Short-time behaviour of the two-dimensional hard-disk model

A. Jaster

Universität - GH Siegen, D-57068 Siegen, Germany

Abstract

Starting from the ordered state, we investigate the short-time behaviour of the hard-disk model. For the positional order, we determine the critical exponents $\eta$ and $z$ from the dynamic relaxation of the order parameter and the cumulant with molecular dynamics simulations. The results are compared with previous Monte Carlo (MC) simulations. The bond orientational order is studied with MC dynamics.

Key words: Hard-disk model; short-time dynamics; critical phenomena

PACS: 64.60.Ht, 82.20.Mj, 05.70.Jk, 64.70.Dv

1 Introduction

For a long time it was believed that universal scaling behaviour can be found only in the long-time regime. Therefore, numerical simulations were performed in the thermodynamic equilibrium. Such simulations in vicinity of the critical point are affected by the critical slowing down. However, recently Janssen, Schaub and Schmittmann [1] showed that universality exists already in the early time of the evolution. They discovered that a system with non-conserved order parameter and energy (model A) quenched from a high temperature state to the critical temperature shows universal short-time behaviour already after a microscopic time scale $t_{\text{mic}}$. Starting from an unordered state with a small value of the order parameter $m_0$, the order increases with a power law $M(t) \sim m_0 t^\theta$, where $\theta$ is a new dynamic exponent. A number of Monte Carlo (MC) investigations [2–4] support this short-time behaviour. These simulations can be also used to calculate the conventional (static and dynamic) exponents as well as the critical point [5]. This may eliminate critical slowing down, since the simulations are performed in the short-time regime.

First simulations of the dynamic relaxation in the short-time regime started from an unordered state. However, short-time dynamical scaling can be also
found starting from the ordered state \((M(t = 0) = 1)\). There exist no analytical calculations for this situation, but several MC simulations were done [6,7,2]. Also, all critical exponents, except for the new exponent \(\theta\), can be calculated starting from the ordered state. Up to now, simulations of the dynamic relaxation have only been performed with MC dynamics. Normally, molecular dynamics (MD) simulations can cause ergodicity problems, since the energy of the system is conserved. However, for the two-dimensional hard-disk model the potential energy of the allowed configurations does not depend on the positions of the particles, but is constant. Therefore, the restriction of energy conservation does not lead to a reduction of possible configurations.

The nature of the two-dimensional melting transition is a longstanding puzzle [8,9]. The Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory [10] predicts two continuous phase transitions. The first transition (dislocation un-binding) at the melting temperature \(T_m\) transforms the solid with quasi-long-range positional order and long-range orientational order into a new hexatic phase that possesses short-range positional order and quasi-long-range orientational order. The disclination unbinding transition at \(T_i\) transforms this hexatic phase into an isotropic phase in which the positional and orientational order are short-range. There are several other theoretical scenarios for the melting transition in two dimensions [8]. Most of them predict a first-order phase transition from the solid to the isotropic phase with a coexistence region instead of a hexatic phase.

Even for the simple hard-disk system no consensus about the nature of the melting transition has been established. A large number of simulations of the two-dimensional hard-disk model in the thermodynamic equilibrium have been performed. A melting transition was first seen in a computer study by Alder and Wainwright [11]. They investigated 870 disks with MD methods (constant number of particles \(N\), volume \(V\) and energy \(E\)) and found the transition to be first order. However, the results of such a small system are affected by large finite-size effects. Recent simulations used MC techniques either in the \(NVT\) ensemble (constant volume) [12–15] or the \(NpT\) ensemble (constant pressure) [16,17]. Unfortunately, the results of these simulations are not compatible.

In this article, we study the short-time behaviour of the two-dimensional hard-disk model starting from the ordered state (perfect crystal). First we examine the positional order parameter \(\psi_{\text{pos}}(t)\) and the cumulant \(\tilde{U}_{\text{pos}}(t)\) with MD simulations. The power law behaviour of these observables is used to determine the critical exponents \(\eta\) and \(z\). The results are compared with those of a previous MC simulation [18]. In the second part we study the bond orientational order parameter \(\psi_{6}(t)\) and the cumulant \(\tilde{U}_{6}(t)\) with MC dynamics. All simulations are performed in a rectangular box with ratio \(2 : \sqrt{3}\), which is necessary for the ordered state, and with periodic boundary conditions. The disk diameter is set equal to one.
2 Positional order

The positional order parameter $\psi_{\text{pos}}$ can be computed via

$$\psi_{\text{pos}}(t) = \left| \frac{1}{N} \sum_{i=1}^{N} \exp(i \vec{G} \cdot \vec{r}_i(t)) \right|, \quad (1)$$

where $\vec{G}$ denotes a reciprocal lattice vector and $\vec{r}_i(t)$ is the position of particle $i$ at time $t$. $\vec{G}$ has a magnitude of $2\pi/a$, where $a = \sqrt{2}/(\sqrt{3} \rho)$ is the average lattice spacing. The direction of $\vec{G}$ is fixed to that of a reciprocal lattice vector of the perfect crystal (which are unique due to the boundary condition of a rectangular box of ratio $2 : \sqrt{3}$). The reason for fixing $\vec{G}$ is that large crystal tilting is not possible since we simulate only the short-time behaviour of the system.

MC simulations of the dynamic relaxation of systems with quasi-long-range order were performed for the 6-state clock model [19], the XY model [20,21], the fully frustrated XY model [3,21], the quantum XY model [22] and the hard-disk model [18]. However, no investigations exist for the relaxation with molecular dynamics. Independent of the dynamics, the scaling form of the second moment of the order parameter at or above $\rho_m$ is

$$\psi_{\text{pos}}^2(t, L) = b^{-\eta} \psi_{\text{pos}}^2(b^{-z}t, b^{-1}L), \quad (2)$$

where $b$ denotes the rescaling factor. This leads for sufficiently large $L$ to a power law time dependence of the form

$$\psi_{\text{pos}}^2(t) \sim t^{-\eta/z}. \quad (3)$$

From a finite-size scaling (FSS) analysis of the time-dependent cumulant

$$\tilde{U}_{\text{pos}}(t) = \frac{\psi_{\text{pos}}^4(t)}{(\psi_{\text{pos}}^2(t))^2} - 1, \quad (4)$$

one obtains

$$\tilde{U}_{\text{pos}}(t) \sim t^{d/z}, \quad (5)$$

where $d$ is the dimension of the system. One can use $\tilde{U}_{\text{pos}}(t)$ to determine the dynamic critical exponent $z$ and then, with $z$ in hand, the static exponent $\eta$ from the behaviour of $\psi_{\text{pos}}^2(t)$. 
In the following we simulate the hard-disk model with molecular dynamics at the melting density $\rho_m \approx 0.933$ [18] (the density is given as usual in reduced units) and in the solid phase ($\rho = 1.0$) to investigate the time evolution of $\psi_{\text{pos}}^2$ and $\tilde{U}_{\text{pos}}$. Since the positional order of the system is quasi-long-range, we expect to find a power law behaviour for $\rho \geq \rho_m$ as in the case of the MC study. Starting from the ordered state ($\psi_{\text{pos}} = 1$), i.e. from a perfect crystal with lattice spacing $a$, we release the system to evolve with molecular dynamics. Solving exactly the simultaneous classical equations of motion for hard-disks means in practice to calculate the next collision point of two particles and their new momenta. The initial components of the momenta are chosen randomly with a distribution proportional $\exp(p_i^2/2)$. Obviously, in the case of a hard-core potential a global change in the kinetic energy just leads to a rescaling of time. We use systems of $16^2$, $32^2$, $64^2$ and $128^2$ hard-disks and measure the observables up to $t = 6$ in time intervals of $\Delta t = 0.04$. The number of independent data sets ranges from $\mathcal{O}(150)$ for $N = 128^2$ to $\mathcal{O}(30000)$ for $N = 16^2$. Statistical errors are calculated by dividing the data into different subsamples. Systematic errors are estimated by least square fits of different system sizes and different time intervals, i.e. the exponent $c$ of the power law behaviour is calculated for each system in small intervals $[t_i, t_j]$. For large enough systems, $c$ is independent of the system size between $t_{\text{min}}$ and $t_{\text{max}}$. The microscopic time scale $t_{\text{min}}$ depends on the microscopic details, but is independent from the system size. In contrast to this, $t_{\text{max}}$ — the time when the system starts to show finite-size effects — scales with the number of particles.

In Fig. 1 we plot the time evolution of $\psi_{\text{pos}}^2$ at the melting density $\rho_m$ for different system sizes in a double logarithmic scale. The figure shows that the power law behaviour starts after a microscopic time scale $t_{\text{mic}}$ of approximately 0.16. For times up to 0.5 the difference between the systems with $64^2$ and $128^2$ hard-disks is negligible. We use these two systems and time intervals of $t = [0.2 \ldots 0.8]$ or smaller for the determination of the critical exponents. Power law fits for the different time intervals and system sizes lead to $\eta/z = 0.201(4)$. The situation in the solid phase at $\rho = 1.0$ is very similar and we get $\eta/z = 0.0695(25)$. To determine $z$ independently, we also measure the time evolution of the cumulant $\tilde{U}_{\text{pos}}$. As before the behaviour can be well described by a power law ansatz. From the slope we get $z = 1.04(3)$ at $\rho_m$, while the analysis for $\rho = 1.0$ yields $z = 1.06(3)$. Thus we get $\eta = 0.194(9)$ at $\rho = 0.933$ and $\eta = 0.0737(49)$ at $\rho = 1.0$, respectively. The values of $\eta$ coincide with the results from the dynamic relaxation with MC dynamics [18] (using the same methods) within statistical errors, as can be seen from Table 1. For comparison we also show the results obtained from conventional FSS [18]. The value of the dynamic critical exponent $z$ changes from $z \approx 2$ for MC dynamics to $z \approx 1$ for MD simulations. These are the usual values for local MC updating schemes — which can be understood as due to the ‘diffusion’ of the changes induced by the local updating — and MD simulations, respectively. The time when the system starts to show finite-size effects scales approximately with $L^z$ for MD.
Fig. 1. Second moment of the positional order parameter $\psi_{\text{pos}}^2$ as a function of time starting from the ordered state at $\rho = 0.933$. $\psi_{\text{pos}}^2(t)$ was calculated in time steps of $\Delta t = 0.04$, where we used MD simulations.

Simulations (as can be estimated from Fig. 1) as well as for MC investigations.

Our results show that the determination of the critical exponents in the short-time region can be done with molecular dynamics at least in the case of hard-core potentials. The disadvantage of the MD simulations compared to the MC investigations with the Metropolis algorithm is the scaling of CPU time with the number of particles. In the Metropolis algorithm the CPU time for a sweep is proportional to the number of particles $N$, i.e. a single step of a disk is independent of $N$. In the MD simulations the number of collisions during a fixed time interval $\Delta t$ scales also with $N$. However, the search for the next two

Table 1

The critical exponents $z$ and $\eta$ determined from the short-time behaviour of $\tilde{U}_{\text{pos}}(t)$ and $\psi_{\text{pos}}^2(t)$ with MD and MC dynamics [16] and the value of $\eta$ measured with FSS methods [16].

| $\rho$  | MD short-time | MC short-time | FSS   |
|---------|---------------|---------------|-------|
|         | $z$           | $\eta$       | $z$   | $\eta$       | $\eta$   |
| 0.933   | 1.04(3)       | 0.194(9)      | 2.01(2)| 0.199(3)      | 0.200(2) |
| 1.0     | 1.06(3)       | 0.0737(49)    | 2.06(4)| 0.0794(29)    | 0.0791(6) |
colliding disks is not independent of $N$. The CPU time for a naive algorithm scales with $N^2$, while an improved version yields a factor $N$. Therefore, also the improved MD algorithm leads to a poorer scaling behaviour as the MC version. However, the MD simulations not only enlarge the knowledge of dynamic relaxation but perhaps also offer a possibility to compare the results with experimental investigations.

3 Bond orientational order

The orientational order of the hard-disk system can be described by the bond orientational order parameter

$$
\psi_6 = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{N_i} \sum_{j=1}^{N_i} \exp(6i \theta_{ij}) .
$$

(6)

The sum on $j$ is over the $N_i$ neighbours of the particle $i$ and $\theta_{ij}$ is the angle between the particles $i$ and $j$ and an arbitrary but fixed reference axis. Two particles are defined as neighbours, if the distance is less than 1.4 times the average lattice spacing $a$. This definition is computationally less expensive than the precise determination with the Voronoi construction [23].

We examine the bond orientational order of the hard-disk model in the liquid regime at $\rho = 0.885$, in vicinity of the transition point $\rho_i \approx 0.899$ [15] at $\rho = 0.9$ and $\rho = 0.905$ and in the solid phase at $\rho = 0.94$. We measure the second moment of the order parameter $\psi_6^2$ and the cumulant $\tilde{U}_6$ as a function of time, where the MC dynamics is given by the Metropolis algorithm [24]. The new positions of the particles are chosen with equal probability within a circle centered about its original position. As before, we start the relaxation process from the perfect ordered crystal ($\psi_6 = \psi_{\text{pos}} = 1$). We use systems of $64^2$ and $128^2$ hard-disks and measure up to 10,000 MC sweeps.

In case of a KTHNY-like scenario $\rho_i$ is the beginning of the hexatic phase, i.e., the lower bond of the critical line which ends at $\rho_m$. Therefore, we expect a power law behaviour similar to Eq. (3) between $\rho_i$ and $\rho_m$ assuming a scaling behaviour of the form (2) for the positional order parameter. The value of the critical exponent $\eta_6$ (at $\rho = \rho_i$) is predicted with 1/4 [10] and was measured with 0.251(36) [15], while the value of the dynamic critical exponent $z$ for the local Metropolis algorithm is normally about two. For a conventional weak first-order phase transition the behaviour of the positional order parameter should be also approximately power-like.

Figure 2 shows the time evolution of $\psi_6^2$ for the different densities. Obviously, the time dependence in vicinity of $\rho_i$ can not be described by a simple power
law behaviour as expected. Therefore, the scaling form of the second moment of the order parameter $\psi_6^2$ is not given by (2). The behaviour of $\psi_6^2(t)$ at $\rho = 0.9$ and 0.905 is also not consistent with a simple weak first-order phase transition. The behaviour in the fluid phase ($\rho = 0.885$) is incompatible with both scenarios, since it is not of the form $t^{-\eta_6/z} \exp(-t/\xi_t)$ [25]. To rule out that the non power law behaviour is just an effect coming from our method determining neighbours, we also make simulations using the precise Voronoi definition. The result for $\psi_6^2(t)$ at $\rho = 0.9$ is visualized in Fig. 3. For small times the difference between both definitions is negligible. At larger times the number of disclinations increase and causes errors in case of using the distance for the determination of neighbours. Therefore, the deviation between the different values of $\psi_6^2$ grows if the time increases. However, also in case of using the Voronoi construction we find no power law dependence.

A possible explanation for the behaviour of $\psi_6^2(t)$ could be a mixing of the order parameters\footnote{A mixing of order parameters was also found for the Ashkin-Teller model [26].}. In the simplest case we expect that the behaviour should be described by the sum of two power law functions. However, we find that the the curves at $\rho = 0.9$ and $\rho = 0.905$ could not be fitted very well by such an ansatz. Nevertheless, we use the almost linear behaviour in the intervals $t_1 = [10, 100]$ and $t_2 = [1000, 10000]$ to determine the values of the exponents,
Fig. 3. Time evolution of the second moment of the bond orientational order parameter $\psi_6^2$ starting from the ordered state at $\rho = 0.9$. The solid curve is the same as in Fig. 2, i.e. neighbours are defined with the distance of the particles. The dashed line shows the behaviour that we obtained using the Voronoi construction for the determination of neighbours.

i.e. we examine if the behaviour in one of these intervals is consistent with a power law coming from the bond orientational order parameter. At $\rho = 0.9$ we get from $\psi_6^2(t)$ the exponent $c_1 = 0.124$ and 0.0264, respectively. The slope of the cumulant $\hat{U}_6(t)$ (which is shown in Fig. 4) gives the exponent $c_U$. This yields $z = 2.12, \eta = 0.262$ (for $t_1 = [10, 100]$) and $z = 4.95, \eta = 0.130$ (for $t_2 = [1000, 10000]$). The first value of $\eta$ is consistent with previous measurements of $\eta_6$ in equilibrium [15], while the value determined in the interval $t_2$ is too small. However, also the behaviour of $\psi_6^2(t)$ in the interval $t_1$ is inconsistent with (2) since the value is not constant in the solid phase. Thus, neither the behaviour in the time interval $t_1$ nor in the interval $t_2$ is compatible with the scaling form (2). Additionally, we try to estimate the dynamic critical exponent $z$ from the exponential behaviour the the fluid phase. But these measurements give also inconsistent results, i.e. we get a value $z \approx 1$. 
Fig. 4. Time dependent cumulant $\tilde{U}_6(t)$ at $\rho = 0.9$ for $N = 64^2$ and $N = 128^2$ for the Metropolis algorithm.

4 Conclusions

We investigated the short-time behaviour of the hard-disk model for the positional and bond orientational order. The positional order parameter was studied with MD simulations at $\rho_m$ and in the solid phase. We determined the critical exponent $\eta$ as well as the dynamic critical exponent $z$ from the power law behaviour of $\psi_{\text{pos}^2}(t)$ and $\tilde{U}_{\text{pos}}(t)$. The values of $\eta$ are in agreement with previous measurements. Our results show that MD simulations can be used for the determination of critical exponents from the short-time behaviour. The dynamic critical exponent changes from $z \approx 2$ for MC to $z \approx 1$ for MD simulations.

The bond orientational order was studied with conventional MC dynamics. The time evolution of the order parameter and the cumulant is not given by a simple power law behaviour, i.e. the scaling behaviour is not of the form (2). This phenomena could not be explained by a weak first-order phase transition or by the way of determining neighbours. A possible mixing of order parameter was discussed.
Acknowledgement

Critical comments by Lothar Schülke are gratefully acknowledged. Especially I benefitted from discussions with Conny Deiters. This work was supported in part by the Deutsche Forschungsgemeinschaft under Grant No. DFG Schu 95/9-1.

References

[1] H.K. Janssen, B. Schaub and B. Schmittmann, Z. Phys. B 73 (1989) 539.
[2] A review of short-time dynamics is given in: B. Zheng, Int. J. Mod. Phys. B 12 (1998) 1419.
[3] H.J. Luo, L. Schülke and B. Zheng, Phys. Rev. E 57 (1998) 1327; Phys. Rev. Lett. 81 (1998) 180.
[4] A. Jaster, J. Mainville, L. Schülke, B. Zheng, J. Phys. A: Math. Gen. 32 (1999) 1395.
[5] L. Schülke and B. Zheng, Phys. Lett. A 215 (1996) 81.
[6] D. Stauffer, Physica A 186 (1992) 197.
[7] Z.B. Li, L. Schülke and B. Zheng, Phys. Rev. E 53 (1996) 2940.
[8] K.J. Strandburg, Rev. Mod. Phys. 60 (1988) 161.
[9] M.A. Glaser and N.A. Clark, Adv. Chem. Phys. 83 (1993) 543.
[10] J.M. Kosterlitz and D.J. Thouless, J. Phys. C 6 (1973) 1181; J.M. Kosterlitz, J. Phys. C 7 (1974) 1046; B.I. Halperin and D.R. Nelson, Phys. Rev. Lett. 41 (1978) 121; A.P. Young, Phys. Rev. B 19 (1979) 1855.
[11] B.J. Alder and T.E. Wainwright, Phys. Rev. 127 (1962) 359.
[12] J.A. Zollweg and G.V. Chester, Phys. Rev. B 46 (1992) 11186.
[13] H. Weber and D. Marx, Europhys. Lett. 27 (1994) 593; H. Weber, D. Marx and K. Binder, Phys. Rev. B 51 (1995) 14636.
[14] A.C. Mitus, H. Weber and D. Marx, Phys. Rev. E 55 (1997) 6855.
[15] A. Jaster, Europhys. Lett. 42 (1998) 277; Phys. Rev. E 59 (1999) 2594.
[16] J. Lee and K.J. Strandburg, Phys. Rev. B 46 (1992) 11190.
[17] J.F. Fernández, J.J. Alonso and J. Stankiewicz, Phys. Rev. Lett. 75 (1995) 3477; Phys. Rev. E 55 (1997) 750.
[18] A. Jaster, Phys. Lett. A 258 (1999) 59.
[19] P. Czerner and U. Ritschel, Phys. Rev. E 53 (1996) 3333.

[20] K. Okano, L. Schülke, K. Yamagishi and B. Zheng, J. Phys. A: Math. Gen. 30 (1997) 4527.

[21] H.J. Luo and B. Zheng, Mod. Phys. Lett. B 11 (1997) 615.

[22] H.P. Ying, H.J. Luo, L. Schülke and B. Zheng, Mod. Phys. Lett. B 12 (1999) 1237.

[23] For a definition of Voronoi cell see: D.P. Fraser, M.J. Zuckerman and O.G. Mouritzen, Phys. Rev. A 42 (1990) 3186.

[24] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.

[25] A. Jaster, Phys. Lett. A 258 (1999) 177.

[26] Z.B. Li, X.W. Liu, Z.G. Pan and L. Schülke, 'Initial order mixing in the kinetic Ashkin-Teller model’, to be published in Communications in Theoretical Physics, International Academic Publishers, Beijing China.