Abstract Submitted for the MAR14 Meeting of The American Physical Society

Theoretical Basis of Monte-Carlo Field Theoretic Simulations DAVID MORSE, University of Minnesota, MARK MATSEN, PAWEL STASIAK, University of Waterloo — Monte-Carlo field theoretic simulations (MC-FTS) of incompressible polymer models rely on a rather poorly understood approximation to the complex-Langevin field theoretic simulation (CL-FTS) method of Fredrickson and coworkers, but yield results that appear to be both surprisingly accurate and much more easily interpreted than the results of CL-FTS simulations. Specifically, two of us (Stasiak and Matsen) have shown [1] that results of CL-FT simulations exhibit a simple dependence on spatial resolution (grid-size) that can analytically corrected for to obtain results that are independent of grid spacing, in which the relationship between the effective χ parameter and the simulation input parameter is given by a simple analytic formula. We give theoretical analysis that explains the accuracy of the method, the nature of its errors, and the reasons for this simple dependence on spatial resolution. We show that a much more complicated dependence on spatial resolution or interaction range is expected in full CL-FT simulations. Our analysis suggests a simple modification of the CL-FT method that should improve its accuracy without effecting its efficiency or other favorable properties. [1] P. Stasiak and M.W. Matsen, Macromolecules 46, 8037 (2013)

> David Morse University of Minnesota

Date submitted: 15 Nov 2013

Electronic form version 1.4