Markov-chain Monte Carlo
and
the hard-disk Universe

Werner Krauth

Laboratoire de Physique, Ecole normale supérieure, Paris, France

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Summer School: Point configurations: Deformations and rigidity

London Mathematical Society, Clay Mathematics Institute, Heilbronn Institute for Mathematical Research

London (United Kingdom)

B. Li, Y. Nishikawa, P. Höllmer, L. Carillo, A. C. Maggs, W. Krauth; arXiv 202207XXXX
Hard-disk computer simulations—a historic perspective

W. Krauth; Front. Phys. (2021)
Event-Chain Monte Carlo: Foundations, Applications, and Prospects

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Metropolis et al. (1953) (1/5)

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.

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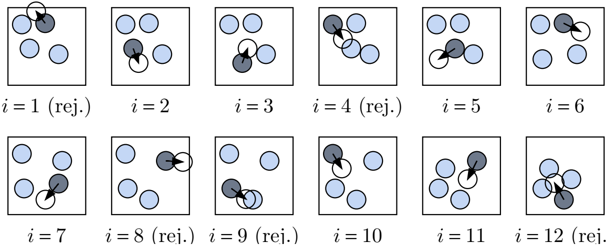
Metropolis et al. (1953) (2/5)



- ‘Metropolis algorithm’

Metropolis et al. (1953) (3/5)

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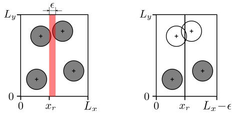
- NB: Equation of state: Pressure as a function of Volume.
- NNB: Pressure: (Rift-Elimination probability)/(rift volume).



- NNNB: Infinite Pressure $\equiv$ Packing problems, energy minimization.

Markov chain, transition matrix

- Sample space $\Omega \leftarrow$ disks in a box.
- Markov chain $\leftarrow$ Moves: Sequence of random variables $(X_0 \sim \pi^{\{0\}}, X_1 \sim \pi^{\{1\}}, X_2 \sim \pi^{\{2\}} \dots)$
  X_{t+1} depends on X_t through a transition matrix P.
- A priori probability$\rightarrow$ split matrix: $P_{ij} = \mathcal{A}_{ij}\mathcal{P}_{ij}$ for $i \neq j$
  $\mathcal{A} \Leftrightarrow$ a priori probability; $\mathcal{P} \Leftrightarrow$ filter
  Examples: Metropolis filter, heatbath filter.
- Monte Carlo rejections $\rightarrow P_{ii} \Leftrightarrow$ (filter) rejection probability.
  NB: Modern MCMC algorithms often have no rejections.

NB: Double role of P:

1. For probability distributions: $\pi^{\{t+1\}} = \pi^{\{t\}} P$ (with $\pi^{\{t\}}, \pi^{\{t+1\}}$ non-explicit objects, often even for $t \rightarrow \infty$).
2. For samples: P_{ij}: explicit probability to move from i to j.

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Irreducibility

- P irreducible $\Leftrightarrow$ any i can be reached from any j.
- $\pi^{\{0\}}$: Initial probability (explicit, user-supplied). Often concentrated on a single sample $x \in \Omega$.
- P irreducible $\Rightarrow$ unique stationary distribution π with

$$\pi_i = \sum_{j \in \Omega} \pi_j P_{ji} \quad \forall i \in \Omega.$$

NB: Transition matrix P is stochastic, that is, $\sum_j P_{ij} = 1$.

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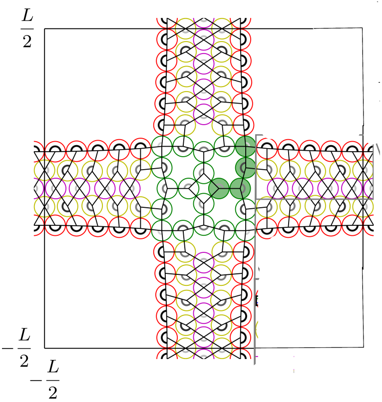
Irreducibility of hard-disk problem

Is the Metropolis algorithm for hard disks irreducible?
Rather not ...



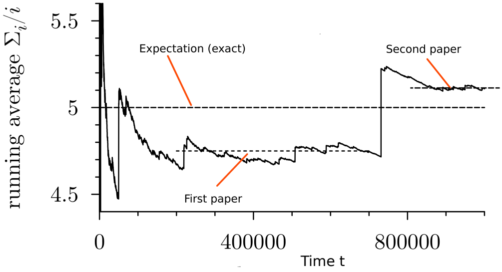
Hoellmer et al. (2022), following Böröczky (1964)

Ergodic theorem

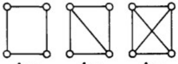
- P irreducible $\Rightarrow$ π unique, but maybe $\pi^{\{t\}} \not\to \pi$ for $t \to \infty$.
- P irreducible $\Rightarrow$ Ergodic theorem ($\mathbb{E}(\mathcal{O}) := \sum_{i \in \Omega} \mathcal{O}_i \pi_i$):

$$\mathbb{P}_{\pi^{\{0\}}} \left[\lim_{t \to \infty} \frac{1}{t} \sum_{i_t} \mathcal{O}(i_t) = \mathbb{E}(\mathcal{O}) \right] = 1$$

(Strong law of large numbers, applied to running average)

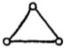


Metropolis et al. (1953) (4/5)



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 $A_{5,5}$.

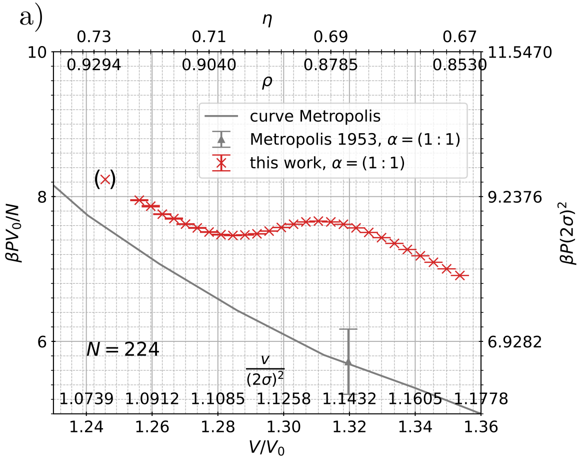
The data on $A_{4,6}$ is quite reliable. We obtained

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.

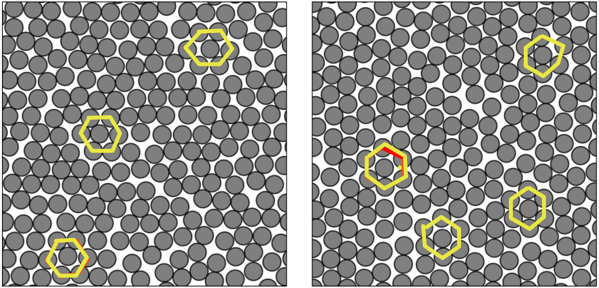
In the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for $A/A_0<1.8$ and with a five-term virial expansion for $A/A_0>2.5$. $\boxed{\text{There is no indication of a phase transition.}}$

Metropolis et al. (1953) (5/5)



‘Base’ and ‘tip’ configurations

$N = 224$ in square box (NB: $224 = 16 \times 14$) with $16\sqrt{3}/2 \simeq 14$.



$$\Psi_6 = \frac{1}{N}\sum_l \frac{1}{\text{nbr}(l)} \sum_{j=1}^{\text{nbr}(l)} \exp\left(6i\phi_{lj}\right),$$

NB: $\mathbb{E}\left(\Psi_6\right) = (0,0)$ (Ergodic theorem as a diagnostic tool).

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Alder–Wainwright (1962) (1/4)

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

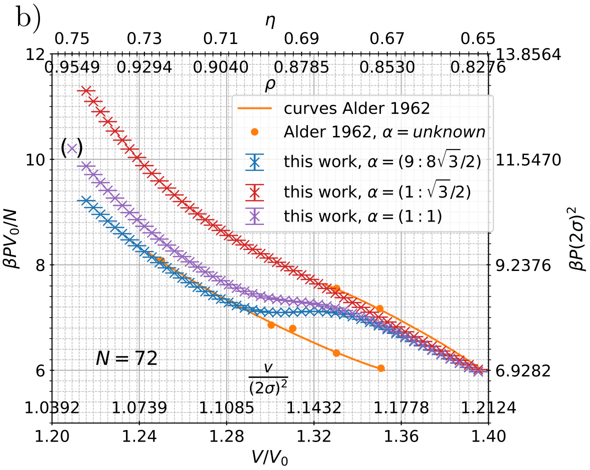
(Received October 30, 1961)

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



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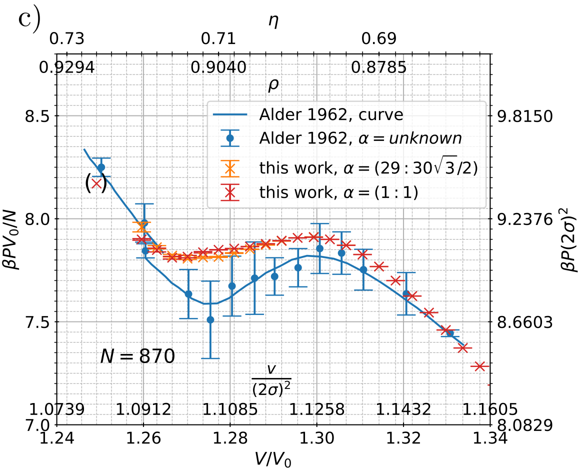
Alder–Wainwright (1962) (3/4)



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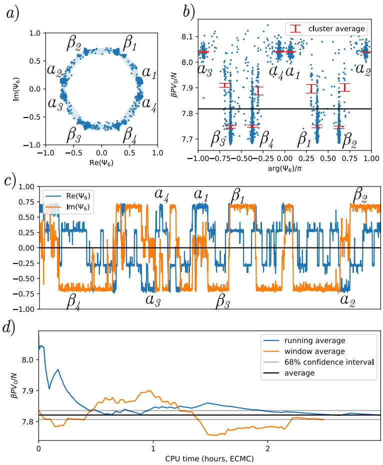
Alder–Wainwright (1962) (4/4)



NB: Three hours on 2022 CPU (best MCMC algorithm) to equilibrate 870 disks in a box.

Probability flows—Global-balance condition

- Global-balance condition:

$$\pi_i = \sum_{j \in \Omega} \underbrace{\overbrace{\pi_j P_{ji}}^{\text{flow } j \to i}}_{\mathcal{F}_{ji}} \qquad \forall i \in \Omega.$$

(NB: This is the steady state of $\pi_i^{\{t+\mathbf{1}\}} = \sum_{j \in \Omega} \pi_j^{\{t\}} P_{ji}$)

- Global-balance condition (second formulation):

$$\pi_i = \overbrace{\sum_{j \in \Omega} \mathcal{F}_{ji}}^{\text{flows entering } i} \qquad \forall i \in \Omega,$$

$$\overbrace{\sum_{k \in \Omega} \mathcal{F}_{ik}}^{\text{flows exiting } i} = \overbrace{\sum_{j \in \Omega} \mathcal{F}_{ji}}^{\text{flows entering } i} \qquad \forall i \in \Omega,$$

(NB: stochasticity condition used $\sum_{k \in \Omega} P_{ik} = 1$).

Reversibility—Detailed-balance condition

- Reversible P satisfies the 'detailed-balance' condition:

$$\overbrace{\underbrace{\pi_i P_{ij}}_{\mathcal{F}_{ij}}}^{\text{flow } i \to j} = \overbrace{\underbrace{\pi_j P_{ji}}_{\mathcal{F}_{ji}}}^{\text{flow } j \to i} \quad \forall i, j \in \Omega.$$

- General P satisfies the 'global-balance' condition

$$\pi_i = \sum_{j \in \Omega} \pi_j P_{ji} \quad \forall i \in \Omega.$$

- Detailed balance implies global balance.
- Global balance:

$$\overbrace{\sum_{k \in \Omega} \mathcal{F}_{ik}}^{\text{flows exiting } i} = \overbrace{\sum_{j \in \Omega} \mathcal{F}_{ji}}^{\text{flows entering } i} \quad \forall i \in \Omega,$$

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Spectrum of reversible transition matrix

- Reversible P:

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \forall i, j \in \Omega.$$

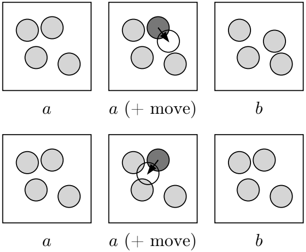
- Reversible P: $A_{ij} = \pi_i^{1/2} P_{ij} \pi_j^{-1/2}$ is symmetric.
- Reversible P:

$$\sum_{j \in \Omega} \underbrace{\pi_i^{1/2} P_{ij} \pi_j^{-1/2}}_{A_{ij}} x_j = \lambda x_i \Leftrightarrow \sum_{j \in \Omega} P_{ij} \left[\pi_j^{-1/2} x_j\right] = \lambda \left[\pi_i^{-1/2} x_i\right].$$

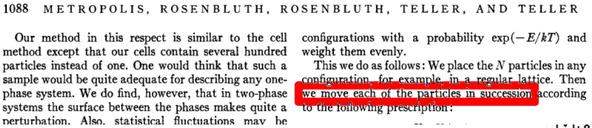
- P and A have same eigenvalues.
- A symmetric: (Spectral theorem): All eigenvalues real, can expand on eigenvectors.
- Irreducible, aperiodic: Single eigenvalue with $\lambda = 1$, all others smaller in absolute value.

Metropolis algorithm / reversibility

1. The Metropolis et al. (1953) algorithm is reversible.



2. The algorithm used by Metropolis et al. (1953) is non-reversible.


1088 METROPOLIS, ROSENBLUTH, ROSENBLUTH, TELLER, AND TELLER

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:

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Total variation distance, mixing time

- Total variation distance:

$$||\pi^{\{t\}} - \pi||_{\mathrm{TV}} = \max_{A \subset \Omega} |\pi^{\{t\}}(A) - \pi(A)| = \frac{1}{2} \sum_{i \in \Omega} |\pi_i^{\{t\}} - \pi_i|.$$

- Distance:

$$d(t) = \max_{\pi^{\{0\}}} ||\pi^{\{t\}}(\pi^{\{0\}}) - \pi||_{\mathrm{TV}}$$

- Mixing time:

$$t_{\mathrm{mix}}(\epsilon) = \min\{t : d(t) \leq \epsilon\} \quad (\epsilon < \frac{1}{2})$$

NB: '$\max_{\pi^{\{0\}}}$' $\equiv$ 'worst initial distribution $\pi^{\{0\}}$'

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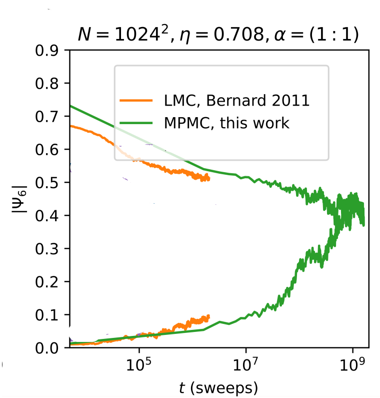
Mixing time (poor man's)



Metropolis algorithm on a single CPU: $\simeq 10^{10}$ moves/hour

- 1 sweep $\simeq 10^6$ moves
- 10^9 sweeps $\simeq 11.4$ years.

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Conductance (bottleneck ratio)

$$\Phi \equiv \min_{S\subset\Omega,\pi_S\leq\frac{1}{2}} \frac{\mathcal{F}_{S\to\overline{S}}}{\pi_S} = \min_{S\subset\Omega,\pi_S\leq\frac{1}{2}} \frac{\sum_{i\in S,j\notin S}\pi_i P_{ij}}{\pi_S}.$$

- Reversible Markov chains:

$$\frac{1}{\Phi} \leq \tau_{\text{corr}} \leq \frac{8}{\Phi^2}$$

('$\leq$': Sinclair & Jerrum (1986), Lemma (3.3))

- Arbitrary Markov chain (see Chen et al. (1999)):

$$\frac{1}{4\Phi} \leq \mathcal{A} \leq \frac{20}{\Phi^2},$$

(set time: Expectation of $\max_S(t_S \times \pi_S)$ from equilibrium)

NB: One bottleneck, not many. Lower and upper bound.

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Lifting (Chen et al. (1999)) (1/2)

- Markov chain $\Pi \Leftrightarrow$ Lifted Markov chain $\hat{\Pi}$
- $\Omega \ni v$ (sample space) $\Leftrightarrow \hat{\Omega} \ni i$ (lifted sample space)
- P (transition matrix) $\Leftrightarrow \hat{P}$ (lifted transition matrix)
- π_v (stationary probability) $\Leftrightarrow \hat{\pi}_i$
- **Condition 1**: sample space is copied ('lifted'), π preserved

$$\pi_v = \hat{\pi}\left[f^{-1}(v)\right] = \sum_{i \in f^{-1}(v)} \hat{\pi}_i,$$

- **Condition 2**: flows are preserved

$$\underbrace{\pi_v P_{vu}}_{\text{collapsed flow}} = \sum_{i \in f^{-1}(v), j \in f^{-1}(u)} \overbrace{\hat{\pi}_i \hat{P}_{ij}}^{\text{lifted flow}} .$$

- Usually: $\hat{\Omega} = \Omega \times \mathcal{L}$, with $\mathcal{L}$ a set of lifting variables σ

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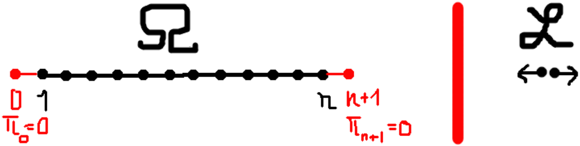
Lifting (Chen et al. (1999)) (2/2)

- Required: Mapping from $\hat{\Omega}$ (lifted sample space) to Ω that preserves stationary probability distribution.
- Required: Lifted transition matrix $\hat{P}$ that preserves flow.
- Optional: $\hat{\Omega} = \Omega \times \mathcal{L}$ (with $\mathcal{L}$: set of lifting variables).
- Optional:

$$\frac{\hat{\pi}(u, \sigma)}{\pi(u)} = \frac{\hat{\pi}(v, \sigma)}{\pi(v)} \quad \forall\ u, v \in \Omega; \forall\ \sigma \in \mathcal{L}. \tag{1}$$

- There are many liftings $\hat{P}$ for a given lifted sample space $\hat{\Omega}$.
- Liftings are popular for transfering parts of the moves into the sample space.
- Lifting do not increase conductance.

Metropolis algorithm on path graph (1/3)

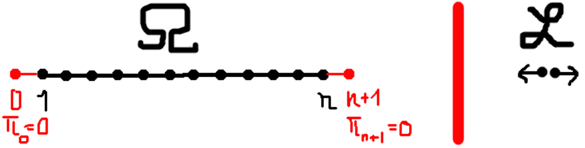


- Sample space = path graph $\Omega = \{1, \ldots, n\}$.
- Phantom vertices and edges.

Metropolis algorithm (NB: $P_{ij} = \mathcal{A}_{ij}\mathcal{P}_{ij}$ for $i \neq j$):

1. Move set $\mathcal{L} = \{+, -\}$.
2. Flat a priori probability $\mathcal{A}$: $\rightarrow \sigma =$ choice($\mathcal{L}$).
3. Metropolis filter: Accept with probability $\min(1, \pi_j/\pi_i)$.
   Reject: Don't move.

Metropolis algorithm on path graph (2/3)



- Detailed balance:

$$\underbrace{\pi_i P_{ij}}_{\mathcal{F}_{ij}} = \underbrace{\pi_j P_{ji}}_{\mathcal{F}_{ji}}$$

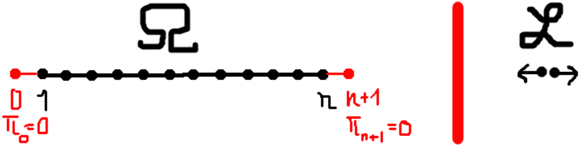
- Metropolis algorithm:

$$\mathcal{F}_{ij} = \frac{1}{2} \min(\pi_i, \pi_j) \Leftrightarrow P_{ij} = \frac{1}{2} \min(1, \pi_j/\pi_i)$$

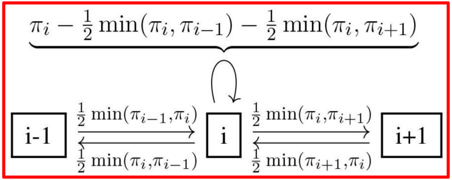
- Metropolis filter (NB: $P_{ij} = \mathcal{A}_{ij}\mathcal{P}_{ij}$):

$$\mathcal{P}_{ij} = \min(1, \pi_j/\pi_i)$$

Metropolis algorithm on path graph (3/3)



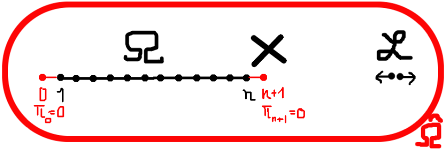
- Global balance ($\pi_i = \sum_j \pi_j P_{ji} = \sum_j \mathcal{F}_{ji}$):



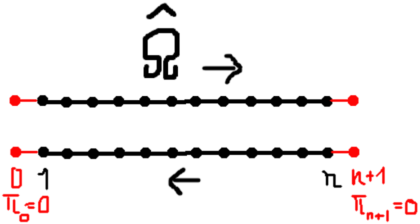
Lifting on the path graph (1/2)

General probability distribution $\pi = (\pi_1, \dots, \pi_n)$

- 'Lifted' sample space $\hat{\Omega} = \{1, \dots, n\} \times \{+, -\}$:



- 'Lifted' non-reversible Markov chain $\hat{\Omega} = \Omega \times \{-, +\}$:



- Diaconis et al. (2000) '

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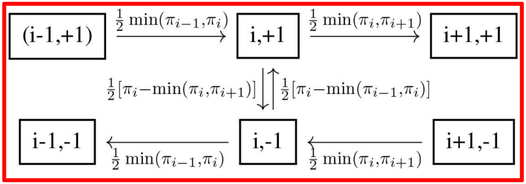
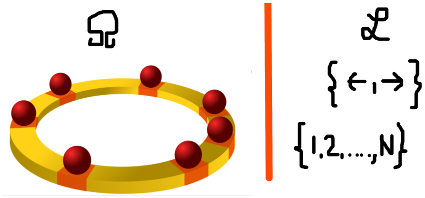
Lifting on the path graph (2/2)

- 'Lifted' non-reversible Markov chain: NB:' only Transport treated



NB: The $\frac{1}{2} \Leftrightarrow \hat{\pi}_{i,\sigma} = \frac{1}{2}\pi_i$

1d hard spheres 1/2



- N spheres, with a sample space Ω, and a move space $\mathcal{L}$.
- Metropolis algorithm samples $\{-,+\} \times \{1,\ldots,N\}$ at each time step.

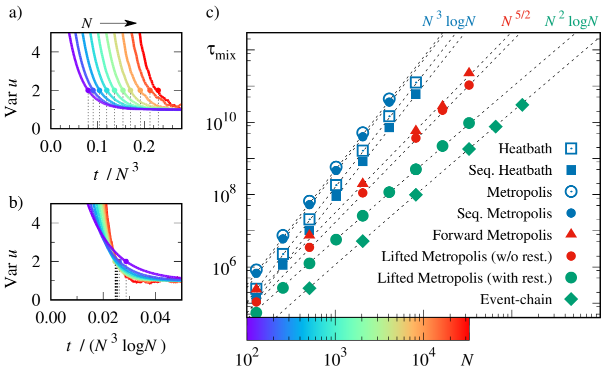
Many choices for non-reversible liftings:

Sequential $\hat{\Omega} = \Omega \times \{1,\ldots,N\}$: Move one disk after the other.

Forward $\hat{\Omega} = \Omega \times \{(-),+\}$: Move only in forward direction.

Particle-lifted forward $\hat{\Omega} = \Omega \times \{1,\ldots,N\} \times \{(-),+\}$: Always move the same disk forward, until it is blocked...

1d hard spheres 2/2



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

- Kapfer—Krauth (2017)

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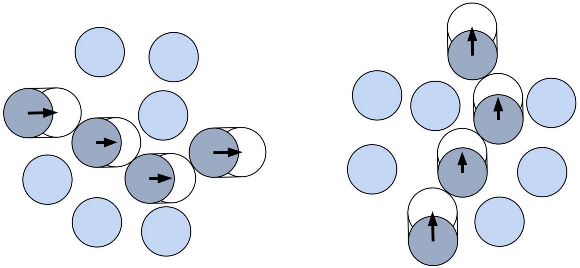
Hard disks: event-chain Monte Carlo (ECMC)



- Bernard, Krauth, Wilson (2009).
- Michel, Kapfer, Krauth (2014) (smooth potentials).
- Many variants.

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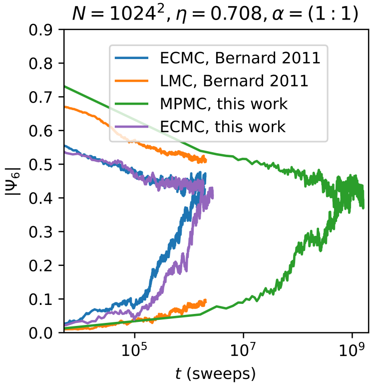
ECMC and the hard-disk model



- 10^9 sweeps $\equiv$ 11.4 years (Metropolis, LMC, MPMC)
- 10^6 sweeps $\equiv$ 4.2 days (Event-chain Monte Carlo)

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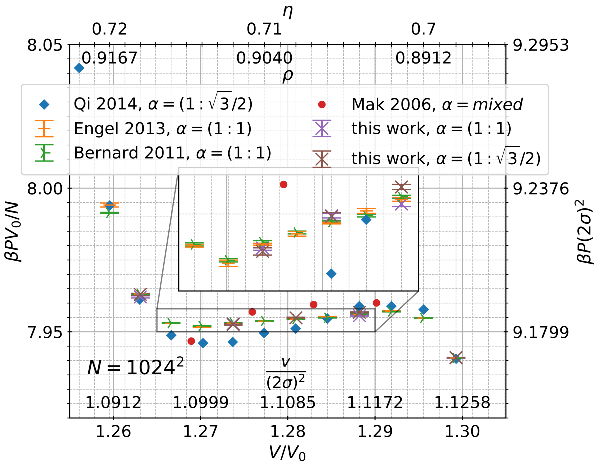
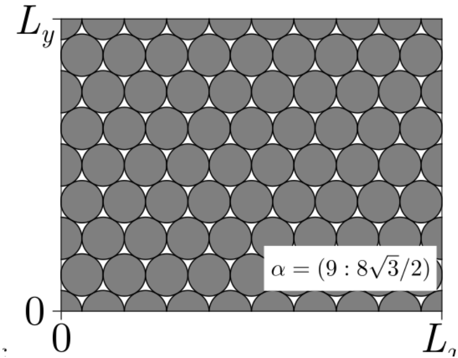
Synopsis large hard-disk system



- Li et al. (2022)

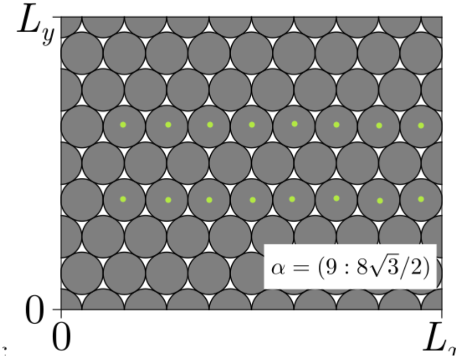
NB: Pressures are required precisely for further analysis.

Hard disks at infinite pressure 1/3



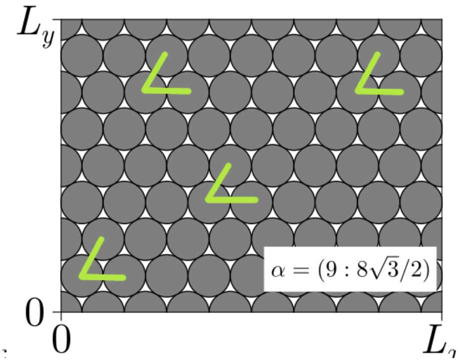
- Infinite-pressure configuration (packing)

Hard disks at infinite pressure 2/3



- Crystal: Positional long-range order

Hard disks at infinite pressure 3/3



- Crystal: Orientational long-range order

No crystal at finite pressure 1/2

R. PEIERLS

Quelques propriétés typiques des corps solides

Annales de l'I. H. P., tome 5, n° 3 (1935), p. 177-222.

C'est à cette circonstance que l'on doit attribuer l'origine de la distinction qualitative qui existe entre les états solide et liquide. Dans un liquide la cohérence ne se conserve pas à longue distance quoique naturellement les atomes voisins forment de préférence les arrangements d'énergie minimum. Dans le cas unidimensionnel la différence entre solide et liquide ne serait que quantitative et, au lieu d'un point de fusion bien déterminé, on aurait là un passage continu.

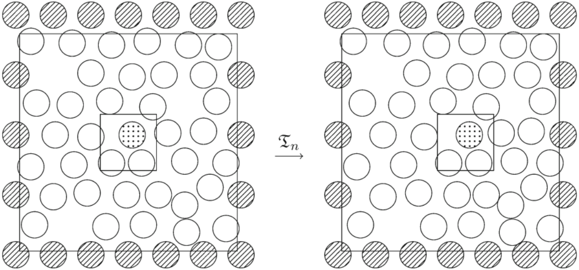
- Classic paper on crystallization.
- No crystal in two dimensions at finite pressure.

No crystal at finite pressure 2/2

Lower Bound on the Mean Square Displacement of Particles in the Hard Disk Model

Thomas Richthammer[1]

Commun. Math. Phys. 345, 1077–1099 (2016)



- No crystal in two dimensions at finite pressure.
- Displacement of center box $\mathfrak{T} \gtrsim \log(N)$.
- Specific to (two-dimensional) hard disks.

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Kosterlitz–Thouless (1973)

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

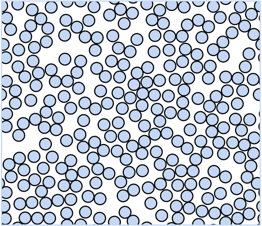
Received 13 November 1972

1. Introduction

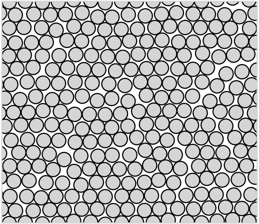
Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the 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 for hard disks



density $\eta = 0.48$



$\eta = 0.72$

Phase	positional order	orientational order
crystal	long-range	long-range [1]
solid	algebraic	long-range (NB: phase not proven to exist)
hexatic	short-range	algebraic (NB: phase not proven to exist)
liquid	short-range	short-range [2]

[1] Feyes (1940), only at $P = \infty$ (Peierls 1935, Richthammer 2016)

[2] Exists at small P (Lebowitz–Penrose 1964)

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Phase diagram for hard disks

, 155704 (2011) PHYSICAL REVIEW LETTERS weel 7 OCT

Two-Step Melting in Two Dimensions: First-Order Liquid-Hexatic Transition

Etienne P. Bernard* and Werner Krauth†

oire de Physique Statistique Ecole Normale Supérieure, UPMC, CNRS 24 rue Lhomond, 75231 Paris Cedex 05

(Received 6 July 2011; published 7 October 2011)

Melting in two spatial dimensions, as realized in thin films or at interfaces, represents one of the most fascinating phase transitions in nature, but it remains poorly understood. Even for the fundamental hard-disk model, the melting mechanism has not been agreed upon after 50 years of studies. A recent Monte Carlo algorithm allows us to thermalize systems large enough to access the thermodynamic regime. We show that melting in hard disks proceeds in two steps with a liquid phase, a hexatic phase, and a solid. The hexatic-solid transition is continuous while, surprisingly, the liquid-hexatic transition is of first order. This melting scenario solves one of the fundamental statistical-physics models, which is at the

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

- Hexatic phase exists.
- Liquid–hexatic transition of first order.
- Hexatic–solid transition of Kosterlitz–Thouless type.

Remarkable results, big & small open problems

Remarkable results:

- D. B. Wilson (1999): Coupling-from-the-past for hard spheres.
- Kannan, Mahoney, Montenegro (2003): Switcheroo hard-disk algorithm with proven $\mathcal{O}(N \log N)$ mixing times.
- Helmuth, Perkins, Petti (2021): Proof that 'algorithm converges fast' $\implies$ 'particle system is fluid'.
- Richthammer (2016): Lone star theorem at high density.

Big & small open problems:

- Existence of crystal at finite pressure in any dimension > 2.
- Existence of solid at finite pressure in dimension 2.
- 'Decent' MCMC algorithm for hard disks at high density.
- Inner workings of lifted Markov chains.