

Melts of unconcatenated polymer rings revisited

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Soft matter systems, such as super-elastic gels, ruled by strong topological interactions may provide new class of materials with distinct structural and dynamical properties. A conceptually simple paradigmatic system with well-controlled topological interactions is provided by melts of unconcatenated and unknotted polymer rings. Despite repeated efforts, both theoretically and numerically, the detailed structure, their form factor, the related self-dissusion and stress relaxation remain debated. Recent computational studies suggest in fact compact ring configurations. This begs the question of whether the irregular surfaces of these compact chains may be characterized by a fractal surface dimension $ds < 3$.

In the first part of our talk, we shall revisit the scaling analysis of the form factor by Halverson *et al.* [J. Chem. Phys. **134**, 204904 (2011)] claiming an exponent $ds = 2.8$. Our analysis [1] suggests that this conclusion might be due to an inappropriate application of the Generalized Porod Law at large wavevectors where length scales other than the total chain size do matter.

We present then in the second part of our talk the “decorated Gaussian loop model” recently proposed by us [2]. In this model, which does not require a fractal surface dimension $ds < 3$, the rings are viewed as random trees of polydisperse Gaussian loops ranging from the entanglement length to a skeleton ring of length $N^{2/3}$. Individual rings are predicted to be **marginally compact** with an average chain size

$$R^2 \sim N^{2/3} (1 - 1/N^{1/3})$$

(all prefactors omitted for clarity). The power laws for asymptotically long rings are shown to necessarily require sluggish corrections to describe experimental data and the computer simulations. The estimated broad crossover functions allow for a satisfactory fit of the published simulation data [2].

References:

[1] J.P. Wittmer, H. Meyer, A. Johner, S. Obukhov, J. Baschnagel, “*Comment on ‘Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Static’ [J. Chem. Phys. 134, 204904 (2011)]*”, JCP **139**, 217101 (2013).

[2] S. Obukhov, A. Johner, J. Baschnagel, H. Meyer, J.P. Wittmer, “*Polymer rings in the melt: The decorated Gaussian loop model*”, EPL **105**, 48005 (2014).

