Variational problems from electrostatics, contact mechanics, and physics of ferromagnetic materials

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Recent Progress on Optimal Point Distributions and Related Fields
ICERM
Jun 3-7 2024

Thermodynamic limits

Goal: study assemblies of large numbers of identical subsystems; characterize them as the number of subsystems goes to infinity (thermodynamic limit).

Practically: given a Hamiltonian on $\mathbb{R}^d$

$$H(p_1, \ldots, p_N, x_1, \ldots, x_N) = U(x_1, \ldots, x_N) + \sum_{i=1}^{N} \frac{p_i^2}{2m},$$

study[1] the asymptotic behavior of its configurational integral,

$$\frac{1}{|\Omega|} \log \frac{1}{N!} \int_\Omega \ldots \int_\Omega exp(-\beta U(x_1, \ldots, x_N)),\, dx_1 \ldots dx_N$$

when

$$\Omega \to \infty$$

(in a sense to be made precise).

[1] Van Hove, Fisher, Ruelle, Dobrushin, and others

Thermodynamic functions

- Other thermodynamic functions and regimes can be considered.

Example: function $\mathfrak{e}$ on configurations $\omega_N = \{x_1, \ldots, x_N\}$ and compact sets $\Omega \in \mathfrak{C}(\mathbb{R}^d)$,

$$\mathfrak{e} : (\mathbb{R}^d)^N \times \mathfrak{C}(\mathbb{R}^d) \to [0, \infty],$$

optimized over $\omega_N \subset \Omega$:

$$\mathfrak{e}(\omega_N^*, \Omega^N) = \inf_{\omega_N} \mathfrak{e}(\omega_N, \Omega^N)$$

- minimizer/maximizer: ω_N^*
- inf / sup can be taken over Ω^N only, if undefined over $(\mathbb{R}^d)^N$.

- Goal: study the asymptotics of optimizers when $N \to \infty$. Set Ω is fixed!

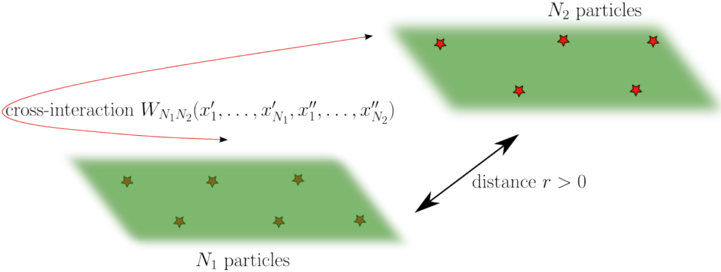
Tempered interactions

The potential energy $U(x_1, \dots, x_N)$ is always translation-independent (possibly isometry-independent), consists of k-(tuple)interactions:

$$U(x_1, \dots, x_N) = \sum_{k \geqslant 2} \sum_{1 \leqslant i_1 \leqslant \dots \leqslant i_k \leqslant N} \Phi_k(x_{i_1}, \dots, x_{i_k})$$

Tempered k-interaction:

$$W_{N_1 N_2}(x'_1, \dots, x'_{N_1}, x''_1, \dots, x''_{N_2}) \leqslant C N_1 N_2 r^{-s}, \qquad s > d.$$



Stable interactions

Fisher and Ruelle prove existence of thermodynamic limits under the assumptions

(i) temperedness: distant particles interact weakly

$$W_{N_1 N_2}(x_1', \ldots, x_{N_1}', x_1'', \ldots, x_{N_2}'') \leqslant C N_1 N_2 r^{-s}, \qquad s > d.$$

(ii) stability: no bounded volume with infinitely many particles

$$U(x_1, \ldots, x_N) \geqslant -cN$$

Stable vs positive definite

For upper-semicontinuous pair interactions,

$$0 \leqslant \sum_{i=1}^{N} \sum_{j=1}^{N} \Phi(x_i - x_j) = N\Phi(0) + 2U(x_1, \ldots, x_N)$$

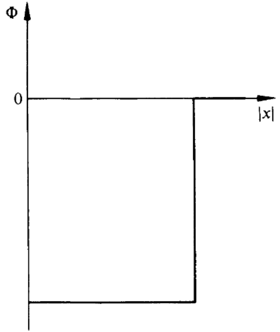
holds for all x_i iff the corresponding $U(x_1, \ldots, x_N) \geqslant -cN$ (is stable).

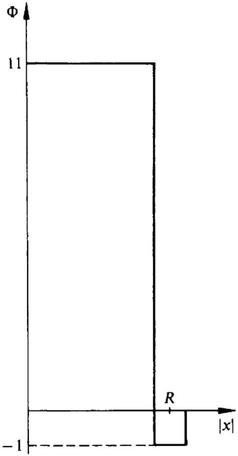
In particular, pair potentials $\Phi(x_1, x_2)$ such that

$$\Phi = \Phi_1 + \Phi_2$$

with Φ_1 <u>positive</u> and Φ_2 <u>positive definite</u> give rise to stable U.

Examples of unstable (catastrophic) interactions





– take R the nearest-neighbor distance in face-centered cubic lattice.

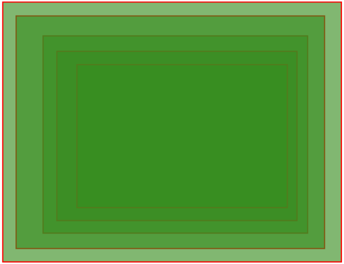
Non-stability of gravity

Figure: Cosmic Cliffs at the edge of the Carina Nebula, by James Webb Space Telescope

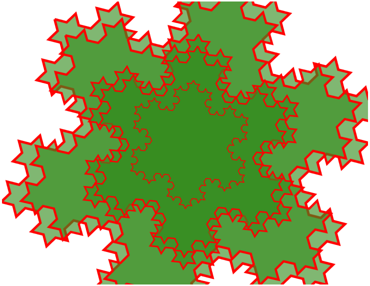
Expanding sequences of sets

Classical mathematical physics results assume boundary regions of the expanding sequence of sets Ω take a small proportion of volume:

Fisher-Ruelle



Hardin-Saff-V



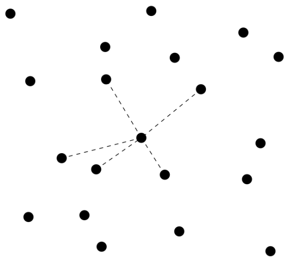
Lieb in Bull. Amer. Math. Soc. 22, 1-49 (1990):

> motivation came from earlier work by Van Hove, Lee and Yang, van Kampen, Wils, Mazur, van der Linden, Griffiths, Dobrushin, and especially Fisher and Ruelle who formulated the problem and showed how to handle certain well chosen, but unrealistic forces.)

Short-range interactions zoo I

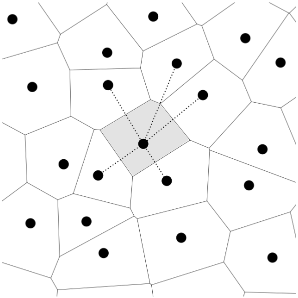
kNN energies

$$\inf_{\boldsymbol{\omega_N}\subset \boldsymbol{A}} \sum_{x\neq y\in\omega_N} w(x)\|x-y\|^{-s}$$



Optimal quantization

$$\inf_{\boldsymbol{\omega_N}} \int \min_{y_i\in\omega_N} \|x-y_i\|^2 \, d\mu(\boldsymbol{x})$$

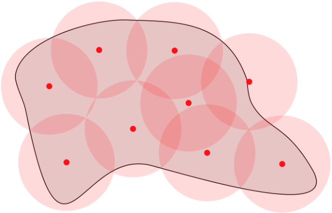


Left: E_s^k, $s>0$ only includes terms for k nearest neighbors of every $x\in\omega_N$.
Right: quadratic quantization error M_2 depends on the second moment of the Voronoi cell of x.

Short-range interactions zoo II

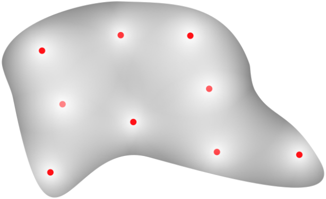
Optimal covering

$$\inf_{\boldsymbol{\omega_N}} \sup_{\boldsymbol{y}\in A} \operatorname{dist}(\boldsymbol{y}, \omega_N)$$

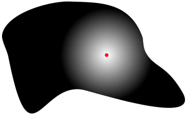


Optimal polarization

$$\sup_{\boldsymbol{\omega_N}} \inf_{\boldsymbol{y}\in A} \sum_{\boldsymbol{x}\in\omega_N} \|\boldsymbol{y}-\boldsymbol{x}\|^{-s}.$$



Left: covering with $N = 9$ points. *Right:* polarizing with $N = 9$ points, $s > 2$.
Below: a single point in a dark set, for comparison.



Persson and Strang's DistMesh

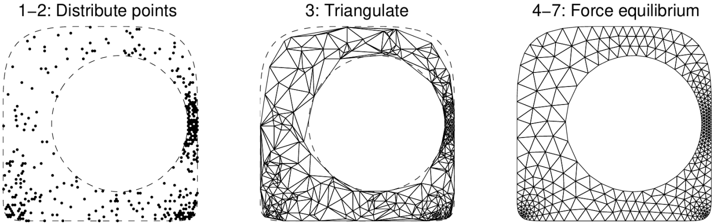
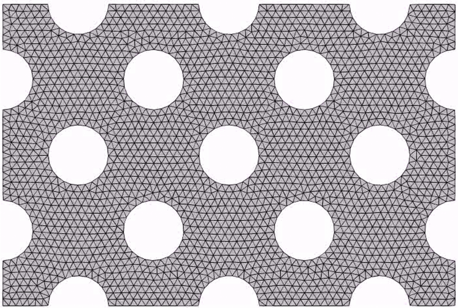
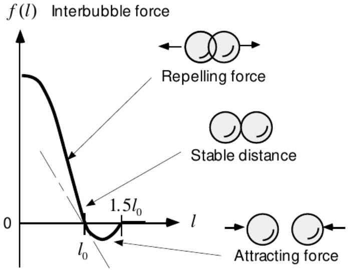


Figure: Persson-Strang (2004)



Shimada-Gossard



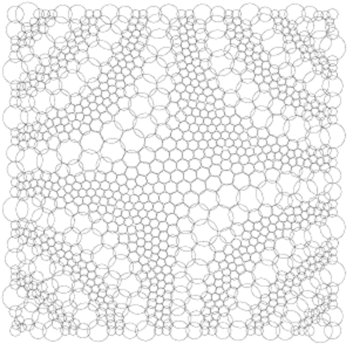
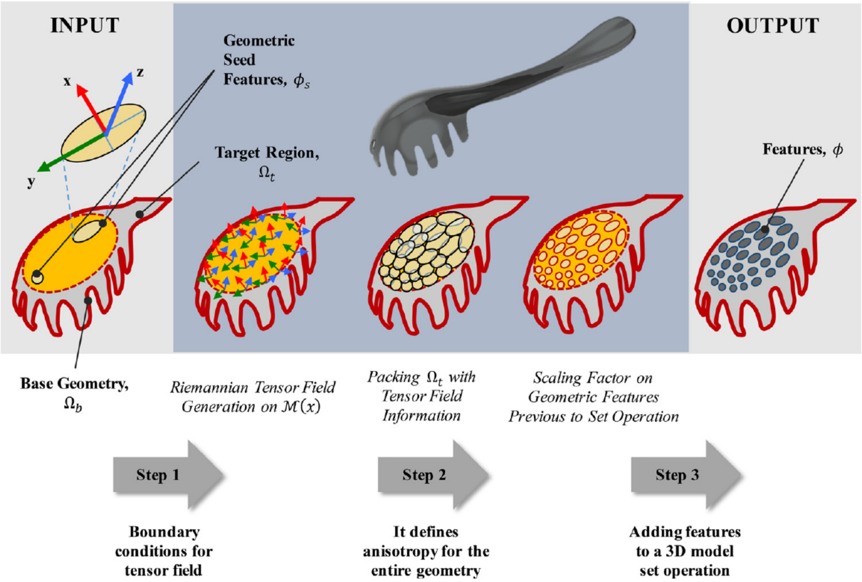


Figure: Shimada-Gossard bubble packing

Andrade-Vyas-Shimada: non-isotropic packing for CAD



Fractals

- A compact $A \subset \mathbb{R}^p$ is a *self-similar fractal* with similitudes $\{\psi_m\}_{m=1}^M$ and their contraction ratios $0 < r_m < 1$, $1 \leqslant m \leqslant M$, if

$$A = \bigsqcup_{m=1}^{M} \psi_m(A).$$

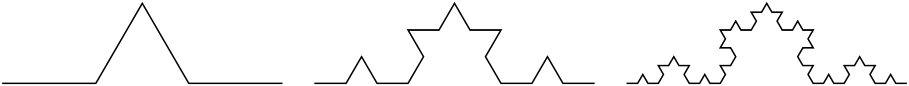


Figure: A Koch snowflake.

- Good fractals satisfy the open set condition: for an open $V \supset A$,

$$\bigsqcup_{m=1}^{M} \psi_m(V) \subset V.$$

- Anderson-Reznikov-V-White: polarization has the thermodynamic limit on good fractals. Also, examples of when this limit does not exist.

Fractals are hard... renewal theory

Theorem (Feller 1966)

Let μ be a probability measure on $[0, \infty)$ and $Z(u)$ be a function defined on $[0, \infty)$. Assume that for some positive constants C, ϵ, and u sufficiently large there holds

$$\left| Z(u) - \int_0^u Z(u-x)\, d\mu(x) \right| \leqslant Ce^{-\epsilon u}.$$

Then $\lim_{u \to \infty} Z(u)$ exists.

- Work with a recursion of the form

$$N(t) = L(t) + \sum_{m=1}^{M} N(tr_m^s)$$

with $r_1, \dots, r_m$ the contraction ratios of the leaves of the fractal. Requires controlling $|L(t)| \leqslant Ct^{d/s-\epsilon}$.

Non-isotropic interactions

- Dipoles are attached to a fixed set of locations, e.g. a lattice.
- Every dipole has a moment vector associated to it: m_i.
- Dipole-dipole interaction:

$$E_{ij} = \frac{m_i \cdot m_j}{\|r_{ij}\|^3} - 3\frac{(m_i \cdot r_{ij})(m_j \cdot r_{ij})}{\|r_{ij}\|^5}$$

  Hamiltonian:

$$\sum_{i \neq j} m_i J_{ij} m_j,$$

  with J_{ij} the 3×3 matrix

$$\frac{1}{\|r_{ij}\|^3}\left(I - 3\frac{r_{ij} \otimes r_{ij}}{\|r_{ij}\|^2}\right)$$

- Stability can be shown – but is it enough?

Aperiodic dipole systems: Penrose

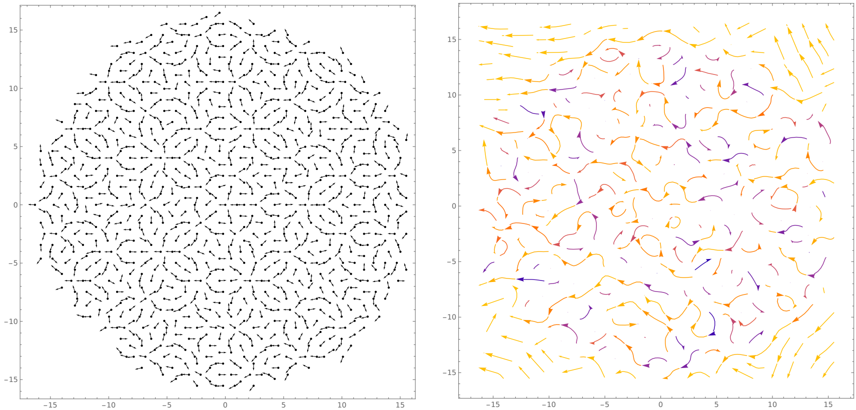


Figure: Left: Somewhat optimized dipoles on the vertices of Penrose tiling. Right: Stream plot of the same configuration.

Aperiodic dipole systems: Ammann tiling

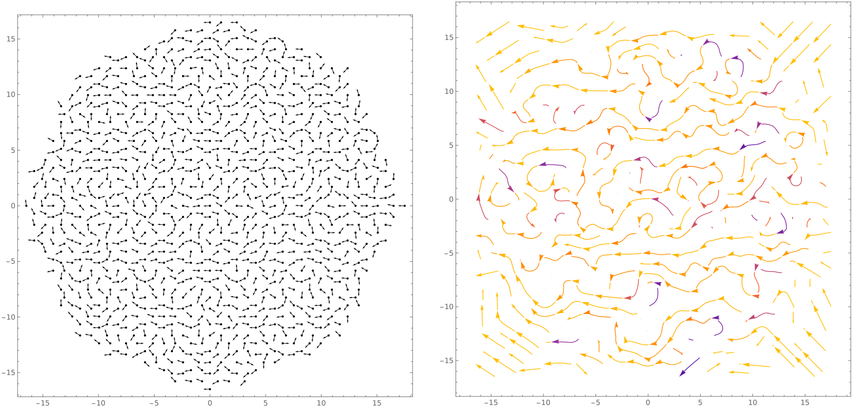


Figure: Left: Somewhat optimized dipoles on the vertices of the aperiodic Ammann tiling.

Ammann vs Penrose

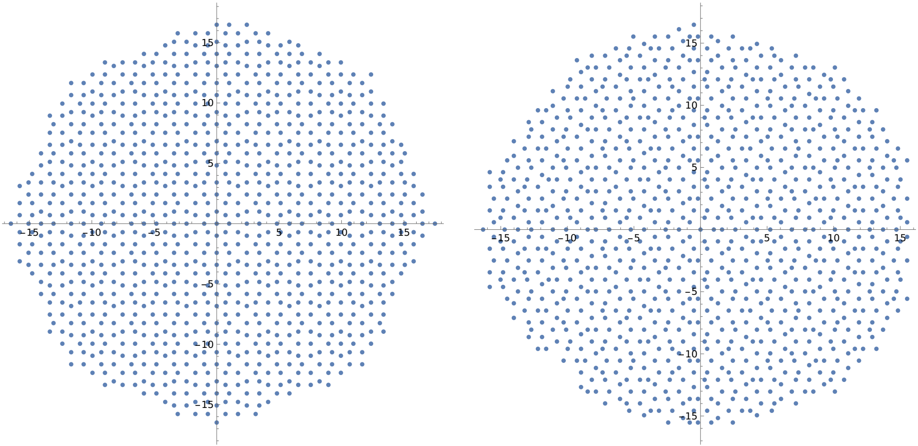
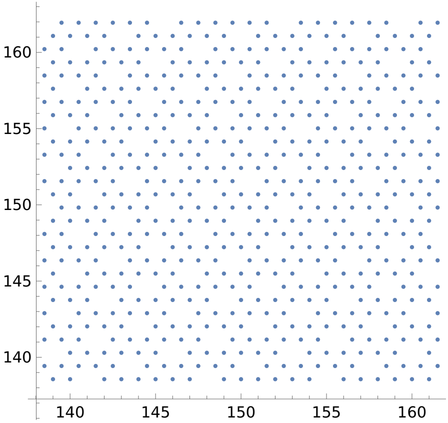
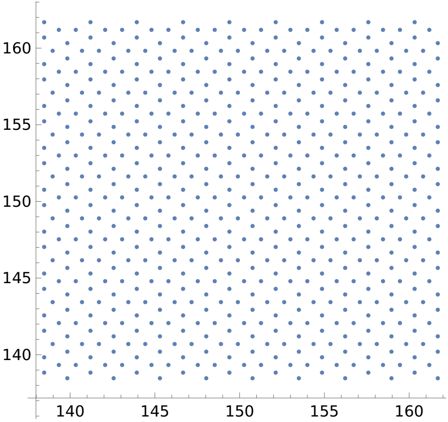


Figure: Left: Ammann. Right: Penrose.

Periodic tilings: snub square and ladybug





Periodic dipole systems: snub square tiling

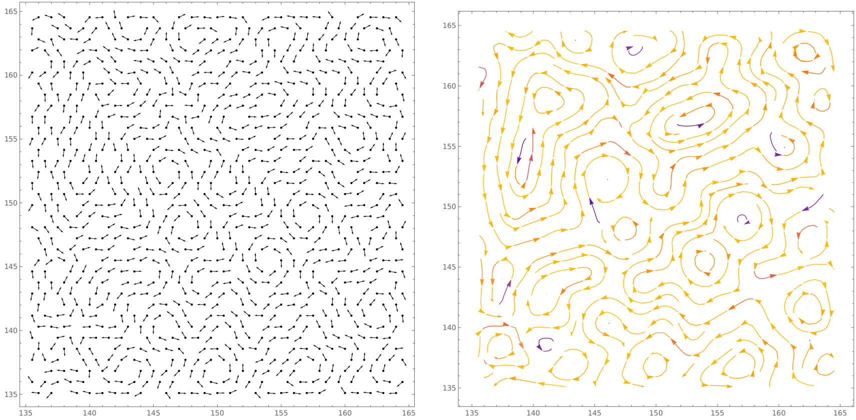


Figure: Left: Somewhat optimized dipoles on the vertices of (a variant of) snub square tiling – a union of several lattices. Right: Stream plot of the same configuration.

Periodic dipole systems: ladybug tiling

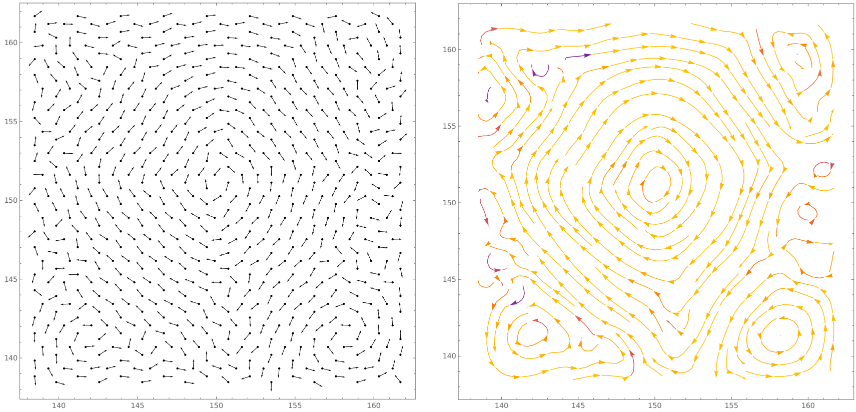
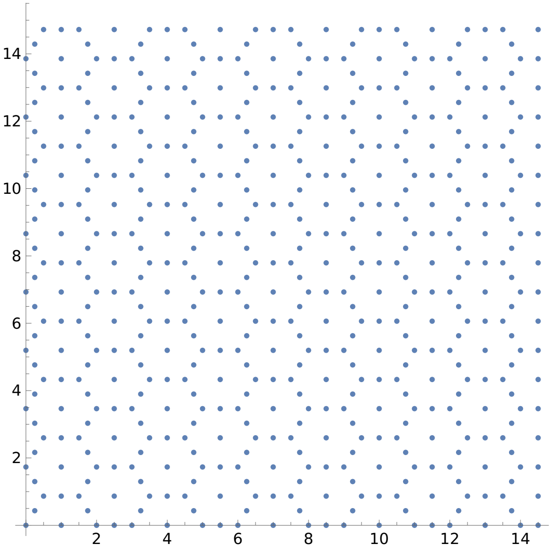


Figure: Left: Somewhat optimized dipoles on the vertices of another snub square tiling. Right: Stream plot of the same configuration.

Triangular Laves tiling



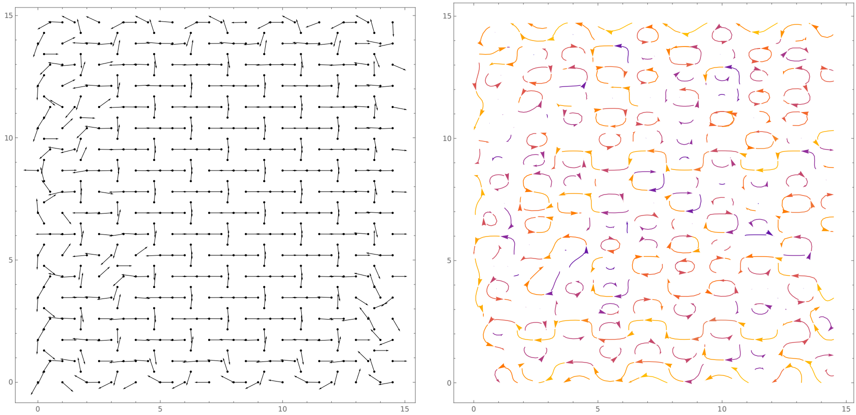


Figure: Dipoles on the vertices of Laves tiling with their stream flow.

Experiments with dipoles on spheres

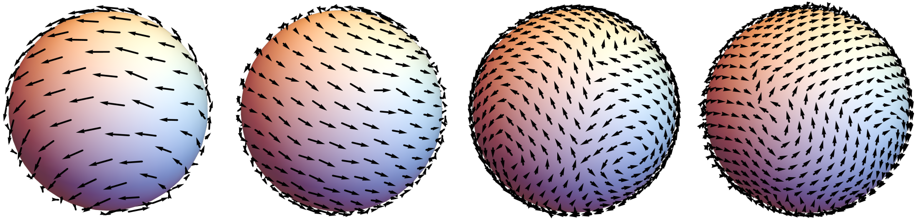


Figure: Left to right: $\{2, 4, 8, 10\} \times 10^2$ dipoles. Locations of the dipoles are produced by minimizing Riesz energy with $s = 3$.

Experiments with dipoles on tori

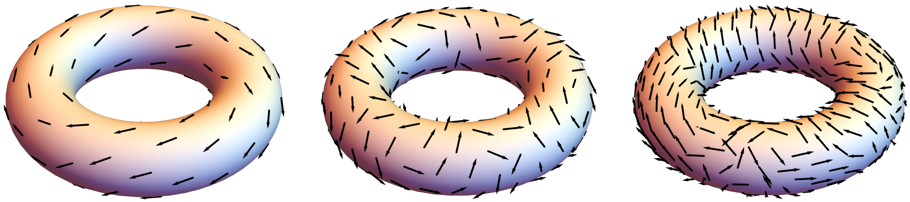


Figure: Left to right: $\{1, 2, 4\} \times 10^2$ dipoles. Locations of the dipoles are produced by minimizing Riesz energy with $s = 3$.

Conclusions and open questions

- Short-range interactions without scale invariance can be subtle, with the limit depending on scaling – see the Lennard-Jones potential

$$\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}.$$

- Tools for exploring particle asymptotics on non-smooth sets: (i) short-range interactions, (ii) renewal theory.

- Thermodynamic limits on fractals are open for most short-range and long-range interactions alike.

- Dynamics of short-range gradient flow: conjectured to converge to the porous medium equation $\partial_t \rho = C_{\mathfrak{e}} \Delta \rho^{1+\sigma}$.

- Geometry of non-isotropic minimizers?

Thank you!