Biassed statistical ensembles for developable ribbons

Dear Editor,

Yong et al. [1] use a numerical method [2] that has previously been shown to be flawed [3] and produce statistical results for developable ribbons that contradict results in the literature [4].

The problem with their numerical method is that it is based on the Frenet frame of tangent, principal normal and binormal of the discrete chains computed for submission to the ensemble averaging. The Frenet frame is well-known to be an improper choice of frame for ribbon modelling [5]: it has the property that it flips at inflection points of the ribbon centreline, i.e., the principal normal and binormal change sign, becoming opposite to the continuous vectors of a material frame. The frame therefore loses contact with the physical deformation of the ribbon.

As explained in [3], the problem can be cured by working with different ranges of angles. Taking advantage of the fact that for developable ribbons the Frenet and material frames are locked/coincident everywhere except at inflection points, one can effectively work with a material frame by defining $-\pi \leq \theta < \pi$, $-\pi/2 \leq \phi < \pi/2$ instead of the choice $0 \leq \theta < \pi$, $0 \leq \phi < 2\pi$ taken in [1, 2]. This eliminates jumps by π in the azimuthal angle ϕ_i (flips) between binormals $\boldsymbol{b}_i$ and instead describes inflections by a sign change of the polar angle θ_i between tangents $\boldsymbol{t}_i$. Doing this, one finds exponential decay of the tangent-tangent correlation function $< \boldsymbol{t}_n \cdot \boldsymbol{t}_0 >$, also found in [4] for developable ribbons, in contrast to the oscillatory decay predicted by Yong et al.

Here we further strengthen our case by performing Monte Carlo simulations to compare results for the two different choices of angles. We take the same parameters as in [1], i.e., $n = 100$, 10^6 sweeps (but 10^7 for $1/\beta = 0.01$), half of which are used for equilibration. $1/\beta$ is temperature in units of energy. No end loads are applied. Results are displayed in Fig. 1.

Fig. 1(*Left*) confirms oscillatory decay of $< \boldsymbol{t}_n \cdot \boldsymbol{t}_0 >$ for the angles in [1] and exponential decay for our angles. The results for $1/\beta = 0.01$ (solid blue curve) give a persistence length $l_p = 91.12$, consistent with the exact asymptotic limit $(32/35)\beta = 91.42$ derived in [3]. Binormal-binormal correlation functions (not shown) are identical for the two choices of angles.

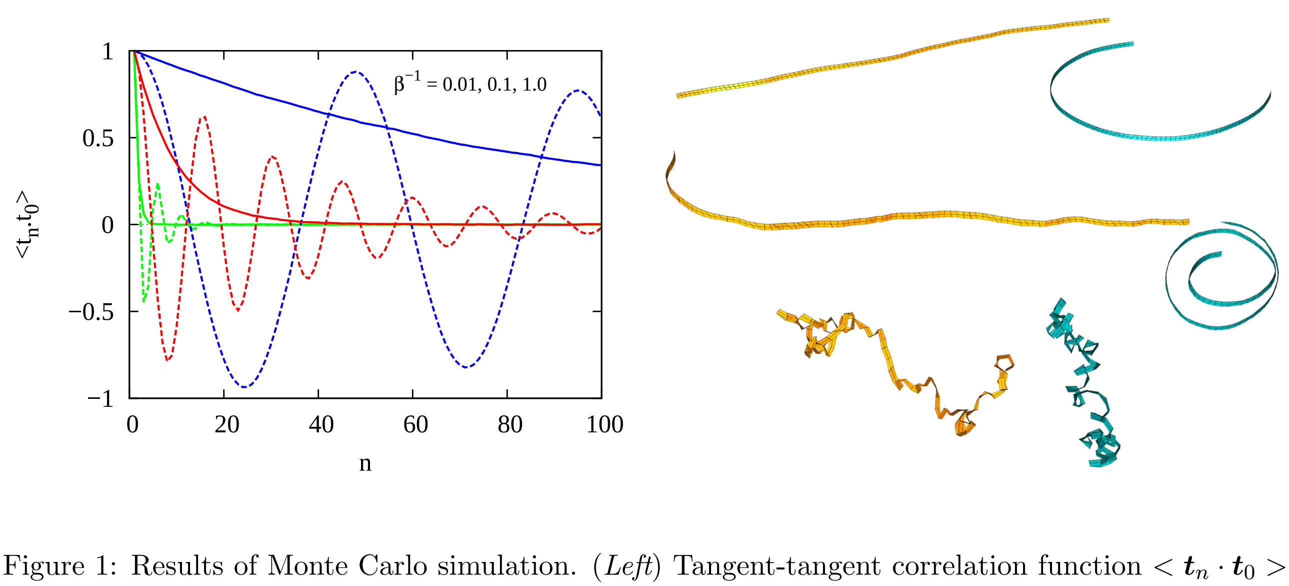

Figure 1: Results of Monte Carlo simulation. (*Left*) Tangent-tangent correlation function $< \boldsymbol{t}_n \cdot \boldsymbol{t}_0 >$ for $1/\beta = 0.01$ (blue), 0.1 (red) and 1.0 (green) for both Yong et al.'s angles (dashed) and our proposed corrections (solid). (*Right*) Typical equilibrated ribbon shapes (blue for Yong et al.'s angles, yellow for corrected angles, for the same $1/\beta$ values, increasing down), drawn with fictitious width. Pairs of solutions are equally scaled, but the scaling varies between pairs.

Fig. 1(*Right*) shows typical equilibrated ribbon shapes for both types of angles. The (unphysical) blue ribbons appear to collapse into a tight coil as temperature decreases but then uncoil and approach the straight configuration in the zero-temperature limit. The blue solutions have no inflections, while the yellow solutions on average have inflections at 50 (out of 100) segments, corresponding to sign changes of the enclosed θ_i. The elastic energy of the ribbon is in both cases identically distributed, with, for $1/\beta = 0.1$, average $Ea/(Bw) = 15$ and standard deviation 1.3.

Yong et al's different results reflect the artificial helical bias built into their statistical ensemble by rejecting inflected ribbon configurations. This bias is not particular to Sadowsky ribbons: use of the Frenet frame similarly causes statistical bias in other ribbon/rod models in which torsion is penalised [6].

[1] E.H. Yong, F. Dary, L. Giomi, L. Mahadevan, Statistics and topology of fluctuating ribbons, *PNAS* **119**, e2122907119 (2022).

[2] L. Giomi, L. Mahadevan, Statistical mechanics of developable ribbons, *Phys. Rev. Lett.* **104**, 238104 (2010).

[3] E.L. Starostin, G.H.M. van der Heijden, Comment on "Statistical Mechanics of Developable Ribbons", *Phys. Rev. Lett.* **107**, 239801 (2011).

[4] B. Mergell, M.R. Ejtehadi, R. Everaers, Statistical mechanics of triangulated ribbons, *Phys. Rev. E* **66**, 011903 (2002).

[5] S.M. Rappaport, Y. Rabin, Differential geometry of polymer models: worm-like chains, ribbons and Fourier knots, *J. Phys. A* **40**, 4455–4466 (2007).

[6] D. Marenduzzo, C. Micheletti, H. Seyed-allaei, A. Trovato, A. Maritan, Continuum model for polymers with finite thickness, *J. Phys. A: Math. Gen.* **38**, L277–L283 (2005).

Sincerely,

G.H.M. van der Heijden
E.L. Starostin