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Complex Langevin Simulation of the Coherent States Formulation of Polymer Field Theory[1] XINGKUN MAN, Chemical Engineering, University of California, Sant Barbara, KRIS DELANEY, Mateirals Research Laboratory, University of Clifornia, Santa Barbara, HENRI ORLAND, Institut de Physique Theorique, CE-Saclay, CEA, GLENN FREDRICKSON, Chemical Engineering, University of California, Sant Barbara — In 1969, Edwards and Freed adapted the "coherent state" methods employed in the second quantization formalism of quantum many-body theory to study polymer networks. Since its introduction into polymer science, this formalism has been largely neglected and to our knowledge, has never been applied as a basis for numerical simulations, even for linear polymers. However, in contrast to the Edwards auxiliary-field framework, this alternative polymer field theory has several attractive features, including an action or effective Hamiltonian with an explicit, finite-order, and semi-local polynomial character. We thus revisited the CS formalism and show that these characteristics have advantages both for analytical and numerical studies of linear polymers at equilibrium. For this purpose, we developed a new Complex Langevin sampling scheme that allows for simulations within the CS formalism with stable and efficient numerical characteristics. We anticipate that this methodology will facilitate efficient simulations of a wide range of systems, including complicated branched and networked polymers and liquid crystalline polymers.

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