Shallow donor in spirally rolled-up quantum well

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Abstract. We study the spectral properties of a shallow donor confined in spirally rolled-up narrow quantum well, in the effective mass approximation. By using the natural curvilinear coordinates, we reduce the problem for the actual system to a two-dimensional wave equation that describes the movement of the electron bound to donor inside the rolled-up well. Solving this equation by means of the double Fourier series expansion method, we found lower donor energies and the density of energy states for different donor positions. Our calculations show that donor energies are very sensible to the variation of the donor position and the geometry of the spiral.

1. Introduction
The basis of microelectronic devices is conducting and dielectric thin films. One of fundamental tasks in their design is the formation of 3D architecture from two-dimensional layers. A promising route, which offers great opportunity to manufacture new materials nanoscale devices, is the self-assembling, based on the self-rolling of layers [1–6]. The progress achieved in the last decade in the rolled-up nanotechnology permits to fabricate nanostructures as promising candidates for applications in advanced energy storage devices ranging from nanofluidics to optics [4–8]. The manufacturing of rolled-up nanostructures has stimulated the theoretical study of spectral properties of quantum wells (QWs) with variable curvature that requires an analyzing of the quantum motion of a particle confined inside a curved quasi-two dimensional region of a small but a finite thickness [9–11].

On the other hand, as the thickness of the layer is very small, the lateral confinement becomes very strong and quantum excitation energies in the normal direction become much higher than in the tangential direction. One can in this case to use an advantage of the adiabatic approximation (AA), which allows us to separate the coordinate that describe the particle motion in the direction normal to the surface and by solving the corresponding one-dimensional Schrödinger equation to find the effective adiabatic potential in curvilinear coordinates for the independent two-dimensional particle motion in the tangential direction [10]. It has been shown that this potential is related to the local radius of the curvature and the quantum mechanics of particles confined within thin curved layers is different from those in a flat plane [9–11]. Particularly, in one-electron QW in a form of an Archimedean spiral appears bound states localized near the points of maximum curvature and the number of bound states is equal to the number of windings of the spiral [11].

Here we concentrate on the problem of the energy spectrum of shallow donors confined in rolled-up QWs, in order to study the effect of doping on the spectral properties of semiconductor curve layers. The energy of the electron delivered from the donor inside the QW is defined mainly
by the interplay between the nanostructure curvature and the Coulomb interaction between the electron and the donor. Therefore, the resulting effective potential in a rolled-up QW unlike the flat layer could have multiple minima along the tangential direction, located at wings adjacent to the donor.

2. Theoretical Model
Following the AA procedure proposed in [10], we derive the Schrödinger equation in natural coordinates for the donor confined in a very thin infinite-barrier QW, which is flat at $z$-direction and rolled-up in $x$-$y$ plane. The natural coordinates system is given in this case by three unit vectors $(\hat{e}_s, \hat{e}_h, \hat{e}_z)$ shown in figure 1(a), which define respectively the tangential direction for the curvilinear coordinate $s$ corresponding to the arc length measured from the beginning of the spiral ($0 < s < s_F$), coordinate $h$ measures the distance from the exterior border of the QW along the normal and the coordinate $z$ that gives the distance from the bottom of the structure ($0 < z < L$). Here and in what follows we denote $s_F$ the arc length of the spiral, $d$ and $L$ the thickness and the height of the QW, respectively. In addition, we assume that in the adiabatic limit ($d \to 0$) the normal coordinate $h = 0$ and the position vectors of the donor and electron are defined as $r_D = (s_D, 0, L/2)$ and $r_e = (s, 0, z)$, respectively.

The aim of this work is to investigate the donor states in a rolled-up QW by using a simple model with a geometry that describes properly a substantial growth of the curvature of actual structures with increase the arc length $s$, measured from the beginning of the spiral. In our model the curvature of the spiral increases by jumps unlike the model of the Archimedean spiral, considered before for one-electron rolled-up QW [10,11]. The spiral consists from semicircle wings of different radii $R_s$. The curvature radius initially keeps the value $R_0$ as the polar coordinate is increased within the interval $0 < \varphi < \pi$ and then at the point of connection of two adjacent semicircles the radius, $R_s$ grows by $\Delta R$, while the center of curvature is displaced to the right in $\Delta R$. As the angle $\varphi$ increasing further reaches the value $\varphi = 2\pi$ the curvature radius grows again by jump and the curvature center shifts to the left. If for such structure with $n_F$ semicircle wings, we denote $k$ the number of the wing $k = 1, 2, \ldots, n_F$ then the radius of the wing of number $k$ is equal to $R_k = R_0 + \Delta R \cdot (k - 1)$ and the length of the spiral from its beginning point up to the final point of the wing number $k$ is equal to $s_k = k \cdot \pi \cdot [R_0 + 0.5(k - 1) \cdot \Delta r]$.

![Figure 1](image_url)

Figure 1: Characteristics of the model: (a) 3D image of donor confined in a rolled-up QW; (b) vertical cross section of system; (c) dependencies of the electron-donor separation, the curvature radius and effective donor potential along the tangential coordinate.

Finally, one can obtain the following relations between cartesian and polar coordinates of the
electron placed in the wing number \( k \) and the donor placed in the wing number \( k_d \):

\[
\begin{align*}
    x(s) &= \Delta_k + R_k \cos \left( \frac{s - s_k}{R_k} \right); \quad y(s) = R_k \sin \left( \frac{s - s_k}{R_k} \right); \quad z = z,
    \\
x_D(s) &= \Delta_{kD} + R_{kD} \cos \left( \frac{s_D - s_{kD}}{R_{kD}} \right); \quad y_D(s) = R_{kD} \sin \left( \frac{s_D - s_{kD}}{R_{kD}} \right); \quad z_D = L/2,
\end{align*}
\]

(1)

Here the displacement of the curvature center \( \Delta_k = 0 \) if \( k \) is even and \( \Delta_k = \Delta R \) otherwise. We use dimensionless units in which distances are measured in the effective Bohr radius \( a_0^* \) which is about 10 nm for GaAs and about 14 nm for InAs, while energies are measured in the effective Rydberg, which is about 6 meV in GaAs and it about 3 meV in InAs QWs. In these units the effective potential energy of the electron delivered from the donor and confined in the rolled-up QW is equal to

\[
V_{pot}(s, z) = \frac{\pi^2}{d^2} - \frac{1}{4R^2(s)} - \frac{2}{\sqrt{[x(s) - x(s_D)]^2 + [y(s) - y(s_D)]^2 + (z - z_D)^2}},
\]

(2)

the first two terms in this expression related to the QW thickness and the curvature result in the framework of the AA after the elimination of the fast electron motion along the normal coordinate [10], while the third term corresponds to the contribution due to the electron-donor attraction.

In figure 1(c) and figure 2 we present examples of dependencies of the potential curves, equation (2), for \( z = z_D \) and for donors located at the beginning and at the middle of the spiral. It is seen that in both cases, the potentials have multiple minima, the deepest one, associated to the configuration with the electron and the donor at the same semicircle wing and other with arrangements in which they are located at neighboring semicircle wings.

Figure 2: The effective donor potential along the tangential coordinate for two different donor positions.

The wave equation describing the electron’s slow motion in the narrow QW has the form [10]:

\[
\hat{H} |\Phi(s, z)\rangle = E |\Phi(s, z)\rangle; \quad \hat{H} = -\frac{\partial^2}{\partial s^2} - \frac{\partial^2}{\partial z^2} + V(s, z); \quad 0 < z < L; \ 0 < s < s_f,
\]

(3)
in addition, the wave function should satisfy the boundary conditions

\[
\Phi(0, z) = \Phi(s_F, z) = \phi(s, -L) = \Phi(s, L) = 0.
\]

(4)
In our numerical work we solve the eigenvalue problem (3) with boundary conditions (4) by using the Fourier series expansion method, in which the wave function is represented as follows:

$$|\Phi(s,z)\rangle = \sum_{m=1}^{N} \sum_{n=1}^{N} c_{n,m} |\sin \left( \frac{\pi ns}{s_f} \right) \rangle |\sin \left( \frac{\pi m z}{L} \right) \rangle,$$  

(5)

here $N$ is the number of terms kept in truncated Fourier series. Considering (5) as a trial function with variational parameters one can obtain in the framework of the Schrödinger variational principle $F[\Phi] = \langle \Phi | H - E | \Phi \rangle \rightarrow \text{min}$, the following secular equation:

$$\sum_{n'=1}^{N} \sum_{m'=1}^{N} \left[ \left( \frac{\pi^2 n'^2}{s_f^2} + \frac{\pi^2 m'^2}{L^2} - E \right) \delta_{n,n'} \delta_{m,m'} + V_{n+n',m-m'} + V_{n+n',m+m'} - V_{n-n',m+m'} - V_{n+n',m-m'} \right] C_{n',m'} = 0,$$  

(6)

the matrix elements $V_{n,\tilde{n}}$ in this expression are defined as follows:

$$V_{n,\tilde{n}} = \frac{1}{s_f L} \int_{0}^{s_f} \frac{\cos \left( \frac{\pi n s}{s_f} \right)}{\cos \left( \frac{\pi \tilde{n} s}{s_f} \right)} ds \int_{0}^{L} \frac{\cos \left( \frac{\pi m z}{L} \right)}{\cos \left( \frac{\pi \tilde{m} z}{L} \right)} V_{\text{pot}}(s,z) dz.$$

(7)

Eigenvalues $E_k < 0$, $k = 1,2,\ldots$ of the secular equation (6) give the energy spectrum of the bound states of the donor; while eigenvectors $c_{mn}^{(k)}$ define the corresponding wave functions $\phi_k(s,z)$ given by the relation (5).

3. Results

In this section, we present results of calculations of the energy spectrum of donors confined in a spiral, where its geometry was described above. Being $s_D$ the length of the spiral between its starting point and the donor location, one can use the ratio $s_D/s_F$ as an appropriate parameter that characterize the donor position in spiral. As this parameter is close to zero, the donor is located at the beginning of the spiral and neighboring minima of the effective potential are found only in semicircle wings of superior radii as it is seen in figure 2(a). As $s_D/s_F$ is increased additional minima of the effective potential appears also in semicircle wings of inferior radii nearer to the beginning of the spiral as it is seen in figure 2(b). Such alteration of the effective donor potential makes the energy spectrum very sensible to the change of the donor position.

In figure 3 we display the dependencies of the donor energies in two rolled-up QWs with different initial radii of spiral on the donor position. It is seen that the energy levels are separated in two groups: five lower energies corresponding to strongly bound states have a significant gaps, while the multiple levels with energies close to cero corresponding to the weakly bounded states form an almost gapless band. Despite of an essential difference in dimensions of the spirals in figures 3(a) and 3(b), one can observe a general similitude in curves of the energies dependencies with only one essential difference: the energies in figure 3(b) are higher than those in 3(a). One can explain this fact comparing the potential curves in figures 2(a) and 2(b); quantum wells in spiral of superior dimension are noticeably narrower than those in the spiral of inferior dimension.
Donor position \((S_D/S_F)\)

Energy \((\text{Ry}^*\) \)

\[(a) \quad R_0 = 1a_0^*, \quad \Delta = 0.1a_0^* \]

\[(b) \quad R_0 = 5a_0^*, \quad \Delta = 0.1a_0^* \]

**Figure 3:** The energies of donor placed in rolled-up QWs with two different initial radii of the spiral as functions of the donor position.

Gaps between energies in the upper part of the spectrum corresponding to states of the electron localized in semicircle wings, remote from the donor position are very small and therefore, it is more appropriate their description by means of curves of the density of electronic states (DOS), \(\rho(E)\). Once the donor energies \(E_k\) are found by solving the eigenvalue problem (3), then the DOS can be calculated as:

\[
\rho(E) = \sum \frac{1}{\pi} \frac{\Gamma}{(E - E_k)^2 + \Gamma^2},
\]

where \(\Gamma\) is the phenomenological natural linewidth for the model of the Lorenzian broadening adopted in our calculations.

\[
\rho(E) = \sum \frac{1}{\pi} \frac{\Gamma}{(E - E_k)^2 + \Gamma^2}, \quad (8)
\]

**Figure 4:** Density of the electronic states for donors with different positions inside Rolled-up QWs with different beginning radii of the spiral.
In figure 4, we show curves of the DOS which illustrates their successive evolution for different donor positions with an increase of the spiral radius. Comparing curves in figures 4(a, b, c) one can observe a continual displacement of peaks corresponding to low-lying levels of the discrete part of the spectrum to right with increase of the spiral radius. We associate this effect with the narrowing of the individual potential wells in figure 2 with increase of the spiral radius. As potential wells in figure 2 becomes narrower the energy levels are pushed up from the lower part of the spectrum toward upper one. Therefore, the low-lying energy levels are displaced to right as the initial radius of the spiral is increased from $R_0 = 1a_0^*$ in figure 4(a) to $R_0 = 5a_0^*$ in figure 4(c).

In figure 4(a) one can observe an essential difference in the lower part of the spectrum of donors placed at the beginning and the middle of spiral. The DOS of the donor located at the middle of the spiral has 5 peaks, whose energies are lower than the energies of 3 peaks for the donor placed at the beginning of the spiral. This fact also agree also with the alteration the shape of the effective potential (2) with the displacement of the donor position from the beginning to the middle of the spiral. On both sides of the central minimum, which with the donor displacement becomes wider, appear two additional minima.

![DOS curves for different donor positions](image)

**Figure 5:** Density of the electronic states for donors with different positions inside rolled-up QWs with different increment $\Delta R$ of the curvature radius in connections.

A similar modification suffer DOS curves as the increment $\Delta R$ of the curvature radius in the connections of the semicircle wings of the spiral grows. In figure 5 we compare curves of DOS in rolled-up QWs with the same initial radius $R_0$ and three different increments $\Delta R$ in the connections of the semicircles. The increase of $\Delta R$ affects more noticeable the DOS of donors located far from the beginning where the curvature radius and the shape of the potential are changed more significantly. It is seen that the DOS of donor placed in rolled-up QW is very sensible to any variation of both the geometry of the structure and the donor location.
4. Conclusions
We propose a simple model, which allows us to analyze effect of the impurity doping on the spectral properties of a spirally rolled-up quantum wells. We have investigated theoretically the effect of the curvature and the location of a single shallow donor on its energies. We have found that the curvature effect results in the appearance of a strong dependence of the energies of the bound states of the donor on its position and in a high sensibility of the curves of the density of the electronic states on the geometry of the structure.

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