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Binding energy of magneto-biexcitons in semiconductor nano-rings

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Abstract

We report a simulation on the magneto-biexciton system of asymmetrical *InAs/GaAs* nano-rings, using a smooth three dimensional confinement potential which realistically describes electronic properties of the rings. In our calculation, we use the Hartree approximation to calculate the self-consistent energy for exciton and biexciton confined in the system. We simulate recombination energy, binding energy and their diamagnetic shifts and compare those results with experimental data obtained from the magneto-photoluminescence measurement. We found that using the realistic geometry and composition of the asymmetric nano-ring in our simulations we are able to reproduce experimental data with good accuracy.

Keywords: magnetoexcitons, nano rings, diamagnetic shift.

1. Introduction

Semiconductor *InAs/GaAs* nano-rings are torus-shaped nano-object recently attracted much attention because of their unusual magnetic properties [1,2]. Nano-rings (like quantum dots) demonstrate atom-like spectra for electrons and holes that makes them interesting for device applications in optoelectronics, quantum information etc. Since excitons determine the optical response of semiconductors, study of the magneto-excitonic spectra in nano-rings can provide the exciting opportunity to observe electronic wave-function phases in magneto-optical experiments [3]. The binding energy of an excitonic complex in quantum dots and nano-rings and their dependencies on external magnetic field are expected to be different compared to the bulk material due to the spatial confinement of electrons and holes. On the other hand, because of the difference in the geometry of quantum dots and nano-rings the study on the magneto-photoluminescence of the nano-rings is bringing new physics in this field. In this paper we simulate the excitonic energies and their diamagnetic shifts within a realistic three dimensional description of the asymmetrical *InAs/GaAs* nano-rings.

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2. Description of the simulation method

For an asymmetric nano-ring in our calculation we first assume that the ring was grown on a substrate parallel to the x - y plane. We model the geometry of the ring by mapping the height of the ring with the function $h(x,y)$ which can be retraced from fitting of known experimental data [1,2]:

$$h(x,y) = h_0 + \frac{\left[h_M \left(1 + \xi \frac{x^2 - y^2}{x^2 + y^2} \right) - h_0 \right] \gamma_0^2}{R^2} \cdot \frac{R^2 - \left(\sqrt{x^2 + y^2} - R \right)^2}{\left(\sqrt{x^2 + y^2} - R \right)^2 + \gamma_0^2}, \sqrt{x^2 + y^2} \leq R; \quad (1)$$

$$h(x,y) = h_\infty + \frac{\left[h_M \left(1 + \xi \frac{x^2 - y^2}{x^2 + y^2} \right) - h_\infty \right] \gamma_\infty^2}{\left(\sqrt{x^2 + y^2} - R \right)^2 + \gamma_\infty^2}, \sqrt{x^2 + y^2} > R,$$

where h_0 , h_M and h_∞ are the heights at the center of the ring, the rim of the ring (at $x^2 + y^2 = R^2$), and far away from the ring correspondingly; γ_0 and γ_∞ stand for the inner and the outer slope near the rim; ξ is the anisotropy of the ring in the x - y plane. On the base of this fit we introduce a three dimensional confinement potential $V_e(x,y,z)$ for electrons in the ring:

$$V_e(x,y,z) = \Delta E_e \left\{ 1 - \frac{1}{4} \cdot \left[1 + \tanh\left(\frac{z-z_0}{a}\right) \right] \cdot \left[1 - \tanh\left(\frac{1-h(x,y)+z_1}{a}\right) \right] \right\}, \quad (2)$$

where $\Delta E_e = V_{max} - V_{min}$ is the electronic band offset in the system, V_{max} is the maximum value of the potential (outside of the object), and V_{min} is the minimum value of the potential (inside the object). The slope of the potential and the range of the potential change at the boundaries of the object are controlled by the parameter a .

On the base of the potential (2) a mapping function $M(x,y,z)$ can be define like the following:

$$M(x,y,z) = 1 - \frac{V_e(x,y,z)}{\Delta E_e}. \quad (3)$$

The mapping function give us information about geometry and position dependent composition of the ring, and then we model the position dependent effective masses for electrons (holes) - $m_{e(h)}^*(x,y,z)$, energy gap - $E_g(x,y,z)$, hole's confinement potential $V_h(x,y,z)$, and the profile of the permittivity of the system - $\varepsilon(x,y,z)$:

$$\begin{aligned} m_{e(h)}^*(x,y,z) &= m_{e(h)(in)}^* \cdot M(x,y,z) + m_{e(h)(out)}^* \cdot [1 - M(x,y,z)], \\ E_g(x,y,z) &= E_{g(in)} \cdot M(x,y,z) + E_{g(out)} \cdot [1 - M(x,y,z)], \\ V_h(x,y,z) &= E_g(x,y,z) - V_e(x,y,z) - E_{g(in)}, \\ \varepsilon(x,y,z) &= \varepsilon_{in} \cdot M(x,y,z) + \varepsilon_{out} \cdot [1 - M(x,y,z)], \end{aligned} \quad (4)$$

where indexes (*in*) and (*out*) indicate the inside (*InAs*) and outside (*GaAs*) regions of the system.

To obtain the ground state energies of an exciton (E_X) and biexciton (E_{XX}) confined in the ring we self-consistently solve a system of the coupled Schrödinger equations for electrons and holes (within the Hartree approximation), including all Coulomb interaction between particles introduced by the solutions of the corresponding Poisson equations:

$$\begin{aligned} \left[H_e^0 - ne\Phi_h - (n-1)e\Phi_e \right] \Psi_e &= E_e \Psi_e, \\ \left[H_h^0 + ne\Phi_e + (n-1)e\Phi_h \right] \Psi_h &= E_h \Psi_h, \\ \nabla_r \varepsilon \nabla_r \Phi_e &= e \frac{|\Psi_e|^2}{\varepsilon_0}, \\ \nabla_r \varepsilon \nabla_r \Phi_h &= -e \frac{|\Psi_h|^2}{\varepsilon_0}, \end{aligned} \quad (5)$$

where n presents of the number of the excitons confined in the system ($n = 1$ for one a single exciton and $n = 2$ for the biexciton), $H_{e(h)}^0$ stand for the Hamiltonians of the non-interacting particles [4] with the mapped parameters (like it was described in Section 2)

$$\hat{H}_{e(h)}^0 = \frac{1}{2} \mathbf{\Pi}_{\mathbf{r}}^{e(h)} \frac{1}{m_{e(h)}^*} \mathbf{\Pi}_{\mathbf{r}}^{e(h)} + V_{e(h)}(\mathbf{r}),$$

$\mathbf{\Pi}_{\mathbf{r}}^{e(h)} = -i\hbar\nabla_{\mathbf{r}} + (-) e\mathbf{A}(\mathbf{r})$ is the momentum operator, $\nabla_{\mathbf{r}}$ stands for the spatial gradient, $\mathbf{r} = \{x, y, z\}$, and $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{B} = \text{curl } \mathbf{A}$, e is the absolute value of the free electron charge. Solutions of the system (5) are related to the ground state energies of a single exciton ($n = 1$) and biexciton ($n = 2$):

$$\begin{aligned} E_X &= E_{g(in)} + E_e + E_h + e \int d\mathbf{r} |\Psi_e(\mathbf{r})|^2 \Phi_h(\mathbf{r}), \\ E_{XX} &= 2(E_{g(in)} + E_e + E_h) + 4e \int d\mathbf{r} |\Psi_e(\mathbf{r})|^2 \Phi_h(\mathbf{r}) + e \int d\mathbf{r} |\Psi_e(\mathbf{r})|^2 \Phi_e(\mathbf{r}) - e \int d\mathbf{r} |\Psi_h(\mathbf{r})|^2 \Phi_h(\mathbf{r}). \end{aligned} \quad (6)$$

The recombination energy E_{Rec} and binding energy E_{Bind} for the biexciton are defined as in [5]

$$\begin{aligned} E_{Rec} &= E_{XX} - E_X, \\ E_{Bind} &= 2E_X - E_{XX}. \end{aligned} \quad (7)$$

3. Simulation results and comparison with experimental data

The self-assembled quantum ring formation process is well-developed. In this study the system growth is performed with partial capping and in-situ annealing of the precursor quantum dots by molecular beam epitaxy [6]. The single ring spectroscopy is achieved in a low-temperature micro-photoluminescence (μ -PL) system combined with a 6 T superconducting magnet. The external magnetic field was directed parallel to the system growth direction (see upper panel in Fig. 1). The single excitons and biexciton emissions are identified by the power dependence of their intensity like it was described in Ref. 7. When the external magnetic field \mathbf{B} is applied to the system the diamagnetic shifts for the energies characterizing the excitonic ground states change can be presented as

$$\Delta E_Y(B) = E_Y(B) - E_Y(0) \approx d_Y \cdot B^2,$$

where Y indicates X , XX , Rec , or $Bind$. For a single exciton in the ground state it has been found from our measurements that $d_X \approx 7.8$ ($\mu\text{eV}/\text{T}^2$) and the emission energy at zero magnetic field was $E_X(0) = 1321.66$ meV. For the recombination energy $d_{Rec} \approx 13.3$ ($\mu\text{eV}/\text{T}^2$) and $E_{Rec}(0) = 1321.33$ meV.

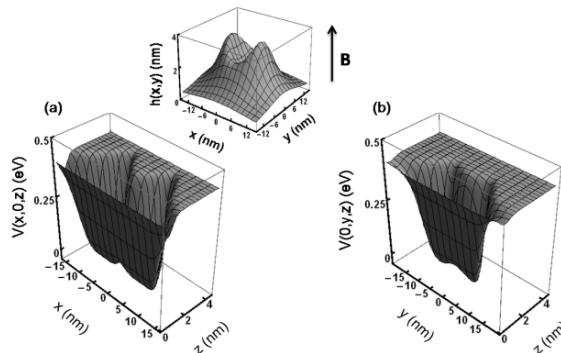


Fig. 1. Confinement potential for the electrons in the ring drawn in $(x, 0, z)$ plane (a) and in $(0, y, z)$ plane (b).

Actual system's parameters used in our simulation we adjusted to the experimental data taken from the measurement performed by us and known from literature [1,2,8,9]. For $In_CGa_{1-C}As/GaAs$ nano-ring we assumed the

In composition in the ring: $C = 0.895$. The realistic semiconductor material parameters for the *InAs/GaAs* heterostructure with complex strained composition were corrected according to Ref. 8. For electrons in the conduction band we use $m_{e(in)}^* = 0.046 m_0$, $m_{e(out)}^* = 0.067 m_0$, $V_{min} = 0.349$ eV, $V_{max} = 0.774$ eV, $\Delta E = 0.425$ eV (m_0 is the free electron elementary mass). For holes we use $m_{h(in)}^* = 0.119 m_0$, $m_{h(out)}^* = 0.5 m_0$. The band gap parameters were taken $E_{g(in)} = 0.913$ eV (*In_CGa_{1-C}As*) and $E_{g(out)} = 1.519$ (GaAs). We also used the following permittivity for the sytem: $\epsilon_{in} = 14.9$ and $\epsilon_{out} = 12.9$. The parameters for $h(x,y)$ simulation were taken: $h_0 = 2$ nm, $h_M = 3$ nm, $h_\infty = 0.2$ nm, $\gamma_0 = 3$ nm, $\gamma_\infty = 5$ nm, $\zeta = 0.2$, $R = 6$ nm, and $a = 0.4$ nm. The calculated full three-dimensional electronic confinement potential in our asymmetrical nano-ring is shown in Fig. 1 in two projections. The system (5) was solved by using by the nonlinear iterative method [10] and Comsol Multiphysics package (www.comsol.com).

The computed single exciton ground state emission energy $E_X(0)$ is 1323.5 meV and $d_X \approx 9.97(\mu\text{eV}/\text{T}^2)$. The recombination energy $E_{Rec}(0)$ was computed as 1322.0 meV and $d_{Rec} \approx 13.8(\mu\text{eV}/\text{T}^2)$. For the diamagnetic shifts of those energies in Fig. 2 we present results of our measurement and simulation results both (the data we present in the average energy of the Zeeman doublets). One can observe a very good agreement between experiment and our theory.

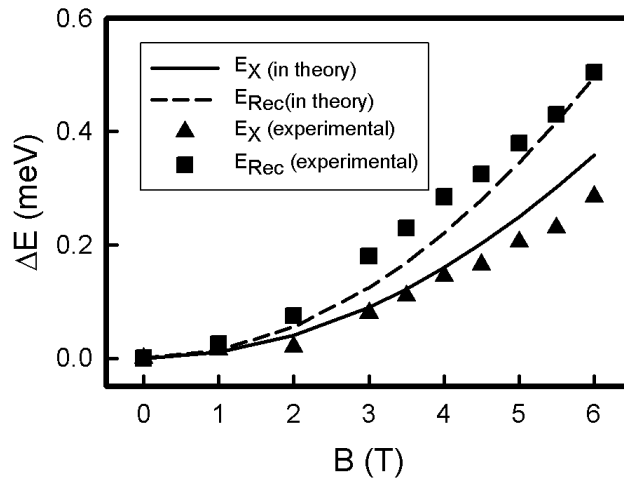


Fig. 2. Diamagnetic shifts of the excitonic energies confined in the nano-ring.

In addition in Fig. 3 we draw the biexciton binding energy shift calculated for our system. The binding energy is small and decreases more as magnetic field increases.

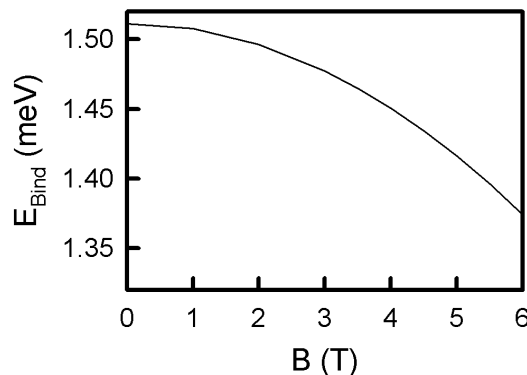


Fig. 3. Biexciton binding energy as a function on magnetic field.

4. Conclusion

In short summary we represent a study on magneto-biexcitons confined in an asymmetric *InAs/GaAs* nano-ring. We performed a simulation of the ring's excitonic properties based on our mapping method. Using the method we are able to build a realistic model of the geometry, structure, and composition of the ring. Comparing with experimental results we are confident that the method allows us accurately and efficiently to simulate magneto-biexcitonic properties of semiconductor nano-objects.

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