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Simultaneous effects of pressure and temperature on excitons in Pöschl–Teller quantum well

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Binding energies of the heavy hole and light hole exciton in a quantum well with Pöschl–Teller (PT) potential composed of GaAs have been studied variationally within effective mass approximation. The effects of pressure and temperature on exciton binding energy are analyzed individually and also simultaneously for symmetric and asymmetric configuration of the well. The results show that exciton binding energy (i) decreases as the well width increases, (ii) increases with pressure and (iii) decreases with temperature. Simultaneous effects of these perturbations lead to more binding of the exciton. The results are compared with the existing literature.

Keywords: Exciton; temperature; pressure; Pöschl–Teller quantum well; binding energy.

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1. Introduction

Studies on low dimensional semiconductor systems with quantum confinement are paid much attention due to their effective applications in electronic and optoelectronic devices. Most of the investigations are carried out with III–V semiconductor heterostructures, mainly with GaAs/GaAlAs. Because of the optical properties, GaAs/GaAlAs structures have become more important in the field of device fabrication. Theoretical investigations on hydrogenic donor and exciton in quantum semiconductor nanostructures play an important role to understand the electrical, magnetic and optical properties of the nanostructures.[1–6] Confinement of excitons

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in semiconductor nanostructures are exploited in the design of novel optoelectronic devices. Various authors have theoretically and experimentally studied the exciton binding energy in cylindrical quantum dot,[7] parabolic quantum wire,[8] spherical quantum dot,[9] triangular quantum well,[10] rectangular quantum well[11,12] and coupled double quantum well.[13]

Band structure and the properties of semiconductor materials can be controlled and altered by the application of pressure and temperature. Hence, an understanding of the effects of pressure and temperature on excitonic binding energy in a quantum well may be useful in the design and preparation of a new generation of efficient semiconductor devices like heterostructure lasers, QLEDs, white light sources, etc.

Raigoza *et al.*[14] have calculated theoretically the effects of hydrostatic pressure and electric field on exciton states in GaAs–GaAlAs quantum well. The combined influences of temperature and hydrostatic pressure on exciton binding energy in a GaAs spherical quantum dot have been investigated by Jeice and Wilson.[9] Effects of temperature and pressure on exciton binding energy in a cylindrical GaAs quantum dot have been studied by Elmeshad *et al.*[7] Moussaouy *et al.*[15] have investigated the temperature and pressure effects on exciton–phonon coupled states in semiconductor quantum dot composed of GaAs–GaAlAs.

Due to the evolution of growth techniques of low dimensional structures, it is possible to alter distinct conduction and valence band potential energy to make different potential profiles of various dimensions. Pöschl–Teller (PT) potential is one among the novel confining potential profiles.[16] An important feature of PT potential is that the degree of asymmetry of the potential is tunable which yields nonlinear optical properties[17,18] such as third-order absorption co-efficient, second-order susceptibility and optical rectification associated with inter-subband optical transitions. By adjusting the characteristic parameters of the potential, there can be a switchover from symmetric to asymmetric configuration.

Studies on such a potential are receiving much attention in the past two decades due to their specific applications like photo detector operations. Barseghyan *et al.*[19] have studied the simultaneous effects of pressure and temperature on the binding energy of a hydrogenic donor impurity in PT quantum well and also investigated the combined effects of pressure, electric and magnetic fields on donor binding energy in InAs PT quantum ring.[20] Mora-Ramos *et al.*[21] have investigated the exciton binding energy in a cylindrical PT GaAs quantum dot. The influence of temperature on exciton binding energy in ZnSe–ZnMgSe PT quantum well has been investigated by Sathiyajothi *et al.*[22] The effects of hydrostatic pressure and temperature on exciton binding energy in a cylindrical quantum dot have been studied by Mora-Ramos *et al.*[23] Optical properties of cylindrical and spherical quantum dots with symmetric or modified PT potential have been studied by Hayrapetyan *et al.*[24,25]

In the present paper, we have investigated the combined effects of pressure and temperature on light hole (lh) and heavy hole (hh) exciton binding energy in PT quantum well formed by GaAs as a function of well width for different symmetric and asymmetric configurations of the quantum well. We have used variational method to compute the binding energy of exciton.

2. Theoretical Framework

2.1. *Hamiltonian and wavefunction of exciton*

The Hamiltonian of an exciton in a quantum well with PT potential composed of GaAs is given in effective-mass approximation and in dimensionless variables as

$$\mathcal{H} = -\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right] - \frac{\mu_{ih}^*}{m_e^*}\frac{\partial^2}{\partial z_e^2} - \frac{\mu_{ih}^*}{m_{ih}^*}\frac{\partial^2}{\partial z_h^2} + V(z_e) + V(z_h) - \frac{2}{r}, \quad (1)$$

where $r = \sqrt{\rho^2 + |z_e - z_h|^2}$ and μ_{ih}^* is the reduced mass of hh- $(i = h)$ exciton or lh- $(i = l)$ exciton given by

$$\frac{1}{\mu_{ih}^*} = \frac{1}{m_e^*} + \frac{1}{m_{ih}^*}. \quad (2)$$

m_e^* and m_{ih}^* are the effective masses of electron and hole, respectively. The effective Bohr radius $(a^* = \hbar^2\varepsilon_0/\mu_{ih}^* e^2)$ and the effective Rydberg $(R^* = \mu_{ih}^* e^4/2\hbar^2\varepsilon_0^2)$ are used as the units of length and energy, respectively.

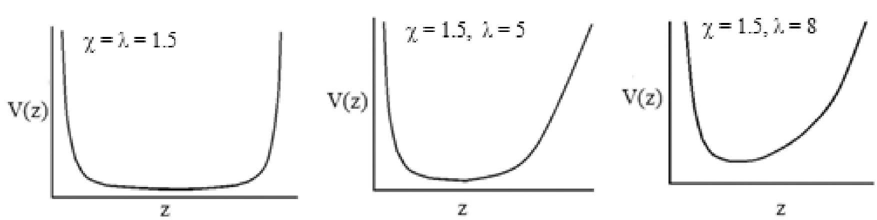
The PT potential for electron $(j = e)$ and hole $(j = ih)$ in quantum well is given by,[20]

$$V_{\mathrm{PT}}(z_j) = \frac{\mu_{ih}^*\eta^2}{m_j^*}\left[\frac{\chi(\chi-1)}{\sin^2\eta z_j} + \frac{\lambda(\lambda-1)}{\cos^2\eta z_j}\right]. \quad (3)$$

χ and λ are the parameters which characterize the asymmetry of the potential. The potential is perfectly symmetric when $\chi = \lambda$. $\eta = \frac{\pi}{2L}$ and L is the well width of the quantum well.

Figure 1 shows the different shapes of the PT potential quantum well with three different asymmetry cases. (a) When $\chi = \lambda = 1.5$, the shape of the quantum well is perfectly symmetric named as modified PT potential.[24,25] The shape of the quantum well is deviated from the symmetric well and becomes asymmetric, when (b) $\chi = 1.5$ and $\lambda = 5$ and (c) $\chi = 1.5$ and $\lambda = 8$.

Since an accurate solution of the Schrödinger equation for the Hamiltonian of Eq. (1) is not possible, a variational method is adopted. The trial wavefunction for



(a) (b) (c)

Fig. 1. PT quantum well according to the asymmetric parameters χ and λ.

excitons within the PT quantum well is taken to be of the form,[20]

$$\Psi = N \sin^{\chi} \eta z_e \cos^{\lambda} \eta z_e \sin^{\chi} \eta z_{ih} \cos^{\lambda} \eta z_{ih} e^{-ar}, \tag{4}$$

where 'N' is normalization constant and 'a' is variational parameter. The expectation value of Hamiltonian $\langle \mathcal{H} \rangle$ with respect to the variational parameter is calculated using the expression

$$\langle \mathcal{H} \rangle = \frac{\int \Psi^* \mathcal{H} \Psi d\tau}{\int \Psi^* \Psi d\tau}. \tag{5}$$

The binding energy of exciton in the PT quantum well is then given by

$$E_B = E_e + E_{ih} - \langle \mathcal{H} \rangle_{\min}, \tag{6}$$

where E_e and E_{ih} are the ground state energies of electron and hole in bare quantum well, respectively, obtained variationally. $\langle \mathcal{H} \rangle_{\min}$ is the minimized value of $\langle \mathcal{H} \rangle$ with respect to the variational parameter a.

2.2. *Effect of temperature and hydrostatic pressure*

The application of temperature and hydrostatic pressure alter the energy gap, effective masses of electron and hole, dielectric constant and well width. Variations of these variables with respect to the applied hydrostatic pressure in kbar and temperature in K are as given below.

The variation of effective-mass of electron in conduction band of GaAs as a function of pressure and temperature is given by the expression[3]

$$m_e^*(P,T) = \frac{m_0}{1 + E_m \left\{ \frac{2}{E_g^{\Gamma}(P,T)} + \frac{1}{E_g^{\Gamma}(P,T) + \triangle_o} \right\}}, \tag{7}$$

where m_0 is free electron mass, $E_m = 7.51$ eV is energy related to the momentum matrix element, $\Delta_o = 0.341$ eV is spin–orbit splitting and $E_g^{\Gamma}(P,T)$ is the energy gap of the GaAs quantum well which depends on both pressure and temperature given by[3]

$$E_g^{\Gamma}(P,T) = E_g^{\Gamma}(0,T) + bP + cP^2, \tag{8}$$

where $b = 1.26 \times 10^{-2}$ eV bar^{-1} and $c = 3.77 \times 10^{-5}$ eV bar^{-2}. $E_g^{\Gamma}(0,T)$ is the energy gap of GaAs as a function of temperature without pressure given by[3]

$$E_g^{\Gamma}(0,T) = 1.519 - \frac{5.405 T^2 \times 10^{-4}}{T + 204}. \tag{9}$$

The valence band effective-mass as a function of temperature and pressure is calculated using the expression[26]

$$m_{ih}^*(P,T) = [m_{ih}^* + x_1 P + x_2 P^2] \frac{E_g^{\Gamma}(0,T)}{1.519}, \tag{10}$$

where $x_1 = -0.1 \times 10^{-3}$ kbar^{-1} and $x_2 = 5.56 \times 10^{-6}$ kbar^{-2} are the pressure coefficients.

The variation of dielectric constant as a function of temperature and pressure is given as,[3]

$$\varepsilon_0(PT) = \begin{cases} 12.74e^{-1.73\times10^{-2}P}e^{9.4\times10^{-5}}(T-75.6), & T \le 200\text{ K}, \\ 13.18e^{-1.73\times10^{-2}P}e^{20.4\times10^{-5}}(T-300), & T > 200\text{ K}. \end{cases} \tag{11}$$

Since the temperature dependence of well width is not available in the literature, variation of well width with pressure alone is considered. The expression for well width as a function of pressure is given by[7]

$$L(P) = L - L(S_{11} + 2S_{12})P, \tag{12}$$

where $S_{11} = 1.16 \times 10^{-3}$ kbar^{-1} and $S_{12} = -3.7 \times 10^{-4}$ kbar^{-1} are the elastic constants of GaAs.

3. Results and Discussion

The material parameters for GaAs[27] used in the calculations are, (i) effective masses of hh, $m^*_{\text{hh}} = 0.34\ m_0$, lh, $m^*_{\text{lh}} = 0.094\ m_0$ and electron, $m^*_e = 0.0665\ m_0$; (ii) reduced masses of lh-exciton, $\mu^*_{\text{lh}} = 0.05562\ m_0$ and hh-exciton, $\mu^*_{\text{hh}} = 0.03895\ m_0$ where m_0 is the free electron mass; (iii) dielectric constant $\varepsilon_0 = 13.2$.

Figure 2 shows the variation of lh-exciton binding energy as a function of well width without applied pressure and temperature for different values of asymmetric parameters χ and λ, which define the shape of PT quantum well. We have calculated the exciton binding energy as a function of well width for four different cases (i) $\chi = \lambda = 1.5$, (ii) $\chi = \lambda = 3$, (iii) $\chi = 1.5$, $\lambda = 3$ and (iv) $\chi = 1.5$, $\lambda = 5$. It is observed that when the well width reduces, the binding energy of lh-exciton increases for all the four cases. The wavefunction of exciton squeezed together in the well, due to the confinement, leads to more binding. This behavior is analogous

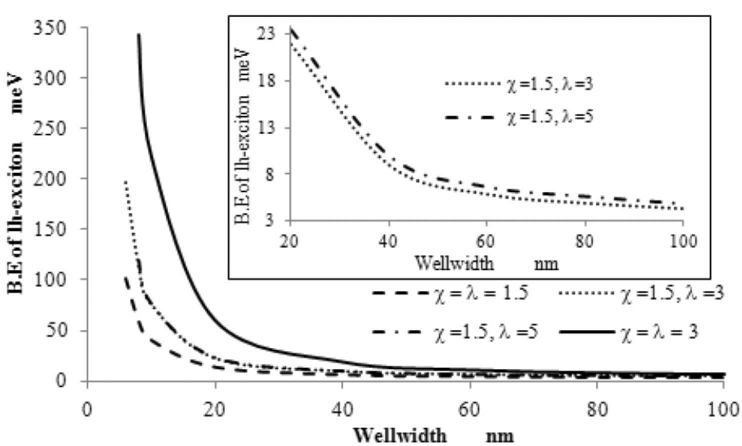


Fig. 2. Binding energy of lh-exciton as a function of well width for different asymmetry parameters.

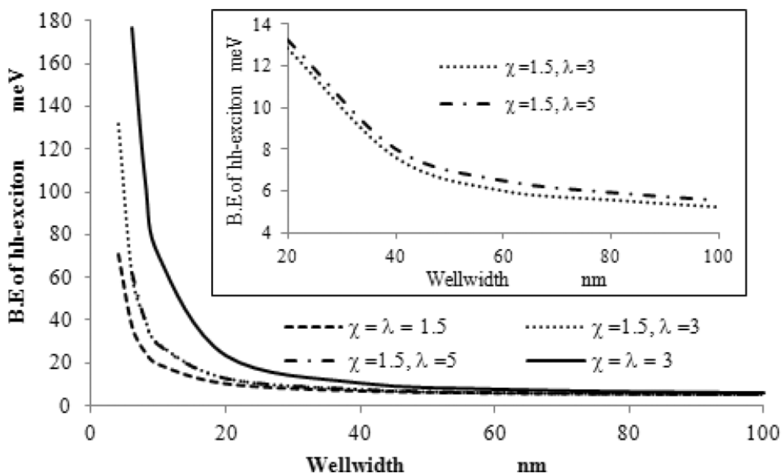


Fig. 3. Binding energy of hh-exciton as a function of well width for different asymmetry parameters.

to the results of Mora-Ramos *et al.*[23] It is also noted that the lh-exciton binding energies increases as the parameters χ and λ increase for zero pressure and zero temperature. As λ increases, keeping χ as a constant, the lh-exciton binding energy increases. But the amount of increase, i.e., the increment decreases as λ increases which is clearly seen from the closeness of curves (iii) and (iv). This behavior may be due to the increase of tendency of the wavefunction to spread out of the well, as λ increases.

In Fig. 3, we show the variation of hh-exciton binding energy in PT quantum well as a function of well width for different combinations of asymmetry parameters without applied pressure and temperature. As in the case of lh-exciton, the hh-exciton binding energy also increases when the well width reduces. It is also observed that the behavior of the hh-exciton binding energy with respect to the asymmetric parameter is same as in case of lh-exciton, but the value of the hh-exciton binding energy is smaller than that of lh-exciton.[10,12]

Figure 4 depicts the variation of lh-exciton binding energy as a function of pressure for different well widths without applied temperature and the value of asymmetry parameters are chosen as $\chi = \lambda = 1.5$ which means that the quantum well is perfectly symmetric. It is observed that for well width $L = 20$ nm, the binding energy of lh-exciton increases with pressure applied to the quantum well. Another significant result from the plot is that the lh-exciton binding energy increases with pressure up to 30 kbar and for well widths such as $L = 6$, 8 and 10 nm, further increase of pressure leads to less binding. This behavior is similar to those observed for a donor by Morales *et al.*[28] This may be due to the penetration of lh-exciton wavefunction through the barrier with small well width under large pressure. So the choice of the pressure level for a particular well width must be given importance during the fabrication of devices.

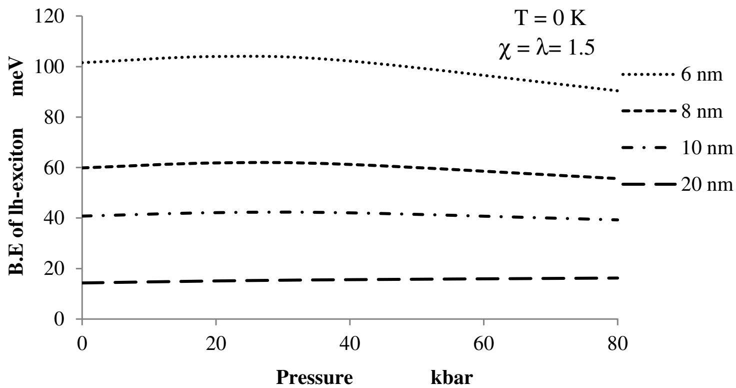


Fig. 4. Binding energy of lh-exciton as a function of pressure for different well widths.

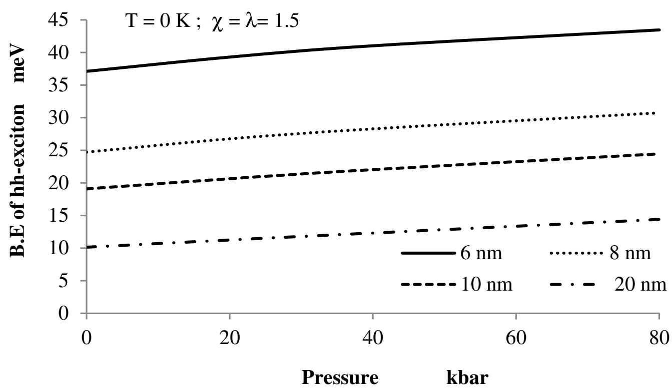


Fig. 5. Binding energy of hh-exciton as a function of pressure for different well widths.

Figure 5 displays hh-exciton binding energy as a function of pressure for different well widths for $T = 0$ K. The asymmetry parameters are considered as $\chi = \lambda = 1.5$. It is noted that the hh-exciton binding energy increases with pressure (up to 80 kbar) for all well widths.[7] This behavior is not similar to that of lh-exciton case presented in Fig. 4. Since the effective-mass of the hh-exciton is greater than that of lh-exciton, the wavefunction of hh-exciton, though compressed together, does not penetrate through the barrier even up to the pressure of 80 kbar.

The results depicted in Figs. 6 and 7 are similar to those in the case of Figs. 4 and 5, respectively, but the PT potential is deformed asymmetrically in the later case by choosing the values of asymmetry parameters as $\chi = 1.5$ and $\lambda = 3$. Comparing Figs. 4 and 6, it is observed that the variation of lh-exciton binding energy with respect to pressure and well width for asymmetric PT quantum well with $\chi = 1.5$ and $\lambda = 3$ is same as in the case of symmetric configuration $\chi = \lambda = 1.5$. However, for all the values of pressure and well width the binding energy in asymmetric case is larger than that in symmetric case ($\chi = \lambda = 1.5$). Similarly, it

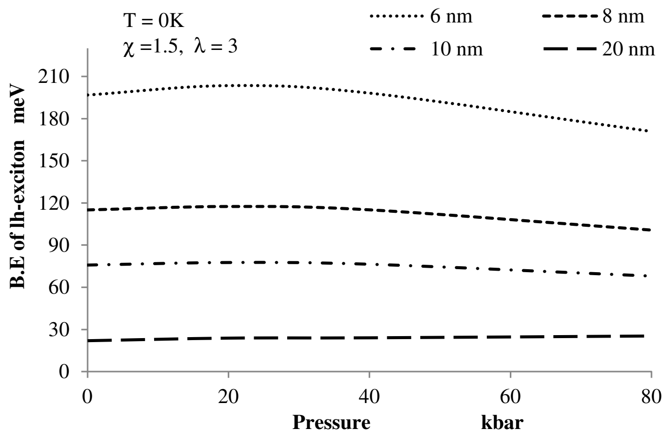


Fig. 6. Binding energy of lh-exciton as a function of pressure for different well widths with $\chi = 1.5$ and $\lambda = 3$.

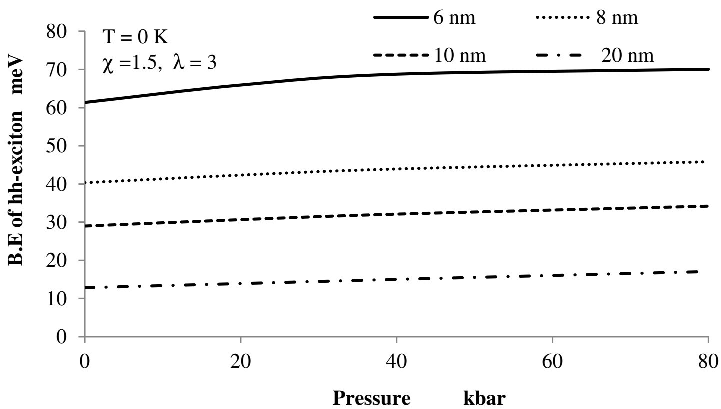


Fig. 7. Binding energy of hh-exciton as a function of pressure for different well widths with $\chi = 1.5$ and $\lambda = 3$.

can be seen from Figs. 5 and 7, the hh-exciton binding energy in symmetric case is smaller than that in asymmetric case $\chi = 1.5$ and $\lambda = 3$.

The variation of lh-exciton and hh-exciton binding energy in GaAs PT quantum well as a function of temperature without applied pressure is presented in Figs. 8 and 9. The PT quantum well is considered as perfectly symmetric with $\chi = \lambda = 1.5$. In both the cases, it is observed that the binding energy decreases with temperature for large well widths $L = 10$, 20 and 80 nm. This behavior agrees with those for a quantum dot reported by Mora-Ramos *et al.*[23] The reason is that the effective mass of the electron and hole diminishes with increase of temperature. Hence the reduced mass of the electron–hole pair also decreases. But for small well widths, the binding energy remains constant when the temperature increases. This may be due to the competitive effects of temperature and confinement.

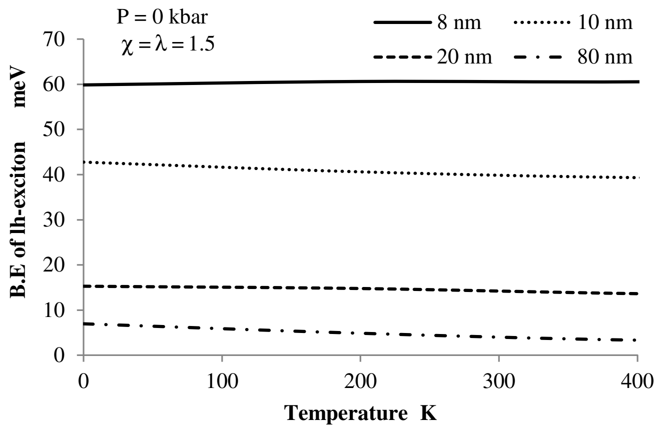


Fig. 8. Binding energy of lh-exciton as a function of temperature for different well widths.

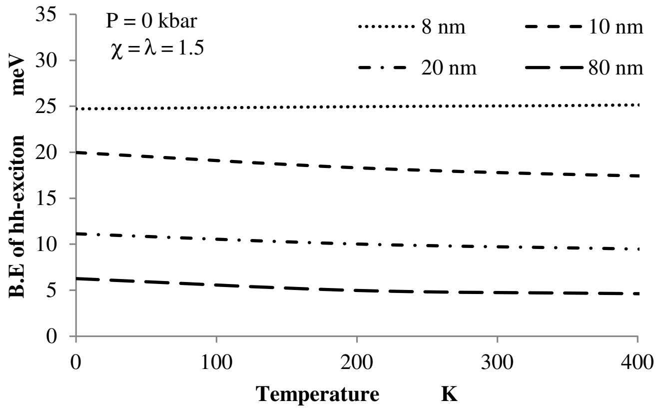


Fig. 9. Binding energy of hh-exciton as a function of temperature for different well widths.

The variation of binding energy of lh-exciton and hh-exciton as a function of temperature for various well widths with asymmetry effect ($\chi = 1.5$, $\lambda = 3$) is shown in Figs. 10 and 11, respectively. It is observed that, the binding energy of lh-exciton and hh-exciton in asymmetric ($\chi = 1.5$, $\lambda = 3$) PT well is larger than that in symmetric ($\chi = \lambda = 1.5$) PT well. It can be seen from Figs. 8 and 10 that the lh-exciton binding energy in asymmetric case increases with temperature for $L = 8$, 10 and 20 nm and decreases with temperature for $L = 80$ nm. This result is quite different from the symmetric case, where the binding energy of lh-exciton increases with temperature for $L = 8$ nm and decreases with temperature for $L = 10, 20$ and 80 nm. This is a consequence of the fact that increase of λ decreases the spatial distance between the electron and hole as depicted in Fig. 1 and the localization of electron and hole states increases in quantum well; hence the coulomb interaction is strengthened which leads to the increase of the exciton binding energy.

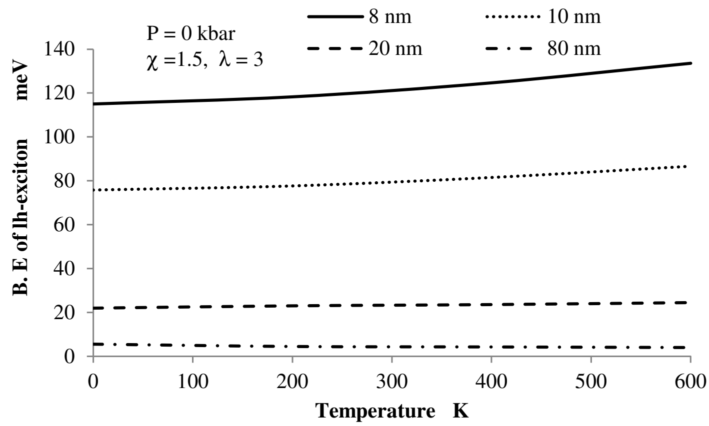


Fig. 10. Binding energy of lh-exciton as a function of temperature for different well widths with $\chi = 1.5$ and $\lambda = 3$.

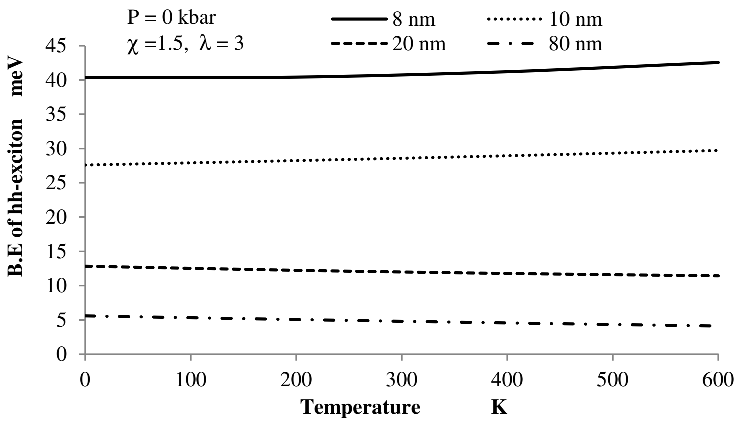


Fig. 11. Binding energy of hh-exciton as a function of temperature for different well widths with $\chi = 1.5$ and $\lambda = 3$.

Comparing Figs. 9 and 11, the hh-exciton binding energy, in symmetric case, increases with respect to temperature for $L = 8$ nm and decreases with temperature for $L = 10, 20$ and 80 nm. But in the case of asymmetric well, the lh-exciton binding energy increases with temperature for well widths $L = 8$ and 10 nm and decreases for $L = 20$ and 80 nm.

The combined effects of asymmetry, temperature and pressure on lh-exciton binding energy in PT quantum well is shown in Fig. 12 for $L = 10$ nm and $T =$ 200 K. It shows that the binding energy increases with pressure up to 30 kbar, beyond that it starts to decrease for all asymmetric cases. It is observed that the binding energy decreases when the value of λ increases with χ kept as a constant. It is also noted that the simultaneous effects of temperature, pressure and asymmetry on lh-exciton leads to increased binding.

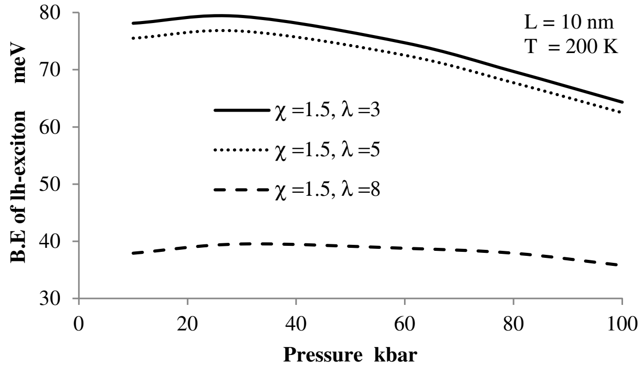


Fig. 12. Binding energy of lh-exciton as a function of pressure for different asymmetric shape of the quantum well with $L = 10$ nm and $T = 200$ K.

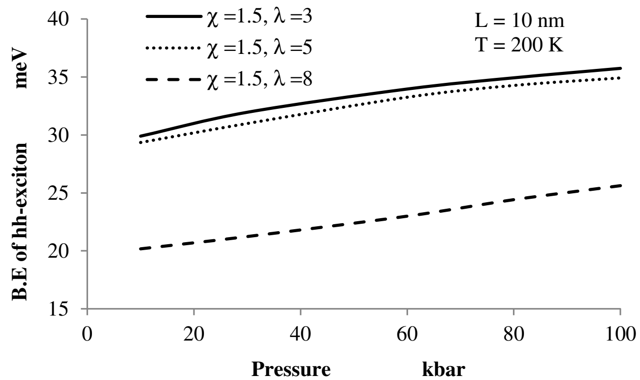


Fig. 13. Binding energy of hh-exciton as a function of pressure for different asymmetric shape of the quantum well with $L = 10$ nm and $T = 200$ K.

Figure 13 presents the results of hh-exciton binding energy as a function of pressure with $L = 10$ nm and $T = 200$ K. The asymmetric PT pattern was chosen with constant $\chi = 1.5$ and three different values of $\lambda = 3, 5$ and 8. It can be seen that, for all asymmetry configurations the binding energy increases with pressure. It is also important to note that, the hh-exciton binding energy decreases when asymmetry parameter λ increases. The hh-exciton binding energy decreases to a large extent when the value of λ goes beyond five. As in the case of lh-exciton, the simultaneous application of pressure, temperature and asymmetry pattern leads to more binding for hh-exciton also.

4. Conclusion

We have investigated the hh- and lh-exciton binding energy under the effects of pressure, temperature and asymmetry pattern of the PT quantum well composed of GaAs as a function of well width by variational method. The following points are noted: (i) increase in the degree of asymmetry of the PT quantum well increases the binding energy of both excitons, (ii) both in symmetric and asymmetric cases, for $L \leq 20$ nm, lh-exciton binding energy increases with pressure up to 30 kbar and decreases for further increase in pressure. But for $L > 20$ nm, it increases with pressure continuously, (iii) hh-exciton binding energy increases with pressure for all well widths (noted up to 80 kbar), (iv) in the asymmetric case, for $L \leq (>) 20$ nm, lh-exciton binding energy increases (decreases) with temperature. But in the symmetric case, the same behavior is observed for $L \leq 8$ nm, (v) similar behavior is observed for hh-exciton binding energy also, in asymmetric case for $L \leq 10$ nm and in symmetric case for $L \leq 8$ nm and (vi) simultaneous effects of pressure, temperature and asymmetry pattern of PT quantum well lead to increased binding of both excitons. The values of pressure and temperature in semiconductor materials for the potential device applications must be properly chosen and our calculations give an idea of the choice of these values which will be surely useful in the preparation of semiconductor devices. However, choice of the wavefunction with two variational parameters as in Mora-Ramos *et al.*[21,23] may give still improved results for the exciton binding energy.

Acknowledgments

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