The hexatic phase
of the two-dimensional hard disk system

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Abstract

We report Monte Carlo results for the two-dimensional hard disk system in the transition region. Simulations were performed in the NVT ensemble with up to $1024^2$ disks. The scaling behaviour of the positional and bond-orientational order parameter as well as the positional correlation length prove the existence of a hexatic phase as predicted by the Kosterlitz-Thouless-Halperin-Nelson-Young theory. The analysis of the pressure shows that this phase is outside a possible first-order transition.

Key words: Hard disk model, Two-dimensional melting, KTHNY theory

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The nature of the two-dimensional melting transition has been an unsolved problem for many years [1,2]. The Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory [3,4,5,6] predicts two continuous transitions. The first transition occurs when the solid (quasi-long-range positional order, long-range orientational order) undergoes a dislocation unbinding transition to the hexatic phase (short-range positional order, quasi-long-range orientational order). The second transition is the disclination unbinding transition which transforms this hexatic phase into an isotropic phase (short-range positional and orientational order). An alternative scenario has been proposed by Chui [7,8]. He presented a theory via spontaneous generation of grain boundaries, i.e. collective excitations of dislocations. He found that grain boundaries may be generated before the dislocations unbind if the core energy of dislocations is sufficiently small, and predicted a first-order transition. This is characterized by a coexistence region of the solid and isotropic phase, while no hexatic phase exists. Another proposal was given by Glaser and Clark [2]. They considered a detailed theory where the transition is handled as a condensation of localized, thermally generated geometrical defects and found also a first-order transition. Calculations based on the density-functional approach were done by Ryzhov and
Tareyeva [9]. They derived that the hexatic phase cannot exist in the hard disk system.

Even for the simple hard disk system no consensus about the existence of a hexatic phase has been established thus far. The melting transition of the hard disk system was first seen in a computer simulation by Alder and Wainwright [10]. They used a system of 870 disks and molecular dynamics methods (NVE ensemble) and found that this system undergoes a first-order phase transition. But the results of such small systems are affected by large finite-size effects. Simulations performed in the last years used Monte Carlo (MC) techniques either with constant volume (NVT ensemble) [11,12,13,14,15,16,17,18,19,20,21] or constant pressure (NpT ensemble) [22,23,24]. Zollweg, Chester and Leung [11] made detailed investigations of large systems up to 16384 particles, but draw no conclusions about the order of the phase transition. The analysis of Zollweg and Chester [12] for the pressure gave an upper limit for a first-order phase transition, but is compatible with all other scenarios. Lee and Strandburg [22] used isobaric MC simulations and found a double-peaked structure in the volume distribution. Lee-Kosterlitz scaling led them to conclude that the phase transition is of first-order. However, the data are not in the scaling region, since their largest system contained only 400 particles. MC investigations of the bond-orientational order parameter via finite-size scaling (FSS) with the block analysis technique of 16384 particle systems were done by Weber, Marx and Binder [13,14]. They also favoured a first-order phase transition. In contrast to this, Fernández, Alonso and Stankiewicz [23,24]¹ predicted a one-stage continuous melting transition, i.e. a scenario with a single continuous transition and consequently without a hexatic phase. Their conclusions were based on the examination of the bond-orientational order parameter of different systems up to 15876 particles and hard-crystalline wall boundary conditions. Mitus, Weber and Marx [15] studied the local structure of a system with 4096 hard disks. From the linear behaviour of a local order parameter they derived bounds for a possible coexistence region. Sengupta, Nielaba and Binder [16] simulated a dislocation free triangular solid of hard disks using a constrained Monte Carlo algorithm and showed that a KTHNY transition preempts a first-order transition. Combining renormalisation groups ideas with MC input they derived also an estimate of \( \rho_m = 0.914(2) \) for a possible hexatic-to-crystal transition [17]. Finally, in [18,19] the present author determined the disclination binding transition density \( \rho_i = 0.899(1) \) from measurements of the bond-orientational correlation length and susceptibility in the isotropic phase as well as the critical exponent \( \eta_6 = 0.25(4) \) from finite-size scaling of systems with up to 16384 particles. The results are in agreement with the KTHNY theory, while a first-order phase transition with small correlation length and a one-stage continuous transition can be ruled out. By studying short-time behaviour and FSS of the positional order [20,21] we also

¹ For a critical discussion of this work see Ref. [25,26].
estimated the dislocation binding density with $\rho_m \approx 0.933$ as well as the critical exponent $\eta \approx 0.200$.

In this letter, we present results obtained through MC simulations in the $NVT$ ensemble to answer the question of the existence of a hexatic phase and therefore the kind of the phase transition. Although we have already shown that the disclination binding density $\rho_i = 0.899(1)$ is lower than the dislocation binding density $\rho_m \approx 0.933$, no direct observation of the hexatic phase so far exists. Therefore, we examine the positional order as well as the orientational order within this region at $\rho = 0.914$ and $\rho = 0.918$. Simulations in the $NVT$ ensemble are computationally less expensive than in the $NpT$ ensemble. The density region is outside a possible first order transition thus there is no necessity to perform constant pressure simulations.

We consider systems of $N = 32^2$ up to $1024^2$ hard disks in a two-dimensional rectangular box with ratio $\sqrt{3} : 2$. Additionally, we studied three systems in a square box to determine the influence of boundary conditions. The disk diameter is set equal to one. For the simulations we used an improved updating scheme [27], in which the conventional Metropolis step of a single particle is replaced by a collective (non-local) step of a chain of particles.

Due to the improved updating scheme, which reduces autocorrelation times, we were able to perform simulations of large systems within the transition region. Although, the scaling behaviour is probably not changed compared to the Metropolis algorithm, the chain algorithm significantly speeds up the simulations. Especially in the hexatic phase with large positional order length, this algorithm is advantageous $^2$.

We measured the $k$th moment of the global bond-orientational order parameter

$$\psi_6^k = \left| \frac{1}{N} \sum_{i=1}^{N} \frac{1}{N_i} \sum_j \exp \left( 6 i \theta_{ij} \right) \right|^k,$$

where the sum on $j$ is over the $N_i$ neighbours of this particle 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 $1.4 a$, where $a = \sqrt{2/\sqrt{3} \rho}$ is the average lattice spacing of a perfect crystal. This definition is computationally less expensive than precise determination by the Voronoi construction. While the values of $\psi_6$ shown in table 1 depend on the definition of neighbours, the conclusions are independent of the method used.

$^2$ The chains or particles moved in a single step are much longer than those observed for $\rho = 0.898$ [27].
The $k$th moment of the positional order parameter is defined as
\begin{equation}
\psi_{\text{pos}}^k = \left| \frac{1}{N} \sum_{i=1}^{N} \exp(i \mathbf{G} \cdot \mathbf{r}_i) \right|^k,
\end{equation}
where $\mathbf{G}$ is a reciprocal lattice vector and $\mathbf{r}_i$ denotes the position of particle $i$. The magnitude of $\mathbf{G}$ is given by $2\pi/a$, while the orientation was determined from the global bond-orientation. With $\psi_6 \sim \exp(6i\theta)$ we defined the angle $\theta (-\pi/6 \leq \theta < \pi/6)$ and therefore the orientation of the crystal and $\mathbf{G}$. The fourth-order cumulant for the positional order is given by
\begin{equation}
U_{\text{pos}} = 1 - \frac{\langle \psi_{\text{pos}}^4 \rangle}{3 \langle \psi_{\text{pos}}^2 \rangle^2}.
\end{equation}

The bond-orientational correlation length $\xi_{\text{pos}}$ was extracted from the ‘zero-momentum’ correlation function of $\psi_{\text{pos}}(x)$
\begin{equation}
g_{\text{pos}}(x) = \left( \frac{1}{N_k} \sum_y \psi_{\text{pos}}(x, y) \right)^* \left( \frac{1}{N_k} \sum_{y'} \psi_{\text{pos}}(0, y') \right),
\end{equation}
by fitting the data with a single cosh, where $N_k$ denotes the number of particles in a stripe between $x + \Delta x/2$ and $x - \Delta x/2$ [19]. The pressure is calculated from the pair correlation function $g(r)$
\begin{equation}
\frac{pA_0}{NkT} = \frac{\sqrt{3}}{2} \rho \left( 1 + \frac{\pi}{2} \rho g(1) \right),
\end{equation}
where $A_0$ is the close-packed area of the system, i.e. $A_0 = N\sqrt{3}/2$.

All simulations of systems in the rectangular box started from the ordered state while we used a closed-packed state as initial condition in case of the square box. Careful attention has been paid to the equilibration of the systems. For that purpose we estimated autocorrelation times from binning.

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\textsuperscript{3} Disordered initial states for the hard disk model at high densities are more difficult to simulate and equilibration is more time consuming.

\textsuperscript{4} We built blocks of subsequent configurations, called bins, and averaged the quantities first in the bin. The obtained bin averages themselves can be considered as the results of single measurements. If the bins are large enough, then the average values in different bins are practically uncorrelated and the obtained statistical errors are correct. All given statistical errors are obtained in this way, i.e. taking correlations into account. This is also a way to estimate the autocorrelation time.
Table 1
The density of three and eight coordinated particles, the pressure, the second moment of the global bond-orientational and positional order parameter, the positional fourth-order cumulant and the positional correlation length for different densities, boundary conditions and system sizes.

| $\rho$ box | N | $n_3 \cdot 10^6$ | $n_8 \cdot 10^5$ | $\frac{N\Delta n}{NKT}$ | $\psi_6^2$ | $\psi_{pos}^2$ | $U_{pos}$ | $\xi_{pos}$ |
|------------|---|----------------|----------------|--------------------------|-----------|-----------|----------|-----------|
| 0.914 rect. | 128$^2$ | 3.76(15) | 4.33(15) | 7.921(6) | 0.5314(20) | 0.15(3) | 0.60(3) | 47(6) |
| 0.914 rect. | 256$^2$ | 4.29(4) | 5.11(4) | 7.968(3) | 0.5181(10) | 0.017(3) | 0.55(2) | 21(3) |
| 0.914 rect. | 512$^2$ | 4.34(4) | 5.21(4) | 7.975(3) | 0.5126(30) | 0.0026(8) | 0.53(2) | 15(3) |
| 0.918 rect. | 32$^2$ | 0.7(4) | 1.3(4) | 7.947(12) | 0.5711(30) | 0.41(4) | 0.66(1) | 17(10) |
| 0.918 rect. | 64$^2$ | 3.0(2) | 3.0(1) | 8.022(5) | 0.5616(10) | 0.33(4) | 0.65(1) | 37(4) |
| 0.918 rect. | 128$^2$ | 3.4(2) | 3.3(1) | 8.050(4) | 0.5558(12) | 0.147(12) | 0.64(1) | 49(4) |
| 0.918 sq. | 128$^2$ | 2.8(1) | 2.8(1) | 8.019(5) | 0.5612(9) | 0.183(8) | 0.65(1) | 52(10) |
| 0.918 rect. | 256$^2$ | 2.7(3) | 2.9(2) | 8.021(10) | 0.5608(16) | 0.117(25) | 0.64(1) | 110(35) |
| 0.918 sq. | 256$^2$ | 3.0(1) | 3.0(1) | 8.029(5) | 0.5592(20) | 0.087(20) | 0.65(1) | 88(30) |
| 0.918 rect. | 512$^2$ | 3.1(1) | 3.1(1) | 8.034(3) | 0.5579(10) | 0.0095(20) | 0.55(3) | 32(8) |
| 0.918 sq. | 512$^2$ | 3.0(1) | 3.1(1) | 8.038(5) | 0.5563(14) | 0.0061(17) | 0.55(4) | 32(6) |
| 0.918 rect. | 1024$^2$ | 3.1(1) | 3.2(1) | 8.041(7) | 0.5561(15) | 0.0020(3) | 0.54(3) | 37(4) |

Table 2
Estimated integrated autocorrelation time measured in units of thousand sweeps of the chain Metropolis algorithm. We used different (optimized) step sizes for each density.

| $\rho$ box | N | $n_3$ | $n_8$ | $\frac{N\Delta n}{NKT}$ | $\psi_6^2$ | $\psi_{pos}^2$ |
|------------|---|--------|--------|--------------------------|-----------|-----------|
| 0.914 rect. | 256$^2$ | <1 | <1 | <1 | 32 | 54 |
| 0.918 rect. | 512$^2$ | <1 | <1 | <1 | 59 | 270 |

Additionally, two systems were studied in detail, i.e. we monitored all quantities and measured the autocorrelation times. We used the defect density as an estimate for the equilibration of dislocations. The results are given in table 2. The autocorrelation times are much smaller than the number of warm-up sweeps, which were at least one million. The number of measurement sweeps ranged from 2 to 20 millions.

For a hexatic phase — as predicted by the KTHNY theory — FSS implies $\psi_6^2 \sim L^{-\eta_6}$ for the orientational order parameter, while the positional order parameter should scale with $\psi_{pos}^2 \sim L^{-2}$ for large enough system sizes ($L \gg \xi_{pos}$). The cumulant $U_{pos}$ should decrease with increasing system size $L$ for $\rho < \rho_m$. 

We measure $\psi_6^2$, $\psi_{\text{pos}}^2$, $U_{\text{pos}}$, $\xi_{\text{pos}}$ and $pA_0/NKT$ as well as the density of three ($n_3$) and eight coordinated particles ($n_8$)\(^5\). We use systems of $N = 32^2, 64^2, 128^2, 256^2, 512^2$ and $1024^2$ particles. All results are given in table 1. Statistical errors have been calculated by binning. We also added systematic errors coming from the interpolation to $g(1)$ for the pressure as well as errors coming from the interval used for fitting in case of the correlation length. Simulations of the hard disk system are not only affected by usual finite-size effects, but also by systematic errors coming from the boundary conditions. Even for a rectangular box of ratio $\sqrt{3}:2$ and (quasi-) long-range order crystal tilting occurs. This leads to large autocorrelation times as well as additional, complicated finite-size effects compared to simple lattice models.

The pressure and positional correlation length at $\rho = 0.918$ are nearly independent for system sizes with $N \geq 64$. The results of $n_3$ and $n_8$ for $N = 32^2$ show the suppression of defects for systems that are too small. Leaving out the data for $N = 32^2$ the results at $\rho = 0.918$ seem to be mostly consistent. The results for $\psi_6^2$ and $\psi_{\text{pos}}^2$ are shown in fig. 1. Obviously, the orientational order is (quasi-) long-range, while the positional order is short-ranged\(^6\) which is confirmed by the decrease of $U_{\text{pos}}$. Deviations are caused by statistical errors coming from large autocorrelation times and systematic errors due to boundary conditions. For example, the increase of $\psi_6^2$ for lower system sizes ($N = 32^2$) and rectangular boundary conditions is caused by stabilization effects. The (quasi-) long-range of the orientational order is consistent with previous measurements \cite{19} where $\rho_i = 0.899(1)$ was determined. The measurements at $\rho = 0.914$ confirm the short-range positional order in this range.

Although, the results should be independent from the initial conditions, our data can differ due to the different boundary conditions used. However, the data should converge for increasing system sizes. Also, for larger systems the correlation length, which is direction dependent for smaller systems, should be isotropic.

A visualisation of the orientational order for a typical configuration at $\rho = 0.918$ with $N = 1024^2$ particles in the rectangular box is shown in fig. 2a and b. We divided the system into $380^2$ subsystems with approximately 7 particles per subsystem and calculated $\psi_6^k$ averaged over the particles inside. The left picture visualises the local orientation. The initial state of a perfect ordered crystal ($\theta = 0$) corresponds to white areas. Areas with $|\theta| > 0$ are grey, where

\(^5\) These values are obtained from the definition for neighbours given above.

\(^6\) We carefully tried to equilibrate the systems. The measurements of the correlation time shows that the only critical point is $N = 1024^2$. However, even a too short equilibration time for the largest system wouldn’t affect our conclusions. The reason is that due to the initial ordered state for the rectangular boxes, a non-equilibrated system would lead to too high values for the order parameter, i.e. the decrease of $\psi_{\text{pos}}^2$ for increasing system sizes would be even larger.
Fig. 1. Double logarithmic plots of the second moment of the bond-orientational (left figure) and the positional order (right figure) parameter at $\rho = 0.918$ as a function of $\sqrt{N}$, which is proportional to the system size $L$. Full symbols are for the rectangular box while open symbols denote square boxes. The lines are guides for the eye.

Fig. 2. Visualisations of the local bond-orientational order parameter $\psi_6$ of a typical configuration with $1024^2$ particles in a rectangular box. In the left picture the amount of black represents the local orientation. White areas correspond to the initial orientation of the perfect ordered system ($\theta = 0$). The larger the absolute value of $\theta$, the darker the areas. The right picture shows the degree of order, i.e. the local value of $0 \leq \psi_6^2 \leq 1$ is visualised. White areas correspond to perfect ordered areas.

the amount of black is proportional $|\theta|$. The case $|\theta| = \pi/6$ corresponds to black regions. The right picture shows the local order, i.e. the amount of black is chosen proportional to $1 - \psi_6^2$. Thus, the initial state of a perfect ordered crystal corresponds to a white area. The two pictures show that areas with orientations significant different from $\theta = 0$ are normally small, i.e. have less than 100 particles.

Our simulations of the hard disk model in the $NVT$ ensemble at $\rho = 0.914$ and $\rho = 0.918$ prove the short-range of the positional order and therefore the existence of a hexatic phase as predicted by the KTHNY theory. The positional correlation length is about 15 at $\rho = 0.914$ and 40 at $\rho = 0.918$, respectively. The orientational order is quasi-long-range. The scaling of $\psi_6^2$ yields $\eta_6 \approx 0.015$ at $\rho = 0.914$ and $\eta_6 = 0.005(3)$ at $\rho = 0.918$, respectively. However, we cannot rule out long-range orientational order. The observed
phase is not within a possible first-order phase transition since the pressure 8.04(1) at \( \rho = 0.918 \) is higher than that of such a transition 7.95(1) [19]. Therefore, a one-stage continuous transition [23,24] as well as a first-order phase transition from the isotropic to the solid phase can be ruled out. Taking the results of previous measurements [18,19] a KTHNY-like phase transition is most likely. However, a first-order phase transition from the isotropic to the hexatic phase with very large orientational order correlation lengths cannot be ruled out. Detailed investigations of the pressure around \( \rho_i \) would be necessary to make a decision. Also, the exact value of \( \rho_m \) and therefore of \( \eta \) as well as the behaviour of \( \eta_6 \) — which should approach zero according to the KTHNY theory — have to be examined in order to reach a final conclusion as to the question of the kind of transition.

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