Effect of radial electrostatic field on optical absorption in semiconductor nanotube

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Abstract. In the effective-mass approximation the single-electron states in a wide-band semiconductor nanocylindrical heterolayer in the presence of strong lateral-radial electrical field are considered. The explicit forms of the energy spectrum and envelope wave functions of single-particle states for charge carriers are obtained using variation approach. Corresponding absorption characteristics of interband and inter-subband optical transitions in the layer in the presence of strong radial field are calculated. The radial field leads to the explicit dependence of absorption intensity on the values of effective masses of charge carriers. It is shown that absorption’s threshold frequencies depend explicitly on geometrical sizes of sample and intensity of external field.

1. Introduction

During the last decade along with various low-dimensional structures, semiconductor nanotubes (SNTs) are one of urgent objects of investigation and had been studied extensively both experimentally and theoretically (see reviews [1-3] and references therein). SNT is an emerging field and possesses potential to provide a wide range of functionalities. The precise controllability of structural and spatial positioning and versatile functionality make SNTs promising candidates for practical application in next generation nanoelectronic and nanophotonic devices. With the progress in synthesis and fabrication of different nanomaterials various kinds of tubular structures, such as CdX, HgX (X=S, Se, Te), compounds II₃-V₃ [4], InGaAs/GaAs, SiGe/Si [5,6], ZnO, GaN, AlN, AlGaN [7], InP/InAs/InP [8], BN, ZnS [9], SiGe/SiO/Ti, SiO₂/SiO₂/TiO₂ [10], SiGe/Si/SiN/Cr [11] and others are obtained and attract a lot of attention. It is necessary to note also that one of the distinctive features of SNTs is the compositional dependence of their electronic, structural and optical properties [12,13].
At the same time, it is now well recognized that the electronic, kinetic, optical and a number of other physical properties of low-dimensional structures (as well as those of bulk samples) are strongly affected by external static fields, in particularly, by the external electrostatic fields. In the previous works of first author with co-authors the influence of external strong homogeneous electrostatic field and the influence of the weak (perturbating ) radial electrostatic fields on the electronic and optical properties of SNTs are examined theoretically [14-18].

In this paper we investigate theoretically the influence of the strong radial electrostatic field on the energy spectrum of charge carriers and on the optical absorption spectrum in wide-band SNTs.

2. General approach and physical model

The system we consider is an infinite tube (along the Z-axis) with cylindrical symmetry. We will take into account the actual thickness of the layer and do not neglect the radial confinement of charge carriers.

Fig.1. shows schematically the composition under consideration. The thickness of layer equals \( 2L \), and the incident light wave \( \vec{A}(r,t) \) is directed along the \( Y \)– axis and is polarized linearly along the \( X \)- axis.

It has been assumed that the confinement potential of quantized heterolayer of the tube can be approximated, in radial direction, by the quantum well “rolled-up into a tube” [14-18]:

\[
U_{\text{conf}}(r) = \begin{cases} 
0, & \text{when } R_1 < r < R_2 \\
\infty, & \text{when } r \leq R_1, r \geq R_2 
\end{cases}
\]  

(1)

It is assumed also that the layer is “thin enough” and lies fairly far from the symmetry axis (Z):

\[
L << R_1, R_2.
\]

(2)

At the same time we will also restrict the analysis with the strong confinement (strong quantization) regime when the Coulomb interaction energy between the electron and hole in the layer can be neglected in comparison with the confinement energies of charge carriers. This means that the “strong quantization regime” takes place in the layer.

In the future, if the material of the quantum well layer has a relatively wide band gap (\( E_g \geq 0.5 \text{ eV} \), for example in compositions CdS / HgS / CdS, CdSe / ZnSe / CdSe), we restrict ourselves to the approximation of isotropic effective mass(\( \mu \)). In the absence of external fields to determine the envelope wave functions and energy spectrum of charge carriers in SNT, one can use the results of Ref[18] :

\[
\psi_{n,m}^{(0)}(r, \varphi, z) = \phi_n^{(0)}(r) f_m(\varphi) w(z) = \frac{2}{L} \sqrt{\frac{\sin \pi n}{\sqrt{r}}} \frac{\sin \pi n}{\sqrt{r}} \frac{r - R_1}{L} \frac{r - R_1}{\sqrt{2 \pi}} \frac{r - R_1}{\sqrt{2 \pi}} \exp \left( i \frac{\pi}{\hbar} p_z z \right),
\]

(3)

\[
E_{n,m}^{(0)}(p_z) = \frac{\pi^2 \hbar^2 n^2}{2 \mu L^2} + \frac{\hbar^2 m^2}{2 \mu R_0^2} + \frac{p_z^2}{2 \mu} = \left( E^{(0)} \right)_{\text{rad}} + \left( E^{(0)} \right)_{\text{ang}} + \left( E^{(0)} \right)_{\nu},
\]

(4)

Here \( n = 1, 2, 3, \ldots; m = 0, \pm 1, \pm 2, \ldots; l \) is the normalizing size of the system along the axis of symmetry, and \( R_0 \) is the effective radius of rotation [18].
3. Single-particle states in the presence of radial field

We will assume that the role of “source” of the radial field in the systems under consideration is played by the homogeneously charged core. Correspondingly, for the potential energy of charge-carriers in the layer we can write now:

\[
U(r) = \begin{cases} 
\infty; & r < R_1; r > R_2; \\
\gamma \ln \frac{r}{R_1}; & R_1 \leq r \leq R_2;
\end{cases}
\]

(5)

where \( \gamma \) is the “interaction constant” between the “source” of the field and charge carrier.

Taking into account the condition (2), and introducing a new variable \( \rho = r - R_1 \) for the electrostatic energy of the particle in the layer we can write:

\[
U(\rho, \gamma) = \begin{cases} 
\infty; & \rho < 0; \rho > L; \\
\gamma \frac{\rho}{R_1}; & 0 \leq \rho \leq L;
\end{cases}
\]

(6)

Later on we will be interested in the case of strong radial field. In this case the field could be considered “strong” if the energy received by the particle from the field \( FL = \gamma L/R_1 \) is much more than the difference between the neighbouring levels of size quantization energy in the quantum well

\[
(\Delta e_{n+1} - \Delta e_n; \Delta e_n = \pi^2 \hbar^2 n^2 / 2 \mu L^2; \ n = 1, 2, 3, \ldots).
\]

From the point of view of size quantization the quantum size effect is most clearly manifested at not much excited levels. Therefore, we present conditions that the external field is strong for the lowest states \( n = 1 \) and \( n = 2 \) since they are of real physical interest.

\[
\frac{\gamma L}{3 \epsilon_1} = \frac{FL}{3 \epsilon_1} \gg 1; \quad \frac{\gamma L}{5 \epsilon_1} = \frac{FL}{5 \epsilon_1} \gg 1
\]

(7)

We will use the variation approach to determine the analytical form of energy spectrum and wave functions of charge carriers in the heterolayer when the conditions (6)-(7) fulfill.

Let us consider now the single-particle states in the layer in the presence of a strong radial field. Using the results of Ref.[19] for the trial wave functions and energy of a particle can be written:

3.1.1. The ground state.

a) \( \gamma < 0 \) (particle is attracted by the core)

\[
\chi_1^{(-)}(\rho) = A \rho \exp \left( -\beta \rho^3 \right)
\]

(8)

b) \( \gamma > 0 \) (particle is repulsed by the core)

\[
\chi_1^{(+)}(\rho) = A (L - \rho) \exp \left[ -\beta (L - \rho)^2 \right]
\]

(9)

3.1.2. First excited state

a) \( \gamma < 0 \) (particle is attracted by the core)

\[
\chi_2^{(-)}(\rho) = B \rho \left( 1 - \lambda \rho^2 \right) \exp \left( -\alpha \beta \rho^2 \right)
\]

(10)

b) \( \gamma > 0 \) (particle is repulsed by the core)
\[
\chi_2^{(\nu)} (\rho) = B(L - \rho) \left[ 1 - \lambda (L - \rho)^2 \right] \exp \left[ -\alpha \beta \frac{(L - \rho)^2}{2} \right]
\]  

(11)

In Exps.(8-11) \( A, B \) are the normalization constants, and \( \alpha, \beta, \lambda \) are variation parameters:

\[
A_{c,v} = 2 \left( \frac{\beta_{c,v}^3}{\pi^2} \right)^{\frac{1}{3}}; \quad \beta_{c,v} = \frac{\pi}{L} \left( \frac{2 FL}{3 \varepsilon_{tc,v}} \right)^{\frac{1}{3}}; \quad B_{c,v} = A_{c,v} \left[ \frac{12 \alpha^2}{5(\alpha^2 + 1) - 2\alpha} \right]^{\frac{1}{2}} \equiv A_{c,v} g;
\]

\[
\lambda_{c,v} = \frac{\beta_{c,v}(1 + \alpha)}{3}; \quad \alpha \equiv 0.814; \quad \varepsilon_{tc,v} = \frac{\pi^2 \hbar^2}{2\mu_{c,v} L^2}; \quad \chi(r) = \frac{\phi(r)}{\sqrt{r}}; \quad \rho = r - R_i;
\]

From where for the energies of radial motion of ground state \( (E_{1\text{rad}}) \) and first excited state \( (E_{2\text{rad}}) \) in SNT we will obtain

\[
E_{1\text{rad}} \approx \frac{3}{\pi^2} \left( \frac{L}{2} \varepsilon_{i} F^2 \right)^{\frac{1}{3}}; \quad E_{2\text{rad}} \approx \frac{4.109}{\pi^{\frac{2}{3}}} \left( \frac{3}{2} \varepsilon_{i} F^2 \right)^{\frac{1}{3}};
\]

(13)

With regard to rotational motion, in the presence of strong radial field the adiabatic approximation holds with even greater accuracy than in the absence of the field. For the effective radius of rotation, averaged over the states (10, 11) we obtain, respectively:

\[
R_{\text{eff}}^2 = \begin{cases} 
R_1^2 \left[ 1 - \frac{4}{\pi} \frac{L}{R_i} \left( \frac{3}{2} \frac{E_{1\text{rad}}}{FL} \right) \right]^{\frac{1}{3}} & \text{when } \gamma < 0; \\
R_2^2 \left[ 1 + \frac{4}{\pi} \frac{L}{R_i} \left( \frac{3}{2} \frac{E_{1\text{rad}}}{FL} \right) \right]^{\frac{1}{3}} & \text{when } \gamma > 0
\end{cases}
\]

(14)

4. Discussion of results

The selection of trial wave functions in the form (8-11) is accurate enough and adequately describes the physical system under consideration. As an example of application of these results let us consider the interband and inter-subband transitions in SNT and examine the influence of strong radial electrostatic field on these transitions.

For the perturbation \( V \), related to the light wave

\[
\tilde{A} (\tilde{r}, t) = \tilde{e} A_0 \exp \left[ i \left( \omega t - \tilde{q} \cdot \tilde{r} \right) \right] + \text{c.c.}
\]

We will have, in dipole approximation [20]:

\[
V = \frac{|\tilde{q}| A_0}{m_e c} (\tilde{e} \cdot \tilde{p})
\]

(15)

Here \( A_0 \) is the amplitude of vector-potential, \( \tilde{p} \) is a 3D operator of momentum, \( m_e \) is the mass of free electron, \( c \) is the wave velocity in free space, and c.c. stands for the complex conjugation. As it was indicated in the beginning, the incident light wave with frequency \( \omega \) is directed along the \( Y \) – axis: \( \tilde{q} = \tilde{q}(0, q, 0) \) and is polarized linearly along the \( X \)- axis: \( \tilde{e} = \tilde{e}(1, 0, 0) \).

4.1. Interband dipole transitions

For the matrix element \( M_{c,c} \) of interband \( |v\rangle \rightarrow |c\rangle \) transitions in the general case we can write:

\[
M_{c,v} = V_{c,v} \int \Psi^*_c (r, \varphi) \Psi_v (r, \varphi) r dr d\varphi,
\]

(16)
where $V_{c,v}$ is the matrix element of operator (15), built on the Bloch amplitudes of $v$ - and $c$- bands. Taking into account the form of angular and radial envelop wave functions from Exp.(3) and Exps.(8-11), respectively, and the corresponding energy values from Exp. (4) and Exp.(13), we will obtain the following expressions for the matrix elements $M_{c,v}$ and threshold frequencies $(\omega_{c,v})$:

4.1.a) Transitions $|1v, m_v\rangle \rightarrow |1c, m_c\rangle$.

$$M_{1,1} = \sqrt{8} V_{1,1} s^2 \left(1 + s^3\right)^{3/2} \delta_{m_v, m_c},$$  \hspace{1cm} (17)

$$\hbar \omega_{1,1} = E_g^L + \left( E_{1v} \right)_{\text{rad}} + \left( E_{1v} \right)_{\text{rad}} + \frac{\hbar^2 m^2 - 1/4}{2 R_i^2} \left( \frac{1}{\mu_v} + \frac{1}{\mu_c} \right);$$  \hspace{1cm} (18)

4.1.b) Transitions $|1v, m_v\rangle \rightarrow |2c, m_c\rangle$.

$$M_{2,1} = \sqrt{8} g V_{2,1} s^2 \left( s^3 - 1 \right) \left( \alpha + s^3 \right)^{5/2} \delta_{m_v, m_c},$$  \hspace{1cm} (19)

$$\hbar \omega_{2,1} = E_g^L + \left( E_{2c} \right)_{\text{rad}} + \left( E_{1v} \right)_{\text{rad}} + \frac{\hbar^2 m^2 - 1/4}{2 R_i^2} \left( \frac{1}{\mu_v} + \frac{1}{\mu_c} \right);$$  \hspace{1cm} (20)

4.1.c) Transitions $|2v, m_v\rangle \rightarrow |1c, m_c\rangle$.

$$M_{1,2} = \sqrt{8} g V_{1,2} s^2 \left( s^3 - 1 \right) \left( 1 + \alpha s^3 \right)^{5/2} \delta_{m_v, m_c},$$  \hspace{1cm} (21)

$$\hbar \omega_{1,2} = E_g^L + \left( E_{1v} \right)_{\text{rad}} + \left( E_{2v} \right)_{\text{rad}} + \frac{\hbar^2 m^2 - 1/4}{2 R_i^2} \left( \frac{1}{\mu_v} + \frac{1}{\mu_c} \right);$$  \hspace{1cm} (22)

4.1.d) Transitions $|2v, m_v\rangle \rightarrow |2c, m_c\rangle$.

$$M_{2,2} = \sqrt{8} g V_{2,2} s^2 \left( \alpha s^3 + \frac{1}{2} \right) \left( 1 + \alpha s^3 \right)^{5/2} \delta_{m_v, m_c},$$  \hspace{1cm} (23)

$$\hbar \omega_{2,2} = E_g^L + \left( E_{2c} \right)_{\text{rad}} + \left( E_{2v} \right)_{\text{rad}} + \frac{\hbar^2 m^2 - 1/4}{2 R_i^2} \left( \frac{1}{\mu_v} + \frac{1}{\mu_c} \right).$$  \hspace{1cm} (24)

In Exps.(17-24) the selection rule $m_v = m_v \equiv m$ takes place, $s = \mu_v / \mu_c$, $E_g^L$ is the band gap of bulk sample from the material of the layer.

As it follows from Exps. (17), (19), (21), (23) the corresponding matrix elements (intensities) of interband transitions do not depend explicitly on the intensity of the external field, but the external field leads to the explicit dependence of transitions’ intensity on the values of charge carriers’ effective masses. The Fig.2. shows the plots of functions $u_{c,v}(s) = \frac{|M_{c,v}|}{\sqrt{8} V_{c,v}} (c, v = 1, 2)$.
4.2. Inter-subband dipole transitions

In the general case we have for the matrix element $D_{f,i}$ of inter-subband $|i\rangle \rightarrow |f\rangle$ transitions

$$D_{f,i} = \int \Psi^*_i(r,\varphi)\Psi_f(r,\varphi)rdrd\varphi$$  \hspace{1cm} (25)

After calculations we obtain the following expressions for the corresponding matrix elements and threshold frequencies:

4.2.a) Transitions $|1c(v), m_i\rangle \rightarrow |2c(v), m_f\rangle$

$$D_{2,1}^{c(v)} = -i\hbar g \frac{|A_0|}{3m_0L} \left( \frac{3 + \alpha}{3} \right) \left( \frac{2}{3} \right) \frac{FL}{\varepsilon_{c(v)}} \frac{1}{3} \frac{\delta_{m_f, m_i+1}}{m_f}$$

$$\frac{D_{2,1}^{c(v)}}{D_{2,1}^{u}} = \frac{\mu}{\mu_c} = \left( \frac{\mu}{\mu_c} \right)^{1/3} = s^{1/3}.$$  \hspace{1cm} (26)
\[ \hbar \omega_{2,1}^{(v)} = \left( E_{2}^{(v)} \right)_{\text{rad}} - \left( E_{1}^{(v)} \right)_{\text{rad}} + \frac{\hbar^2 (2|m|+1)}{2\mu_{(v)} R^2}; \quad (m \equiv m_v) \quad (27) \]

As one can see, in this case the selection rule \( m_v = m \pm 1 \) takes place. The absorption intensity of direct inter-subband transitions in the layer depends explicitly on the intensity of external field. The absorption increases with the increasing of external field. At the same time inter-subband absorption depends explicitly also on the values of effective masses of charge carriers.

5. Conclusions
On the results obtained in this study we can conclude the following:
- the suggested theoretical model is physically adequate to the system under consideration and allows to get results in analytical form;
- the external strong radial electrostatic field leads to a significant spatial separation of opposite charge carriers, which reduces the probability of radiative recombinination of electron and hole;
- it is possible to modify the optical-energy parameters of the system by variation of geometrical sizes of the sample and the intensity of external field in a controlled manner;
- at the same time the dependence of absorption parameters upon effective masses of carriers opens a possibility to define its values experimentally in the presence of external radial electric field.

As a consequence, we can conclude that if the material and geometrical sizes of SNT are known, the results of above theoretical calculations could be used to carry out appropriate experiments.

In the application plan there is a real opportunity to use the theoretical results obtained for the geometrical and electrical tuning of optical and other parameters of SNT.

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