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Electron energy states in a strongly oblate asymmetric ellipsoidal InAs quantum dot in the presence of an axial magnetic field

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Abstract. Within the framework of the adiabatic approximation, the electron's energy spectrum in a strongly oblate asymmetric ellipsoidal quantum dot, in the presence of an axial magnetic field, has been investigated. It has been shown that in the QD's section plane, for relatively low energy levels, the confining potential of the system can be described within the framework of a two-dimensional asymmetric oscillator. The electron's axial and planar energies have been defined, and the electron's energy dependencies on the geometrical parameters as well as the magnitude of the magnetic field have been studied.

Keywords: adiabatic approximation, asymmetric ellipsoidal quantum dot, magnetic field

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1. Introduction

Semiconductor structures with complex geometries are the subject of extensive investigation, as the presence of numerous geometrical parameters in the studied samples enables flexible control over the system's energy levels [1]. Modern techniques for growing quantum dots (QDs) allow for the experimental realization of pyramidal, conical, lens-shaped, and ellipsoidal structures [2 − 7]. The complexity of QD geometry necessitates solving the Schrödinger equation under non-trivial boundary conditions. Even in the single-particle case, these equations typically require numerical methods for solution. However, obtaining analytical representations of Schrödinger equation solutions allows for a deeper analysis of various physical characteristics of the studied structures, including their optical, kinetic, and tunneling properties. Therefore, developing approximate analytical models for describing QDs remains a relevant and active area of research in modern quantum dot physics. Alongside methods such as the variational approach and perturbation theory, the adiabatic approximation offers an effective means of describing quantum systems. This method is based on representing the system's Hamiltonian as the sum of Hamiltonians corresponding to the fast and slow subsystems [8].

Experimental studies of the optical properties of strongly oblate, asymmetric lens-shaped QDs [9, 10] have demonstrated that the adiabatic approach is quite effective for describing both one-particle and many-particle systems in such structures. It is important to note, however, that most research on electron and hole states in strongly oblate ellipsoidal and lens-shaped QDs has focused on structures with circular cross-sections. Yet, structures with asymmetric cross-sections can also be realized — for example, when considering ellipsoids with unequal semi-axes.

Previous studies have examined one-electron and many-electron states in strongly oblate asymmetric QDs [11, 12]. In particular, it has been shown that, for relatively low energy levels, the confining potential of the slow subsystem can be described using a two-dimensional asymmetric oscillator model. Notably, applying an axial magnetic field to a strongly oblate asymmetric ellipsoidal QD creates additional opportunities for manipulating charge carriers' energy levels, which in turn affects various physical properties of these systems. This motivates further theoretical investigation of electron states in strongly oblate asymmetric ellipsoidal QDs (SAEQD) in the presence of a homogeneous axial magnetic field.

2. Theory

Let us discuss the electron energy states in the strongly oblate asymmetric ellipsoidal quantum dot in the presence of an axial magnetic field. The problem scheme is presented below (Fig.1).

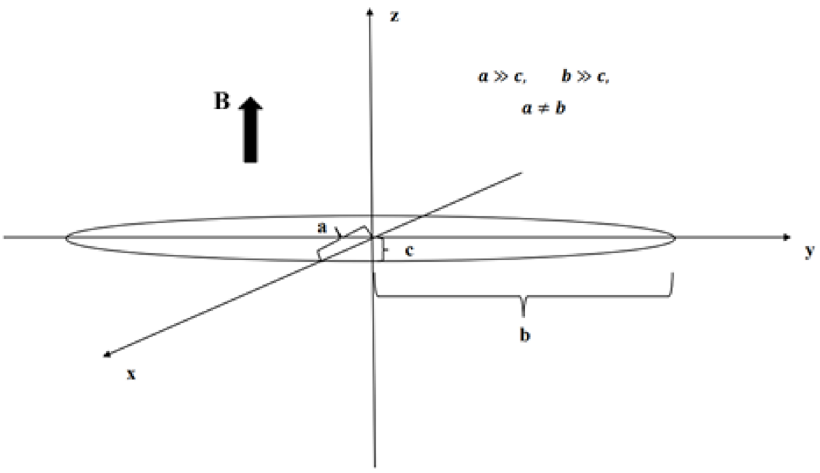

Fig. 1. Schematic view of QD.

Considering the magnetic field B, directed along the OZ axis, the Schrodinger equation of the system can be presented in the following form:

$$\left[\frac{1}{2\mu}(\mathbf{p}-\frac{e}{c}\mathbf{A})^2+V_{\text{conf}}(x,y,z)\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}), \tag{1}$$

where $\mu=0.026m_0$ – the effective mass of the electron in InAs (m_0 is the mass of the free electron) and the gauge of the vector potential is $\mathbf{A}=B\left\{-\frac{y}{2},\frac{x}{2},0\right\}$.

The confining potential of the system is introduced below:

$$V_{\text{conf}}(x,y,z)=\begin{cases}0, e^- \in \text{SAEQD},\\ \infty, e^- \notin \text{SAEQD}.\end{cases} \tag{2}$$

The considered system is under a strong quantization regime along the axial direction, allowing the application of the adiabatic approximation method in solving the problem. Within this framework, the motion of the electron can be viewed in two perpendicular directions: along the axis and in the plane. The first direction represents the fast subsystem, while the second represents the slow subsystem. Consequently, the wave function of the system $\Psi(\mathbf{r})$ can be expressed as the product of two wave functions that describe the fast subsystem $\left(\psi_f(z;(x,y))\right)$ and the slow subsystem $\left(\psi_s(x,y)\right)$:

$$\Psi(\mathbf{r}) = \psi_f(z;(x,y))\psi_s(x,y). \tag{3}$$

In the axial direction (fast subsystem), the particle is in the one-dimensional infinitely deep potential well. The Schrodinger equation of the fast subsystem has the form:

$$\left[\frac{1}{2\mu}p_z^2 + V_{\text{conf}}^z(z;(x,y))\right]\psi_f(z;(x,y)) = E_f\psi_f(z;(x,y)). \tag{4}$$

The solution to that problem is well-known and has the form introduced below:

$$\begin{gathered}\psi_f(z;(x,y)) = \sqrt{\frac{2}{L(x,y)}}\sin\left(\frac{\pi n_z}{L(x,y)}z + \delta_{n_z}\right),\\ E_f \equiv E_{n_z} = \frac{\pi^2\hbar^2}{2\mu L^2(x,y)}n_z^2,\end{gathered} \tag{5}$$

where n_z – the axial quantum number, δ_{n_z} – the initial phase of the particle's wave function, $L(x,y)$ – the width of the potential well, that parametrically depends on the in-plane coordinates x and y.

As the system has the form of the ellipsoid, $L(x,y)$ can be presented by the following expression:

$$L(x,y) = 2c\sqrt{1 - \frac{x^2}{a^2} - \frac{y^2}{b^2}}. \tag{6}$$

Considering here the confining effect of the walls of QD on the electron, we can assume that the particle will be concentrated mainly around the geometrical center of the system, the result of which will be the realization of these conditions: $x \ll a$ and $y \ll b$. This makes possible the expansion of the relation (6) in the Taylor series by the small parameters x/a and y/b, after which we get the new expression for $L(x,y)$:

$$\frac{1}{L^2(x,y)} \approx \frac{1}{4c^2}\left(1 + \frac{x^2}{a^2} + \frac{y^2}{b^2}\right). \tag{7}$$

Substituting (7) into (5) for the energy spectrum E_{n_z} of the system we obtain the following relation:

$$E_{n_z} = \frac{\pi^2\hbar^2}{8\mu c^2}n_z^2 + \frac{\mu\omega_x^2(n_z)}{2}x^2 + \frac{\mu\omega_y^2(n_z)}{2}y^2, \tag{8}$$

where $\omega_x(n_z) = \frac{\pi\hbar}{2\mu ac} n_z$, $\omega_y(n_z) = \frac{\pi\hbar}{2\mu bc} n_z$.

Due to the strong quantization regime in the axial direction, the particle can be considered in the ground state along the OZ axis, so that $n_z = 1$, hence $\omega_x(1) = \frac{\pi\hbar}{2\mu ac}$ and $\omega_y(1) = \frac{\pi\hbar}{2\mu bc}$. Substituting E_{n_z} into (1) and making some transformations, we obtain the two-dimensional Schrodinger equation in the form presented below:

$$\frac{1}{2\mu}\left[p_x^2 + \Omega_1^2 x^2 + p_y^2 + \Omega_2^2 y^2 + \mu\omega_c\left(yp_x - xp_y\right)\right]\psi_s(x,y) = \mathrm{E}\psi_s(x,y), \tag{9}$$

where $\Omega_{1(2)}^2 = \mu^2\left(\omega_{x(y)}^2(1) + \frac{1}{4}\omega_c^2\right)$, $\omega_c = eB/\mu\mathrm{c}$, $\mathrm{E} = E - \frac{\pi^2\hbar^2}{8\mu c^2}$.

Further, using the transformations presented in the article [13], the equation (9) can be expressed in the new variables:

$$\frac{1}{2\mu}\left[\alpha_1^2 p_1^2 + \alpha_2^2 p_2^2 + \beta_1^2 q_1^2 + \beta_2^2 q_2^2\right]\psi_s(q_1,q_2) = \mathrm{E}\psi_s(q_1,q_2), \tag{10}$$

with these designations:

$$\begin{aligned} \alpha_1^2 &= \frac{\Omega_1^2 + 3\Omega_2^2 + \Omega_3^2}{2\left(\Omega_1^2 + \Omega_2^2\right)}, & \beta_1^2 &= \frac{1}{4}\left(3\Omega_1^2 + \Omega_2^2 + \Omega_3^2\right), \\ \alpha_2^2 &= \frac{3\Omega_1^2 + \Omega_2^2 - \Omega_3^2}{2\left(\Omega_1^2 + \Omega_2^2\right)}, & \beta_2^2 &= \frac{1}{4}\left(\Omega_1^2 + 3\Omega_2^2 - \Omega_3^2\right). \end{aligned} \tag{11}$$

Solving the latter equation for q_1 and q_2 we'll eventually obtain the two-dimensional energy spectrum:

$$E_{n_x,n_y} = \hbar\omega_1\left(n_x + \frac{1}{2}\right) + \hbar\omega_2\left(n_y + \frac{1}{2}\right), \tag{12}$$

where $\omega_1 = \alpha_1\beta_1/\mu$, $\omega_2 = \alpha_2\beta_2/\mu$ and $n_x, n_y = 0,1,2,\ldots$ are quantum numbers of the particle in the OX and OY directions, respectively.

Thus, in the general case, we get the following form of the system's energy spectrum:

$$E_{n_x,n_y,n_z} = \frac{\pi^2\hbar^2}{8\mu\mathrm{c}^2} n_z^2 + \hbar\omega_1\left(n_x + \frac{1}{2}\right) + \hbar\omega_2\left(n_y + \frac{1}{2}\right), \tag{13}$$

However, in our further calculations, we'll assume again, that the particle is on the ground state along the axial direction, so that $n_z = 1$.

3. Results and Discussions

In this section, the dependences of the system's energy spectrum on the geometrical parameters a, b and c of the QD and on the magnitude of the magnetic field B is discussed.

The following material parameters have been used in the calculations: $a = 5a_B$, $b = 7a_B$, $c = a_B$ – the geometrical parameters of QD along OX , OY and OZ respectively, and the magnetic field B has been changed in the range of $1T - 15T$.

In fig.2a, b, and c the dependences of the system's energy on the QD's geometrical parameters are shown in the case of the fixed value of the magnetic field B equal to $1T$. Considering the specific geometry of the QD—namely, the strong oblateness along the OZ axis, due to the strong quantization regime in that direction—a stronger dependence of the energy E_{n_x,n_y,n_z} on the small semi-axis c can be anticipated, compared to the other two parameters, a and b. Nevertheless, it can be seen from fig.2, that the system's energy decreases with the increase of each geometrical parameter of QD. One can also see that the overall values of energy in the case of the first set of quantum numbers $\{n_x, n_y, n_z\} = \{1,2,1\}$ are less than in the second case $\{n_x, n_y, n_z\} = \{2,1,1\}$. This can be explained by the fact that frequency ω_1, which is determined via α_1 and β_1, is greater than ω_2 determined by α_2 and β_2. Therefore, although in the first case the quantum number n_x is less than n_y, nevertheless, the inequality of the frequencies has greater effect on the energy.

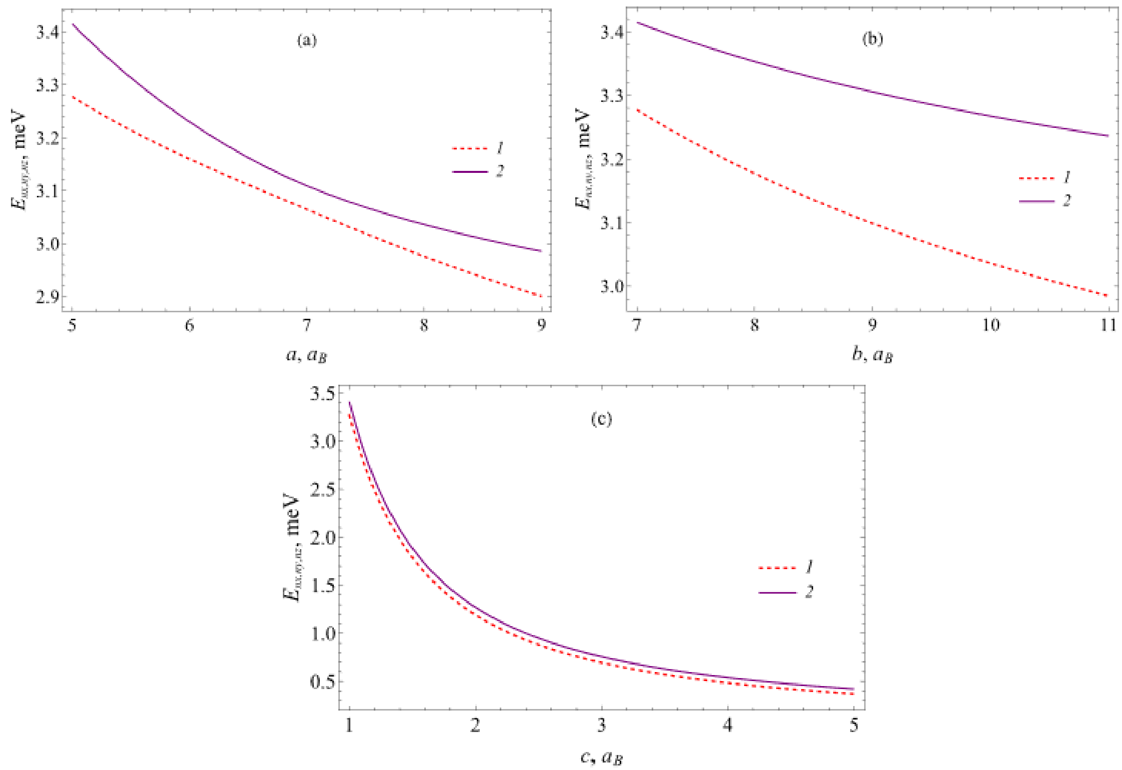

Fig. 2. The system's energy E_{n_x,n_y,n_z} dependence on the geometrical parameters $a, b,$ and $c.$ The energy levels considered are: $\{n_x, n_y, n_z\} = \{1,2,1\}$ (curve 1), $\{n_x, n_y, n_z\} = \{2,1,1\}$ (curve 2). The magnetic field B in all cases is equal to $1T$.

In Fig.3 the energy E_{n_x,n_y,n_z} dependency on the magnetic field B is displayed for the fixed values of the semi-axes a, b, and c equal to $5a_B$, $7a_B$, and $1a_B$ respectively. In this case, the energy increases with the increase of the magnetic field. The figure illustrates that the effect of the magnetic field on energy is compatible with that in the case of geometrical parameters a and b in the XOY plane, still, it is much less pronounced compared with the effect of the small semi-axis c of the QD on the energy states. This is attributed to the strong quantization regime in the axial direction, which significantly impacts the energy states than the magnetic field.

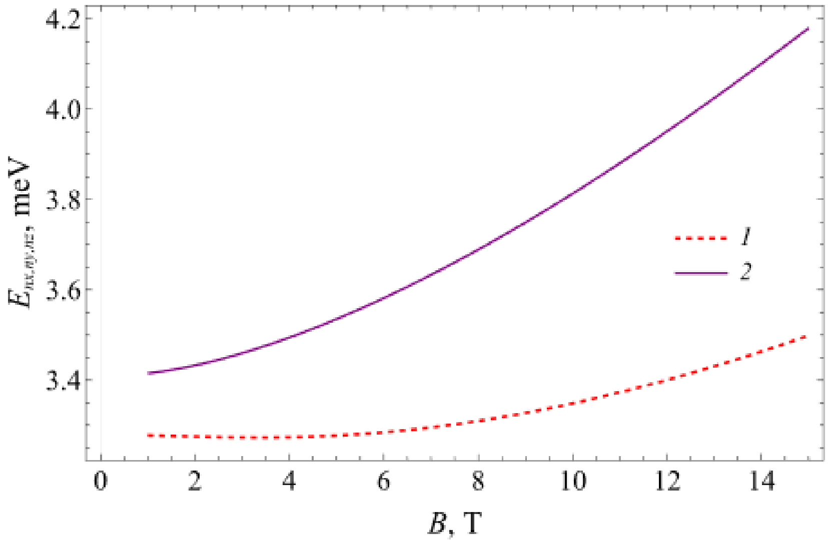

Fig. 3. The system's energy E_{n_x,n_y,n_z} dependence on the magnetic field B, for the fixed values of geometrical parameters $a=5a_B$, $b=7a_B$ and $c=a_B$. The energy levels considered are: $\{n_x,n_y,n_z\}=\{1,2,1\}$ (curve 1), $\{n_x,n_y,n_z\}=\{2,1,1\}$ (curve 2).

3. Conclusions

The electron's energy decreases with the increase in QD's geometrical parameters. On the other hand, with the rise in the magnetic field due to magnetic quantization strengthening, the energy levels increase. At the same time, the system's energy is more sensitive to the change in the axial semi-axis, as the influence of walls in that direction is significantly stronger compared to the other two.

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