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Physica E 32 (2006) 37–40
PHYSICA E
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Impurity effects in the optical absorption of quantum rings

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Available online 2 February 2006

Abstract

We study the interplay between impurity scattering and Coulomb interaction effects in the absorption spectrum of neutral bound magnetoexcitons confined in quantum-ring structures. Impurity scattering breaks the rotational symmetry of the ring system, introducing characteristic features in the optical emission. Signatures of the optical Aharonov–Bohm effect are still present for weak scattering and strong Coulomb screening. Furthermore, an impurity-induced modulation of the absorption strength is present even for a strong impurity potential and low screening. This behavior is likely responsible of recent experimental observations in quantum-ring structures.

PACS: 73.21.La; 21.60.Jz; 65.80.+n

Keywords: Quantum rings; Aharonov–Bohm effect; Impurities; Optical properties; Quantum dots

Considerable attention has been given to the study of the optical Aharonov–Bohm effect (ABE) in neutral and charged excitons in semiconductor quantum rings [1–5,7,8]. In contrast to the cumulative-phase ABE in electronic systems, [9] the optical ABE originates from the difference between phases acquired by the electron and hole wave functions as the magnetic flux threads the ring. Such phase differences can be probed by standard photoluminescence (PL) experiments [7,8] since the change in phase is accompanied by a change in the exciton's total angular momentum, which makes the optical emission field-dependent through dipole selection rules [1–4].

It has been shown [1] that the AB effect is weak when both the electron and the hole forming the neutral exciton are confined within the same ring geometry. However, an enhancement of this effect is expected when the exciton is *radially polarized* by an asymmetry in the effective confinement for electrons and holes [3–5]. In this case, differences in the valence and conduction band profiles, lead to different *effective* ring radii for holes and electrons, and therefore distinct magnetic flux, giving rise to a field-dependent *phase difference* between the electron and hole wave functions. A less studied but relevant issue in such systems is the role of symmetry-breaking potentials. The presence of charge impurities [5] or piezoelectric fields [6] break the confining potential's rotational symmetry, relaxing the selection rules for optical emission.

We have shown recently that the optical absorption in semiconductor quantum rings is governed by the interplay between Coulomb interactions and the excitonic radial polarization [4]. In this paper, we extend this analysis by studying the effect of impurity scattering in these systems. An impurity-induced modulation in the optical absorption as a function of magnetic field appears, even for very weak scattering potentials. Such modulations remain even for strongly bound excitons, when AB oscillations in the absorption peak are suppressed. For weakly bound excitons, AB oscillations in the ground state are modified by the presence of impurities.

Model: We approximate the confining potential of the electron and hole forming the exciton as one-dimensional (1D) concentric rings with radii R_e and R_h, respectively. We also include the scattering of the electron and hole due to localized impurities located along the rings at an angle θ_{imp} [5]. The model Hamiltonian for the exciton is given by $H = H_{eh} + H_{imp} + H_{field}$ where H_{eh} describes the ring-confined electron–hole pair, H_{imp} is the Hamiltonian for

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1386-9477/$ - see front matter
doi:10.1016/j.physe.2005.12.011

the impurity and H_{field} is the coupling to the external electric field, namely:

$$H_{\text{eh}} = \sum_{l} \Big[\big[\varepsilon_{\text{e}}(l+\phi_{\text{e}})^2 + E_{\text{g}}\big] a_l^{\dagger} a_l + \varepsilon_{\text{h}}(l-\phi_{\text{h}})^2 b_l^{\dagger} b_l \Big] - \sum_{ll'q} v_q a_{l+q}^{\dagger} b_{l'-q}^{\dagger} b_{l'} a_l,$$

$$H_{\text{imp}} = \sum_{ll'} U_{\text{e}}(l,l') a_l^{\dagger} a_{l'} + U_{\text{h}}(l,l') b_l^{\dagger} b_{l'},$$

$$H_{\text{field}} = -\mu E(t) \sum_{l} (a_l^{\dagger} b_{-l}^{\dagger} + h.c.). \tag{1}$$

The operator a_l (b_l) annihilates an electron (hole) with integer-valued angular momentum l, $\varepsilon_i = \hbar^2/(2m_i R_i^2)$ ($i = \text{e, h}$) is the size-quantization energy for each ring, $\phi_i = \pi R_i^2 B/\phi_0$ is the magnetic flux through the ith ring in units of $\phi_0 = he/c$, B is the magnetic field. The impurity potential $U_{\text{e(h)}}(l,l') \equiv \exp \text{i}(l-l')\theta_{\text{imp}}^{\text{e(h)}}$ scatters electrons (holes), changing the angular momentum from l to l', thus coupling the different $|l\rangle$ states. $E(t) = E_0 \cos \omega t$ is the electric field of incident light, μ is the interband matrix element, and E_{g} is the optical bandgap.

Light absorption (emission) is determined by the optical polarization due to excitation of an electron–hole pair with zero total angular momentum ($L \equiv l_{\text{e}} + l_{\text{h}} = 0$), namely, $P(t) = 2\mu \sum_l P_{l(-l)}(t) = 2\mu \sum_l \langle b_{-l} a_l \rangle$ [11].

For rotationally invariant systems, we obtain the microscopic polarization components $P_{l(-l)}$ from the equation of motion (EOM) for the operator $b_{-l}a_l$ [4,11]. However, the rotational symmetry of the Hamiltonian (1) is broken by H_{imp} and we use the EOM for the more general operator $b_{l'}a_l$, giving a set of coupled equations for the components $P_{ll'} \equiv \langle b_{l'} a_l \rangle$. In the rotating wave approximation, the frequency-dependent components $P_{ll'}(\omega)$ are determined from

$$[\Omega + i\gamma - \varepsilon_{\text{e}}(l+\phi_{\text{e}})^2 - \varepsilon_{\text{h}}(l'-\phi_{\text{h}})^2 + E_{\text{g}}]P_{ll'} - \left(\sum_{l''} U_{\text{e}}(l,l'')P_{l''l'} + U_{\text{h}}(l',l'')P_{ll''} \right) + \sum_q v_q P_{(l-q)(l'+q)} = -\delta_{l(-l')}\mu E_0/2, \tag{2}$$

where $\Omega = \omega - E_{\text{g}}$, and γ describes homogeneous broadening. The electron–hole interaction is given by $v_q = (e^2/\pi\varepsilon_{\text{r}}\bar{R})K_0[(q+1/2)d/\bar{R}]$ where $d = |R_{\text{h}} - R_{\text{e}}|$, $\bar{R} = \sqrt{R_{\text{e}}R_{\text{h}}}$ is the geometrical average radius, ε_{r} is the dielectric constant of the environment, and $K_0(x)$ is the modified Bessel function [4,10].

The solution of the system of coupled equations given by Eq. (2) determines the absorption coefficient,

$$\alpha(\omega, B) = \frac{8\pi\mu\omega}{n\varepsilon_{\text{r}}E_0} \text{Im} \sum_l P_{l(-l)}(\omega, B), \tag{3}$$

which is a function of the incident light frequency ω, and of the magnetic field B. Note that resonances of $\alpha(\omega, B)$ occur at frequency values corresponding to exciton eigenstates which are directly coupled to radiation (dipole active), i.e. states with zero total angular momentum ($l_{\text{e}} = -l_{\text{h}}$).

We calculate the absorption coefficient $\alpha(\omega, B)$ for different systems. In the following, we have set $\gamma = 0.05$ meV and $E_{\text{g}} = 1.5$ eV, which are in the range of actual experimental values. For concreteness, we take the electron effective mass to be $m_{\text{e}} = 0.073m_0$ (InP value) and set $m_{\text{h}} = 3.5m_{\text{e}}$. The E_0 and μ values determine the amplitude of the absorption coefficient, so that α is reported in those units. For simplicity, we take the impurity position to be $\theta_{\text{imp}}^{\text{e(h)}} = 0$ so that $U_{\text{e(h)}}$ is independent of l, l'.

The relative strength of the Coulomb interaction, given by the effective dielectric constant ε_{r}, strongly affects the optical properties of the system. Fig. 1 shows $\alpha(\omega, B)$ for $\varepsilon_{\text{r}} = 10$, a value close to the bulk value in semiconductor structure, henceforth referred to as a "fully interacting exciton" regime. When no impurities are present ("clean" system), the exciton energy spectrum consists of a set of parabolas (one for each value of L), depicted as solid curves in Fig. 1a.

In a polarized quantum-ring exciton ($R_{\text{e}} \neq R_{\text{h}}$), the ABE manifests itself as a periodic change of the ground-state angular momentum [3]. In particular, the first $L = 0$ state, which is the ground state for $B = 0$, becomes higher in energy than the first $L = 1$ state at a certain magnetic field ($B \approx 5$ T for the parameters of Fig. 1a). As the magnetic field is further increased, this $L = 1$ ground state is replaced by a $L = 2$ state and so on. Since only $L = 0$ states are optically active, the ground state goes from "bright" to "dark" as a function of the magnetic field. The absorption peak shows a uniform diamagnetic blueshift, following the lowest $L = 0$ state, with no oscillatory behavior.

This picture is strongly modified when impurities are present. For low values of the impurity potential $U_{\text{e(h)}}$,

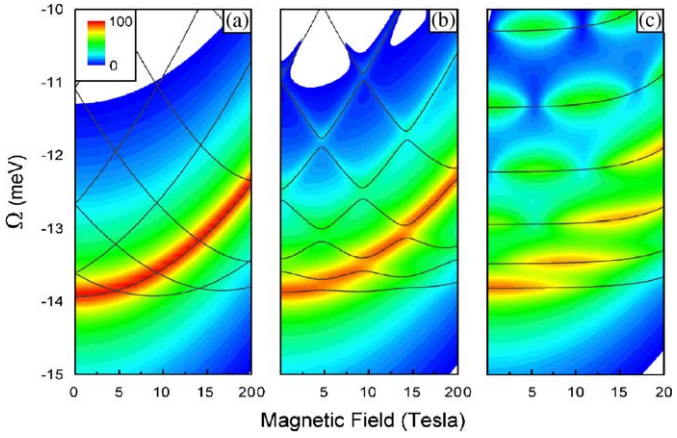

Fig. 1. Optical absorption, shown as a color map, for the fully interacting regime ($\varepsilon_{\text{r}} = 10$) with $R_{\text{e}} = 16$ nm and $R_{\text{h}} = 20$ nm and increasing impurity potential strength. The lines correspond to the energy eigenvalues calculated by direct diagonalization. (a) No impurity scattering ($U_{\text{e(h)}} = 0$). (b,c) $U_{\text{e(h)}} = 0.05\varepsilon_{\text{e(h)}}$ and $2\varepsilon_{\text{e(h)}}$, respectively. Notice anti-crossings in the energy levels, optical emission from "dark" states due to impurity scattering, and energy and absorption strength oscillations with field. Scale is normalized to the highest absorption value (= 100).

anticrossings in the spectrum appear due to the coupling between states with different L (Fig. 1b) [5]. Most importantly, this coupling also results in the appearance of *new* absorption peaks, at energies corresponding to otherwise "dark" states. In particular, the main absorption peak splits at the magnetic field values where the anticrossings occur, generating an impurity-induced *modulation* of the absorption strength as a function of magnetic field. This splitting is further enhanced for larger values of $U_{e(h)}$ (Fig. 1c). In this case, the dependence of the energy levels with magnetic field is essentially parabolic due to the strong localization of the exciton wave function in the ring by the impurity potential [5]. In addition to the large splittings in the main absorption peak, a series of secondary peaks appear and disappear as a function of magnetic field, their positions following the ground and excited states energies.

Results for the ground-state absorption for the exciton in the weakly bound regime are shown in Fig. 2. This regime is characterized by a large dielectric constant ($\varepsilon_r = 30$), and corresponds to the case where the effective screening of the Coulomb interaction caused by metal contacts and nearby image charges is much larger than the bulk dielectric screening of the material. In the "clean" (no impurity scattering) case, the absorption peak follows the low-lying $L = 0$ ("bright") state, as expected. In contrast to the fully interacting case, oscillations in the excitonic energy levels (solid curves) are seen superimposed to the usual parabolic structure. The absorption peak shows oscillations in both position *and* height (Fig. 2a). These oscillations in energy and absorption strength constitute the signature of the optical ABE and have been studied previously [3–5].

Figs. 2b and c show how such oscillations are modified by the impurity scattering. Albeit L is no longer a good quantum number, the main peak still follows the state with larger $L = 0$ component (Fig. 2b) for relatively low values of $U_{e(h)}$, but the modulation in absorption amplitude as a function of field is much more pronounced. For even larger values of $U_{e(h)}$ (Fig. 2c), the absorption peaks appear in "steps," following the flat energy levels, with an oscillating amplitude as a function of field.

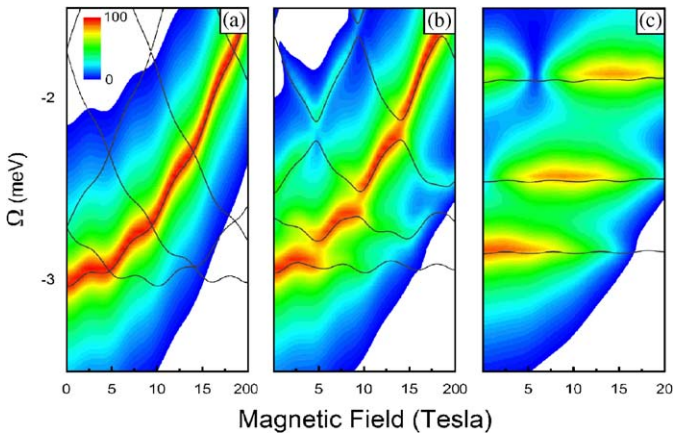

Fig. 2. Same as Fig. 1 for the weakly bound regime ($\varepsilon_r = 30$). (a) No impurity scattering ($U_{e(h)} = 0$). The absorption peak follows the lowest $L = 0$ state and oscillates with field, a signature of the optical AB effect. (b,c) $U_{e(h)} = 0.05\varepsilon_{e(h)}$ and $\varepsilon_{e(h)}$, respectively.

This interesting result shows that, although a strong impurity scattering "kills" the AB oscillations in the energy levels as a function of field, a strong modulation in the absorption remains and constitutes a signature of the optical ABE, which could be experimentally accessed.

To summarize, we have shown that, as impurity scattering breaks the original rotational symmetry of the system, it couples excitonic states with distinct angular momenta L. The absorption, given by the $L = 0$ component of the optical polarization, shows flux-related features. In clean systems, the absorption displays peaks at the energies corresponding to the optically active $L = 0$ states. Important qualitative differences arise as the Coulomb interaction screening is stronger or weaker. For excitons in the strongly interacting regime, absorption oscillations are suppressed due to the Coulomb locking of the electron and hole in the lowest optically active state, whereas the AB effect is manifested in a bright $\rightarrow$ dark transition in the ground state as the magnetic field increases. In contrast, AB oscillations in the low-lying optically active states appear for weakly bound excitons.

The presence of impurities changes this picture qualitatively, introducing anticrossings in the spectrum and splittings in the main absorption peak, as well as secondary peaks with energies corresponding to otherwise dark states. The change in the absorption strength at the anticrossings leads to an impurity-induced modulation of the absorption as a function of the magnetic field, much stronger than the one observed in the clean case.

Even very weak impurity potentials produce such field modulations in the optical absorption/emission strength. In experimental systems, some degree of localization of the wave functions is expected, either due to impurity scattering or to piezoelectric potentials [6], and observation of this effect is anticipated. Field modulations in the PL emission intensity of quantum-ring magnetoexcitons have been observed [8], which could be related to some degree on the localization in the ring.

We thank A. Govorov for valuable conversations and suggestions; support from NSF-IMC and NIRT Grants at OU, and NSF DMR-0305557 and NUE-0407108, and ARL Grant DAAD19-01-2-0014 at JSU.

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