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Electronic and magnetic states in core multishell nanowires: Edge localization, Landau levels and Aharonov-Bohm oscillations

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Abstract. We study the electronic states of hexagonal core multishell semiconductor nanowires, including the effect of magnetic fields. We find that the two dimensional electron states formed at the interface between different layers are mostly localized at the six edges of the hexagonal prism, and behave as a set of quasi-1D quantum channels. They can be manipulated by magnetic fields either parallel or perpendicular to the wire axis. These results can be rationalized in terms of Aharonov-Bohm oscillations or Landau level formation. We also show that inter-channel coupling and magnetic behavior is influenced by the geometric details of the nanowires.

1. Introduction

New inorganic semiconductor systems are emerging where carriers are confined in non-planar two dimensional electron states (2DESs). Among these nano-structures, we study the properties of 2DESs formed in multishell semiconductor nanowires (NWs) with hexagonal cross-section. Samples of this type have been recently realized experimentally [1, 2]. The 2DES is obtained in coaxial structures which are fabricated similarly to standard layered heterostructures, but using a hexagonal substrate, provided by a free standing NW, rather than the usual planar substrate, for multilayer overgrowth of lattice matched materials. The resulting 2DESs have a diameter in the tens of nm range and a cross-section shape determined by the NW used as a substrate.

The application of a magnetic field in the axial direction induces Aharonov-Bohm (AB) oscillations of the energy of the system, due to the enclosing of the magnetic flux through the shells. Since the semiconductor NWs have relative large diameters, the measure of such effect is quite accessible [3, 4]. The magneto-transport properties of similar systems, with a cylindrical cross-section, have been also investigated by applying a magnetic field perpendicular to the tube axis. Peculiar magneto-resistance properties emerged, that have no correspondence in similar planar structures [5].

2. Edge localization

In order to properly describe 2DESs with hexagonal cross-sections, the 2D quantum equation of motion for carriers on curved surfaces has been adopted. In fact, it can be derived by a limiting procedure starting from the full 3D Schrödinger equation [6, 7]. This technique allows

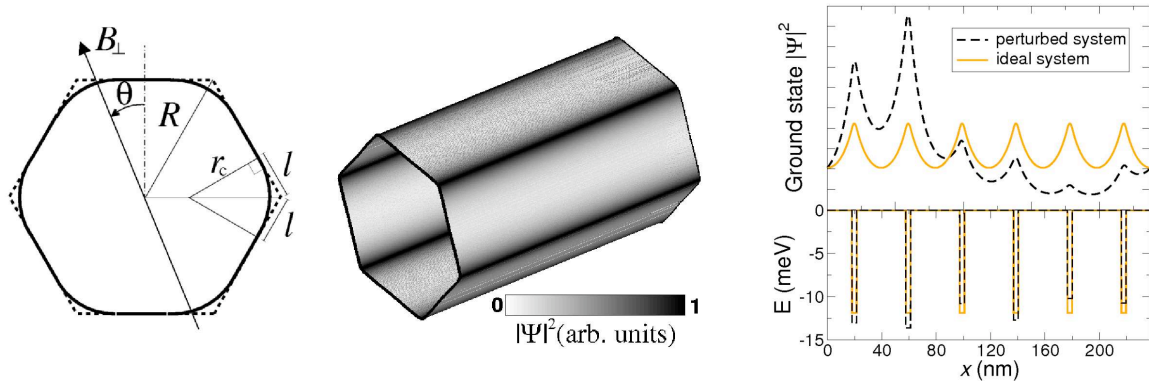


Figure 1. Left: the cross-section of an hexagonal NW is modeled from a regular hexagon (dashed line). The radius of the circumscribed circle is R . Each edge is rounded for a length l and with a constant radius of curvature r_c . A transverse magnetic field B_{\perp} forms an angle θ with a line normal to a facet. The azimuthal position on the rounded polygon (solid line) is given by an x coordinate. Center: charge density of the ground state of a carrier in a core multishell NW (gray scale), showing preferential localization along the edges (darker regions). The state shown here is for a GaAs-based nanostructure. Right: confining potential $V_{geo}(x)$ (bottom panel) and charge density $|\Psi|^2$ of the ground state, shown both for the ideal case (solid line) with all the wells of equal depth, and for a perturbed system (dashed line) with values for each well of chosen randomly between $\pm 15\%$.

to model the effective attractive potential arising in the curved regions of 2D nanostructures [2]. The left panel of Fig. 1 shows the model of the system, whose cross-section results to be a rounded-hexagon. Electrons are strictly confined to the perimeter of the hexagon. In order to simulate the round-off of the edges of realistic devices, the full length of the side of the hexagon is R , but a piece of length l is removed at every side of each edge, and replaced by a round corner with a constant radius of curvature $r_c = \sqrt{3}l$. This finite curvature gives rise to an attractive potential [6, 7], whose intensity is given by

$$V_{geo} = -\frac{\hbar^2}{8m^*r_c^2}, \quad (1)$$

resulting, for the present model, in a set of six square wells located at the edges, as shown in the bottom of the right panel of Fig. 1. In the above formula, m^* is the effective mass, that has been taken to be that of a GaAs shell. The parameters for the rounded-hexagonal cross-section have been taken from Ref.[2], that is $R = 40$ nm and $l = 2$ nm, so that the resulting wells of Fig. 1 are 11.9 meV deep and 4 nm wide. This description corresponds to an ideal case, where the growth of the NW and the overgrowth of the shells is perfectly homogeneous all around the wire. The magnetic states of this ideal case have been studied in detail in Ref.[8]. In real cases, it is most likely that fluctuations may occur in the growth, so that the corner sharpness or the shell thickness might be inhomogeneous, breaking the 6-fold symmetry of the system.

In order to study the effect of the above symmetry breaking, we have randomly varied the depth of the wells, and kept the width unaltered (as shown in the right panel of Fig. 1), and then studied the effect on the electronic and magnetic states. The upper graph of the right panel of Fig. 1 shows the square moduli of the eigen-functions corresponding to the ground states. Due to the presence of the wells at the corners, the probability-density of the ground state shows maxima in the edges, this leading to the formation of six 1D channels in the hexagonal 2DES with higher probability density in the edges. We note how the random perturbation of the well

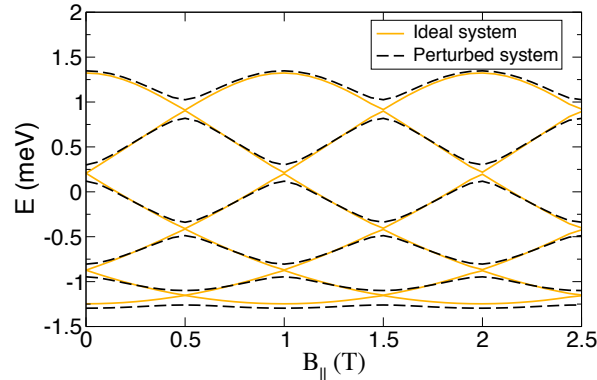


Figure 2. Magnetic levels as a function of an axial magnetic field. In the ideal case (solid line) the AB oscillations affect groups of six levels that cross each other while oscillating, while in the perturbed case (dashed line) the energy degeneracy occurring at $\Phi = (n + 1/2)\Phi_0$ ($n = 0, 1, 2, \dots$) is removed and each level oscillates with the AB period Φ_0 .

depths changes the relative probabilities of finding the carrier in each edge, but still preserves overall the edges as regions of preferential localization. The same edge-localization has been demonstrated also for other materials and shapes of the NWs [8].

3. Axial field B_{\parallel}

When a magnetic field is introduced, the expression of the Schrödinger equation on a curved surface should be derived with attention. In fact, a proper choice of the gauge allows to decouple the dynamics on the surface from the perpendicular one and to avoid couplings between the curvature and the field in the dynamical equation [9]. Solving the proper surface Schrödinger equation, we observe that, by applying an axial magnetic field, the energies show AB oscillations with respect to the field intensity as expected, and that the effect of the hexagonal cross-section is still present and important. Figure 2 shows the first six energy levels as a function of the applied field B_{\parallel} , both in the ideal and perturbed cases, so that we can recognize the different behaviors depending on the symmetry of the shell. In the ideal case, the levels oscillate in bunches of six levels crossing each other [8], while, in the perturbed case, the introduction of the random potential breaks the grouping, and the level crossing is split, so that each level oscillates without crossings. In both cases, however, the period of the oscillation is the AB period Φ_0 . Note that only the first six levels are shown in Fig. 2; for an analysis of the higher energy levels see Ref.[8].

4. Transverse field B_{\perp}

The analysis of the effect of the magnetic field can be repeated for a field B_{\perp} perpendicular to the NW axis. We showed in a previous work [10] that in cylindrical systems a strong transverse magnetic field induces the formation of Landau levels in the regions of the 2DES orthogonal to the direction of the field. Therefore, these regions behave as 1D channels where the carriers tend to localize. This mechanism is competing with the edge-localization described in Section 2, hence, depending on the orientation θ of the facets with respect to the field direction: the perpendicular magnetic field can be used as a tool to enhance the localization in the edges (Landau levels for $\theta = \pi/6$) or to extract carriers from the wells (for $\theta = 0$), as shown in Fig. 3. In the central panel of the latter figure, we show the density of states (DOS) for the ideal GaAs shell described in the previous sections, when B_{\perp} is applied with an orientation θ with respect to the facets. If the field is sufficiently strong to induce Landau localization [10], the edge-localized

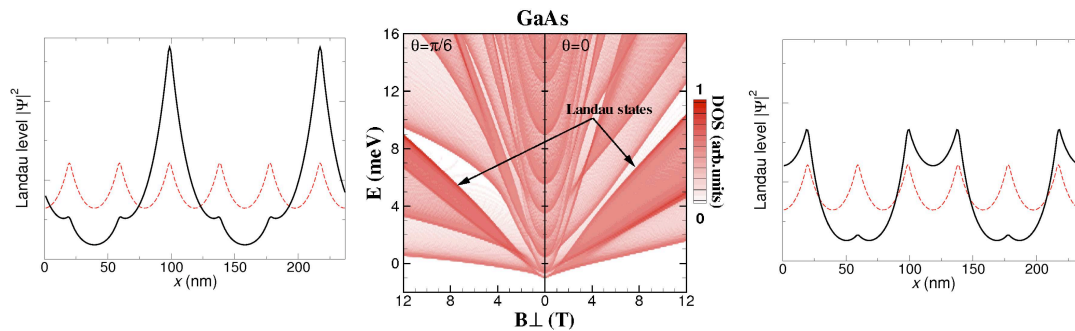


Figure 3. Results are shown for the ideal case with an unperturbed 6-fold symmetry. Center: DOS as a function of a perpendicular magnetic field and energy, shown for two different orientations θ of the facets with respect to the field direction. Darker color correspond to higher DOS. The states corresponding to the Landau levels are indicated by the arrows. Left: carrier probability density of a Landau state for $\theta = \pi/6$, showing a localization increase in two of the six edges. Right: carrier probability density of a Landau state for $\theta = 0$, showing a depletion of the edge-localized states. The zero-field ground state (dashed line) is shown as a comparison.

states can be depleted or further filled, depending on θ , as shown in the side panels of Fig. 3 for $\theta = \pi/6$ (left panel, enhancement) and $\theta = 0$ (right panel, depletion).

5. Conclusions

We have calculated the eigen-functions, energies and DOS of carriers in a shell of a core-multishell NW with rounded-hexagonal cross-section. We have shown that the edges are regions of preferential localization: this effect is persistent also against fluctuations of the edge sharpness and shell width. When an axial magnetic field is applied, the energy of the system oscillates with the AB period, corresponding to the quantum flux, and the crossing of the levels reflects the symmetry of the NW and the defects in the shell homogeneity. On the other hand, a magnetic field applied perpendicularly to the NW axis can be used to control the edge localization, allowing to strengthen or weaken it.

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