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# Quantum effective potential, electron transport and conformons in biopolymers

Rossen Dandoloff<sup>1</sup> and Radha Balakrishnan<sup>2</sup>

<sup>1</sup> Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, F-95302 Cergy-Pontoise, France

<sup>2</sup> The Institute of Mathematical Sciences, Chennai 600113, India

E-mail: [rossen.dandoloff@ptm.u-cergy.fr](mailto:rossen.dandoloff@ptm.u-cergy.fr) and [radha@imsc.res.in](mailto:radha@imsc.res.in)

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## Abstract

In the Kirchhoff model of a biopolymer, conformation dynamics can be described in terms of solitary waves, for certain special cross-section asymmetries. Applying this to the problem of electron transport, we show that the quantum effective potential arising due to the bends and twists of the polymer enables us to formalize and quantify the concept of a *conformon* that has been hypothesized in biology. Its connection to the soliton solution of the cubic nonlinear Schrödinger equation emerges in a natural fashion.

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Geometry and topology of long chain biopolymers such as proteins and DNA play a significant role [1] during processes such as replication and transcription. Interesting experiments for studying the conformation and elastic properties of a *single* polymer by bending or twisting it have been devised [2]. The static properties of semi-flexible biopolymers such as actin which have only bending energy, are described by the well-known wormlike chain (WLC) model [3] with a single elastic constant, the bending modulus. In contrast, the static DNA with its double-helix structure is described by the wormlike rod chain (WLRC) model [4] with an additional elastic constant, the twist rigidity. Although considerable work has been done on various equilibrium properties of both these elastic models, their intrinsic dynamical properties have not been studied so far. The latter play a crucial role in the mechanisms of energy and information propagation along a biopolymer, an issue of vital interest to biologists, chemists and physicists alike. The equilibrium properties have been studied in [3, 4]. The study of intrinsic static and dynamical properties of biopolymers, taking into account their geometry, is a subject of great importance [5, 6]. Such issues are of vital interest in biology as well as physics, since they would help us understand the mechanisms of storage and transport of energy and charge along a biopolymer.

In this paper, we describe a biopolymer using the Kirchhoff model [5]. This model starts with equations that govern the dynamics of a thin rod that in fact characterizes a polymer in the

well-established WLRC model mentioned above. We are interested in its intrinsic dynamics, as well as its effect on electron transport, since the measured electrical conductivities of certain polymers are seen to be much larger than expected due to conventional mechanisms [7]. Under certain conditions, polymer conformations take on the form of spatially localized nonlinear excitations. Applying this to the problem of electron transport, we show that the quantum effective potential arising due to the bends and twists of the polymer enables us to formalize and quantify the concept of a *conformon* that has been put forward in biology [7, 8]. It is expected to play an important role in statics and dynamics of biopolymers in general. Its connection to the soliton solution of the cubic nonlinear Schrödinger equation emerges in a natural fashion.

We consider the biopolymer to be a very thin elastic filament (or rod) modelled by a *strip* [6], which is defined as a space curve  $\mathbf{R}(s, t)$ , along with a smooth unit vector field  $\mathbf{d}_2$ , perpendicular to the curve. Here  $s$  denotes the arc length of the polymer and  $t$  is the time. The unit tangent to the curve is given by  $\mathbf{d}_3$  and the third unit vector of the triad is defined as  $\mathbf{d}_1 = \mathbf{d}_2 \times \mathbf{d}_3$ , so that the triad  $(\mathbf{d}_3, \mathbf{d}_2, \mathbf{d}_1)$  forms a right-handed, orthonormal frame at every point on the curve.

The space derivatives of the vectors of the frame can be shown to be given by the compact expression

$$\mathbf{d}_{i,s} = \mathbf{k} \times \mathbf{d}_i, \quad (1)$$

where  $i = 1, 2, 3$ , the subscript  $s$  stands for  $\frac{d}{ds}$ , and  $\mathbf{k}$ , the Darboux vector or ‘twist’ vector is given by

$$\mathbf{k}(s, t) = k_1 \mathbf{d}_1 + k_2 \mathbf{d}_2 + k_3 \mathbf{d}_3. \quad (2)$$

Its components  $k_i$ ,  $i = 1, 2, 3$ , can be expressed as a function of the curvature  $k$ , the torsion  $\tau$  and the angle  $\phi$  between the principal normal to the curve and  $\mathbf{d}_1$ , the normal to the strip:

$$(k_1, k_2, k_3) = (k \sin \phi, k \cos \phi, \tau + \phi_s). \quad (3)$$

Here,

$$k = |\mathbf{d}_{3,s}| \quad (4)$$

and

$$\tau = \mathbf{d}_3 \cdot (\mathbf{d}_{3,s} \times \mathbf{d}_{3,ss}) / k^2. \quad (5)$$

The Kirchhoff equations that govern the dynamics of the biopolymer (modelled as a thin elastic rod) are given (in their dimensionless form) by [5, 9]

$$\mathbf{g}_s = \mathbf{R}_{tt} \quad (6)$$

and

$$\mathbf{m}_s + \mathbf{d}_3 \times \mathbf{g} = a \mathbf{d}_1 \times \mathbf{d}_{1,tt} + \mathbf{d}_2 \times \mathbf{d}_{2,tt}, \quad (7)$$

with

$$\mathbf{m} = k_1 \mathbf{d}_1 + a k_2 \mathbf{d}_2 + b k_3 \mathbf{d}_3, \quad (8)$$

where the subscript  $t$  stands for the time derivative  $\frac{d}{dt}$ . In these equations  $\mathbf{g}(s, t)$  and  $\mathbf{m}(s, t)$  represent the force (or tension) and the torque acting on each cross-section of the rod. The equations are obtained from the conservation of linear and angular momentum. The parameter  $a$  ( $0 < a \leq 1$ ) is a measure of the bending asymmetry of its cross-section.  $b = 2a/(1 + \sigma)(1 + a)$ ,  $\sigma$  being the Poisson ratio, is a measure of the change in volume of the rod as it is stretched.

First we consider the static version of the Kirchhoff equations (6)–(8). Using the general expression

$$\mathbf{g} = g_1 \mathbf{d}_1 + g_2 \mathbf{d}_2 + g_3 \mathbf{d}_3 \quad (9)$$

leads to the following system of equations<sup>3</sup>:

$$g_{1,s} + k_2 g_3 - k_3 g_2 = 0 \quad (10)$$

$$g_{2,s} + k_3 g_1 - k_1 g_3 = 0 \quad (11)$$

$$g_{3,s} + k_1 g_2 - k_2 g_1 = 0 \quad (12)$$

$$g_2 = k_{1,s} + (b - a)k_2 k_3 \quad (13)$$

$$g_1 = -ak_{2,s} + (b - 1)k_1 k_3 \quad (14)$$

$$bk_{3,s} + (a - 1)k_1 k_2 = 0. \quad (15)$$

For all  $\phi = n\pi/2$ ,  $n$  an integer, using equation (3) in equation (15) shows that

$$k_3 = \tau = \tau_0. \quad (16)$$

Thus the torsion of the polymer is a *constant*, denoted by  $\tau_0$ . As an example, we first take  $\phi = \pi$  in equation (3) and analyse equations (10)–(15). We find  $b = 2a$ . This implies  $a = -1/(1 + \sigma)$ . Further,

$$\mathbf{g} = a k_s \mathbf{d}_1 + (a - b)\tau_0 k \mathbf{d}_2 + a\left(-\frac{1}{2}k^2 + C_2\right) \mathbf{d}_3, \quad (17)$$

where  $C_2$  is an integration constant. To understand its physical significance, note that for  $k = 0$  (a straight polymer),  $\mathbf{g} = a C_2 \mathbf{d}_3$ . This essentially means that  $C_2$  represents the tension in the polymer.

With this result, equation (10) leads to the following equation for the curvature  $k$ :

$$k_{ss} + \frac{k^3}{2} = (C_2 - \tau_0^2)k. \quad (18)$$

Equation (18) has two trivial solutions: the straight line  $k = 0$ , and the circular helix  $k = \sqrt{2(C_2 - \tau_0^2)}$ . More interestingly, it admits the following nontrivial solution:

$$k = 2\sqrt{C_2 - \tau_0^2} \operatorname{sech} \sqrt{C_2 - \tau_0^2} s, \quad (19)$$

where, as already stated,  $\tau_0$  and  $C_2$  are constants.

For  $\phi = \frac{\pi}{2}$ , following the same procedure, we get  $b = 2$ . This implies  $a = -(1 + \sigma)/\sigma$ . We can show that  $k$  satisfies an equation of the same form as equation (18). In fact, we can verify that for all  $\phi = n\pi/2$ ,  $n$  any integer, the curvature has the form given in equation (19), and as already found,  $\tau$  is just a constant,  $\tau_0$ . Since the curvature must be real, equation (19) shows that  $C_2$  must be always greater than  $\tau_0^2$ . In the case of a planar polymer,  $\tau_0 = 0$ . Thus physically, a larger tension is needed to get a twisted polymer, for the case under discussion.

Turning our attention to dynamical solutions, it has been noted in [5] that the Kirchhoff equations (6) and (7) can support travelling wave solutions for the curvature  $k$ , called *Kovalevskaya waves*. These are of the same form as the static solution (19), where now  $s$  is replaced by  $\xi = (s - vt)$ , with  $v$  the speed of these spatially localized, solitary waves, which propagate without change of form. These arise due to a certain nontrivial scaling property [9] satisfied by the Kirchhoff equations.

<sup>3</sup> Note that in equation (14), we have corrected a typographical error which we found in the corresponding equation obtained in [5].

We will consider possible quantum mechanical implications of this nontrivial solution for  $k$ , with regard to electron transport on a biopolymer. It has been shown by [10–12] that a quantum particle in a thin tube whose axis follows a space curve with curvature  $k$  and constant torsion  $\tau_0$  (as in our case) *feels* an effective potential [12] of the form

$$V_{\text{eff}}(s) = \frac{\hbar^2}{2m} \left[ -\frac{k^2(s)}{4} + \frac{\tau_0^2}{2} \right]. \quad (20)$$

Writing down the Schrödinger equation for an electron in the presence of the above effective potential, and making a gauge transformation of the wavefunction  $\psi_1$ , by using the following appropriate phase factor  $\psi_1(s, t) = \psi(s, t) \exp(-i\hbar \frac{\tau_0^2}{4m} t)$ , we obtain

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial s^2} + \frac{k^2(s)}{4} \right) \psi(s, t) = i\hbar \frac{\partial}{\partial t} \psi(s, t). \quad (21)$$

After rescaling the time such that  $\frac{\hbar}{4m} t \rightarrow u$  and the coordinate  $s \rightarrow \sqrt{2}s_1$ , the Schrödinger equation reads

$$i\psi_u + \psi_{s_1 s_1} + \frac{k^2}{2} \psi = 0, \quad (22)$$

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

Looking for solutions of equation (22) of the form

$$\psi(s_1, u) = k(s_1) \exp(i\alpha u), \quad (23)$$

we get

$$\left( k_{s_1 s_1} + \frac{k^3}{2} \right) = \alpha k. \quad (24)$$

This equation has the same form as equation (18), provided

$$\alpha = (C_2 - \tau_0^2). \quad (25)$$

Using the solution given in equation (19) (with  $s$  replaced by  $s_1$ ) in equation (23), we get

$$\psi(s_1, u) = 2\sqrt{\alpha} \operatorname{sech} \sqrt{\alpha} s_1 \exp(i\alpha u), \quad (26)$$

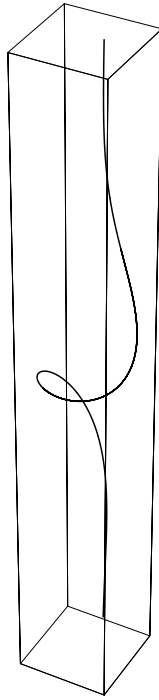
where  $\alpha \geq 0$ . It is readily seen that the wavefunction of the electron is *localized* around that point on the polymer where the maximum of its curvature is located. Further, it has a simple sinusoidal time dependence like a *breather*.

Since  $\alpha = k^2(s=0)/4 = k_0^2/4$ , equation (25) leads to

$$\frac{k_0^2}{4} + \tau_0^2 = C_2. \quad (27)$$

This leads to an interesting *constraint* between the maximum curvature  $k_0$  and the constant torsion  $\tau_0$  of the polymer,  $C_2$  being the constant representing tension.

We choose various values of  $\alpha$  and  $\tau_0$  that satisfy this constraint. Note that  $\alpha \leq C_2$ , from equation (25). The actual conformation of the polymer, which has a space-dependent curvature  $k = 2\sqrt{\alpha} \operatorname{sech} \sqrt{\alpha} s_1$  and a constant torsion  $\tau = \tau_0$ , can be found by integrating equations (1). Typically, we find that polymer has a single non-intersecting twisted loop, centred around  $s_1 = 0$ . It straightens out as  $s_1 \rightarrow \pm\infty$ , as it should, since its curvature is readily seen to vanish in those limits. Figure 1 gives an example of such a conformation, for  $C_2 = 2$ , with  $\alpha = 1$  and  $\tau_0 = 1$ . For the same  $C_2$ , smaller values of torsion, e.g.,  $\tau_0 = 0.7$ , make the loop curve more around the centre, while for larger values, e.g.,  $\tau_0 = 1.23$ , the opposite happens, and the loop starts ‘unravelling’ and straightens out more. Our results show how the above



**Figure 1.** Polymer conformation for curvature  $k$  as given in equation (19) with  $(C_2 - \tau_0^2) = \alpha = 1$  and torsion  $\tau = \tau_0 = 1$ . Note the localized twisted loop on the polymer.

conformation of a polymer that emerges directly from static Kirchhoff equations, can lead to electron localization, i.e., ‘trapping’ of an electron around the maximum curvature point on the twisted loop that develops mid-way on the polymer. As already mentioned, the dynamical solutions for the curvature  $k$  are just Kovalevskaya travelling waves, given by

$$k(s_1, u) = k(s_1 - vu) = 2\sqrt{\alpha} \operatorname{sech}[\sqrt{\alpha}(s_1 - vu)]. \tag{28}$$

For this case, the wavefunction of the electron is to be found as the solution of the corresponding time-dependent Schrödinger equation (22), where now  $k = k(s_1 - vu)$  is given in (28). Thus for this dynamical case, we look for a solution of the form

$$\psi(s_1, u) = k(s_1 - vu) \exp i[\lambda s_1 + \mu u], \tag{29}$$

where  $\lambda$  and  $\mu$  are to be found by substituting equation (29) into equation (22), with  $k$  as in (28). After some algebra, we find

$$\lambda = (v/2), \quad \mu = (\alpha - \lambda^2) = \left[ C_2 - \tau_0^2 - \frac{v^2}{4} \right], \tag{30}$$

on using equation (25). Substituting for  $\lambda$  and  $\mu$  from equation (30) and  $k(s_1 - vu)$  from equations (28), (29) becomes

$$\psi = 2\sqrt{\alpha} \operatorname{sech}[\sqrt{\alpha}(s_1 - vu)] \exp i \left[ \frac{v}{2} s_1 + \left( \alpha - \frac{v^2}{4} \right) u \right]. \tag{31}$$

This is identical to the *envelope soliton* solution of the following, completely integrable [13] cubic nonlinear Schrödinger equation (CNLSE),

$$i\psi_u + \psi_{s_1 s_1} + \frac{|\psi|^2}{2} \psi = 0. \tag{32}$$

This is as expected, because for solution (29) that we have considered,  $k^2 = |\psi|^2$ , so that equation (22) reduces to equation (32).

From equation (31), it is clear that the envelope soliton has a localized profile: its modulus travels with *envelope velocity*  $V_e = v$ , while its phase has a *carrier velocity*  $V_c$  given by

$$V_c = -(\mu/\lambda) = \frac{(v^2 - 4\alpha)}{2v} = \frac{[v^2 - 4(C_2 - \tau_0^2)]}{2v}. \quad (33)$$

This leads to the well-known inequality  $v[v - 2V_c] \geq 0$  between these two velocities of the CNLSE soliton on the polymer. From equation (33), we see that for a given  $v$ ,  $V_c$  depends on the tension and torsion of the polymer.

Incorporating the additional phase factor  $\exp(-i\tau_0^2 u)$  due to the gauge transformation we had made earlier, we finally obtain the following travelling wave solution for the wavefunction  $\psi_1(s_1, u)$ :

$$\psi_1(s_1, u) = 2\sqrt{\alpha} \operatorname{sech}(\sqrt{\alpha}(s_1 - vu)) \exp i[vs_1 + (C_2 - 2\tau_0^2 - v^2)u], \quad (34)$$

where  $\alpha$  is defined in equation (25). It is easy to see that in this case, the electron gets trapped by a *moving* potential well, which travels along the polymer. To understand the conformation here, we note that the polymer now has a curvature which is a Kovalevskaya solitary wave, travelling without change of form:  $k = 2\sqrt{\alpha} \operatorname{sech}(\sqrt{\alpha}(s_1 - v u))$ . The conformation is again a twisted loop, but now it *travels* with a constant velocity  $v$ . Thus the electron gets trapped in the loop, and is transported along with it, on the polymer. As we have seen, its transport is soliton-like in this case.

We believe that our results provide a precise dynamical underpinning for the *conformon* concept hypothesized by various authors [8, 14, 15] to play an important role in biology. Green and Ji [8] state that a conformon is a localized packet of energy (and genetic information). It is an energy packet associated with a conformational strain, which is localized in a region much shorter than the length of the molecule [7]. We find the curvature  $k$  to be a localized function. Since the energy density on the polymer is proportional to  $k^2$ , this leads to a localized packet of energy.

Volkenstein [14] suggests that a conformon is like an ‘electron plus conformational change’. Kemeny and Goklany [15] remark that ‘in some sense, the conformon is a generalization of a polaron’. As is well known, a polaron is a localized electronic bound state in a discrete lattice, which is not perfectly periodic. It is formed by the *trapping* of the electron due to the *nonlinearities* arising from its strong coupling to the lattice (phonons). Here, we mention that in the specific context of an  $\alpha$ -helical protein, starting with a quantum mechanical *discrete lattice* model, and invoking electron–phonon coupling, a CNLSE has been derived in the continuum approximation, by Davydov [16].

On the other hand, our work deals with conformational aspects. Using the Kirchhoff model (which is a continuum model per se), we have shown that a localized electronic state arises in the *curved and twisted* polymer. This is essentially because its curvature and torsion ‘interact’ with the electron by inducing a potential well, which *traps* it, in addition to creating a *nonlinearity* in its Schrödinger equation. While this scenario is indeed somewhat analogous to the polaron picture described above, the origin of the two mechanisms are quite distinct, with the curved geometry of the polymer playing a key role in the creation of a conformon. We conjecture that the moving soliton solution that arises, along with its robust propagation can provide an explanation for the unexpectedly high electrical conductivity (around  $10^{22} \text{ } \Omega^{-1} \text{ cm}^{-1}$ ) found in certain biopolymers. It represents a novel mechanism of charge transport without dissipation which is not restricted to low temperatures.

Finally, we have shown how the geometry of polymers, nonlinearity and quantum particle transport are intimately related. Thus our results are also likely to be of significance in other kinds of transport phenomena in molecular biology.

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