Zero-free regions for repulsive gasses

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Outline

A **classical model** from statistical physics

Some history and a **major open problem**

Classical results and some analogies to spin systems

New results from ideas of the program

Some manageable **open problems**

Some themes of the program

Relationships between approaches to approximate counting:

Markov chains, correlation decay, polynomial interpolation

Influence of different fields on each other:

algorithms, geometry, statistical physics, combinatorics

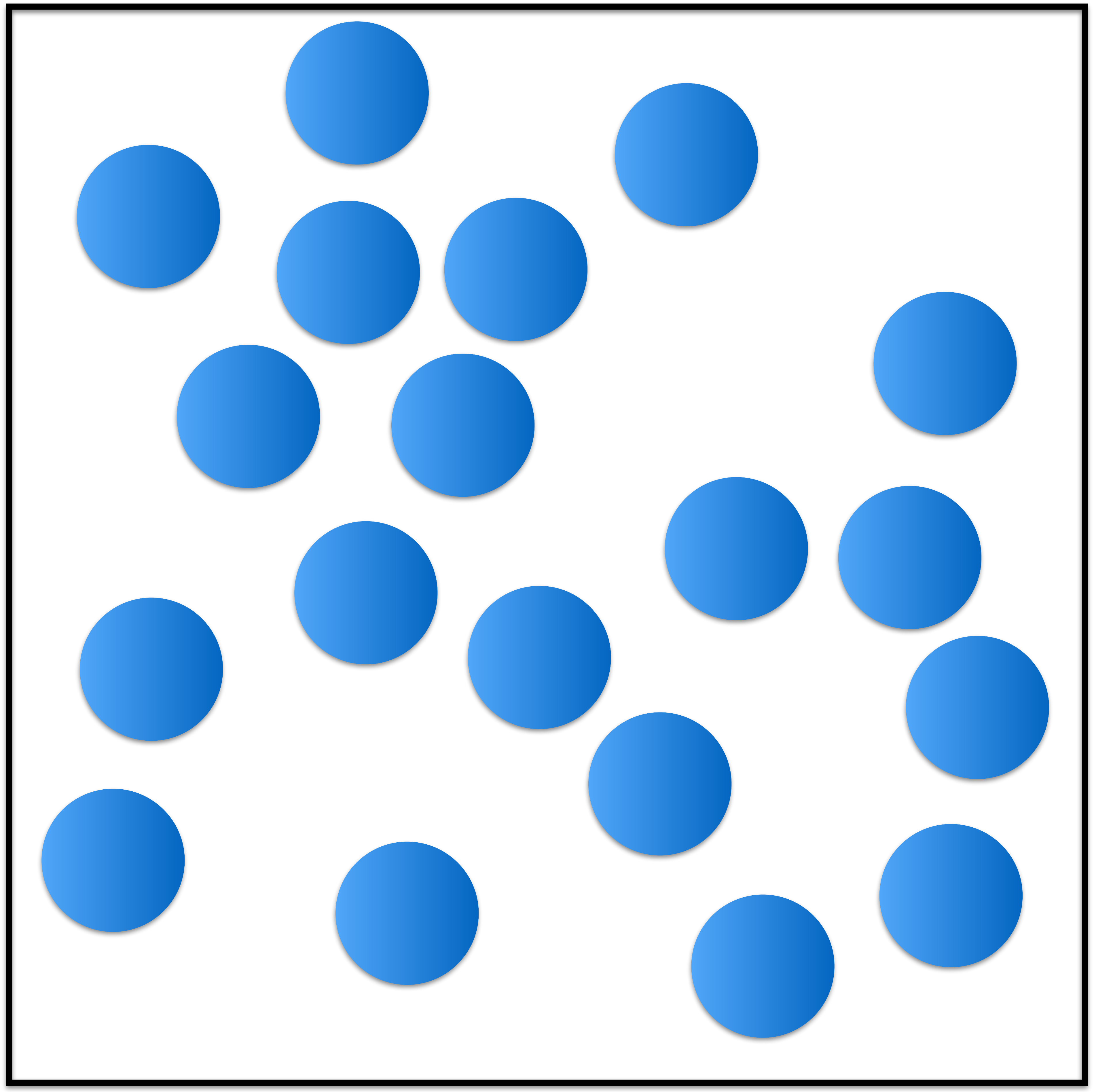
Classical statistical mechanics

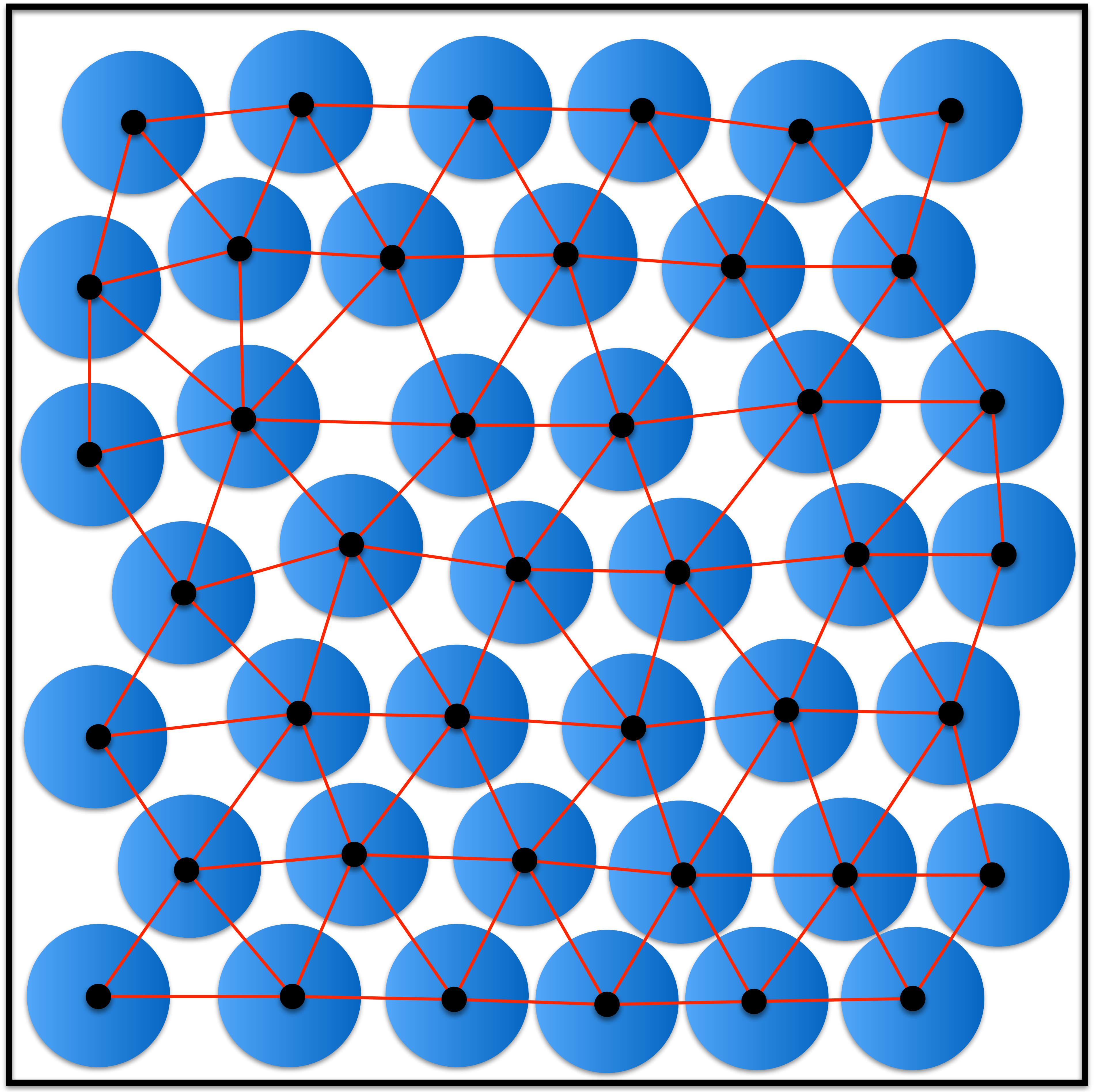
Goal: derive the **macroscopic properties** of fluids (gasses, liquids, solids) from their **microscopic interactions**

This dates back to **Maxwell**, **Boltzmann**, **Gibbs** in the 1800's

Many foundational mathematical results proved in the 1960's: **Penrose**, **Ruelle**, **Lebowitz**, **Groeneveld**, **Lieb**… and earlier: **Mayer**, **Lee**, **Yang**

Classical statistical mechanics





The model

Energy function H from finite point sets in $\mathbb{R}^d$ to $\mathbb{R} \cup \{+\infty\}$

$\Lambda \subset \mathbb{R}^d$ a bounded region

$\lambda > 0$ the **activity parameter**, $\beta > 0$ the **inverse temperature**

Define the **Gibbs point process** as the point process on Λ with density $e^{-\beta H(\cdot)}$ against the Poisson process of intensity λ on Λ

Pair potentials

Most studied class of energy functions: sum of **pairwise interactions**

$\phi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$

$$H(x_1, \ldots, x_k) = \sum_{1 \leq i < j \leq k} \phi(x_i - x_j)$$

The potential is **repulsive** if $\phi \geq 0$

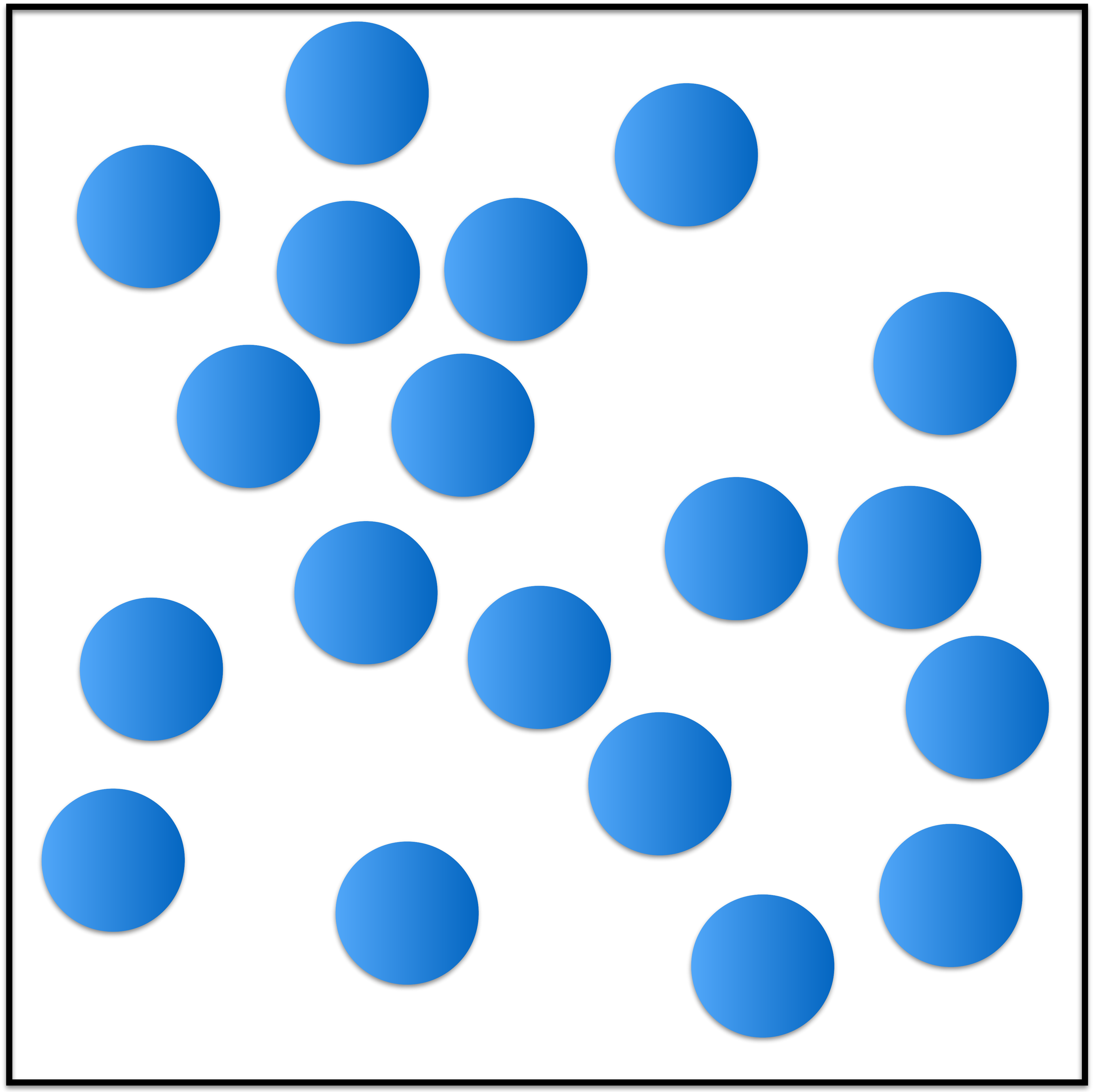
Hard sphere model

Important special case (and our initial motivation)

$\phi(x) = +\infty$ if $||x|| < r$ and 0 otherwise

Only interaction is a **hard-core repulsion**; the point process represents the centers of a packing of spheres of radius r/2

This is a **hard-core model** on an infinite graph



Hard sphere model

Perhaps the original statistical mechanics model, studied mathematically as far back as **van der Waals** and **Boltzmann** (1890's)

Long association with computer science: **Metropolis algorithm** was invented to sample from the 2-d hard disk model

Physicists believe it has a **crystallization phase transition** in dimension 3

Dimension 2 is more subtle, with recent predictions of a `**hexatic phase**' given by Event-chain Monte Carlo (**Bernard-Krauth**)

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THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

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.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed, only two-body forces are considered, and the potential field of a molecule is assumed spherically symmetric.

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† containing N particles. In order to minimize the surface effects we suppose the complete substance to be periodic, consisting of many such squares, each square contain-

PRL **107,** 155704 (2011) PHYSICAL REVIEW LETTERS week ending 7 OCTOBER 2011

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

Etienne P. Bernard* and Werner Krauth†
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(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 root of a large body of theoretical, computational, and experimental research.

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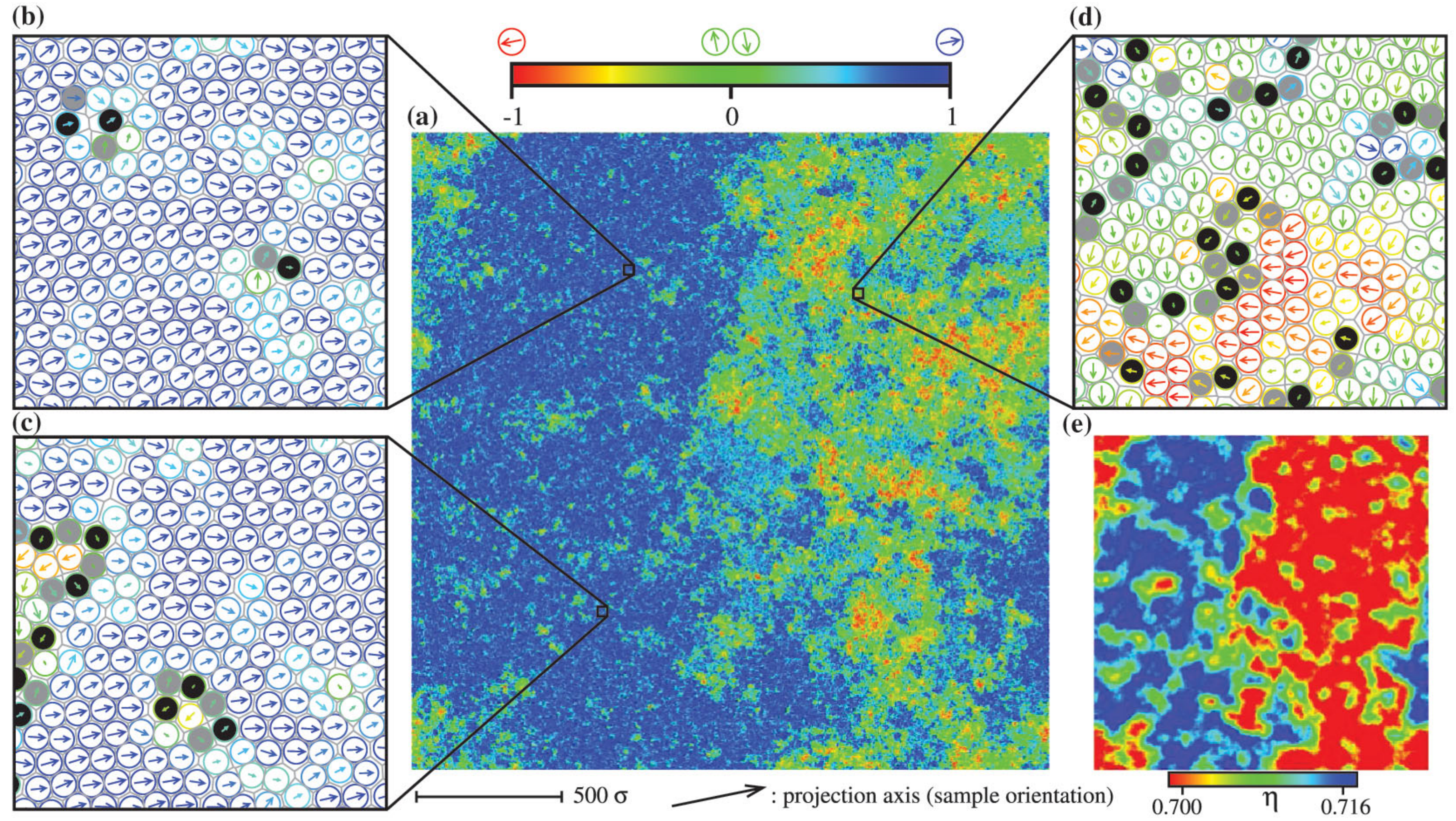
PRL **107,** 155704 (2011) PHYSICAL REVIEW LETTERS week ending 7 OCTOBER 20



Questions

Is the Gibbs point process a reasonably accurate **model of a fluid**? Does it exhibit the phase transitions real fluids do (gas/liquid/solid)

What choices of pair potentials are physically realistic? (**Lennard-Jones**,…)

What **mathematical properties** of the model define the different states of matter? Correlation decay, mixing times,…

Can these properties be **proved rigorously**?

Classical results

Mathematically, **phase transitions** only happen in the infinite volume limit

Partition function: $Z_\Lambda(\lambda) = \sum_{k \geq 0} \frac{\lambda^k}{k!} \int_{\Lambda^k} e^{-\beta H_\phi(x_1, \ldots, x_k)} \, dx_1 \cdots dx_k$

Infinite volume **pressure**: $p(\lambda) = \lim_{\Lambda \to \mathbb{R}^d} \frac{1}{|\Lambda|} \log Z_\Lambda(\lambda)$

Non-analyticities of $p(\lambda)$ on the positive real axis mark **phase transitions**

Phase transitions

Believed that a large class of pair potentials ϕ exhibit phase transitions - the **Crystallization Conjecture**

No phase transition is proved in any monatomic classical gas interacting via a pair potential!

Some special **multi-type** or **multi-body** models have been proved to have a phase transition (e.g. **Widom-Rowlinson** model)

Phase transitions

Major Open Problem

Prove the existence of a phase transition in a classical continuum model of a gas.

Failure to prove this (along with computational issues) led to the popularity of **lattice models** (Ising model, hard-core lattice gas, monomer-dimer model etc.). For many of these models the **Peierls' argument** (1936) can be used to prove the existence of a phase transition

Most results about continuum models pertain to the **gaseous state** (absence of phase transition at low activity / high temperature)

Classical results

PHYSICAL REVIEW VOLUME 87, NUMBER 3 AUGUST 1, 1952

Statistical Theory of Equations of State and Phase Transitions. I. Theory of Condensation

C. N. YANG AND T. D. LEE
Institute for Advanced Study, Princeton, New Jersey

(Received March 31, 1952)

A theory of equations of state and phase transitions is developed that describes the condensed as well as the gas phases and the transition regions. The thermodynamic properties of an infinite sample are studied rigorously and Mayer's theory is re-examined.

I. INTRODUCTION

THIS and a subsequent paper will be concerned with the problem of a statistical theory of equations of state and phase transitions. This problem has always interested physicists both from the practical viewpoint

difference lay, not in the difference of the models, but in the inadequacy of Mayer's method for dealing with a condensed phase. This led to a study of the analytical behavior of the grand partition function of an assembly of interacting atoms, and we were able, as in the special

Zero-free regions imply the absence of phase transition

Classical results

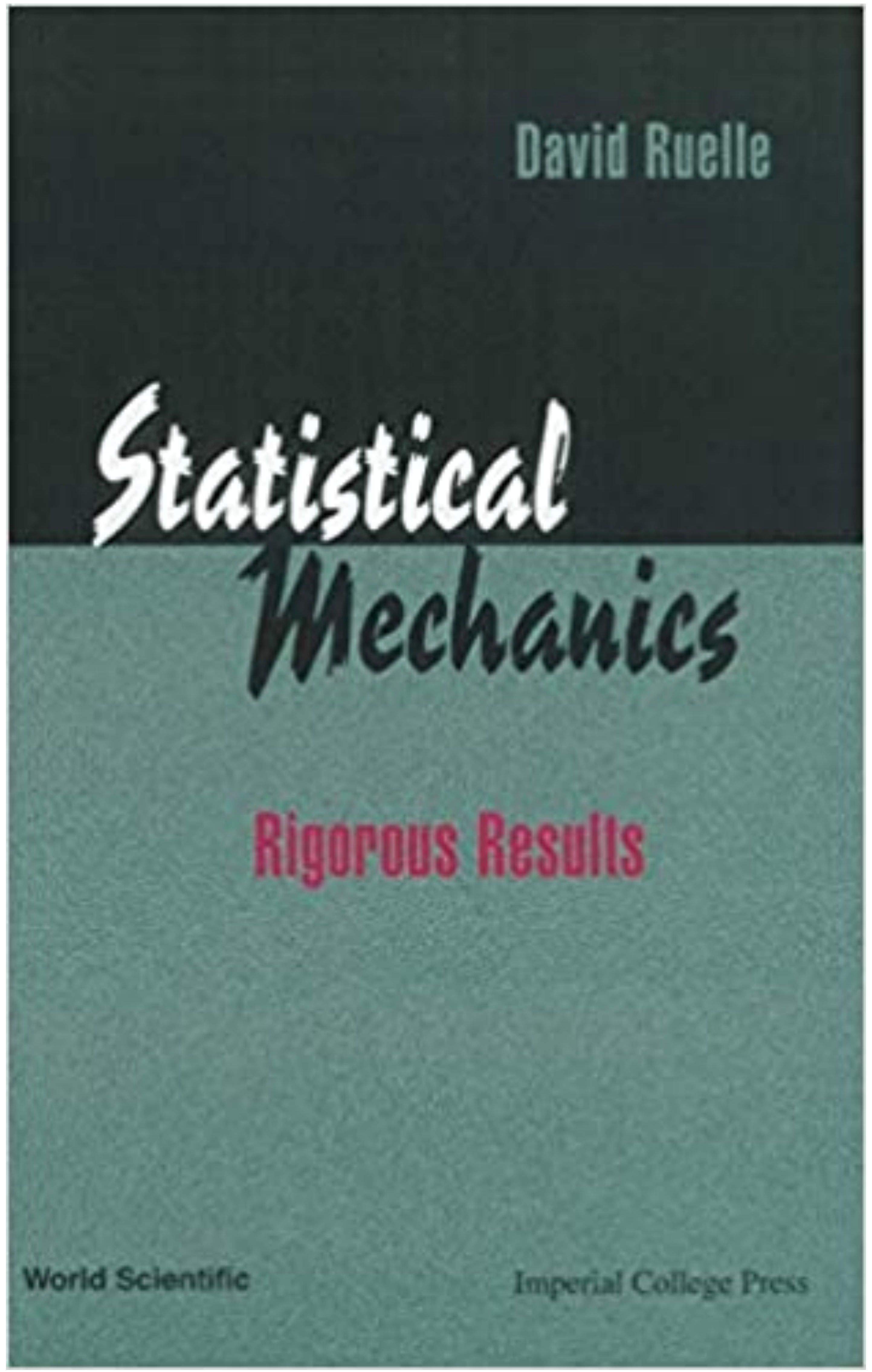
Realistic potentials are **strongly repulsive** at short range, **weakly attractive** at long range

Stable: $\sum_{x,y \in A} \phi(x-y) \geq -B|A|$ for some constant $B \geq 0$. Can take

$B = 0$ for repulsive potentials.

Tempered: $C_\phi := \int_{\mathbb{R}^d} \left| 1 - e^{-\phi(x)} \right| \, dx < \infty$

Classical results



Many results and proofs collected in Ruelle's classic book, mostly still up-to-date!

(Though statisticians have since studied sampling from these processes)

Classical results

Most general result on analyticity and uniqueness: **Penrose**, **Ruelle**: for any stable, tempered potential, $p(\lambda)$ is analytic when $|\lambda| < \dfrac{1}{e^{2B+1}C_\phi}$.

For repulsive potentials ($B = 0$) this is $|\lambda| < \dfrac{1}{eC_\phi}$, proved by **Groeneveld**

Classical results

Proofs via **convergence of the cluster expansion** (power series for log Z around $\lambda = 0$) and **Kirkwood-Salsberg equations**

For repulsive potentials, **Groeneveld** showed that cluster expansion cannot converge for $|\lambda| > \dfrac{1}{C_\phi}$

Closest singularity is on the **negative real axis** and thus not physical. How to avoid this?

Recent results

Probabilistic approaches (for hard spheres):

Disagreement percolation (**Hofer-Temmel**, **Dereudre**)

Markov Chain mixing (**Kannan-Mahoney-Montenegro**, **Hayes-Moore**, **Guo-Jerrum**, **Helmuth-P.-Petti** after **Vigoda**)

The last improves the classical bound for analyticity by a factor $2e$, but only for hard spheres

Analogies to discrete models

Discrete	**Continuous**
2-spin model	Monatomic gas
Hard-core model	Hard-sphere model
Shearer disk, $1/(e\Delta)$	Cluster expansion convergence, $1/(eC_\phi)$
Anti-ferromagnetic	Repulsive
Ferromagnetic	??
hard-core on 2^d-regular graph	d-dimensional hard sphere
Path coupling, $1/\Delta$	Path coupling, $1/C_\phi$ (hard spheres)
Optimized metric, $2/\Delta$	Optimized metric, $2/C_\phi$ (hard spheres)
Weitz, e/Δ	???

New result

Theorem (Michelen-P. ‘20+) A classical gas with a repulsive, tempered potential ϕ exhibits uniqueness and analyticity for $\lambda < \dfrac{e}{C_\phi}$.

Beats the known limit of cluster expansion convergence by factor e and the previous best for the special case of hard spheres by a factor $e/2$

Ideas

Adapt the **Weitz argument** to the continuous setting (strong spatial mixing?)

For infinite-range potentials we needed to go via **zero-freeness**: connection between correlation decay on the infinite tree and zeroes (**Peters-Regts**, **Liu-Sinclair-Srivastava** (x2), **Shao-Sun**)

Difficulties

The building block of correlation decay is the **recursion** for ratios of spin probabilities. Is there an analogue for continuous models?

What is the `**infinite tree**’ for a continuous model?

How to do an **inductive argument**?

Tools

Work in the **multivariate setting**: activity function $\lambda : \mathbb{R}^d \to [0,\infty)$,

$$Z_\Lambda(\lambda) = \sum_{k\geq 0} \frac{1}{k!} \int_{\Lambda^k} \lambda(x_1)\cdots\lambda(x_k) e^{-\beta H(x_1,\ldots x_k)} dx_1 \cdots dx_k$$

Work with **densities** $\rho_\lambda(x)$: the function that computes the expected number of points in a region when integrated

Need 1) a connection between the **partition function** and **densities** and 2) a **recursion** for densities

Densities

Several ways to define **densities** (and k-point densities) but we want one that can be generalized to **complex** activity functions

$$\rho_\lambda(x) = \lambda(x) \cdot \frac{Z(\lambda e^{-\phi(x-\cdot)})}{Z(\lambda)}$$

Definition works for complex λ if $Z(\lambda) \neq 0$

Totally zero-free

We say an activity function $\boldsymbol{\lambda}$ is **totally zero-free** if $Z(\boldsymbol{\lambda}') \neq 0$ for all $\boldsymbol{\lambda}' = \boldsymbol{\lambda}\boldsymbol{\alpha}$, $\boldsymbol{\alpha} \in [0,1]$ (pointwise contractions)

We will prove that if $\boldsymbol{\lambda}(x)$ lies in a small neighborhood of $[0, e/C_\phi - \epsilon)$ then $\boldsymbol{\lambda}$ is totally zero-free.

Integral identity for log Z

Lemma. If λ is totally zero-free, then

$$\log Z(\lambda) = \int_{\mathbb{R}^d} \rho_{\hat{\lambda}_x}(x)\, dx$$

where $\hat{\lambda}_x(y) = \begin{cases} 0 \text{ if } y \in \Lambda_x \\ \lambda(y) \text{ if } y \notin \Lambda_x \end{cases}$ and $\Lambda_x = \{y \in \mathbb{R}^d : \|y\| < \|x\|\}$

Discrete recursion

Recall the basic building block of the **Weitz** argument:

$R_v = \frac{\rho_v}{1 - \rho_v}$ where ρ_v is the probability v is occupied.

On a tree, $R_v = \frac{\lambda}{\prod_{i=1}^{\Delta} (1 + R_{v_i}^{T_i})}$

Continuous recursion

Theorem. Suppose λ is **totally zero-free**. Then for all x,

$$\rho_{\boldsymbol{\lambda}}(x) = \boldsymbol{\lambda}(x) \cdot \exp\left(- \int_{\mathbb{R}^d} \rho_{\boldsymbol{\lambda}_{x \to w}}(w)(1 - e^{-\phi(x-w)})\, dw \right),$$

where $\lambda_{x \to w}(y) = \begin{cases} \boldsymbol{\lambda}(y) e^{-\phi(x-y)} \text{ if } \|x - y\| < \|x - w\| \\ \boldsymbol{\lambda}(y) \text{ if } \|x - y\| \geq \|x - w\| \end{cases}$

Contraction

The recursion defines a functional:

$$F(\lambda, \boldsymbol{\rho}) = \lambda \cdot \exp\left(-\int \boldsymbol{\rho}(x)(1 - e^{-\phi(x)})\, dx\right)$$

This is **contractive** (after applying a potential function) for $\lambda < e/C_\phi$

Zero-freeness

The **contraction** tells us that if densities and activity lie in a certain complex neighborhood, applying the functional keeps us in this neighborhood (just as in **Peters-Regts**).

Our `**induction**' starts with the identically 0 activity function and moves up to show that λ is **totally zero-free** if it pointwise lies in a complex neighborhood of $[0, e/C_\phi - \epsilon)$.

Open Problems

Extend to **stable, tempered potentials**. Includes e.g. Lennard-Jones. (Not clear what to aim for, but the identities go through)

Deterministic algorithms?

Algorithmic applications of **Kirkwood-Salsberg** equations?

Analogue of a **random graph** for continuous particle models?

Thank you!

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