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Polaron Effects of Exciton in ZnSe/ZnS Parabolic Quantum Wells

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Abstract: ZnSe-related quantum well structures have attracted much interest with regard to their optoelectronic application. They have large optical nonlinearity due to the large exciton binding energy compared with the Ⅲ-Ⅴ compound semiconductors. The ZnSe/ZnS quantum well structure is a promising material for fabricating laser diodes since they have a direct band gap with wide band gap energy up to 3.75 eV at room temperature. The purpose of the present work is to investigate the polaron effects of the exciton in the ZnSe/ZnS parabolic quantum well (PQW). We assume the trial function has a simple form with the variables describing the motion within the quantum well plane separated from those describing the motion along the growth axis. The interaction of the charged particles with bulk longitudinal optical(LO) phonons is considered only, and the energy of the system is obtained by using a variational method developed by Lee, Low and Pines. The results showed that the ground state energy and the binding energy of the exciton with LO-phonon decrease rapidly with increasing the well width L at the beginning, then decreases very slowly with increasing L. In contrast to our previous work, it can be found that the exciton in the ZnSe/ZnS PQWs is more strongly bound than that in the GaAs/$\mathrm{Ga}_{1-x}\mathrm{Al}_x$As PQWs.

Key words: exciton; polaron; parabolic quantum well
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1 Introduction

Because of several characteristic features, in contrast to rectangular quantum wells, the PQWs have attracted considerable interest. These interesting features include, apart from obvious equidistant energy separation of eigenvalues, a weak dependence of the eigenenergies on the barrier height and well width for PQWs with the same value of the curvature parameter. This possibly makes an accurate determination of the band offset parameters[1~4]. On the experimental side, optical properties of the real PQW structures are usually good, indeed with rich spectra revealed by various methods. It is possible, for example, to observe 1s, 2s, 3s exciton states[5]. Therefore, one can study the energy of various excitonic states confined in PQWs in details. This enables various theories of confined excitons to be put to a stringent test.

Up to now, the polaron effects of exciton in the ZnSe/ZnS PQW have few been studied. ZnSe related quantum structures have attracted much interest with regard to the optoelectronic application, such as laser diodes covering the blue to the ultraviolet spectral region. Also, they have large optical nonlinearity due to the large exciton binding energy compared with the Ⅲ-Ⅴ compound semiconductors. This gives the possibility of application as an optical modulator for second harmonic generation of lasers. Therefore, great effort has been made to fabricate ar-

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tificial structures with these ZnSe-related materials. The ZnSe/ZnS quantum well structure is a promising material for fabrication of laser diodes since they have a direct band gap with wide band gap energy up to 3.75 eV at room temperature [6]. In all probability, ZnSe/ZnS PQWs have very characteristic features.

The purpose of this paper is to investigate the polaron effects of the exciton in the ZnSe parabolic quantum well. The energies of exciton in the ZnSe/ZnS PQW have been calculated by using the variational procedure with the separable wave function. The interaction of the electron and hole with bulk LO-phonons is considered only.

2 Theory

We consider the interaction of exciton in an infinitely deep PQW with LO-phonons. The Hamiltonian of the system can be written as

$$H = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_h}\nabla_2^2 - \frac{e^2}{\varepsilon_\infty |\boldsymbol{r}_1 - \boldsymbol{r}_2|} + V_e(z_1) + V_h(z_2) + \sum_q \hbar\omega a_q^+ a_q + \sum_q [V_q a_q (e^{i\boldsymbol{q}\cdot\boldsymbol{r}_2} - e^{i\boldsymbol{q}\cdot\boldsymbol{r}_1} + h\cdot c],$$

$$V_j(z_j) = V_j^0 (z_j/b)^2, \tag{1}$$

In Eq. (1), m_e (m_h) is the effective mass of the electron (hole), $V_e(z_1)$, $V_h(z_2)$ are the effective parabolic potential, ω is the frequency of LO-phonon, a_q^+ (a_q) is the creation (destruction) operator of the phonon. The coefficient of electron-phonon coupling is given by

$$V_q = i\left[\frac{2\pi e^2}{V}\frac{\hbar\omega}{q^2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\right]^{1/2},$$

We introduce center-of-mass coordinate and relative coordinate

$$\boldsymbol{R} = \beta_1 \boldsymbol{r}_1 + \beta_2 \boldsymbol{r}_2,$$
$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2,$$

here $\beta_1 = m_e/M$, $\beta_2 = m_h/M$, $M = m_e + m_h$, and adopt cylindrical polar coordinates due to the symmetry of our problem, the Hamiltonian of (1) becomes

$$H = -\frac{\hbar^2}{2M}\nabla_{R\parallel}^2 - \frac{\hbar^2}{2\mu}\nabla_{r\parallel}^2 - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_1^2} - \frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_2^2} - \frac{e^2}{\varepsilon_\infty r} + V_e(z_1) + V_h(z_2) + \sum_q \hbar\omega a_q^+ a_q + \sum_q [V_q a_q e^{i\boldsymbol{q}_\parallel\cdot\boldsymbol{R}_\parallel}(e^{-i\beta_1\boldsymbol{q}_\parallel\cdot\boldsymbol{r}_\parallel} e^{iq_\perp z_2} - e^{i\beta_2\boldsymbol{q}_\parallel\cdot\boldsymbol{r}_\parallel} e^{iq_\perp z_1}) + h\cdot c], \tag{2}$$

where μ is the reduced mass. In the case of weak or intermediate electron-phonon interaction, we can use Lee, Low and Pines variational method[7~10] to introduce two successive unitary transformations: the first unitary operator is to eliminate the center-of-mass coordinate of exciton in the well plane,

$$U_1 = \exp[i(\boldsymbol{K}_\parallel - \sum_q \boldsymbol{q}_\parallel a_q^+ a_q)\cdot \boldsymbol{R}_\parallel],$$

After the first transformation we have

$$H^* = U_1^{-1} H U_1 = \frac{\hbar^2}{2M}\left(\boldsymbol{K} - \sum_q q_\parallel a_q^+ a_q\right)^2 - \frac{\hbar^2}{2\mu}\nabla_{r\parallel}^2 - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_1^2} - \frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_2^2} - \frac{e^2}{\varepsilon_\infty r} + V_1(z_1) + V_2(z_2) + \sum \hbar\omega a_q^+ a_q + \sum [V_q a_q (e^{-i\beta_1\boldsymbol{q}_\parallel\cdot\boldsymbol{r}_\parallel} e^{iq_\perp z_2} - e^{-i\beta_2\boldsymbol{q}_\parallel\cdot\boldsymbol{r}_\parallel} e^{iq_\perp z_1}) + h\cdot c], \tag{3}$$

The second one is to displace the phonon coordinate

$$U_2 = \exp[\sum_q (a_q^+ f_q - a_q f_q^*)],$$

where the displacement amplitude can be determined (and its conjugate complex), similarly to the works of [11,12], as

$$f_q = -\frac{2M}{\hbar^2}\frac{W_q^*}{u^2 + q^2},$$
$$W_q = V_q (e^{-i\beta_1\boldsymbol{q}_\parallel\cdot\boldsymbol{r}_\parallel} e^{iq_\perp z_2} - e^{-i\beta_2\boldsymbol{q}_\parallel\cdot\boldsymbol{r}_\parallel} e^{iq_\perp z_1})$$
$$\frac{\hbar^2 u^2}{2M} = \hbar\omega, \tag{4}$$

By the very complex compute, the effective Hamiltonian of the system is

$$H_{eff} = \langle 0 | U_2^{-1} H^* U_2 | 0 \rangle = -\frac{\hbar^2}{2\mu}\nabla_{r\parallel}^2 - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_1^2} - \frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_2^2} + V_e(z_1) + V_h(z_2) - 2\alpha\hbar\omega\left(1 - \frac{2\beta_1^2 + 2\beta_2^2 + 1}{12\beta_1\beta_2}\right) - \frac{e^2}{\varepsilon_0 r} - \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\frac{e^2}{r}e^{-ur} + 2\alpha\hbar\omega\left(\frac{1}{ur}\right)^3\left[1 - \frac{1}{4}(ur + 2)e^{-ur}\right], \tag{5}$$

In Eq. (5), we have ignored the interaction between virtual phonons with different wave vectors emitted by recoiling hole and electron, and assume the momentum of the exciton $\boldsymbol{K}_\parallel = 0$. In the right side of (5), the 6th term is self-energy of the exciton, and the constant of electron-phonon interaction

$$\alpha = (\mathrm{M}e^2/\hbar^2 u)(1/\varepsilon_\infty - 1/\varepsilon_0),$$

the rest parts are effective potential between the electron and the hole, induced by the coupling of the electron and the hole with the phonons.

We use a variational approach to resolve the Schrodinger equation of the Hamiltonian of (5), the trial wave function is

$$\psi = \exp(-\xi z_1^2)\exp(-\eta z_2^2)\exp(-\zeta\rho),$$

where ξ, η, ζ are the variational parameters, and $\rho^2 = x^2 + y^2$. The form of the separable wave function is more convenient for actual calculations than that of the non-separable function[13].

The ground state energy $E_{\min}$ of the exciton is determined by minimizing the energy E

$$E = \frac{\langle\psi | H_{\mathrm{eff}} | \psi\rangle}{\langle\psi | \psi\rangle},$$

$$\frac{\partial E}{\partial\xi} = \frac{\partial E}{\partial\eta} = \frac{\partial E}{\partial\zeta} = 0,$$

The binding energy is then

$$E_{\mathrm{b}} = E_0 + \alpha_{\mathrm{e}}\hbar\omega + \alpha_{\mathrm{h}}\hbar\omega - E_{\min},$$

E_0 is the energy of free exciton, and the Hamiltonian of the free exciton is

$$H_0 = \frac{\hbar^2}{2m_{\mathrm{e}}}\frac{d^2}{dz_1^2} - \frac{\hbar^2}{2m_{\mathrm{h}}}\frac{d^2}{dz_2^2} + V_{\mathrm{e}}(z_1) + V_{\mathrm{h}}(z_2),$$

and we choose the trial wave function as

$$\psi_0 = \mathrm{e}^{-\xi z_1^2}\mathrm{e}^{-\eta z_2^2},$$

The energy of a free exciton in a PQW is

$$E_0 = \langle\psi_0 | H_0 | \psi_0\rangle / \langle\psi_0 | \psi_0\rangle,$$

3 Numerical Results and Discussion

We have calculated the ground state energy and the binding energy of the exciton in the ZnSe/ZnS PQW. We assume that the effective mass and the dielectric constant are the same values throughout the whole structure. For the exciton in the ZnSe PQW, we use the effective Bohr radius $a_0 = \frac{\varepsilon_0\hbar^2}{\mu e^2}$ as the length unit and the effective Rydberg $R_y = \frac{\mu e^4}{2\hbar^2\varepsilon_0^2}$ as the energy unit. The parameters[6,13] used in our calculation are $m_{\mathrm{e}} = 0.17m_0$, $m_{\mathrm{h}} = 0.15m_0$, $\hbar\omega = 31$ meV, $\varepsilon_0 = 8.10$, $\varepsilon_\infty = 5.9$, where m_0 as the free-electron mass. $R_y = 16.57$ meV, $a_0 = 5.377$ nm. The numerical results are illustrated in Fig. 1 and Fig. 2.

Fig. 1 shows the exciton ground state energy as a function of the ZnSe PQW size L. It is found that the ground state energy of the exciton with LO-phonon decreases rapidly with increasing the well width (L) at first and then decreases slowly with increasing L.

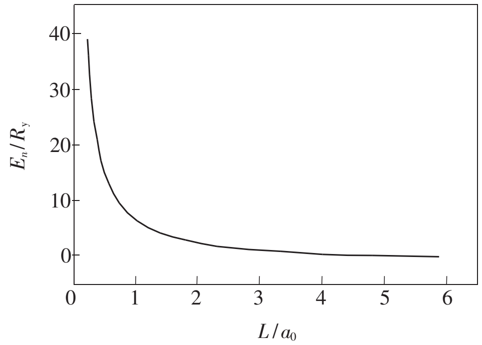

Fig. 1 The ground state energy of exciton as a function of the well size. The electron- and hole-phonon interactions are considered.

Fig. 2 shows the result we have obtained for the exciton binding energy which is plotted as a function of the ZnSe PQW thickness L. The binding energy of the exciton with LO-phonon decreases with increasing L. Through the photoluminescence measurement of ZnSe/ZnS single quantum wells, S. K. Chang *et al*[6]. observed clear shifts of the excitons to higher energies with decreasing well width. The experimental results are in qualitative agreement with our theoretical results.

From the two figures we can see that our result is almost the same as one of the results obtained by

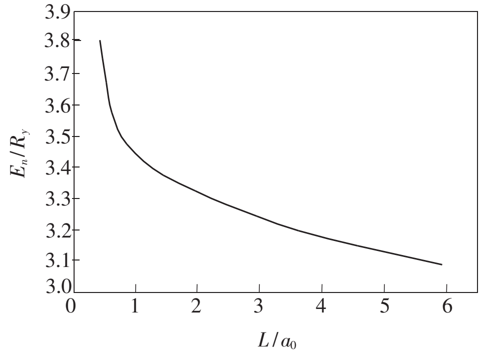

Fig. 2 The binding energy of exciton as a function of the well size. The electron- and hole-phonon interactions are considered.

us in the GaAs/$Ga_{1-x}Al_xAs$ PQWs[14] by qualitative analysis, although we use a different trial function and different materials. But it is different by quantitative analysis. The binding energy of exciton with LO-phonon in the ZnSe PQW is higher than that in the GaAs PQW. This shows that the ZnSe/ZnS PQWs result in a stronger localization of the exciton than that in GaAs/$Ga_{1-x}Al_xAs$ PQWs.

4　Conclusion

We study theoretically the polaron effects of the exciton in ZnSe/ZnS PQWs by using a developed LLP method to deal with the interaction between charged particles and phonons. The ground state energy and binding energy of exciton are obtained. The results show that the energy of the exciton with LO-phonon decreases rapidly with increasing well width *L* at the beginning, then decreases very slowly with increasing *L*. In contrast to our previous work, it can be found that the exciton in the ZnSe/ZnS PQWs is more strongly bound than that in the GaAs/$Ga_{1-x}Al_xAs$ PQWs.

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ZnSe/ZnS 抛物量子阱中激子的极化子效应

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摘要：采用推广的 LLP 方法研究了 ZnSe/ZnS 抛物量子阱中激子的极化子效应。考虑电子和空穴与 LO 声子的相互作用，得到了激子基态能量和结合能随阱宽的变化关系。结果表明，阱宽较小时，能量随着阱宽的增大而急剧减小；阱宽较大时，能量减小的比较缓慢。和我们以前的工作对比，我们发现 ZnSe/ZnS 抛物量子阱对激子的束缚强于 GaAs/Ga$_{1-x}$Al$_x$As 抛物量子阱。

关 键 词：激子；极化子；抛物量子阱

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