

Multiple Relaxation Times in the Gibbs Ensemble Monte Carlo Simulation of Phase Separation

Authors : Bina Kumari, Subir K. Sarkar, Pradipta Bandyopadhyay

Abstract : The autocorrelation function of the density fluctuation is studied in each of the two phases in a Gibbs Ensemble Monte Carlo (GEMC) simulation of the problem of phase separation for a square well potential with various values of its range. We find that the normalized autocorrelation function is described very well as a linear combination of an exponential function with a time scale τ_2 and a stretched exponential function with a time scale τ_1 and an exponent α . Dependence of (α, τ_1, τ_2) on the parameters of the GEMC algorithm and the range of the square well potential is investigated and interpreted. We also analyse the issue of how to choose the parameters of the GEMC simulation optimally.

Keywords : autocorrelation function, density fluctuation, GEMC, simulation

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