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Coherent electron transport in a helical nanotube

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HIGHLIGHTS

- Fano resonance induced by the geometric potential of a helical nanotube is analyzed.
- Symmetry blocking in a bent cylindrical surface is found and proved.
- The transport of double-degenerate mode in a helical nanotube is reminiscent of the Zeeman coupling.
- New plateau in conductance appears for a helical nanotube with suitable length.

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ABSTRACT

The quantum dynamics of carriers bound to helical tube surfaces is investigated in a thin-layer quantization scheme. By numerically solving the open-boundary Schrödinger equation in curvilinear coordinates, geometric effect on the coherent transmission spectra is analysed in the case of single propagating mode as well as multimode. It is shown that, the coiling endows the helical nanotube with different transport properties from a bent cylindrical surface. Fano resonance appears as a purely geometric effect in the conductance, the corresponding energy of quasibound state is obviously influenced by the torsion and length of the nanotube. We also find new plateaus in the conductance. The transport of double-degenerate mode in this geometry is reminiscent of the Zeeman coupling between the magnetic field and spin angular momentum in quasi-one-dimensional structure.

1. Introduction

The realization of growing quasi-two-dimensional surfaces of arbitrary shape in nanoscale helps people find new physical effects which are originated from the topology. Many intriguing phenomena associated with the surface curvatures, such as electron localization [1–3], Aharonov–Bohm oscillations [4,5] and anisotropic magnetoresistance [6], have been investigated. Briefly speaking, in both theoretical and experimental fields scientists have accomplished essential developments for the curved two-dimensional (2D) systems.

To describe a particle confined to a curved surface, there is a triumphant approach that is introduced by Jensen and Koppe [7] and da Costa [8] (JKC). In this approach a confining potential is introduced to squeeze [9] the particle on curved surface. The introduced potential gives rise to that the quantum excitation energies in the direction normal to the surface are substantially larger than those in the tangential directions. Hence one can reasonably neglect the particle motion in the normal direction, and focus on the effective and dimensionally reduced equation. It is a great achievement to the JKC method that a curvature-induced potential appears in the effective 2D equation. The induced potential is the well-known geometric potential. The JKC approach has been successfully applied to many nanostructures with different geometries, such as rolled-up nanotubes [6,10], Möbius stripes [3,11] and helicoidal ribbon [12]. And the method is also proved by experimental results [13–15], such as the geometric effects on electron states [15], on proximity effects [16], and on the transport in photonic topological crystals [17].

In past decades, various interesting properties in carbon nanotubes have been widely and deeply studied, such as quantum transport and conductance [18–24], size effects [25–27]. Quantum transmission is a natural property of nanostructure devices, in

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which the topological effect is considerable. Recently, the geometric effects on the coherent electron transport have been investigated in bent cylindrical surfaces [28], and in the surface of a truncated cone [29]. Additionally, the curvature effects on vitrification behavior has been discussed for polymer nanotubes [30]. In the nanotubes the geometrical curvature plays an important role to influence their quantum properties. At the same time, in twisted nanoscale systems some quantum properties and phenomena have been studied, such as bound states [31–33], coherent electron transport [32,34], spin–orbit coupled electron [35]. In terms of those investigations, one can realize that the torsion-induced effect is significant to the quantum properties of the twisted systems. Consequently, in the present study we will investigate the coherent electron transport in helically coiled nanotubes (hereafter referred to as helical nanotubes) with finite length.

In this work, we treat the electron states in the effective mass approximation, which is valid for the conventional semiconducting nanotubes. The ballistic 1D transport in nanotubes has been demonstrated by several experiments [36–38]. In the case of semiconducting helical nanotubes, by taking into account the local change of electronic property [39,40] induced by geometric deformation, the envelope-function approach can still be used. Electron localization caused by the mixing of σ and π states are presented by the effective geometric potential in this approach. We will employ quantum transmitting boundary method (QTBM) [41] to numerically solve the transmission probability. This method is capable of solving open-boundary transmission problems for arbitrary internal geometries, since it can be generalized to include the metric tensor of the system [28,32]. In the calculational procedure, it is treated as that the two components of effective mass tensor [42,43] in two directions on the surface of 2D nanotubes are equal. To avoid misunderstanding, we stress that in our analysis, only the geometric chirality associated with torsion is considered and discussed, the effect of the chirality of atomic structure is ignored.

This work is structured as follows. In Section 2, we outline the mathematical description of an electron confined to the surface of a helical tube, and analyse the geometric potential and modes in leads. In Section 3, we numerically calculate the transmission probability in helical nanotubes and discuss the relationship between the transport and the symmetries in the helical system. In Section 4, the conductance at zero temperature is presented. Finally, in Section 5, we have a brief summary.

2. Model

2.1. Quantum dynamics of a particle constrained on a helical tube surface

One can construct a helical tube (as shown in Fig. 1) by moving a disk with radius ρ_0 along a helical line parametrized as $\mathbf{x}(s)$. To describe this geometry we introduce the Frenet frame vectors $\mathbf{t}$, $\mathbf{n}$ and $\mathbf{b}$ which satisfy

$$\begin{pmatrix}\dot{\mathbf{t}}\\ \dot{\mathbf{n}}\\ \dot{\mathbf{b}}\end{pmatrix}=\begin{pmatrix}0 & \kappa(s) & 0\\ -\kappa(s) & 0 & \tau(s)\\ 0 & -\tau(s) & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}, \tag{1}$$

where $\mathbf{t}$, $\mathbf{n}$ and $\mathbf{b}$ are the unit tangent vector, normal vector and binormal vector of $\mathbf{x}(\mathbf{s})$, respectively, the dot denotes derivative with respect to the natural parameter s, and $\kappa(s)$ and $\tau(s)$ are the curvature and torsion of $\mathbf{x}(s)$, respectively. During the disk moving along $\mathbf{x}(s)$, the disk is always orthogonal to $\mathbf{t}$, on the disk plane $\mathbf{n}$ and $\mathbf{b}$ shift due to $\tau(s)$. It is convenient to define two new vectors

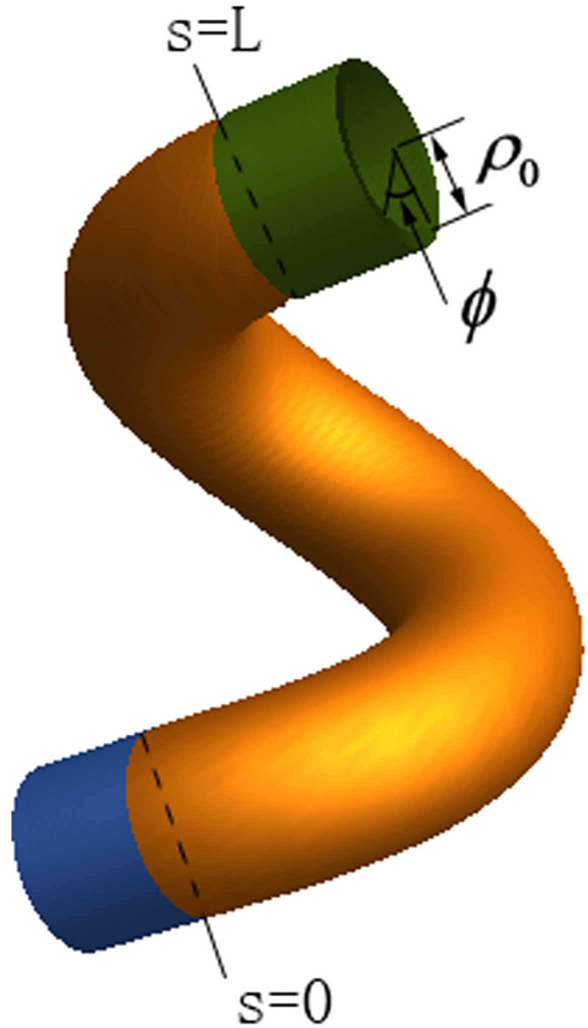

Fig. 1. Surface of a helical tube with two straight cylinders at the two ends. The geometry is parametrized by s and ϕ.

$$\mathbf{N}=\cos\theta(s)\mathbf{n}+\sin\theta(s)\mathbf{b}, \tag{2}$$

$$\mathbf{B}=-\sin\theta(s)\mathbf{n}+\cos\theta(s)\mathbf{b}, \tag{3}$$

where the angle $\theta(s)=-\int_{s_0}^{s}\tau(s')ds'$.

In this new frame, $\mathbf{N}$ and $\mathbf{B}$ are fixed on the disk. The relation equation (1) becomes

$$\begin{pmatrix}\dot{\mathbf{t}}\\ \dot{\mathbf{N}}\\ \dot{\mathbf{B}}\end{pmatrix}=\begin{pmatrix}0 & \xi(s) & -\eta(s)\\ -\xi(s) & 0 & 0\\ \eta(s) & 0 & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{N}\\ \mathbf{B}\end{pmatrix}, \tag{4}$$

where $\xi(s)=\kappa(s)\cos\theta(s)$, $\eta(s)=\kappa(s)\sin\theta(s)$. Consequently, points on the tube surface can be parametrized as

$$\mathbf{R}(s,\phi)=\mathbf{x}(s)-\rho_0[\sin(\phi)\mathbf{B}+\cos(\phi)\mathbf{N}], \tag{5}$$

where ϕ is the angular position of the point on the edge of the disk.

It is straightforward now to get the metric tensor of the tube surface by using the definition $g_{ij}=\frac{\partial\mathbf{R}}{\partial q^i}\cdot\frac{\partial\mathbf{R}}{\partial q^j}$ and the relation equation (4),