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

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Motivation

Proton number fluctuations in heavy-ion collisions are a prime observable in the search for the QCD critical point and the associated first-order phase transition. This is motivated by the equilibrium expectations of large critical fluctuations of baryon density near the critical point. However, it remains a non-trivial task to understand the development of critical point signatures.To shed light on this question, we explore the behavior of critical point fluctuations in a framework of molecular dynamics with Lennard-Jones (LJ) potential.

Molecular dynamics of the Lennard-Jones fluid

We solve the classical N-body problem by performing molecular dynamics simulations of the LJ fluid in a box with periodic boundary conditions. The LJ interaction potential reads

$$V_{\mathrm{LJ}}(\tilde{r})/\varepsilon = 4\left[\left(\frac{\sigma}{r}\right)^{6} - \left(\frac{\sigma}{r}\right)^{12}\right] = 4(\tilde{r}^{-12} - \tilde{r}^{-6}), \tag{1}$$

where the first and second terms correspond to short-range repulsion and intermediate-range attraction, respectively. We use reduced variables ($\mathbf{r}^* = \mathbf{r}/\sigma,\ T^* = T/(\varepsilon),\ n^* = n\sigma^3,\ p^* = p\sigma^3/\varepsilon,\ \tilde{t} = t\sqrt{\varepsilon/(m\sigma^2)}$) as well as normalized relative to the critical point location ($\tilde{\mathbf{r}} = \mathbf{r}^*,\ \tilde{T} = T^*/T^*_{\mathrm{c}}, \tilde{n} = n^*/n_{\mathrm{c}},\ \tilde{p} = p^*/p^*_{\mathrm{c}}$).

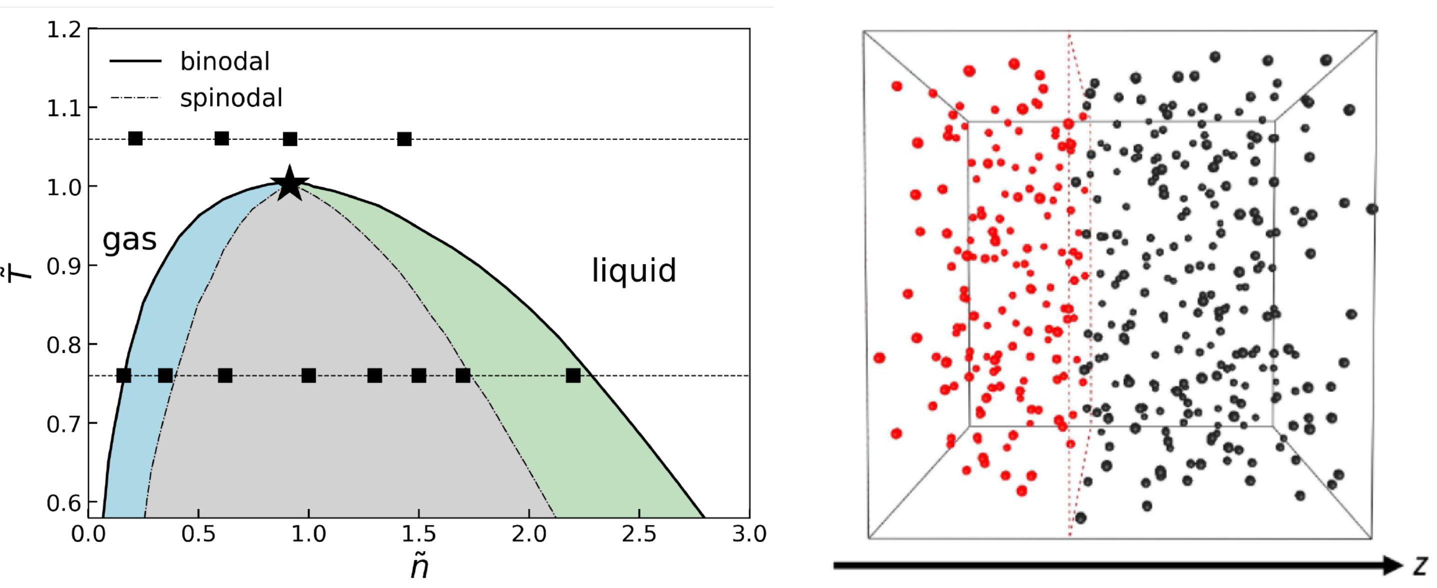

Figure 1: (Left): (T, n) phase diagram in liquid-gas region. (Right): subensemble in simulation.

Ergodic hypothesis: Observables can be calculated as time averages

$$\langle A\rangle = \frac{1}{\tilde{\tau}}\int_{\tilde{t}_{\mathrm{eq}}}^{\tilde{t}_{\mathrm{eq}}+\tilde{\tau}} A(\{\tilde{\mathbf{r}}_i(\tilde{t}), \tilde{\mathbf{v}}_i(\tilde{t})\})\, d\tilde{t}, \tag{2}$$

Pressure (virial theorem):

$$\tilde{p} = \tilde{n}\tilde{T} + \frac{\sum_{i=1}^{N}\sum_{j=i+1}^{N}\tilde{\mathbf{r}}_{i,j}\cdot\tilde{\mathbf{f}}_{i,j}}{3\tilde{L}^3}. \tag{3}$$

Scaled variance of particle number fluctuations in a subvolume:

$$\tilde{\omega} = (1-\alpha)^{-1}\frac{\langle N^2\rangle - \langle N\rangle^2}{\langle N\rangle}. \tag{4}$$

Here α is observed volume fraction and the factor $(1-\alpha)^{-1}$ is a correction for global conservation [3].
Grand-canonical limit:

$$\omega_{\mathrm{gce}} = \tilde{T}\left(\frac{\partial\tilde{p}}{\partial\tilde{n}}\right)^{-1}_{\tilde{T}}, \qquad \omega_{\mathrm{gce}} \to \infty \text{ at the critical point.} \tag{5}$$

Results

Pure phase (crossover region)

We study fluctuations along a supercritical isotherm $T = 1.06T_c$, where the system is in a pure phase.

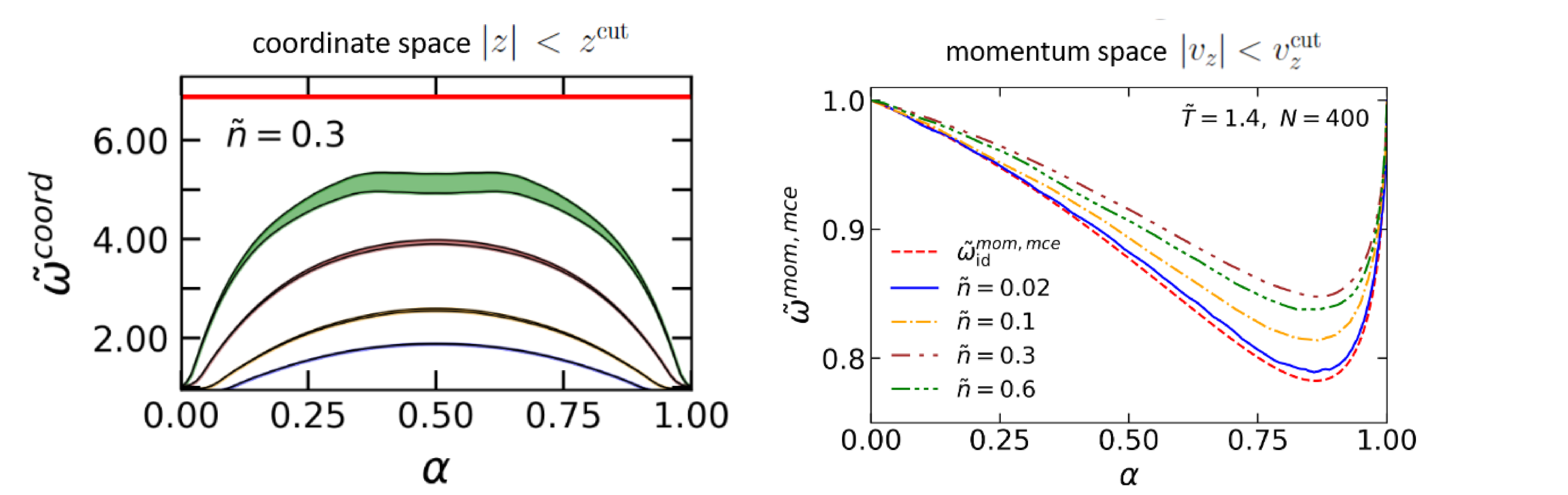

Figure 2: Corrected scaled variance $\tilde{\omega}$ of particle number fluctuations near the critical point from a crossover side ($T = 1.06T_c$, $n \approx n_c$) in (left) coordinate and (right) momentum space subvolumes.

Conclusion: We observe large fluctuations associated with the critical point in coordinate space subvolumes, but in the absence of collective flow, these signals are washed out when momentum cuts are imposed instead.

Mixed phase

Here we study fluctuations along a subcritical isotherm $T = 0.76T_c$.

Results

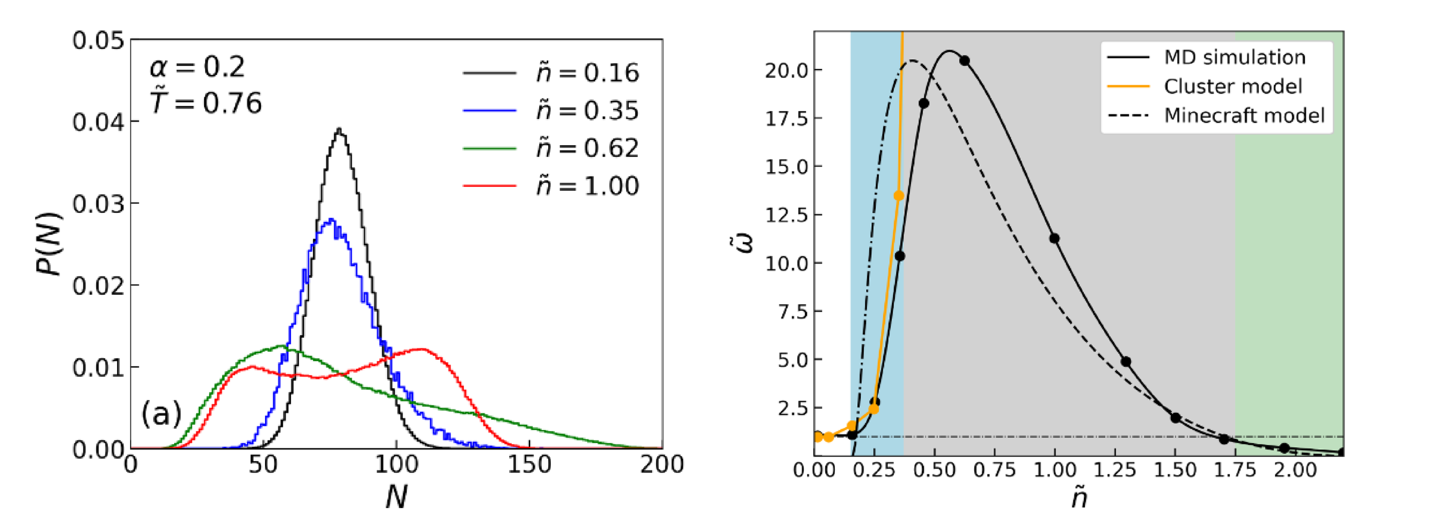

Figure 3: (Left): $P(N)$ distribution at mixed phase. (Right): Fluctuations at mixed phase. Here $\alpha = 0.2, N = 400$.

Conclusion: We observe large particle number fluctuations in the nucleation region $\tilde{n} \leq 0.35$, where *cluster model* can be used,

$$Z_{\mathrm{GCE}} = \prod_{k\geq 1}\exp\left[V(2\pi kmT)^{3/2}g(k)\exp\left\{\frac{\mu k}{T}\right\}\right], \tag{6}$$

and in the spinodal decomposition region at $\tilde{n} > 0.35$ where we use the so-called Minecraft model (see [2] for explicit formulas).

Outlook

- Fluctuations in expanding systems as appropriate for heavy-ion collisions.
- Precise study of fluctuations in the mixed phase region, dependence on system size and subvolume form, and test of the thermodynamic limit.

References

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[2] Volodymyr A. Kuznietsov, Oleh Savchuk, Roman V. Poberezhnyuk, Volodymyr Vovchenko, Mark I. Gorenstein **and** Horst Stoecker. "Molecular dynamics analysis of particle number fluctuations in the mixed phase of a first-order phase transition". **in** *Phys. Rev. C*: 107 (2023).

[3] Volodymyr Vovchenko, Oleh Savchuk, Roman V. Poberezhnyuk, Mark I. Gorenstein **and** Volker Koch. "Connecting fluctuation measurements in heavy-ion collisions with the grand-canonical susceptibilities". **in** *Physics Letters B*: 811 (2020).