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Effect of geometry on the excitonic diamagnetic shift of nano-rings

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We simulate magneto-excitons confined in asymmetrically wobbled three-dimensional *InAs/GaAs* nano-rings. The wobbling asymmetry reproduces realistic experimental geometry of the rings and generates an asymmetry in the side valleys of the three dimensional confinement potential. Using our mapping method and the exact diagonization approach we calculated the excitonic diamagnetic shift and found that even a small wobbling asymmetry can drastically change the diamagnetic shift coefficient.

1 Introduction The single *InAs/GaAs* nano-ring's (see for instance [1,2] and references therein) magneto-exitonic emission demonstrates an interesting discrepancy with the conventional theory. Recently it was found that the diamagnetic shift of a single exciton's peak is considerably smaller than that expected from traditional theory [3]. It was also found that a perfect in geometry wobbled symmetric nano-ring is particularly hard to achieve [2]. In this work we theoretically demonstrate the impact of the wobbling asymmetry of nano-rings on the diamagnetic shift of the single exciton's peak. To make a link to realistic three-dimensional shapes of the rings we use our mapping method [4], which makes it possible to project the ring's actual geometry onto the position dependent effective masses, energy gap, band offsets of electrons and holes confined in the ring. Using the exact diagonalization method we simulate magneto-excitons and the diamagnetic shift and demonstrate that even a small wobbling asymmetry strongly effects the diamagnetic shift.

2 Simulation method We assume that the *InAs/GaAs* nano-ring was grown on a substrate surface (*x*-*y* plane) and the external magnetic field is applied in *z*-direction. In our simulation we map the wobbled ring geometry [4] for the case when the ring's height *h(x,y)* is asymmetrical along *x*-axis (see Fig. 1(a)). We fit the height as the following [2,4]:

where the difference between parameters a_{in} and a_{out} represents the wobbling asymmetry along *x*-direction, and *b* controls the range of the wobbling asymmetry.

On the base of (1) we can (as it was described in [4])

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

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

introduce a three-dimensional electronic confinement potential:

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

where $\Delta E_e = V_{max} - V_{min}$ is the electronic band offset of the system, V_{max} is the maximum value of the potential, V_{min} is the minimum value of the potential (inside the ring), and a controls the range on the potential boundaries of the ring.

From $V_e(x,y,z)$ we define the mapping function $M(x,y,z)$ as the following [4]:

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

The mapping function projects the ring geometry onto the position dependent parameters: electron's (hole's) effective mass - $m^*_{e(h)}(x,y,z)$, energy gap - $E_g(x,y,z)$, hole's confinement potential $V_h(x,y,z)$, and permittivity $\varepsilon(x,y,z)$:

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

where the subscripts (*in*) and (*out*) indicate the bulk material parameters for the inside (*InAs)* and outside (*GaAs*) regions.

Using the parameters mapped above we perform simulation of the ground state excitonic energy of the ring. To obtain wave functions and energies of non-interacting electrons and holes (see [4] and reference therein), we solve the following Schrödinger equations

$$\begin{aligned} &\hat{\boldsymbol{H}}_{e(h)}\Psi_{e(h)} = E_{e(h)}\Psi_{e(h)}, \\ &\hat{\boldsymbol{H}}_{e(h)} = \frac{1}{2}\boldsymbol{\Pi}_{\boldsymbol{r}}^{e(h)}\frac{1}{m^*_{e(h)}(\boldsymbol{r})}\boldsymbol{\Pi}_{\boldsymbol{r}}^{e(h)} + V_{e(h)}(\boldsymbol{r}), \end{aligned} \quad (5)$$

where $\boldsymbol{\Pi}^{e(h)}_{\mathbf{r}} = -ih\boldsymbol{\nabla}_{\mathbf{r}} + (-)\,e\mathbf{A}(\mathbf{r})$ is the momentum operator, $\boldsymbol{\nabla}_{\mathbf{r}}$ represents the spatial gradient, $\mathbf{r} = \{x, y, z\}$, $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{B}$ = curl $\mathbf{A}$, and e is the absolute value of the free electron charge. Having solutions for the non-interacting electrons and holes we then simulate the exciton ground state energy and exciton ground state wave function through the exact diagonalization method (see [5-7]). Our calculation was running under COMSOL multiphysics package (www.comsol.com).

3 Calculation results The material and geometry parameters for our simulation were taken from [2,3,7,8] and adjusted to the realistic semiconductor material parameters for *InAs/GaAs* with complex strained composition in [8]. For instance for $In_CGa_{1-C}As/GaAs$ nano-ring we assumed that the *In* content inside the ring is $C = 0.895$. For the electrons in the conduction band we used $m^*_{e(in)} = 0.046\ m_0$, $m^*_{e(out)} = 0.067\ m_0$, $V_{min} = 0.349$ eV, $V_{max} = 0.774$ eV, $\Delta E = 0.425$ eV (m_0 is the free electron mass). For the holes we admitted $m^*_{h(in)} = 0.119\ m_0$, $m^*_{h(out)} = 0.5\ m_0$. 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: $\varepsilon_{in} = 14.9$ and $\varepsilon_{out} = 12.9$. To quantify the wobbling asymmetry we introduce the following asymmetry parameter

$$\delta_h = \frac{h_+ - h_-}{h_-}\cdot 100\%, \quad (6)$$

where h_+ is the maximal value of the rim height for positive x and h_- represents the opposite one. The mapping function of the rings was defined with: $h_0 = 2$ nm, $h_M = 3$ nm, $h_\infty = 0.2$ nm, $\gamma_0 = 3$ nm, $\gamma_\infty = 5$ nm, $\xi = 0.2$, R = 6 nm, a = 0.4nm, and b = 5nm. To achieve desired geometry within this mapping we choose correspondingly (see Fig 1(b): $a_{in} = 0$, and $a_{out} = 0$ ($\delta_h = 0\%$, $h_+ = h_- = 3.6$ nm, no asymmetry); $a_{in} = 0.123$ and $a_{out} = 0.054$ ($\delta_h \approx 5.5\%$, $h_+ \approx 3.8$ nm, $h_- = 3.6$ nm); and $a_{in} = 0.247$ and $a_{out} = 0.120$ ($\delta_h \approx 11\%$ ($h_+ \approx 4.0$ nm, $h_- = 3.6$ nm). Using these three different geometries we map for each of them the electronic confinement potential accordingly. The potential profiles for different asymmetry parameters are shown in Fig. 2.

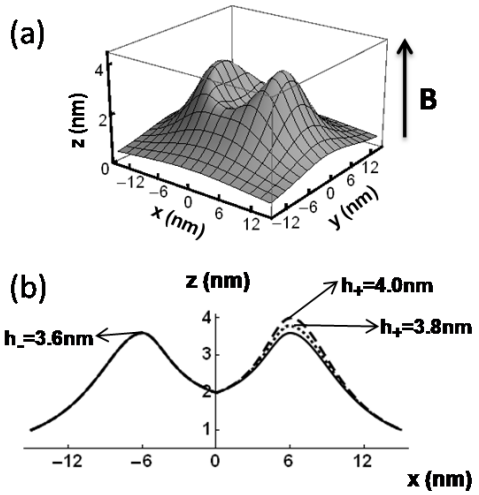

Figure 1 (a) Geometry of the asymmetrically wobbled *InAs/GaAs* nano-ring for $\delta_h \approx 5.5\%$. (b) Projection of the ring height onto the *x-z* plane for: $\delta_h = 0\%$ (solid curve); $\delta_h \approx 5.5\%$ (dotted curve); $\delta_h \approx 11\%$ (dashed curve).

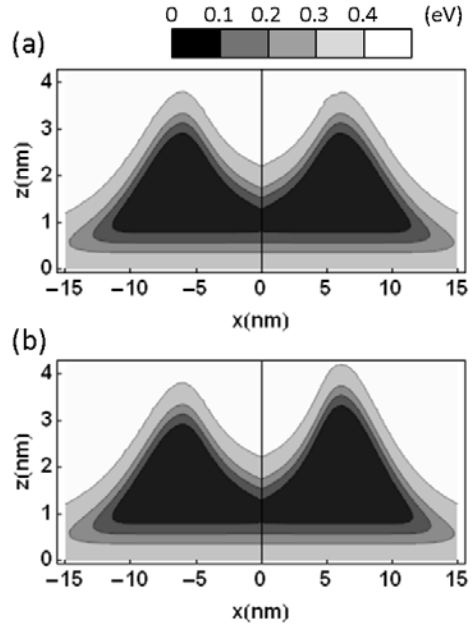

Figure 2 The electronic confinement potential projected onto *x*-*z* plane for (a) $\delta_h = 0\%$ and (b) $\delta_h \approx 11\%$.

We define the diamagnetic shift of the energy of the exciton confined in the ring as the following [4]

$$\Delta E_X = E_X(B) - E_X(0) \approx d_X \cdot B^2, \tag{7}$$

where $E_X(B)$ is the magnetic field dependent exciton's ground state energy and d_X is the diamagnetic shift coefficient. The simulation results (averaged by the Zeeman splitting) are shown in Fig. 3. Those read: $d_X \approx 10$ μeV/T^2 for $\delta_h = 0\%$ and 9 μeV/T^2 for $\delta_h \approx 5.5\%$, and 8 μeV/T^2 for $\delta_h \approx 11\%$ The last one is close to the experimental data: 6.8 μeV/T^2 [3].

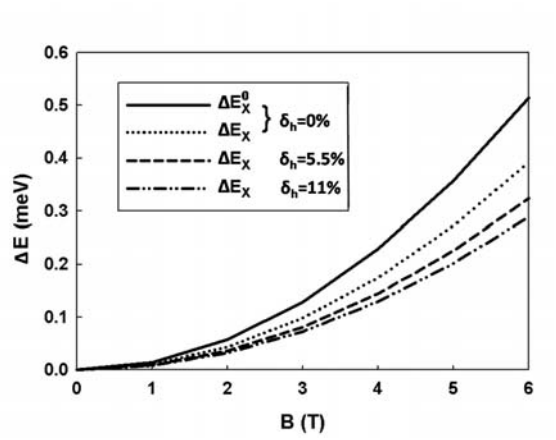

Figure 3 Diamagnetic shift of the ground state energy of the exciton confined in the ring for different wobbling asymmenries (ΔE_X^0 presents the optical transition energy diamagnetic shift for non-interacting electrons and holes).

We found that the excitonic wave function is equally distributed in both side of the ring along *x*-direction when $\delta_h = 0\%$. At the same time if δ_h exceeds 10% the wave function is already localized in the potential valley at the positive *x*-side. This is a clear reason for the suppression of the diamagnetic shift since the diamagnetic shift coefficient is defined by the wave function distributions.

4 Conclusion We simulated the excitonic diamagnetic shift of the asymmetrically wobbled *InAs/GaAs* nanorings. Using our mapping method and direct diagonalization approach we managed to obtain an accurate explanation for the experimental data on the reduction of the diamagnetic shift coefficient. We argue that the diamagnetic shift's suppression reproduces actual asymmetry in the ring geometry.

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