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The energy spectrum of a twisted flexible string under elastic relaxation

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Abstract. A full investigation of the energy spectrum of a twisted flexible string under elastic relaxation is presented and discussed in detail for the first time. New polynomial expressions for critical energy states are derived and the whole spectrum of critical states (minima, maxima and inflexion points) of the elastic energy is found and discussed in relation to superhelicity and elastic characteristics of the string. The study is carried out in the context of the theory of linear elasticity and the thin rod approximation. The relaxation mechanism is studied by using conservation of linking difference (by the formula $\Delta Lk = Wr + \Delta Tw$). We show how specific geometric quantities, such as pitch angle, writhe and twist contributions, as well as physical quantities, such as torsional and bending energy, depend on superhelicity (given by the specific linking difference) and elastic characteristics of the string (given by bending and torsional rigidity). These quantities, expressed per unit length, are examined and compared at each critical energy state. Starting from a supertwisted configuration, we show that the string relaxes (by twist reduction) through two different intermediate helical states (which correspond to different local minima), to reach the lowest minimum energy state in a supercoiled configuration. The case of a generic kink formation (and consequent passage through an inflexional configuration) is then examined and new expressions for the energy change in the vicinity of the inflexion point are derived.

1. Introduction

In this paper we present a number of results concerning the elastic energy of an initially twisted flexible string when it is relaxed to a minimum energy state. Geometric and energetic estimates associated with intermediate maximum and minimum energy configurations realized during the relaxation process are presented for the first time with a discussion of the corresponding configurational change from an initial supertwist state to a supercoil end state, and new expressions for the energy change associated with an isolated generic kink formation are derived. These results have a wide range of applications in many physical contexts, where we make use of elastic string models. Examples include the mechanics of thin elastic rods, the kink instability of fibres and cables, the DNA supercoiling and the processes of protein folding in biochemistry (see, for example, Dean *et al* 1985, Wadati and Tsuru 1986, Schlick and Olson 1992, Klapper and Tabor 1994, Shi and Hearst 1994). Moreover, information about geometric and topological aspects of twisted strings (presence of writhe and twist in the filament, distribution of superhelicity), and physical aspects (influence of elastic characteristics of the string on linking and kink formation, distribution of bending energy and torsional energy, etc) are extremely important in the general study of the structural mechanics of fibres, yarns and fabrics (Hearle *et al* 1969). In this paper some of these aspects are investigated and clarified by studying the relaxation

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mechanism of a twisted elastic string in isolation. In doing this, we improve and extend the study done by Hunt and Hearst (1991) on DNA supercoiling, presenting the whole spectrum of critical energy states (minima, maxima and inflexion states) for different elastic characteristics and examining in detail the energy change associated with a generic kink formation in the string. The results of the present work can then be applied to the study of more complex physical situations, where, for example, highly entangled structures are present (as in polymer physics; see, for example, Kantor and Hassold 1988) and estimates of the configurational energy of the system are much harder. Let us first consider an elastic string model.

The string is given by a slender tube (a filament) of length L and uniform circular cross section of area $A = \pi a^2$ such that $a/L \ll 1$. Let the filament axis C be a smooth, simple, closed curve $\boldsymbol{X} = \boldsymbol{X}(s)$ (s is the arc length), with curvature $c = c(s)$ and torsion $\tau = \tau(s)$, and let $(\boldsymbol{t}, \boldsymbol{n}, \boldsymbol{b})$ be the unit tangent, normal and binormal vector to $\boldsymbol{X}$. A twisted string is simply modelled by assuming that the filament is made of a bundle of infinitesimal fibres uniformly twisted about the filament axis, each fibre C^* being described by $\boldsymbol{X}^*(s) = \boldsymbol{X}(s) + \epsilon \boldsymbol{N}(s)$, where $\epsilon \in [0, a]$ is the distance of the fibre from the filament axis along the direction of a unit normal vector $\boldsymbol{N}(s) = \boldsymbol{n}\cos\Theta(s) + \boldsymbol{b}\sin\Theta(s)$ orthogonal to $\boldsymbol{X}$. The total twist number Tw, which is a measure of the winding of each fibre about $\boldsymbol{X}$ as we move along the axis, is given by

$$Tw \equiv \frac{1}{2\pi}\oint_C \Omega(s)\,\mathrm{d}s = \frac{1}{2\pi}\oint_C \left(\boldsymbol{N} \times \frac{\mathrm{d}\boldsymbol{N}}{\mathrm{d}s}\right)\cdot \boldsymbol{t}\,\mathrm{d}s \tag{1}$$

where $\Omega(s)$ denotes the angular twist rate (Love 1944). By direct evaluation of the last integral, we can express the total twist as the sum of the normalized total torsion and the intrinsic twist $\mathcal{N} = [\Theta]_C/2\pi$, i.e.

$$Tw = \frac{1}{2\pi}\oint_C \left[\tau(s) + \frac{\mathrm{d}\Theta(s)}{\mathrm{d}s}\right]\mathrm{d}s = \frac{1}{2\pi}\oint_C \tau(s)\,\mathrm{d}s + \frac{1}{2\pi}[\Theta]_C\,.$$

The total twist is a geometric property of the string and varies continuously during evolution.

A second geometric quantity, which measures the folding of the string axis, is the writhing number Wr defined by

$$Wr \equiv \frac{1}{4\pi}\oint_C\oint_C \frac{[\mathrm{d}\boldsymbol{X}(s) \times \mathrm{d}\boldsymbol{X}^*(s)]\cdot[\boldsymbol{X}(s) - \boldsymbol{X}^*(s)]}{|\boldsymbol{X}(s) - \boldsymbol{X}^*(s)|^3}\,. \tag{2}$$

This quantity admits a physical interpretation in terms of the algebraic sum of positive and negative crossings of the plane projection of C, averaged over all projections (Fuller 1971, Moffatt and Ricca 1992).

For topologically complex structures, topological quantities such as linkage and knot type, are invariant of the evolution and act as physical constraints. In this paper, we rely on the known invariance of the (Călugăreanu) linking number Lk, defined as the limiting form of the (Gauss) linking number of C^* with C, a quantity that is associated with the degree of knottedness of the string. This topological invariant relates the writhing number of the string with the total twist number by the simple formula $Lk = Wr + Tw$ (Călugăreanu 1961, White 1969, see also Moffatt and Ricca 1992 for further references). In particular, changes in linking number ΔLk (assumed here always positive) from the equilibrium linking number Lk_0, will result in changes in writhe Wr and total twist ΔTw, according to the equation (Fuller 1971)

$$\Delta Lk = Wr + \Delta Tw\,. \tag{3}$$

A string with a surplus (or a deficit) of linking number (a state which is referred to as *superhelicity*) has a net amount of writhe and twist distributed between its bending and torsional deformation. When superhelicity is solely due to net internal twist of fibres (i.e. $[\Theta]_C \neq 0$ with no curvature and torsion effects) we have a 'supertwist' configuration (see the inset in figure 1(*b*)). On the other hand, when net twist effects are negligible compared to net writhe ($\Delta Lk \approx Wr$), we have a 'supercoil' configuration (see the inset in figure 1(*e*)).

2. Elastic energy and configurational states in the relaxation mechanism

The string is assumed to be uniform, homogeneous, and linearly elastic. The elastic characteristics of the string are given by the (Young) modulus of elasticity Y and the modulus of rigidity G, and these can be related to a third quantity, the modulus of compressibility κ, by the relation (Love 1944) $Y = 9\kappa G/(3\kappa + G)$. Fundamental physical facts pose limits on the values taken by the elastic characteristics (Landau and Lifshitz 1959); in the limiting case of an incompressible medium, as $\kappa \to \infty$, $Y \to 3G$, and in general we have $2 \leqslant Y/G \leqslant 3$. Under the assumption of a uniform, thin filament, the bending rigidity K_b and the torsional rigidity K_t of the string are then given by (Love 1944):

$$K_b = \tfrac{1}{4}\pi a^4 Y \qquad K_t = \tfrac{1}{2}\pi a^4 G\,. \tag{4}$$

For our purpose it is convenient to refer to the rigidity ratio $\chi = K_b/K_t = Y/2G$, and parametrize the physical characteristics of the elastic string by $\chi \in [1, 1.5]$.

Let us now consider the elastic energy E of the string. For a linearly elastic inextensible string this is just the sum of two terms, the bending energy E_b and the torsional energy E_t, given by (Landau and Lifshitz 1959)

$$E_b = \oint_C \tfrac{1}{2}K_b[c(s)]^2\,\mathrm{d}s \qquad E_t = \oint_C \tfrac{1}{2}K_t[\Omega(s) - \Omega_0]^2\,\mathrm{d}s \tag{5}$$

where Ω_0 is the (natural) angular twist rate of the generating fibres.

Before going further a word of warning about the validity of the linear elastic approximation for the range of configurations examined below is perhaps necessary. It is known that the stress–strain relation may well lead to the quadratic form of the deformation energy per unit length $\mathcal{E}(c, \Omega) = \frac{1}{2}(K_b c^2 + K_t\Omega^2)$ only for small deformations (see, for example, the discussion in Dill 1992). More generally, it is known that a Taylor expansion of the strain energy function $\mathcal{E}$ can be expressed in powers of the components of the angular rotation rate vector of the deformation. Now, from inspection of the energy functional and the assumption of elastic isotropy for directions perpendicular to the string axis (so that $\mathcal{E}$ depends only on c and Ω), we have that the quadratic part of the expansion indeed retains the conventional form given by the integrands in (5) (Landau and Lifshitz 1959, Fuller 1971). Note that in many cases even this second-order approximation is not sufficient for an accurate theory, and further assumptions on hyper-elasticity for the constitutive relations are necessary to take account of nonlinear effects (Stoker 1968, Ogden 1984). Here, however, the motivation for the present study is to find a first-order magnitude information on the energy spectrum and relative energy redistribution for different string configurations. Hence, the use of the (first-order quadratic form) energy functional given by (5) is fully justified.

By taking into account the invariance of the linking number, Fuller (1971) showed that at critical energy states (when, for example, the elastic energy takes maximum or minimum values) the bending and torsional energies per unit length become

$$\tilde{E}_b = \tfrac{1}{2}K_b[c(s)]^2 \qquad \tilde{E}_t = \frac{2\pi^2 K_t}{L^2}(\Delta Tw)^2 = 2\pi^2 K_t\big(\Delta\tilde{L}k - \tilde{W}r\big)^2 \tag{6}$$

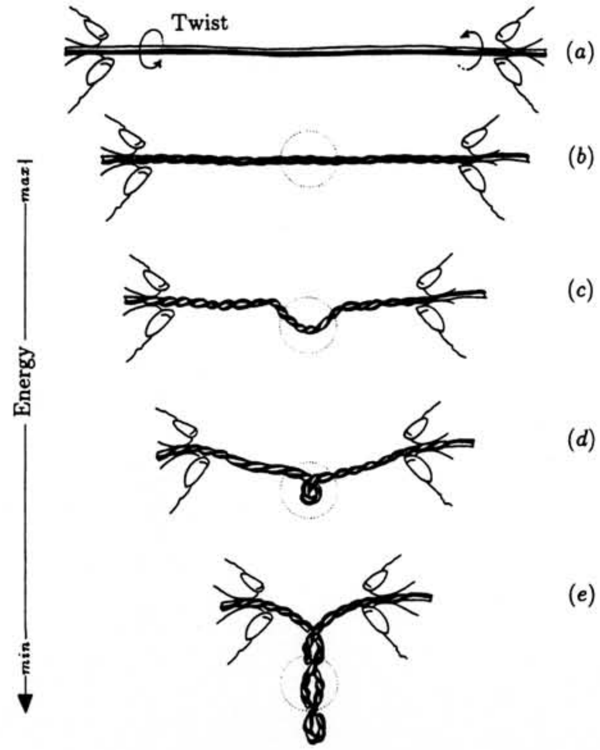

Figure 1. (a) A flexible elastic string can relax to a minimum energy state, (b) starting from a supertwist configuration (obtained by injection of pure internal twist), (c), (d) passing through a spectrum of intermediate helical states and (e) attaining the lowest energy state in a supercoil configuration.

where $\Delta\tilde{L}k$ denotes the specific linking difference and over-tildes denote quantities per unit length (with respect to L).

We now wish to consider the relaxation of the twisted flexible string under elastic tension. The basic mechanism (well known at a phenomenological level) is sketched in figure 1, where, for the sake of example, the relaxation of an extensible twisted string is shown. Figure 1(a) shows the original string when it is pulled tight: here L denotes the distance between the two marked ends (for a closed string imagine that the two ends are joined together at infinity). Let us first consider the supertwist case: by keeping L fixed, we inject superhelicity simply by increasing pure internal twist ($\Delta Lk = \Delta Tw > 1$ well above Zajac's (1962) critical twist value; see figures 1(a) and (b)); as internal twist increases, both elastic tension and total energy will increase to a certain value. Now let us relax the string by allowing the two marked ends to approach each other: a change in the string geometry then becomes visible, with the development of helical states (figure 1(c)) and consequent kink formation (figure 1(d)). Here, a decrease in length will correspond to a reduction in tension (tension is proportional to extension) with a reduction of specific net twist and a decrease in elastic energy. As the relaxation mechanism proceeds further, the string evolves to form a supercoil, with a continuous redistribution of internal twist into writhe and a continuous production of new coils (figure 1(e)).

For the moment we do not consider the mechanism of the transition from one state to the other (the energetics of kink formation is discussed in section 4), but we merely compare the elastic energy associated with each critical state. This is done by considering all quantities per unit length and conservation of arc length. (If we were to take into account stretching, we would have a decrease in torsional energy as well as in potential energy associated with the stretching, both contributing to the relaxation mechanism; Love (1944), Stoker (1968).) In order to estimate the energy associated with each critical state at different $\Delta\tilde{L}k$, we need to estimate curvature and writhing number corresponding to the different geometric configurations. Let us examine the following three particular cases.

Supertwist configuration

In this case there are no curvature and torsion effects present. Hence, by (3), $\Delta\tilde{T}w = \Delta\tilde{L}k$, with no contribution to bending energy. Therefore, the specific total energy is given simply by

$$\tilde{E}^{(\mathrm{st})} = 2\pi^2 K_\mathrm{t}(\Delta\tilde{L}k)^2 . \tag{7}$$

Helical configuration

A helical string (axis) has curvature and torsion constant, with

$$c = \frac{\cos^2\alpha}{r} \tag{8}$$

where α and r denote, respectively, the helix pitch angle and the radius of the circular cylinder on which the helical axis is inscribed. The specific writhing number is evaluated by using a theorem originally put forward by Fuller (1978) (see the appendix, case (a)), which gives

$$\tilde{W}r = \frac{(1-\sin\alpha)\cos\alpha}{2\pi r} . \tag{9}$$

Thus, by (6), we have

$$\tilde{E}^{(\mathrm{h})} = \frac{K_\mathrm{b}\cos^4\alpha}{2r^2} + 2\pi^2 K_\mathrm{t}\left[\Delta\tilde{L}k - \frac{(1-\sin\alpha)\cos\alpha}{2\pi r}\right]^2 . \tag{10}$$

On the other hand, the pitch p of the helix is given by $p = 2\pi r\tan\alpha$, and, alternatively, this can be written as (see figure 2) $p = 2(a+h)/\cos\alpha$, where $h = O(a)$, with $0 \leqslant h \ll L$ (since ideally the helix has an infinite number of turns). By equating the two expressions above, we have

$$\alpha = \sin^{-1}\left(\frac{a+h}{\pi r}\right) \tag{11}$$

and by substituting the equation above into (10) and taking $\rho = r/(a+h)$, we have

$$\tilde{E}_\mathrm{b}^{(\mathrm{h})} = \frac{K_\mathrm{b}}{2(a+h)^2\rho^2}\left(1 - \frac{2}{\pi^2\rho^2} + \frac{1}{\pi^4\rho^4}\right) \tag{12}$$

for the bending energy, and

$$\tilde{E}_\mathrm{t}^{(\mathrm{h})} = 2\pi^2 K_\mathrm{t}\left[\Delta\tilde{L}k - \frac{1}{2\pi(a+h)\rho}\left(1 - \frac{2}{\pi\rho} + \frac{2}{\pi^3\rho^3} - \frac{1}{\pi^4\rho^4}\right)^{1/2}\right]^2 \tag{13}$$

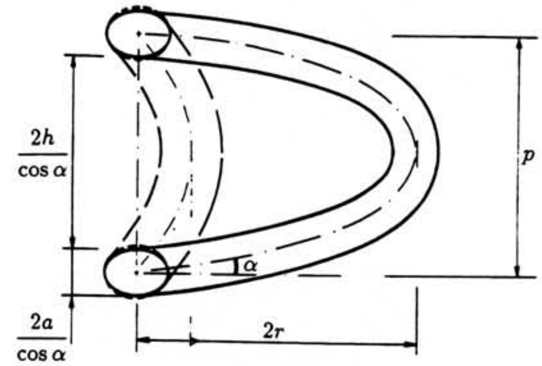

Figure 2. A family of helical tubes of given pitch (p = constant) is obtained by varying the pitch angle α and cylindrical radius r according to the relation $p = 2\pi r \tan\alpha$.

for the torsional energy. Critical states of the elastic energy are given by setting $\partial\tilde{E}^{(h)}/\partial r = (a+h)^{-1}\partial\tilde{E}^{(h)}/\partial\rho$ to zero. Thus, by combining (12) and (13) and differentiating, we have

$$\frac{\partial\tilde{E}^{(h)}}{\partial r} = 0 \quad \Rightarrow \quad H^2\rho^6A^2 - 4B\,(A+\chi C)^2 = 0 \tag{14}$$

where

$$A = \rho^4 - \frac{3}{\pi}\rho^3 + \frac{5}{\pi^3}\rho - \frac{3}{\pi^4} \qquad B = \rho^4 - \frac{2}{\pi}\rho^3 + \frac{2}{\pi^3}\rho - \frac{1}{\pi^4} \qquad C = \rho^4 - \frac{4}{\pi^2}\rho^2 + \frac{3}{\pi^4}$$

and $H = 2\pi(a+h)\Delta\tilde{L}k$. Equation (14) is a polynomial of 14th order in ρ and will be solved numerically for given $H = H(\Delta Lk)$ and χ (see below for a discussion of the numerical results). The writhe and the net total twist are also expressed as function of ρ. By equation (9), we have

$$Wr = \frac{L}{2\pi^3(a+h)}\frac{[(\pi\rho-1)^3(\pi\rho+1)]^{1/2}}{\rho^3} \tag{15}$$

and by (3) $\Delta Tw = \Delta Lk - Wr$. The fraction of elastic energy that goes in bending energy (relative bending energy) is given by

$$\%\tilde{E}_b^{(h)} = \frac{\tilde{E}_b^{(h)}}{\tilde{E}^{(h)}} = \frac{\chi\left(\pi^2\rho^2-1\right)^2}{\chi\left(\pi^2\rho^2-1\right)^2 + \pi^4H^2\rho^6\left(1-\frac{Wr}{\Delta Lk}\right)^2} \tag{16}$$

with the rest going in torsional energy. For the sake of comparison, it is convenient to normalize the energy with respect to a reference energy. Taking

$$\tilde{E}_0^{(st)} = \tilde{E}^{(st)}(\Delta Lk = 1) = \frac{2\pi^2K_t}{L^2} \tag{17}$$

we have the normalized elastic energy given by

$$\tilde{E}_0^{(h)} = \frac{\tilde{E}^{(h)}}{\tilde{E}_0^{(st)}} = \frac{\chi}{H^2\rho^2}\left(1-\frac{1}{\pi^2\rho^2}\right)^2 + (\Delta Lk - Wr)^2\,. \tag{18}$$

Supercoil configuration

In this case two helical strands are closely interwound with high pitch angle β ($\beta > \pi/4$), so that a good approximation is to take $r = a$ and

$$c = \frac{\cos^2\beta}{a}. \tag{19}$$

Application of Fuller's theorem to the supercoil case (see the appendix again, case b) gives

$$\tilde{W}r = \frac{\sin\beta\cos\beta}{2\pi a}. \tag{20}$$

Note that this writhing number measures the folding of the two interwound helical strands and differs (evidently) from that of a helix of high pitch (cf equation (9) with $\alpha > \pi/4$). The energy per unit length of the double strand supercoil is thus given by

$$\tilde{E}^{(\mathrm{sc})} = \frac{K_\mathrm{b}\cos^4\beta}{2a^2} + 2\pi^2 K_\mathrm{t}\left[\Delta\tilde{L}k - \frac{\sin\beta\cos\beta}{2\pi a}\right]^2. \tag{21}$$

Critical states of the elastic energy are found by setting $\partial\tilde{E}^{(\mathrm{sc})}/\partial\beta = 0$. After some straightforward algebra, we have

$$\frac{\partial\tilde{E}^{(\mathrm{sc})}}{\partial\beta} = 0 \quad\Rightarrow\quad \tan^4\beta - \frac{1}{H}\tan^3\beta - \frac{2\chi-1}{H}\tan\beta - 1 = 0 \tag{22}$$

whose solutions will be analysed and discussed below for given $H = H(\Delta Lk)$ and χ. For each critical state, the writhing number is given by

$$Wr = \frac{L}{2\pi(a+h)}\frac{\tan\beta}{1+\tan^2\beta} \tag{23}$$

and, similarly as we did for the helical state, we calculate relative energies and normalized energies. For example, the relative bending energy is given by

$$\%\tilde{E}_\mathrm{b}^{(\mathrm{sc})} = \frac{\chi}{\chi + H^2\left(1 - \frac{Wr}{\Delta Lk}\right)^2(1+\tan^2\beta)^2} \tag{24}$$

and the normalized total energy by

$$\tilde{E}_0^{(\mathrm{sc})} = \frac{\tilde{E}^{(\mathrm{sc})}}{\tilde{E}_0^{(\mathrm{st})}} = \chi\left(\frac{L}{2\pi(a+h)}\right)^2\left(\frac{1}{1+\tan^2\beta}\right)^2 + (\Delta Lk - Wr)^2 \tag{25}$$

which will be estimated and compared with the results for the helical case.

3. Spectrum of critical energy states: analytical and numerical results

A full investigation of the whole spectrum of critical energy states of helical and supercoil configurations is carried out for different values of specific linking difference and elastic characteristics, taking $\Delta Lk \in (0, 30]$, $\chi \in [1, 1.5]$ and $2\pi(a+h)/L = 0.1$.

The critical energy states of the helical configurations are found by solving the polynomial in (14). A detailed numerical investigation shows that this polynomial has 12 real roots (and two complex conjugate roots) throughout the whole range of values considered. By examining the behaviour of the second derivative at each critical state, we find that the polynomial has four minima, four maxima and four inflexional states, with two minima and two maxima of physical relevance. The pitch angle and the writhing number corresponding to the minima are plotted versus ΔLk in figure 3, for $\chi = 1$ and $\chi = 1.5$ (the curves of physical interest, $h1_{\min}$ and $h2_{\min}$, are plotted as full curves). Note how the α-curve $h2_{\min}$ (figure 3(*a*)), which is slightly decreasing in both diagrams (passing from $\approx 89°$ to $\approx 86.5°$ at $\chi = 1.0$), gives a writhing number that is negligible at $\chi = 1.0$ and rather relevant in the incompressible case ($\chi = 1.5$) (figure 3(*b*)); the relative behaviour of the writhing number for $h1_{\min}$ and $h2_{\min}$ as ΔLk increases is also noteworthy, as this will have important implications on the redistribution of twist (see the discussion below).

For the sake of comparison, before examining some energy aspects associated with the helical configuration (and indeed also with the supertwist and the supercoil configuration), we wish to consider, for the moment, the case of the supercoil. In this case, the critical energy states are given by solving the polynomial in (22). By substituting $\beta = \tan^{-1}[(1/4\pi) + y]$, the polynomial takes the normal form

$$y^4 - \frac{3}{8H^2}y^2 - \frac{1}{H}\left(\frac{1}{8H^2} + 2\chi - 1\right)y - \left[\frac{3}{(4H)^4} + \frac{2\chi - 1}{4H^2} + 1\right] = 0 \tag{26}$$

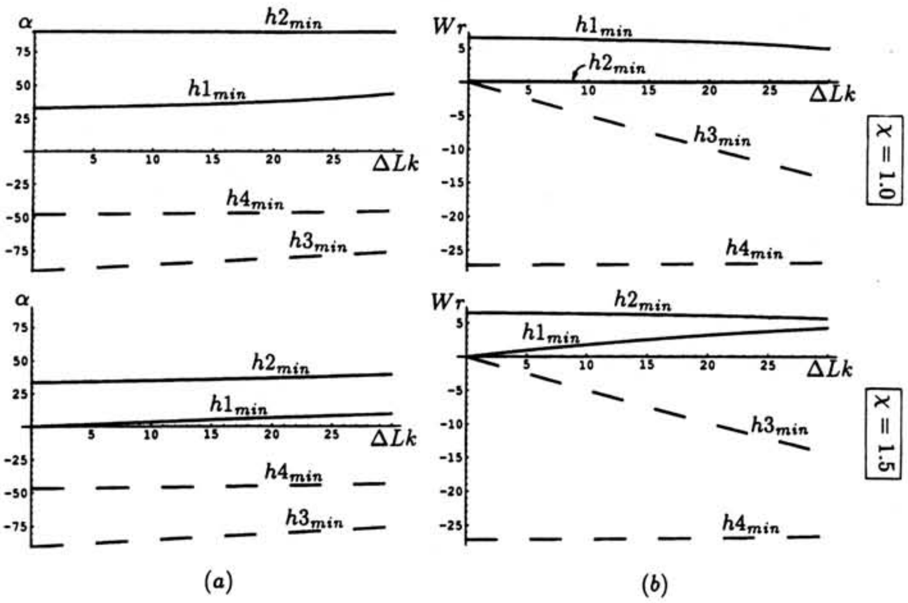

Figure 3. (*a*) Pitch angle and (*b*) writhing number versus ΔLk, corresponding to several minima energy state for helical configuration. Top diagrams refer to the case $\chi = 1.0$. Bottom diagrams refer to the case $\chi = 1.5$, in the incompressible limit. Curves of physical interest are the full curves.

with cubic resolvent in z

$$z^3 - \frac{3}{4H^2}z^2 + \left(\frac{3}{(2H)^4} + \frac{2\chi - 1}{H^2} + 4\right)z + \frac{1}{H}\left(\frac{1}{8H^2} + 2\chi - 1\right) = 0\,. \tag{27}$$

The behaviour of the solutions depends on the sign of the discriminant $D = (P/3)^3 + (Q/2)^2$, where

$$P = \frac{2\chi - 1}{H^2} + 4 \qquad Q = \frac{1}{64H^6} + \frac{2\chi - 1}{4H^2} + \frac{1}{8H^3} + \frac{1}{H^2} + \frac{2\chi - 1}{H}\,.$$

Since $P > 0$ always, then $D > 0$ and the cubic resolvent always has one real solution. This means that the quartic (26) (as well as the original polynomial) always has two real solutions (and two complex conjugate solutions). The real solutions can be calculated analytically by standard techniques (see Bronshtein and Semendyayev 1985). An inspection of the second derivative of the energy shows that the two critical states correspond to a maximum and a minimum.

Geometric and energetic properties of the supercoil minimum energy state are shown in figure 4, where pitch angle, writhe, twist, and relative bending and torsional energies are plotted against ΔLk and χ. For very large linking difference the pitch angle results are bounded from above (cf equation (22), taking the limit as $H \to \infty$), so that $\pi/4 < \beta \leqslant \pi/2$.

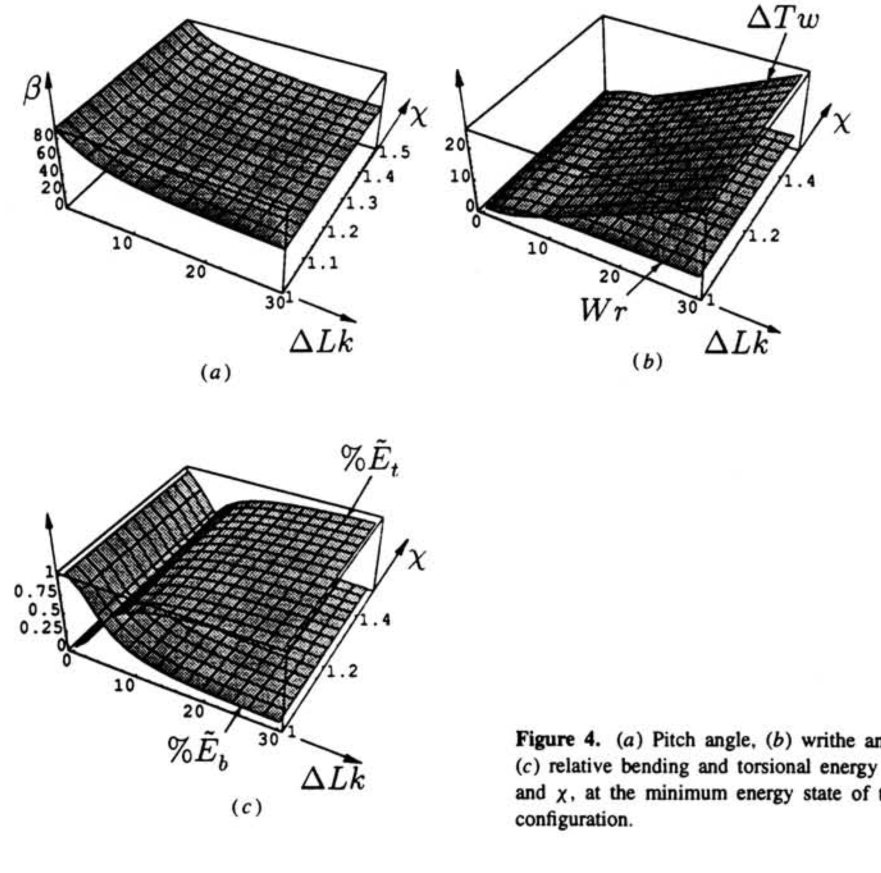

Figure 4. (a) Pitch angle, (b) writhe and twist, and (c) relative bending and torsional energy versus ΔLk and χ, at the minimum energy state of the supercoil configuration.

This implies that $Wr \to L/[4\pi(a+h)] =$ constant as $\Delta Lk \to \infty$ (cf equation (23)), so that $\Delta Tw \propto \Delta Lk$ for very large ΔLk. Therefore, for very large linking difference the elastic energy is transformed almost entirely in torsional energy (cf equations (24) and (25)), with the normalized bending energy that takes the (upper bound) limiting value $\tilde{E}_{b0} \to \chi L^2/[4\pi(a+h)]^2$ as $\Delta Lk \to \infty$. As we shall see below, this limit on the bending energy has interesting implications in the spectrum of minimum energy states. Note the two particular cases for which $Wr = \Delta Tw$ (figure 4(*b*)) and $\%\tilde{E}_b^{(sc)} = \%\tilde{E}_t^{(sc)} = 0.5$ (figure 4(*c*)). In the first case, using (23), we have

$$Wr = \Delta Tw \quad \Rightarrow \quad \tan^4\beta - 2\chi\tan^2\beta - 2\chi + 1 = 0 \tag{28}$$

so that (by choosing positive values for the pitch angle) we have an equal share of writhe and net twist when

$$\beta = \tan^{-1}(2\chi+1)^{1/2} \qquad \Delta Lk = \frac{2\pi(a+h)}{L}\frac{(2\chi+1)^{1/2}}{\chi+1}. \tag{29}$$

Similarly, by (24) and after some algebraic manipulation, we have

$$\%\tilde{E}_b^{(sc)} = \%\tilde{E}_t^{(sc)} = 0.5 \quad \Rightarrow \quad \tan^2\beta - 2\chi^{1/2}\tan\beta - 1 = 0 \tag{30}$$

which gives (again, by choosing positive pitch angles)

$$\beta = \tan^{-1}\left[\chi^{1/2} + (\chi+1)^{1/2}\right] \qquad \Delta Lk = \frac{2\pi(a+h)}{L}\frac{2\chi^{1/2}+(\chi+1)^{1/2}}{2(\chi+1)+2\left[\chi(\chi+1)\right]^{1/2}}. \tag{31}$$

We can now make a full comparison of minima and maxima (chain curves) of the normalized total energy. The whole spectrum of critical energy states for the three geometric configurations is shown in figure 5. For $\Delta Lk \in (0, 30]$ and for both $\chi = 1.0$ and $\chi = 1.5$, the lowest energy state is attained by the supercoil configuration (curve $sc1_{min}$). As energy increases in the range $16 < \Delta Lk < 30$, above the supercoil minimum energy state we have the minima for the helical configuration (curves $h1_{min}$ and $h2_{min}$), and above that energy level we have the supertwist curve (*st* curve). This means that for large linking difference, the relaxation mechanism must pass through two (different) intermediate helical minimum energy states (with geometry and writhing number given by diagrams in figure 3) before attaining the supercoil lowest energy state. Notice here that a lower intermediate helical state corresponds (cf figure 3) to a helical tube of lower pitch angle. In the incompressible case ($\chi = 1.5$) in particular, this means that the transition from a supertwist state passes first through an intermediate helical minimum (of approximately 35° pitch angle) and then through a second intermediate helical minimum (of approximately 5° pitch angle—almost a kink) before attaining the supercoil lowest energy state. (This mechanism, sketched intuitively in figure 1, can be observed by direct experience with a twisted elastic (rubber) string.)

A different situation is visible in the range $1 < \Delta Lk < 15$. At $\chi = 1.0$ the minimum helical state is attained only by the curve $h2_{min}$, which in the top diagram of figure 5 appears to be indistinguishable from the *st* curve. However, a close-up view (figure 6(*b*), $\chi = 1.0$) shows that the helical minimum energy state is placed decidedly between the supercoil lowest minimum energy state and the *st* curve (as it should be). In the incompressible case ($\chi = 1.5$), on the other hand, the transition passes through a different helical minimum state, given by the curve $h1_{min}$ (see also the bottom diagram of figure 6(*b*)), at much lower pitch

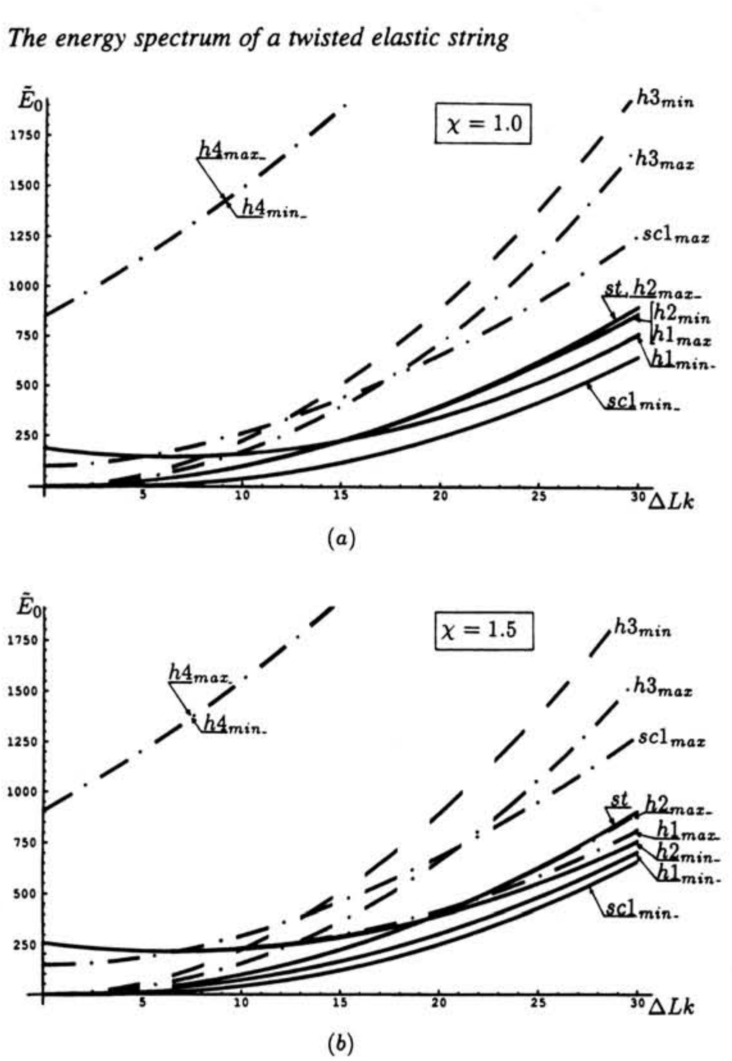

Figure 5. Spectrum of minima (full and broken curves) and maxima (chain curves) of the normalized elastic energy for different configurational states and elastic characteristics.

angle but now certainly with non-negligible writhing number (cf figure 3 again). Therefore, for relatively low ΔLk (but well above the writhing instability) the twisted string relaxes through only one of the two intermediate helical states, determined by the specific physical (elastic) properties.

The normalized bending energy relative to different minimum energy states is shown in figure 6(*a*). As was pointed out earlier on, remember that the writhing number of the supercoil configuration is bounded from above by $Wr \to L/[4\pi(a+h)] = \text{constant}$ as $\Delta Lk \to \infty$, which poses an upper bound to the corresponding bending energy. As a consequence, a helical state, while having more curvature for small writhing numbers, can attain larger writhing numbers (for a given aspect ratio) than the supercoil configuration. This means that, comparatively, more bending energy can be absorbed in the helical state than in the supercoil state, and therefore the helical state can reach lower energy levels for very large linking numbers. This behaviour is particularly evident when we compare the lower-energy helical state ($h1_{\text{min}}$) with the supercoil minimum energy state (see figure 7) in

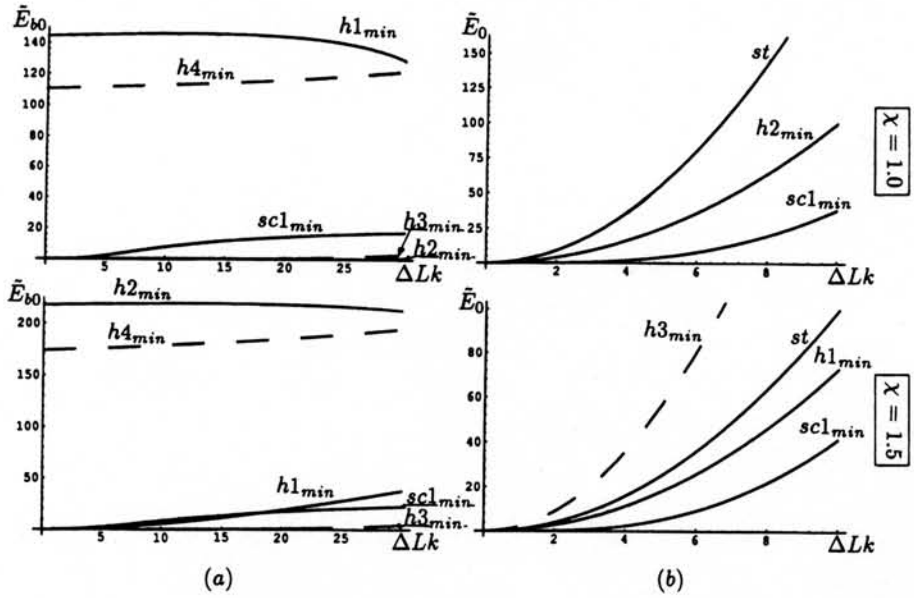

Figure 6. (*a*) Normalized bending energy and (*b*) elastic energy versus ΔLk, for different configurational states at minimum energy.

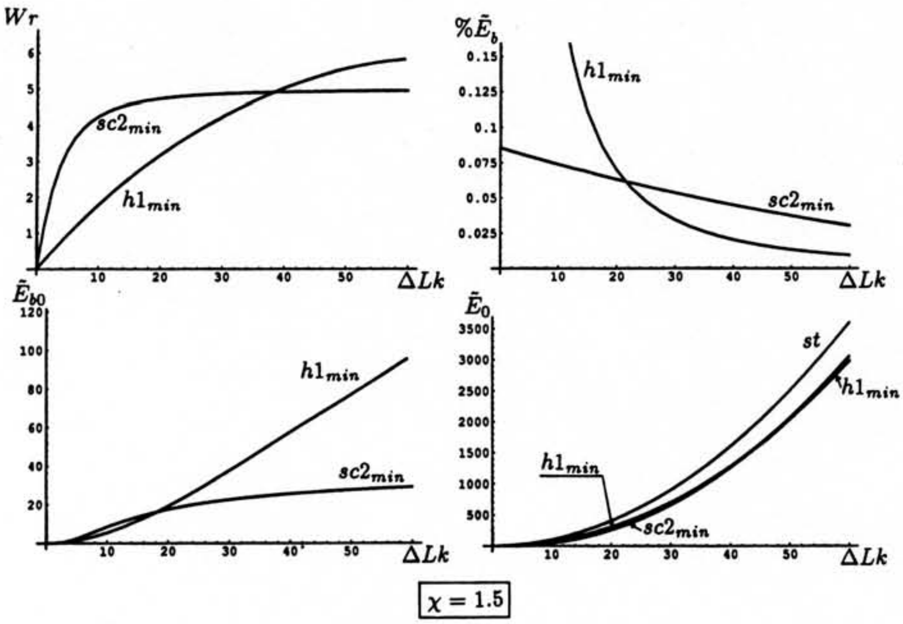

Figure 7. Comparison of writhing number (top left), relative bending energy (top right), normalized bending energy (bottom left) and total elastic energy (bottom right) for the lower helical energy state ($h1_{\min}$) and the supercoil minimum energy state ($sc1_{\min}$) in the incompressible limit ($\chi = 1.5$). Note (in the bottom right diagram) the transition of the helical energy state ($h1_{\min}$) to the lowest minimum energy state for $\Delta Lk > 50$.

the incompressible case ($\chi = 1.5$) and for large specific linking differences. A comparison of writhing numbers (top left diagram of figure 7) shows that indeed the helical case can attain larger writhing numbers at increasing ΔLk, and this results in higher values of (relative and normalized) bending energy absorbed in the helical configuration (diagrams at the top right- and bottom left-hand corners of figure 7), allowing further reduction in twist and consequential decrease in total energy. In the incompressible case, a close inspection of the curves $h1_{\min}$ and $sc1_{\min}$ (bottom right-hand diagram of figure 7) shows that indeed for $\Delta Lk > 50$ the lowest energy state is achieved by the helical configuration, confirming the predictions of Fuller (1971) and Hunt and Hearst (1991).

4. Energy change associated with a kink formation

The case of a formation of an isolated kink in the string (for example by twist reduction, to attain a lower energy state) is particularly interesting, since it is invariably associated with the initial development of a supercoil state. From a purely topological viewpoint, the development of a kink by continuous deformation of the string is equivalent to performing a Reidemeister type I move on the string (Kauffman 1991) (see figure 8). As pointed out by Ricca and Moffatt (1992), any deformation whose projection on any plane involves a Reidemeister type I move must involve passage through an inflexional configuration (i.e. through a state that does contain a point of inflexion, with $c = 0$). The emergence of a kink (by 'ambient isotopy') does therefore typically involve such a passage and consideration of corresponding changes in bending and torsional energy is of particular interest.

Let us consider the case $\Delta Tw = +1$, $Wr = 0$ (see figure 8(a)). As the kink develops, the string axis passes through an inflexional state (say at $s = 0$ and $t = 0$, t parametrizing the deformation), with decrease in ΔTw and equal and opposite increase in Wr (for the conservation of the linking number, cf equation (3)). Thus $0 < Wr < 1$ (figure 8(b)). Let us assume that arc length is locally preserved during the deformation and suppose that in the neighbourhood where $s \in [-s_0, s_0]$ (for $s_0 = O(a)$) there is only one point of inflexion. During this process, the generic behaviour of the string axis in the vicinity of the inflexion point is given by the parametrized twisted cubic (Ricca and Moffatt 1992, Moffatt and Ricca 1992)

$$X(s,t) = \left(s - \tfrac{2}{3}t^2 s^3, -ts^2, s^3\right) \tag{32}$$

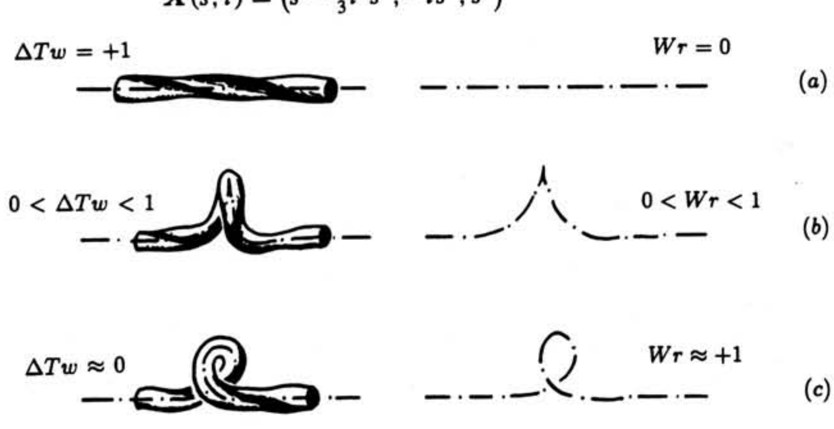

Figure 8. The development of a kink in the string is associated with a topological transformation known as Reidemeister type I move: in this case, a continuous change of (a) twist to (c) writhe is attained by a sequence of (b) intermediate helical states, with the appearance of an inflexional configuration (i.e. a state that does contain a point of inflexion).

with curvature and torsion given by

$$c(s,t) \sim 2\left(t^2+9s^2\right)^{1/2} \qquad \tau(s,t) \sim \frac{-3t}{t^2+9s^2} \tag{33}$$

for $|s|$ and $|t|$ ($t \in [-t_0, t_0]$, $s_0 \gg |t|$) small. Note the singular behaviour of $\tau(s,t)$ at the inflexion point as t passes through zero.

In the vicinity of the inflexion point the quadratic form of the energy functional gives a first-order approximation to estimate the energy change. Hence, the bending and torsional energy per unit length associated with uniform share of torsional stress can be estimated (to leading order in $|s|$ and $|t|$) as

$$\tilde{E}_b(s,t) = \tfrac{1}{2}K_b[c(s,t)]^2 \sim 2K_b\left(t^2+9s^2\right) \tag{34}$$

and (see the appendix, case (c))

$$\tilde{E}_t(s,t) = \frac{2\pi^2 K_t}{L^2}(\Delta Lk - Wr)^2 \sim \frac{2\pi^2 K_t}{L^2}\left(1-\frac{t}{T}\right)^2 \tag{35}$$

where $T > t_0$. The change in energy in the neighbourhood of the inflexion point is thus given by

$$\frac{\partial \tilde{E}_b}{\partial t} \sim 4K_b t \tag{36}$$

and

$$\frac{\partial \tilde{E}_t}{\partial t} \sim -\frac{4\pi^2 K_t}{L^2}\frac{\partial Wr}{\partial t} \tag{37}$$

where the dependence of writhe on deformation can be evaluated more accurately by using the formula (Klapper and Tabor 1994)

$$\frac{\partial Wr}{\partial t} = -\frac{1}{2\pi}\int_{-s_0}^{s_0} c\left(\frac{\partial q_b}{\partial s} + \tau q_n\right) \mathrm{d}s \tag{38}$$

with $q_b = (\partial \boldsymbol{X}/\partial s)\cdot \boldsymbol{b}$ and $q_n = (\partial \boldsymbol{X}/\partial s)\cdot \boldsymbol{n}$. Hence, by (32) and the expressions above, we have a change in bending energy given by

$$\frac{\partial\,(\delta E_b)}{\partial t} \sim 8K_b t s_0 \tag{39}$$

and a change in torsional energy given by

$$\begin{aligned}\frac{\partial\,(\delta E_t)}{\partial t} &\sim -\frac{24\pi K_t}{L^2}\int_0^{s_0}\left[3s^2 + \frac{s^2\left(t^2-9s^2\right)}{t^2+9s^2}\right]\mathrm{d}s \\ &= -\frac{16\pi K_t}{L^2}\left\{s_0^3 + \frac{t^2}{3}\left[s_0 - \frac{t}{3}\tan^{-1}\left(\frac{3s_0}{t}\right)\right]\right\}.\end{aligned} \tag{40}$$

Equations (39) and (40) express respectively the increase in bending energy and the (corresponding) decrease in torsional energy associated with the inflexional configuration as a kink develops. Note that as the string axis passes through the inflexional configuration the energy functional remains continuous, with $\partial(\delta E_b)/\partial t = 0$ and $\partial(\delta E_t)/\partial t = -16\pi K_t s_0^3/L^2$, at $t = 0$.

5. Conclusions

In recent years, new applications of geometric and topological techniques have been used successfully in the solution of many physical problems involving twisting, kinking and entanglement of topologically complex structures (Sumners 1992).

In this paper, a combined use of these techniques has been applied to study the elastic relaxation of a twisted flexible string and the corresponding energy spectrum. The study has been carried out in the context of the theory of linear elasticity and the thin rod approximation (which is known to give correct first-order magnitude information) and the relaxation mechanism is studied by using conservation of linking difference by the formula $\Delta Lk = Wr + \Delta Tw$. New polynomial expressions for critical energy states have been derived and the whole spectrum of critical states (minima, maxima and inflexion points) of the elastic energy has been found. Specific geometric quantities, such as pitch angle, writhe and twist contributions, as well as physical quantities, such as torsional and bending energy, have been closely examined at each minimum energy state. Starting from a supertwisted configuration (which has maximum elastic energy), we have shown that the string relaxes (by twist reduction) through two different intermediate helical states (which correspond to different local minima), to reach the lowest energy state in a supercoiled configuration.

In the case of very high superhelicity, we have shown that the writhing number of the supercoil configuration is bounded from above by $Wr \to L/[4\pi(a+h)] =$ constant as $\Delta Lk \to \infty$, which poses an upper bound to the corresponding bending energy. In the incompressible case we have proved Fuller's original conjecture (1971), explaining why for very high linking difference the helical configuration, and not the supercoil, attains the lowest energy state. Finally, the case of a kink formation and the associated passage through a generic inflexional configuration has been discussed and new expressions for the corresponding change in bending and torsional energy valid in the vicinity of the inflexion point have been derived. The equations describe the increase in bending energy and decrease in torsional energy as the kink develops and an example of the corresponding change in writhing number is given in the appendix.

The results presented in this paper are quite general and can be usefully applied to a variety of mathematical and physical problems, from the study of knotted elastic strings and defect lines (Langer and Singer 1984, Ricca 1993, 1994a) to the problem of protein folding (De Santis *et al* 1986, Bednar *et al* 1994). Evaluation of the energy change associated with kink formation and the development of supercoil state is also important in the study of evolution of twisted magnetic flux tubes in ideal magnetohydrodynamics (Berger and Field 1984, Moffatt and Ricca 1992, Ricca 1994b). We wish to extend this approach to study energetic aspects of structures geometrically and topologically more complex and we hope to carry out this programme in the near future.

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Appendix

The writhing number of a curve can be interpreted in terms of spherical area and calculated according to the following result (Fuller 1978, Aldinger *et al* 1994):

Theorem. For any closed space curve $\boldsymbol{X}(s)$ of class C^3 the tangents $\boldsymbol{t}$ trace out a space curve $\mathcal{C}(s)$ on the unit sphere which is piecewise of class C^2 ($\mathcal{C}$ may lose differentiability at inflexion points of $\boldsymbol{X}$). After giving the curve an orientation, divide it into a finite family of non-self-intersecting closed piecewise C^2 space curves. Each curve of this family then encloses a domain Ω_i defined in such a manner that the geodesic normal points into its interior; let A be the sum of the areas of these domains (some components of this area might be counted with multiplicity determined by how often the corresponding domains are encircled by the curve). Then we obtain the following characterization of the writhe:

$$1 + Wr(\boldsymbol{X}) = \frac{A}{2\pi} \pmod 2 .$$

The writhing number for the helix and the supercoil can be evaluated as follows (see also Fuller 1971 and Tanaka and Takahashi 1985):

(*a*) *Writhing number of the helix*

Consider an infinite helix $\boldsymbol{X}(\mathcal{H})$ of m turns and pitch angle α which is closed at infinity by a smooth curve (possibly a point) (see figure A1(*a*)). The helix $\boldsymbol{X}(\mathcal{H})$ is mapped to the curve $\mathcal{C}(\mathcal{H})$ on the unit sphere by the tangent indicatrix $\boldsymbol{t}(\mathcal{H})$. The spherical area enclosed by $\mathcal{C}(\mathcal{H})$ is given by the hemisphere of area 2π plus m times a spherical cap of area $2\pi(\operatorname{signum}\alpha - \sin\alpha)$ (asymptotically). By applying the theorem above we have that the writhing number $Wr(\mathcal{H})$ is given by $Wr(\mathcal{H}) = \pm m(1-\sin\alpha) \pmod 2$. Since $Wr(\mathcal{H}) \to 0$ as $\alpha \to \pi/2$, by a continuity argument we have $Wr(\mathcal{H}) = \pm m(1 - \sin\alpha)$. The length of a helical turn is $2\pi r/\cos\alpha$, therefore (taking the positive value) the writhe of the helix per unit length (m turns) is given by $\tilde{W}r(\mathcal{H}) = (1 - \sin\alpha)\cos\alpha/2\pi r$.

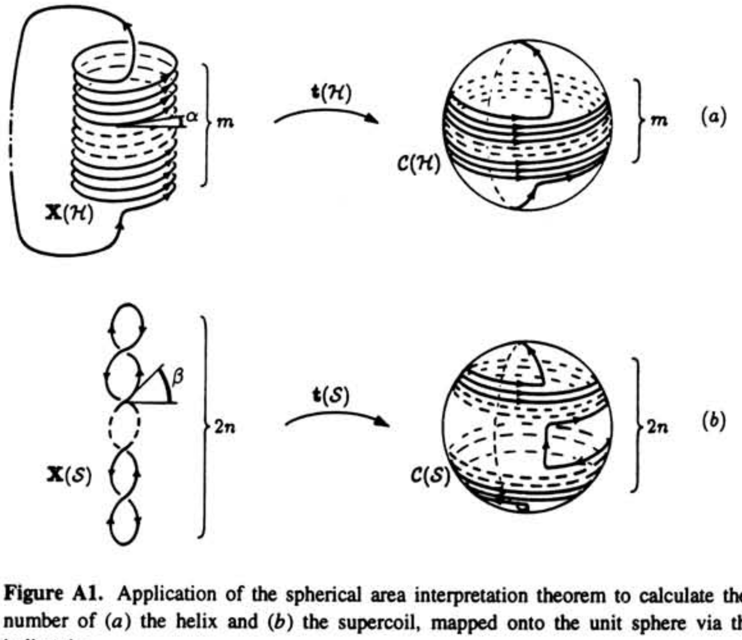

Figure A1. Application of the spherical area interpretation theorem to calculate the writhing number of (*a*) the helix and (*b*) the supercoil, mapped onto the unit sphere via the tangent indicatrix.

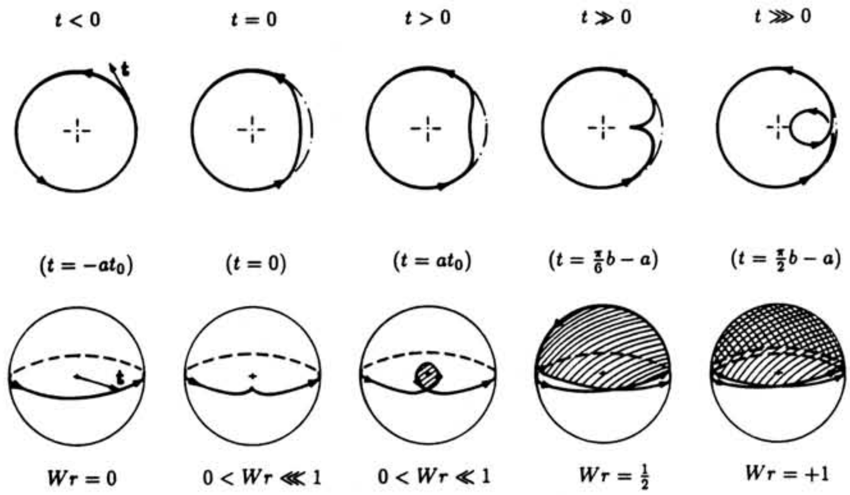

Figure A2. Deformation of a closed curve developing a kink. As the positive kink develops, the writhing number increases, due to the increase of the spherical area encircled by the curve mapped via the tangent indicatrix.

(*b*) *Writhing number of the supercoil*

Now consider an infinite supercoil $\boldsymbol{X}(\mathcal{S})$ of n turns and pitch angle β which is closed on itself smoothly (see figure A1(a)). The supercoil $\boldsymbol{X}(\mathcal{S})$ is mapped to the curve $\mathcal{C}(\mathcal{S})$ on the unit sphere by the tangent indicatrix $\boldsymbol{t}(\mathcal{S})$. The spherical area enclosed by $\mathcal{C}(\mathcal{S})$ is given by the hemisphere of area 2π plus n times a spherical cap (counted with multiplicity and orientation) of area $2\pi(\text{signum}\beta - \sin\beta)$ (asymptotically). Again applying the above theorem we have that the writhing number $Wr(\mathcal{S})$ is given by $Wr(\mathcal{S}) = \mp 2n(\sin\beta) \pmod 2$. Since $Wr(\mathcal{S}) \to 2n$ as $\beta \to \pi/2$, by a continuity argument we have $Wr(\mathcal{S}) = \mp 2n(1 - \sin\beta)$. The length of a helical turn is $2\pi r/\cos\beta$, therefore (taking the positive value and $r = a$) the writhe of the supercoil per unit length ($2n$ turns) is given by $\tilde{W}r(\mathcal{S}) = \sin\beta\cos\beta/2\pi a$.

(*c*) *Writhing number of a curve developing a kink*

Application of the spherical area interpretation theorem to the case of a curve developing a kink is illustrated in figure A2, in which the curve (representative of the string axis) is mapped to the unit sphere. Note how the sperical area (measure of the writhing number) changes as the kink develops. For example, if we take $0 < t_0 < T = bt_0$, then $A(t) = 2\pi + 2\pi\sin\Gamma(t)$ (t parametrizes the deformation), where $\Gamma(t) = (t + at_0)/(bt_0)$ and $a \ll b$, so that, by continuity, we have $Wr[t] = \sin\Gamma(t)$. Hence as t increases, we have $Wr[t = -at_0] = 0$ $(t < 0)$, $0 < Wr[t] \ll 1$ $(t \in [-t_0, t_0])$, $Wr[t = \pi/6b - a] = \frac{1}{2}$ $(t > 0)$ and $Wr[t = \pi b/2 - a] = 1$ $(t \gg 0)$, as shown in the sequence in figure A2.

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