Effect of conformations on charge transport in a thin elastic tube

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Abstract

We study the effect of conformations on charge transport in a thin elastic tube. Using the Kirchhoff model for a tube with any given Poisson ratio, cross-sectional shape and intrinsic twist, we obtain a class of exact solutions for its conformation. The tube’s torsion is found in terms of its intrinsic twist and its Poisson ratio, while its curvature satisfies a nonlinear differential equation which supports exact periodic solutions in the form of Jacobi elliptic functions, which we call \textit{conformon lattice} solutions. These solutions typically describe conformations with loops. Each solution induces a corresponding quantum effective periodic potential in the Schrödinger equation for an electron in the tube. The wave function describes the delocalization of the electron along the central axis of the tube. We discuss some possible applications of this novel mechanism of charge transport.

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1. Introduction

Nanotubes and nanowires have attracted considerable attention due to their potential technological applications [1]. Carbon nanotubes and DNA are well known examples. One important problem is to understand their mechanical properties. Another is to gain some insight into the effect of quantum confinement on electronic transport in such nanostructures.

One striking observation concerning the DNA molecule is that its central axis can take on various curved conformations. Similarly, nanotubes need not always be straight. Helix-shaped nanotubes have been observed by Volodin \textit{et al} [2]. One way to theoretically model these twisted thin tubes (wires) would be to assume that they are elastic filaments described within the framework of the Kirchhoff rod model [3], derive the various possible curved
conformations that can arise from it, and see if they are in accordance with the shapes actually observed. This would also help in studying the elastic properties of these structures within this model. [4] The natural question that arises is how the confinement of a particle to a curved path would affect its transport.

Now, the problem of quantum transport of a free particle in a thin curved tube has been studied by several authors [5–7]. They have shown that the curved geometry of the tube essentially induces a potential in the path of the particle, thereby affecting its transport properties.

In a recent paper [8], we analysed the case when the thin tube is made of elastic material, and applied it to electron transport in a biopolymer. We analysed the statics and dynamics of the thin elastic tube using the Kirchhoff model [3]. Under certain conditions, the curvature function of the tube supports a spatially localized travelling wave solution called a Kovalevskaya solitary wave [9,10]. We showed that this solution corresponds to a conformation which is a localized twisted loop travelling along the tube [8]. The localized bend induces a quantum potential well in the Schrödinger equation for an electron in the tube [5–7], which traps it in the twisted loop, resulting in its efficient motion, without change of form, along the polymer. Our result formalizes the concept of a conformon that has been hypothesized in biology [11–13].

The motivation for this paper is as follows. Firstly, the analysis of the Kirchhoff model given in [8, 10] had assumed that the elastic tube had no intrinsic twist. It was therefore not strictly applicable either to DNA (which has an intrinsic twist of about $10^\circ\text{Å}$, even in the straight relaxed state) or to the class of intrinsically twisted nanotubes. In what follows, we present a more general analysis of the Kirchhoff model, by incorporating an intrinsic twist in the tube, and point out the nontrivial role that it plays in determining the geometrical shape of the axis of the tube. Further, our analysis is valid for any general value of the Poisson ratio. Secondly, we show that the nonlinear differential equation for the curvature function obtained from the static Kirchhoff equations can, in addition to the localized solution discussed in [8], also support a class of spatially periodic solutions in the form of Jacobi elliptic functions. We call them conformon lattice solutions. Each such solution induces a quantum periodic potential. Finally, we show explicitly that the Schrödinger equation supports an exact solution, which corresponds to the electron getting delocalized along the axis of the quantum wire, even in the static case. Thus this mechanism for electron transport in a quantum nanotube is distinct from the conformon mechanism discussed in [8].

2. The Kirchhoff model

We consider a thin elastic rod [3] whose central axis is described by a space curve $\mathbf{R}(s, t)$. Here, $s$ denotes the arc length of the curve and $t$ the time. Let the rod remain inextensible with time evolution, with the unit tangent to its axial curve given by $\mathbf{t} = \mathbf{R}_s$. (The subscript $s$ denotes the derivative with respect to $s$). In the plane perpendicular to $\mathbf{t}$, we define as usual [14], two orthogonal unit vectors $\mathbf{n}$ and $\mathbf{b}$, where the principal normal $\mathbf{n}$ is the unit vector along $\mathbf{t}_s$, and the binormal $\mathbf{b} = (\mathbf{t} \times \mathbf{n})$. The rotation of the Frenet frame $(\mathbf{t}, \mathbf{n}, \mathbf{b})$ as it moves along the curve, is given by the well known Frenet–Serret equations, $\mathbf{t}_s = k\mathbf{n}$, $\mathbf{n}_s = -kt + \tau\mathbf{b}$ and $\mathbf{b}_s = -\tau\mathbf{n}$, where the curvature $k = |\mathbf{t}_s|$ and the torsion $\tau = \mathbf{t} \cdot (\mathbf{t}_s \times \mathbf{t}_{ss})/k^2$.

For elastic tubes, instead of $\mathbf{n}$ and $\mathbf{b}$, it is more natural to use ‘material’ orthogonal unit vectors $\mathbf{d}_1$ and $\mathbf{d}_2$ lying on the cross-section of the tube, perpendicular to its axial curve. For example, they could lie along the principal axes of inertia of the cross-section. Let $\mathbf{d}_1$ make an angle $\phi$ with $\mathbf{n}$. Hence we get $\mathbf{d}_1 = n \cos \phi + b \sin \phi$ and $\mathbf{d}_2 = -n \sin \phi + b \cos \phi$. Denoting the tangent $\mathbf{t}$ by $\mathbf{d}_1$, and using the Frenet–Serret equations, it is easy to show that the rotation
of the ‘material’ frame \((d_1, d_2, d_3)\) along the curve is given by
\[ d_{i,s} = k \times d_i, \]  
(1)
where \(i = 1, 2, 3\), and the vector \(k\) is given by
\[ k = k_1d_1 + k_2d_2 + k_3d_3. \]  
(2)

Here
\[(k_1, k_2, k_3) = (k \sin \phi, k \cos \phi, \tau + \phi_s). \]  
(3)
Let the internal elastic force (or tension) and the total torque, that act on each cross-section of the rod be given by \(g\) and \(m\), respectively. The Kirchhoff equations that result from the conservation of linear and angular momentum at every point \(s\) are given in dimensionless form by [9, 10]
\[ g_s = R_{tt} \]  
(4)
and
\[ m_s + d_3 \times g = ad_1 \times d_{1,tt} + d_2 \times d_{2,tt}, \]  
(5)
where the subscript \(t\) stands for the derivative with respect to time. The internal force is written in general form as
\[ g = g_1d_1 + g_2d_2 + g_3d_3. \]  
(6)
We take into account the intrinsic twist \(k_3^0\) of the elastic tube, by writing the constitutive relation for the internal torque \(m\) as
\[ m = k_1d_1 + ak_2d_2 + b(k_3 - k_3^0)d_3. \]  
(7)
In the equations above, the parameter \(a\) is a measure of the bending rigidity of the cross-section of the rod. It is the ratio \(I_1/I_2\) of the two moments of inertia of the cross-sections of the nanotube in the directions \(d_1\) and \(d_2\). These are conventionally oriented such that \(I_1 \leq I_2\). Hence \(0 < a \leq 1\). (For a circular cross-section, \(a = 1\).) \(b\) is a measure of the twisting rigidity of the rod. It is given in terms of \(a\) and the Poisson ratio \(\sigma\), which is a measure of the change in the volume of the rod as it is stretched:
\[ b = 2a/[1(1 + \sigma)(1 + a)] \]  
(8)
In [8, 10], the term involving \(k_3^0\) in equation (7) is absent. Hence the analysis given there is valid for tubes without an intrinsic twist. In the next section, we analyze the Kirchhoff equations (4) and (5) with \(k_3^0 \neq 0\). Our analysis will be valid for general values of \(a\) and \(\sigma\).

3. Role of the intrinsic twist
We first analyze the static conformations. Substituting equations (6) and (7) in equations (4) and (5), we get
\[ g_{1,s} + k_2g_3 - k_3g_2 = 0, \]  
(9)
\[ g_{2,s} + k_3g_1 - k_1g_3 = 0, \]  
(10)
\[ g_{3,s} + k_1g_2 - k_2g_1 = 0, \]  
(11)
\[ g_3 = k_{1,s} + (b - a)k_2k_3 - bk_3^0k_1, \]  
(12)
\[ g_1 = -ak_{2,s} + (b - 1)k_1k_3 - bk_3^0k_1 \]  
(13)
The internal elastic force is found to be

\[ bk_{3,4} + (a - 1)k_3k_2 = 0. \] (14)

As is clear from equation (3), the equations above represent a set of nonlinear coupled differential equations involving \( k, \tau \) and \( \phi \).

To understand the role played by the intrinsic twist, we proceed as in [8, 10], and look for solutions that correspond to \( \phi = \frac{1}{2}n\pi, \; n = 0, 1, \ldots \). Using this in equation (3), we see that equation (14) yields

\[ \tau = \tau_0. \] (15)

Thus the torsion of the tube, which is a measure of its nonplanarity, is an arbitrary constant, to be determined consistently. We focus on nontrivial conformations with a nonvanishing \( \tau_0 \).

Two cases arise in the analysis of equations (9)–(13):

**Case (i).** \( \phi = j\pi, \; j = 0, 1; \; k_1 = 0; \; k_2 = (-)^j k \).

We find in this case

\[ (b - 2a) \tau_0 = b k^0_3. \] (16)

Using equation (8) in this equation, we get

\[ \tau_0 = -k^0_1/[a + \sigma(a + 1)]. \] (17)

The internal elastic force is found to be

\[ g = (-1)^j a(\tau_0 k d_2 - k_1 d_1) + (C - \frac{1}{2} ak^2) d_3, \] (18)

where the constant \( C \) represents the tension in the rod when it is straight.

**Case (ii).** \( \phi = (j + \frac{1}{2})\pi, \; j = 0, 1; \; k_1 = (-)^j k; \; k_2 = 0 \).

We now obtain

\[ (b - 2) \tau_0 = b k^0_3. \] (19)

As before, using equation (8) in this equation yields

\[ \tau_0 = -ak^0_3/[1 + \sigma(a + 1)]. \] (20)

The elastic force is determined as

\[ g = (-1)^j[(\tau_0 k d_1 + k_3 d_2) + (C - \frac{1}{2} k^2) d_3]. \] (21)

We now show that the intrinsic twist indeed plays a nontrivial role in determining the torsion \( \tau_0 \) of the conformation of the elastic tube.

First, if \( k^0_3 = 0 \), then equations (16) and (19) yield \( b = 2a \) and \( b = 2 \), respectively, because \( \tau_0 \neq 0 \). Putting in these two values of \( b \) in equation (8) successively, we get \( \sigma = -1/(1 + a) \) and \( \sigma = -a/(1 + a) \), respectively. Since \( 0 < a \leq 1 \), it follows that the Poisson ratio \( \sigma \) has to be negative, and in the range \(-1 < \sigma \leq -\frac{1}{2} \) and \(-\frac{1}{2} \leq \sigma < 0 \), respectively, for the two cases. Although thermodynamic stability arguments [15] merely restrict \( \sigma \) to the range \(-1 \leq \sigma \leq \frac{1}{2} \), and while \( \sigma \) can indeed be negative for some biopolymers [10], for most elastic media one finds that \( 0 < \sigma < \frac{1}{2} \).

Thus, for both cases (i) and (ii), setting \( k^0_3 = 0 \) determines the numerical value of \( \sigma \), which turns out to be negative for any \( a \). Further, \( \tau_0 \) can take on any arbitrary value in this instance.

In contrast, if \( k^0_3 \neq 0 \), the corresponding torsion \( \tau_0 \) is not arbitrary, but is determined in terms of \( k^0_3, a \) and \( \sigma \) (which are material properties), as we may expect on physical grounds. This dependence can be seen from equations (17) and (20). These equations also show that positive as well as negative values of \( \sigma \) are allowed in this instance, which is a desirable feature. We may note that when \( \sigma > 0 \), the torsion \( \tau_0 \) and the intrinsic twist \( k^0_3 \) have opposite signs. In addition, on imposing the condition \( 0 < \sigma \leq 1 \), both equations (17) and (20) lead to the same inequality, \( \sigma < -k^0_3/\tau_0 \leq 2\sigma + 1 \).
4. Exact conformations

In the last section, we found the solutions for the torsion $\tau_0$. Using equation (18) in equation (9), and equation (21) in equation (10), respectively, we can derive the nonlinear differential equation for the curvature $k$ in cases (i) and (ii). They are seen to have the same form

$$k'' + \frac{1}{2}k^3 = (C_2 - \tau_0^2)k,$$

(22)

where $C_2 = C/a$ for case (i), while $C_2 = C$ for case (ii).

Note that equation (22) has the same form as that obtained earlier [8, 10], for the case $k_0^3 = 0$ as well, but with the important difference that $\tau_0$ is not arbitrary any more, but depends on $k_0$ as shown in the last section. Equation (22) has a solution of the form

$$k(s) = 2(C_2 - \tau_0^2)^{1/2} \text{sech} \left[\left(C_2 - \tau_0^2\right)^{1/2} s\right],$$

(23)

for $(C_2 - \tau_0^2) > 0$.

This represents a static conformon. Now, due to scale and galilean invariance [9] of the dynamic Kirchhoff equations (4) and (5), travelling wave solutions are possible for $k$, with $s$ replaced by $(s - vt)$ in equation (23). Here $v$ represents the velocity of the wave. This leads to a moving conformon [8], which is like a solitary wave.

Now, in general, we find that the nonlinear differential equation (22) supports solutions of the form

$$k(s, \kappa) = 2\sqrt{C_2 - \tau_0^2} \frac{1}{2 - \kappa^2} \text{dn} \left(\sqrt{C_2 - \tau_0^2} s, \kappa\right),$$

(24)

where $\text{dn}$ is the usual Jacobi elliptic function, with modulus $\kappa$ in the range $0 \leq \kappa < 1$ [16]. For $\kappa = 1$, solution (24) becomes (23), which was considered in [8]. But in contrast to that solution, which was spatially localized, solution (24) is a spatially periodic function, with a finite period $2K(\kappa)$ for all $\kappa \neq 1$. Here $K(\kappa)$ is the complete Jacobi integral of the first kind, which tends to infinity for $\kappa = 1$. Thus we call equation (24) for all $\kappa \neq 1$, a conformon lattice solution.

In figures 1–5, we have displayed the conformations of a thin elastic tube (rod) that correspond to the conformon lattice solutions for the curvature, given in equation (24), for various values of $\kappa$, and constant torsion $\tau_0 = 0.5$. In all the plots, $\sqrt{(C_2 - \tau_0^2)}$ has been set equal to unity, since its inverse merely scales the length.

For $\kappa = 1$, the conformation is given in figure 1, and it corresponds to a single loop or conformon. Its shape is (as expected) different from that obtained in [8] for $\tau_0 = 1$.

We find that even a slight decrease to $\kappa = 0.995$ leads to a fairly large change in the conformation, with two loops, and a partially complete loop, as seen in figure 2. From $\kappa = 0.995$ to $\kappa = 0.75$, there are steady changes in the conformation. In contrast, below $\kappa = 0.75$, the conformational changes are much slower as $\kappa$ varies, as seen by comparing figure 3 ($\kappa = 0.75$) with figure 4 ($\kappa = 0.25$), which differ very slightly.

For $\kappa = 0$, the curvature becomes a constant independent of $s$. Hence this conformation represents a structure in which the axis of the tube is coiled into a helix, with a constant curvature and torsion. This is displayed in figure 5. We parenthetically remark that while this helical tube was essentially the only conformation considered in [4] in the context of the Kirchhoff model, we see that a wide class of coiled conformations corresponding to nonzero $\kappa$ are supported by the model.

As explained below solution (23) for the conformon, it is possible to have travelling wave solutions (24) with $s$ replaced by $(s - vt)$.
Figure 1. Conformation corresponding to curvature $k$ as given in equation (24) for $\kappa = 1$. Note the localized twisted loop formed by the axis of the tube.

Figure 2. Conformation corresponding to curvature $k$ as given in equation (24) for $\kappa = 0.995$. Note the appearance of two loops and a partially complete loop.

We conclude this section with the remark that the solutions for the curvature (equation (24)) will also be applicable for a closed tube of length $L$ satisfying periodic boundary conditions. We get $L \sqrt{(C_2 - \tau_0^2)/(2 - \kappa^2)} = 2mK(\kappa)$, where $m$ is an integer.

5. Quantum mechanical charge transport in a tube

In this section, we consider the implications of the conformon lattice solution (24) for electron transport along a nanotube. We recall some salient steps given in [8], where we discussed the conformon, for the sake of completeness.

As has been shown [6, 7], a thin tube with curvature $k(s)$ and torsion $\tau_0$ induces a quantum potential $V_{\text{eff}}(s) = (\hbar^2/2\mu)(-k^2/4 + \tau_0^2/2)$ for an electron moving on it. Here $\mu$ is the mass of the electron. In the time-dependent Schrödinger equation with the above potential, we can eliminate the constant torsion $\tau_0$ using a simple gauge transformation.
There are three twisted loops of unequal sizes, and a bend.

Using the transformation $(t, s) \rightarrow ((4 \mu / \hbar) u, \sqrt{2}s_1)$, equation (25) becomes

\[ i \psi_u + \psi_{s_1 s_1} + \frac{k^2}{2} \psi = 0, \tag{26} \]

where $k = k(s_1)$, and the subscripts $s_1$ and $u$ stand for the partial derivatives $\partial/\partial s_1$ and $\partial/\partial u$. 

\[ \psi_1 = \psi(s, t) \exp(-i\frac{\tau_0^2 t}{4 \mu}). \]

This leads to

\[ i \hbar \frac{\partial}{\partial t} \psi(s, t) = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial s^2} + \frac{k^2(s)}{4} \right) \psi(s, t). \tag{25} \]
Looking for stationary solutions of the Schrödinger equation (26) in the form
\[ \psi(s_1, \kappa, u) = k(s_1) \exp(-iE u), \] (27)
we get
\[ \left( k_{s_1} + \frac{k^3}{2} \right) = -E k. \] (28)
Comparing this with equation (22), for self-consistency, we must have
\[ E = -(C_2 - \tau_0^2), \] (29)
which is negative. We write equation (28) in the form of a time-independent Schrödinger equation with a potential term \[ V = \kappa(s, \kappa) k = E k. \] (30)
On using equation (24), we see that the potential is given by
\[ V(s, \kappa) = -2(C_2 - \tau_0^2) \sqrt{C_2 - \tau_0^2 - \kappa^2} \delta(s_1, \kappa), \] (31)
which is negative as well. Since \( \delta^2(s, \kappa) \leq 1 \) for all \( s \) and \( \kappa \), the minimum value of the potential in equation (28) is
\[ V_{\text{min}} = -\left( C_2 - \tau_0^2 \right) \sqrt{1 - \frac{\kappa^2}{2}}. \] (32)
Thus we have the inequality \( 0 \geq E \geq V_{\text{min}} \). On using equation (24) and equation (29) in equation (27), the exact stationary solution of the time dependent Schrödinger equation for the electron (equation (26)) is of the form
\[ \psi(s_1, \kappa, u) = 2\sqrt{\frac{C_2 - \tau_0^2}{2 - \kappa^2}} \delta\left( C_2 - \tau_0^2 s_1, \kappa \right) \exp(i(C_2 - \tau_0^2)u). \] (33)
Hence we see that the conformation lattice solution, a spatially periodic solution for \( k(s_1) \) given in equation (24), which determines the conformation of the elastic tube, is also the amplitude of the electron wave function in (33).
Note that when $\kappa$ goes to 1, the amplitude of the above solution reduces to equation (23), which corresponds to the static conformation in figure 5. This would in turn localize the electron at the centre of the loop.

However, as we explained below equation (23), a dynamical solution with $s$ replaced by $(s - vt)$ is possible for the Kirchhoff equations (4) and (5), which would describe a moving loop. Turning to electron transport on a tube, we showed in [8] that the quantum effective potential induced by the above (moving) curvature traps the electron, which then travels with it along the tube. This is the conformon mechanism described in [8] and applied to a biopolymer.

Now, we see that the conformon lattice solution for the curvature (equation (24)) leads to a different type of charge transport mechanism. While for $\kappa = 1$, it was the motion of the conformon that led to electron transport, we see that for $\kappa \neq 1$, even the static conformon lattice contributes to electron transport. This happens because the electron wave function equation (33) corresponds to a spatially delocalized state, due to the finite periodicity of $d_n$. Indeed, equation (33) shows that since for any $\kappa$, $d_n(s, \kappa)$ does not vanish for any $s$, the probability of finding the electron on the polymer, $d_n^2(s, \kappa)$, is nonvanishing for all $s$. Note that the period of $d_n(s, \kappa)$ increases as $\kappa$ increases, and tends to infinity as $\kappa$ tends to 1. Further, $d_n(s, \kappa)$ itself goes to unity for all $s$ as $\kappa$ tends to zero. The conformon lattice mechanism therefore contributes towards enhancing electron transport along the nanotube as $\kappa$ is decreased from 1 to 0.

6. Discussion

With regard to applications, let us first consider carbon nanotubes. It has been shown using Green function techniques in the context of an ‘arm chair’ carbon nanotube that bending of a nanotube increases its electrical resistance [17]. This agrees with our finding that a single bend (as in figure 1) would cause localization of the electron wave function. Thus although the phenomenological model we have presented is a highly idealized continuum model in the sense that it ignores details such as electronic structure, it is able to capture the essence of the curved geometric effects quite succinctly. Its merits include the use of a realistic elastic model that takes into account an intrinsic twist and a possible asymmetry in the bending rigidities. We have obtained a helical conformation (figure 5) which has been observed experimentally. While the fact that a helical solution per se can be supported by the Kirchhoff model is well known [18], here it emerges as a special case of an elliptic function solution. It would be interesting to experimentally measure its electrical resistance as a function of the number of coils. We conjecture that the resistance of nanotubes where the coils appear very close to each other may be less than that in which the coils are far apart, since the delocalization of the electron will be very efficient in the former case. Hence design of suitable experiments to verify the above would be of interest.

More importantly, we have shown that in addition to the helical conformation, the Kirchhoff model supports shapes such as those given in figures 1–4, which have constant torsion but varying curvature. While we have seen in [8] that a static loop conformation (figure 1) localizes the charge on the loop, the new multiloop solutions (figures 2–5) are shown to lead to delocalization of the wave function, which provides a novel mechanism for charge transport.

Conformations corresponding to closed tubes are also possible. First, the simplest case of a circular ring (and hence planar) solution is easily obtained by setting the curvature $k$ to be a constant $K_0$, and the torsion $\tau_0 = 0$ in the basic equations (9)–(14). We obtain $K_0 = \sqrt{2C_2}$. This is the same as the solution of $k$ found from equation (22) by inspection in this case. In addition, closed tube conformations for the general elliptic function solution (24) exist when
its length $L$ is such that $L \sqrt{(C_2 - \tau_0^2)/(2 - \kappa^2)}$ is an integral multiple of its period, $2K(\kappa)$, with periodic boundary conditions $R(L) = R(0)$.

In the context of DNA, Shi and Hearst [19] have analysed the Kirchhoff equations, by treating DNA as a thin elastic rod with a circular cross-section, to obtain exact solutions of curvature and torsion. They have plotted closed tube configurations of a supercoiled DNA in the form of a toroidal helix. Our analysis and plots are for open tubes with noncircular cross-section, the helix being a special case.

Over the years, physicists have used various types of experiments to measure DNA conductivity, but the results contradict each other [20]. Bioscientists have employed other types of methods [21] such as oxidative damage in DNA, to study charge transport. They have firmly established that there is definitely an efficient transport of electrons (or holes) through the DNA base pair stack, which proceeds over fairly long molecular distances ($\sim 200$ Å) under ordinary thermal conditions. Since the central axis of DNA can take on curved conformations, especially when it interacts with various proteins during replication and transcription, the quantum mechanical motion of the electron is not always along a straight line, but rather, on a curved path. This curvature perhaps plays a role in charge transport, since the sensitivity of transport to sequence-dependent conformations as well as local flexibility and distortions of the soft DNA chain have been noted in experiments [21, 22].

It is indeed not easy to measure coherent charge transport in DNA, because of effects due to temperature, disorder, dissipation and interaction with molecular vibrations, etc [20]. In addition, issues connected with the source of the charge, whether it is transport between the leads or due to a donor–acceptor scenario, will need careful experimental scrutiny. But we believe that irrespective of how the charge gets injected, given the same ambient conditions like temperature, a coiled elastic nanotube induces a quantum potential in its path, while a straight tube of the same length does not, and this should lead to observable effects on charge transport.

We note that the formation of DNA loops (such as in figures 1–5) has been frequently observed [23], and is considered to be an important biological mechanism for regulating gene expression. Thus the exact conformations that we have obtained using the elastic model indeed seem to have physical significance. In view of the above, systematic experiments should be designed to study the dependence of charge transport on DNA conformations.

We suggest that in such experiments, long molecules (with length greater than the persistence length of 50 nm) which are not stretched out or attached to a surface, but rather in their more natural, free curved conformation (with loops, if possible) should be used to investigate for what kinds of conformations there would be either enhancement or depletion of charge migration.

In summary, as a result of an intricate interplay between classical elasticity of the nanotube and quantum motion of the electron in it, certain conformations with constant torsion are shown to lead to a class of corresponding exact electronic wave functions. This suggests a charge transport mechanism that underscores the role played by the curved geometry of the axis of the tube, and in particular, the nonlinear differential equation satisfied by the curvature function. Hence curved geometry should be taken into account in order to obtain a full understanding of charge conduction in nanotubes. Our work should be regarded as a first step in this direction.

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