Hard-disk packings, fast Markov chains, and the two phase transitions of two-dimensional particle systems

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B. Li, Y. Nishikawa, P. Höllmer, L. Carillo, A. C. Maggs, W. Krauth arXiv:2202(1).XXXX
Hard-disk computer simulations—a historic perspective

P. Hoellmer, N. Noirault, B. Li, A. C. Maggs, W. Krauth arXiv:2109.13343 (2021)
Sparse hard-disk packings and local Markov chains

E. P. Bernard, W. Krauth, D. B. Wilson, PRE (2009)
Event-chain algorithms for hard-sphere systems

E. P. Bernard, W. Krauth, PRL (2011)
Two-Step Melting in Two Dimensions: First-Order Liquid-Hexatic Transition

Work supported by A. v. Humboldt Foundation

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Hard-disk packings 1/4

Über einen geometrischen Satz.

Von

L. Fejes in Budapest.

Wir beweisen im folgenden den Satz: *Es sei* $\mathfrak{S}_2, \mathfrak{S}_3, \ldots, \mathfrak{S}_n, \ldots$ *eine Folge von Punktsystemen, die beziehentlich aus* 2, 3, …, n, … *Punkten bestehen und die sämtlich in einem Gebiet mit dem Flächeninhalt* T *liegen. Dann läßt sich von jedem* $\mathfrak{S}_n$ *ein Punktpaar mit dem Abstand* d_n *derart herausgreifen, daß* $\overline{\lim_{n\to\infty}}\, n d_n^2 \leq \frac{2\sqrt{3}}{3} T$ *ausfällt.* Die Konstante $\frac{2\sqrt{3}}{3}$ läßt sich dabei durch keine kleinere ersetzen[1]).

- This is Fejes (1940) proving optimal disk packing in 2D.
- There is also Thue (1910), but it seems to be wrong.
- Conway & Sloane (1999): 'This result has a long history - see especially Thue's 1910 paper [Thu 1] and the proof given by Fejes Toth in 1940' ...
- Question: Is Thue's proof correct or is it wrong, and does anyone (in the audience) have a copy of the paper?

Hard-disk packings 2/4

ÜBER STABILE KREIS- UND KUGELSYSTEME

Von

K. BÖRÖCZKY

Lehrstuhl für Geometrie, Eötvös Loránd Universität, Budapest

(Eingegangen am 28. September 1964)

Eine Packung von Kreisen bzw. Kugeln heißt *stabil*, wenn jeder Kreis bzw. jede Kugel durch die nachbarenen festgehalten ist, d. h. kein Kreis bzw. keine Kugel lassen sich ohne gleichzeitige Bewegung der anderen bewegen.[1]

Zum Schluß bemerken wir, daß man „periodische" stabile Kreissysteme mit beliebig kleiner positiver Dichte auf ähnliche Weise konstruieren kann, aber dann muß man die Asymptote der von unten gesehen konvexen Kurve ein „bisschen" unten von g_2 aufnehmen (Figur 5).

- This is Böröczky's (1964) paper showing sparse 'locally' stable packings in 2D (and also in higher dimensions).
- Hoellmer et al (2021) follows in its footsteps, provides an open-source arbitrary-precision implementation.

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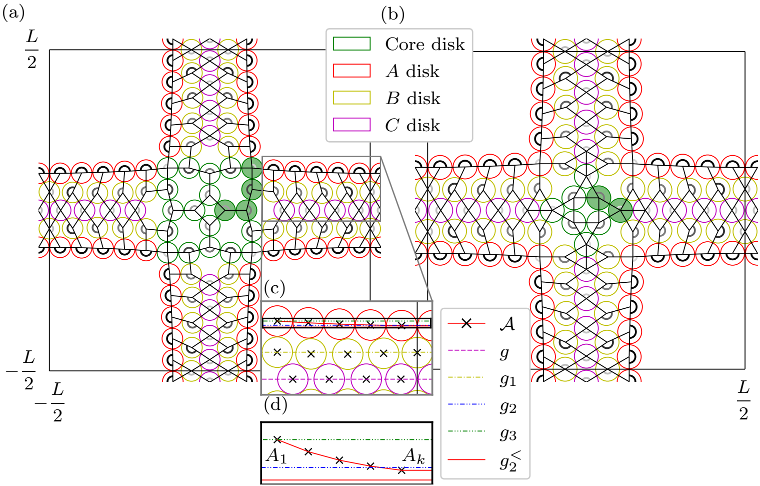
Hard-disk packings 3/4



- Böröczky packings in a periodic square box.
- see Hoellmer et al. (2021).

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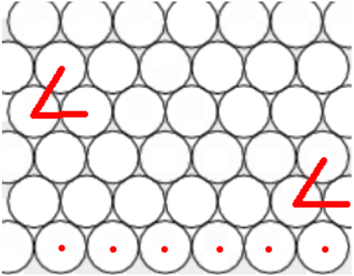
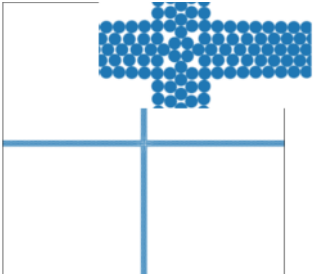
Hard-disk packings 4/4





- Long-range positional order.
- Long-range orientational order.

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Hard disks away from close packing (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.

- A one-d (two-d) hard-sphere system cannot have positional long-range order.
- A three-d hard-sphere system can have positional long-range order

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Hard disks away from close packing (2/2)

PHYSICAL REVIEW VOLUME 176, NUMBER 1 5 DECEMBER 1968

Crystalline Order in Two Dimensions*

N. D. Mermin†
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York

(Received 1 July 1968)

If N classical particles in two dimensions interacting through a pair potential $\Phi(\vec{r})$ are in equilibrium in a parallelogram box, it is proved that every $\vec{k}\neq 0$ Fourier component of the density must vanish in the thermodynamic limit, provided that $\Phi(\vec{r})-\lambda r^2|\nabla^2\Phi(\vec{r})|$ is integrable at $r=\infty$ and positive and nonintegrable at $r=0$, both for $\lambda=0$ and for some positive λ. This result excludes conventional crystalline long-range order in two dimensions for power-law potentials of the Lennard-Jones type, but is inconclusive for hard-core potentials. The

(d) The weakness of the instability suggests that some kind of ordering may still be present. An example of this is provided by the two-dimensional harmonic lattice. If the supposed equilibrium sites are $\vec{R}=n_1\vec{a}_1+n_2\vec{a}_2$ and the actual instantaneous position of the ions $\vec{r}(\vec{R})=\vec{R}+\vec{u}(\vec{R})$, then the absence of long-range crystalline order is reflected in the divergence of the displacement autocorrelation function:

$$\langle[\vec{u}(\vec{R})-\vec{u}(\vec{R}')]^2\rangle \sim \ln|\vec{R}-\vec{R}'|\,,\ |\vec{R}-\vec{R}'|\to\infty\ . \quad (32)$$

This reveals that positional long-range order does not exist. However *directional* long-range order is transmitted infinitely far, as revealed by a calculation of

$$\langle[\vec{r}(\vec{R}+\vec{a}_1)-\vec{r}(\vec{R})]\cdot[\vec{r}(\vec{R}'+\vec{a}_1)-\vec{r}(\vec{R}')]\rangle\ . \quad (33)$$

- A $2d$ particle system cannot be a crystal.
- $2d$ harmonic model: long-range orientational order.

Metropolis et al (1953) (1/3)

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

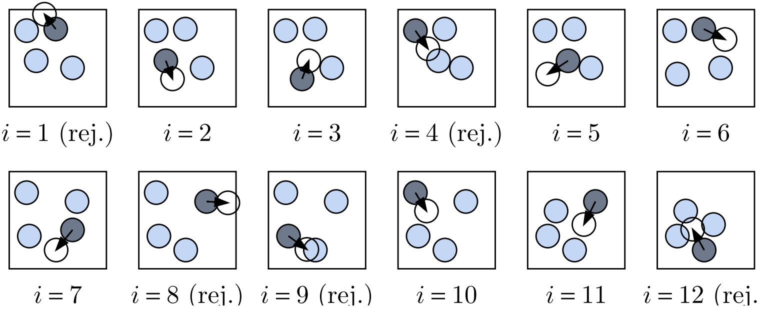
AND

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

(Received March 6, 1953)

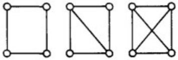
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional 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) (2/3)



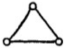
- Metropolis et al. (1953) introduced reversible MCMC.
- They also introduced non-reversible MCMC (sic).

Metropolis et al (1953) (3/3)



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.

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Alder–Wainwright (1962) (1/2)

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) (2/2)

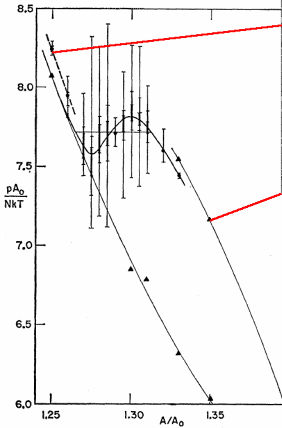
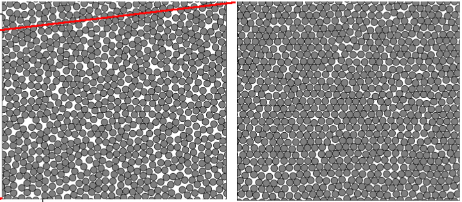
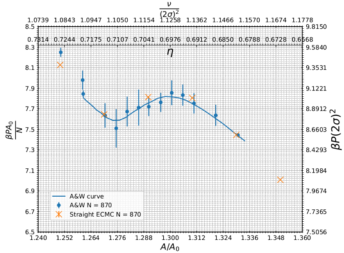


FIG. 1. The equation of state of hard disks in the phase transition region.





Box size 29 x 30 sqrt(3)/2
N=870 = 29x30

Li et al (2022, in prep.)

- Alder–Wainwright (1962) revisited by Li et al. (2022)

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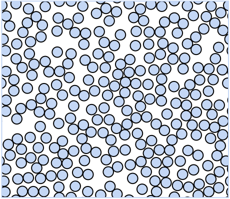
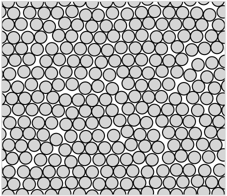
2D melting transition



density $\eta = 0.48$



$\eta = 0.72$

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

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

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

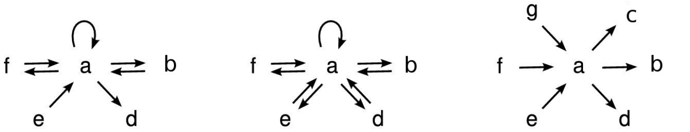
Received 13 November 1972

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

Detailed balance - global balance



global balance | detailed balance | maximal global balance

- flow into a = Boltzmann weight $\pi(a)$ (global balance condition):

$$\underbrace{\sum_k \pi^{(t-1)}(k) p(k \to a)}_{\text{flow into } a \sum_k \mathcal{F}(k \to a)} = \pi^{(t)}(a)$$

- flow $\mathcal{F}(a \to b) \equiv$ flow $\mathcal{F}(b \to a)$ (detailed balance condition):

$$\underbrace{\pi(b)p(b \to a)}_{\text{flow from } b \text{ to } a \mathcal{F}(b \to a)} = \underbrace{\pi(a)p(a \to b)}_{\mathcal{F}(a \to b) \text{ flow from } a \text{ to } b}$$

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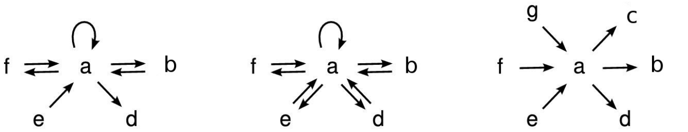
Detailed balance - global balance



global balance | detailed balance | maximal global balance

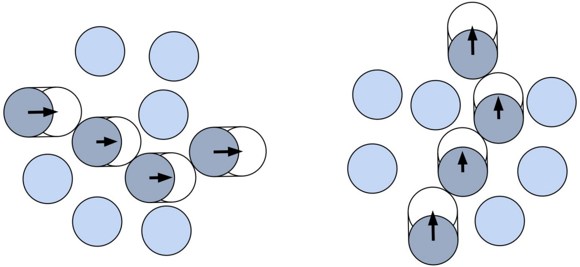
- flow into a = Boltzmann weight $\pi(a)$ (global balance condition):

$$\underbrace{\sum_k \pi(k) p(k \to a)}_{\text{flow into } a \sum_k \mathcal{F}(k \to a)} = \pi(a)$$

- flow $\mathcal{F}(a \to b) \equiv$ flow $\mathcal{F}(b \to a)$ (detailed balance condition):

$$\underbrace{\pi(b) p(b \to a)}_{\text{flow from } b \text{ to } a \mathcal{F}(b \to a)} = \underbrace{\pi(a) p(a \to b)}_{\mathcal{F}(a \to b) \text{ flow from } a \text{ to } b}$$

Faster algorithm: (Straight) Event-chain Monte Carlo



- Bernard, Krauth, Wilson (2009): Non-reversible, continuous-time.
- Infinitesimal moves: No multiple overlaps, consensus.
- Michel, Kapfer, Krauth (2014) (smooth potentials).
- Other versions of ECMC: ‘Straight’ (2009), ‘Reflective’ (2009), ‘Forward’ (Michel et al. 2020), ‘Newtonian’ (Klement et al. 2020).
- New world of MCMC (Review: Krauth (2021)).

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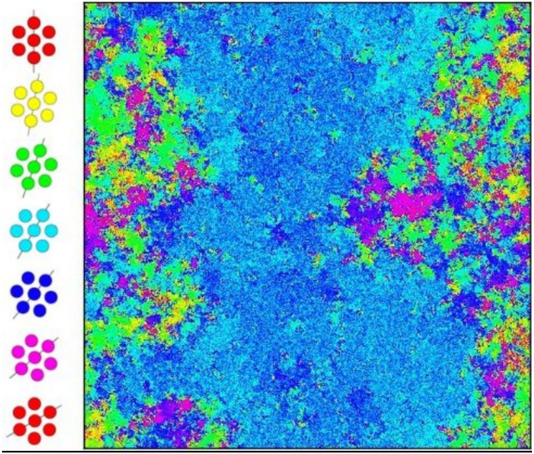
Hard-disk configuration



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

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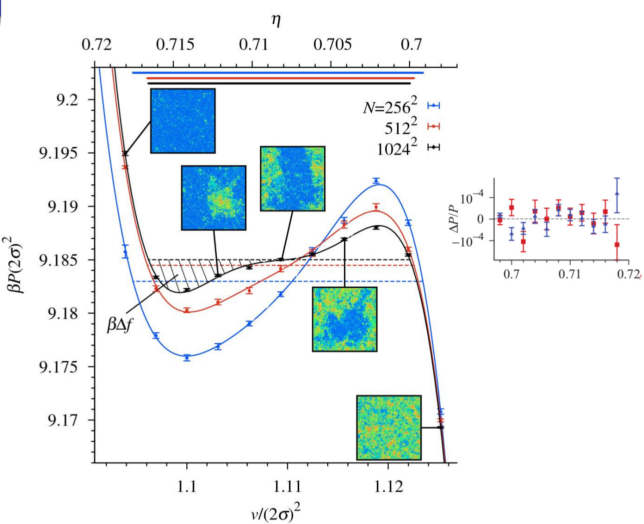
Equilibrium equation of state



- 1st-order liquid–hexatic (Bernard & Krauth, PRL (2011)).
- Many confirmations (Engel, Anderson, Glotzer, Isobe, Bernard, Krauth, PRE Milestone (2013)).

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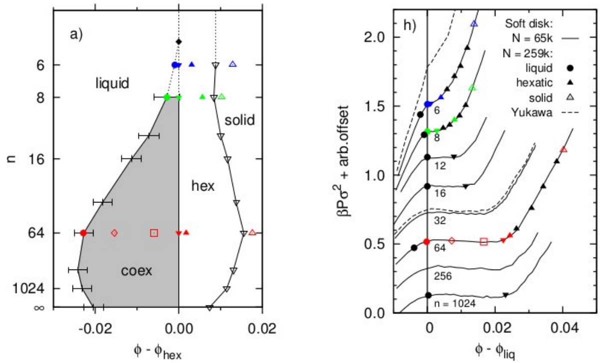
Soft disks

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



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

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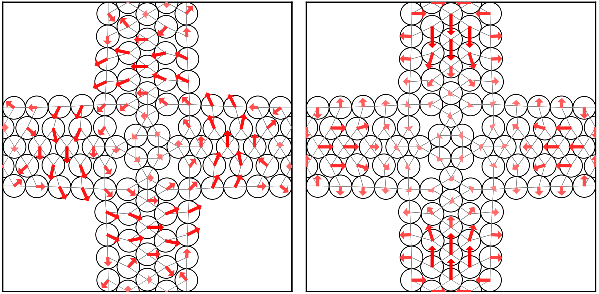
Local Markov chains and packings (1/4)



- Sparse packings are only ‘locally’ stable.
- They trap local Markov chains that move single disks.
- They are a ‘lower-dimensional’ manifold.
- Can they break the connectivity of sample space?

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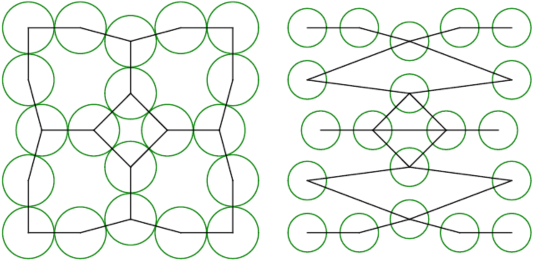
Local Markov chains and packings (2/4)



- Böröczky packing $\Longrightarrow$ ϵ-relaxed Böröczky configuration.
- They no longer trap local Markov chains that move single disks.
- They correspond to a finite portion of sample space.
- For small ϵ, the relaxed Böröczky configurations are 'tough cookies'.

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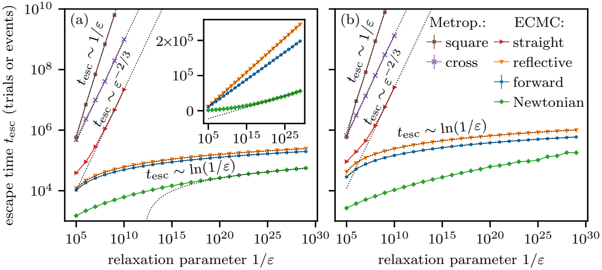
Local Markov chains and packings (3/4)



- Exact scaling prediction from an ϵ-relaxed Böröczky configuration.
- Scaling as a function of ϵ, not of system size N.
- Enormous differences in escape times between local Metropolis algorithm and Event-chain Monte Carlo.
- Enormous differences in escape times between ECMC variants.

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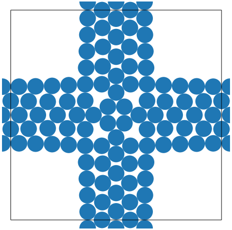
Local Markov chains and packings (4/4)



- Packing $\equiv \infty$-Pressure configuration.
- In an *NPT* MCMC algorithm, pressure is constant, not the box volume.
- Homothetic expansion of box (volume V, side L) part of move set. Scaling as a function of ϵ, not of system size N

$$\frac{\Delta L}{L} \sim \epsilon \sim \frac{1}{\beta P V_{\text{cut}}} \quad \text{(fixed configuration)}. \tag{1}$$

- See Höllmer et al. (2021).

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Conclusions

- Packings, from low to high densities.
- Local Markov chains.
- Hard-disk model.
- NB: Help with Thue (1910)? (Really needed)

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