Phase Transition in 2-Dimensional Hard Disk Fluid

Project Report - CHM684A

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Contents

Problem Statement

In this project, we studied phase transition using a two dimensional hard disk fluid by applying the Monte Carlo (MC) method.

1 Introduction

1.1 RDF

The potential energy of hard disk system is given by:

$$V(r_1, r_2, ..., r_n) = \sum_{i}^{N-1} \sum_{j>1} v(r_{ij})$$

with $v(r_{ij}) = 0$ if $r_{ij} \leq \sigma$ and equal to ∞ otherwise. Here $r_{ij}$is the inter-particle distance. Diameter of the disk is given by σ. In condensed matter system the local structure around any particle can be understood from the Radial Distribution Function (RDF). Generally, RDF is defined by the notation g(r). It is actually a pair correlation function. It defines the probability of finding a particle at distance r from a reference particle with respect to ideal system. g(r) gives the distribution of particles i.e how many particles are within a distance r to r+dr away from a reference particle. g(r) can be computed by:

$$g(r) = \frac{\sum_{j=1}^{N} \sum_{i=1}^{T} n_{ij}(r)}{2\pi r dr (N-1) T \rho}$$

where, N is number of particles, T is the number of configurations, ρ is the number density & n_{ij} is the number of particles in the shell r and r+dr from atom j in the frame i.

1.2 Equation of State

The hard sphere equation of state can be calculated from the following equation:

$$\frac{\beta p}{\rho} = 1 + B_2 \rho g(\sigma)$$

where, $\beta = \frac{1}{k_B T}$,ρ is the number density and B_2 is the second virial coefficient. B_2 is expressed as:

$$B_2 = \frac{2\pi}{3} \sigma^3$$

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2 Methods

2.1 Subprograms

We used 3 modules in this program and one main program file as follows.

- main program
- module mc
- module gr
- module variables

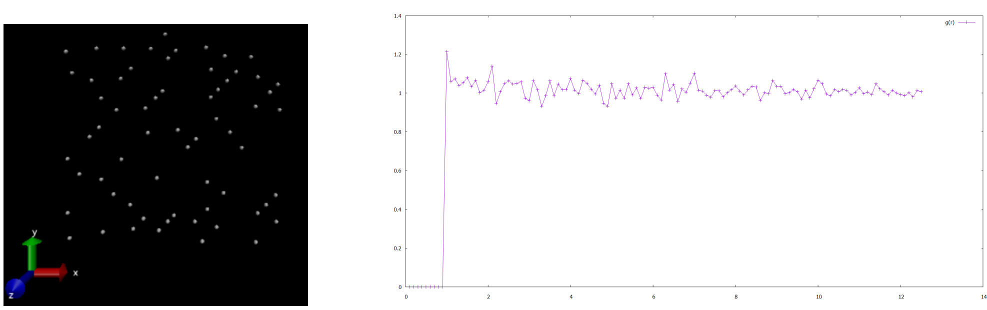
2.2 Procedure

1. First we called SUBROUTINE create_lattice() to create initial lattice structure. This subroutine takes ρ as input and calculate box size and thus creates lattice.
2. After creating lattice program takes stepsize and number of steps as input from user. Now, program call SUBROUTINE mc_step(). This routine displaces the randomly chosen particle with random perturbation. It also checks for overlaps and apply PBC to each particle. This is repeated nstep times.
3. Each accepted step is printed in .xyz file.
4. Now, g(r) is calculated using MODULE gr and calling SUBROUTINE calculate_gr(). This step returns value of $g(\sigma)$ and g(r) is also plotted using GNU plot.
5. At last step we calculated $\frac{\beta p}{\rho}$ using SUBROUTINE calculate_betap().
6. We repeated all the above mentioned steps for $\rho = 0.1, 0.2, 0.3$ upto 0.94 and plotted $\frac{\beta p}{\rho}$ Vs ρ.

3 Results

3.1 Snapshots and RDF

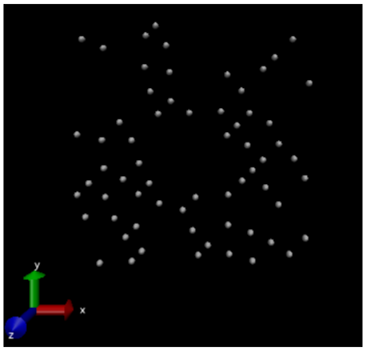
Snapshots for last accepted configuration for different rho is as shown in the following figures 1 to 10:



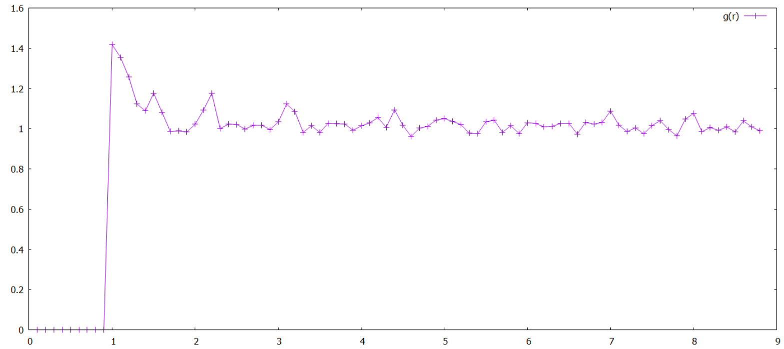
(a) Snapshot of last accepted configuration

(b) Plot of RDF function

Figure 1: For $\rho = 0.1$

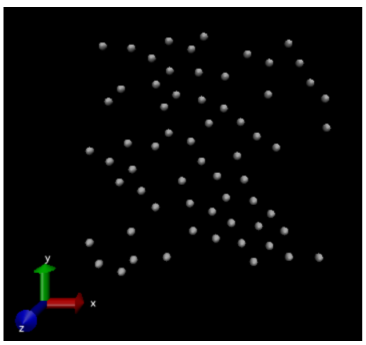


(a) Snapshot of last accepted configuration

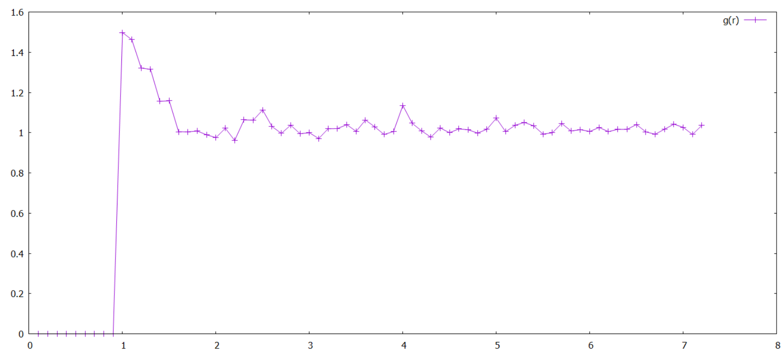


(b) Plot of RDF function

Figure 2: For $\rho = 0.2$

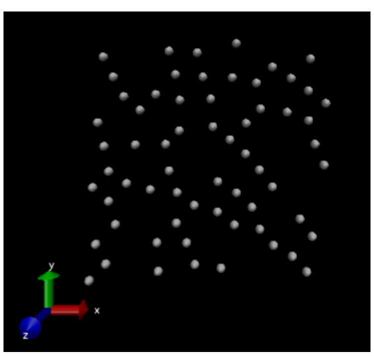


(a) Snapshot of last accepted configuration

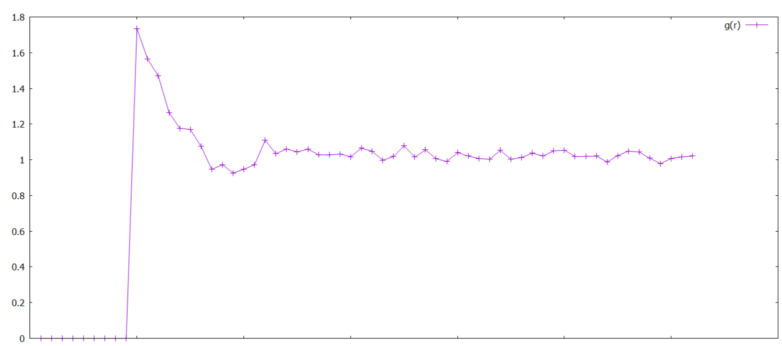


(b) Plot of RDF function

Figure 3: For $\rho = 0.3$

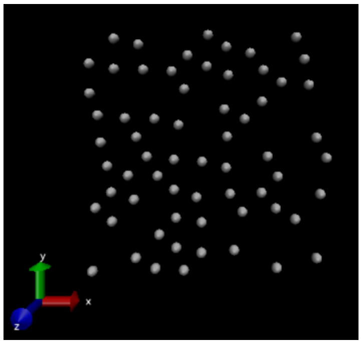


(a) Snapshot of last accepted configuration

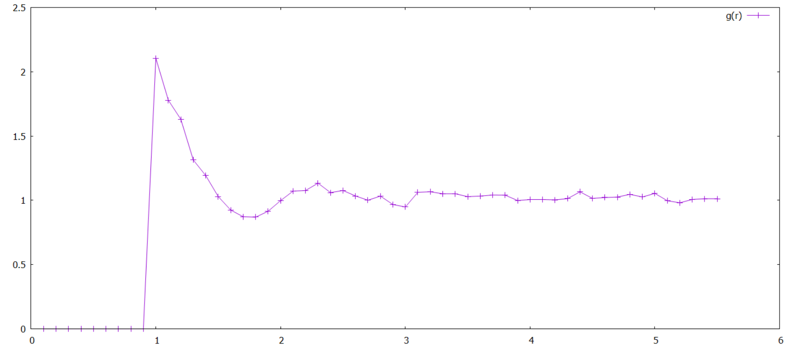


(b) Plot of RDF function

Figure 4: For $\rho = 0.4$

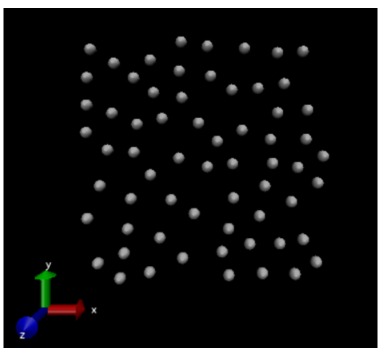


(a) Snapshot of last accepted configuration

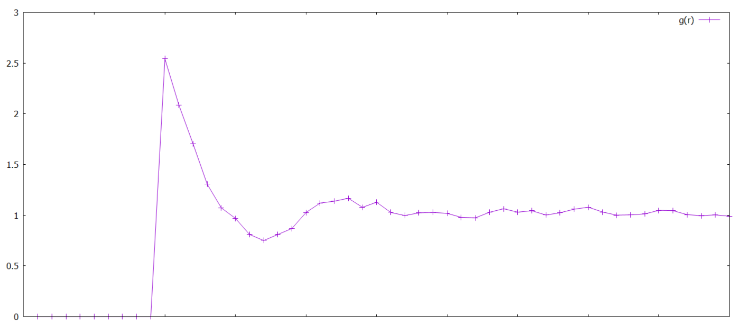


(b) Plot of RDF function

Figure 5: For $\rho = 0.5$

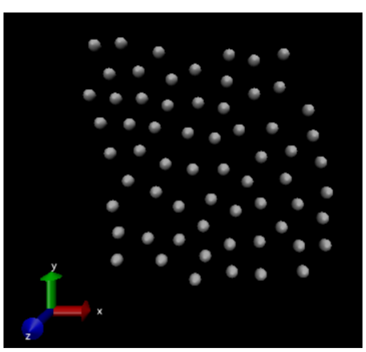


(a) Snapshot of last accepted configuration

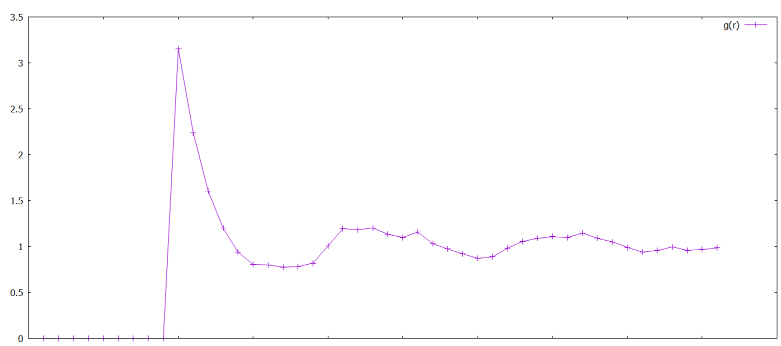


(b) Plot of RDF function

Figure 6: For $\rho = 0.6$

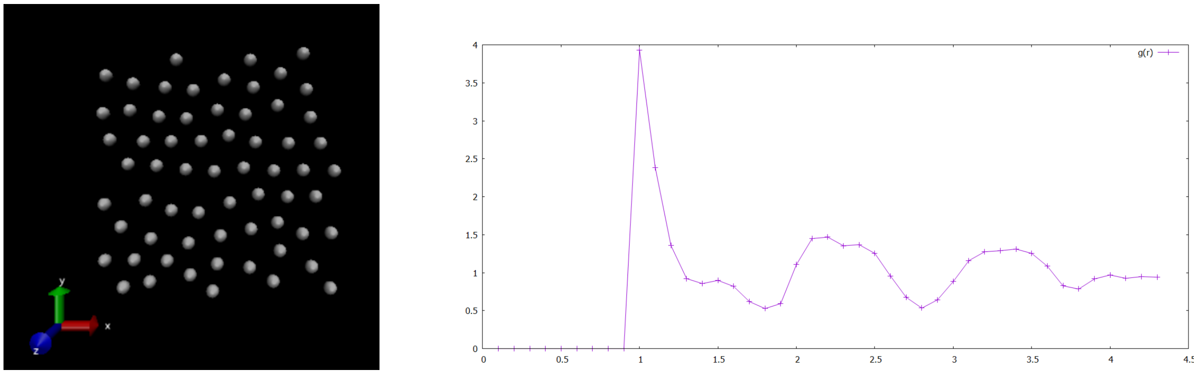


(a) Snapshot of last accepted configuration



(b) Plot of RDF function

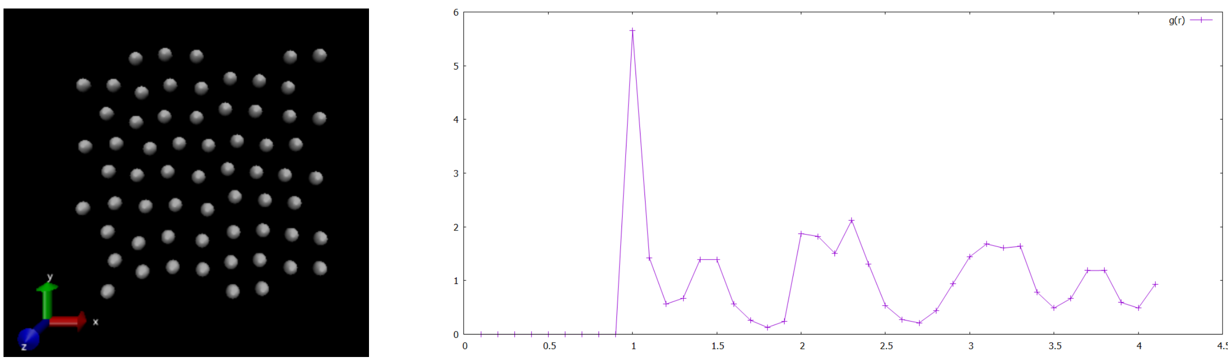
Figure 7: For $\rho = 0.7$



(a) Snapshot of last accepted configuration

(b) Plot of RDF function

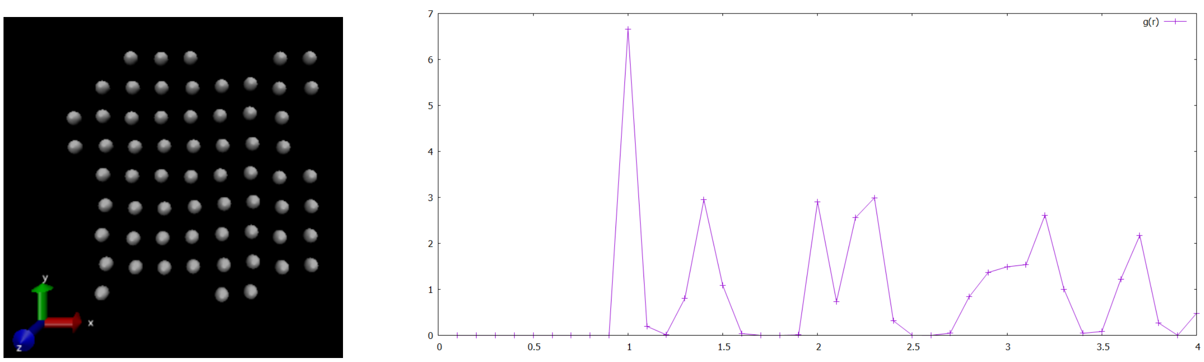
Figure 8: For $\rho = 0.8$



(a) Snapshot of last accepted configuration

(b) Plot of RDF function

Figure 9: For $\rho = 0.9$



(a) Snapshot of last accepted configuration

(b) Plot of RDF function

Figure 10: For $\rho = 0.94$

3.2 Table of $g(\sigma)$ and $\frac{\beta p}{\rho}$ for every rho

Calculated value of $g(\sigma)$ and $\frac{\beta p}{\rho}$ for each rho is given in the table in figure 11.

ρ	$g(\sigma)$	$\frac{\beta p}{\rho}$
0.1	1.213659	1.254188
0.2	1.418178	1.594045
0.3	1.498124	1.941299
0.4	1.735248	2.453718
0.5	2.105144	3.204502
0.6	2.543027	4.195662
0.7	3.153873	5.623819
0.8	3.929018	7.583133
0.9	5.652230	11.654202
0.94	6.664213	14.120046

Figure 11: $g(\sigma)$ and $\frac{\beta p}{\rho}$ for each ρ

3.3 Plot of $\frac{\beta p}{\rho}$ Vs ρ

Obtained plot of $\frac{\beta p}{\rho}$ Vs ρ is as shown in figure 12:

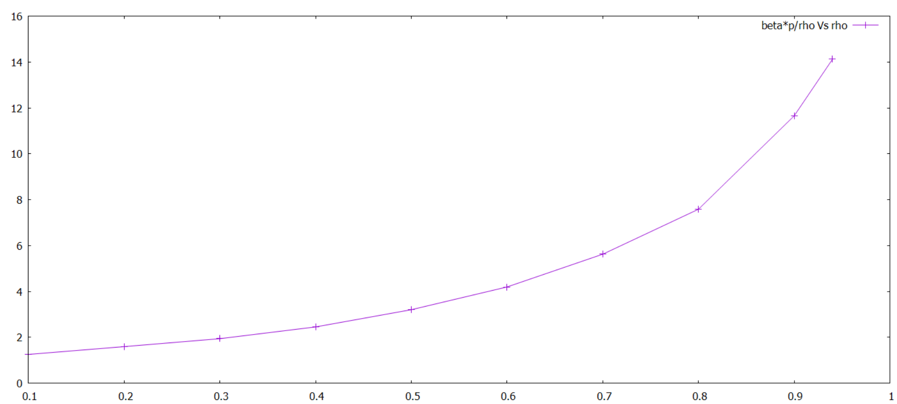


Figure 12: Plot of $\frac{\beta p}{\rho}$ Vs ρ

4 Conclusion

In this project we have studied the equation of state of 2D hard disk system and verified it from the plot of $\frac{\beta p}{\rho}$ vs ρ. We studied RDF for different densities and plotted them individually. Phase transition of Hard disk system has been studied. From the all data we recorded, we conclude that phase transition of fluid from liquid to solid between $\rho = 0.8$ to $\rho = 0.94$.

Acknowledgement

We would like to thank Prof. Nisanth Nair and Dr. Saurabh Srivastav for Motivating and guiding us throughout the project.

Appendix

Complete updated code is available at : Phase-Transition-in-2D-Hard-Disk