Optimal and Disordered Hyperuniform Point Configurations

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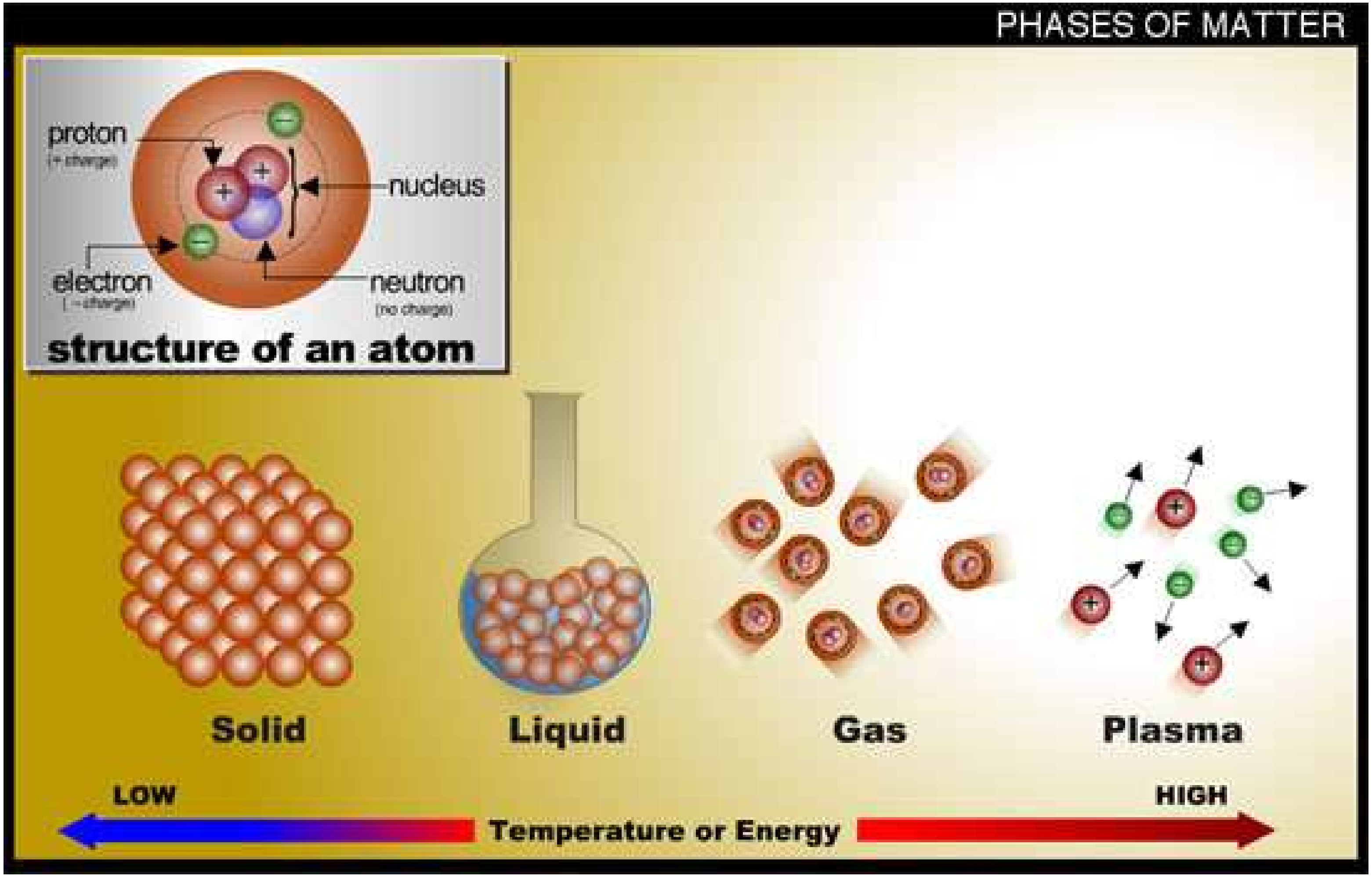
States (Phases) of Matter



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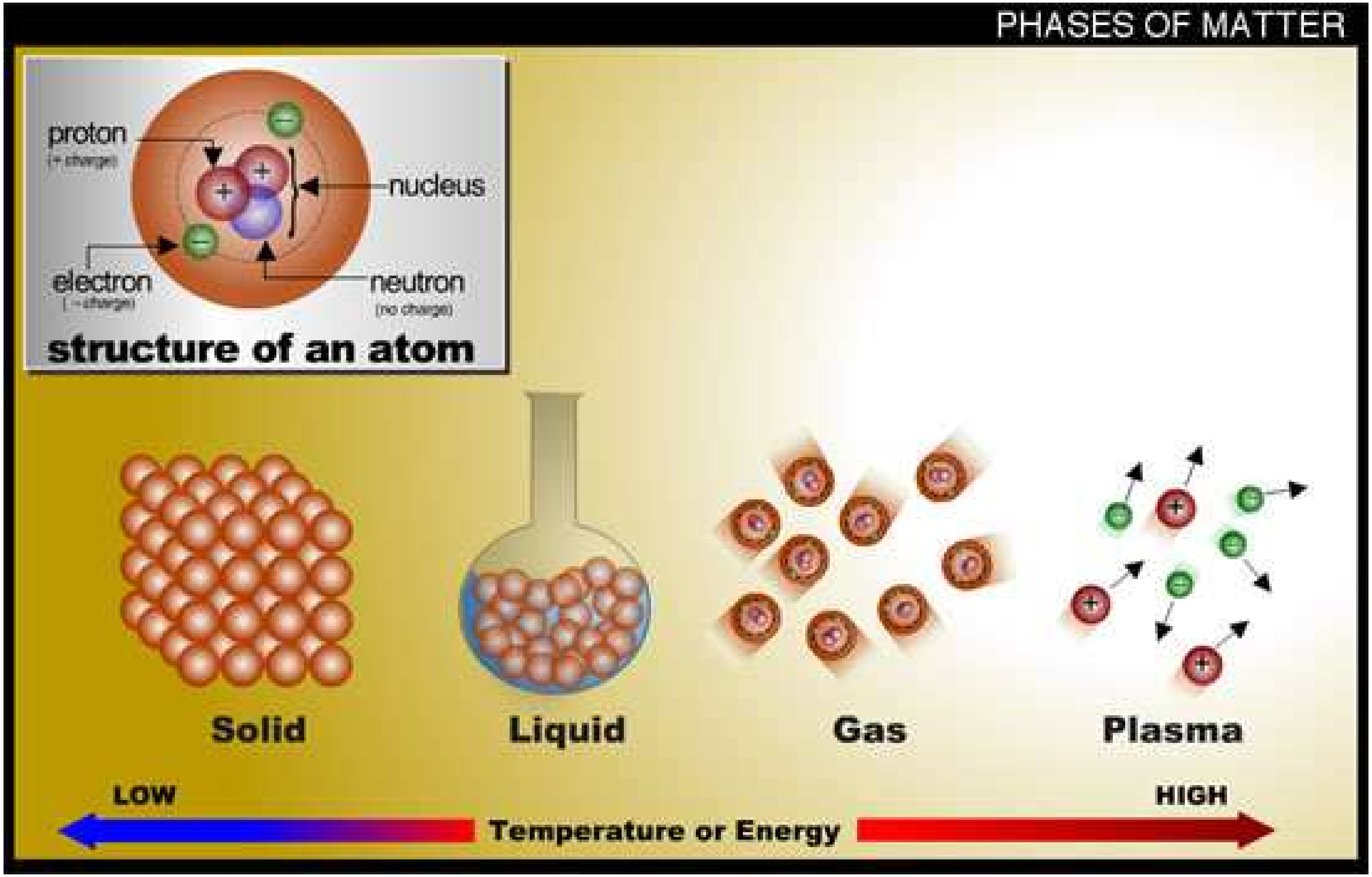

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- **We now know there are a multitude of distinguishable states of matter, e.g., quasicrystals and liquid crystals, which break the continuous translational and rotational symmetries of a liquid differently from a solid crystal.**

What Qualifies as a Distinguishable State of Matter?

Traditional Criteria

- **Homogeneous phase in thermodynamic equilibrium**
- **Interacting entities are microscopic objects, e.g. atoms, molecules or spins**
- **Often, phases are distinguished by symmetry-breaking and/or some qualitative change in some bulk property**

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Broader Criteria

- Reproducible quenched/long-lived metastable or nonequilibrium phases, e.g., spin glasses and structural glasses
- Interacting entities need not be microscopic, but can include building blocks across a wide range of length scales, e.g., colloids and metamaterials
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New states of matter become more compelling if they:

- Give rise to or require new ideas and/or experimental/theoretical tools
- Technologically important

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- **Disordered hyperuniform many-particle systems can be regarded to be new ideal states of disordered matter in that they**

  (i) *behave more like crystals or quasicrystals in the manner in which they suppress large-scale density fluctuations, and yet are also like liquids and glasses because they are statistically isotropic structures with no Bragg peaks*;

  (ii) *can exist as both as equilibrium and quenched nonequilibrium phases*;

  (iii) *and, appear to be endowed with unique bulk physical properties*.

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Understanding such states of matter, which have technological importance, require new theoretical tools.

- **All perfect crystals (periodic systems) and quasicrystals are hyperuniform.**

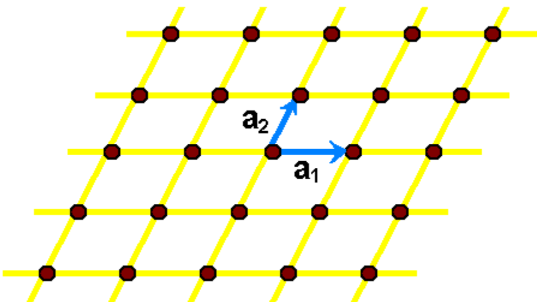
- **Thus, hyperuniformity provides a unified means of categorizing and characterizing crystals, quasicrystals and such special disordered systems.**

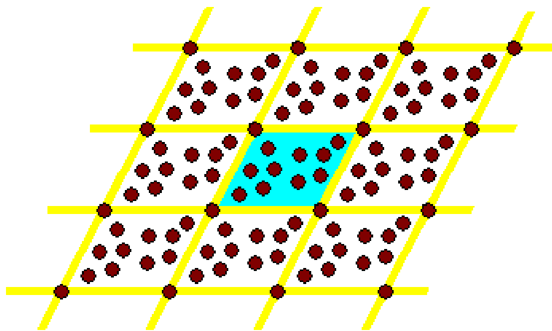
Definitions

- A **point process** in d-dimensional Euclidean space $\mathbb{R}^d$ is a distribution of an infinite number of points in $\mathbb{R}^d$ with configuration $\mathbf{r}_1, \mathbf{r}_2, \ldots$ with a well-defined number density ρ (number of points per unit volume). This is statistically described by the n-**particle correlation function** $g_n(\mathbf{r}_1, , \ldots, \mathbf{r}_n)$.
- A **lattice** L in d-dimensional Euclidean space $\mathbb{R}^d$ is the set of points that are integer linear combinations of d basis (linearly independent) vectors $\mathbf{a}_i$, i.e.,

$$\{n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \cdots + n_d\mathbf{a}_d \mid n_1, \ldots, n_d \in Z\}$$

The space $\mathbb{R}^d$ can be geometrically divided into identical regions F called **fundamental cells**, each of which contains just one point. For example, in $\mathbb{R}^2$:





- Every lattice L has a **dual (or reciprocal)** lattice L^*.
- A **periodic** point distribution in $\mathbb{R}^d$ is a fixed but arbitrary configuration of N points ($N \geq 1$) in each fundamental cell of a lattice.

Definitions

- For statistically homogeneous and isotropic point processes in $\mathbb{R}^d$ at number density ρ , $g_2(r)$ is a nonnegative radial function that is proportional to the probability density of pair distances r.

- We call

$$h(r) \equiv g_2(r) - 1$$

the total correlation function.

- When there is no long-range order in the system, $h(r) \longrightarrow 0$ [or $g_2(r) \longrightarrow 1$] in the large-r limit. We call a point process disordered if $h(r)$ tends to zero sufficiently rapidly such that it is integrable over all space.

- The nonnegative structure factor $S(k)$ is defined in terms of the Fourier transform of $h(r)$, which we denote by $\tilde{h}(k)$:

$$S(k) \equiv 1 + \rho\tilde{h}(k),$$

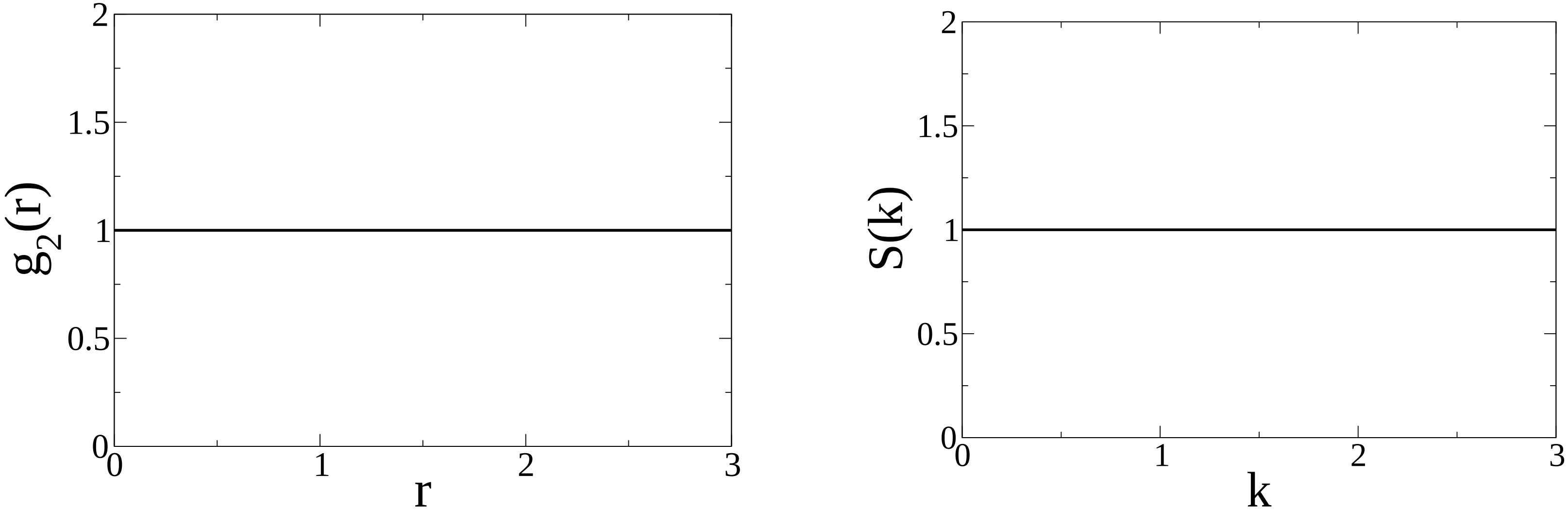
where k denotes wavenumber.

- When there is no long-range order in the system, $S(k) \longrightarrow 1$ in the large-k limit, the dual-space analog of the aforementioned direct space condition.

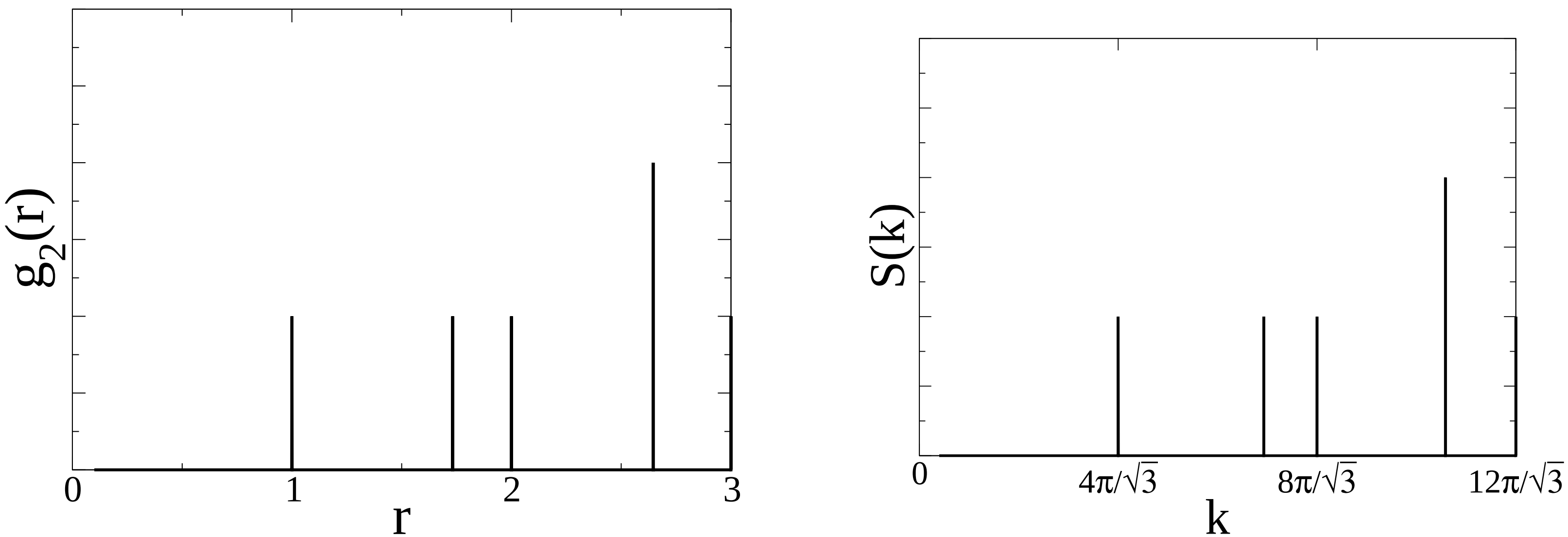
- In some generalized sense, $S(k)$ can be viewed as a probability density of pair distances of "points" in reciprocal space.

Pair Statistics for Spatially Uncorrelated and Ordered Point Processes

Poisson Distribution (Ideal Gas)

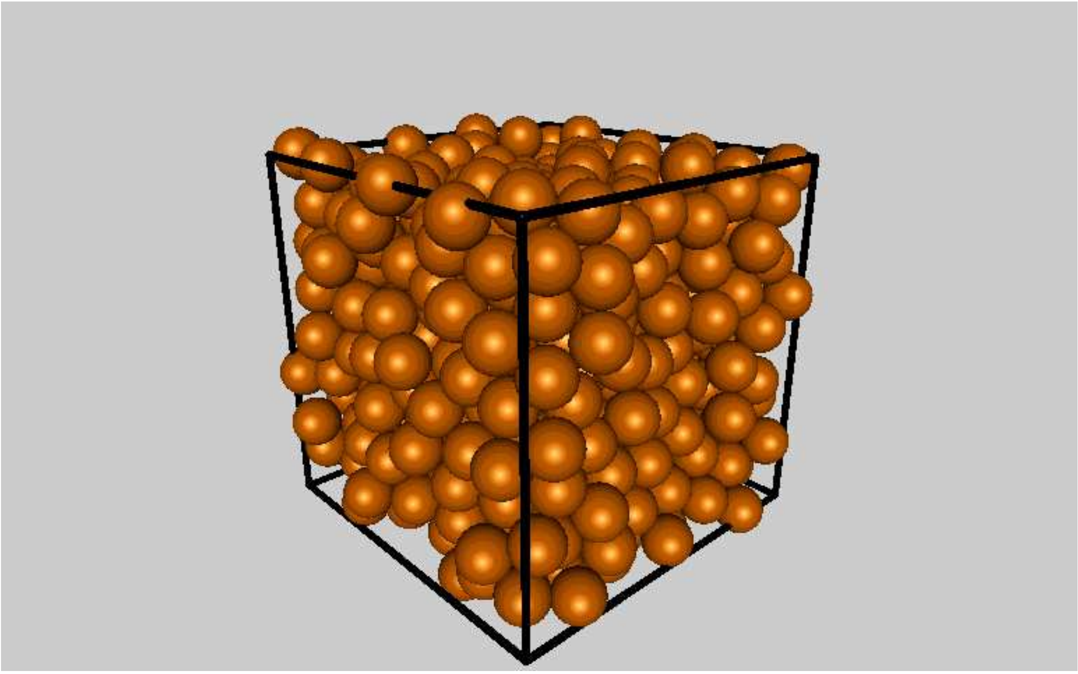


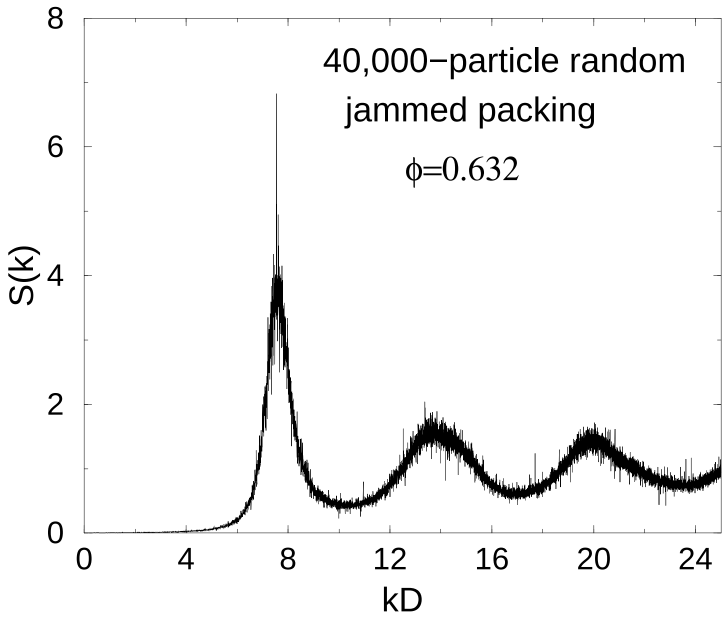
Lattice



Curiosities

- **Disordered jammed packings**





$S(k)$ appears to vanish in the limit $k \to 0$: very unusual behavior for a disordered system.

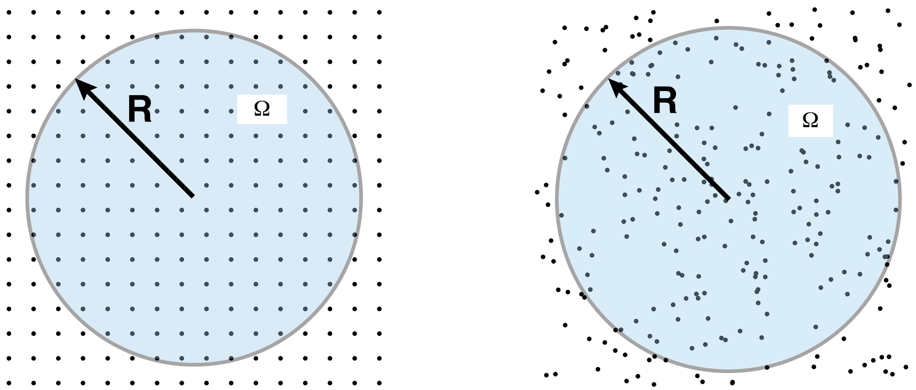
- **Harrison-Zeldovich spectrum for density fluctuations in the early Universe: $S(k) \sim k$ for sufficiently small k.**

Gabrielli et al. (2003)

Local Density Fluctuations for General Point Patterns

Torquato and Stillinger, PRE (2003)

- **Points can represent molecules of a material, stars in a galaxy, or trees in a forest. Let Ω represent a spherical window of radius R in d-dimensional Euclidean space $\mathbb{R}^d$.**



Average number of points in window of volume $v_1(R)$: $\langle N(R)\rangle = \rho v_1(R) \sim R^d$

Local number variance: $\sigma^2(R) \equiv \langle N^2(R)\rangle - \langle N(R)\rangle^2$

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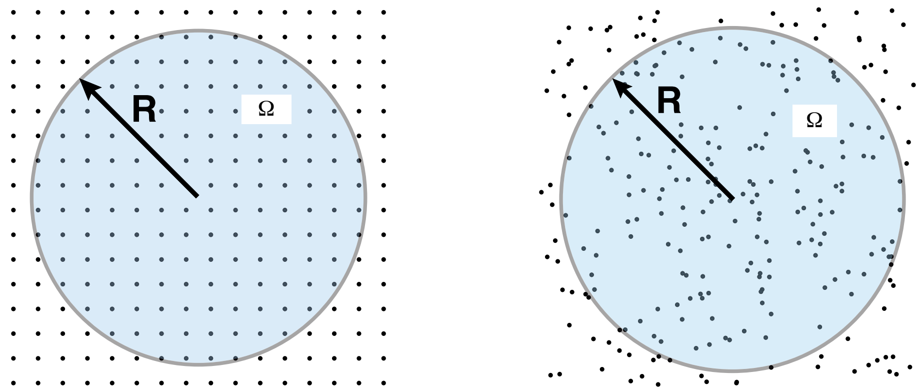

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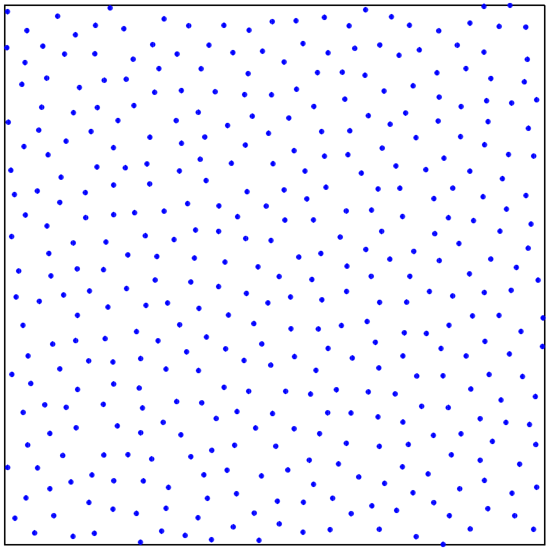
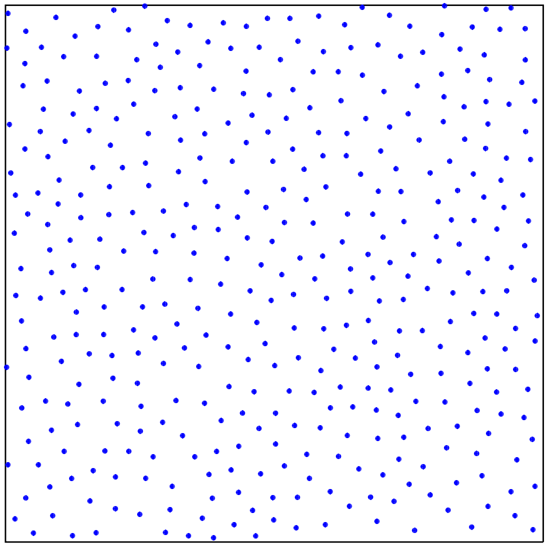
- For a Poisson point pattern and many disordered point patterns, $\sigma^2(R) \sim R^d$.
- We call point patterns whose variance grows more slowly than R^d (window volume) hyperuniform . This implies that structure factor $S(k) \to 0$ for $k \to 0$.
- All perfect crystals and perfect quasicrystals are hyperuniform such that $\sigma^2(R) \sim R^{d-1}$: number variance grows like window surface area.

Hyperuniformity is aka superhomogeneity: Gabrielli, Joyce & Sylos Labini, Phys. Rev. E (2002)

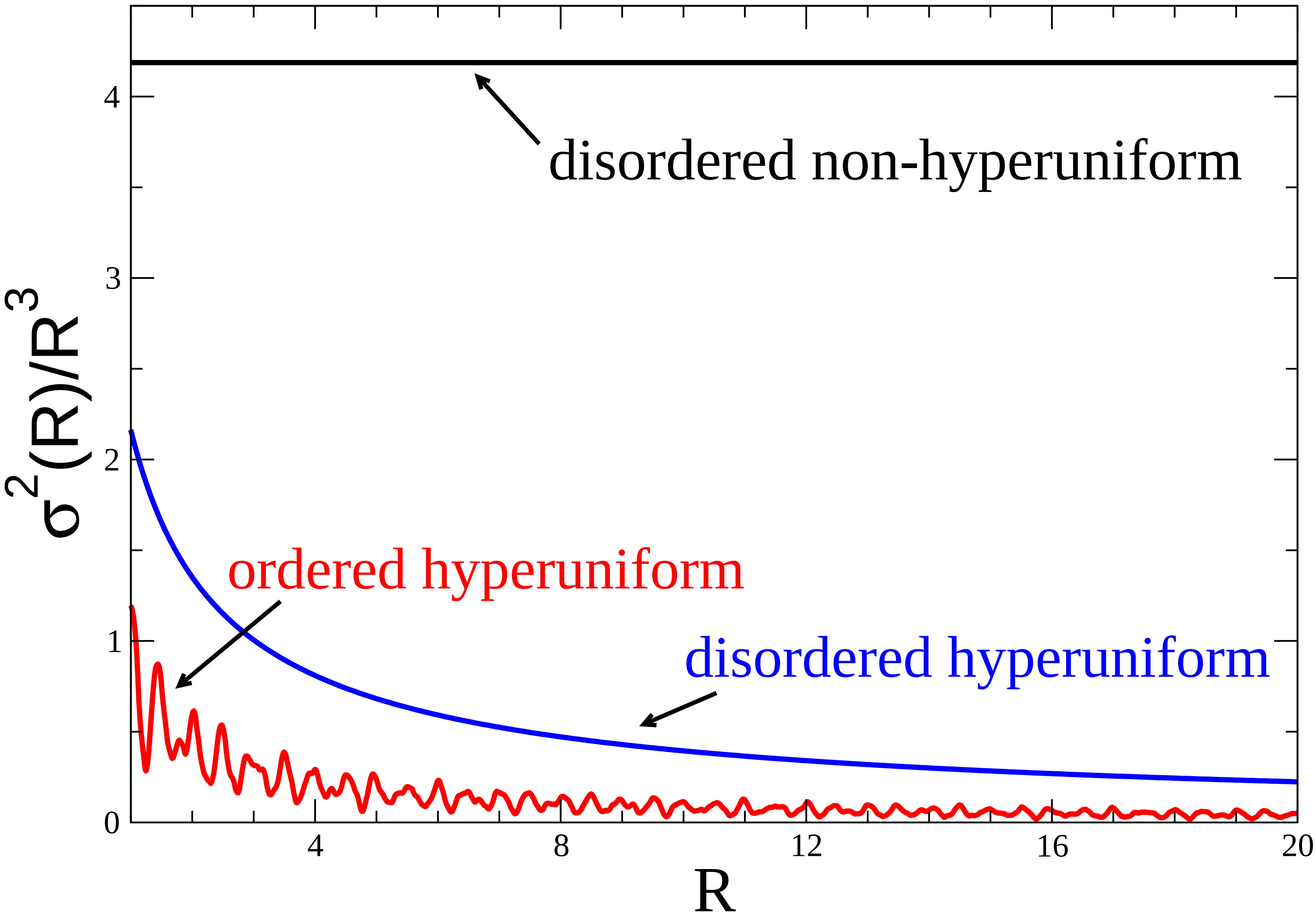
Hidden Order on Large Length Scales





Which is the hyperuniform pattern?

Scaled Number Variance for 3D Systems at Unit Density



Outline

- Hyperuniform Point Configurations: History and Recent Developments
- Connections to Sphere Packing, Covering and Quantizer Problems

Running themes:

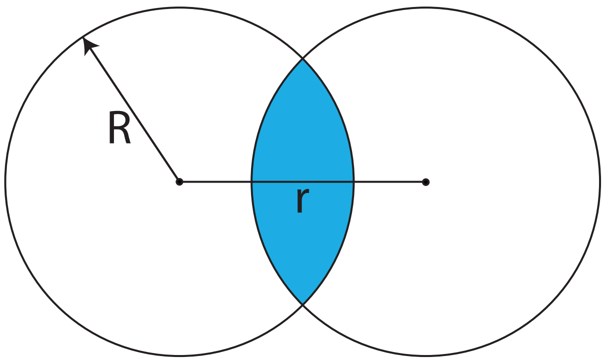
1. **All of these problems can be cast as optimization tasks; specifically energy-minimizing point configurations.**
2. **Optimal solutions can be both ordered and disordered.**

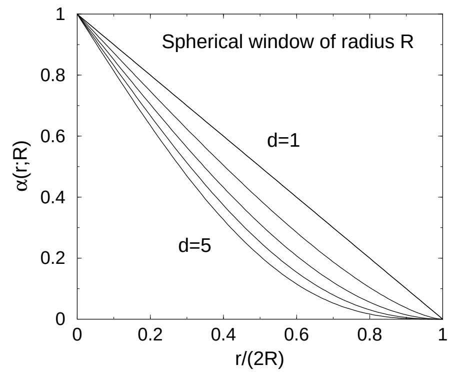
ENSEMBLE-AVERAGE FORMULATION

- **For a translationally invariant point process at number density ρ in $\mathbb{R}^d$:**

$$\sigma^2(R) \quad = \quad \langle N(R) \rangle \Big[1 + \rho \int_{\mathbb{R}^d} h(\mathbf{r}) \alpha(\mathbf{r}; R) d\mathbf{r} \Big]$$

$\alpha(\mathbf{r}; R)$**- scaled intersection volume of 2 windows of radius R separated by $\mathbf{r}$**





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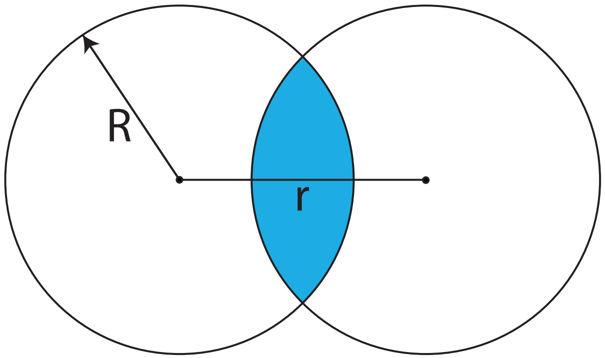

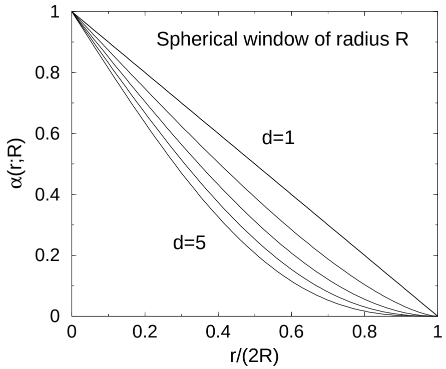

- **For large R, we can show**

$$\sigma^2(R) = 2^d \phi \Big[A \left(\frac{R}{D} \right)^d + B \left(\frac{R}{D} \right)^{d-1} + o \left(\frac{R}{D} \right)^{d-1} \Big],$$

where A and B are the "volume" and "surface-area" coefficients:

$$A = S(\mathbf{k} = \mathbf{0}) = 1 + \rho \int_{\mathbb{R}^d} h(\mathbf{r}) d\mathbf{r}, \qquad B = -c(d) \int_{\mathbb{R}^d} h(\mathbf{r}) r d\mathbf{r},$$

D**: microscopic length scale,** ϕ**: dimensionless density**

- **Hyperuniform: $A = 0$, $B > 0$**

INVERTED CRITICAL PHENOMENA: Ornstein-Zernike Formalism

- $h(\mathbf{r})$ can be divided into direct correlations, via function $c(\mathbf{r})$, and indirect correlations:

$$\tilde{c}(\mathbf{k}) = \frac{\tilde{h}(\mathbf{k})}{1 + \rho\tilde{h}(\mathbf{k})}$$

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- **For any hyperuniform system, $\tilde{h}(\mathbf{k}=\mathbf{0}) = -1/\rho$, and thus $\tilde{c}(\mathbf{k}=\mathbf{0}) = -\infty$. Therefore, at the "critical" reduced density ϕ_c, $h(\mathbf{r})$ is short-ranged and $c(\mathbf{r})$ is long-ranged.**

- **This is the inverse of the behavior at liquid-gas (or magnetic) critical points, where $h(\mathbf{r})$ is long-ranged (compressibility or susceptibility diverges) and $c(\mathbf{r})$ is short-ranged.**

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- For sufficiently large d at a disordered hyperuniform state, whether achieved via a nonequilibrium or an equilibrium route,

$$c(\mathbf{r}) \sim -\frac{1}{r^{d-2+\eta}} \qquad (r \to \infty), \qquad c(\mathbf{k}) \sim -\frac{1}{k^{2-\eta}} \qquad (k \to 0),$$

$$h(\mathbf{r}) \sim -\frac{1}{r^{d+2-\eta}} \qquad (r \to \infty), \qquad S(\mathbf{k}) \sim k^{2-\eta} \qquad (k \to 0),$$

where η is a new critical exponent.

- One can think of a hyperuniform system as one resulting from an effective pair potential $v(r)$ at large r that is a generalized Coulombic interaction between like charges. Why? Because

$$\frac{v(r)}{k_B T} \sim -c(r) \sim \frac{1}{r^{d-2+\eta}} \qquad (r \to \infty)$$

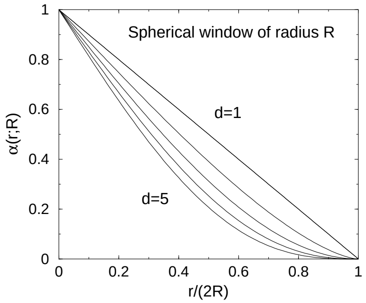
- However, long-range interactions are not required to drive a nonequilibrium system to a disordered hyperuniform state.

SINGLE-CONFIGURATION FORMULATION & GROUND STATES

- **We showed**

$$\sigma^2(R) = 2^d\phi\left(\frac{R}{D}\right)^d\left[1 - 2^d\phi\left(\frac{R}{D}\right)^d + \frac{1}{N}\sum_{i\neq j}^{N}\alpha(r_{ij};R)\right]$$

where $\alpha(r;R)$ can be viewed as a repulsive pair potential:



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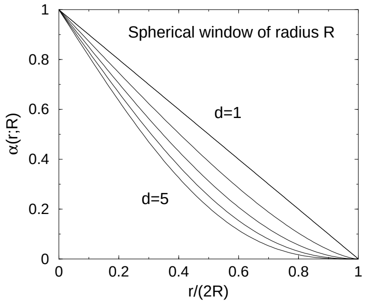

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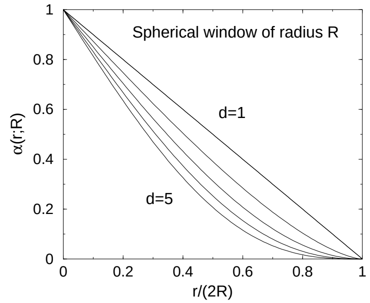
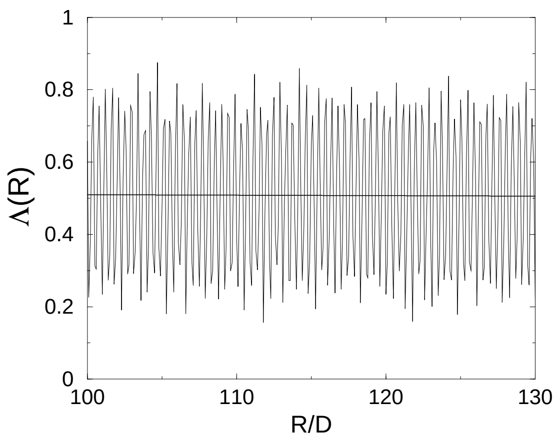


- **Finding global minimum of $\sigma^2(R)$ equivalent to finding ground states (energy minimizing configurations).**
- **For large R, in the special case of hyperuniform systems,**

$$\sigma^2(R) = \Lambda(R)\left(\frac{R}{D}\right)^{d-1} + \mathcal{O}\left(\frac{R}{D}\right)^{d-3}$$

Triangular Lattice (Average value=0.507826)



Hyperuniformity and Number Theory

- **Averaging fluctuating quantity $\Lambda(R)$ gives coefficient of interest:**

$$\overline{\Lambda} = \lim_{L\to\infty} \frac{1}{L} \int_0^L \Lambda(R) dR$$

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- **Averaging fluctuating quantity $\Lambda(R)$ gives coefficient of interest:**

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- **We showed that for a lattice**

$$\sigma^2(R) = \sum_{\mathbf{q}\neq\mathbf{0}} \left(\frac{2\pi R}{q}\right)^d [J_{d/2}(qR)]^2, \qquad \overline{\Lambda} = 2^d \pi^{d-1} \sum_{\mathbf{q}\neq\mathbf{0}} \frac{1}{|\mathbf{q}|^{d+1}}.$$

- **Epstein zeta function for a lattice is defined by**

$$Z_Q(s) = \sum_{\mathbf{q}\neq\mathbf{0}} \frac{1}{|\mathbf{q}|^{2s}}, \qquad \textbf{Re } s > d/2.$$

  Summand can be viewed as an inverse power-law potential. For lattices, minimizer of $Z_Q(d+1)$ is the lattice dual to the minimizer of $\overline{\Lambda}$.

- **Surface-area coefficient $\overline{\Lambda}$ provides useful way to rank order crystals, quasicrystals and special correlated disordered point patterns.**

Quantifying Suppression of Density Fluctuations at Large Scales: 1D

- **The surface-area coefficient $\overline{\Lambda}$ for some crystal, quasicrystal and disordered one-dimensional hyperuniform point patterns.**

Pattern	$\overline{\Lambda}$
Integer Lattice	$1/6 \approx 0.166667$
Step+Delta-Function g_2	3/16 =0.1875
Fibonacci Chain*	0.2011
Step-Function g_2	$1/4 = 0.25$
Randomized Lattice	$1/3 \approx 0.333333$

*Zachary & Torquato (2009)

Quantifying Suppression of Density Fluctuations at Large Scales: 2D

- **The surface-area coefficient $\overline{\Lambda}$ for some crystal, quasicrystal and disordered two-dimensional hyperuniform point patterns.**

2D Pattern	$\overline{\Lambda}$
Triangular Lattice	0.508347
Square Lattice	0.516401
Honeycomb Lattice	0.567026
Kagomé Lattice	0.586990
Penrose Tiling*	0.597798
Step+Delta-Function g_2	0.600211
Step-Function g_2	0.848826

*Zachary & Torquato (2009)

Quantifying Suppression of Density Fluctuations at Large Scales: 3D

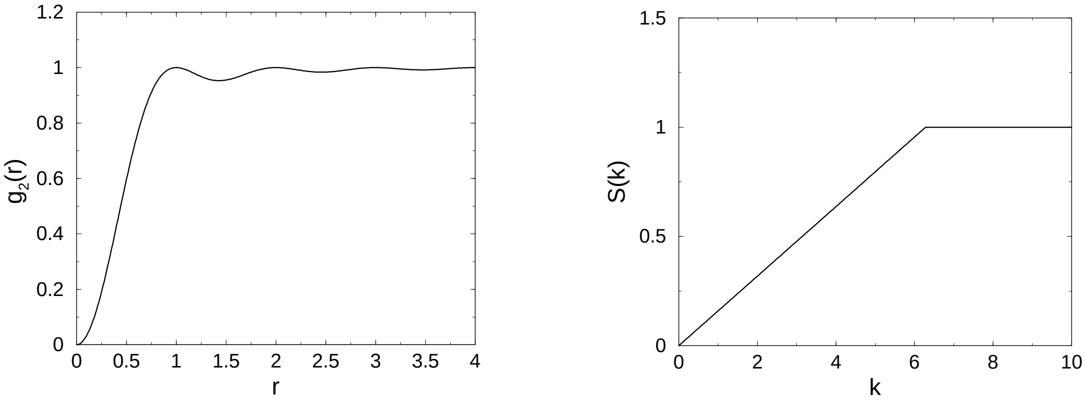
- **Contrary to conjecture that lattices associated with the densest sphere packings have smallest variance regardless of d, we have shown that for $d = 3$, BCC has a smaller variance than FCC.**

Pattern	$\overline{\Lambda}$
BCC Lattice	1.24476
FCC Lattice	1.24552
HCP Lattice	1.24569
SC Lattice	1.28920
Diamond Lattice	1.41892
Wurtzite Lattice	1.42184
Damped-Oscillating g_2	1.44837
Step+Delta-Function g_2	1.52686
Step-Function g_2	2.25

- **Carried out analogous calculations in high d (Zachary & Torquato, 2009), of importance in communications. Disordered point patterns may win in high d (Torquato & Stillinger, 2006).**

1D Translationally Invariant Hyperuniform Systems

- **An interesting 1D hyperuniform point pattern is the distribution of the nontrivial zeros of the Riemann zeta function (eigenvalues of random Hermitian matrices and bus arrivals in Cuernavaca): Dyson, 1970; Montgomery, 1973; Krbàlek & Šeba, 2000;** $g_2(r) = 1 - \sin^2(\pi r)/(\pi r)^2$



1D point process is always negatively correlated, i.e., $g_2(r) \leq 1$ **and pairs of points tend to repel one another, i.e.,** $g_2(r) \to 0$ **as** r **tends to zero.**

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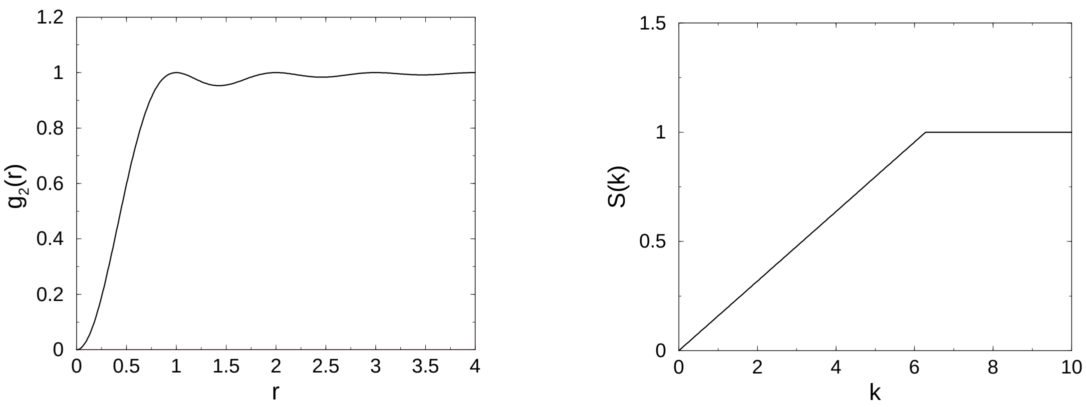

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- **Dyson mapped this problem to a 1D log Coulomb gas at positive temperature:** $k_B T = 1/2$**. The total potential energy of the system is given by**

$$\Phi_N(\mathbf{r}^N) = \frac{1}{2}\sum_{i=1}^{N}|\mathbf{r}_i|^2 - \sum_{i\leq j}^{N}\ln(|\mathbf{r}_i - \mathbf{r}_j|)\,.$$

Sandier and Serfaty, Prob. Theory & Related Fields (2015)

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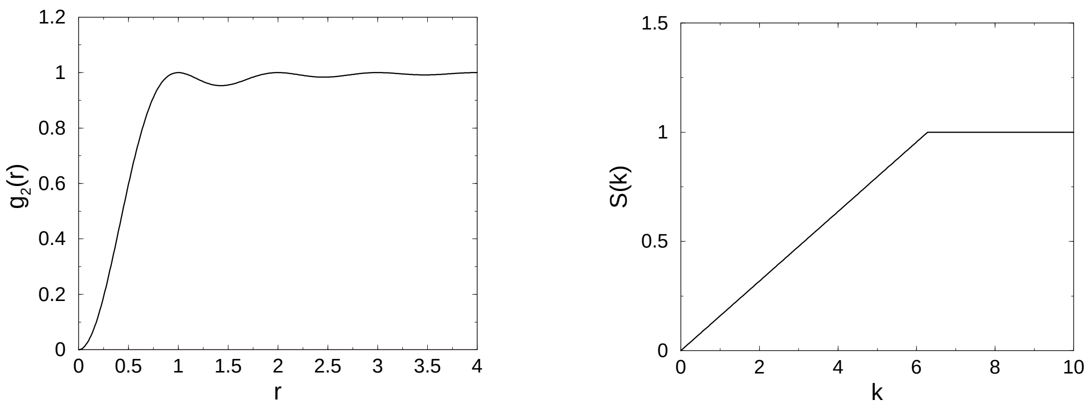
- **An interesting 1D hyperuniform point pattern is the distribution of the nontrivial zeros of the Riemann zeta function (eigenvalues of random Hermitian matrices and bus arrivals in Cuernavaca): Dyson, 1970; Montgomery, 1973; Krbàlek & Šeba, 2000; $g_2(r) = 1 - \sin^2(\pi r)/(\pi r)^2$**



1D point process is always negatively correlated, i.e., $g_2(r) \leq 1$ and pairs of points tend to repel one another, i.e., $g_2(r) \to 0$ as r tends to zero.

- **Dyson mapped this problem to a 1D log Coulomb gas at positive temperature: $k_B T = 1/2$. The total potential energy of the system is given by**

$$\Phi_N(\mathbf{r}^N) = \frac{1}{2}\sum_{i=1}^{N} |\mathbf{r}_i|^2 - \sum_{i \leq j}^{N} \ln(|\mathbf{r}_i - \mathbf{r}_j|)\,.$$

Sandier and Serfaty, Prob. Theory & Related Fields (2015)

- **Constructing and/or identifying homogeneous, isotropic hyperuniform patterns for $d \geq 2$ is more challenging. We now know of many more examples.**

More Recent Examples of Disordered Hyperuniform Systems

- **Fermionic point processes**: $S(k) \sim k$ **as** $k \to 0$ **(ground states and/or positive temperature equilibrium states): Torquato et al. J. Stat. Mech. (2008)**
- **Maximally random jammed (MRJ) particle packings:** $S(k) \sim k$ **as** $k \to 0$ **(nonequilibrium states): Donev et al. PRL (2005)**
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- **Avian Photoreceptors (nonequilibrium states): Jiao et al. PRE (2014)**
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Nearly Hyperuniform Disordered Systems

- **Amorphous Silicon** (nonequilibrium states): Henja et al. PRB (2013)
- **Structural Glasses** (nonequilibrium states): Marcotte et al. (2013)

Hyperuniformity and Jammed Packings

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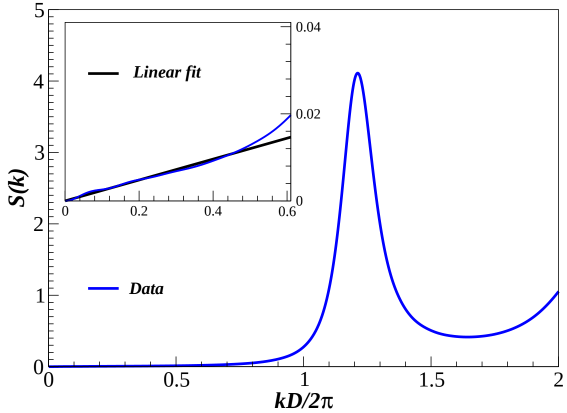
- **Such packings of identical spheres have been shown to be hyperuniform with quasi-long-range (QLR) pair correlations in which $h(r)$ decays as $-1/r^4$ (Donev, Stillinger & Torquato, PRL, 2005).**



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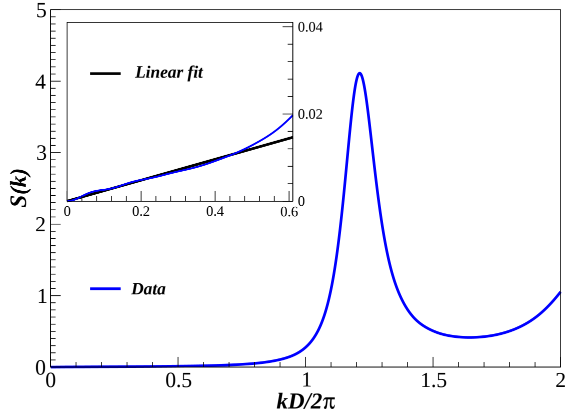

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- **Apparently, hyperuniform QLR correlations with decay $-1/r^{d+1}$ are a universal feature of general MRJ packings in $\mathbb{R}^d$.**

Zachary, Jiao and Torquato, PRL (2011): ellipsoids, superballs, sphere mixtures

Berthier et al., PRL (2011); Kurita and Weeks, PRE (2011) : sphere mixtures

Jiao and Torquato, PRE (2011): polyhedra

In the Eye of a Chicken: Photoreceptors

- **Optimal spatial sampling of light requires that photoreceptors be arranged in the triangular lattice (e.g., insects and some fish).**
- **Birds are highly visual animals, yet their cone photoreceptor patterns are irregular.**

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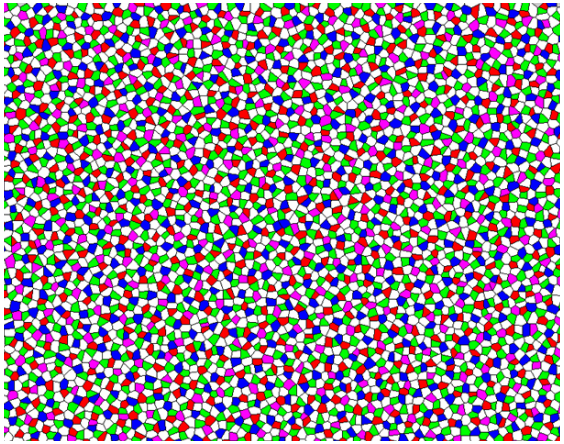
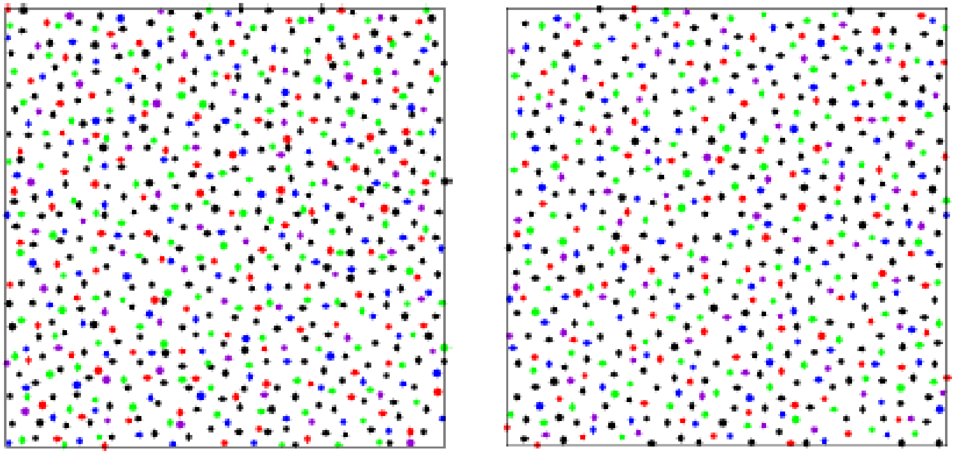


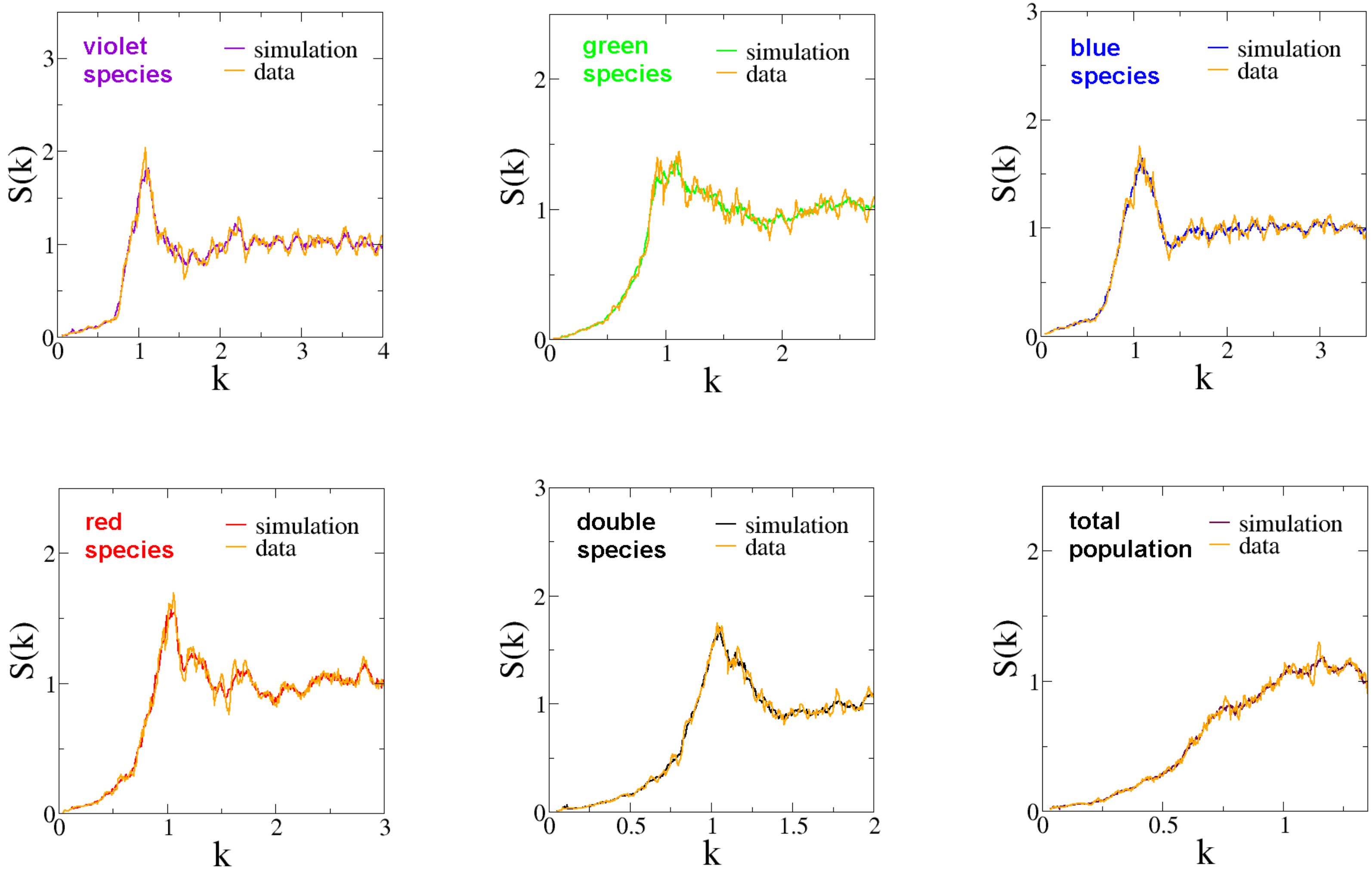
5 Cone Types



Jiao, Corbo & Torquato, PRE (2014).

Avian Cone Photoreceptors

- **Disordered mosaics of both total population and individual cone types are effectively hyperuniform, which has been never observed in any system before (biological or not). We term this multi-hyperuniformity.**



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Hyperuniformity, Free Fermions & Determinantal Point Processes

- **One can map random Hermitian matrices (GUE), fermionic gases, and zeros of the Riemann zeta function to a unique hyperuniform point process on $\mathbb{R}$.**

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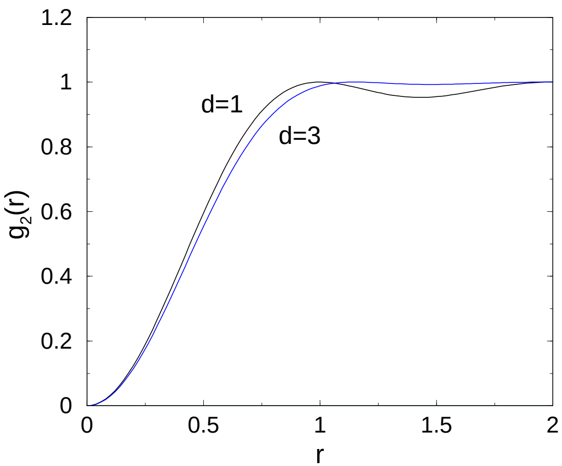
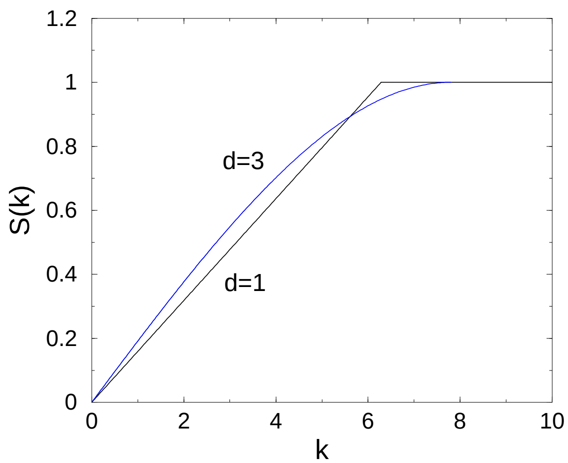
- **We provide exact generalizations of such a point process in d-dimensional Euclidean space $\mathbb{R}^d$ and the corresponding n-particle correlation functions, which correspond to those of spin-polarized free fermionic systems in $\mathbb{R}^d$.**





$$g_2(r) = 1 - \frac{2\Gamma(1+d/2)\cos^2\left(rK - \pi(d+1)/4\right)}{K\,\pi^{d/2+1}\,r^{d+1}} \qquad (r \to \infty)$$

$$S(k) = \frac{c(d)}{2K}k + \mathcal{O}(k^3) \qquad (k \to 0) \qquad (K: \text{Fermi sphere radius})$$

Torquato, Zachary & Scardicchio, J. Stat. Mech., 2008

Scardicchio, Zachary & Torquato, Phys. Rev., 2009

Hyperuniformity, Free Fermions & Determinantal Point Processe

- Let $H(\mathbf{r}) = H(-\mathbf{r})$ be a translationally invariant Hermitian-symmetric kernel of an integral operator $\mathcal{H}$. A translationally invariant **determinantal point process** in $\mathbb{R}^d$ exists if the the n-particle density functions for $n \geq 1$ are given by the following determinants:

$$g_n(\mathbf{r}_{12}, \mathbf{r}_{13}, \ldots, \mathbf{r}_{1n}) = \text{det}[H(\mathbf{r}_{ij})]_{i,j=1,\ldots,n} \quad \text{with} \quad H(\mathbf{0}) = 1.$$

- By virtue of the nonnegativity of the ρ_n and relation above, it follows that $H(\mathbf{r})$ is positive semidefinite with a **nonnegative Fourier transform** $\tilde{H}(\mathbf{k})$ and with the condition $H(\mathbf{0}) = 1 = \int_{\mathbb{R}^d} \tilde{H}(\mathbf{k}) d\mathbf{k}$ implies that $\tilde{H}(\mathbf{k}) \leq 1$, i.e.,

$$0 \leq \tilde{H}(\mathbf{k}) \leq 1 \quad \text{for all } \mathbf{k}.$$

- Such a kernel describes a determinantal point process with a pair correlation function

$$g_2(\mathbf{r}) = 1 - |H(\mathbf{r})|^2,$$

such that

$$0 \leq g_2(\mathbf{r}) \leq 1 \qquad \text{and} \qquad g_2(\mathbf{0}) = 0.$$

Macchi, Adv. Appl. Prob. (1975); Soshnikov, Russ. Math. Surveys (2000)

Hyperuniformity, Free Fermions & Determinantal Point Processe

- **For 1D GUE, we make the simple observation that $S(k)$ is determined by the intersection volume of two intervals of radius π whose centers are separated by a distance k, and hence**

$$g_2(r) = 1 - \sin^2(\pi r)/(\pi r)^2$$

- **A natural d-dimensional extension is to replace 1D intersection volume in Fourier space with its d-dimensional generalization, yielding**

$$g_2(r) = 1 - 2^d \Gamma(1 + d/2)^2 \, \frac{J_{d/2}^2(Kr)}{(Kr)^d}.$$

where $K = 2\sqrt{\pi}\,[\Gamma(1 + d/2)]^{1/d}$ ensures determinantal point process for any d.

- **We then showed that this special determinantal point process corresponds exactly to the ground-state non-interacting gas of spin-polarized fermions in $\mathbb{R}^d$, $d \geq 1$.**

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One-Component Plasma (OCP): Ginibre (1965) Ensemble

- A hyperuniform determinantal point process is generated by 2D OCP: particles of charge e interacting via the Coulomb potential immersed in a rigid, uniform background of opposite charge.

Sandier and Serfaty, Annals Prob. (2015)

- For a special coupling constant $\Gamma = e^2/k_B T$ equal to 2, the total correlation function $h(r)$ and $S(k)$ have been ascertained exactly by Jancovici (Phys. Rev. Lett, 1981):

$$h(r) = -\exp\left(-\pi r^2\right)$$
$$S(k) = 1 - \exp[-k^2/(4\pi)]$$

Hence,

$$S(k) \sim k^2 \qquad (k \to 0)$$

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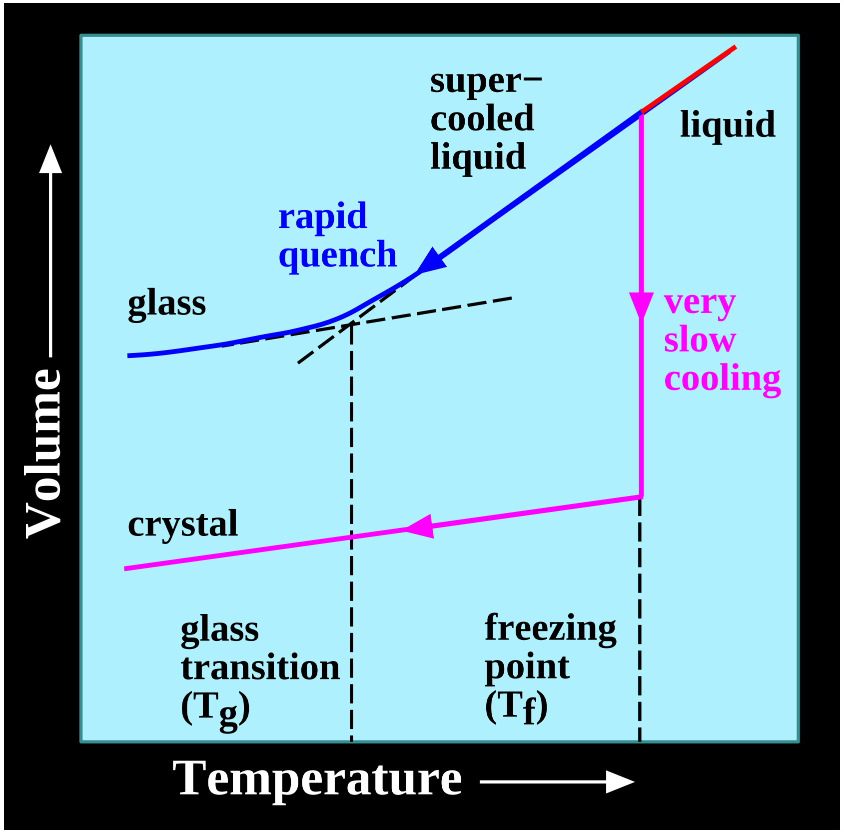

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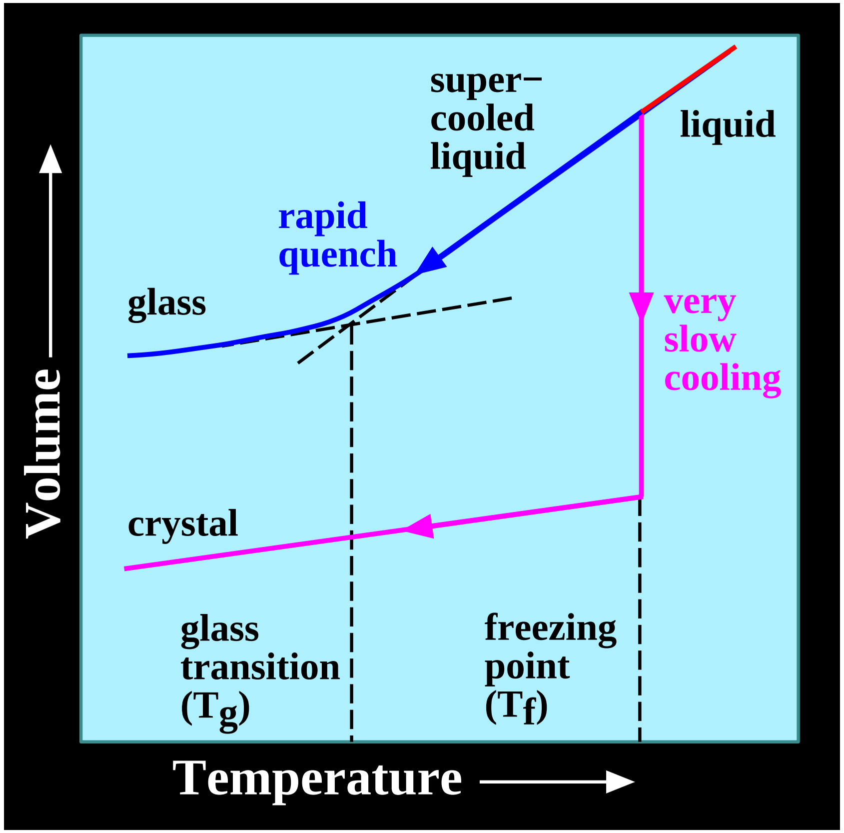

- **Typically, ground states are periodic with high crystallographic symmetries.**
- **Can classical ground states ever be disordered?**

Creation of Disordered Hyperuniform Ground States

Uche, Stillinger & Torquato, Phys. Rev. E 2004

Batten, Stillinger & Torquato, Phys. Rev. E 2008

Collective-Coordinate Simulations

- **Consider a system of N particles with configuration $\mathbf{r}^N$ in a fundamental region Ω under periodic boundary conditions) with a pair potentials $v(\mathbf{r})$ that is bounded with Fourier transform $\tilde{v}(\mathbf{k})$.**

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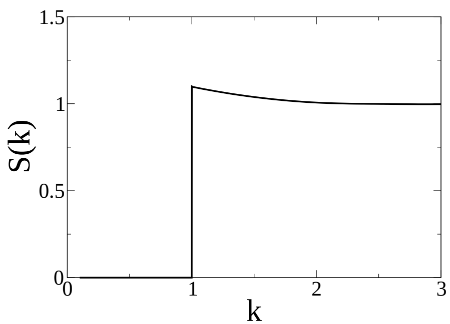
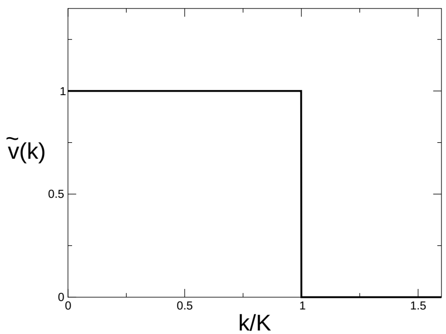
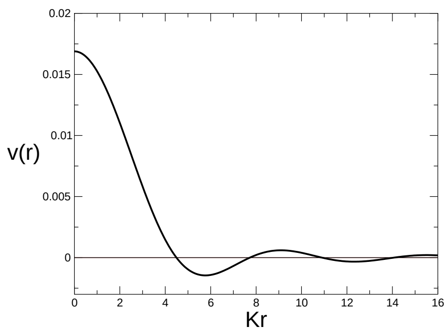
The total energy is

$$\Phi_N(\mathbf{r}^N) = \sum_{i<j} v(\mathbf{r}_{ij})$$
$$= \frac{N}{2|\Omega|}\sum_{\mathbf{k}} \tilde{v}(\mathbf{k})S(\mathbf{k}) + \text{ constant}$$

- **For $\tilde{v}(\mathbf{k})$ positive $\forall\ 0 \le |\mathbf{k}| \le K$ and zero otherwise, finding configurations in which $S(\mathbf{k})$ is constrained to be zero where $\tilde{v}(\mathbf{k})$ has support is equivalent to globally minimizing $\Phi(\mathbf{r}^N)$.**







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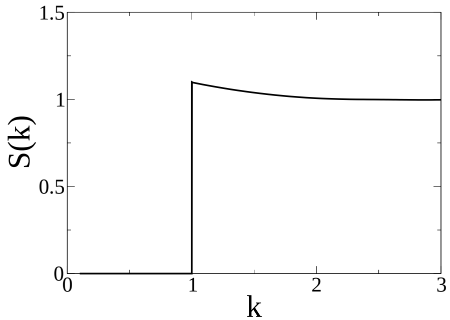

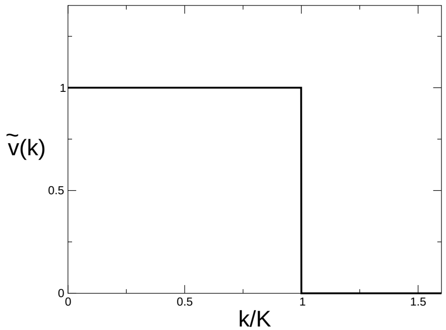

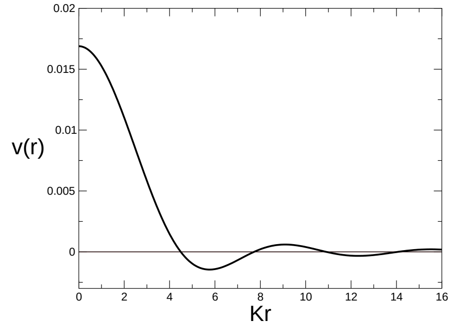

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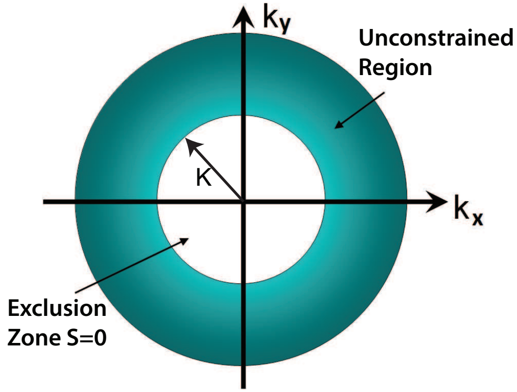
- **Stealthy patterns can be tuned by varying the parameter χ: ratio of number of constrained degrees of freedom to the total number of degrees of freedom, $d(N-1)$.**

Creation of Disordered Stealthy Ground States



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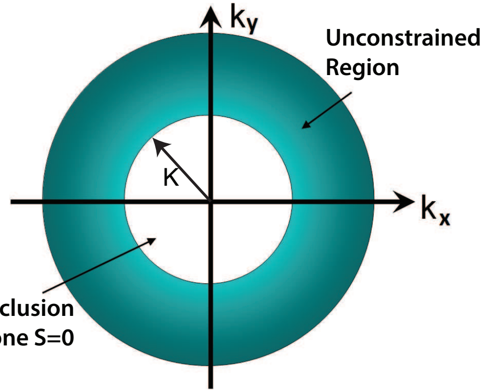
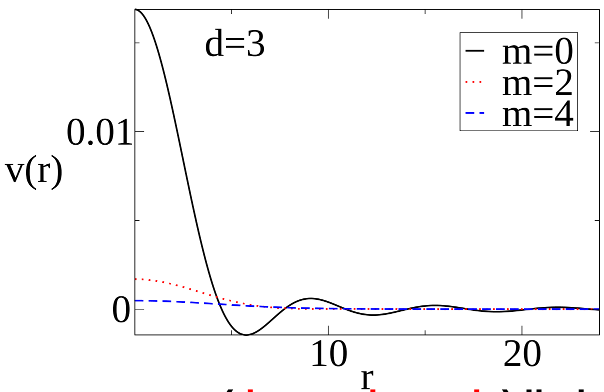
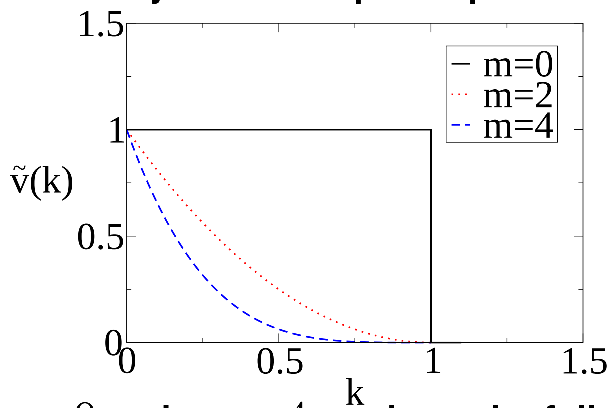


- **One class of stealthy potentials involves the following power-law form:**

$$\tilde{v}(k) = v_0(1 - k/K)^m \, \Theta(K - k),$$

where n is any whole number. The special case $n = 0$ is just the simple step function.





- **In the large-system (thermodynamic) limit with $m = 0$ and $m = 4$, we have the following large-r asymptotic behavior, respectively:**

$$v(r) \sim \frac{\cos(r)}{r^2} \qquad (m = 0)$$

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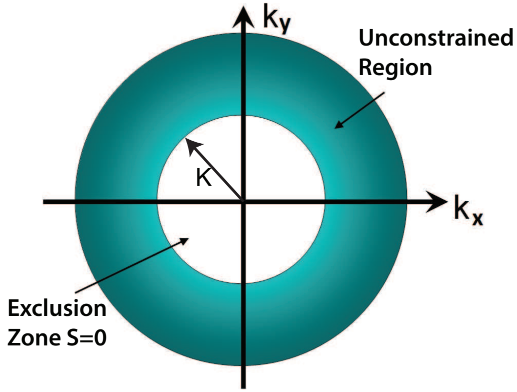

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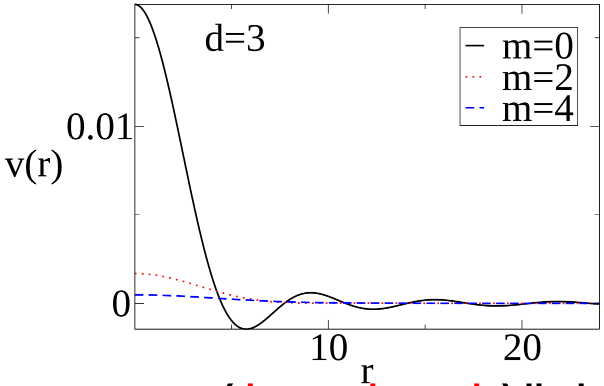

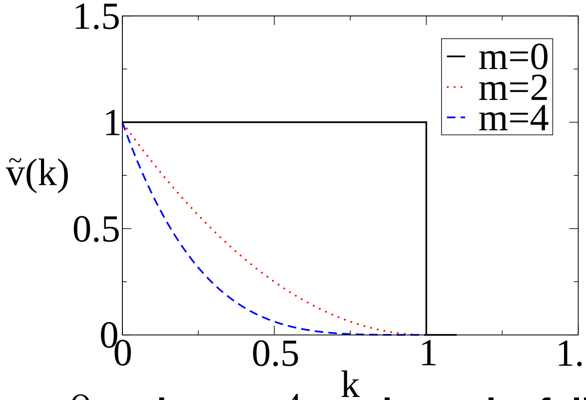

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- **While the specific forms of these stealthy potentials lead to the same convergent ground-state energies, this may not be the case for the pressure and other thermodynamic quantities.**

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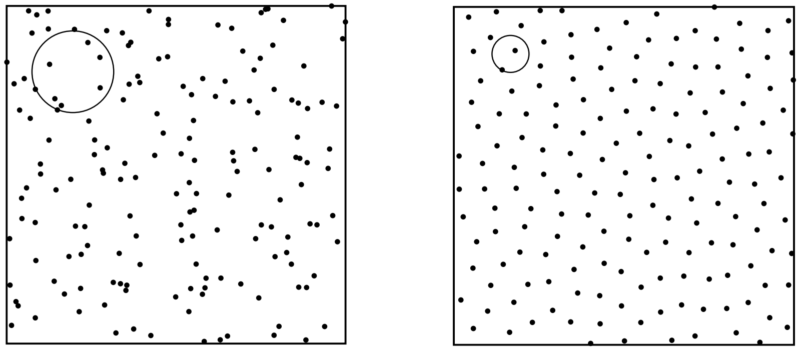

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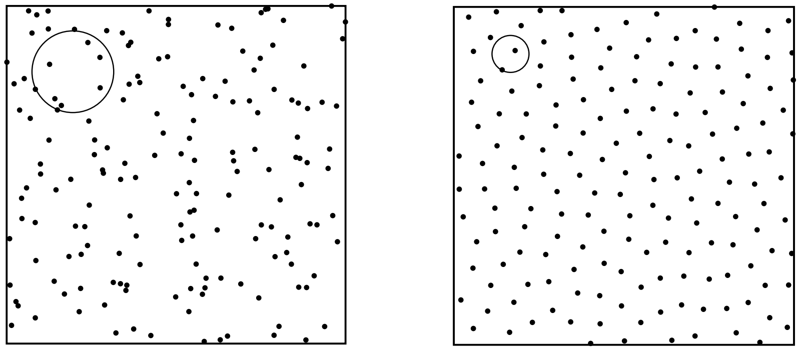

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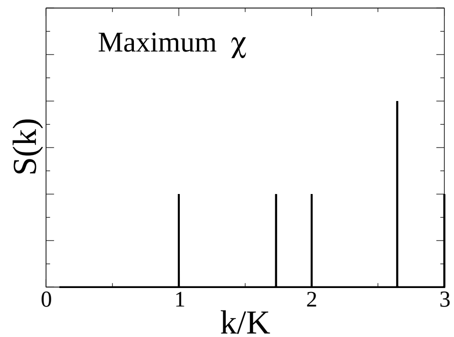
- **For $\chi > 1/2$, the system undergoes a transition to a crystal phase and the energy landscape becomes considerably more complex.**



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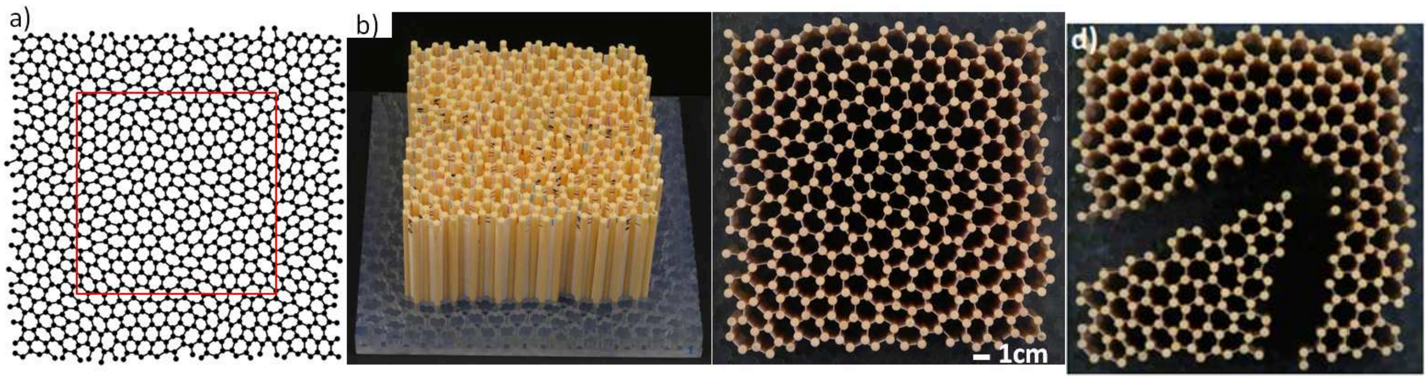

Because band gaps are **isotropic**, such photonic materials offer advantages over photonic crystals (e.g., **free-form waveguides**).

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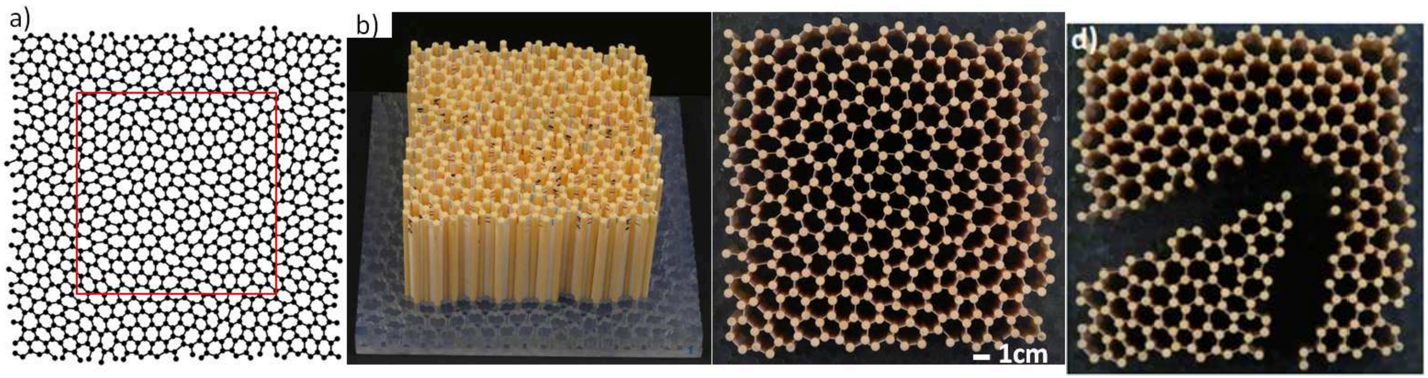

  Because band gaps are isotropic, such photonic materials offer advantages over photonic crystals (e.g., free-form waveguides).

- Other applications include new phononic devices.

Ensemble Theory of Disordered Ground States

Torquato, Zhang & Stillinger, Phys. Rev. X, 2015

- **Nontrivial: Dimensionality of the configuration space depends on the number density ρ (or χ) and there is a multitude of ways of sampling the ground-state manifold, each with its own probability measure Which ensemble? How are entropically favored states determined?**
- **For some ensemble at fixed density ρ, the average energy per particle u for radial potentials in the thermodynamic limit is given by**

$$u \equiv \langle \frac{\Phi(\mathbf{r}^N)}{N} \rangle = \frac{\rho}{2} \int_{\mathbb{R}^d} v(r) g_2(r) d\mathbf{r}$$

$$= \frac{\rho}{2} \tilde{v}(k=0) - \frac{1}{2} v(r=0) + \frac{1}{2(2\pi)^d} \int_{\mathbb{R}^d} \tilde{v}(k) S(k) d\mathbf{k}.$$

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- **Consider the same class of "stealthy" radial potential functions $\tilde{v}(k)$ in $\mathbb{R}^d$. Whenever particle configurations in $\mathbb{R}^d$ exist such that $S(k)$ is constrained to be its minimum value of zero where $\tilde{v}(k)$ has support, the system must be at its ground state or global energy minimum:**

$$u = \frac{\rho}{2} v_0 - \frac{1}{2} v(r=0)$$

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- **In the thermodynamic limit, parameter χ is related to the number density ρ in any dimension d via**

$$\rho\,\chi = \frac{V_1(K)}{2d\,(2\pi)^d},$$

where $V_1(K)$ is the volume of a d-dimensional sphere of radius K.

Remarks: We see that χ and ρ are inversely proportional to one another. Thus, for fixed K and d, as χ tends to zero, ρ tends to infinity, which corresponds counterintuitively to the uncorrelated ideal-gas limit (Poisson distribution). As χ increases from zero, the density ρ decreases.

Ensemble Theory of Disordered Ground States

- **Any periodic crystal with a finite basis is a stealthy ground state for all positive χ up to a maximum χ_{max} (ρ_{min}) determined by its first positive Bragg peak (minimal vector in Fourier space).**

  - **Lemma: At fixed K, a configuration comprised of the union of m different stealthy ground-state configurations in $\mathbb{R}^d$ with $\chi_1, \chi_2, \ldots, \chi_m$, respectively, is itself stealthy with a value χ value given by**

$$\chi = \left[\sum_{i=1}^{m} \chi_i^{-1}\right]^{-1},$$

    which is the harmonic mean of the χ_i divided by m.

- **These last two facts can be used to show how disordered patterns are possible ground states.**

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Table 1: **Periodic stealthy ground states in $\mathbb{R}^2$ with $K = 1$.**

Structure	χ_{max}	ρ_{min}
Kagomé crystal	$\frac{\pi}{3\sqrt{12}} = 0.3022\ldots$	$\frac{3\sqrt{3}}{8\pi^2} = 0.06581\ldots$
Honeycomb crystal	$\frac{\pi}{2\sqrt{12}} = 0.4534\ldots$	$\frac{\sqrt{3}}{4\pi^2} = 0.04387\ldots$
Square lattice	$\frac{\pi}{4} = 0.7853\ldots$	$\frac{1}{4\pi^2} = 0.02533\ldots$
Triangular lattice	$\frac{\pi}{\sqrt{12}} = 0.9068\ldots$	$\frac{\sqrt{3}}{8\pi^2} = 0.02193\ldots$

Canonical Ensemble Theory of Disordered Ground States

- We consider the Gibbs canonical ensemble in which the partition function Z is a function of ρ and absolute temperature T. Our main interest is in a theory in the limit $T \longrightarrow 0$, i.e., the entropically favored ground states in the canonical ensemble.

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Ground-State Pressure and Isothermal Compressibility

- **Energy Route: The pressure in the thermodynamic limit at $T = 0$ can be obtained from the energy per particle (taking $v_0 = 1$) via the relation**

$$p = \rho^2 \left(\frac{\partial u}{\partial \rho} \right)_T .$$

Therefore, for stealthy potentials,

$$p = \frac{\rho^2}{2}.$$

- **The isothermal compressibility $\kappa_T \equiv \rho^{-1} \left(\frac{\partial \rho}{\partial p} \right)_T$ of such a system is**

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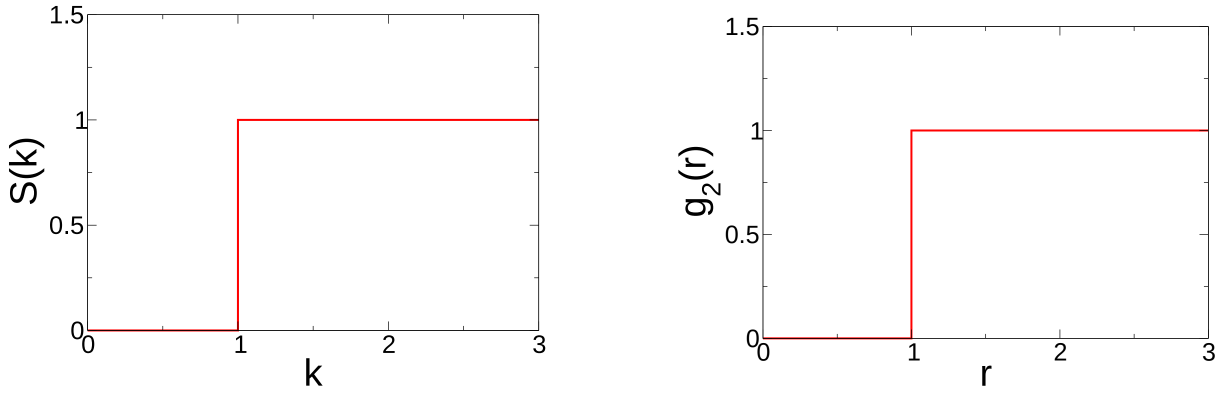
- Virial Route: An alternative route to the pressure is through the "virial" equation, which at $T = 0$ is given by

$$\begin{aligned} p &= -\frac{\rho^2}{2d} s_1(1) \int_0^\infty r^d \, \frac{dv}{dr} g_2(r) dr \\ &= -\frac{\rho^2}{2d} \left[\tilde{f}(k=0) + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \tilde{f}(k) \, \tilde{h}(k) d\mathbf{k}\right] \end{aligned}$$

where $\tilde{f}(k)$ is the Fourier transform of $f(r) \equiv r dv/dr$, when it exists.

Pseudo-Hard Spheres in Fourier Space

- **From previous considerations, we see that that an important contribution to $S(k)$ is a simple hard-core step function $\Theta(k-K)$, which can be viewed as a disordered hard-sphere system in Fourier space in the limit that χ tends to zero, i.e., as the number density ρ tends to infinity.**



- **That the structure factor must have the behavior**

$$S(k) \rightarrow \Theta(k-K), \qquad \chi \rightarrow 0$$

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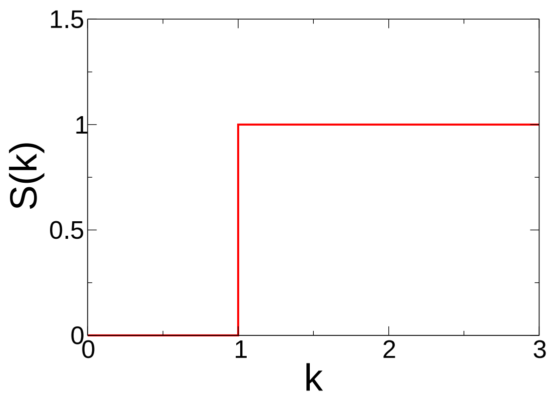

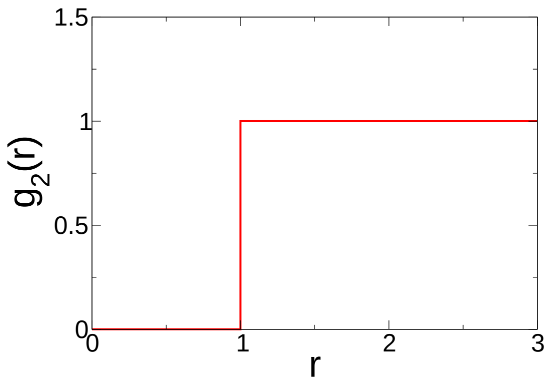

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- **Imagine carrying out a series expansion of $S(k)$ about $\chi = 0$. We make the ansatz that for sufficiently small χ, $S(k)$ in the canonical ensemble for a stealthy potential can be mapped to $g_2(r)$ for an effective disordered hard-sphere system for sufficiently small density.**

Pseudo-Hard Spheres in Fourier Space

Let us define

$$\tilde{H}(k) \equiv \rho \tilde{h}(k) = h_{HS}(r = k)$$

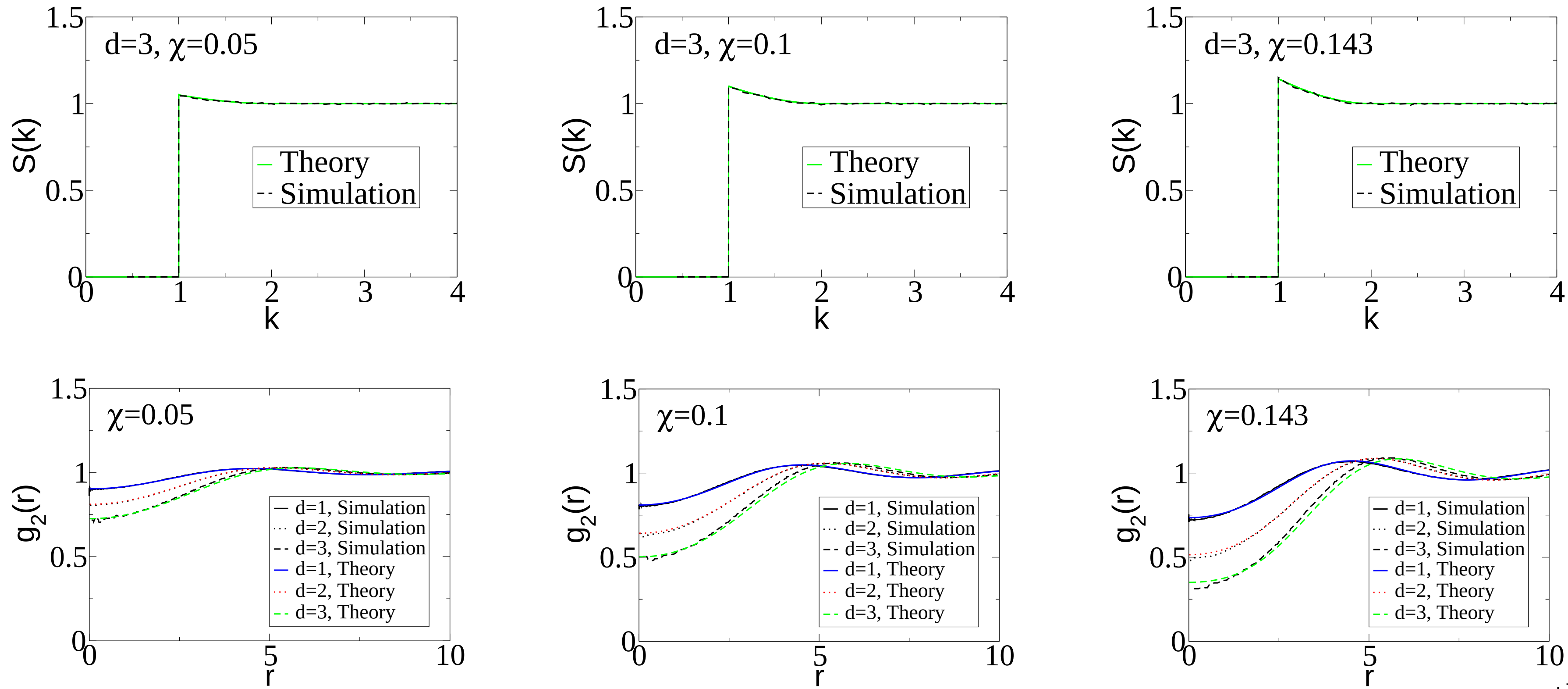
There is an Ornstein-Zernike integral eq. that defines FT of appropriate direct correlation function, $\tilde{C}(k)$:

$$\tilde{H}(k) = \tilde{C}(k) + \eta\, \tilde{H}(k) \otimes \tilde{C}(k),$$

where η is an effective packing fraction. Therefore,

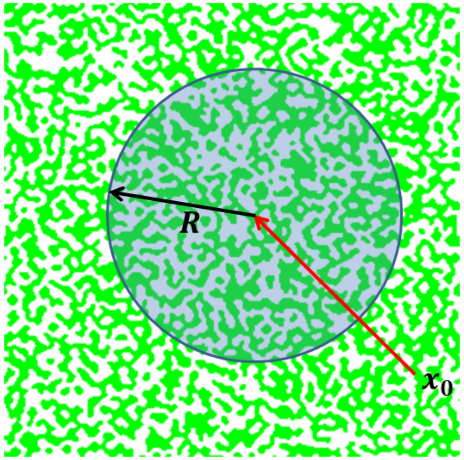
$$H(r) = \frac{C(r)}{1 - (2\pi)^d\, \eta\, C(r)}.$$

This mapping enables us to exploit the well-developed accurate theories of standard Gibbsian disordered hard spheres in direct space.



Hyperuniformity of Disordered Two-Phase Materials

- The hyperuniformity concept was generalized to the case of two-phase heterogeneous materials (Zachary and Torquato, 2009).
- Here the phase volume fraction fluctuates within a spherical window of radius R, which can be characterized by the volume-fraction variance $\sigma_V^2(R)$.



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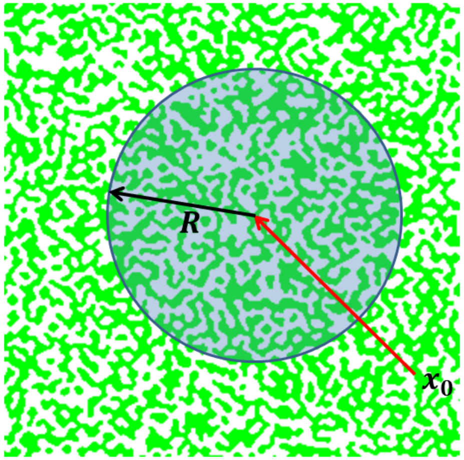
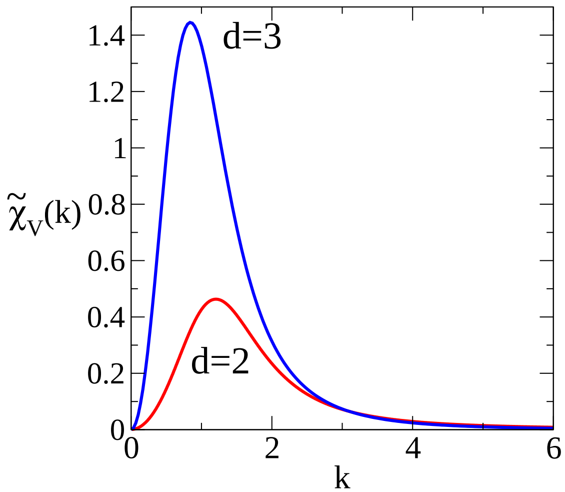


- **For typical disordered two-phase media, the variance $\sigma_V^2(R)$ for large R goes to zero like R^{-d}.**
- **For hyperuniform disordered two-phase media, $\sigma_V^2(R)$ goes to zero faster than R^{-d}, equivalent to following condition on spectral density $\tilde{\chi}_V(\mathbf{k})$:**

$$\lim_{|\mathbf{k}|\to 0} \tilde{\chi}_V(\mathbf{k}) = 0.$$

Designing Disordered Hyperuniform Heterogeneous Materials

- **Disordered hyperuniform two-phase systems can be designed with targeted spectral functions (Torquato, 2016).**
- **For example, consider the following hyperuniform functional forms in 2D and 3D:**



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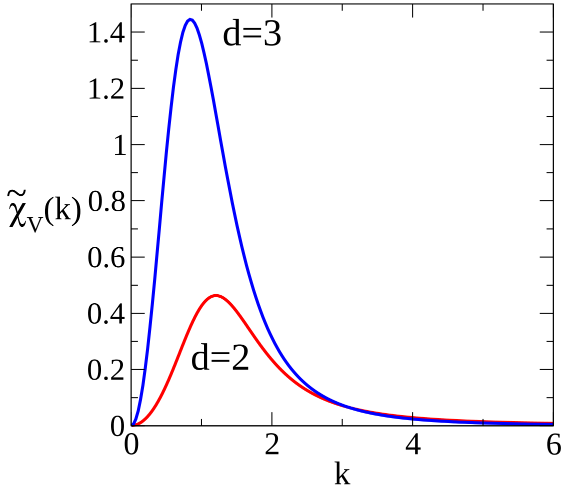
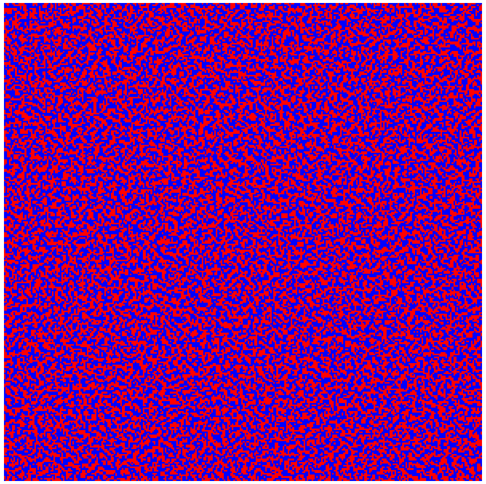


- **The following is a 2D realization:**



CONCLUSIONS

- Disordered hyperuniform materials can be regarded to be new ideal states of disordered matter.
- Hyperuniformity provides a unified means of categorizing and characterizing crystals, quasicrystals and special correlated disordered systems.
- The degree of hyperuniformity provides an order metric for the extent to which large-scale density fluctuations are suppressed in such systems.
- Disordered hyperuniform systems appear to be endowed with unusual physical properties that we are only beginning to discover.
- Hyperuniformity has connections to physics and materials science (e.g., ground states, quantum systems, random matrices, novel materials, etc.), mathematics (e.g., geometry and number theory), and biology.
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Collaborators

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