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Quantitative test of polymer field theories by fast lattice Monte Carlo simulations XINGHUA ZHANG, Department of Chemical and Biological Engineering, Colorado State University, PENGFEI ZHANG, BAOHUI LI, Institute of Physics, Nankai University, Tianjin, P. R. China, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Recently, one of us proposed the so-called fast lattice Monte Carlo (FLMC) simulations,[1] where, instead of the self- and mutual-avoiding walks used in conventional lattice Monte Carlo simulations, multiple occupancy of lattice sites is allowed with a proper Boltzmann weight. FLMC simulations give orders of magnitude faster/better sampling of configurational space for multi-chain polymeric systems, and further allow stringent test, without any parameter-fitting, of the widely used polymer field theories. Taking homopolymer solutions and brushes as examples, we formulate the field theories (the self-consistent field theory, Gaussian-fluctuation theory, and the self-consistent Hartree approximation) on the same lattice and with the same Hamiltonian as used in FLMC simulations. Direct comparisons between the simulations and theories therefore unambiguously and quantitatively reveal the consequences of approximations used in the latter.

[1] *Q. Wang*, **Soft Matter, 5**, 4564 (2009).

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