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ORIGINAL PAPER

# Excitonic susceptibility in near triangular quantum wells

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**Abstract:** Diamagnetic susceptibility and binding energy of an exciton in a near triangular quantum well, with potential profile proportional to $|z|^{2/3}$ composed of GaAs/$Ga_{1-x}Al_xAs$ and ZnO/$Zn_{1-x}Mg_xO$ are calculated as a function of the wellwidth and concentration of Al and Mg respectively varying the magnetic field applied along growth direction (i.e. $z$-axis). Diamagnetic susceptibility of light hole exciton and heavy hole exciton, shows inverse behaviors in the two materials below 20 nm wellwidth and the binding energy of both excitons increases, as the magnetic field increases. The results obtained, are compared with those of quantum wells with varied potential profiles and the experimental results reported in the literature.

**Keywords:** Quantum wells; Exciton; Binding energy; Diamagnetic susceptibility; Magnetic field

**PACS Nos.:** 73.21.Fg; 71.35.-y; 71.35.Ji

## 1. Introduction

Advanced semiconductor growth techniques such as molecular beam epitaxy, chemical lithography and etching have made it possible to fabricate quantum wells with varied potential profiles [1]. Owing to the numerous advantages for device applications, quantum wells are fabricated with different materials such as GaAs/$Ga_{1-x}Al_xAs$ [2–13] and ZnO/$Zn_{1-x}Mg_xO$ [14–17] and investigated extensively. Studies on excitons play an important role in the development of optoelectronic devices. Excitons in rectangular quantum wells (RQW) [2–6], parabolic quantum wells (PQW) [7–9], triangular quantum wells (TQW) [10], surface quantum wells (SQW) [11], near triangular quantum wells (NTQW) with potential profile proportional to $|z|^{2/3}$ [12, 13] have been studied theoretically and experimentally by many authors.

Effect of magnetic field on a material is widely used in Nuclear Magnetic Resonance to identify the chemical and geometrical structure. Diamagnetic susceptibility is one of the important parameters to analyze the magnetic response of a material. Binding energy and diamagnetic susceptibility of a hydrogenic donor in GaAs/$Ga_{1-x}Al_xAs$ low dimensional semiconducting systems with rectangular profile have been reported by Nithiananthi and Jayakumar [18]. Effect of the nitrogen concentration and magnetic field on diamagnetic susceptibility and the binding energy of a hydrogenic donor in $Ga_xIn_{1-x}N_yAs_{1-y}$/GaAs RQW have been studied by Kilicarslan et al. [19]. Edelshtein has theoretically proved that the diamagnetic susceptibility of an exciton molecule does not differ greatly from double the susceptibility of a single exciton [20]. Studies on the diamagnetic susceptibility of an exciton in quantum wells especially in ZnO/$Zn_{1-x}Mg_xO$ quantum wells are reported less in literature.

In this paper, the binding energy and diamagnetic susceptibility of light hole exciton (lh-exciton) and heavy hole exciton (hh-exciton) in NTQW formed by GaAs/$Ga_{1-x}Al_xAs$ and ZnO/$Zn_{1-x}Mg_xO$ are calculated as a function of width of the well as well as Al and Mg concentrations respectively. The results are compared with the available experimental data and also with the results for various potential profiles.

## 2. Theory

The Hamiltonian for an exciton in a quantum well with an applied magnetic field $\boldsymbol{B}$ along the growth direction ($z$-axis) is given in the effective mass approximation as [21],

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$$\mathcal{H} = \frac{1}{2m_e^*}\left(p + \frac{eA}{c}\right)^2 + \frac{1}{2m_{ih}^*}\left(p - \frac{eA}{c}\right)^2 - \frac{e^2}{\varepsilon_o r} + V_e(z_e) + V_h(z_h) \quad (1)$$

where e is the electronic charge, c is the velocity of light and $\varepsilon_o$ is the dielectric constant. $m_{ih}^*$ is the effective mass of the hole, i = h for heavy hole or i = l for light hole and $m_e^*$ is the effective mass of the electron.

The vector potential $\boldsymbol{A}$ can be written in the cylindrical gauge [22] as

$$\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r} \quad (2)$$

where $r = \sqrt{\rho^2 + |z_e - z_h|^2}$ and ρ is the distance in x–y plane [21].

Using the cylindrical co-ordinate system, the Hamiltonian for an exciton can be written as [13, 22]

$$\mathcal{H} = -\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right] - \frac{\mu_{ih}^*}{m_e^*}\frac{\partial^2}{\partial z_e^2} - \frac{\mu_{ih}^*}{m_{ih}^*}\frac{\partial^2}{\partial z_h^2} + V_e(z_e) + V_{ih}(z_{ih}) - \frac{2}{r} + \gamma\left(\frac{m_{ih}^* - m_e^*}{m_e^* + m_{ih}^*}\right)L_z + \frac{1}{4}\gamma^2\rho^2 \quad (3)$$

$\mu_{ih}^*$ is the reduced effective mass of the exciton given by [13],

$$\frac{1}{\mu_{ih}^*} = \frac{1}{m_e^*} + \frac{1}{m_{ih}^*} \quad (4)$$

The effective Bohr radius ($a^* = \hbar^2\varepsilon_o/\mu_{ih}^* e^2$) and the effective Rydberg ($R^* = \mu_{ih}^* e^4/2\hbar^2\varepsilon_o^2$) are used as the units of length and energy respectively. In Eq. (3), $L_z$ is the z-component of the angular momentum and γ is the dimensionless measure of the magnetic field, defined as $\gamma = \frac{e\hbar B}{2\mu_{ih}^* c R^*}$.

The potential profile for the electron and hole in NTQW [12] is given by

$$V_j(z_j) = \begin{cases} V_{oj}\left|\frac{z_j}{L/2}\right|^{\frac{2}{3}} & |z_j| < L/2 \\ V_{oj} & |z_j| > L/2 \end{cases} \quad (5)$$

where $V_{oj}$ is the barrier height, which depends on the composition x of Al or Mg and j = e for electron or lh for light hole or hh for heavy hole.

The trial wavefunction for the exciton in the NTQW with applied magnetic field is taken to be of the form [13, 22]

$$\Psi = \begin{cases} N e^{-\alpha_e^2 z_e^2} e^{-\alpha_h^2 z_h^2} e^{-ar} e^{-\lambda\rho^2} & |z| < L/2 \\ N_1 e^{-\beta_e|z_e|} e^{-\beta_h|z_h|} e^{-ar} e^{-\lambda\rho^2} & |z| > L/2 \end{cases} \quad (6)$$

where $\alpha_e, \alpha_h, \beta_e, \beta_h, a$ and $\lambda$ are variational parameters. The wavefunction for the NTQW is chosen to be that of a PQW with $\alpha_e, \alpha_h, \beta_e$ and $\beta_h$ as variational parameters, which are constants in PQW [8, 9]. $e^{-ar}$ and $e^{-\lambda\rho^2}$ are the parts of the wavefunction for the electron–hole interaction with $r = \sqrt{\rho^2 + |z_e - z_h|^2}$ and for the applied magnetic field respectively. N is the normalization constant. The continuity conditions for wavefunction and its derivative at $z_e = L/2$ and $z_h = L/2$ relate the normalization constants N and $N_1$. $\langle\mathcal{H}\rangle$ is evaluated as a function of the variational parameters using the Hamiltonian in Eq. (3) and the trial wavefunction in Eq. (6) as,

$$\langle\mathcal{H}\rangle = \frac{\int \Psi^* \mathcal{H} \Psi d\tau}{\int \Psi^* \Psi d\tau} \quad (7)$$

The binding energy ($E_B$) of the exciton is then given by

$$E_B = E_e + E_h + \gamma - \langle\mathcal{H}\rangle_{min} \quad (8)$$

where $E_e$ and $E_h$ are the ground state energies of electron and hole respectively in bare NTQW given in Eq. (5) obtained variationally. $\langle\mathcal{H}\rangle_{min}$ is the minimized value of $\langle\mathcal{H}\rangle$ with respect to the variational parameters.

Diamagnetic susceptibility of an exciton in a quantum well is given by [19]

$$\chi_{dia} = \frac{-e^2}{6\mu_{ih}^* \varepsilon_0 c^2}\langle\rho^2\rangle \quad (9)$$

where c = 137, e = 1 and $m_o = 1$ in a.u. and $\langle\rho^2\rangle$ is the mean square distance between electron and hole.

## 3. Results and discussion

All the material parameters used in our calculations such as effective masses of heavy hole, light hole and electron; reduced masses of lh-exciton and hh-exciton; dielectric constants of GaAs and ZnO are given in Table 1.

The total bandgap difference $\Delta E_g$ between GaAs and $Ga_{1-x}Al_xAs$ is calculated from the equation [22],

$$\Delta E_g = 1.155x + 0.37x^2 \, \text{eV} \quad (10)$$

$\Delta E_g$ between ZnO and $Zn_{1-x}Mg_xO$ is determined by the following expression [17],

**Table 1** Material parameters used in the calculations

| Parameters | GaAs | ZnO |
|---|---|---|
| $m_e^*$ | 0.0665 $m_0$ [13] | 0.21 $m_0$ [17] |
| $m_{hh}^*$ | 0.34 $m_0$ [13] | 0.78 $m_0$ [16] |
| $m_{lh}^*$ | 0.094 $m_0$ [13] | 0.59 $m_0$ [17] |
| $\mu_{hh}^*$ | 0.05562 $m_0$ | 0.165 $m_0$ |
| $\mu_{1h}^*$ | 0.03895 $m_0$ | 0.155 $m_0$ |
| $\varepsilon_0$ | 13.2 [13] | 8.1 [16] |

Where $m_0$ is the free electron mass

$$\Delta E_g = 1.93x + 1.57x^2 \text{ eV} \quad (11)$$

The barrier height $V_{oe}$ or the conduction band discontinuity is taken to be 0.65 $\Delta E_g$ for GaAs/$Ga_{1-x}Al_xAs$ [22] and 0.60 $\Delta E_g$ for ZnO/$Zn_{1-x}Mg_xO$ [16] quantum well. The effects due to the effective mass mismatch, conduction band nonparabolicity and dielectric constant mismatch are not considered, since they are expected to be small in the $E_B$ calculations [13], which is the difference between the eigenvalues of two Hamiltonians each having to have the above features.

Figure 1 shows the variation of $E_B$ of lh-exciton in NTQW formed by GaAs/$Ga_{0.7}Al_{0.3}As$ as a function of wellwidth L for various values of γ. The barrier heights of conduction band and valence band are calculated as 246.87 and 132.93 meV respectively. For lh-exciton in GaAs, the magnetic field $\gamma = 1$ corresponds to a magnetic field of about 20.45 kG. For comparison, we have also displayed the variation of $E_B$ as a function of wellwidth without magnetic field i.e. $\gamma = 0$ [13]. Increase in magnetic field leads to more binding between electron and light hole. But as the magnetic field increases, the increase in $E_B$ decreases.

As the wellwidth L is reduced, $E_B$ slowly increases until it reaches a maximum at certain value of L. As L is reduced further, $E_B$ decreases rapidly due to the tunnelling of trial wavefunction through the barrier and the unbounding of electron and hole. For all magnetic fields, the maximum $E_B$ of lh-exciton is observed at L = 20 nm.

In Fig. 2 we display the variation of $E_B$ of hh-exciton in NTQW composed of GaAs/$Ga_{0.7}Al_{0.3}As$ as a function of wellwidth L for different magnetic field parameters γ. As in the case of lh-exciton, the presence of magnetic field increases the electron–hole binding. For hh-exciton in GaAs, the magnetic field parameter $\gamma = 1$ corresponds to the magnetic field of about 41.76 kG. The behaviour of $E_B$ of hh-exciton is similar to the case of lh-exciton. The maximum $E_B$ occurs at 16 nm for all magnetic field

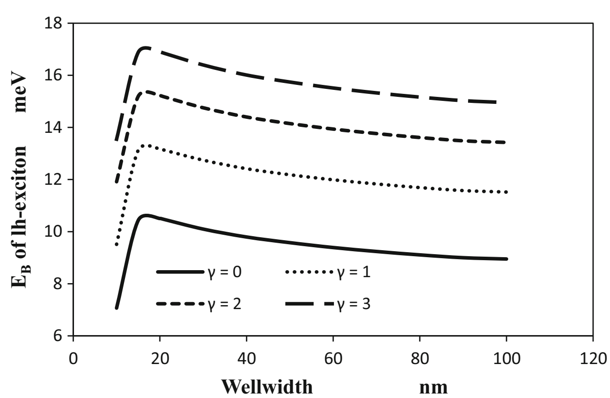


**Fig. 1** Variation of the binding energy of lh-exciton in NTQW formed by GaAs/$Ga_{0.7}Al_{0.3}As$ as a function of wellwidth L for different magnetic fields

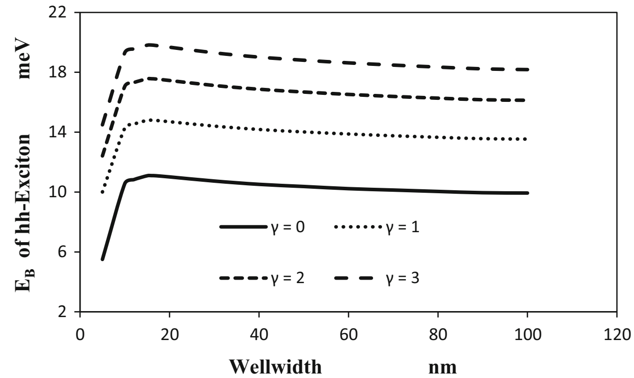


**Fig. 2** Variation of the binding energy of hh-exciton in NTQW formed by GaAs/$Ga_{0.7}Al_{0.3}As$ as a function of wellwidth L for different magnetic fields

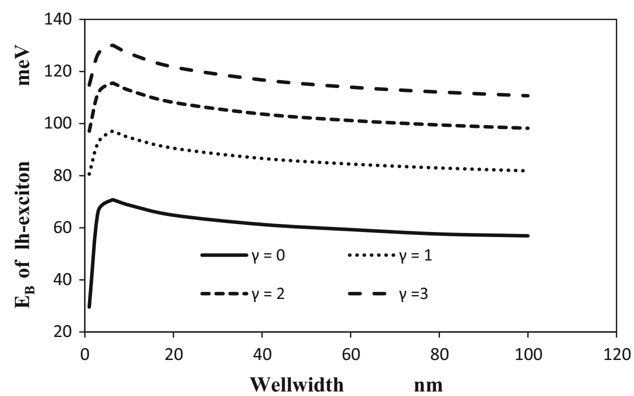


**Fig. 3** Variation of the binding energy of lh-exciton in NTQW formed by ZnO/$Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth L for different magnetic fields

parameters. $E_B$ of hh-exciton is greater than that of lh-exciton. The behaviour of $E_B$ is qualitatively similar to those of exciton in RQW [2–6], PQW [8, 9], TQW [10] and SQW [11]. But the values of $E_B$ in NTQW are quantitatively larger compared to those in quantum wells of other profiles. Hence the use of NTQW will be better in optical devices than the use of quantum wells of other shapes.

In Figs. 1 and 2, the plots for $\gamma = 0$ are similar to those presented in Fig. 3 of Arulmozhi and Balasubramanian [13] after conversion of units (from effective Rydberg to meV and from effective Bohr radius to nm). The small variations are due to the difference in the values of the parameters used (Experimental values from Ref. [12] are used in Ref. [13]). The effect of magnetic field on the exciton binding energy in NTQW is previously reported by the authors [23] with the Zeeman term in the Hamiltonian inversely proportional to the reduced effective mass of the exciton i.e. $\left(\propto \frac{1}{\mu_{ih}}\right)$. But in the present work, due to the opposite charge sign of electron and hole, this Zeeman term in the Hamiltonian is taken to be proportional to the difference between the inverted mass of hole and inverted mass of electron $\left(\propto \frac{1}{m_e} - \frac{1}{m_{ih}}\right)$. The variations found in the results of the present work and Ref. [23] may be due to the inclusion of this effect.

Figure 3 describes the behaviour of $E_B$ of lh-exciton in NTQW composed of $ZnO/Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth L for different magnetic fields. For ZnO, 432.18 and 288.12 meV are the barrier heights of conduction band and valence band respectively. For lh-exciton in ZnO, the magnetic field parameter $\gamma = 1$ corresponds to the magnetic field of about 861.3 kG. In the presence of magnetic field, lh-exciton is more bounded than that in the absence of magnetic field. The variation of $E_B$ with wellwidth in ZnO is similar to the case of GaAs. The maximum $E_B$ is observed at L = 6 nm for all magnetic fields. $E_B$ is much larger, but the turnover wellwidth is smaller in ZnO quantum well than that in GaAs quantum well.

In Fig. 4, we present the variation of $E_B$ of hh-exciton in NTQW formed by $ZnO/Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth for different magnetic fields. From this plot, it is observed that the hh-excitons are more bounded than the lh-excitons for all magnetic fields. The magnetic field parameter $\gamma = 1$ is about 976 kG. When the wellwidth increases, $E_B$ initially increases rapidly, reaches its maximum and then starts to decrease gradually. For all magnetic fields, the maximum value of $E_B$ occurs at 4 nm. As mentioned earlier, the reason for the decrease of $E_B$ for L < 4 nm is the penetrating of the trial wavefunction into the barrier, so that the excitons are less bounded. The peak values of $E_B$ of both excitons without magnetic field in $ZnO/Zn_{0.7}Mg_{0.3}O$ are larger than the experimental data reported for Mg concentration x = 0.27 and for other potential profiles [14, 16]. This again confirms that excitons are more stable in NTQW than other profiles which leads to the realization of excitonic opto-electronic devices.

Figure 5 shows the behaviour of $E_B$ of lh-exciton and hh-exciton in NTQW composed of $GaAs/Ga_{1-x}Al_xAs$ as a function of Aluminium composition x with the magnetic field parameter $\gamma = 1$ and L = 20 nm. It is observed that the increase in Al composition leads to increased binding, because the barrier height increases as Al composition increases [3–5]. In this case, $E_B$ of hh-exciton is more than that of lh-exciton.

In Fig. 6, we display the variation of $E_B$ of lh-exciton and hh-exciton in $ZnO/Zn_{1-x}Mg_xO$ NTQW for various Mg compositions x with $\gamma = 1$ and L = 20 nm. As in the case of GaAs/GaAlAs quantum well, $E_B$ increases with the increase of barrier height or Mg composition. Comparison of $E_B$ of lh-exciton and hh-exciton shows that hh-exciton is more bounded than lh-exciton.

In Fig. 7 and 8, we present the variation of diamagnetic susceptibility of lh-exciton and hh-exciton in NTQW formed by $GaAs/Ga_{0.7}Al_{0.3}As$ as a function of wellwidth for different magnetic fields. For lh-exciton, it is observed that the diamagnetic susceptibility increases with decrease of the wellwidth, reaches a maximum and then decreases. But for $\gamma > 3$, it continuously increases as wellwidth decreases. For hh-exciton, it increases as the wellwidth

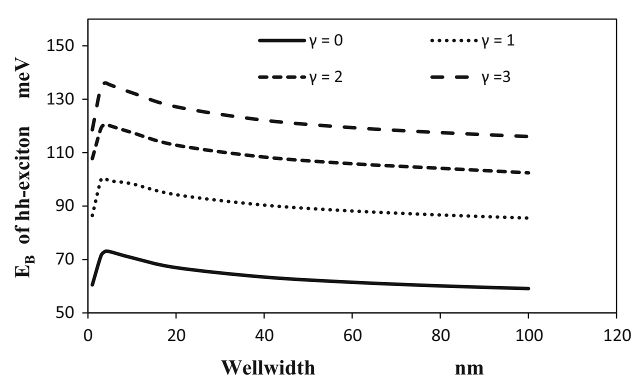


**Fig. 4** Variation of the binding energy of hh-exciton in NTQW formed by $ZnO/Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth L for different magnetic fields

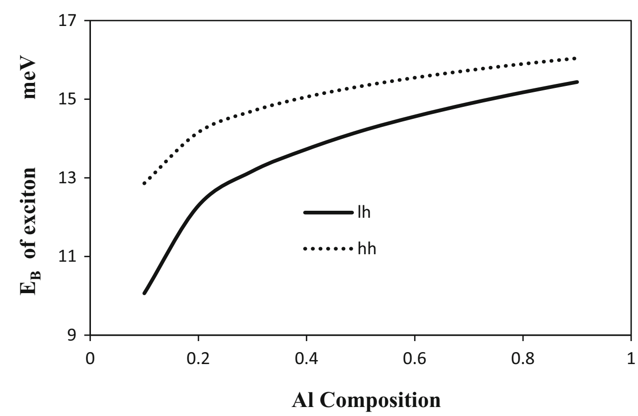


**Fig. 5** Variation of the binding energy of lh-exciton and hh-exciton in NTQW formed by $GaAs/Ga_{1-x}Al_xAs$ as a function of x for $\gamma = 1$

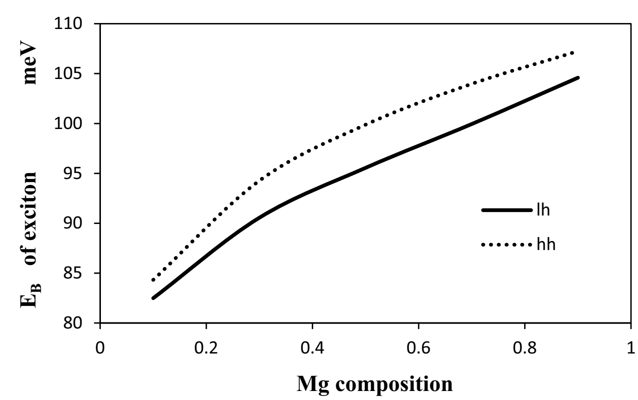


**Fig. 6** Variation of the binding energy of lh-exciton and hh-exciton in NTQW formed by $ZnO/Zn_{1-x}Mg_xO$ as a function of x for $\gamma = 1$

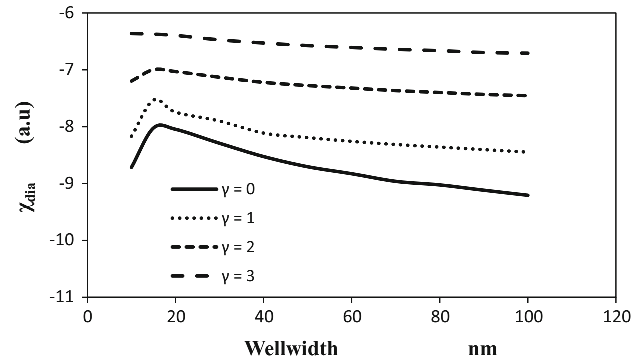


**Fig. 7** Variation of the diamagnetic susceptibility of lh-exciton in NTQW formed by $GaAs/Ga_{0.7}Al_{0.3}As$ as a function of wellwidth L for different magnetic fields

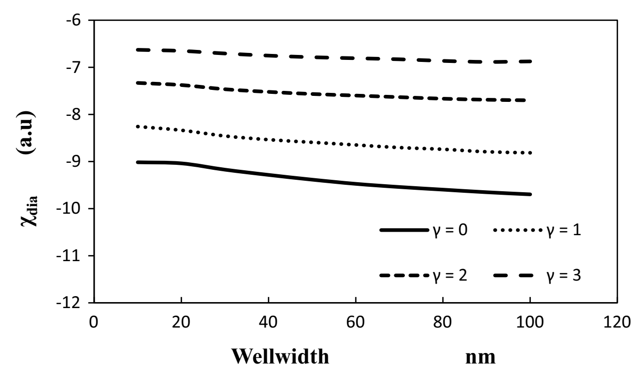


**Fig. 8** Variation of the diamagnetic susceptibility of hh-exciton in NTQW formed by $GaAs/Ga_{0.7}Al_{0.3}As$ as a function of wellwidth L for different magnetic fields

decreases for all magnetic fields. This behaviour is similar to diamagnetic susceptibility of hydrogenic donor in RQW [19, 20]. The diamagnetic susceptibility of hh-exciton is greater than that of lh-exciton.

We present the variation of diamagnetic susceptibility of lh-exciton and hh exciton in NTQW composed of $ZnO/Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth for various magnetic fields in Figs. 9 and 10 respectively. From both graphs, it is observed that the diamagnetic susceptibility of lh-exciton and hh-exciton decreases as wellwidth increases. Diamagnetic susceptibility has greater value in ZnO/ZnMgO quantum well than in GaAs/GaAlAs quantum well.

Figure 11 shows the variation of diamagnetic susceptibility of lh-exciton and hh-exciton in NTQW formed by $GaAs/Ga_{1-x}Al_xAs$ and $ZnO/Zn_{1-x}Mg_xO$ as a function of x for $\gamma = 1$ and L = 20 nm. When the Al/Mg composition or barrier height increases, the diamagnetic susceptibility increases in all the cases. At present, there are no theoretical or experimental data to compare our results for the

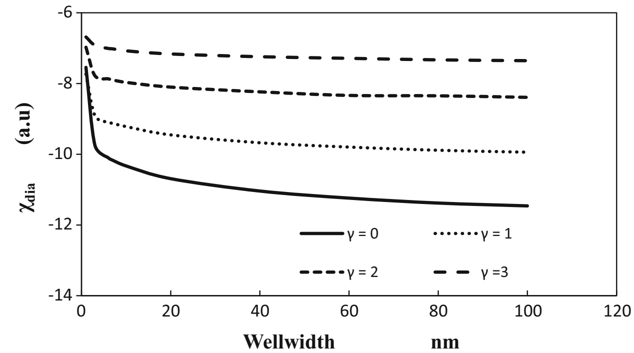


**Fig. 9** Variation of the diamagnetic susceptibility of lh-exciton in NTQW formed by $ZnO/Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth L for different magnetic fields

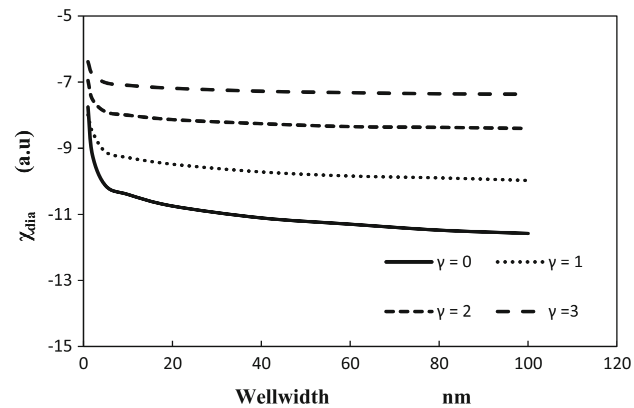


**Fig. 10** Variation of the diamagnetic susceptibility of hh-exciton in NTQW formed by $ZnO/Zn_{0.7}Mg_{0.3}O$ as a function of wellwidth L for different magnetic fields

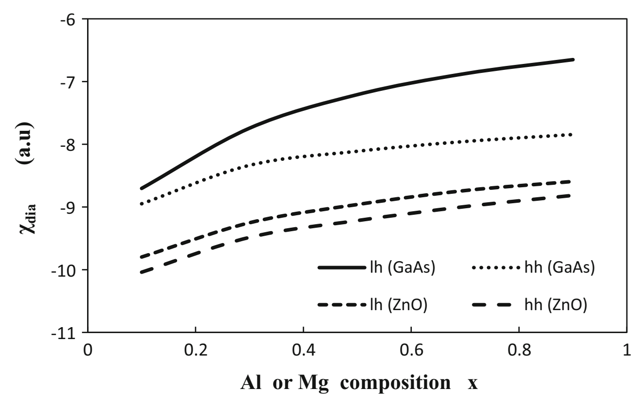


**Fig. 11** Variation of the diamagnetic susceptibility of lh-exciton and hh-exciton in NTQW formed by $GaAs/Ga_{1-x}Al_xAs$ and $ZnO/Zn_{1-x}Mg_xO$ as a function of x for $\gamma = 1$

diamagnetic susceptibility of exciton in $ZnO/Zn_{1-x}Mg_xO$ NTQW. However, in future our calculation may support the experimental work.

## 4. Conclusions

We have studied the diamagnetic susceptibility and binding energy of lh-exciton and hh-exciton in NTQW formed by GaAs/GaAlAs and ZnO/ZnMgO as a function of wellwidth and Al/Mg composition. The diamagnetic susceptibility and the binding energy increases when the applied magnetic field increases. Excitons in ZnO/ZnMgO quantum well have larger binding energy than in GaAs/GaAlAs quantum well which leads to higher stability of the exciton in this quantum well and enhancement of the performance of ZnO based excitonic devices. Diamagnetic susceptibility is larger in ZnO/ZnMgO quantum well than in GaAs/GaAlAs quantum well, which implies ZnO to be more promising for magnetic field applications.

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