Magnetoexciton in nanotube under external electric field

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Abstract. We study the Aharonov-Bohm oscillation of the energy levels of an electron-hole pair confined in a narrow nanotube in the presence of the magnetic field applied along the symmetry axis. We show that the electric field applied at the same direction makes the oscillation more pronounced.

1. Introduction
The Aharonov-Bohm (AB) effect of an exciton confined in a ring-like nanostructure, related to the interaction of the external magnetic field with the induced tunnelling current through the electron-to-hole rotation, has been studied both experimentally and theoretically [1, 2]. At the same time the theoretical analysis showed that tunnelling through potential barriers in electron-hole relative rotation is very feebre and there is no AB oscillation in ground state energy of the exciton [3, 4]. Yet, AB effect in a ring-like structure can be enhanced when the exciton is polarized in the radial or axial directions [5]. A quantum nanotube (NT), where the exciton could be polarized additionally at the axial direction by the application of an external electric field, is a possible structure for observing a stable AB effect of an electron-hole composite system. The sophisticated techniques of crystal growth developed recently permit to fabricate narrow NTs and to observe the oscillation of photoluminescence peak energies due to the AB effect of a charged exciton in a quantum tube [6, 7].

Above we present a theoretical analysis of spectral properties of the electron-hole pair confined in a very thin ideally cylindrical NT structure in the presence of electric and magnetic fields, applied along the symmetry axis. We show that the AB effect is strongly affected by the external electric field. Our calculations show that the external electric field increases the separation between electron and hole in a narrow NT, restoring an independent rotation of the particle at opposite directions and making possible the AB oscillation of the ground state level, especially for quantum NTs with a large radius.

2. Theoretical model
We consider a model of an endlessly long and very thin cylindrical nanotube, whose thickness \( w \) is much smaller than the centreline radius, in accordance to dimensions of experimentally fabricated tubes are essentially smaller than their radius [8]. Moreover, this condition allows us to reduce the number of variables in the Schrödinger equation describing in this case the electron and hole positions by means of only four cylindrical coordinates \(-\pi \leq \theta_e, \theta_h < \pi, -\infty < z_e, z_h < +\infty\), neglecting the particles displacements at radial direction \( \rho_e \approx \rho_h \approx R \). By using the centre-of-mass coordinates,

\[
Q = \frac{m_e q_e + m_h q_h}{m_e + m_h}; \quad q = q_e - q_h; \quad Z = \frac{m_e z_e + m_h z_h}{m_e + m_h}; \quad z = z_e - z_h
\]

In this coordinates the dimensionless electron-hole Hamiltonian acquires the following form:
\[ H = H_{\text{cm}} + H_{\text{rel}}; \quad H_{\text{cm}} = -\frac{\mu}{(m_e + m_h)} \left[ \frac{\partial^2}{R^2 \partial \Theta^2} + \frac{\partial^2}{\partial Z^2} \right]; \quad H_{\text{rel}} = -\frac{\partial^2}{\partial z^2} + \left( \frac{i}{R} \frac{\partial}{\partial \Theta} + \frac{\gamma R}{2} \right) - \beta \cdot z + V_{\text{eh}}(z, \Theta) \]

(2)

Here we use the effective atomic units, in which the effective Bohr radius \( a_e^* = \frac{e^2}{\mu e^2} \), the effective Rydberg \( R_y^* = e^2 / 2a_e^* \), parameters \( \gamma = e B / 2\mu e^2 \gamma \) and \( b = ea_e^*/R_y^* \) are used as units of length, energy and the dimensionless magnetic and electric fields, being the electron, hole and reduced effective masses, respectively \( m_e^*, m_h^* \) and \( \mu = m_h^* m_e^* / (m_h^* + m_e^*) \). In our calculations we adopt a simple model, in which the confinement potential is supposed to be equal to zero inside a narrow NT region and to infinity otherwise, while the energy of the electron-hole interaction can be approximated by the expression [9]:

\[ V_{\text{eh}}(z, \Theta) = -2\sqrt{\frac{z^2 + 4R^2 \sin^2 \Theta / 2 + (0.2w)^2 \frac{\pi}{2}}{z_c - z_h}; \quad \Theta = \Theta_e - \Theta_h} \]

(3)

Where \( w \) thickness is the thickness the layer. Eigenvalues of the Hamiltonian (2), \( E_{X} = E_{X,M} + E_{n,m}^{\text{rel}} \) corresponding to the exciton energies depend on four quantum numbers, the axial centre of mass and relative quantum numbers \( N,n = 1,2,... \) and corresponding quantum numbers of angular momenta \( (m,M = 0, \pm 1, \pm 2,...) \). The centre of mass energy can be found explicitly:

\[ E_{X,M}^{\text{cm}} = \frac{\mu}{(m_e + m_h)} \left[ M^2 / R^2 + \pi^2 N^2 / L^2 \right]; \quad N = 1,2; \quad M = 0, \pm 1, \pm 2, \]

(4)

On the contrary, the energy of the relative motion \( E_{n,m}^{\text{rel}} \) can be found only numerically. But, the numerical procedure may be simplified taking advantage of the adiabatic approximation based on the fact that the rotation around the axis is significantly faster than the displacement along the \( z \) axis. In framework of this approximation, the eigenfunctions \( \psi_{n,m}^{\text{rel}} = u_n(z, \Theta) \cdot \phi_{m,n}(\Theta) \) and eigenenergies \( E_{n,m}^{\text{rel}} \) of the Hamiltonian \( H_{\text{rel}} \) can be found by using the following two-step numerical procedure:

\[ -\frac{d^2 u_n(z, \Theta)}{dz^2} + V_{\text{eff}}(z, \Theta) u_n(z, \Theta) = E_{n}^{\text{fast}}(\Theta) u_n(z, \Theta); \quad V_{\text{eff}}(z, \Theta) = -\beta \cdot z + V_{\text{eh}}(z, \Theta) \quad (5a) \]

\[ \left( i \frac{1}{R} \frac{d}{d \Theta} - \frac{\gamma R}{2} \right) \phi_{m,n}(\Theta) + E_{n}^{\text{fast}}(\Theta) \cdot \phi_{m,n}(\Theta) = E_{n,m}^{\text{rel}} \cdot \phi_{m,n}(\Theta) \quad (5b) \]

In our numerical work we first solve Equation (5a) by using the trigonometric sweep method [9] in order to find the adiabatic potential \( E_{n}^{\text{fast}}(\Theta) \) for 181 different angles \( \Theta = \pi (i - 1) / 180, i = 1,2,...,181 \) and for two lower axial quantum numbers \( n = 1,2. \) Afterwards, we use the found values of the function \( E_{n}^{\text{fast}}(\Theta) \) in order to solve the eigenvalue problem (5b) via Fourier series expansion method. The periodic shape of the adiabatic potential \( E_{n}^{\text{fast}}(\Theta) = E_{n}^{\text{fast}}(\Theta + 2\pi) \) allows us to analyse qualitatively properties of the solutions of the Equation (5b) by using the Bloch's theorem. Really, via the substitution \( \phi_{m,n}(\Theta) = \exp\left( i \gamma R^2 \Theta / 2 \right) \psi_n(\Theta) \), Equation (5b) is reduced to 1D Schrödinger equation,
\[
-\frac{1}{R^2} \frac{d^2\psi_n(\theta)}{d\theta^2} + E_{n}^{\text{fast}}(\theta)\cdot\psi_n(\theta) = E_{n,m}^{\text{rel}}\cdot\psi_n(\theta) 
\]

(6)

As the adiabatic potential has the period \(2\pi\), Equation (6) has formally the Bloch-type solutions \(\psi(\theta) = e^{i\theta}\chi_{k,\gamma}(\theta)\) with \(0 < k \leq 1\) and a periodic function \(\chi_{k,\gamma}(\theta)\) with the same period.

3. Results and discussion

Below, we present results of calculations, obtained by numerical solution of differential Equations (5a) and (5b) for NTs with the height \(L = 10a_0^*\), the width \(w = 0.4a_0^*\), and two different centreline radius \(R = 1a_0^*\) and \(R = 4a_0^*\). In our calculations we use typical for GaAs material parameters, effective Bohr radius 10nm, effective Rydberg 6meV and dimensionless magnetic field \(\gamma = 1\) corresponds approximately to \(B \approx 7T\). In Figure 1 we present results of calculation for zero electric field case. At the left side we display the adiabatic potentials found from Equation (5a) for states with axial quantum numbers \(n = 1\) and \(n = 2\), marked by solid and dashed lines, respectively. Additionally, by horizontal lines are indicated the edges of two lowers subbands in NT of radius and three lowers subbands in NT of radius \(4a_0^*\). Comparing curves in Figures 1(a) and (c) one can see that the barriers between periodical potential wells become higher and the separation between them becomes larger as the NT radius increases from \(1a_0^*\) to \(4a_0^*\). Consequently, in a NT of large radius the electron-to-hole tunnelling through barriers is weaker and subbands are narrower than those in a NT of small radius.

At right side of Figure 1, we display some lower energy \(E_{n,m}^{\text{rel}}(\gamma)\) as functions of the magnetic field found from Equation (5b) for states with axial quantum numbers \(n = 1\), (solid lines) and \(n = 2\) (dashed lines). The meaning of these curves as we point out above is related to the fact that their shapes within the interval \(0 < \gamma \leq 2/R^2\) coincide with the dispersion curves of the energy bands corresponding to electron-hole relative rotation around the symmetry axis. It is seen that these curves exhibit oscillations with the period \(T = 2/R^2\) and crossovers of the energy levels, typical for AB effect beginning from the second level in NT of radius \(1a_0^*\) and beginning from the third level in NT of radius \(4a_0^*\). There is an only one localized energy level \(N_1\) in NT of radius \(1a_0^*\) and there are three localized levels \(N_1, N_2, N_3\) in NT of radius \(4a_0^*\), which are arranged below the set of superior intersected curves.

**Figure 1.** (a), (c) Adiabatic periodical potentials for relative electron-hole rotation and (b), (d) lower energies of the electron-hole pair as functions of the magnetic field for zero-case electric field and for two different axial quantum numbers, \(n = 1\) (solid lines) and \(n = 2\) (dash lines).

The deeper the energy level in Figures 1(a) and (c), the narrower is the correspondent subband and larger is the amplitudes of oscillations in Figures 1(b) and (d). In the case of the small NT radius for both lower \(N_1\) and \(N_2\) are located only partially below the barrier top, therefore the tunnelling in these
states is strong and the amplitude of the AB oscillation is large. Conversely, for NT of radius $4a_0^*$ both lower subbands $N_1$ and $N_2$ in Figure 1(c) are located completely below the barrier top, the tunnelling is very weak and the amplitude of the AB oscillations in the corresponding curves of Figure 1(d) is almost zero.

The comparison of two lower curves $N_1$ and $N_2$ in Figures 1(c) and (d) show clearly that an increase of the NT radius yields a successive quenching of their AB oscillations, related to transition of the electron-hole complex to a Wigner-molecule-like state with practically frozen relative rotation [10]. This transition is resulted from a competition between the kinetic energy $\left( K \propto 1/R^2 \right)$, assisting to tunnelling and the Coulomb attraction $\left( V \propto -1/R \right)$, which impedes the tunnelling. For NTs of large radius the Coulomb attraction becomes dominating and an almost independent electron-to-hole gas-like rotation, typical for NTs of small radius, is transformed into oscillation of a structure with a molecule-like arrangement. The independence of the energy levels $N_1$ and $N_2$ in Figure 1(d) on the magnetic field proves that their configurations are similar to Wigner molecule, for which the tunnelling in these states is very weak.

Such transition should be reflected in the fluorescence spectrum of NTs, presenting a drastic change in a structuring and a blue shift of the spectral lines with increase of the NT radius. A specific interest of this effect is related to a possibility to control the amplitude of the oscillation of the energy levels by means of application of the external electric field along the symmetry axis. In the presence of a strong external electric field the separation between electron and hole grows, the energy of the attraction between them is diminished making instalable the electron-hole the bound state.

We have performed similar calculations for magnetoexcitons confined in NTs in the presence of the external electric field, applied along the symmetry axis. In order to give a simple explanation of the effect of the electric field on magnetoexciton energies let us first to analyse induced by it the dipole moment and the polarizability. The dipole moment of electron-hole pair $p_{n,m}$ in the state with the relative energy $E_{n,m}^{rel}$ one can calculate as $p_{n,m} = dE_{n,m}^{rel}/dF$ and the polarizability as $\alpha_{n,m} = dp_{n,m}/dF$. In our calculations we found that dependencies of both the dipole moment and the polarizability on the electric field are very similar for different values of the magnetic field and different energy states. Therefore, in Figure 2 we present as examples of such dependencies for NTs of radius $R = 1a_0^*$ and $R = 4a_0^*$, only for the ground state $(n = 1, m = 0)$ and the magnetic field $\gamma = 0$.

One can see that the separation between the electron and the hole and the polarization of the exciton induced by the electric field are increased successively while electric field grows up the value about 2kV/cm and afterwards, the dipole moment of magnetoexcitons in NTs of radius becomes almost unchanging while the polarizability tends to zero. According to this estimation, the electron-
hole separation in NTs of radius $R = 1a^*_0$ and $R = 4a^*_0$ under electric field $\varepsilon = 15 \text{kV/cm}$, for which we below in Figure 3 present results of calculations, becomes such large that their relative movement can be considered as almost independent.

At left side of Figure 3 we display the adiabatic potentials for states with axial quantum numbers $n = 1$ and $n = 2$, marked by solid and dashed lines, respectively, while horizontal lines indicate positions of the lowest subbands bottoms. Comparing curves in Figures 3(a) and (c) with those in Figures 1(a) and (c), one can see that in the presence of the electric field of 15 kV/cm the heights of barriers are reduced in about 100 times, while their widths become essentially narrower, independently on the NT radius size.

**Figure 3.** The same as in Figure 1 but for the electric field 15 kV/cm.

Consequently, electric field facilitates electron-to-hole tunnelling through barriers, enlarges the widths of subbands, originating their overlapping and the multiple crossovers between curves of the energies dependencies on the magnetic field on the right side of Figure 3. These curves have a behaviour typical for one-particle system in a nanostructure with a ring-like geometry, AB oscillation of the ground state with minima at the points $T = 2n/R^2; n = 1, 2, 3$, multiple crossovers between curves at the points $T = (2n-1)/R; n = 1, 2, 3$, a successive increase of the amplitudes of oscillation of the excited states and the absence of low-lying states whose energies are independent on the magnetic field. Thus, the external electric field which has a large effect on the Coulomb interaction between the electron and the hole, changing essentially the spectral properties of the magnetoexciton confined in NT.

4. Conclusions

We propose a simple procedure for solving two-particle wave equation describing the exciton confined in a nanotube in the presence of the external magnetic and electric fields applied along the symmetry axis. For zero-electric-field case we found clearly distinct dependencies of lower energy levels on the magnetic field for nanotubes with small and large radius, provided by a transformation of the relative electron-hole arrangement, from the gas-like configuration to the Wigner-like one, with an increase of the nanotube's radius. We find that in the presence of a strong electric field, applied along the symmetry axis, the two-dimensional configuration and the AB oscillations in these states are restored partially or totally, due to the polarization of the exciton in the vertical direction. Our calculations for the dipole moment and the polarizability of the exciton as functions of the electric field show that the ground state configuration of the exciton in nanotubes of large radius undergoes a significant modification under external electric field. Particularly, for the electric field of several kV/cm, the separation between the electron and hole in the axial direction becomes such large that the relative rotation around the axis is “defrosted”. Our estimation show that the height of the barriers of the effective potential corresponding to the relative rotation responsible for the AB oscillation of the exciton energies is lowered in 100 times while the electric field is increased up to 15kV/cm. Therefore in this regime the rotation of the electron and the hole around the axis can be considered as almost independent.
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