Electrostatic multipoles created by electron localized in narrow-band cylindrical nanolayer

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Abstract. The problem of definition and control of electrostatic field, created by electron, localized in cylindrical nanolayer from InSb is considered. The average values of quadrupole and dipole moments have been calculated and the appropriate corrections in the potential and the electric field strength have been found. The obtained results can be applied in single-electron transistors, where role of the active functional element will play an InSb cylindrical quantum layer.

1. Introduction

The possibility of the flexible manipulating of the energy levels of charge carriers in the layered nanostructures allows to use them in different devices of semiconductor nanoelectronics. One of the most intensively investigated devices in the modern nanoelectronics is one-electron transistor, also called one-electron switch [1–5]. This device works on the base of coulomb electron blockade effect by injection quantum dot (QD), containing one or several electrons, into emitter–collector space. Electron, located inside the QD, creates repulsive coulomb field, which blocks the penetration of external electron inside the QD, that is what was called coulomb blockade. Last circumstance allows to realize one particle transitions via QDs, containing one or several electrons. The problem of interaction of electron, localized inside the QD, with external electron can be reduced to the problem of interaction of electron, restricted in spherical quantum well with external electron. Taking into account that electron localization area in the QD is of order of its effective de Broglie wavelength, the consideration of such an electron as a point charge is unacceptable [6]. It is necessary to take into account the spatial distribution of the electron, localized inside nanolayer. This circumstance leads to the necessity to take into account the electrostatic multipoles contribution to the field potential expression.

In this paper we calculate the electrostatic potentials of the electron in the narrow-gap InSb cylindrical nanolayer. We also account, that electron dispersion law is non-parabolic and described in terms of two-band Kane model, where energy depends on momentum analogous to relativistic form [7]:

\[ E = \sqrt{P^2 s^2 + \mu^2 s^4} - \mu s^2 \]  \hspace{1cm} (1)
where $s$ is parameter of nonparabolicity ($s = 10^8$ cm/s), $\mu$ is electron effective mass ($\mu = 0.018m_0$).

2. Energetic spectrum and wave function

Let’s consider an InSb cylindrical core/shell/shell quantum dot with the confining potential

$$U_{\text{conf}}(r) = \begin{cases} 
0, & R_1 < r < R_2, |z| < \frac{L}{2} \\
\infty, & r \leq R_1, r \geq R_2, |z| \geq \frac{L}{2}.
\end{cases} \quad (2)$$

where $R_1$ and $R_2$ are the inner and the outer radiuses respectively, $L$ is the height of the studied structure (figure 1).

![Figure 1. Geometrical shape of cylindrical core/shell/shell quantum dot.](image)

The behavior of the electron in this structure is described by a stationary Schrodinger type equation, to which we will come in view of no nparabolicity of dispersion law. It has the next form:

$$-\frac{1}{2\mu} \left( \frac{\hbar^2}{c^2} + \frac{1}{c} \nabla - A \right)^2 \Psi = E \Psi, \quad (3)$$

where $E = \left( \frac{E_{n,m_n} + \mu s^2}{2\mu s^2} \right)^2 - \mu^2 s^4$, and the wave function $\Psi$ has the following form [8]

$$\Psi_{n,m_n}(r, \varphi, z) = \frac{1}{\sqrt{2\pi}} e^{i\mu r} \sqrt{\frac{2}{L}} \left\{ \sin \frac{\pi n}{L} z (n = 2k) \cos \frac{\pi n}{L} z (n = 2k + 1) \right\} f(r), \quad (4)$$

where $m = 0; \pm 1; \pm 2; \ldots$ The gauge of the vector potential $\vec{A}$ is selected as follows:

$$\vec{A} = \left\{ A_\rho = A_z = 0, A_\varphi = \frac{H \rho}{2} \right\}. \quad (5)$$

The radial wave function $f(r)$ is as follows [8]

$$f(r) = r^m e^{-\frac{m^2}{2\alpha_n^2}} \left\{ C_1 F_i \left( -\left( \beta - \frac{m+1}{2} \right), m+1, \frac{r^2}{2\alpha_n^2} \right) + C_2 U \left( -\left( \beta - \frac{m+1}{2} \right), m+1, \frac{r^2}{2\alpha_n^2} \right) \right\}. \quad (6)$$
The energy spectrum can be determined from the boundary conditions, i.e. from the requirement of the wave function being zero for \( r = R_1 \) and \( r = R_2 \) [8]:

\[
E_{n,m} = \hbar \omega_n \left( \beta + \frac{m}{2} \right) + E_n
\]  

(7)

where \( E_n = \frac{\pi^2 \hbar^2 n^2}{2 \mu L^2} \) is the energy of quantization in \( z \) direction. Then for \( E_{n,m,n_r} \), we have

\[
E_{n,m,n_r} = \sqrt{\mu^2 s^4 + 2 \mu s^2 \left( \hbar \omega_n \left( \beta + \frac{m}{2} \right) + E_n \right) - \mu s^2}
\]  

(8)

3. Multipoles

Now let’s turning to a problem of determination of electrostatic field, created by an electron, localized in the considered system. This problem is reduced to definition of average values of dipole and quadrupole momentums of electron in core/shell/shell system [9]. First, we consider dipole momentum.

The average values of components of dipole momentum vector is defined from the expression

\[
\langle P_i \rangle = \int \Psi^* P_i \Psi dV,
\]  

(9)

where \( i = 1, 2, 3 \). In view, that \( P_i = e x_i \), by substitution of corresponding expression for the wave function \( \Psi \), expressions for coordinates in cylindrical system and integration over the whole volume attributable of the area of layer and by taking into account that starting point of reference on \( z \) axis we choose the center of cylindrical nanolayer it could be shown, that all three values in expression (9) are equals to zero:

\[
\langle P_x \rangle = \langle P_y \rangle = \langle P_z \rangle = 0.
\]  

(10)

Now let’s consider the quadrupole momentum. General expression for components of quadrupole momentum has the form [6]:

\[
Q_{ik} = 3 x_i x_k - r^2 \delta_{ik}.
\]  

(11)

Presenting \( Q_{ik} \) in cylindrical coordinates and making averaging over the wave functions (4 and 6), it could be shown, that the average values of non-diagonal components \( Q_{ik} \) turn to zero:

\[
\langle Q_{xy} \rangle = \langle Q_{yz} \rangle = \langle Q_{xz} \rangle = 0.
\]  

(12)

On the other hand, for diagonal components we have the following relations:

\[
\langle Q_{xx} \rangle = \langle Q_{yy} \rangle = -\frac{1}{2} \langle Q_{zz} \rangle.
\]  

(13)

So, the average values of the components of the tensor of quadrupole momentum could be presented in the next form:

\[
\langle Q_{ik} \rangle = \begin{pmatrix}
-\frac{1}{2} & 0 & 0 \\
0 & -\frac{1}{2} & 0 \\
0 & 0 & 1
\end{pmatrix}.
\]  

(14)
In other words, the task of the definition of quadrupole momentum reduces to the calculation of 
\( \langle Q_{zz} \rangle \). Using (4) one can obtain

\[
\langle Q_{zz} \rangle = \frac{1}{L^2 \pi} \int_{-L/2}^{L/2} \int_{0}^{R_2} \int_{r_i}^{r_f} \sin \left( \frac{\pi n}{L} z \right) \left( 2z^2 - r^2 \right) f^2(r) r dr d\varphi dz .
\]

(15)

On the figures 2 and 3 the dependences of quadrupole momentums of electron on the values of the outer and the inner radiuses are shown for quantum numbers \( n = 1, \ h = 1, m = 1 \). As it could be seen from these figures with the increasing of \( R_2 \) and \( R_1 \) for fixed values of \( R_1 \) and \( R_2 \) respectively the absolute value of quadrupole momentum increases. It is due to the fact that the most probable region of electron’s localization moves away from the geometrical center of the system. This leads to increasing of absolute value of quadrupole momentum of system in both cases.

**Figure 2.** Dependence of quadrupole momentum of electron on outer radius for fixed value of inner one equals to \( R_1 = 2a_0 \) for state \( n = 1, \ h = 1 \), \( n_r = 1 \), when \( \overline{H} = 10^4 \text{g}^2 \cdot \text{cm}^{-1} \cdot \text{s}^{-1} \).

**Figure 3.** Dependence of quadrupole momentum of electron on inner radius for fixed value of outer one equals to \( R_2 = 3a_0 \) for state \( n = 1, \ h = 1 \), \( n_r = 1 \), when \( \overline{H} = 10^4 \text{g}^2 \cdot \text{cm}^{-1} \cdot \text{s}^{-1} \).

Here and further \( a_0 = 530 \text{Å} \) is Bohr radius of electron in InSb.
4. Electrostatic field

Now let’s turn to the calculation of electrostatic potential \( \Phi(r) \). In the approximation of two first terms in its multipole expansion [9] we obtain

\[
\Phi(r) = \frac{q}{\varepsilon \sqrt{z^2 + r^2}} + \frac{q}{2\varepsilon \left(\sqrt{z^2 + r^2}\right)^3} \left( \sum_k \sum_i \langle Q_{ik} \rangle x_i x_k \right). \tag{16}
\]

By taking into account (14) from (16) for \( \Phi(r) \) we find

\[
\Phi(r) = \frac{q}{\varepsilon \sqrt{z^2 + r^2}} + \frac{q \langle Q_{zz} \rangle}{2\varepsilon \left(\sqrt{z^2 + r^2}\right)^3} \left( z^2 - \frac{1}{2} r^2 \right). \tag{17}
\]

The dependence (17) is given on figure 4.

Figure 4. Dependence of electrostatic potential of electron on radial coordinate for \( n = 1, m = \pm 1, \; n_z = 1, \; z = 0, \; R_1 = 2a_0, \; R_2 = 3a_0 \),

\[
\vec{H} = 10^4 \text{ g}^2 \text{cm}^{-2} \text{s}^{-1}.
\]

As we can see the absolute value of the electrostatic potential decreases with the increase in the radial coordinate.

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