Comment on "Elasticity Model of a Supercoiled DNA Molecule"

Bouchiat and Mézard[1] have proposed a "worm-like 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 this model has exceptional physical behavior: The continuum limit is singular and linear response theory can not be used in the absence of a cut-off to calculate the experimental curves: For example the curves of extension versus torsion flatten in the continuum limit.

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

$$\chi_W^C = \frac{1}{2}\int_0^L \frac{\mathbf{r}(\mathbf{s})-\mathbf{r}(\mathbf{s}')}{|\mathbf{r}(\mathbf{s})-\mathbf{r}(\mathbf{s}')|^3}\cdot\frac{\mathrm{d}\mathbf{r}(\mathbf{s})}{\mathrm{d}s}\times\frac{\mathrm{d}\mathbf{r}(\mathbf{s}')}{\mathrm{d}s}\,\mathrm{d}s\,\mathrm{d}s', \quad (1)$$

where $\mathbf{r}(\mathbf{s}) = \int_\mathbf{0}^\mathbf{s} \mathbf{t}(\mathbf{s}')\,\mathrm{d}\mathbf{s}'$ 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 $\mathbf{t}(\mathbf{s})$ on the sphere[4], is in certain cases equal to χ_W^C. The general relation between Fuller's and Călugăreanu's formulas is expressed by:

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

Fuller's result, expressed as a local integral, was used in [1]. The authors justify the use of χ_W^F to interpret experiments on *open* chains with a topological argument [5] and find that the probability distribution $p(\chi_W^F)$ varies as $1/\left(\chi_W^F\right)^2$ for large χ_W^F due to winding of trajectories about the south pole of the sphere.

We have performed a simulations to directly compare the distribution of writhe implied by each formulation: We numerically generate a large equilibrated ensemble of semiflexible chains of eight times the persistence length, made of $8N$ straight links with $\mathbf{t}(\mathbf{0})$ and $\mathbf{t}(\mathbf{L})$ parallel. This assures that the path of $\mathbf{t}(\mathbf{s})$ 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 in the directions $-\mathbf{t}(\mathbf{0})$ and $\mathbf{t}(\mathbf{L})$ and then join the two extremities with an arc of a circle; the contribution from the exterior is important in order to preserve the modulo equality eq. (2); it is this augmented version of eq. (1) which determins 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 $P(\chi_W) = \int_{-\infty}^{\chi_W} p(\chi)\mathrm{d}\chi$. For the Cauchy distribution, one thus obtains $\chi_W^F \sim \frac{1}{1-P}$ for large values of χ_W^F.

Results are displayed in fig. 1. The curves of P as a function of χ_W^F indeed depend on discretization. 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.

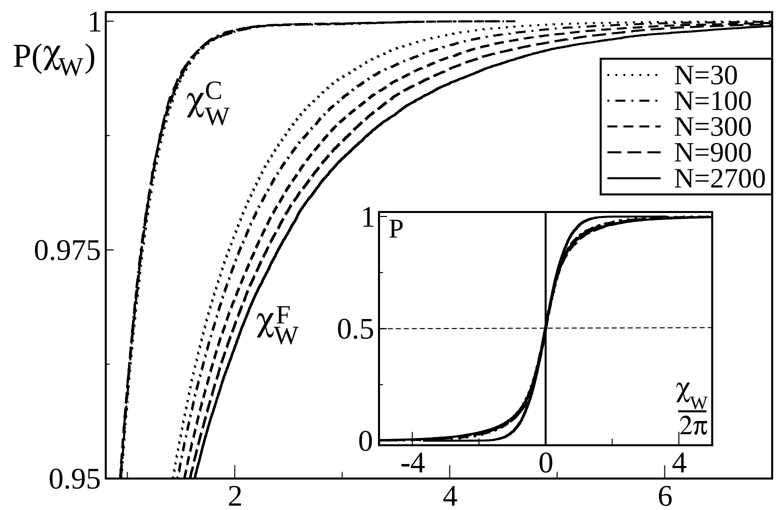

FIG. 1: Inset: The integrated writhe distribution function $P(\chi_W)$ computed with two different formulations of the writhe. χ_W^C not computed for $N = 2700$ due to computer limitations. The main figure is a zoom of the top right corner of the inset. One can compare the continuous evolution of χ_W^F 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.

To conclude we believe that torsional fluctuations of a semiflexible chains are not divergent when going to the continum limit. A DNA chain has a persistence length of order 50 times its radius so; it is in a regime where eq. (1) has reached the continuum limit to a very good approximation.

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