Irreversible Markov chains with fast mixing - Application to particle systems

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S. C. Kapfer, W. Krauth: Phys. Rev. Lett. 119, 240603 (2017)
Z. Lei, W. Krauth: EPL 121 10008 (2018)
Z. Lei, W. Krauth: EPL 124 20003 (2018)

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Metropolis et al (1953) 1/4

URNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUN

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

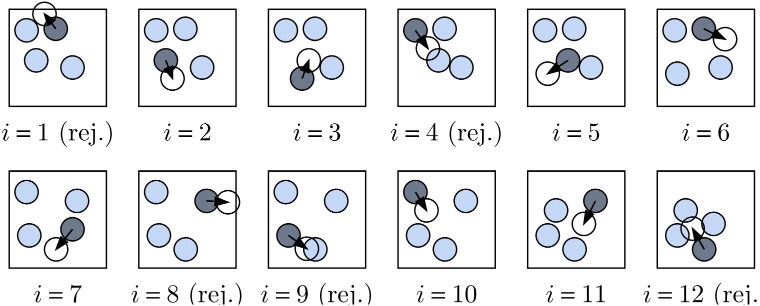
AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

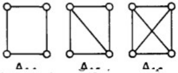
(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

Metropolis et al (1953) 2/4

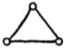


Metropolis et al (1953) 3/4



distinguished by primes. For example, A_{33} is given schematically by the diagram

$A_{3,3}$:



and mathematically as follows: if we define $f(r_{ij})$ by

$$f(r_{ij})=1 \quad \text{if} \quad r_{ij}<d,$$
$$f(r_{ij})=0 \quad \text{if} \quad r_{ij}>d,$$

then

$$A_{3,3}=\frac{1}{\pi^2 d^4}\int\cdots\int dx_1dx_2dx_3dy_1dy_2dy_3(f_{12}f_{23}f_{31}).$$

The schematics for the remaining integrals are indicated in Fig. 6.

The coefficients $A_{3,3}$, $A_{4,4}$, and $A_{4,5}$ were calculated

were put down at random, subject to $f_{12}=f_{23}=f_{34}=f_{15}=1$. The number of trials for which $f_{45}=1$, divided by the total number of trials, is just $A_{5,5}$.

The data on $A_{4,6}$ is quite reliable. We obtained

VI. CONCLUSION

The method of Monte Carlo integrations over configuration space seems to be a feasible approach to statistical mechanical problems which are as yet not analytically soluble. At least for a single-phase system a sample of several hundred particles seems sufficient. In the case of two-dimensional rigid spheres, runs made with 56 particles and with 224 particles agreed within statistical error. For a computing time of a few hours with presently available electronic computers, it seems possible to obtain the pressure for a given volume and temperature to an accuracy of a few percent.

In the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for $A/A_0<1.8$ and with a five-term virial expansion for $A/A_0>2.5$. There is no indication of a phase transition.

Alder Wainwright (1962)

PHYSICAL REVIEW VOLUME 127, NUMBER 2 JULY 15, 1962

Phase Transition in Elastic Disks*

B. J. ALDER AND T. E. WAINWRIGHT
University of California, Lawrence Radiation Laboratory, Livermore, California

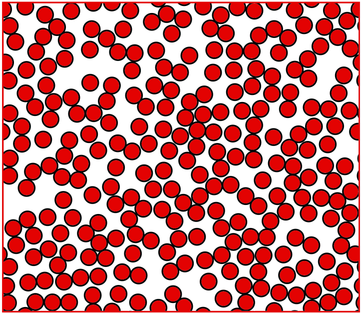
(Received October 30, 1961)

The study of a two-dimensional system consisting of 870 hard-disk particles in the phase-transition region has shown that the isotherm has a van der Waals-like loop. The density change across the transition is about 4% and the corresponding entropy change is small.

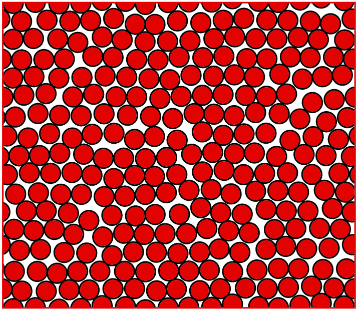
A STUDY has been made of a two-dimensional system consisting of 870 hard-disk particles. Simultaneous motions of the particles have been calculated by means of an electronic computer as described previously.[1] The disks were again placed in a periodically repeated rectangular array. The computer program interchanges it was not possible to average the two branches.

Two-dimensional systems were then studied, since the number of particles required to form clusters of particles of one phase of any given diameter is less than in three dimensions. Thus, an 870 hard-disk system is

$2D$ melting transition

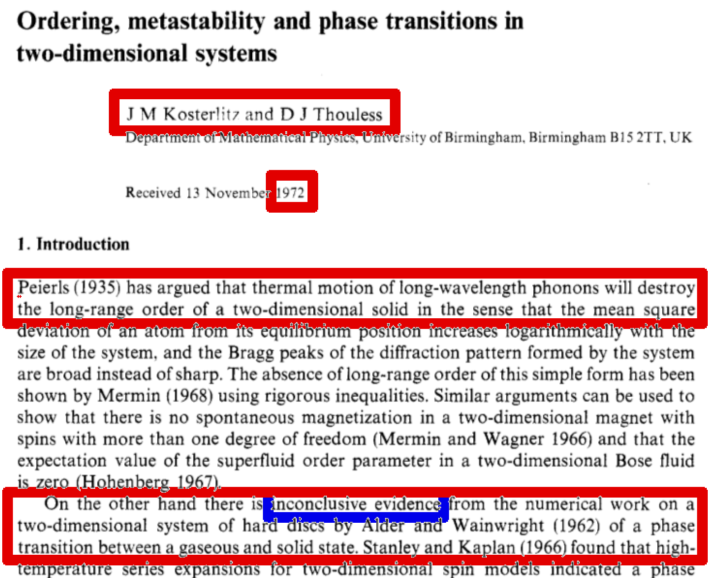


$\eta = 0.48$



$\eta = 0.72$

- Generic 2D systems cannot crystallize (Peierls, Landau 1930s) but they can turn solid (Alder & Wainwright, 1962).
- Nature of transition disputed for decades.


Ordering, metastability and phase transitions in two-dimensional systems

J M Kosterlitz and D J Thouless
Department of Mathematical Physics, University of Birmingham, Birmingham B15 2TT, UK

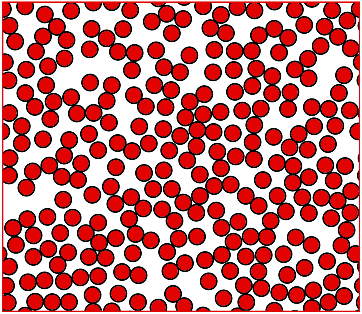
Received 13 November 1972

1. Introduction

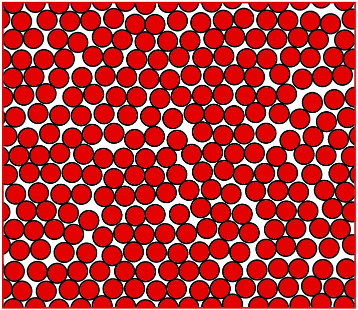
Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the diffraction pattern formed by the system are broad instead of sharp. The absence of long-range order of this simple form has been shown by Mermin (1968) using rigorous inequalities. Similar arguments can be used to show that there is no spontaneous magnetization in a two-dimensional magnet with spins with more than one degree of freedom (Mermin and Wagner 1966) and that the expectation value of the superfluid order parameter in a two-dimensional Bose fluid is zero (Hohenberg 1967).

On the other hand there is inconclusive evidence from the numerical work on a two-dimensional system of hard discs by Alder and Wainwright (1962) of a phase transition between a gaseous and solid state. Stanley and Kaplan (1966) found that high-temperature series expansions for two-dimensional spin models indicated a phase

Possible phases in two dimensions



$\eta = 0.48$



$\eta = 0.72$

Phase	positional order	orientational order
solid	algebraic	long-range
hexatic	short-range	algebraic
liquid	short-range	short-range

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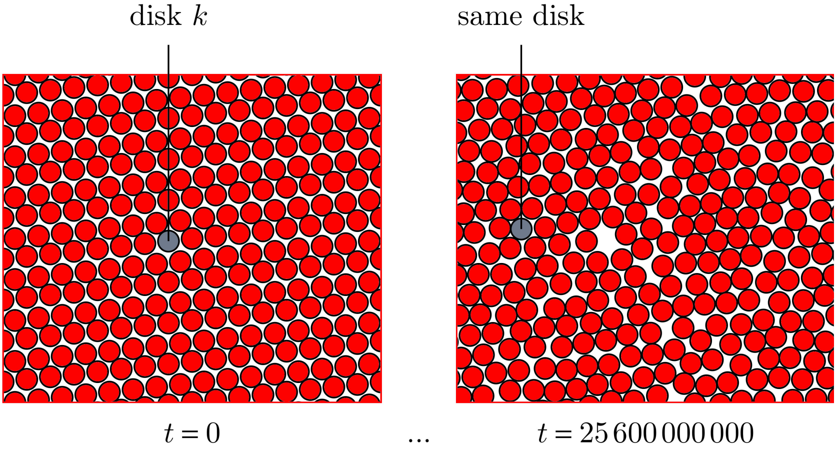
Correlation time in larger simulations



- τ exists, but it is large ($\tau \gg 25\,600\,000\,000$).

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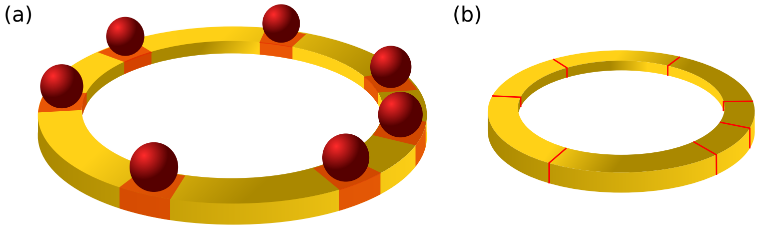
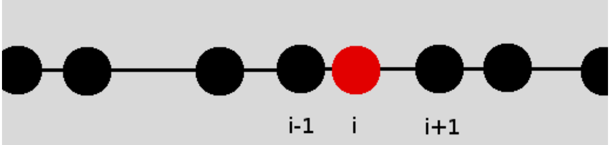
$1D$ $1d$ hard spheres with periodic boundary conditions



- N spheres, diameter σ, interval L, $\pi(a) = 1 \quad \forall a$
- N spheres, diameter 0, interval $L - N\sigma$.
- Equivalent if local moves (no change of order).

Reversible Metropolis algorithm, 1d (detailed balance)



- Local Metropolis: $x_i \to x_i + \text{ran}[-1, 1]$ (reject if overlap)
- Detailed balance:

$$\pi_a p(a \to b) = \pi_b p(b \to a)$$

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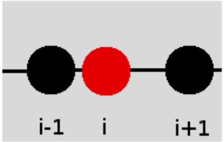
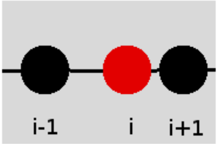
Reversible Metropolis algorithm, 1d (detailed balance)





- Local Metropolis: $x_i \to x_i + \text{ran}[-1, 1]$ (reject if overlap)
- Detailed balance:

$$\pi_a p(a \to b) = \pi_b p(b \to a)$$

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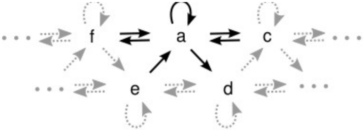
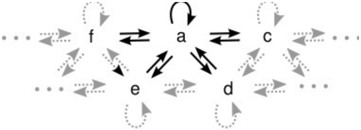
Detailed balance and global balance



global balance



detailed balance

$$\pi_a p(a \to b) = \pi_b p(b \to a) \quad \text{detailed balance}$$

$$\mathcal{F}_a \equiv \sum_b \pi_b p(b \to a) = \pi_a \quad \text{global balance}$$

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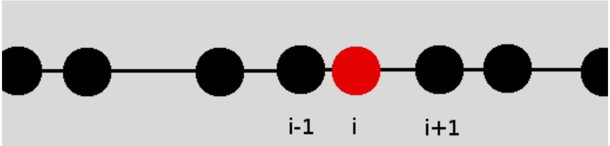
Reversible Metropolis algorithm



- Reversible Metropolis: $x_i \to x_i + \text{ran}[-1, 1]$ (reject if overlap)
- Global balance:

$$\mathcal{F}_a^{\text{rev}} = \frac{1}{2N} \sum_i \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_i^+ + \mathcal{A}_i^- + \mathcal{R}_i^-\right)}_{= 2 \text{ for any } \epsilon} = 1.$$

- NB: $\mathcal{A}_i^+(\epsilon) + \mathcal{R}_i^-(\epsilon) = 1$ also $\mathcal{A}_i^-(\epsilon) + \mathcal{R}_i^+(\epsilon) = 1$.

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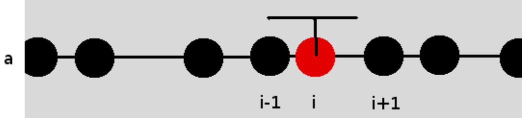
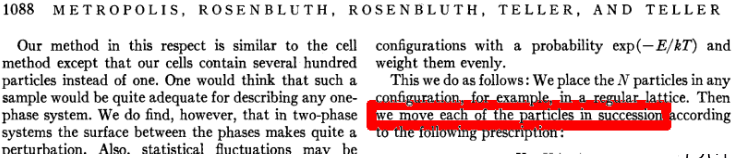
Sequential Metropolis algorithm



- Sequential Metropolis: Update 0, then 1, then 2, ...
- Global balance:

$$\mathcal{F}_a^{\text{seq}} = \frac{1}{2}\left(\mathcal{A}_i^+ + \mathcal{R}_i^+ + \mathcal{A}_i^- + \mathcal{R}_i^-\right) = 1.$$



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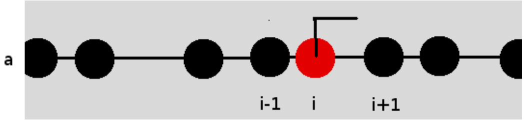
Our method in this respect is similar to the cell method except that our cells contain several hundred particles instead of one. One would think that such a sample would be quite adequate for describing any one-phase system. We do find, however, that in two-phase systems the surface between the phases makes quite a perturbation. Also, statistical fluctuations may be

configurations with a probability $\exp(-E/kT)$ and weight them evenly.

This we do as follows: We place the N particles in any configuration, for example, in a regular lattice. Then we move each of the particles in succession according to the following prescription:

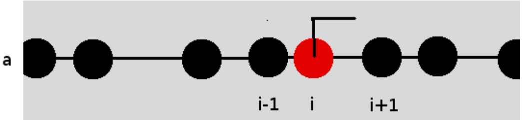
Forward Metropolis algorithm



- Forward Metropolis: $x_i \to x_i + \mathrm{ran}[0,1]$ (reject if overlap)
- $$\mathcal{F}_a^{\mathrm{forw}} = \frac{1}{N}\sum_i \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_{i-1}^+\right)}_{=1 \text{ for any } \epsilon} = 1,$$
- NB: Forward sequential Metropolis is wrong (but there is a variant that is OK)

Lifted Forward Metropolis algorithm (infinite chain)

- Move i forward until it is rejected by $i+1$.
- Then move $i+1$ forward until it is rejected, etc.



- $\mathcal{F}^{\text{lift}}_{(a,i)} = \mathcal{A}^{+}_{i} + \mathcal{R}^{+}_{i-1} = 1.$
- NB: 1 time step: 1 particle move OR 1 lifting move

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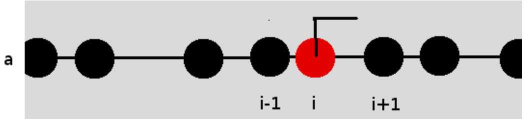
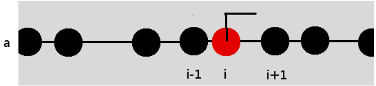
Lifted Forward Metropolis algorithm (with restarts)

- uniformly sample starting sphere i
- sample chain length $M \propto N$
- Then perform the lifted forward Metropolis algorithm



Infinitesimal Lifted Forward Metropolis algorithm ≡ event-chain algorithm

- In the lifted forward Metropolis, take $\epsilon \to 0$, $M \to \infty$, $\ell = \epsilon M \sim N\text{const}$



Synopsis (Irreversible Markov chains in 1d)

Algorithm	mixing	discrete analogue
Rev. Metropolis	$N^3 \log N$	Symmetric SEP
Forward Metropolis, Lifted (∞)	$N^{5/2}$	TASEP
Event-chain, Lifted (restarts)	$N^2 \log N$	lifted TASEP

- For Symmetric SEP mixing cf Lacoin (2014).
- For TASEP mixing cf Baik & Liu (2016).
- All others cf Kapfer & Krauth (2017).
- Proofs for event-chain cf Lei & Krauth (2018b).

NB: All algorithms converge towards equilibrium.

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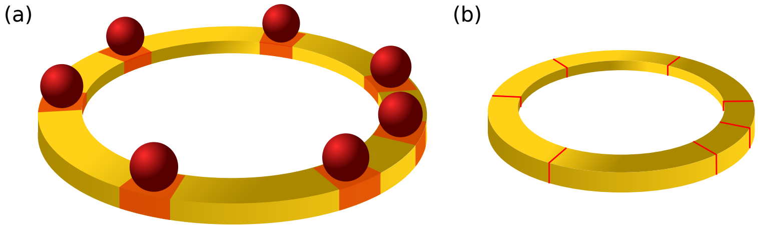
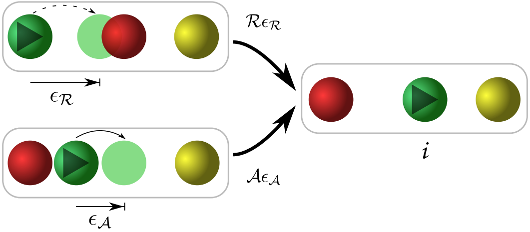


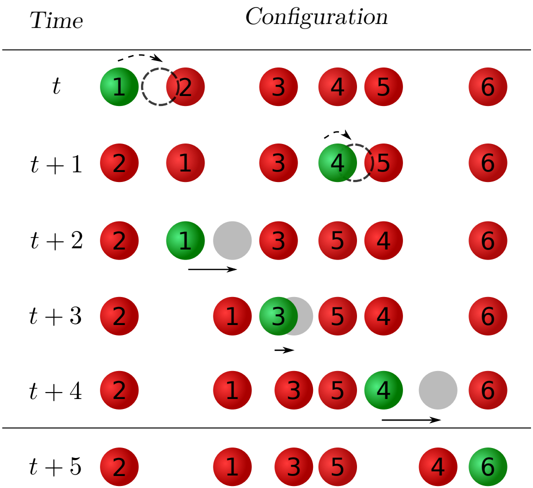
- Event-chain with chain length $=$ ran$[0, L - N\sigma]$.
- Obtains perfect sample in $\mathcal{O}\left(N^2 \log N\right)$ steps.
- The logarithm $\equiv$ Coupon collector.
- Lei & Krauth (2018)

Postscriptum 2/3 (Irreversible Markov chains in 1d)



- Relabeling algorithm, can be used sequentially.
- Obtains perfect sample in $\mathcal{O}\left(N^2\right)$ steps.
- No logarithm $\equiv$ No coupon collector.
- Lei & Krauth (2018)

Postscriptum 3/3 (Irreversible Markov chains in 1d)



- Arbitrary sequences are OK
- Lei & Krauth (2018)

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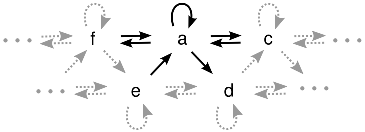
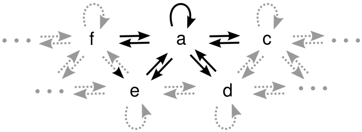
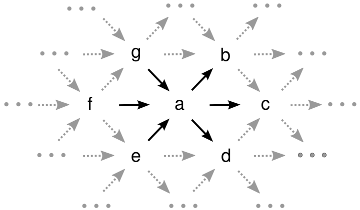
Detailed balance and global balance again 1/3



global balance

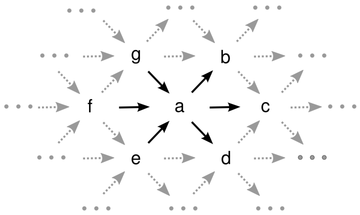


detailed balance



maximal global balance

Detailed balance and global balance again 2/3



maximal global balance

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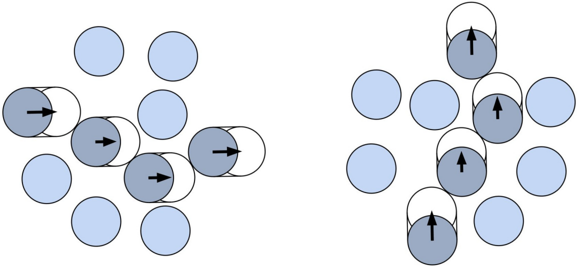
Detailed balance and global balance again 3/3

$$\cdots \dashrightarrow f \longrightarrow a \longrightarrow c \dashrightarrow \cdots$$

maximal global balance

Faster algorithm: Event-chain algorithm again



- Bernard, Krauth, Wilson (2009).
- Infinitesimal moves: No multiple overlaps, consensus.
- Global balance, lifting (Diaconis, Holmes, & Neal (2000))
- $1d$: $\sim$ TASEP ('lifted' TASEP) Kapfer, Krauth (2017).
- Michel, Kapfer, Krauth (2014) (smooth potentials).

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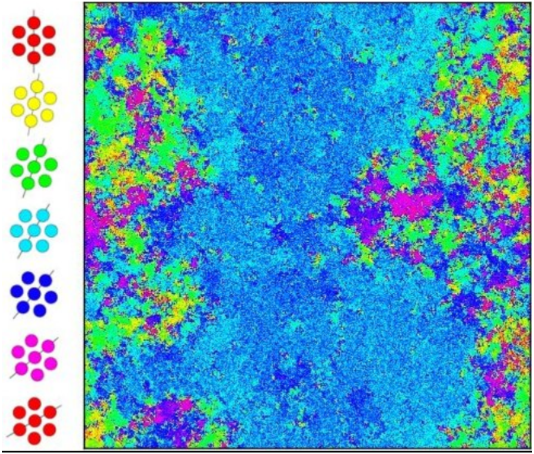
Hard-disk configuration



- 1024^2 hard disks
- Bernard, Krauth (PRL 2011)

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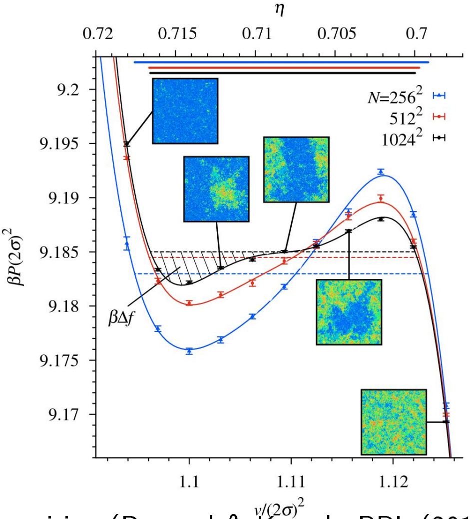
Equilibrium equation of state



- First-order transition (Bernard & Krauth, PRL (2011)).
- Many confirmations.

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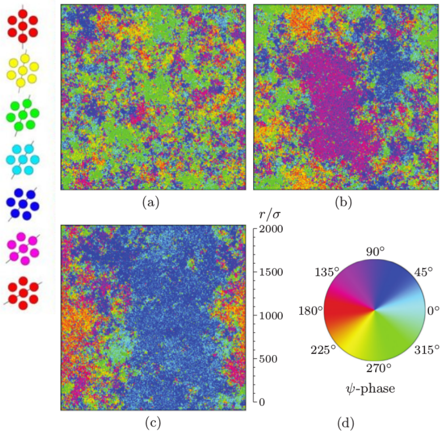
Phase coexistence in hard disks



- 1024^2 systems.
- Densities $\eta = 0.700$ (a), $\eta = 0.704$ (b), $\eta = 0.708$ (c).
- Phase coexistence $\Longrightarrow$ Coarsening $\Longrightarrow$ Slow dynamics.
- cf. Engel et al (2013).

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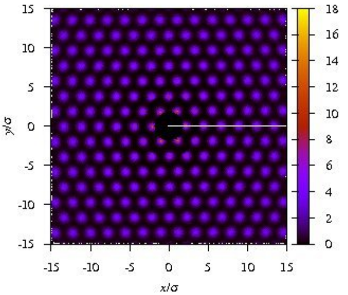
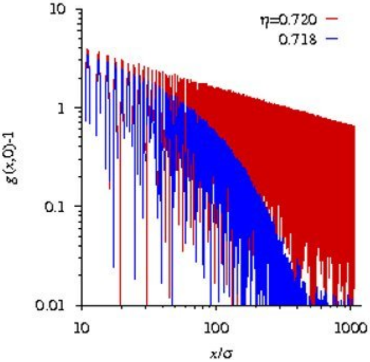
Possible phases (again)

Phase	positional order	orientational order
solid	algebraic	long-range
hexatic	short-range	algebraic
liquid	short-range	short-range

Spatial correlations at $\eta = 0.718$ and 0.720

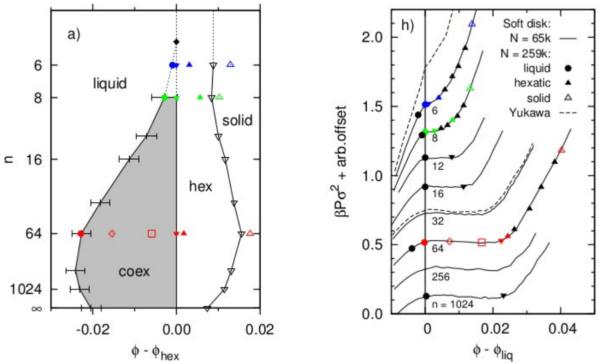




- Two-dimensional pair correlations, sample-averaged.
- At $\eta = 0.718$; hexatic: First-order liquid-hexatic transition.
- At $\eta \sim 0.720$: KT-type hexatic-solid transition.
- Bernard & Krauth (PRL 2011).
- Many confirmations.

Soft disks

- Soft disks: $V \propto (\sigma/r)^n$.



- Kapfer & Krauth (PRL 2015).
- Two melting scenarios depending on softness n of potential.

Discussion

Berni Alder and Phase Transitions in Two Dimensions (2016)

J. Michael Kosterlitz

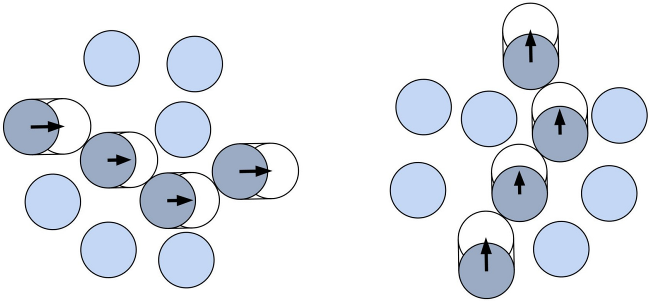
I do not know Berni Alder as a person, but I feel that I know him well through his seminal paper "Phase Transition in Elastic Disks" by B. J. Alder and T. E. Wainwright [1962], which was essential in motivating David Thouless and myself to think about phase transitions in two dimensional systems with a continuous symmetry. In the early 1970's, the conventional wisdom was that a crystalline solid could not exist in a

transition resulting in the expected isotropic fluid phase. These results hold for a crystal described by standard elasticity theory, but of course, no crystal is completely described by elasticity theory alone and there are all sorts of extra excitations such as vacancies and interstitials which are ignored in a purely elastic theory but can affect the order of a transition. These can explain the first order nature of the second hexatic/isotropic fluid transition found by Alder and Wainwright in 1961 and Bernard and Krauth in 2011.

NO!

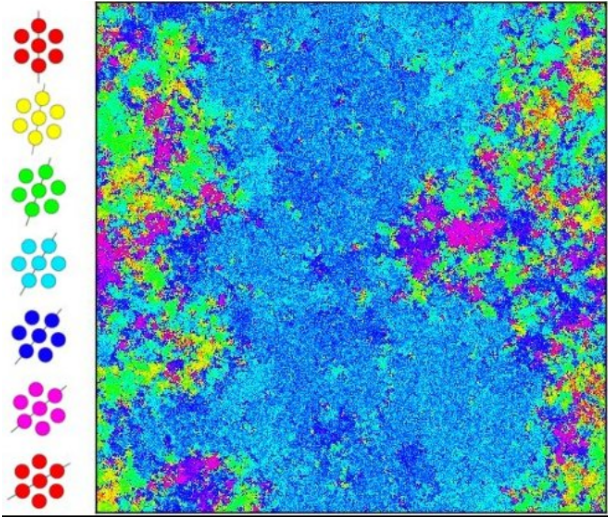
- IMHO: Elasticity theory does describe 2D melting...
- See: Krauth (2017, soon)

Conclusion 1/6



- cf Bernard, Krauth, Wilson (2009).
- NB: Uniform distribution from non-equilibrium (irreversibility)

Conclusion 2/6



- cf Bernard & Krauth (2011).

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Conclusion 3/6

"Metropolis" paradigm
(Metropolis et al, 1953)

- **Detailed balance** — vanishing probability flows
- **Metropolis algorithm** — energy driven
- **Rejections** — finite random moves

"Beyond-Metropolis" paradigm
(Michel , Kapfer & Krauth, 2014)

- **Global balance** — steady-state probability flows
- **Factorized Metropolis algorithm** — consensus driven
- **Liftings** — infinitesimal persistent moves

- Metropolis algorithm

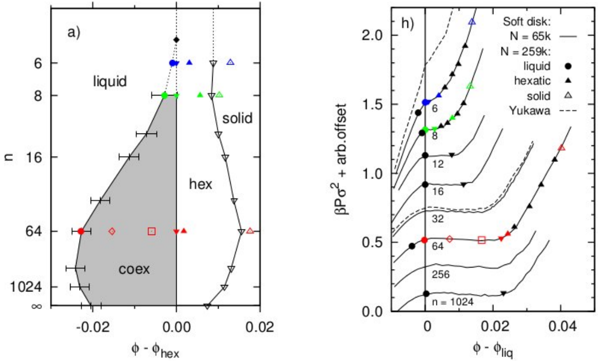
$$p^{\mathrm{Met}}(a \to b) = \min \left[1, \prod_{i<j} \exp\left(-\beta \Delta V_{i,j}\right) \right]$$

- Factorized Metropolis algorithm (Michel, Kapfer, Krauth 2014)

$$p^{\mathrm{Fact.}}(a \to b) = \prod_{i<j} \min\left[1, \exp\left(-\beta \Delta V_{i,j}\right)\right].$$

$$X^{\mathrm{Fact.}}(a \to b) = X_{1,2} \wedge X_{1,3} \wedge \cdots \wedge X_{N-1,N}$$

- Soft disks: $V \propto (\sigma/r)^n$.



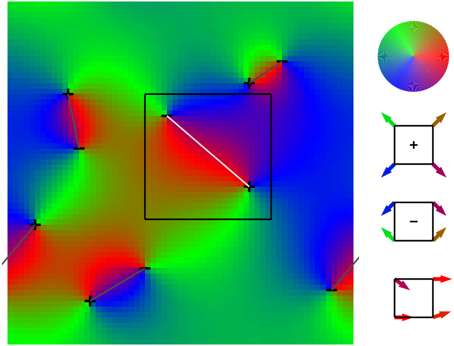
- cf Kapfer & Krauth (2015).

Conclusion 5/6

Algorithm	mixing	discrete analogue
Heatbath, Metropolis	$N^3 \log N$	Symmetric SEP
Forward Metropolis, Lifted (∞)	$N^{5/2}$	TASEP
Event-chain, Lifted (term)	$N^2 \log N$	lifted TASEP
Event-chain (relabel)	N^2	?

- cf Kapfer & Krauth (2017).
- cf Lei & Krauth (2018).

Conclusion 6/6 (XY model)



- Irreversible MCMC great for spin waves and phonons.
- Local algorithm, moves topological excitations step by step.
- cf Lei, Krauth (2017).

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