Electronic States in Nanowires with Hexagonal Cross-Section

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Abstract—The electron spectrum in a uniform nanowire with a hexagonal cross-section is calculated by means of a numerical diagonalization of the effective-mass Hamiltonian. Two basis sets are utilized. The wave-functions of low-lying states are calculated and visualized. The approach has an advantage over mesh methods based on finite-differences (or finite-elements) schemes: non-physical solutions do not arise. Our scheme can be easily generalized to the case of multi-band (Luttinger or Kane) \( k \cdot p \) Hamiltonians. The external fields (electrical, magnetic or strain) can be consistently introduced into the problem as well.

Keywords: nanowire, electronic states, effective mass approximation, numerical diagonalization

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1. INTRODUCTION

Semiconductor nanowires (NWs) are currently of great interest due to the possibility of their application in electronics. NWs can be used as a work item of field-effect transistors [1, 2], photodetectors [3]. Moreover, there is a wide variety of NW-based photonic devices including light-emitting diodes, chemical and gas sensors, waveguides, solar cells and nonlinear optical converters [4, 5]. The NW-based structures are also of fundamental interest. The topological states of the matter and Majorana fermions are realized in NWs due to the proximity effect [6–9].

Usually, NWs of III–V materials with a zinc-blende lattice are grown in [111] crystal direction, that leads to the hexagonal shape of NW’s cross-section (Fig. 1a). Early, simple models of NW with circular or square cross-sections were used for the calculation of the charge carrier spectrum and wave functions. However, for optical and transport applications it is necessary to know the carrier subband spectrum with higher precision, i.e., take into account a real NW’s shape.

The NW’s translation invariance in longitudinal direction simplifies the problem: one needs simply to solve the spectral problem for a two-dimensional electron bounded in a hexagon. Usually, the finite-difference (or finite elements) method is used for this purpose [10–12]. This problem is nontrivial even for the case of the electron in a non-degenerate band described by the scalar effective mass. We propose an alternative approach based on the numerical diagonalization of the matrix Hamiltonian written in an appropriate basis.

2. HAMILTONIAN AND BASIS FUNCTIONS

The effective potential barrier bounding an electron in NW is equal to the electron affinity \( \chi \) (several eV). Within the effective mass approximation, such a
height is equivalent to an infinite barrier. To find electronic states in NW with a hexagonal cross-section we propose to use the matrix mechanics. It is convenient to choose the eigenfunctions of the Hamiltonian $H_0$, which describes electrons in NW with a circular or rectangular cross-section, as the basis functions. The corresponding circle or rectangle is chosen to be circumscribed around the hexagon (see Figs. 1b, 1c). The spectral problem is reduced to the problem with the Hamiltonian $H = H_0 + V(r)$, where $V(r)$ is nonzero in shaded areas of Figs. 1b, 1c. The height of this potential cannot be chosen infinite at calculation, however, we do not make a big mistake putting it to be finite but high, e.g., $V_0 \sim \chi$. The envelope function approximation in a single band with a scalar effective mass $m^*$ is used. The spin-dependent terms are excluded from consideration.

The eigenfunctions and eigenenergies for the electron in the infinite circular potential well of radius $R$ are well-known

$$\Psi_{mn}^0(r, \varphi) = \frac{\sqrt{2}}{R J_{|m|+1}(r)} J_m \left( \frac{r}{R} \right) \frac{1}{\sqrt{2\pi}} e^{im\varphi},$$

(1)

$$E_{mn}^0 = \frac{\hbar^2 J_{mn}^2}{2m^* R^2},$$

(2)

where $m = 0, \pm 1, \pm 2, \ldots, n = 1, 2, \ldots; J_m(x)$ is the first kind Bessel function, and $j_{mn}$ is the $n$th zero of $J_m(x)$.

In the case of a potential well of rectangular shape circumscribing the same hexagon, the eigenfunctions and eigenenergies are given by

$$\Psi_{mn}^0(x, y) = \frac{\sqrt{2}}{3^{1/4} R} \sin \left( \frac{\pi mx}{2R} \right) \sin \left( \frac{\pi ny}{\sqrt{3} R} \right),$$

(3)

$$E_{mn}^0 = \frac{\pi^2 \hbar^2}{8m^* R} \left( m^2 + \frac{4}{3} n^2 \right)$$

(4)

with $m, n = 1, 2, \ldots$. We will search for the electron wavefunctions in hexagonal NW (h-NW) as a series in above basis sets

$$\Psi_j(r) = \sum_{mn} C_{mn}^j \Psi_{mn}^0(r).$$

(5)

The spectral problem is reduced to finding the eigenvalues of the Hamiltonian $H = H_0 + V(r)$ matrix. For the matrix elements we have, $\langle m'n'|H|mn \rangle = E_{mn}^0 \delta_{mn} + \langle m'n'|V(r)mn \rangle$. The latter term is proportional to the overlap integral $I_{m'n';mn}$ of the basis functions in the single barrier segment.

We can use some symmetry arguments for the matrix elements calculation. They are given by

$$\langle m'n'|V(r)mn \rangle = 6V_0 \delta_{mn} \delta_{n'1} + 6M M' I_{m'n';mn},$$

(6)

and

$$\langle m'n'|V(r)mn \rangle = 4V_0 \delta_{m'n';m+2M} \delta_{n'1} + 6N N' I_{m'n';mn},$$

(7)

for the case of a circular and rectangular basis, respectively. Here $M, N = 0, \pm 1, \pm 2, \ldots$. In the latter case the overlap integral can be found analytically, but in the former, only numerically.
3. NUMERICAL DIAGONALIZATION

For the numerical diagonalization of derived matrix Hamiltonians one needs to truncate the matrix dimension. At the same time, we have to choose a matrix size so as to ensure acceptable accuracy. The maximal values of \(m_{\text{max}}\) and \(n_{\text{max}}\) determine the size of the truncated matrix. In the circular basis the matrix dimension is \((2m_{\text{max}} + 1)n_{\text{max}}\), while in rectangular one we have \(m_{\text{max}}n_{\text{max}}\). The position of calculated subband bottoms in h-NW is depicted in the central section of Fig. 2a. The results are depicted for the truncated matrix of dimension 775 × 775 and 1000 × 1000 for circular and rectangular bases, respectively. This corresponds to the choice of \(m_{\text{max}} = 15\), \(n_{\text{max}} = 25\) and \(m_{\text{max}} = 40\), \(n_{\text{max}} = 25\), respectively. The energies are scaled to the value \(E_0 = \hbar^2/2m^*R^2\), that for the case of GaAs NW \((m^* = 0.067m_0)\) with \(R = 20\) nm is equal to 1.41 meV. The barrier height \(V_0\) was set to \(10^3E_0\).

The energy levels are a single or twofold degenerate (excluding spin). This is especially easy to trace when considering a circular basis. In this case the degenerate states arise even at diagonalization of the Hamiltonian matrix of small size, which does not provide a good precision. In this sense the use of Cartesian basis is more appropriate (there are no degenerate states) in order to track the convergence of the method with the growing matrix dimension. Nonetheless, the use of a Cartesian basis requires a larger matrix size to attain the same precision as for a circular basis. Moreover, for the case of a non-degenerate Cartesian basis, the real twofold degeneracy of states is reached only in the limit of \(V_0 \to \infty\), \(m_{\text{max}}n_{\text{max}} \to \infty\). This is due to the lack of 6th order symmetry axis in the model described in Fig. 1c compared to that in Fig. 1b.

The calculated coefficients \(C_{jm}^i\) give us the opportunity to find the spatial behavior of wave functions (see Eq. (5)). The electron distributions \(|\Psi|^2\) corresponding to energy levels of Fig. 2a (central panel) are depicted in Fig. 2b. The wave functions of degenerate states calculated in the Cartesian basis, in general, do not possess hexagonal symmetry. However, the total electron density at degenerate levels has this property.

4. CONCLUSIONS

In conclusion, the electronic states in h-NW are calculated. Corresponding wave functions are numerically found and visualized. The given approach can be generalized onto the case of the hole quantization in NWs or the more general case of a multi-band Hamiltonian. In the same manner the external fields can be introduced into the problem. The core-shell (or core-multi-shell) structures with a hexagonal cross-section of the core and shells can be considered by analogy with circular ones [14, 15]. This approach is attractive because there is no need to impose boundary conditions at the heterointerfaces, which is usually the case when calculating electronic and hole states in heterostructures using wave mechanics [16]. Moreover, nonphysical solutions do not arise in our approach compared to other ones.

CONFLICT OF INTEREST

The author declares that he has no conflict of interest.

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