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► **To cite this version:**

Vincent Rossetto, A. C. Maggs. Comment on "Elasticity Model of a Supercoiled DNA Molecule". Physical Review Letters, 2002, 88, pp.089801. 10.1103/PhysRevLett.88.089801 . hal-00372278

HAL Id: hal-00372278

<https://hal.science/hal-00372278>

Submitted on 1 Oct 2021

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Comment on “Elasticity Model of a Supercoiled DNA Molecule”

Bouchiat and Mézard [1] have proposed a “wormlike rod chain model” to describe recent experiments on DNA mechanics [2]. Their model can be solved using an analogy with quantum mechanics, thanks to the *local* nature of the effective Hamiltonian. The Letter concluded that the continuum limit of DNA elasticity is singular and linear response theory cannot be used in the absence of a cut-off: For example, the curves of extension versus torsion flatten in the continuum limit. We show here that this singular behavior is an artifact of an inexact formulation of the writhing geometry. An exact formulation of the experimental geometry needs no extra regularization.

The writhe, $Wr = \chi_W^C/2\pi$, of a closed chain is given by the Călugăreanu-White formula [3]

$$\chi_W^C = \frac{1}{2} \iint_0^L \frac{\mathbf{r}(s) - \mathbf{r}(s')}{|\mathbf{r}(s) - \mathbf{r}(s')|^3} \cdot \frac{d\mathbf{r}(s)}{ds} \times \frac{d\mathbf{r}(s')}{ds} ds ds', \quad (1)$$

where $\mathbf{r}(s) = \int_0^s \mathbf{t}(s') ds'$ is the position in space and L is the length of the chain. Fuller showed that if we represent the tangent vector \mathbf{t} by a point on the unit sphere the area, χ_W^F , enclosed by $\mathbf{t}(s)$ on the sphere [4], is related to χ_W^C . The relation between Fuller’s and Călugăreanu’s formulas is

$$\chi_W^F \equiv \chi_W^C \pmod{4\pi}. \quad (2)$$

Fuller’s result, expressed as a local integral, was used in [1] to calculate the writhe. The authors find a Cauchy probability distribution, $p(\chi_W^F)$, varying as $1/(\chi_W^F)^2$ for large χ_W^F due to winding of trajectories about the south pole of the sphere. It is this broad distribution of probability which leads to the breakdown of linear response. We proceed by examining numerically the distribution function for writhe in the two formulations.

We numerically generate a large equilibrated ensemble of open semiflexible chains of 8 times the persistence length, made of $8N$ straight links with $\mathbf{t}(0)$ and $\mathbf{t}(L)$ parallel. This assures that the path of $\mathbf{t}(s)$ on the sphere is a closed loop. In order to use the Călugăreanu-White formula, the chain must also be closed in real space. To do this we extend the chain at each end with a long straight segment [5] in the directions $-\mathbf{t}(0)$ and $\mathbf{t}(L)$ and then join the two extremities with an arc of a circle, effectively closing the chain at infinity; it is this augmented version of Eq. (1) which determines the rotation angle measured in experiments on open chains. We calculate χ_W^F and χ_W^C for each chain from our ensemble and plot the integrated probability $P(\chi_W) = \int_{-\infty}^{\chi_W} p(\chi) d\chi$. For the Cauchy distribution, one expects $\chi_W^F \sim \frac{1}{1-P}$ for large values of χ_W^F .

Results are displayed in Fig. 1. The curves of P as a function of χ_W^F depend on discretization and converge to a

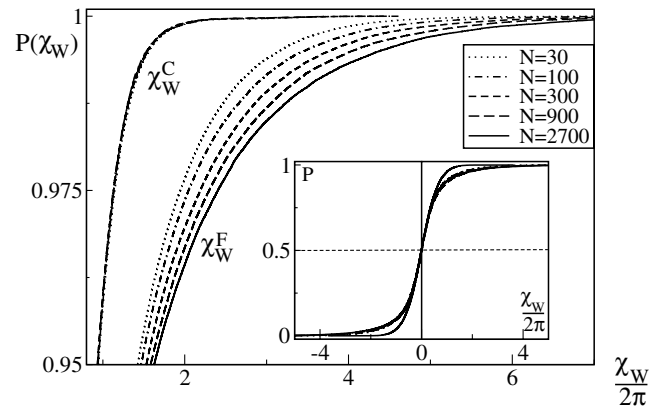


FIG. 1. Inset: The integrated writhe distribution function $P(\chi_W)$ computed with two different formulations of the writhe. χ_W^C is not computed for $N = 2700$ due to computer limitations. The main figure is a zoom of the top right corner of the inset. One can compare the continuous evolution of χ_W^F as N grows with the stability of χ_W^C in the same limit. An asymptote in $\chi_W^F \sim \frac{1}{1-P}$ observed in this figure corresponds to the Cauchy distribution. The singularity of χ_W^C is clearly weaker than $\frac{1}{1-P}$. Statistical fluctuations of the curves are smaller than their width.

Cauchy tail. We have additionally verified that the curves of χ_W^F scaled by the factor $\sqrt{\ln N}$ converge very accurately to a master curve as predicted in [1]. On the other hand, χ_W^C converges to a limiting curve as N grows. We find no evidence of divergence of χ_W^C as $\frac{1}{1-P}$ nor evidence of scaling with $\sqrt{\ln N}$. From Fig. 1 we see that even for N small, the Fuller formulation strongly overestimates the statistical weight of large writhe fluctuations.

To conclude, we believe that fluctuations of semiflexible chains are not divergent when going to the continuum limit. A DNA chain has a persistence length of order 50 times its radius; it is in a regime where Eq. (1) has reached the continuum limit to a very good approximation. The singular limit emphasized in [1] is due to the ambiguity introduced by the modulo relation Eq. (2).

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Received 11 January 2001; published 11 February 2002

DOI: 10.1103/PhysRevLett.88.089801

PACS numbers: 87.15.By, 61.41.+e

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