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Self-consistent field theory for polymer dynamics
DOUG GRZETIC, ROBERT WICKHAM, Department of Physics, University of Guelph, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University — We develop a self-consistent field theory (SCFT) for polymer dynamics. We reformulate a Rouse model for interacting monomers as a dynamical functional integral over field variables, using standard techniques. Novel aspects include our use of the functional Fokker-Planck equation to describe single-chain dynamics, and our extremization of the functional integral, resulting in a set of self-consistent equations for the time-dependent monomer density and the mean force field on a monomer. Our theory is distinct from published dynamical SCFTs that combine elements of equilibrium SCFT with phenomenological dynamical evolution schemes. The time scale in our theory is known exactly; no phenomenological kinetic coefficient needs to be introduced. Dynamical quantities in our theory have analogs in equilibrium SCFT, allowing sophisticated numerical techniques developed for equilibrium SCFT to be applied directly to study the dynamics. Our approach is flexible and can be used, for example, to study polymer melt dynamics. To test the self-consistent nature of the theory in space-time, we examine the simple case of the dynamics of trapped, interacting particles, and binary mixtures, in one dimension.

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