Critical point particle number fluctuations from molecular dynamics

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29.11.2022
Plan

- Introduction
- Molecular Dynamics simulation
- Fluctuations
- Results
- Summary and discussions
QCD matter

Figure from Bzdak et al., Phys. Rept. 2020
Fluctuations as CP signature

In GCE density cumulants shows singularity behaviour in the critical point.

\[
\ln Z^{gce}(T, V, \mu) = \ln \left[ \sum_N e^{\mu N} Z^{ce}(T, V, N) \right], \quad \text{(1)}
\]

\[
\kappa_n \approx \frac{\partial^n (\ln Z^{gce})}{\partial (\mu N)^n}. \quad \text{(2)}
\]

The real expression for \(Z^{gce}\) is unknown in QCD matter.
## Connection to the experiment

| Theory                                                                 | Experiment                                      |
|-----------------------------------------------------------------------|-------------------------------------------------|
| Coordinate and/or momentum space                                      | Momentum space                                  |
| In contact with the heat bath                                         | Expanding in vacuum                             |
| Conserved charges                                                     | Non-conserved particle numbers                  |
| Uniform                                                               | Inhomogenous                                    |
| Fixed volume                                                          | Fluctuating volume                              |

*Need dynamical model description*
The Lennard-Jones potential reads

\[ V_{\text{LJ}} = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^6 - \left( \frac{\sigma}{r} \right)^{12} \right], \quad (3) \]

In reduced dimensionless variables it can be rewritten as

\[ \tilde{V}_{\text{LJ}} = 4[\tilde{r}^{-12} - \tilde{r}^{-6}], \quad (4) \]

where the reduced variables are used: \( \tilde{r} = r/\sigma \) and \( \tilde{V}_{\text{LJ}} = V_{\text{LJ}}/\varepsilon \).
In the critical point two equations must be satisfied

\[ \frac{\partial p}{\partial n} = 0, \quad \frac{\partial^2 p}{\partial n^2} = 0. \] (5)

The CP location has been estimated from numerous MD simulations, yielding (here \( \tilde{T} = T/\varepsilon \) and \( \tilde{n} = n\sigma^3 \))

\[ \tilde{T}_c = 1.321 \pm 0.007, \quad \tilde{n}_c = 0.316 \pm 0.005, \quad \tilde{\rho}_c = 0.129 \pm 0.005. \] (6)
Details of simulation

The simulations are done for a system of N particles with periodic boundary conditions by solving a system of classical Newton equations.

\[ m \frac{d^2 \vec{r}_{ij}}{d\tilde{t}^2} = -\nabla \tilde{V}_{\text{LJ}}(\vec{r}_{ij}) \]  \hspace{1cm} (7)

\[ \langle A \rangle = \frac{1}{\tilde{\tau}} \int_{\tilde{t}_\text{eq}}^{\tilde{t}_\text{eq}+\tilde{\tau}} A(\{\vec{r}_i(\tilde{t}), \vec{v}_i(\tilde{t})\}) d\tilde{t}. \]  \hspace{1cm} (8)

The simulations are performed on GPU. Code is available at: https://github.com/vlvovch/lennard-jones-cuda
Equation of state at $\tilde{T} = 1.4 = 1.06 T_c$
Scaled variance of particle number fluctuations in the grand-canonical ensemble reads

$$\omega = \frac{\langle \Delta N^2 \rangle}{\langle N \rangle} = T \left[ \frac{\partial P}{\partial n} \right]^{-1}_T \quad (9)$$
Subensemble method

In the case of interacting system (V Vovchenko O. Savchuk, R. Poberezhnyuk, M. Gorenstein, V. Koch, Phys. Let. B, 2020) one can find

\[ \kappa_1 = \alpha VT^3 \chi_1, \quad \kappa_2 = \alpha (1 - \alpha) VT^3 \chi_2. \]  

(10)

By definition in cumulants formalism

\[ \omega_{\text{coord}} = \frac{\kappa_2}{\kappa_1} = (1 - \alpha) \cdot \frac{\chi_2}{\chi_1} = (1 - \alpha) \cdot \omega. \]  

(11)

Finally, one can introduce

\[ \tilde{\omega}_{\text{coord}} \equiv \omega_{\text{coord}} / (1 - \alpha). \]  

(12)
Coordinate space subsystem \((\tilde{T} = 1.4 = 1.06 T_c)\)
Momentum space subsystem \((\tilde{T} = 1.4 = 1.06 T_c)\)

\[
\tilde{\omega}_{id}^{\text{mom}, \text{mce}} = 1 - \frac{2[\text{erf}^{-1}(\alpha)]^2 e^{-2[\text{erf}^{-1}(\alpha)]}}{3\pi \alpha (1 - \alpha)}
\]  
(13)

\[
\alpha = \frac{\langle N^{\text{acc}} \rangle}{N}, \quad |v_z| < v_z^{\text{cut}}
\]  
(14)
Summary

1. Molecular dynamics simulations of the Lennard-Jones fluid provide a microscopic approach to studying critical point fluctuations;
2. Scaled variance of particle number is computed along the supercritical isotherm $\tilde{T} = 1.06 T_c$ in a periodic box setup;
3. Large fluctuations are observed near the critical point when calculated in coordinate space, but washed out when momentum cuts are imposed instead

Outlook

- Fluctuations in expanding systems with the collective flow, ensemble averaging;
- Fluctuations and cluster formation and distributions in mixed-phase;
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THANK YOU FOR ATTENTION!

Questions?