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FRACTAL DIMENSION MEETS TOPOLOGY: STATISTICS OF COLLAPSED POLYMERS AND BEYOND

SERGEI NECHAEV

LPTMS, Université Paris Saclay, 91405 Orsay Cedex, France
E-mail: serguei.nechaev@universite-paris-saclay.fr

ABSTRACT

We consider statistical and topological properties of fractional Brownian polymers, equipped with short-range volume interactions [1]. The attention is paid to statistical properties of collapsed conformations with the fractal dimension $D_f \geq 2$ in 3D, which are analyzed both numerically and via the mean-field Flory approach. Our study is motivated by an attempt to mimic the conformational statistics of collapsed unknotted polymer rings, which are known to equilibrate into the compact hierarchical crumpled globules (CG) with $D_f = 3$ at large scales. Replacing the topologically stabilized CG state by a self-avoiding fractal path adjusted to the fractal dimension $D_f \approx 3$, we tremendously simplify the problem of generating the CG-like conformations since we wash out the topological constraints from the consideration. We show that, with the increase of D_f, typical conformations become more territorial and less knotted. Distributions of the knot complexity, $P(\chi)$, for collapsed ring chains with $D_f \geq 2$ suggest a direct correspondence between the fractal dimension and knotting of fractal paths. We extend the found results to the investigation of braiding of directed polymers near curved surfaces where the statistics of random walks becomes non-Gaussian [2].

[1] Astakhov, A.M., Avetisov, V.A., Nechaev, S.K. and Polovnikov, K.E. 2021 Fractal dimension meets topology: statistical and topological properties of globular macromolecules with volume interactions. *Macromolecules* **54**, 1281.

[2] Valov, A., Avetisov, V., Nechaev, S. and Oshanin, G. 2020 Field-driven tracer diffusion through curved bottlenecks: fine structure of first passage events. *Phys. Chem. Chem. Phys*. **22**, 18414.