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Molecular dynamics analysis of particle number fluctuations of a first-order phase transition

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We study the critical point effects on particle number fluctuations both in the crossover ($T > T_c$) and mixed phase ($T < T_c$) regions by means of molecular dynamics simulations of a Lennard-Jones fluid, motivated by the ongoing search for the QCD critical point in heavy-ion collisions.

In the crossover region, we find large fluctuations associated with the critical point in coordinate space, but in the absence of collective flow and expansion, they are essentially washed out when momentum cuts are imposed instead.

In the mixed phase region, the behavior depends on whether the system is in a metastable nucleation or cavitation region, or in the spinodal decomposition region, and can be interpreted in terms of simplified analytic models. For the case of nucleation, we find that fluctuations are qualitatively described by a non-interacting cluster model.

The spinodal decomposition, on the other hand, leads to large fluctuations in coordinate space, which can be understood to arise due to the interplay between the size of the acceptance region and that of the liquid phase.

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