BITS Pilani K.K Birla Goa Campus

Monte-Carlo Simulation of 2-Dimensional Fluid in the presence of substrate potential

by

George Joseph

Study Project Report

Under the guidance of

Dr. Toby Joseph
Department of Physics
BITS Goa

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Abstract

This report describes the results obtained from a Metropolis simulation of interacting particles under the effects of a substrate. Random samples of points are taken for generating data about the system. This data is used to calculate various metrics to verify the observed results.

Acknowledgements

I owe a great thanks to Dr. Toby Joseph, Department of Physics, BITS Pilani K.K Birla Goa Campus, Zuarinagar for imparting his valuable guidance and encouragement throughout this work. Without his continued interest, immense help and stimulating suggestions, my endeavour to have a successful project would not be fruitful.

George Joseph

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Chapter 1

Introduction

Studying the interaction of particles at the solid liquid interface has been a difficult process as the **R-Y** Theory[1] that describes this process requires the two point correlation function which is extremely difficult to obtain via experiments. As an alternative, it can be calculated using computational techniques like Metropolis simulations [2].

This project describe the simulation of a system of particles under the influence of a substrate potential using Metropolis simulations. This data is used to calculate correlation and density function of the particles. Finally the two point correlation function is obtained which can be plugged into **R-Y** Theory.

Chapter 2

Metropolis Hastings algorithm

The Metropolis-Hastings Algorithm is a type of Markov chain Monte Carlo method which is used to generate random samples from a probability distribution. The main advantage of this algorithm is that to simulate a probability density $\mathbf{P(x)}$ only a function $\mathbf{f(x)}$ which is proportional to $\mathbf{P(x)}$ is needed. This greatly simplifies the process of simulating a probability density as calculating the normalization factor is quite arduous in practice.

The Algorithm can be described as follows:

- Choose a random point x_0 to be the initial point
- For every step, choose a random point $\acute{x}$ that suggests the next candidate. The $\acute{x}$ is chosen such that it is close to previous point x.
- Calculate
$$\alpha = \frac{P(x)}{P(x)} = \frac{f(x)}{f(x)}$$
. This removes the need for the normalization factor.
- If $\alpha > 1$ $\acute{x}$ is more likely that x and thus is accepted.
- If $\alpha < 1$ $\acute{x}$ is randomly chosen with probability α.
- This process is repeated multiple times to generate random samples.

Chapter 3

Probability density for 2-D Fluids

To simulate a fluid, we consider a system of N particles that interact with each other, the interaction potential between the particles is given by,

$$U = C\frac{e^{\frac{-r}{\lambda}}}{r}$$

Where r is the distance between the particles. λ determines the strength of the potential. C is a proportionality constant.

This is used to calculate the total energy E of the system. The probability density of the system is given by

$$D = e^{\frac{-\delta E}{k_B T}}$$

This is used as the probability density function in the Metropolis algorithm described in the previous chapter. Initially, the N particles are added to random locations in a 2-D plane. The energy of the system is calculated. Then a random particle is moved to another random point. If the total energy **E** decreases, the change is accepted. Else, the change is accepted with a given probability. This procedure mimics the systems tendency to move to a lower energy state.

Chapter 4

The Substrate Potential

The system also contains a substrate which can be considered as a fixed 2D mesh with particles at every intersection. We assume that the substrate particles dont interact with each other, as they are fixed in their positions. However, they do interact with the fluid particles. The potential of the substrate - particle interaction is given by,

$$U = C\frac{e^{-\frac{r}{\lambda}}}{r}$$

Where, **r** is the distance between the fluid particle and the substrate particle. λ determines the strength of the potential. C is a proportionality constant.

The total energy required by the Metropolis method is obtained from the potentials of both the particle-particle potential and the particle substrate potential.

Chapter 5

The Simulation

The system was simulated using the technique described by Sri Krishna Yasaswi[3] as part of his thesis. The following section will describe his method in brief.

The system is modeled by using a **LxL** matrix with N particles. The substrate particles are arranged in a rigid square mesh with the four closest substrate particles at a distance **l** from it.

Since the substrate potential does not change at a point during the simulation, the potential can be pre calculated and stored in a table. During the simulation, only a table look-up is necessary. This heuristic greatly speeds up the Metropolis steps.

To further speed up the steps, the interaction of particles beyond a certain threshold is ignored as they are very small anyway.

The **LxL** grid is wrapped around at the edges to create the effect of an infinite plane. This also adds periodic boundaries where if a particle crosses the edge, it reappears on the opposite edge.

Chapter 6

Metrics:

6.0.1 Correlation Function

This is a histogram of all the possible distances between particles. At every 10^{th} iteration, the distance between each particle pair is calculated and the corresponding bin is updated by one.

6.0.2 Density function

This is a 2D matrix that represents the density of the fluid particles in between the substrate particles. Since the substrate particles form a square of length **l**, a **lxl** matrix is initialized with all zeros. At every 10th iteration, an update is made for each particle in its corresponding bin depending on its position.

6.0.3 Two point Correlation Function

In the presence of an external substrate potential, the liquid in no longer isotropic. A two point correlation is required to represent the function. A four dimensional matrix is used to store this information. For every particle, first the location of the square in which it is present is determined with its x, y coordinates. These form the first two dimensions.

Then the distance between every pair of particles is determined, which form the next two dimensions. After every ten steps, the cell for the calculated index is updated by one.

Chapter 7

Results:

The following section will describe the results obtained from the simulations for different values of $\beta = \frac{1}{k_b T}$. Larger the value of β, colder the system is.

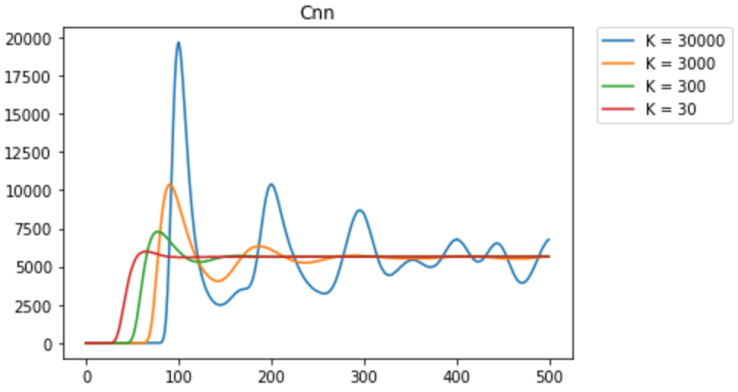

FIGURE 7.1: Correlation Function for different values of β

From the above plot the following observations can be made:

- For high temperatures the particles are almost equally distributed.
- For lower temperatures, there is a peak at 100, which corresponds to a particle in the opposite square at a distance of **l**.
- At lower temperatures, the particles get confined to the center of the square as the substrate particles are present in the corner.
- The second peak corresponds to a the particle in the diagonal box at a distance of $\sqrt{2}l$

The density of particle at different values of β are shown below. The substrate particles are located on the four corners of the square. As the system gets colder, the kinetic energy of the particles decrease and they get localized due to the substrate potential.

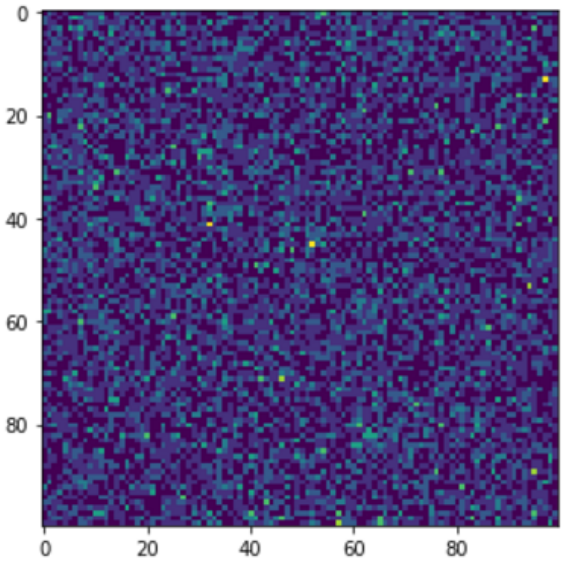

FIGURE 7.2: Density of particles between the substrate particles for $\beta = 30$

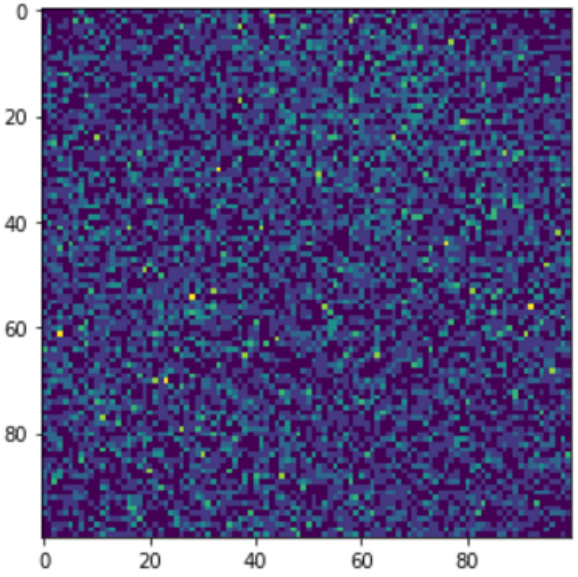

FIGURE 7.3: Density of particles between the substrate particles for $\beta = 300$

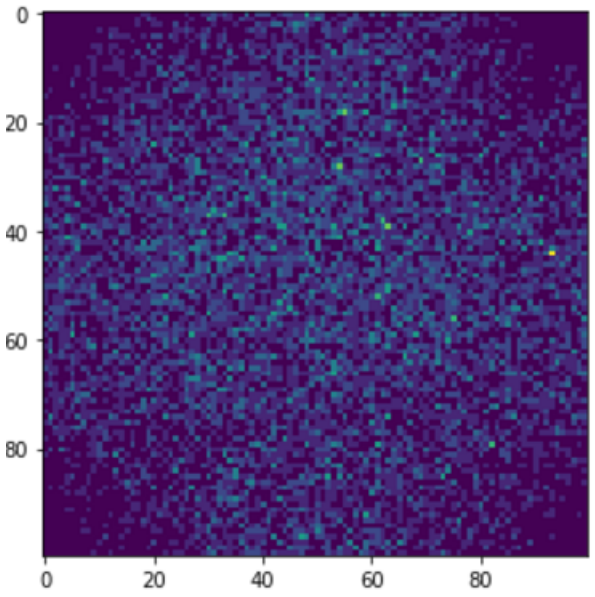

FIGURE 7.4: Density of particles between the substrate particles for $\beta = 3000$

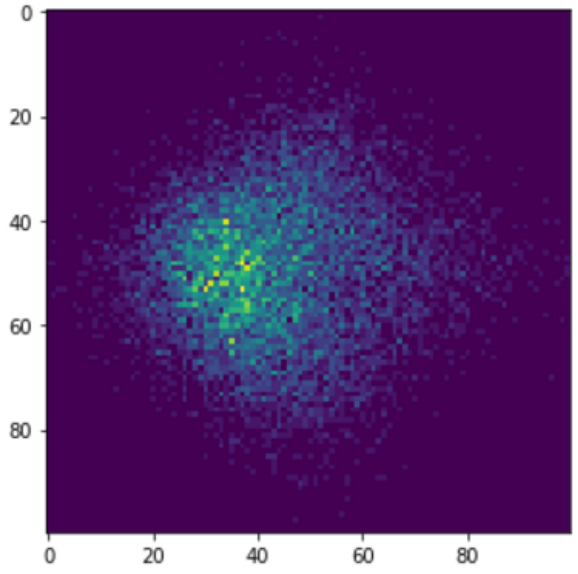

FIGURE 7.5: Density of particles between the substrate particles for $\beta = 30000$

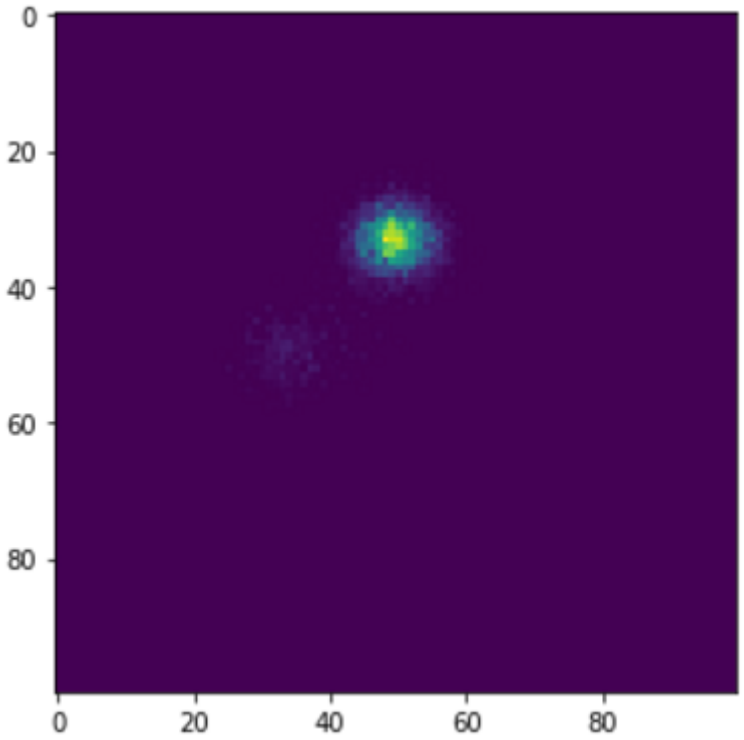

FIGURE 7.6: Density of particles between the substrate particles for $\beta = 300000$

To find the transition point from solid to liquid, β was plotted against the variance of energy normalized by temperature square [2]. This plot will peak at the transition point as observed below.

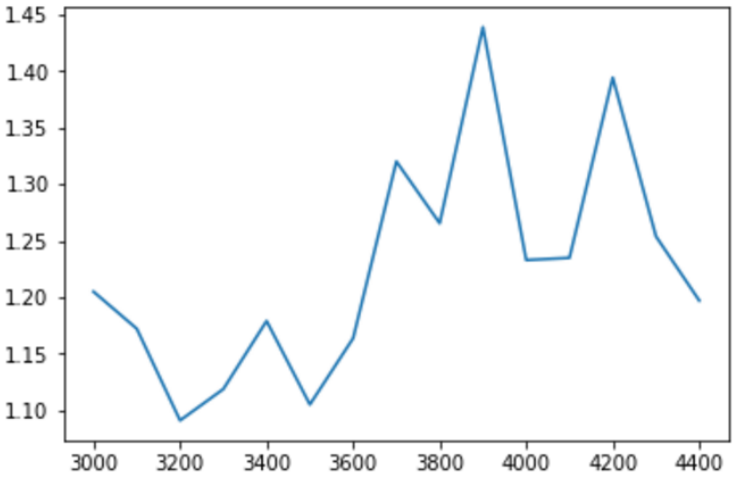

FIGURE 7.7: Finding the transition point for the system.

Chapter 8

Conclusion

It is clear from the graphs that as the temperature is reduced, the particles get confined to a specific location in the matrix. This represents the formation of crystals from the particles. The transition point of the system has also been found from the graphs.

Further work will include using the two point correlation data obtained from these simulations in **R-Y** Theory to study the properties of particles in the solid liquid interface.

Bibliography

[1] T. V. Ramakrishnan and M. Yussouff. First-principles order-parameter theory of freezing. 1979. URL https://journals.aps.org/prb/abstract/10.1103/PhysRevB.19.2775.

[2] A. D. J. Haymet and David W. Oxtoby. A molecular theory for the solid liquid interface. 1981. URL http://aip.scitation.org/doi/abs/10.1063/1.441326.

[3] T. Sri Krishna Yasaswi. Estimation of correlation function for a 2 dimensional fluid in the presence of substrate potential. May 2015.