in these quantum well structures. Miller *et al.* [5] measured the increase in the exciton binding energy in these structures while Bastard *et al.* [1] and Greene and Bajaj [6] theoretically calculated the binding energy of the exciton using a variational technique and assuming confinement of the carriers in either an infinite or finite square well potential. Miller *et al.* [8, 9] have observed room temperature exciton effects in quantum well systems and increased optical nonlinearities which they have attributed to the screening of the Coulomb interaction between the electron-hole pair by the free carriers created while Chemla *et al.* [10, 11] have observed a large shift in the exciton peak with electric field which has been proposed for use in optical switching and light beam modulation devices [12, 13]. Spector *et al.* [2], Ping *et al.* [14] have calculated the effect of screening on the binding energy of the purely 2D exciton using a variational method while Edelstein and Spector [3] did a similar calculation by numerically solving the Schrödinger equation for the screened 2D Coulomb potential. Ping and Xiang [14] used a variational-perturbation method to study the effect of charge carrier screening on the exciton binding energy in quantum wells. However, they used the 3D screened Coulomb interaction in their Hamiltonian which may be valid if the screening length is smaller than the well width but is certainly questionable when the screening length is larger than the well width. Pikus [15] solved Poisson's equation for the screening potential due to a 2D degenerate electron to obtain the effect of screening on the exciton binding energy and oscillator strength. He also took account of phase space filling which is important for a degenerate electron gas but does not play a role when the electron gas is nondegenerate. However, in his calculation he used a purely 2D variational wave function to obtain the effect of screening on the exciton binding energy. Henriques [16] has taken into account the finite width of the well in calculating screening potential which he obtained from the solution of Poisson's equation.

However, it is still of interest to see how screening would effect the binding energy of a quasi-two dimensional exciton when we use variational wave functions which take account

of the quasi-3D nature of the exciton. In this paper we propose to do such a calculation. In Sec. II of this paper, we used three different models, starting with the simpler ones. Our first calculation is performed using the trial variational wave functions of Bastard *et al.* [1], which were referred to as Type 1 and Type 2 wave functions. For Type 3 we used the more accurate two-parameter trial wave function of Shinozuki and Matsuuara [7]. For the Type 1 wave function, the atomic part of the wave function is taken to be a 2D ground state hydrogenic wave function while for the Type 2 wave function, the atomic part of the wave function is taken to be a 3D ground state hydrogenic wave function. The two parameter variational wave function of Shinozuki and Matsuuara [7] reduces to the trial wave functions of Bastard *et al.* [1] when the one of the variational parameters is equal to zero or the two variational parameters are taken equal to each other. The numerical results for the binding energy of the screened exciton as a function of the screening parameter and the well width are presented in Sec. III of this paper, where the results are discussed.

2. Theory

The model we will use in our calculations is that of electrons and holes confined to move in a square well potential along the z direction and interacting with each other via an attractive Coulomb potential. The Hamiltonian for our system is

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V_S(r) + V_{SW}(z_1) + V_{SW}(z_2), \quad (1)$$

where m_1 and m_2 are the effective masses of the electrons and holes respectively, $V_S(r)$ is the screened Coulomb potential and $V_{SW}(z_i)$ are the square well potentials which confine the motion of the electrons and holes along the z direction. The motion of the electrons and holes is not confined in the xy plane except by the Coulomb interaction between them. For a quasi-two dimensional gas of electrons and holes, the screened Coulomb interaction potential between the electrons and holes is given by [2, 17, 18]

$$V_S(r) = \frac{-e^2}{\varepsilon}\int_0^\infty dq \frac{qJ_0(q\rho)\exp(-q|z_1 - z_2|)}{(q+q_s)}, \quad (2)$$

where q_s is the screening parameter of the electron-hole plasma, ε is the static dielectric constant of the semiconductor, $J_0(x)$ is the Bessel function of order zero and argument x and $\rho = (x^2+y^2)^{1/2}$ is the magnitude of the position vector in the plane of the quantum well. Of course, the density of screening carrier gas should not be high enough so that the electrons become degenerate. As it is usual, since the binding energies of screened excitons are very small (with a small associated rotation frequency), we have used a model of static screening for excitons as an approximation of the more general models of dynamic screening. This degeneration occurs when the Fermi energy E_f is of order of the thermal energy k_BT. For example for a purely $2D$ electron gas $E_f \propto N/A$ where N is the total number of electron and A is the area the system and for a $3D$ electron gas, $E_f \propto (N/V)^{2/3}$ where V is the volume of the system. For simplicity, we will assume in our calculations that the electrons and holes are confined by an infinite square well potential

$$V_{SW}(z_i) = \begin{cases} 0, & |z_i| < L/2, \\ \infty, & |z_i| > L/2. \end{cases} \quad (3)$$

This type of infinite confinement is not a good one for narrow wells since in a real system the electron or the hole can get out of the well but it is a convenient confinement from the mathematical point of view. In Fig. 1 we show schematically our system, that is, an electron and a hole in an infinite quantum well in the presence of screening charges. Since the Hamiltonian given by Eq. (1) is not separable, we will use a variational approach to obtain an upper bound on the exciton energy of the quasi-two dimensional screened exciton. In our variational calculations, we will use three types of variational wave functions. The first one , which was denoted as Type 1 by Bastard *et al.* [1] but which we will denote as Model I, has as its atomic part a 2D hydrogenic wave function and has been shown to give good results for the binding energy of the unscreened quasi-two dimensional exciton for narrow wells.

$$\Psi = \left(\frac{2}{\pi}\right)^{\frac{1}{2}}\left(\frac{\beta}{L}\right)\cos(\pi z_1/L)\cos(\pi z_2/L) \times \exp(-\beta\rho/2) \quad (4)$$

Using the trial wave function given by Eq. (4), the expectation value of the Hamiltonian is given by

$$E(\beta) = \frac{\pi^2\hbar^2}{2\mu L^2} + \frac{\hbar^2\beta^2}{8\mu} - \frac{4e^2\beta^3}{\varepsilon L^2} \times \int_0^\infty \frac{dqq}{(q^2+\beta^2)^{3/2}(q+q_s)\left(q^2+\left(\frac{2\pi}{L}\right)^2\right)} \times \left\{\frac{3qL}{4} + \frac{2\pi^2}{qL} - \left(\frac{2\pi}{qL}\right)^4 \frac{\exp\left(-\frac{qL}{2}\right)\sinh\left(\frac{qL}{2}\right)}{1+\left(\frac{2\pi}{qL}\right)^2}\right\}, \quad (5)$$

where L is the width of the well, β is the variation parameter in the wave function and μ is the appropriate exciton reduced mass. The binding energy of the exciton is the difference in energy between the free and bound electron-hole pairs

$$E_B = \frac{\pi^2\hbar^2}{2\mu L^2} - E(\beta), \quad (6)$$

where the first term in Eq. (6) represents the sums of the lowest subband energies for the free electrons and holes in the infinite confining potential well model. The exciton binding energy as defined above is positive and therefore, our

variational approach will yield a lower limit on this binding energy. A similar approach to the one used here has been used by Brum *et al.* [19] to calculate the binding energy of screened hydrogenic impurities in a quantum well structure.

The screening parameter itself is a function of the electron density,temperature and width of the well. Under conditions where the carriers occupy the lowest subbands (or in the case of holes, the highest subband), we can use the screening parameter for the 2D electron-hole gas [20, 21] which is what we have done in our calculations here. A Debye model yields the following expression for the screening parameter of a $2D$ electron gas [22, 23]

$$q_s = (2/a_e)\left[1-\exp\left(-\pi\hbar^2 n_{2D}/m_e k_B T\right)\right], \qquad a_e = \varepsilon\hbar^2/m_e e^2, \tag{7}$$

which gives the screening parameter as a function of the temperature T and the electron density per unit area for a $2D$ system, n_{2D}. In the last expression we have chosen electronic screening but could also have screening by holes. Here a_e is an effective Bohr radius with a reduced mass μ equal to the electronic effective mass m_e. When both electrons and holes contribute to the screening of the Coulomb interaction between the electron-hole pair, as would be the case when the free carriers arise from the dissociation of the exciton, the electron and hole contributions to the screening parameter q_s will be additive. When the concentrations of the electrons and holes are equal to n, the screening parameter is given by

$$q_s = (2/a)\left\{m_e\left[1-\exp\left(-\pi\hbar^2 n/m_e k_B T\right)\right]/\mu + m_h\left[1-\exp\left(-\pi\hbar^2 n/m_h k_B T\right)\right]/\mu\right\}, \tag{8}$$

where $a = \varepsilon\hbar^2/\mu e^2$ is the effective Bohr radius of the exciton with a reduced mass μ, and m_e and m_h are the effective masses of the electron and hole, respectively. The binding energy of atomic hydrogen is $-e^4 m/2\hbar^2$ in CGS where m is the bare electronic mass. In a semiconductor we replace e^2 by e^2/ε. For semiconductor materials the typical values are $a = 100\ A$ and .001x10^{-3} Ry or more for the exciton energy. Therefore the absolute value of the exciton groundstate energy is

$$(e^2/\varepsilon)/2a_e = \mu e^2/\left(m\varepsilon^2 2a\right) = 13.6eV\mu/\left(m\varepsilon^2\right)$$

and it is called excitonic Rydberg.

It has been shown [24, 25] that the absorption at the exciton peak is directly proportional to $|\Psi(0)|^2$ which in this case is proportional to β^2 so a plot of this quantity will show how the intensity at the exciton peak change with screening parameter and well width for the screened exciton.

The second trial wave function, which was denoted as Type 2 by Bastard *et al.* [1], but which we will denote as Model II, has as its atomic part a 3D hydrogenic 1s wave function and has been found to give excellent results for the exciton binding energy in the infinite potential well for all well widths, yielding both the 3D binding energy when $L \to \infty$ and the 2D binding energy when $L \to 0$. This trial wave function is given by

$$\Psi(r) = N\cos(\pi z_1/L)\cos(\pi z_2/L)\exp(-\beta r/2), \tag{9}$$

where $r = \left[\rho^2 + (z_1 - z_2)^2\right]^{1/2}$ and

$$N^{-2} = F_1(\beta) = \frac{2\pi}{\beta^2 + \left(\frac{2\pi}{L}\right)^2}\left\{\frac{4\pi^2}{L\beta} + \frac{3\beta L}{2} - \frac{32\pi^4}{L^4\beta^2}\frac{\exp\left(-\frac{\beta L}{2}\right)\sinh\left(\frac{\beta L}{2}\right)}{\beta^2 + \left(\frac{2\pi}{L}\right)^2}\right\}$$
$$+\frac{\pi}{\beta^2 + \left(\frac{2\pi}{L}\right)^2}\left\{\frac{8\pi^2}{L\beta^3} + \frac{16\pi^4}{L^3\beta^3}\frac{\exp\left(-\frac{\beta L}{2}\right)\cosh\left(\frac{\beta L}{2}\right)}{\beta^2 + \left(\frac{2\pi}{L}\right)^2}\right\} - \frac{32\pi^5}{L^4\beta^4\left(\beta^2 + \left(\frac{2\pi}{L}\right)^2\right)^3}$$
$$\times\left\{\left(5\beta^2 + \frac{12\pi^2}{L^2} + \frac{\beta L}{2}\left(\beta^2 + \left(\frac{2\pi}{L}\right)^2\right)\right)\exp\left(-\frac{\beta L}{2}\right)\sinh\left(\frac{\beta L}{2}\right)\right\}. \tag{10}$$

The intensity at the exciton peak using this wave function is directly proportional to $N^2 = F_1(\beta)^{-1}$. Using the trial wave function given by Eq. (9) to evaluate the expectation value of the Hamiltonian in Eq. (1), we obtain

$$E(\beta) = \frac{\pi^2\hbar^2}{2\mu L^2} + \frac{\hbar^2\beta^2}{8\mu} - \frac{e^2\beta}{4\pi\varepsilon_0\kappa F_1(\beta)}\int_0^\infty \frac{dqq}{(q^2+\beta^2)^{3/2}(q+q_s)}\left[qF_0(\gamma) + \left(q^2+\beta^2\right)^{1/2}\gamma F_1(\gamma)\right], \tag{11}$$

where $\gamma = q + \left(q^2 + \beta^2\right)^{1/2}$ and

$$F_0(\gamma) = \frac{\pi}{\gamma^2 + \left(\frac{2\pi}{L}\right)^2} \left\{ \frac{4\pi^2}{L\gamma^2} + \frac{3L}{2} - \frac{32\pi^4}{L^4\gamma^3\left[\gamma^2 + \left(\frac{2\pi}{L}\right)^2\right]} \exp\left(-\frac{\gamma L}{2}\right) \sinh\left(\frac{\gamma L}{2}\right) \right\}. \quad (12)$$

In evaluating the expectation value of the screened Coulomb potential given by Eq. (2), we have used the integral [26]

$$\int_1^\infty dt \exp(-at) J_0\left(b\sqrt{t^2-1}\right) = \frac{\exp\left[-\left(a^2+b^2\right)^{1/2}\right]}{\left(a^2+b^2\right)^{1/2}}, \quad (13)$$

where $J_0(x)$ is the Bessel function of the first kind of order zero and argument x.

The third trial wave function we will use in our variational calculations of the binding energy of the screened exciton is a two parameter wave function proposed by Shinozuki and Matsuuara [7], which we will denote as Model III, is .

$$\Psi(r) = N \cos(\pi z_1/L) \cos(\pi z_2/L) \times \exp\left\{-\left[\beta^2\rho^2 + \alpha^2(z_1 - z_2)^2\right]^{1/2}/2\right\}, \quad (14)$$

where $N^{-2} = (\alpha/\beta)^2 F_1(\alpha)$. When $\alpha = 0$, this wave function reduces to Bastard's Type 1 wave function while when $\alpha = \beta$, it reduces to his Type 2 wave function. Obviously, we expect this two-parameter trial function to yield better results than the former Model I and Model II. Model I gives a 2D description of the electron and hole relative coordinates since the wave function depends only on ρ, whereas Model II gives a 3D description of the electron and hole relative coordinates since the wave function depends only on r and it exhibits spherical symmetry. In contrast Model III gives a better description since the wave function exhibits ellipsoidal symmetry. Using this trial wave function, the expectation value of the Hamiltonian is given by

$$E(\alpha,\beta) = \frac{\pi^2\hbar^2}{2\mu L^2} + \frac{\hbar^2\beta^2}{8\mu} - \frac{e^2\beta^3}{4\pi\varepsilon_0\kappa\alpha^2 F_1(\alpha)} \times \int_0^\infty \frac{dqq}{\left(q^2+\beta^2\right)^{3/2}(q+q_s)} \times \left[qF_0(\delta) + \frac{\alpha}{\beta}\left(q^2+\beta^2\right)^{1/2}\delta F_1(\delta)\right] \quad (15)$$

where $\delta = q + (\alpha/\beta)\left(q^2+\beta^2\right)^{1/2}$. The use of the variational wave functions given in Eqs. (4), (9) and (14) should be valid as long as the density of screening carrier gas is not high enough so that the electrons become degenerate.

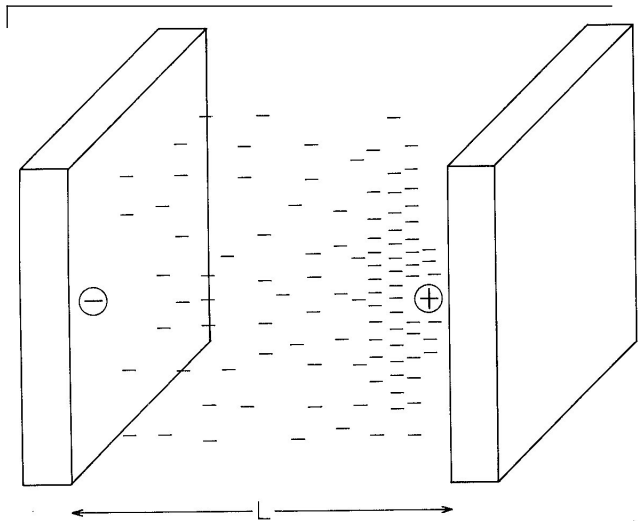

FIGURE 1. Schematically depicted system showing two parallel infinite walls as confining potential (which are shown as finite walls for visual purposes. Localized electron and hole that form an exciton are encircled and the density of screening particles (in this case electrons) is represented by a different concentration near the electron and hole. This representation exhibits the physical concept of the screening despite the fact that each particle spreads out occupying the available space.

3. Discussion

The binding energy can be obtained by minimizing the energies given by Eqs. (5), (11) and (15) with respect to the variational parameters. The results are shown in Figs. 2, 3, 4 and 5 where the binding energy in each of these three models using the three types of variational wave functions is shown as a function of the well width for various values of the screening parameter q_s. In these figures, the binding energy is given in exciton Rydberg units, the width of the well in exciton Bohr radii and the screening parameter in inverse exciton Bohr radii. For all three models and the various values of the screening parameter q_s, the binding energy decreases with increasing well width. The typical energies of excitons in a semiconductor in the absence of screening is of order of a few meV . Since the interlevel energies (using the infinite well model) are $E = \pi^2\hbar^2/2\mu L^2$, then these energies would be of order of 1 meV when L is of order of 800 angstroms if μ is of the order of 0.05 m. Therefore, our assumption of only employing groundstate wavefunctions to account for the confinement is valid for values of L less than 0.1 micron.

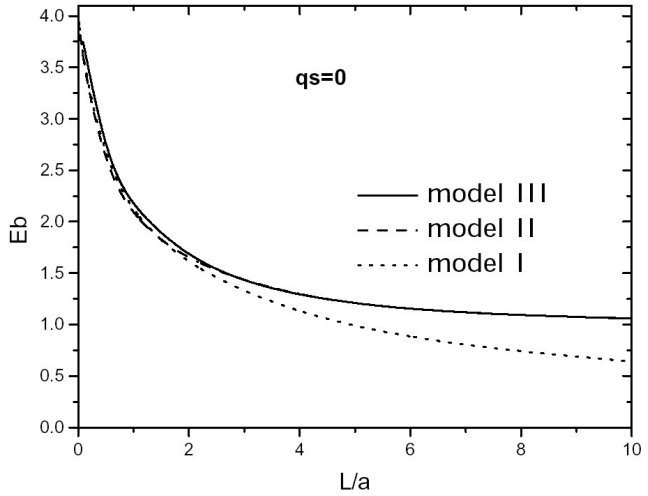

FIGURE 2. The binding energy in exciton Rydberg units is shown as a function of well width in exciton Bohr radii for Models I, II and III in the absence of screening where $q_s = 0$.

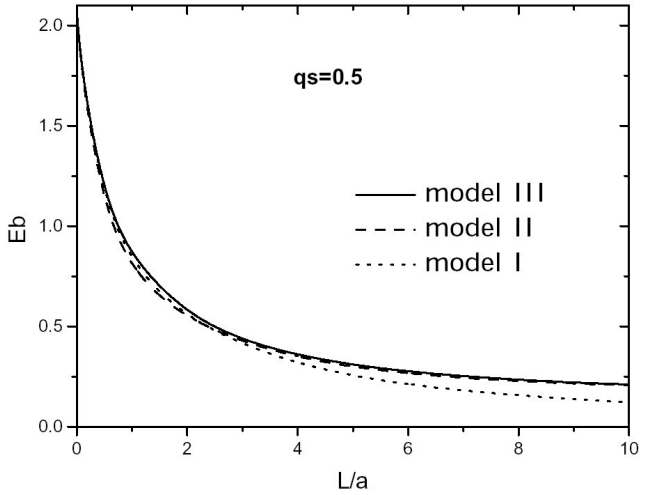

FIGURE 3. The binding energy in exciton Rydberg units is shown as a function of well width in exciton Bohr radii for Models I, II and III for the value of the screening parameter $q_s = 0.5$, where q_s is given in inverse exciton Bohr radii.

In Fig. 2, where the binding energy is shown as a function of well width in the absence of screening, we can see that Model III, using the variational wave function of Shinozuki and Matsuuara [7], gives the largest binding energy at all values of the well width. The binding energy given bye Model II, which uses the Type 2 variational wave function, merges into the results for Model III as the well width becomes much larger than an exciton Bohr radius a, while the results of Model I, which uses the Type 1 variational wave function, does not approach the 3D limit for increasing well width. As the well width becomes much smaller than an exciton Bohr radius, the results for all three models are close with Model III giving the highest binding energy. From Figs. 3, 4 and 5, we see that as the screening parameter becomes larger, the values of the binding energy become smaller. This is because the screening reduces the attractive Coulomb interaction which binds the electron and hole into the exciton. With increased screening, Model III still gives the highest binding energies for the exciton but the difference in the binding energies for the three models becomes smaller and smaller as the screening becomes larger and larger. The results using Model II are close to the results using Model III for all well widths and values of the screening parameter while the results using Model I are only close to those of Model III for small well widths and/or large values of the screening parameter. The largest differences in the binding energy between the predictions of Models II and III occur for well widths between one and two exciton Bohr radii. For all three models, the exciton remains bound as the value of the screening parameter increases, even though the value of the binding energy decreases (or equivalently, the groundstate energy approaches zero from below). Thus, taking into account the finite width of the well does not alter the conclusions of Refs. 2,3 and 14 using a purely 2D model for the screened exciton which is that the exciton remains bound for very large screening in narrow wells.

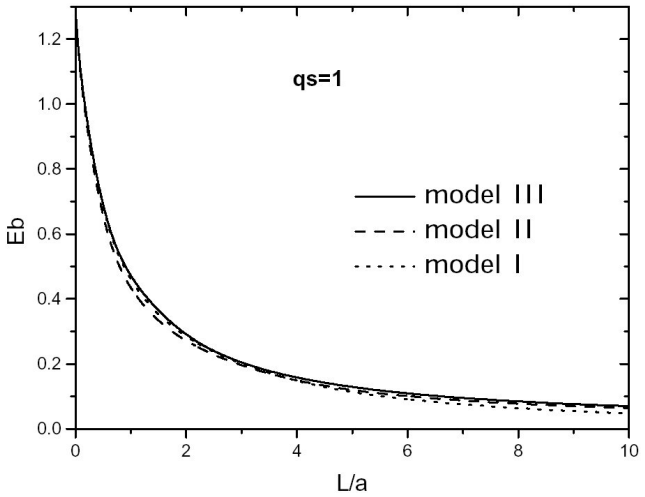

FIGURE 4. Same as Fig. 3 with $q_s = 1.0$.

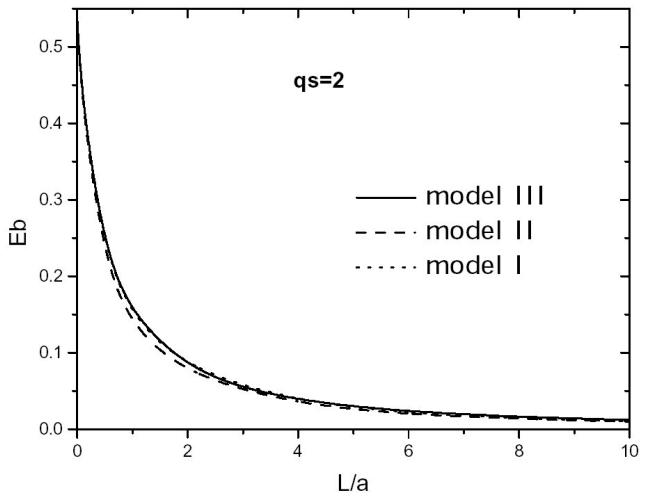

FIGURE 5. Same as Fig. 3 with $q_s = 2.0$.

In Figs. 6 and 7, the variational parameter βa in the Models I and II are shown as a function of the well width for various values of the screening parameter q_s. The well width is given in exciton Bohr radii while the screening parameter is given in inverse exciton Bohr radii. For both models, the variational parameter βa decreases with increasing well width. However, in the absence of screening, the variational parameter βa for Model I continues to decrease as the well width increases while for Model II, it saturates at a value of 2 with increasing well width. In the presence of screening, the variational parameter βa decreases from its value in the absence of screening and continues to decrease with increasing well width for both models. This reflects the fact that as the binding of the electron and hole into the exciton becomes weaker, the exciton wave function becomes more spread out in space. Since in Model I, the absorption at the exciton peak is directly proportional β^2, this indicates that the optical absorption will decrease with increasing screening as the electron and hole become less likely to be found in the same region of space.

In Figs. 8 and 9, the variational parameters βa and αa are shown as a function of well width for various values of the screening parameter q_s using the Model III wave function. In the absence of screening, the parameter βa decreases from a value of 4 for small well widths to a value of 2 for large well widths while the variational parameter αa initially decreases and then increases approaching the value of 2 for large well widths. Also when q_s increases yielding a weaker electron-hole interaction an a larger exciton size, α and β approach their $3D$ bulk value $\alpha = \beta$ at larger values of L. Interestingly enough, the variational parameter αa never goes to zero as the well width decreases. Therefore, the wave function maintains a quasi-3D behavior even for small well widths. With increasing screening, the variational parameter βa decreases with the decrease becoming larger as the screening parameter becomes larger. However, the variational parameter, although decreasing with increasing screening, does not change as dramatically with increasing well width as it does in the absence of screening.

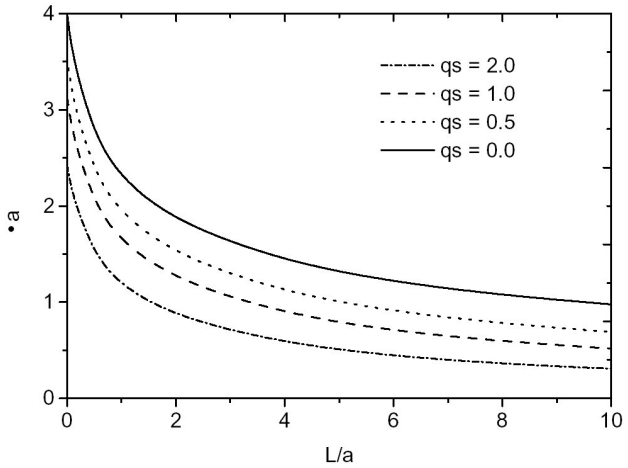

FIGURE 6. The variational parameter βa in the Model I type wave functions is shown as a function of the well width for various values of the screening parameter q_s. The well width is given in exciton Bohr radii while the screening parameter is given in inverse exciton Bohr radii.

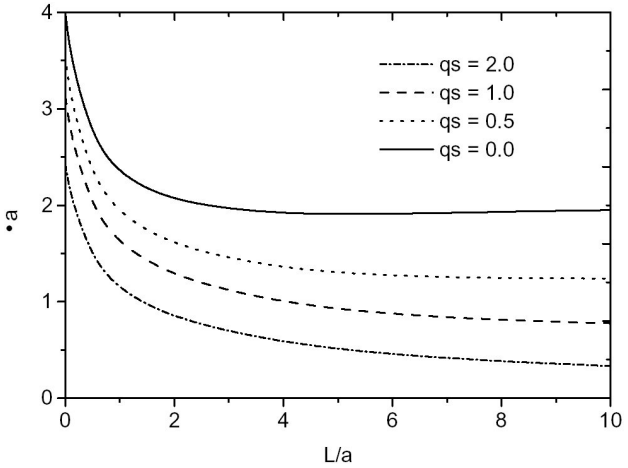

FIGURE 7. Same as Fig. 6 for Model II type wave functions.

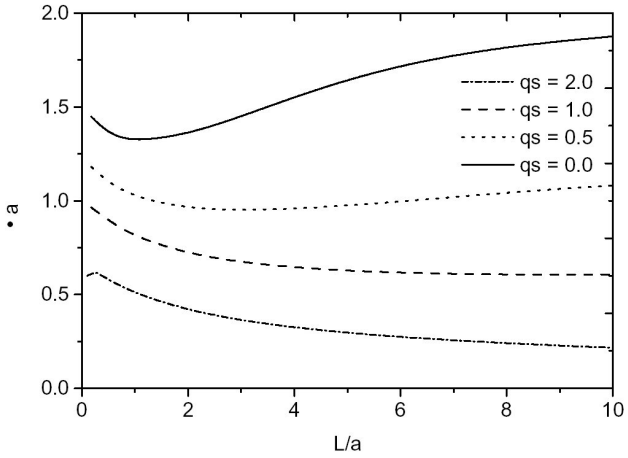

FIGURE 8. Same as Fig. 6 for Model III type wave functions.

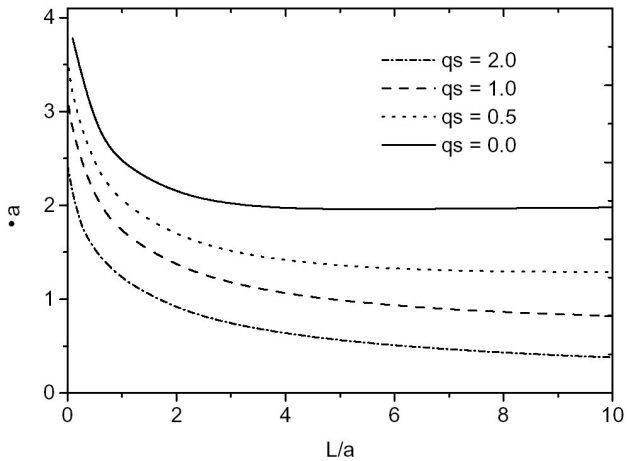

FIGURE 9. The variational parameter αa is shown as a function of the well width for various values of the screening parameter q_s using the Model III wave functions. The well width is given in exciton Bohr radii while the screening parameter is given in inverse exciton Bohr radii.

Our calculations show that the binding energy is the largest using the two variational parameter wave function of Model III for all values of the well width and the screening parameter. However, the difference in the binding energy calculated using the three models becomes smaller as the screening parameter increases. In addition, when we take the finite width of the well into account, the exciton remains bound for narrow wells. Also, for all three models, the wave function becomes more spread out as the screening becomes stronger which should lead to a decrease in the optical absorption with increasing screening.

In summary, our theoretical calculations using all three of our model wave functions show that although the binding energy of the exciton decreases with increasing screening, the exciton still remains bound even when we take into account the finite width of the well. Also, since the exciton wave function becomes more spread out with increasing screening, the effect of the screening is to reduce the optical absorption due to the exciton. We show that the highest binding energy of the exciton is given by the two parameter variational wave function of Shinozuki and Matsuuara [7]. Since we employed a $2D$ screening formalism our results are not a good description of the exciton when L is very large (or when the screening effects are very small, that is, whenever q_s is small). On the other hand, for large values of L our model is not accurate and it should include confinement excited states or higher confinement subbands. Therefore our results are expected to be reasonable only for intermediate values of L, where the range intermediate depends on the value of the screening parameter q_s. Larger values of q_s imply that results for larger values of L are reasonable since they correspond to larger exciton sizes.

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