2D melting: Slowdown of equilibration

P. Hartmann, A. Derzsi, Z. Donkó
Institute for Solid State Physics and Optics, Wigner Research Centre, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary

Introduction:
The equilibrium solid-liquid phase transition in two dimensions is subject of ongoing controversy, largely enhanced by the application of computer simulations to this field since the 1970's. Serious independent studies concluded first-order, second-order, single step continuous and two-step continuous (KTHNY-like) phase transition for the same system. Recent simulations, using particle numbers in the 10^10 range, tend to support the two-step picture, where the solid and liquid phases are separated by a third, so called hexatic phase. Here we show, that simply increasing the particle number in particle simulations not necessarily results in more definite conclusions, the studied time domain needs to be extended as well, as thermalization of large systems takes longer.

The level of equilibration can be quantified in different ways, based on the velocity distribution, configurational properties, or correlation functions. In general we can expect from a system in thermal equilibrium that all observable quantities are stationary, exhibiting only fluctuations but no systematic time evolution. If we further assume Maxwell-Boltzmann type equilibrium (lowest order approach), quantitative measures can be defined based on the moments of the velocity distribution function.

The simulation:
We have performed classical molecular dynamics simulations using point particles interacting via the Yukawa pair potential
\[ \Phi(r) = \frac{G}{r^{\delta}}e^{-r/\lambda} \]
with a screening parameter \( \kappa = a/\lambda = 2 \). Periodic boundary conditions and rectangular simulations cells were applied. In the following we compare equilibration studies on systems with three different sizes between 2000 and 740000 particles.

Time is measured in units of the inverse nominal plasma frequency:
\[ \omega_p^2 = \frac{2\pi N e^2}{\varepsilon_0 \hbar a^2} \]
The simulations start from perfect hexagonal lattice configuration. Initial thermostat is realized by simple velocity back-scaling.

The time evolution of the different observed quantities is assumed to exponentially approach the equilibrium values, thus can be approximated in the form:
\[ y(t) = y_0 + A \exp \left( -t/\tau \right) \]
where \( \tau \) is the characteristic relaxation time.

Results:
1. Moments of the velocity distribution (N = 184400 & 7520):
The figure shows the value of the different moments of the measured velocity distribution function relative to the theoretical value derived from the Maxwell distribution. The initial velocities are uniformly sampled.

System size and temperature dependence could not be observed. The relaxation time was found to be \( \tau = 3.5 \) in all cases.

2. Configurational temperature:
At fixed system size (N = 184400) the relaxation time has a significant temperature dependence in the vicinity of the solid-liquid phase transition. A typical value of \( \tau_{eq} = 55 \) is found in the liquid near the phase transition, but it is expected to be sensitive to the specific form of the interaction potential.

At fixed temperature, on the other hand, the relaxation time does not show a significant system size dependence.

3. Long range correlations:
From point of view of the solid-liquid phase transition, the long-range behavior of the orientational and translational correlation functions are of fundamental importance. The following figures present the correlation functions measured during \( \tau_{eq} = 500 \); data collection was preceded by equilibration phases of different lengths, \( \tau_{eq} \) as indicated.

In large systems, which provide correlation data at long distances, the time needed for equilibration can be extremely long (several million simulation time-steps). Using long enough equilibration the power-law type decay approaches simple exponential type.

Conclusions:
During the equilibration of an interacting many-particle system we have identified three different stages of relaxation:
1. The velocity distribution does approach the Maxwellian distribution within a few plasma oscillation cycles. In the close vicinity of the melting transition the speed of this process is independent of temperature and system size.
2. The configurational temperature (determined by the local neighborhood within the range of the inter-particle interaction potential) relaxes at time scales about ten times longer. There is no significant system size, but strong temperature dependence of this process.
3. The equilibration of the long range correlations is significantly slower and does depend strongly on the system size (larger systems need longer time).

From this study we can conclude, that increasing the systems size in particle simulations alone (an attractive choice made possible by the rapid evolution of the computational resources) can be insufficient and can result in misleading conclusions, as additionally, the length of the equilibration period plays a crucial role in building up correlations.

Acknowledgements:
This work was supported by OTKA grants K-77653 and PD-75113