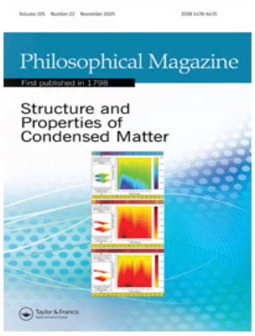

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Electric field effect on the anisotropic optical properties of elliptical nanotubes

V. V. Yarema, V. A. Holovatsky and N. H. Holovatska

Yuriy Fedkovych Chernivtsi National University, Chernivtsi, Ukraine

ABSTRACT

The energy spectrum and wave functions of an electron in elliptical nanotubes with hard walls under the influence of an electric field directed along the major or minor axis of the ellipse were studied within the framework of the effective mass approximation using the finite element method. The considered nanotubes have equal thickness along the major and minor axes. The dependence of energy levels and oscillator strengths on the nanotube ellipticity and the strength of the external electric field was calculated. It was shown that the selection rules for quantum transitions of an electron depend on the nanotube ellipticity, the magnitude and direction of the electric field, and the orientation of the linear polarisation of the electromagnetic wave. It has been shown that the selection rules for quantum transitions of an electron depend on the nanotube ellipticity, the magnitude and direction of the electric field, as well as the orientation of the linear polarisation of the electromagnetic wave. Conditions under which the probability of electron quantum transitions to high-energy excited states increases have been determined. The obtained results are also applicable to the corresponding elliptical nanorings and can be useful for designing optoelectronic devices with specified energy and polarisation properties.

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Elliptical nanotubes; quantum transitions; oscillator strengths; electric field; finite element method; selection rules

1. Introduction

The development of technologies for growing quantum nanostructures plays a key role in modern semiconductor device engineering. Different types of nanostructures, such as quantum dots, wires, and rings, are used not only to improve the characteristics of existing semiconductor devices – light sources, electromagnetic radiation detectors, solar cells – but also to create fundamentally new single-photon devices focussed on the needs of quantum computing and sensors [1,2].

The controlled formation of wave functions and the energy spectrum of quasiparticles in quantum nanostructures opens up new opportunities for the creation of highly sensitive and highly efficient devices with specified characteristics. Optimization of nanostructure geometries, including multilayered quantum dots, nanowires, and nanorings, allows to achieve specific effects of quantum confinement, which significantly affect their optical

CONTACT V. A. Holovatsky v.holovatsky@chnu.edu.ua Yuriy Fedkovych Chernivtsi National University, 2 Kotsubynsky str, Chernivtsi 58012, Ukraine

properties. Elliptical semiconductor nanostructures attract special attention, which are less studied compared to spherical and cylindrical ones, but demonstrate unique polarisation properties due to their asymmetric shape. In particular, ellipticity provides the possibility of generating and absorbing photons with a given polarisation, which is important for creating polarisation-sensitive quantum optoelectronic devices [3,4]. In the study [5], the operation of polarisation photodetectors based on elliptical nanowires was demonstrated, which provide polarisation separation of images without the use of polarisation filters. The use of elliptical nanowires in solar cells allows to significantly increase their efficiency, which makes this technology promising for improving solar cells [6].

Thus, theoretical investigations of the anisotropic optical properties of elliptical nanosystems represent a relevant direction in modern physics. Currently, elliptical quantum wires and nanotubes [7–11], as well as elliptical quantum dots and nanorings [12–17], are being actively studied. Most theoretical studies of the optical properties of nanosystems are performed in the effective mass approximation, which allows solving the Schrödinger equation and obtaining the energy spectrum and wave functions of quasiparticles by various methods. For example, exact solutions of the Schrödinger equation for an electron in an elliptical wire can be obtained by the method of separation of variables in an elliptic coordinate system [8–10]. Based on these solutions, an orthogonal basis that satisfies the boundary conditions of the problem was constructed in [11], and the effect of a uniform electric field on the intensity of the quantum transition oscillator was investigated using the matrix method [11–13].

For multilayer elliptical nanosystems, exact solutions are available only for confocal elliptical surfaces [8–10]. These elliptical nanotubes have a distinctive cross-section, with the thickness along the minor semi-axis of the ellipse being greater than that along the major semi-axis. This asymmetry significantly influences the quantum states in such tubes or nanorings [9].

In many theoretical investigations of elliptical nanosystems that do not allow exact solutions of the Schrödinger equation, various numerical methods are employed [14–21]. One of the most widely used and reliable numerical methods is the finite element method (FEM) [22], which is implemented in COMSOL Multiphysics [23]. Studies [24,25] have demonstrated that the electron energies in nanosystems calculated using the matrix method and FEM agree with high precision. Using the finite element method [17–19,26–28] the authors investigated the influence of the geometric shape of elliptical rings on the energy spectrum and electron density distribution. Vinasco et al. investigated elliptical quantum rings with a constant radial width but varying axial profiles [17], as well as rings with non-uniform radial width [18]. In both types of elliptical nanosystems, a quasi-degeneracy of the ground and first excited energy levels is observed. In the case of an elliptical ring with varying width in different radial directions, the localisation of the electron in the ground state is determined by the direction of the weakest confinement, and the degeneracy appears at small ellipticities [18]. On the contrary, for a ring with constant width, the ground-state electron is distributed nearly uniformly along the ring [17], and quasi-degeneracy occurs only at high ellipticity, when the aspect ratio of the ellipse exceeds 2.

A similar quasi-degeneracy of the ground and excited states is observed for elliptical rings with confocal ellipses [9] and for the rings studied in [26], where the confining potential in the xy-plane combines an inverse square potential function acting at small distances from the ring centre with a parabolic function at larger distances, resulting from an increase in the width of the rings along the major axis of the ellipse.

We note that the results obtained for elliptical nanostructures may also be relevant to circular systems in which the anisotropy of the effective mass plays a significant role. The electron density distribution in a circular quantum ring with anisotropic effective mass is equivalent to that in an elliptical ring [28]. In such nanosystems, the ground state of the electron is also quasi-degenerate.

It has been shown that in elliptical nanosystems, quantum transitions from the ground to the first excited state can have high probability due to the large dipole moment. However, the energy of such transitions is close to zero as a result of quasi-degeneracy [9,18,19].

From this perspective, it is of particular interest to study the optical properties of elliptical rings and nanotubes with uniform width or thickness, where the ground state is not quasi-degenerate. Such elliptical rings have been partially investigated by Vinasco et al. in [17], where the dependence of the energy spectrum on ellipticity was studied. However, the probabilities of quantum transitions under different light polarisations–which determine the anisotropic optical response–remain unexplored.

In the present work, the oscillator strengths of quantum transitions are studied for this type of nanosystem (elliptical quantum rings and nanotubes) under different light polarisations, as well as the influence of a uniform electric field on these transitions.

2. Theoretical model

Our model system consists of an electron confined by two hard walls of an elliptical GaAs nanotube. The Oz axis coincides with the nanotube axis, and the Ox axis aligns with the major axis of the ellipse. Then the potential energy of the electron in the nanotube, expressed in the Cartesian coordinate system, takes the form:

$$U(x,y)=\begin{cases}0, & \frac{x^2}{a_0^2}+\frac{y^2}{b_0^2}>1 \quad \cap \quad \frac{x^2}{a_1^2}+\frac{y^2}{b_1^2}\leq 1\\ \infty, & \frac{x^2}{a_0^2}+\frac{y^2}{b_0^2}\leq 1 \quad \cup \quad \frac{x^2}{a_1^2}+\frac{y^2}{b_1^2}\geq 1,\end{cases} \tag{1}$$

where a_0, b_0 and a_1, b_1 – the semi-axes of the inner and outer ellipses, respectively. To ensure equal wall thickness in two mutually perpendicular directions, these semi-axes are related by the conditions $a_1-a_0=b_1-b_0=d$. The focal lengths of elliptical surfaces $f_0=\sqrt{a_0^2-b_0^2}$, $f_1=\sqrt{a_1^2-b_1^2}$ satisfy the relation $f_1^2-f_0^2=2db_1(\chi-1)$, where $\chi=a_1/b_1$. Therefore f_0= f_1 only when $\chi=1$, i.e. in the case of a circular cylinder.

In the direction of the Oz axis (along the nanotube), the electron moves freely. The electric field is directed perpendicular to the Oz axis at an angle φ to the semi-major axis of the ellipse. Part of the energy of the electron due to longitudinal motion $E_z=\hbar^2k_z^2/2\mu$, while the energy of the transverse motion and the wave functions of the electron are determined from the solution of the Schrödinger equation, which in the general case takes the form

$$\frac{-\hbar^2}{2\mu}\Delta\Psi_f(x,y)+|e|F(x\cos\varphi+y\sin\varphi)\Psi_f+U(x,y)\Psi_f(x,y)=E_f\Psi_f(x,y). \tag{2}$$

Energy spectrum E_f and wave functions of an electron in an elliptical nanotube $\Psi_f(x, y)$ at different values and direction of electric field intensity $\overrightarrow{F}$ are calculated using the finite element method.

In the case of an elliptical quantum ring, which is additionally bounded along the Oz axis by planes $z = 0$ and $z = h$, the axial part of the wave function is given by $\Phi_{n_z}(z) = \sqrt{2/h}\sin(n_z \pi z/h)$, and the energy of the axial motion of an electron is $E_{n_z} = \frac{\hbar^2\pi^2 n_z^2}{2\mu h^2}$. Wave functions $\Phi_{n_z}(z)$ orthonormal $\int_0^h \Phi_{n_z}(z)\Phi_{n_z'}(z) = \delta_{n_z n_z'}$.

Based on functions $\Psi_f(x, y)$ it is possible to study the influence of the electric field and the cross-sectional shape of the nanotube or nanoring on the oscillator strengths of quantum intersubband transitions

$$F_{ff'}^{x(y)} = \frac{2m}{\hbar^2}(E_f - E_{f'})|M_{ff'}^{x(y)}|^2, \tag{3}$$

where $M_{ff'}^x = \langle f|x|f'\rangle$ and $M_{ff'}^y = \langle f|y|f'\rangle$ – dipole moments of quantum transitions $f \to f'$ at x- and y-polarisation of the electromagnetic wave.

3. Calculation results and their discussion

Numerical calculations were performed using the parameters of the semiconductor material GaAs. The effective mass of the electron was assumed to be $\mu = 0.069m_e$, (m_e is the mass of a free electron). The values of the semi-axes of the external elliptical surface a_1 and b_1 were selected so that when the ratio $\chi = a_1/b_1$ changes, the area of the outer ellipse remained constant and equal to the area of a circle with radius $r_1 = 10nm$. The thickness of the nanotube is $d = 5nm$. The cross-sectional area of a nanotube, $S_\chi = \pi(a_1b_1 - a_0b_0)$, increases slightly with increasing ellipticity χ. For example, at $\chi = 1.3$ the area S_χ is only 1.1% larger than the area of a circular nanotube (S_1), and at $\chi = 1.5$ we have $S_\chi/S_1 = 1.027$.

Figure 1 shows the wave functions and energies of the first five electron states in nanotubes with different ellipticities ($\chi = 1, 5; 1.3; 1.1$).

The blue colour of the wave function corresponds to its negative values, and red to its positive values. By analogy with the wave functions of an electron in an elliptical nanotube formed by confocal ellipses [9], wave functions that are symmetric about the horizontal axis will be called even, and those that are antisymmetric will be called odd. In [9], even and odd states are obtained based on Mathieu's even and odd functions, respectively, which are analytical solutions of the Schrödinger equation in the elliptic coordinate system. As can be seen from Figure 1, the ground state of the electron (f = 1) is even. When $\chi < 1.5$, states $f = 2, 4, 6$ are also even, and states $f = 3, 5, 7$ – odd. The energies of the $f = 2$ and $f = 3$ states, which are degenerate at $\chi = 1$, become nearly identical again at $\chi = 1.5$. This effect was not observed in nanotubes with confocal elliptical surfaces [9]. The dependence of the energy spectrum on the semi-axis ratio χ is shown in Figure 2. For convenience, the graphs are accompanied by insets depicting the shape of the wave functions in various states. At $\chi = 1$, the energies of the corresponding even and odd states coincide, as there is no preferred direction. At low ellipticity ($\chi < 1.5$), the even state $f = 2$ has a lower energy than the odd state $f = 3$, but at $\chi = 1.5$ their energies become approximately equal (quasi-degeneracy). In this case, an anticrossing of energy levels occurs, and the states exchange the wave function forms.

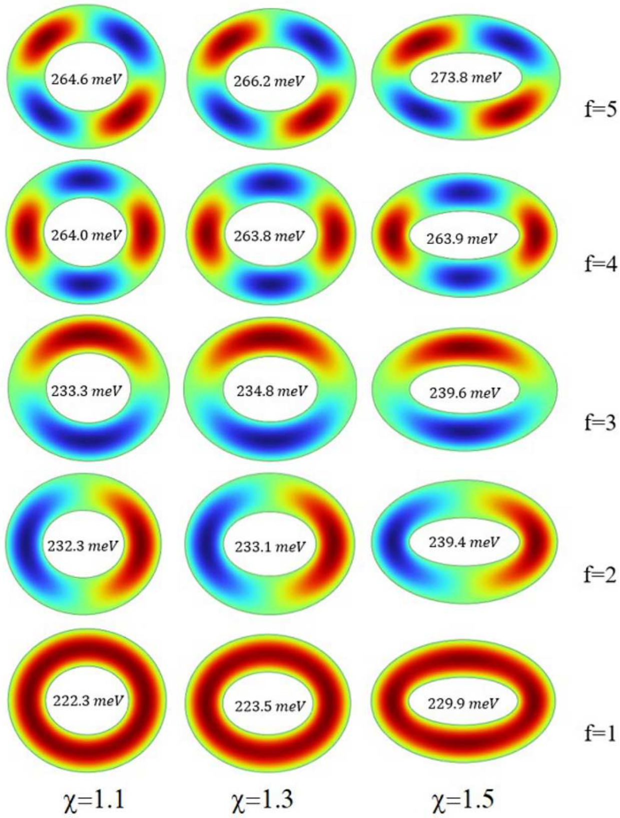

Figure 1. Electron wave functions in GaAs nanotubes at $\chi = 1.5, 1.3, 1.1$.

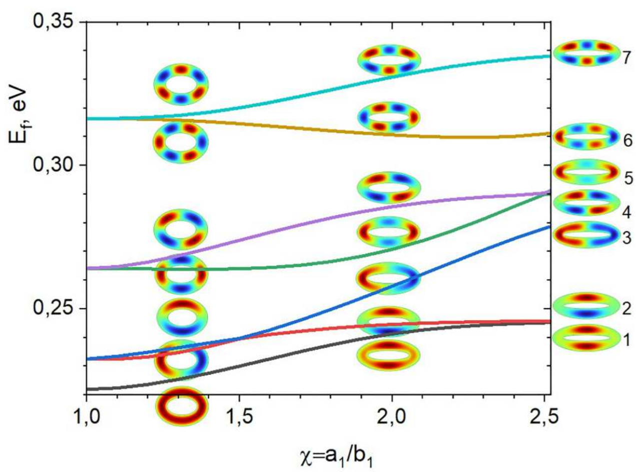

Figure 2. Dependence of the electron energy spectrum on $\chi = a_1/b_1$.

At $\chi > 1.5$, the energy of the lowest odd state increases slowly, approaching saturation, and finally coincides with the energy of the ground state. Although the wave functions of these states differ in parity, the electron density distribution ($|\Psi_f(x, y)|^2$) for them at high ellipticity are identical. A similar phenomenon was observed in the corresponding dependences given in [8,9].

In addition, as shown in Figure 2, despite the increase in the cross-sectional area of the nanotube with an increase in its ellipticity, the energies of all states rise. The effects of anticrossing of energy levels are also observed for higher even and odd states, indicating a complex interaction between the levels as the geometry of the nanotube changes.

Figure 3 shows the dependence of the energy levels on the electric field strength for two orientations: $\varphi = 0^\circ$ (Figure 3(a)) and $\varphi = 90^\circ$ (Figure 3(b)). The wave functions of the electron in the corresponding states at $F = 100$ kV/cm are shown to the right of the graphs. It can be seen that the energies of the two lower states decrease rapidly with increasing electric field strength. This behaviour is attributed to the tilting of the potential well, causing significant shifts in the electron density distribution within the nanosystem, particularly for the lower-energy states. The remaining electronic states exhibit a non-monotonic dependence on the electric field strength. Due to the distinct responses of even and odd states to the field, regions of energy level anticrossing are observed.

To determine the most probable quantum transitions from the ground state to excited states (via photon absorption) and from excited states to the ground state (via electromagnetic wave emission), the oscillator strengths for intraband quantum transitions of an electron in a nanotube with varying ellipticity under a transverse electric field were calculated. The results are shown in Figures 4 and 5.

Figure 4 shows the dependence of the oscillator strengths for quantum transitions on the ellipticity of the quantum wire for x- and y-polarised electromagnetic waves. The graphs indicate that the dependence on the nanotube's ellipticity varies significantly between different light polarisations.

In the case of $\chi = 1$, only quantum transitions defined by the selection rules for cylindrical nanosystems are allowed. From the ground state, an electron can undergo a transition only to states with $m = \pm 1$. These conditions are satisfied by states: $f = 2$ $(n = 1, m = 1)$, $f = 19$ $(n = 2, m = 1)$ and $f = 3$ $(n = 1, m = -1)$, $f = 20$ $(n = 2, m = -1)$ (the quantum numbers of states in the cylindrical nanosystem are indicated in parentheses). Quantum transitions 1→2 and 1→19 correspond to x-

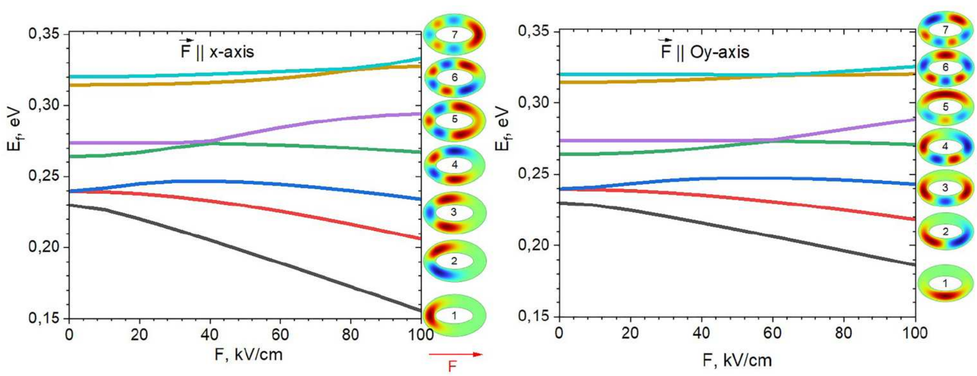

Figure 3. Dependence of energies E_1 to E_7 on F at $\chi = 1.5$ and $\varphi = 0$ (a), $\varphi = 90^\circ$(b).

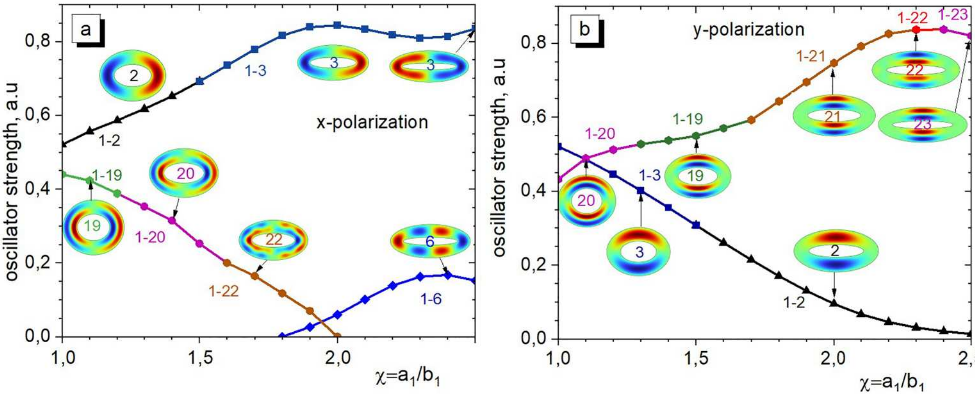

Figure 4. Dependence of the oscillator strengths of quantum transitions on the ellipticity of the quantum wire: (a) *x*-polarisation; (b) *y*-polarisation.

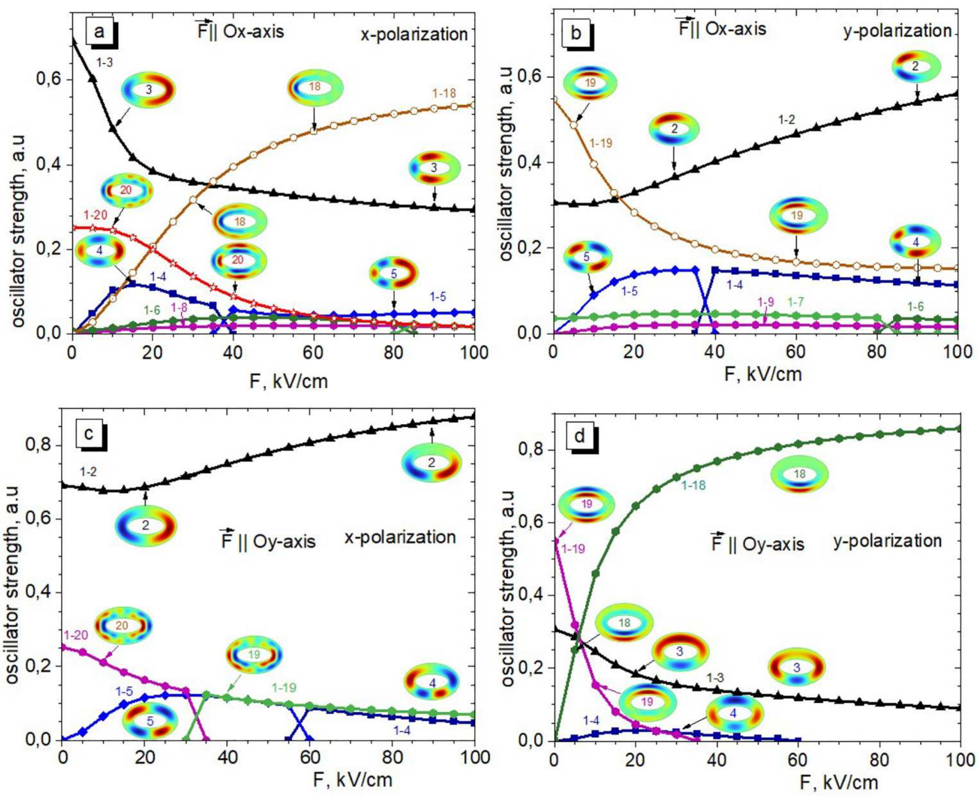

Figure 5. Dependencies of the oscillator strengths of electron quantum transitions $F_{1f}^{x(y)}$ on the electric field intensity: (a), (b) – $\varphi = 0°$; (c), (d) – $\varphi = 90°$; (a), (c) *x*-polarisation; (b), (d) *y*-polarisation.

polarisation, while transitions 1→3 and 1→20 correspond to *y*-polarisation of light. The probability of quantum transitions to low-excited states ($f = 2$, $f = 3$) slightly exceeds the probability of transitions to high-energy states ($f = 19$, $f = 20$).

As the ellipticity of the nanotube increases, the selection rules for quantum transitions change. For x-polarised light, quantum transitions are allowed only to states that are odd with respect to the y-axis ($\Psi_f(x, y) = -\Psi_f(-x, y)$) and even with respect to the x-axis ($\Psi_f(x, y) = \Psi_f(x, -y)$). The probability of quantum transitions to low-lying excited states ($f = 2$, $f = 3$) increases, while the probability of transitions to higher excited states ($f = 19$, $f = 20$) decreases with increasing ellipticity χ.

In contrast, for y-polarised light, quantum transitions are allowed only to states that are odd with respect to the x-axis and even with respect to the y-axis. In this case, an increase in the ellipticity of the nanotube reduces the probability of quantum transitions to low-lying excited states, while the oscillator strengths of transitions to higher excited states increase.

The effect of a static electric field on the probability of electron quantum transitions was analysed for an elliptical nanotube with a semi-axis ratio of $\chi = 1.5$. Figure 5 shows the dependence of the oscillator strengths of electron quantum transitions on the electric field strength for x- and y-polarisations of the electromagnetic wave, considering two electric field orientations along the Ox and Oy axes.

Figures 5(a,c) show that for an x-polarised electromagnetic wave, in the absence of an electric field, quantum transitions from the ground state to the first and second excited states ($1 \rightarrow 2$ and $1 \rightarrow 3$) exhibit the highest oscillator strengths. Although the energy of these transitions is relatively small (around 10 meV), it increases under the influence of an electric field, reaching approximately 50 meV at $F = 100$ kV/cm (Figure 6(a)).

The electric field has a significant effect on the oscillator strengths of transitions $1 \rightarrow 2$ and $1 \rightarrow 3$. When the electric field is oriented parallel to the major axis of the ellipse, the oscillator strength of transition $1 \rightarrow 3$ decreases, and for $F > 35$ kV/cm the quantum transition to the state $f = 18$ becomes the most probable. Furthermore, as shown in Figure 6(a), the energy of the quantum transition $1 \rightarrow 18$ shows weak dependence on the electric field strength, stabilising at approximately 0.7 eV. Conversely, when the electric field is aligned parallel to the minor axis of the ellipse, the quantum transition $1 \rightarrow 2$ remains the most probable under excitation by an x-polarised electromagnetic wave, with its oscillator strength increasing as the electric field strength increases. For a y-polarised electromagnetic wave, as the intensity of the electric field parallel to the major axis of the ellipse increases, the oscillator strength of the most probable quantum transition $1 \rightarrow 19$

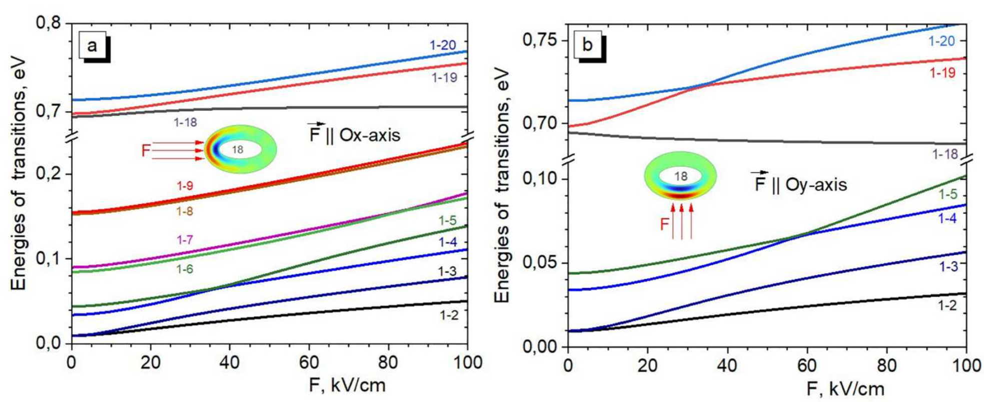

Figure 6. Dependences of the energies of electron quantum transitions (1–f) on the F.

rapidly decreases. At F>20 kV/cm, the transition 1→2 becomes the most probable quantum transition. In contrast, for an electric field parallel to the minor axis of the ellipse, excitation by a y-polarised electromagnetic wave results in quantum transitions to the highly excited states f = 18 and f = 19 becoming the most probable.

Conclusions

In this paper, within the framework of the effective mass approximation, the energy spectrum, wave functions, and oscillator strengths of electron quantum transitions in elliptical nanotubes under the influence of an electric field oriented along the major or minor axis of the ellipse were studied using the finite element method.

It has been demonstrated that the selection rules and oscillator strengths of quantum transitions are influenced by the ellipticity of the nanotube, the strength and orientation of the electric field, and the direction of linear polarisation of the exciting electromagnetic wave.

In the absence of an electric field, quantum transitions to low-energy states are most probable for x-polarised electromagnetic waves, whereas transitions to high-energy states are more likely for y-polarised waves.

When the static electric field is aligned with the linear polarisation of the exciting electromagnetic wave (along the Ox or Oy axis), allowed quantum transitions occur to states symmetric with respect to the axis of the ellipse parallel to the electric field. In this case, quantum transitions of the electron to high-energy states are most probable. Conversely, when the electric field is perpendicular to the linear polarisation of the electromagnetic wave, allowed quantum transitions occur to states antisymmetric with respect to the ellipse's axis parallel to the electric field. In this case, transitions to the lowest excited states are the most probable.

The obtained results provide valuable information for the creation of optoelectronic devices with desired energy and polarisation characteristics.

Disclosure statement

No potential conflict of interest was reported by the author(s).

ORCID

V. V. Yarema http://orcid.org/0009-0003-0024-3635
V. A. Holovatsky http://orcid.org/0000-0002-5573-2562
N. H. Holovatska http://orcid.org/0000-0002-2051-9454

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