

Unknown

Ze-Yang Li

School of Physics, Peking University, Beijing 100871, P. R. China,

In this report I briefly present the results of pressure-time curve simulation, pressure-volume curve simulation of Lennard-Jones potential based on package `lammers`[1]. A different pressure-volume feature with respect to temperature chosen is observed, indicating a phase transition at the critical temperature.

I. INTRODUCTION

The Lennard-Jones potential is given by

$$U(r) = 4\epsilon \left\{ \left[\frac{\sigma}{r} \right]^{12} - \left[\frac{\sigma}{r} \right]^6 \right\}$$

with rescaled parameter

$$T^* = k_B T / \epsilon, \quad \rho^* = \rho \sigma^3, \quad p^* = p \sigma^3 / \epsilon$$

I choose $\sigma = 1, \epsilon = 1$ with a cutoff to save computation resource

$$U(r) = \begin{cases} 4\epsilon \left\{ \left[\frac{\sigma}{r} \right]^{12} - \left[\frac{\sigma}{r} \right]^6 \right\} & \Rightarrow 4 \left\{ \left[\frac{1}{r} \right]^{12} - \left[\frac{1}{r} \right]^6 \right\} & r < \text{cutoff} = 2.5 \\ 0 & & \text{otherwise} \end{cases}$$

II. PRESSURE-TIME RESULTS

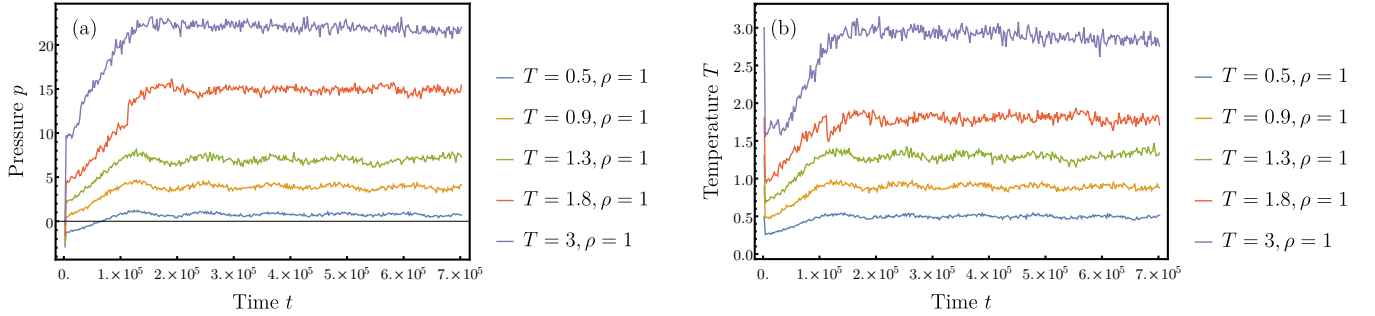


FIG. 1: (a) Pressure-time results for different initial-set temperature with same density (volume), (b) the equilibrium is examined by the temperature-time simulation

Here I present the simulation results of pressure-time curve, where an equilibrium is observed as expected (Fig. 1). I here define a parameter of the validity of the results. First we define an average of pressure while dropping calculations of first t from total τ simulation results

$$Q(t) = \frac{1}{\tau - t} \int_t^\tau p(t') dt', \quad t < \tau$$

where the validity is defined as mean deviation of the function (sequence as discrete time point)

$$v = \frac{|\langle Q(t) - \bar{Q} \rangle|}{|\bar{p}|}$$

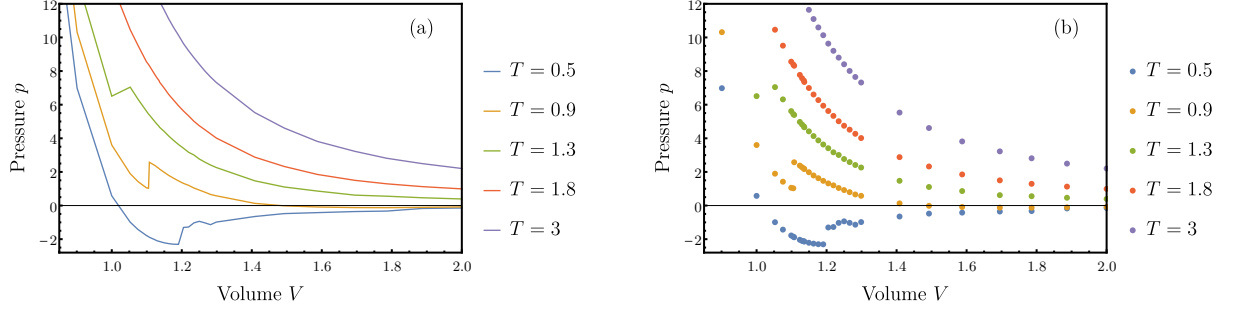


FIG. 2: (a) ListpLinePlot and (b) ListPlot of pressure-volume simulation result for different temperature $T = 0.5, 0.9, 1.3, 1.8, 3$. The phase transition happens only if $T < T_c$, where $T_c \approx 1.3$ in this case (1.326 ± 0.002 in [2]). Different temperature has different phase transition volume, which for $T = 0.5, V_c \sim 1.2$; $T = 0.9, V_c \sim 1.1$ and $T = 1.3, V_c \sim 1.0$. Besides, for ultra low temperature, the detailed fluctuation and positive correlation between pressure and volume is observed in $T = 0.5$.

0.5	0.53	0.56	0.59	0.63	0.67	0.71	0.77	0.78	0.79	0.8
0.81	0.82	0.83	0.84	0.85	0.86	0.87	0.88	0.881	0.885	0.89
0.903	0.905	0.91	0.93	0.95	1.0	1.11	1.25	1.43	1.67	2.0

TABLE I: Range of ρ .

III. PRESSURE-VOLUME RESULT

By varying the density ρ the volume $V = 1/\rho$ is obtained, the relation between pressure and volume as well. It is shown in Fig. 2 that at low temperature the pressure-temperature is not continuous, and there exists a sharp jump at some particular volume, indicating a phase transition. At high temperature, this sharp noncontinuity vanishes as expected (like critical point for water's liquid-gas phase transition).

Appendix A: Validity examination

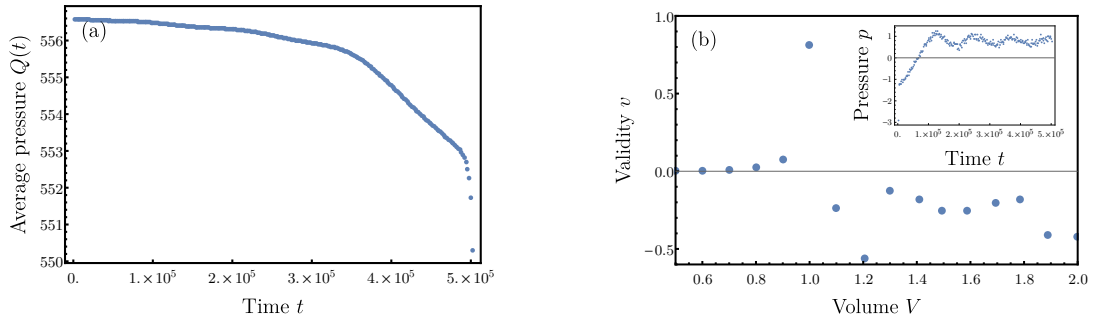


FIG. 3: (a) Example of $Q(t)$ with validity $v = 0.00161451 \ll 1$. In this case, $\rho = 2.0, T = 0.5$, (b) validity v of different volume V at $T = 0.5$, inset shows an extraordinary large v at $\rho = 1.0$ case's $p(t)$ figure. The final estimation of \bar{p} is somehow questionable.

Appendix B: Sampling method

I chose ρ in the Table. I to achieve the goal of covering almost every physically significant region, where the phase transition volume is changed as a function of temperature is not considered.

-
- [1] S. Plimpton, Journal of computational physics **117**, 1 (1995).
 - [2] J. Caillol et al., Journal of Chemical Physics **109**, 4885 (1998).