In contrast to equilibrium systems, seeking a statistical mechanics description and a corresponding thermodynamics picture for non-equilibrium system is still an unresolved issue. Many experiments, both practical and simulative, have been carried out to investigate its properties. Yet, a general framework to describe non-equilibrium system is still far from obtainable. In this project, numerical simulations have been made on a drive-diffusive lattice gas model contacting with a fixed chemical potential equilibrium system. The geometry of the contact area between the two systems is believed to be a crucial factor on the final steady state of the system.

Introduction

The driven lattice gas model was originally proposed to simulate ionic conduction system [1]. The model has then been widely used as a prototype to investigate non-equilibrium system. Many surprising and non-trivial behaviors have been discovered about this system and also its extensions [2, 3, 4]. The lattice is assumed to be connected to a heat bath. With a presence of driving field, the particles in the system have a preference to jump along the direction of the field. This leads to an unequal transition rate for particle’s jumping, and thus produces a flux of particle moving along the field direction. The detailed balance is broken so that the usual equations/laws for thermodynamics do not hold in this system anymore.

This project followed the earlier work by P. Pradhan, R. Ramsperger and U. Seifert, in order to investigate the possibility of zeroth law of thermodynamics in non-equilibrium system [5]. In their simulation, a driven lattice gas system was allowed to touch with an equilibrium lattice gas system by defining a contacting area among the two systems. The density of the equilibrium system was fixed so that it acted as a particle reservoir. The chemical potential of the particle reservoir is known to be determined from its density. The temperature of the heat bath was higher than the critical temperature, the system was then set into disorder state and so the ordering of the particles were not a concern in this project. Also, periodic boundary condition is imposed in this case.

In their simulation, the role of the contact area between the two systems was not well justified. It was found in many literatures that the correlation in longitudinal and transverse direction is different [6, 7]. The long range parallel correlation is positive while the transverse correlation showed an anti-correlation. The particles in the contact area are interacting with the system through the correlation of the particles around them, so this discrepancy in correlation will possibly lead to a different exchange rate of particles between the two systems and thus a steady state with different density. It was found that the power law decay in long range correlations is a common feature in many different types of non-equilibrium system [8]. Equilibrium system is actually a special case where the correlation decays exponentially. Therefore, equilibrium system can be divided into a smaller subsystem without changing its
macroscopic properties. This feature, however, is not generally true in non-equilibrium system. Any small change in the contact point between two non-equilibrium systems would propagate and spread to the whole system, and should have a decisive effect on the final steady state. In our simulation, the geometry of the contact area is varied. The first simulation was carried out with the contact area in rectangle shape, with the longer sides parallel to the driving field. The same contact area and shape were used in the second simulation, but this time, the longer side was perpendicular to the transverse field. This should have a small, but observable effect on the final steady state.

Result and Discussion

It was found that the increase of strength of driving field leads to a drop of density in attractive interaction case, but an increase or decrease of density in repulsive case, depending on the value of other parameters ( etc. chemical potential of the particle reservoir, interaction strength). The main reason for the change of density was the suppression of nearest neighbor interaction. The drive acts as an extra noise in breaking bonds, so that the effective strength of the nearest neighbor coupling is reduced. The paper by C.Hill, R.K.P.Zia and B.Schmittmann [6] provides an insight on how the driving field changes the correlation of particles among the system.

It was then successfully shown that there was a discrepancy between the two steady state systems of different geometry of contact area. The final steady state density was found to be higher when the contact area is perpendicular to the driven field. Yet, the determining factors, which leads to the result that the perpendicular case has a higher density than the parallel case, were still unknown.

Conclusion

It was shown that the contact dynamics will have a small impact on the final steady state when two systems, if at least one of it is in non-equilibrium, are allowed to exchange particles. Therefore, a complete description should include the contact mechanism if non-equilibrium system is allowed to contact with other systems in experiments. A more rigorous simulation can be done to obtain a more reliable and accurate result. The jamming effect of the system is not possible to be eliminated, and has to be carefully examined of its role in the mechanism [9]. Also, the choice of transition rule was found to have a crucial effect on the correlation [10, 11], and so possibly also on the finally steady state in this experiment. The same procedure can be repeated on two steady systems in contact to further investigate the properties of contact dynamics. A more general approach to determine the final steady state is still being searched by physicists [12, 13, 14]. Variational principle on entropy production rate was proposed as one of the possible methods [15, 16]. Also, a simpler model can be designed to investigate further the role of the contact dynamics on other steady state behaviors, for instance, the shift of critical temperature. Last but not least, the finite size effect is very important in statistical mechanic system simulation, but this was not well examined due to the limitation of time.
1. "Nonequilibrium steady states of stochastic lattice gas models of fast ionic conductors" Sheldon Katz, Joel L. Lebowitz and Herbert Spohn


5. "Approximate thermodynamic structure for driven lattice gases in contact" Punyabrata Pradhan, Robert Ramsperger, and Udo Seifert


7. "Long range correlations for stochastic lattice gases in a non-equilibrium steady state" Herbert, Spohn

8. "Long-range correlations for conservative dynamics" P. Garrido, J. Lebowitz, C. Maes, H. Spohn


10. "A remark on the choice of stochastic transition rates in driven non-equilibrium systems" Hal Tasaki


12. “Intensive thermodynamic parameters in non-equilibrium systems” Eric Bertin, Kirsten Martens, Olivier Dauchot and Michel Droz

13. “The large deviation approach to statistical mechanics” Hugo Touchette

14. “The steady state distribution of the master equation” Mitsusada M Sano

15. “Entropy Production in Non-equilibrium Systems at Stationary States” Tania Tome and Mario J. de Oliveira