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Curvature-induced quantum behaviour on a helical nanotube

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ABSTRACT

We investigate the effect of curvature on the behaviour of a quantum particle bound to move on a surface shaped as a helical tube. We derive and discuss the governing Schrödinger equation and the corresponding quantum effective potential which is periodic and points to the helical configuration as more energetically favorable as compared to the straight tube. The exhibited periodicity also leads to energy band structure of pure geometrical origin.

Recent developments in nanotechnology [1] made it possible to grow quasi-two-dimensional surfaces of arbitrary shape where quantum and curvature effects play a major role [2]. Examples include single crystal $NbSe_3$ Möbius strips [3], spherical CdSe–ZnS core-shell quantum dots [4], Si nanowire, nanoribbon transistors [5], quantum waveguides [6] and nanotorus [7]. Several publications [8–14] have treated the constrainment of quantum-mechanical particles (with applications in, e.g. standard Schödinger equation problems [15] and relativistic Dirac equation problems [16,17]) to a two-dimensional surface since the original works by Jensen and Koppe, da Costa [18–20]. Since two-dimensional systems are an a priori idealization it is reasonable to quantize before constraining the particle to the nanotube. As a result a quantum particle confined to a two-dimensional surface embedded in $\mathbb{R}^3$ experiences a potential that is a function of the Mean and the Gauss curvatures of the surface [19,20]. This curvature-induced quantum potential is a geometric invariant, a property that led the authors [21] to pose the inverse differential geometrical problem: what curved surfaces produce prescribed curvature-induced potential.

Possible physical applications of the above include the geometric interaction between defects and curvature in thin layers of superfluids, superconductors, and liquid crystals deposited on curved surfaces [22]; the curvature of a semiconductor surface determines also an interesting mechanism of spin–orbit interaction of electrons [23]; a charged quantum particle trapped in a potential of quantum nature due to bending of an elastically deformable thin tube travels without dissipation like a soliton [24]; the twist of a strip plays a role of a magnetic field and is responsible for the appearance of localized states and an effective transverse electric field thus reminisces the quantum Hall effect [25].

Now let us turn our attention to the geometrical realization of the helical tube. One can associate with a space curve $\vec{\mathbf{x}}(s)$ at any point s along it a moving frame consisting of three vectors $\vec{\mathbf{t}}$—tangent, $\vec{\mathbf{n}}$—normal and $\vec{\mathbf{b}}$—binormal and evolving along the curve according to the Frenet–Serret equations:

$$\dot{\vec{\mathbf{t}}} = \vec{\omega} \wedge \vec{\mathbf{t}}, \qquad \dot{\vec{\mathbf{b}}} = \vec{\omega} \wedge \vec{\mathbf{b}}, \qquad \dot{\vec{\mathbf{n}}} = \vec{\omega} \wedge \vec{\mathbf{n}}, \tag{1}$$

where $\vec{\omega}$ is the instantaneous angular velocity of the Frenet–Serret frame where the arclength s plays the role of time. Hereafter the dot denotes derivation with respect to the natural parameter s. Here $\kappa(s)$ and $\tau(s)$ are the curvature and torsion of the space curve.

Since $\vec{\omega}$ has a component along $\vec{\mathbf{t}}$ we redefine the frame vectors

$$\vec{\mathbf{N}} = \cos\theta(s)\vec{\mathbf{n}} + \sin\theta(s)\vec{\mathbf{b}}, \qquad \dot{\vec{\mathbf{N}}} = \vec{\Omega} \wedge \vec{\mathbf{N}}, \tag{2}$$

$$\vec{\mathbf{B}} = -\sin\theta(s)\vec{\mathbf{n}} + \cos\theta(s)\vec{\mathbf{b}}, \qquad \dot{\vec{\mathbf{B}}} = \vec{\Omega} \wedge \vec{\mathbf{B}}. \tag{3}$$

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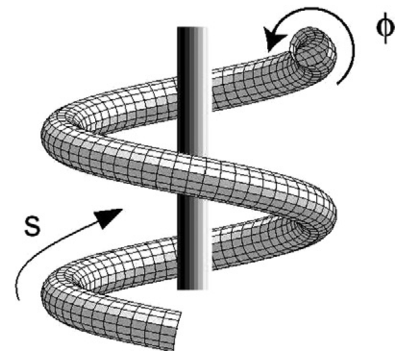

Fig. 1. The geometry of an infinite helical tube may be parametrized by two families of space curves (see Eq. (5) and text).

We choose $\theta(s)$ so that $\vec{\Omega}$ has no component in the direction of $\vec{\mathbf{t}}$. A brief calculation yields [26]

$$\theta(s) = -\int_{s_0}^{s} ds'\,\tau(s'). \tag{4}$$

Now let us mount a disc D rigidly in the reference frame [31] where $\vec{\mathbf{N}}$ and $\vec{\mathbf{B}}$ are at rest, i.e. the Fermi–Walker frame. The points on the surface may be parametrized by

$$\vec{\mathbf{X}}(s,\phi) = \vec{\mathbf{x}}(s) - \rho_0\{\sin\phi\,\vec{\mathbf{B}} + \cos\phi\,\vec{\mathbf{N}}\}. \tag{5}$$

The two families of space curves weaving the above surface in $\mathbb{R}^3$ are the following. The first is a circle parametrized by the angle ϕ and is actually the rim of the disc that is rigidly mounted to the tangent $\vec{\mathbf{t}}(s)$ of the helical curve $\vec{\mathbf{x}}(s)$ at each point in space. The tangent $\vec{\mathbf{t}}(s)$ coincides with the normal of the disk. The tip of the vector in the disc from the central axis to the rim is denoted by $\rho_0\cos\phi\,\vec{\mathbf{N}} + \rho_0\sin\phi\,\vec{\mathbf{B}}$. Its origin coincides with the helical space curve $\vec{\mathbf{x}}(s)$. The second is given by the curves whose tangents are passing through each point of the first family. Refer to Fig. 1 for the visual expression of the above construction.

In this article we will study the properties of the Schrödinger equation on the helical tube shown in Fig. 1.

The line element is

$$|d\vec{\mathbf{X}}|^2 = d\varphi^2 + h^2\,ds^2, \tag{6}$$

where

$$h(s,\phi) = 1 + \rho_0\kappa(s)\cos\left[\theta(s) + \frac{\varphi}{\rho_0}\right] \tag{7}$$

and

$$\varphi = \rho_0\phi \tag{8}$$

has a dimension of length.

If we change the parametrization $s \to -s$ and $\varphi \to -\varphi$ this would mean that we evolve the surface backward from a certain arbitrary point s_0 of the infinite space line $\vec{\mathbf{x}}(s)$. The torsion τ exhibits invariance $\tau(s) = \tau(-s)$ and the surface element must remain unchanged:

$$\theta(-s) + \left(-\frac{\varphi}{\rho_0}\right) \to -\left[\theta(s) + \frac{\varphi}{\rho_0}\right], \qquad h(s) \to h(-s).$$

Thus we show that the line element is indeed invariant

$$\left|d\vec{\mathbf{X}}(s,\varphi)\right|^2 = \left|d\vec{\mathbf{X}}(-s,-\varphi)\right|^2.$$

From formulas (2) and (3) we see that at $\theta(s) = 0$, that is at $s = 0$ if $s_0 = 0$ (see (4)), we have the coincidence $\vec{\mathbf{N}} \equiv \vec{\mathbf{n}}$ and $\vec{\mathbf{B}} \equiv \vec{\mathbf{b}}$. The normal $\vec{\mathbf{n}}$ always points towards the axis around which the helix is wound, i.e. it points inward. From (7) it is clear that $h(0,0) = 1 + \rho_0\kappa(0) > 1 - \rho_0\kappa(0) = h(0,\pi)$. The surface is stretched more on the outside thus we have a natural choice of the origin (the outer intersection of the ray through $\vec{\mathbf{n}}$ and the cross-section of the tube) for the two families of curves (see Fig. 2).

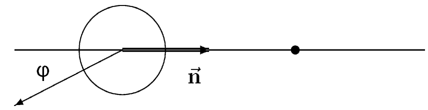

Fig. 2. The cross-section of the nanotube in Fig. 1.

Introducing the normal to the surface $\vec{\nu}$ from the Gauss triad $\vec{\nu} = \partial_\varphi\vec{\mathbf{X}} \wedge \partial_s\vec{\mathbf{X}}|\partial_\varphi\vec{\mathbf{X}} \wedge \partial_s\vec{\mathbf{X}}|^{-1/2}$ we can compute the linear Weingarten map [27]

$$\begin{pmatrix} \partial_\varphi\vec{\nu} \\ \partial_s\vec{\nu} \end{pmatrix} = W \begin{pmatrix} \partial_\varphi\vec{\mathbf{X}} \\ \partial_s\vec{\mathbf{X}} \end{pmatrix},$$

where W is the matrix realizing the map of the tangent space in itself:

$$W = \begin{pmatrix} \rho_0^{-1} & 0 \\ 0 & \kappa(s)\cos[\theta(s) + \frac{\varphi}{\rho_0}]h^{-1} \end{pmatrix}. \tag{9}$$

With the help of (9) we may compute

$$M = \frac{\kappa_1 + \kappa_2}{2} = -\frac{\mathrm{tr}(W)}{2}, \qquad K = \kappa_1\kappa_2 = \det(W), \tag{10}$$

the Mean and the Gauss curvatures of the surface respectively, where κ_1 and κ_2 are the principal curvatures of the surface. They are also the eigenvalues of the Weingarten matrix (9). Thus we obtain

$$\kappa_1 = \frac{1}{\rho_0}, \qquad \kappa_2 = \kappa(s)\cos\left[\theta(s) + \frac{\varphi}{\rho_0}\right]h^{-1}. \tag{11}$$

Since we study the resulting Schrödinger equation for a particle confined to move on that surface and following da Costa an effective potential appears in the Schrödinger equation which has the following form:

$$V_{\mathrm{curv}} = -\frac{\hbar^2}{2\mu}\left(M^2 - K\right), \tag{12}$$

where μ is the effective particle's mass, $\hbar$ is Planck's constant; V_{curv} depends on s and φ which appear as the generalized coordinates on the surface; M and K are the Mean and the Gauss curvatures given in (10). For the surface (5) we obtain

$$V_{\mathrm{curv}}(s,\varphi) = -\frac{\hbar^2}{8\mu}\frac{1}{\rho_0^2}\frac{1}{h^2}. \tag{13}$$

From Eqs. (6) and (7) it follows that the surface is more stretched on the outside, that is at $\varphi = 0$ (see Fig. 2), because $h(0,0) > h(0,\pi)$. The Heisenberg uncertainty principle states that a particle would have a lower energy where the line element is bigger. Our expectation is that the probability to find a particle on the outer rim of the surface is maximal. This guiding principle will allow us to interpret the appropriate effective Schrödinger equation whose potential possesses the above property.

The Laplace–Beltrami operator (the quantum mechanical kinetic term) in the coordinate system (5) can be written as follows:

$$\begin{aligned} -\Delta_{s,\varphi}\Psi = {} & -\frac{1}{h^2}\frac{\partial^2\Psi}{\partial s^2} - \frac{\partial^2\Psi}{\partial\varphi^2} + \kappa\sin\left(\theta + \frac{\varphi}{\rho_0}\right)\frac{1}{h}\frac{\partial\Psi}{\partial\varphi} \\ & + \rho_0\dot{\kappa}(s)\cos\left(\theta(s) + \frac{\varphi}{\rho_0}\right)\frac{1}{h^3}\frac{\partial\Psi}{\partial s} \\ & - \rho_0\dot{\theta}(s)\kappa(s)\sin\left(\theta(s) + \frac{\varphi}{\rho_0}\right)\frac{1}{h^3}\frac{\partial\Psi}{\partial s}. \end{aligned} \tag{14}$$