Orientational order of the two-dimensional hard-disk system

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Abstract. – We report Monte Carlo results for the two-dimensional hard-disk system. Simulations were performed in the NVT ensemble with up to 65 536 disks, using a new updating scheme. We analyze the bond orientational order parameter and correlation length in the isotropic phase and the scaling behaviour of the bond orientational order parameter in the transition region. The data are consistent with predictions of the Kosterlitz-Thouless-Halperin-Nelson-Young theory, while a first-order phase transition is unlikely and a one-stage continuous transition can be ruled out.

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] 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). There are several other theoretical approaches for the transition. One alternative scenario has been proposed by Chui [4]. He presented a theory via spontaneous generation of grain boundaries, i.e. collective excitations of dislocations, and predicted a conventional first-order phase transition from the solid to the isotropic phase. In this case there exists a region where both phases coexist instead of a hexatic phase. Even for the simple hard-disk system no consensus about the existence of a hexatic phase has been established.

The melting transition of the hard-disk system was first seen in a computer simulation by Alder and Wainwright [5]. They used a system of 870 disks and molecular-dynamics methods (constant volume \( V \), energy \( E \) and number of particles \( N \) simulations) 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. Recent simulations used Monte Carlo (MC) techniques either with constant volume (NVT ensemble) [6], [7] or constant pressure (NpT ensemble) [8], [9]. Lee and Strandburg [8] 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 with the block analysis technique of 16 384-particle systems
were done by Weber, Marx and Binder [7]. They also favoured a first-order phase transition.
In contrast to this, Fernández, Alonso and Stankiewicz [9] predicted a one-stage continuous
melting transition, i.e. a scenario without a hexatic phase. Their conclusions were based on the
examination of the bond orientational order parameter in very long runs of different systems
up to 15 876 particles and hard-crystalline wall boundary conditions. The analysis of Zollweg
and Chester [6] for the pressure gave an upper limit for a first-order phase transition, but is
compatible with all other scenarios.

In this letter, we present results obtained through MC simulations in the NVT ensemble

to answer the question of the kind of the phase transition. We consider systems of
$N = 32^2$, $64^2$, $128^2$ and $256^2$ hard disks in a two-dimensional square box. We find that finite-size effects
with these boundary conditions are not substantially larger than in a rectangular box with
ratio $\sqrt{3}:2$, furthermore no simulations in the solid phase were made. The disk diameter is
set equal to one. For the simulations a new updating scheme was developed [10], in which the
conventional Metropolis step of a single particle is replaced by a collective (non-local) step of
a chain of particles. A cell structure was chosen such that one cell can only be occupied by
a single disk. In all updatings, the random number generator proposed by Lüscher [11] was
applied. The simulations were performed on a Silicon Graphics workstation and a CRAY T3E.
In the latter case, we used the different nodes of the parallel machine to generate independent
data sets. Statistical errors have been calculated by binning. Additionally, we performed a
jackknife analysis of the different data sets from the different nodes. Careful attention has
been paid to the equilibration of all systems. For example, we performed $3 \times 10^5$ “sweeps”
for $N = 256^2$ at $\rho = 0.890$ with the improved (chain) metropolis updating scheme to warm
up the system and $1.9 \times 10^6$ “sweeps” to measure the expectation values (for 6 independent
data sets). The acceptance rate for this run was about 54%. Further details will be published
later [12].

Simulations were performed in the isotropic phase and in the phase transition region. In
the isotropic phase we measured the (global) bond orientational order parameter $\psi_6$ and the
correlation length of the bond orientation $\xi_6$. The local value of $\psi_6$ for a particle $i$ located at
$x = (x, y)$ is given by

$$
\psi_6(x) = \frac{1}{N_i} \sum_j \exp[6i \theta_{ij}],
$$

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. Neighbours are obtained in a usual
way by the Voronoi construction. The (global) bond orientational order parameter is just the
absolute value of the average over all particles:

$$
\psi_6 = \left| \frac{1}{N} \sum \psi_6(x) \right|.
$$

The bond orientational correlation length was extracted from the “zero-momentum” correlation
function of $\psi_6(x)$

$$
g_6(x) = \left< \left( \frac{1}{N_k} \sum_y \psi_6(x, y) \right)^* \left( \frac{1}{N_k} \sum_{y'} \psi_6(0, y') \right) \right>.
$$
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 \( x - \Delta x/2 \). This method allows a precise measurement of \( \psi_6 \) apart from some systematical errors, which will be large —compared to our statistical errors— for small values of \( \xi_6 \) (for details see [12]). Additionally, we calculated the radial bond orientational correlation function

\[ g_6(r) = \langle \psi_6^*(0) \psi_6(r) \rangle / g(r), \tag{4} \]

and extracted the correlation length from an Ansatz of the form \( g_6(r) \sim r^{-1/2} \exp[-r/\xi_6] \), where \( g(r) \) is the pair correlation function. In all simulations of the isotropic phase we used systems of at least \( N = 64^2 \) particles and chose the box length to satisfy \( L > 7 \xi_6 \). In these cases, within statistical errors, we found no finite-size effects on the bond orientational correlation length and on the susceptibility

\[ \chi_6 = N \langle \psi_6^2 \rangle . \tag{5} \]

Equation (5) differs from \( \chi_6 = N(\langle \psi_6^2 \rangle - \langle \psi_6 \rangle^2) \) by a factor \( 1 - 2/\pi \) in the thermodynamic limit. Due to the new updating scheme, which reduces the autocorrelation time, we were able to perform simulations with large correlation lengths, namely close to the disclination binding transition point \( \rho_i \).

The KTHNY scenario predicts an exponential singularity for the correlation length

\[ \xi_6(t) = a_\xi \exp \left[ b_\xi t^{-1/2} \right] \tag{6} \]

and the susceptibility \( \chi_6 \)

\[ \chi_6(t) = a_\chi \exp \left[ b_\chi t^{-1/2} \right] \tag{7} \]

if \( t = \rho_i - \rho \to 0^+ \). The critical exponent \( \eta_6 \), defined by

\[ \chi_6 \sim \xi_6^{2-\eta_6} \tag{8} \]

is given by \( \eta_6 = 1/4 \), while \( b_\chi \) is a non-universal constant and

\[ b_\chi = (2 - \eta_6)b_\xi . \tag{9} \]

We analyzed the critical behaviour of \( \xi_6 \) and \( \chi_6 \) by performing least-square fits according to eqs. (6) and (7). Typically, statistical errors of \( \xi_6 \) and \( \chi_6 \) are in the range \( 1\%-5\% \). Errors for the fitting parameter were computed by performing fits on data sets being Gaussian distributed around the expectation value. If we used all 12 different measurement points with \( 0.82 \leq \rho \leq 0.89 \) we got a \( \chi^2/d.o.f. = 0.75 \) for \( \xi_6(t) \) and 0.65 for \( \chi_6(t) \), i.e. the data are in very good agreement with an exponential singularity of the KTHNY type. The critical values of \( \rho \) were given by \( \rho_i = 0.9017(7) \) and 0.9002(3), respectively. The results for the susceptibility are shown in fig. 1. Data far away from the transition (in particular for the correlation length) are affected by systematical errors. Therefore, fits were also performed omitting some data at low densities. For example, for the eight points with \( 0.855 \leq \rho \leq 0.89 \) (for \( \xi_6 \geq 3.0 \)) we got \( \chi^2/d.o.f. = 0.23 \) and \( \rho_i = 0.9006(8) \) for \( \xi_6(t) \) and \( \chi^2/d.o.f. = 0.58 \), \( \rho_i = 0.9000(4) \) for \( \chi_6(t) \). The critical exponent \( \eta_6 \) is calculated using eq. (9), yielding \( \eta_6 = 0.451(21) \) and 0.349(44), respectively. A detailed analysis shows that the value of \( \eta_6 \) decreases if \( t \to 0^+ \). This can be seen, if we use eq. (8) and plot \( \ln(\chi_6/\xi_6^{7/4}) \) vs. \( \ln(\xi_6) \). For the predicted value \( \eta_6 = 1/4 \) we should see a horizontal line. A different value of \( \eta_6 \) would correspond to a straight line with a non-zero slope. Indeed, there is a negative slope for small
Fig. 1. – Susceptibility as a function of the density. The curve shown is the best fit for a KTHNY behaviour. The critical value of \( \rho \) is visualized by a vertical line.

Fig. 2. – Test of the scaling relation \( \chi_6 \sim \xi_6^{7/4} \). The slope gives the deviation from \( \eta_6 = 1/4 \).

values of \( \xi_6 \), as can be seen in fig. 2. Nevertheless, in the limit \( \xi_6 \to \infty \) the data are compatible with \( \eta_6 = 1/4 \). A fit with the last six data points gives \( \eta_6 = 0.251(36) \).

We now come to the simulations with \( \rho \approx \rho_i \). Finite-size scaling (FSS) implies \( \chi_6 \sim L^{2-\eta_6} \) at \( \rho = \rho_i \) for large enough systems. For \( \rho < \rho_i \), corrections for finite correlation lengths of \( O(L/\xi_6) \) have to be taken into account. For \( \rho_i < \rho \leq \rho_m \), \( \eta_6 \) is a function of the density. As \( \rho \) approaches the melting density \( \rho_m \), i.e. at the end of the hexatic phase, \( \eta_6 \to 0^+ \). Figure 3 shows \( \ln(\chi_6/L^{7/4}) \) vs. \( \ln(L) \) for various \( \rho \). The slope was extracted from linear fits and gives the deviation from \( \eta_6 = 1/4 \). Using the FSS behaviour to locate \( \rho_i \), the requirement \( \eta_6(\rho_i) = 1/4 \) yields \( \rho_i = 0.899(1) \). This value is in agreement with that obtained from the singularities of \( \xi_6(t) \) and \( \chi_6(t) \). A slightly different value of \( \eta_6 \) would not alter this situation. Moreover, our

Fig. 3. – Finite-size scaling of the susceptibility for various densities. The slope gives the deviation from \( \eta_6 = 1/4 \). The lines are guides to the eye.
estimates of $\rho_i$ agree with Weber et al. [7] who used the fourth-order cumulant intersection ($\rho_i = 0.8985(5)$). However, it differs from their value obtained using the singularity of $\chi_6$ ($\rho_i = 0.913$). The result $\rho_i = 0.916(4)$ of Fernández et al. [9] is not compatible with our value.

Our MC data suggest that the orientational order behaves as predicted by the KTHNY theory. A one-stage continuous transition [9] can be ruled out, since $\rho_m \geq 0.910$ (obtained from $\eta(\rho_m) = 0$) is away from $\rho_i$ in this work. Also our data are not compatible with a first-order phase transition with small correlation lengths, since we find no deviation from the predicted singularities of $\chi_6$ and $\xi_6$ up to $\xi_6 \approx 38$. (Alternative approaches for the singularities result in large $\chi^2$/d.o.f. For example, a conventional second-order behaviour with a power law singularity of the form $\ln(\xi_6) = a - \nu \ln(t)$ yields $\chi^2$/d.o.f. = 4.1.) We have also examined FSS of the fourth-order cumulant $U = 1 - \langle \psi^4 \rangle^2/3(\psi^2)^2$. In the hexatic phase, FSS implies scale invariance of $U$. The narrowness of such a scale-invariant region was one argument in ref. [7] against the existence of a hexatic phase. Unfortunately, statistical errors in our data are too large to answer this question. Although our data cannot rule out a first-order phase transition with very large orientational order correlation lengths, a KTHNY-like phase transition seems to be more likely.

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