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Minimum Energy Configurations of a Twisted Flexible String under Elastic Relaxation

Following our recent investigation [1] on the energy spectrum of closed, twisted, flexible strings under elastic relaxation, we compare and analyse further the minimum energy states attained by relaxed strings in helical and supercoiled configuartion. We show that for very high values of specific linking difference (high superhelicity) the writhing number of the supercoil state tends to a limit (independent of the elastic charateristics of the string), which yields upper bounds on the bending energy of the string. By this mechanism we can explain Fuller's [2] conjecture on the limit behaviour of helical and supercoiled configurations at minimum energy states.

1. Helical and supercoil states attained by relaxed twisted strings

In our recent work [1] we found the whole spectrum of critical states (minima, maxima and inflexion points) for the elastic energy of closed, twisted, flexible strings under relaxation. The study was carried out in the context of linear elastic theory and thin rod approximation. The relaxation mechanism (which is naturally driven by elastic tension) was studied by using conservation of linking difference by the formula $\Delta Lk = Wr + \Delta Tw$, where ΔLk denotes net linking difference (superhelicity), Wr writhing number and ΔTw net twist (for a mathematical definition of these quantities see [1]). Starting from a supertwisted configuration (with net twist well above Zajac's [3] critical value; see inset in figure 1a) at maximum elastic energy, we showed that the string relaxes (by twist reduction) through two different intermediate helical states (which correspond to different local minima $h1_{min}$, $h2_{min}$; figure 1b, c), to attain the lowest energy state in a supercoiled configuration ($sc1_{min}$; figure 1d). These critical states were found by solving (analytically and numerically) polynomial expressions for helical and supercoiled configurations, for $\Delta Lk \in (0, 30]$ and $\chi = (K_b/K_t) \in [1, 1.5]$ (K_b and K_t being the bending and torsional rigidity of the string). Specific geometric quantities, such as pitch angle, writhe and twist contributions, as well as physical quantities, such as torsional and bending energy, were also examined at each minimum energy state.

The spectra of the (normalised) specific elastic energy $\tilde{E}_0$ (sum of normalised bending and torsional energy per unit length) relative to the helical and supercoil states are shown in the diagrams of figure 1 in the elastic limits at $\chi = 1$ and $\chi = 1.5$. The curves $h1_{min}$ and $h2_{min}$ correspond to families of helices of different pitch angle α, where in general $\alpha(h1_{min}) < \alpha(h2_{min})$ ($32° < \alpha(h1_{min}) < 47°$ at $\chi = 1$, and $1° < \alpha(h1_{min}) < 8°$ at $\chi = 1.5$; see [1]). The lowest minimum energy state is given by the supercoiled configuration for $\Delta Lk \in (0, 30]$ and independently of the elastic characteristics of the string. Before attaining the lowest energy state, however, the string relaxes through two local minima given by helical states. Note that at $\chi = 1$, i.e. in the incompressible limit, and for $1 < \Delta Lk < 15$,

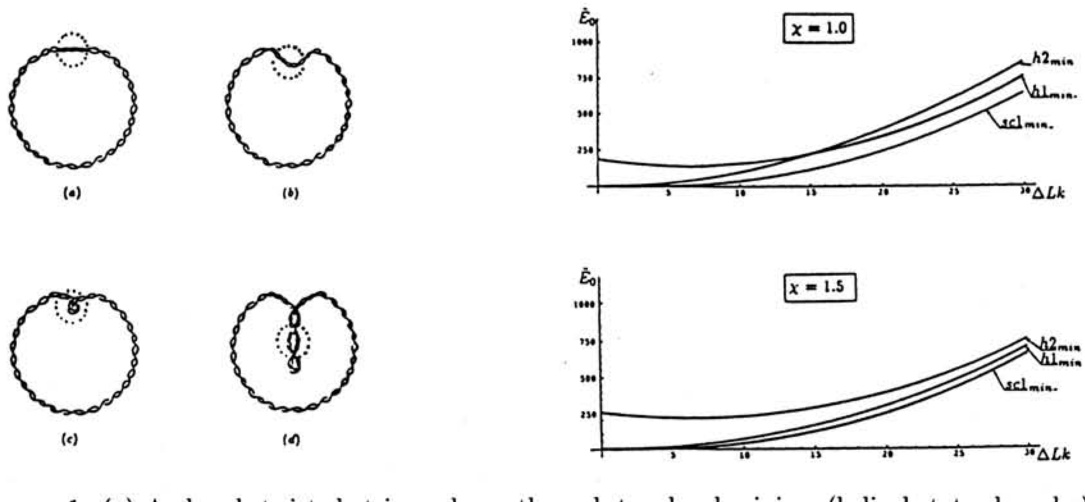

Figure 1. (a) A closed, twisted string relaxes through two local minima (helical states b and c), to attain the lowest minimum energy state (d) in a supercoiled configuration. The energy spectra corresponding to the three critical energy states ($h1_{min}$, $h2_{min}$ and $sc1_{min}$) are shown at $\chi = 1$ and $\chi = 1.5$ (incompressible limit).

the string relaxes first through a low-pitch helical state ($h1_{min}$) and then through a high-pitch helical state ($h2_{min}$), whereas for $\Delta Lk > 15$ is the low-pitch helical state $h1_{min}$ (which corresponds to a helical kink, like in the inset of figure 1c) remains always well below the high-pitch helical state given by the curve $h2_{min}$.

2. Limit behaviour of minimum energy states at high linking numbers

Fuller [2] conjectured that for very high values of linking number (high superhelicity) the helical state could become more energetically favourable than that in the supercoiled configuration. Our analysis shows that in the supercoil (sc) state we have

$$\lim_{\Delta Lk \to \infty} Wr^{(sc)} = h, \qquad \text{and} \qquad \lim_{\Delta Lk \to \infty} \tilde{E}_{b0}^{(sc)} = \chi h,$$

where h (= cst.) is a parameter that depends only on the geometry of the rod model (total length, cross-sectional radius, etc...) and $\tilde{E}_{b0}^{(sc)}$ is the normalised specific bending energy. Note that since $1 \le \chi \le 1.5$, $\tilde{E}_{b0}^{(sc)}$ is also bounded. This means that during relaxation only a limited amount of bending energy can be absorbed into the supercoiled string, being the energetic surplus entirely transformed into torsional energy. Such a limit on bending energy doesn't exist for the helical state, where energy due to curvature effects can be absorbed indefinitely.

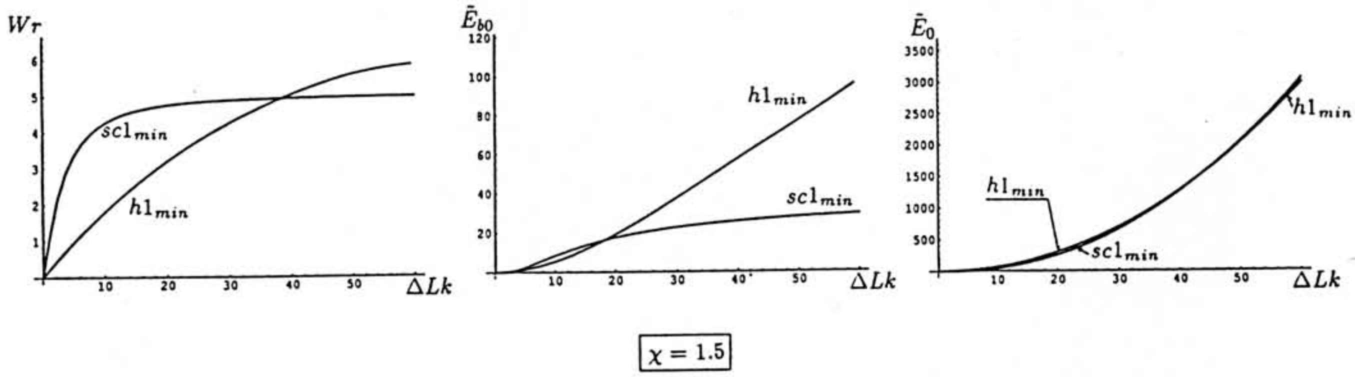

Figure 2. Comparative behaviour of writhing number (left), normalised specific bending energy (centre) and normalised specific total elastic energy (right) for the lower helical energy state ($h1_{min}$) and the supercoil minimum energy state ($sc1_{min}$) in the incompressible limit. Note in the right diagram the transition of the helical energy state to the lowest minimum energy state.

In the incompressible case, for example, a direct comparison of writhing numbers (figure 2, left diagram) shows that indeed the helical state can attain larger writhing numbers (at high ΔLk) in comparison with the supercoil state. Higher writhing numbers induce higher values of (normalised) bending energy (central diagram), allowing further absorption and re-distribution of energy in the helical state. Because of the limiting value of $\tilde{E}_{b0}^{(sc)}$ as $\Delta Lk \to \infty$, the helical state becomes then energetically more favourable, with transition to the lowest minimum energy state at about $\Delta Lk \approx 50$.

These results are rather general and can find useful application in many different contexts, from the mechanics of cables and wires, to the biochemical processes involving protein folding and DNA supercoiling.

Acknowledgements

Financial support from The Leverhulme Trust is kindly acknowledged.

3. References

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