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On the Anomalous Diffusion of a Polymer Chain in an Unentangled Melt

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The dynamics of polymer chains in unentangled melts is commonly described by the Rouse model. However, various experimental and simulation studies show that certain dynamical phenomena in unentangled melts cannot be explained by the Rouse theory. One of the puzzling observations is the anomalous diffusion of the center-of-mass (CM) of a polymer chain for times $t < t_N$, where $t_N \propto N^2$ is the Rouse time of a polymer consisting of N monomers. We explore two attempts to explain this observation: (i) an approach based on the effective interactions between the CMs in the melt and (ii) an approach based on the hydrodynamic flow and viscoelasticity of the melt. For approach (i) we find a partial success [1]: The theory accounts for the anomalous motion by yielding a negative power-law tail for the CM velocity autocorrelation function (CM VAF), $C_{\mathrm{cm}}(t) \propto -N^{-1}t^{-5/4}$. This prediction is in good agreement with molecular-dynamics (MD) simulations utilizing Langevin dynamics with a strong damping constant. On the other hand, for simulations with momentum conserving dynamics (i.e., the experimentally relevant situation) the prediction of approach (i) is qualitatively incorrect. In the latter case, the CM VAF rather scales as $C_{\mathrm{cm}}(t) \propto -N^{-1/2}t^{-3/2}$. This behavior can be rationalized by approach (ii). The predictions of approach (ii) are found to be good quantitative agreement with the MD simulations [2].

[1] J. Farago, A. N. Semenov, H. Meyer, J. P. Wittmer, A. Johner and J. Baschnagel, Phys. Rev. E **85**, 051806 (2012).
[2] J. Farago, H. Meyer, J. Baschnagel and A. N. Semenov, Phys. Rev. E **85**, 051807 (2012).

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