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Electron conductance in curved quantum structures

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ABSTRACT

A differential-geometry analysis is employed to investigate the transmission of electrons through a curved quantum-wire structure. Although the problem is a three-dimensional spatial problem, the Schrödinger equation can be separated into three general coordinates. Hence, the proposed method is computationally fast and provides direct (geometrical) parameter insight as regards the determination of the electron transmission coefficient. We present, as a case study, calculations of the electron conductivity of a helically shaped quantum-wire structure and discuss the influence of the quantum-wire centerline radius of curvature and pitch length for the conductivity versus the chemical potential.

1. Introduction

In recent years, growth methods have allowed rather general and complicated nanowire structures to be developed in laboratories and characterized in terms of electronic and optical properties [1]. This calls for a better understanding of the importance of size and shape of nanostructures for physical properties and eventually device characteristics [2–4]. Differential-geometry methods are convenient for addressing nanostructure shape and size properties. Examples of differential-geometry applications exist for studies of lipid molecule structures [5] and carbon nanotubes [6,7]. In the present work, a differential-geometry analysis is employed to computationally effectively obtain the electron transmission coefficient or equivalently the electron conductivity for a nanowire semiconductor structure characterized by a generally varying curvature as a function of the centerline coordinate. We shall assume the nanostructure to be composed of three regions where regions 1 and 3 are straight cylinder sections but the central section (region 2) is arbitrarily curved. An electron propagates from region 1 towards region 2 and the transmission coefficient, defined as the ratio of wave amplitudes

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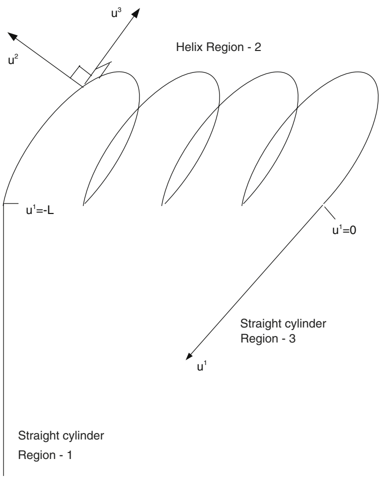

Fig. 1. Schematic drawing of the complete structure. Region 2 is the helical region while regions 1, 3 are straight cylinder sections.

in regions 3 and 1, is determined. In the case where the cross-sectional dimensions are small as compared to the centerline length of the full quantum-wire structure, the complete three-dimensional problem reduces to a separable problem in all three coordinates. The two ordinary differential equations in the in-plane coordinates can be solved immediately analytically while the latter ordinary differential equation in the centerline coordinate can be solved either analytically or numerically using a simple one-dimensional second-order differential equation. The method allows easy access to the importance of geometrical parameters such as curvature, centerline length, and in-plane dimensions for the electron conductivity.

2. Theory

Consider a curved quantum-wire structure composed of three regions. Region 1 is a straight cylinder, region 2 a curved cylinder, i.e., the cylinder centerline is characterized by a (possibly) varying curvature as a function of the centerline coordinate u^1, and region 3 is a straight cylinder. The cylinder cross-sectional dimensions, parametrized by u^2 and u^3, respectively, are constant as a function of the centerline coordinate for the whole structure.

In the first part of this section, we shall assume that the parametrization of region 2 can be done using an arc-length parametrization $\mathbf{r}(s)$, i.e., the tangent vector $\mathbf{t}(s) = \mathbf{r}'(s) = \mathrm{d}\mathbf{r}/\mathrm{d}s$ is a unit vector field along the curve and we can augment it with vector fields $\mathbf{p}(s)$ and $\mathbf{q}(s)$ along the curve such that $\mathbf{t}(s), \mathbf{p}(s), \mathbf{q}(s)$ constitutes an orthonormal frame at each point $\mathbf{r}(s)$ along the axis.

Assume that the electron is moving from region 1 towards region 2. At the interface between region 1 and 2, if region 2 is curved, partial reflection of the electron wave takes place. In region 3 the transmitted wave propagates towards infinity away from the interface between region 2 and region 3. We assume that the parameter range for the structure centerline is $-\infty < u^1 < \infty$ with the region 1–region 2 interface at $u^1 = -L$ and the region 2–region 3 interface at $u^1 = 0$ (see Fig. 1).

The Schrödinger equation in the u^1 coordinate for an electron with mass m and energy E reads (applying to zeroth order in u^1 and u^2) in the wavefunction χ [8]

$$\frac{-\hbar^2}{2m}\left(\partial_1^2\chi + \partial_2^2\chi + \partial_3^2\chi + \frac{\kappa(u^1)^2}{4}\chi\right) + V(u^1, u^2, u^3)\chi = E\chi, \tag{1}$$

where κ is the curvature of the nanowire centerline, which is a function of u^1 only. The potential V is assumed zero within the quantum-wire structure and infinite outside the quantum-wire structure.