Crystallization in two dimensions

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Motivation:
1. Derivation of
2. Coupling between
continuum models from/and atomistic systems.

Today:
Ground states of pair interaction models
Pair energy models

\[ E_N(\{y\}) = \sum_{x,x'\neq 1}^N V(|y(x) - y(x')|), \]

\( \{y(x)\}_{x\in\{1,\ldots,N\}} \in \mathbb{R}^d, \quad d \in \{1, 2, 3\} \) are the positions of \( N \) particles.

Popular choice for \( V \):

\[ V_{LJ}(r) = r^{-12} - r^{-6} \text{ (Lennard-Jones)} \]

describes van-der-Waals interactions at long distances.
Why are pair-energy models interesting?

- Simple evaluation → efficient simulation
- Finite temperature, phase transitions
- Interesting critical points: dislocations
- Unusual interaction between local and global phenomena

Ground state energy $E_{min} = -8.642719e+01$ for $N = 121$. 
Why are pair-energy models interesting?

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Ground state energy \( E_{\text{min}} = -8.642719 \times 10^1 \) for \( N = 121 \).
Invariances

The pair interaction energy satisfies

$$E(\{Ry(P(\cdot)) + t\}) = E(\{y(\cdot)\})$$

for all

- $t \in \mathbb{R}^d$ (translations),
- $R \in SO(d)$ (rotations),
- $P \in \Pi(N)$, the group of permutations of $N \in \mathbb{N}$ symbols.
Numerical observations (YBL, 2003: $d = 2, V = V_{LJ}$)

- The ground state $\left\{ y_{\text{min}}^N(x) \mid x \in \{1, \ldots, N\}\right\} \subset \mathbb{R}^2$ is approximately a subset of the two-dimensional triangular Bravais-lattice

$$A_2 = \left\{ \left(k_1 + \frac{1}{2}k_2, \frac{\sqrt{3}}{2}k_2\right) \mid k \in \mathbb{Z}^2 \right\}$$

up to rotations, translations and dilations $\forall N \in \mathbb{N}$.

Two-dimensional Bravais-lattice $A_2$  

Typical groundstate for $N = 35$
Main result

**Theorem A.** (Ground state energy)
Let $d = 2$. There exists a number $\alpha > 0$ such that for all potentials $V \in C^2(0, \infty)$ with the properties $V(1) = -1$, $\lim_{r \to \infty} V(r) = 0$, and

\[
V(r) \geq \alpha^{-1} \quad \text{if } 0 < r < 1 - \alpha,
\]

\[
V''(r) \geq \alpha^{-\frac{1}{2}} \quad \text{if } r \in [1 - \alpha, 1 + \alpha],
\]

\[
V(r) \geq -\frac{1}{2} \quad \text{if } r \in (1 + \alpha, \sqrt{2}),
\]

\[
|V''(r)| \leq \alpha r^{-4} \quad \text{if } r \geq \sqrt{2}
\]

the identity

\[
\liminf_{N \to \infty} \min_{y \in \mathbb{R}^{2 \times N}} \frac{1}{N} E_N\{y\} = E_* = \frac{1}{2} \min_{r > 0} V^*(r) = \frac{1}{2} V^*(r^*)
\]

holds.
The renormalized potential 

\((r^*, E^*)\) is the minimizer of the renormalized potential 

\[ E^* = V^*(r^*) = \min_r \sum_{x \in \mathbb{Z}^2 \backslash \{0\}} V(r | \mathcal{L}x|). \]

Triangular lattice: \(\mathcal{L} = \frac{1}{2} \left( \begin{array}{c} 2 \\ 0 \sqrt{3} \end{array} \right)\), cubic lattice: \(\mathcal{L} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}\).

Example: \(V_1(r) = r^{-12} - r^{-6}\), \(V_2(r) = r^{-12} + \tanh(4r - \frac{13}{2}) - 1\).
**Theorem B.** (Ground states)
Let $\mathcal{A} \subset A_2$ be finite and assume that $y : A_2 \to \mathbb{R}^2$ is a ground state of

$$\sum_{x \in \mathcal{A}, \ x' \in A_2} V(|y(x) - y(x')|)$$

subject to the constraint $y(x) = r^*x$ for all $x \in A_2 \setminus \mathcal{A}$. Then

$$\{y(x) \mid x \in A_2\} = A_2.$$
Previous mathematical results

\( d = 1 \): The minimizers are periodic up to a boundary layer. (Radin '79, Ping Lin '01, LeBris-Blanc '02)

\( d = 2 \): The minimizers are rotated and translated subsets of \( r^*A_2 \) provided that \( V \) is given by

No long-range interaction! (Gardener, Heitmann, Radin, Schulman, Wagner '79-'83)

\( d = 3 \): Open.
Sketch of the proof

**Step 1:** Upper bound for the number of nearest neighbor-interactions.
Ground state energy $E_{\text{min}} \sim N$ (number of particles), not $N^2$ (number of bonds).

**Step 2:** Rigidity
Lower bound for the energy of defect-free regions.

**Step 3:** Defect energy
Show that summation errors are smaller than defect energy.
Step 1: \( \{x, x'\} \in B \iff |y(x) - y(x')| \in (1 - \alpha, 1 + \alpha) \)

Combinatorics:

\( \#B \leq 3N - \frac{1}{2} \#\partial X \), where

\[ \mathcal{N}(x) = \{x' \in X \mid \{x, x'\} \in B\} \] (neighbors) and

\[ \partial X = \{x \in X \mid \#\mathcal{N}(x) \neq 6\} \] (defects).
Step 2: Represent long-range interactions in terms of renormalized short range interactions.

- Defect free patches can be imbedded into $A_2$ → Induced metric on label space
- Sum over equilateral triangles
- Approximation: weighted volume form
Error control

Use geometric rigidity of the system in order to control errors:

If the small triangles are undistorted, then the big triangle is undistorted

Quantitative version:

Lemma. Let $y : A_2 \to \mathbb{R}^2$ and $T \subset A_2$ such that $|z - z'| = \lambda$ for all $\{z, z'\} \subset T$. Then

$$\sum_{\{z,z'\} \subset T} \left| |y(z) - y(z')| - \lambda \right|^2 \leq C \log(\lambda) \sum_{S \subset A_2, \text{diam}(S) = 1} \sum_{\{x,x'\} \subset S} \left| |y(x) - y(x')| - 1 \right|^2$$
Continuum rigidity results

\[ u \in C^1(\Omega, \mathbb{R}^d), \ \Omega \subset \mathbb{R}^d. \]

- If \( \nabla u \in SO(d) \Rightarrow \nabla u = \text{const} \) (Liouville).
  

- If \( |(\nabla u)^T \nabla u - \text{Id}| \ll 1 \Rightarrow Du \) is almost constant (Reshetnyak, 1967).

- \[ \int |\nabla u - R|^2 \, dx \leq C \int |\nabla u - SO(d)|^2 \, dx \]
  
  (Friesecke, James & Müller, CPAM 2002).
Outlook

Three dimensions

1. More than one lattice: stacking sequence

2. Finite temperature: Dual lattice possible due to entropic effects

3. Quantum-mechanical version

\[ E(\Psi) = \int_{\mathbb{R}^{3N}} \left( \sum_{l=1}^{N} \frac{\hbar}{2} |\nabla_{x_l} \Psi|^2 + |\Psi|^2 \sum_{l,l'=1 \atop l \neq l'}^{N} V(|x_l - x_{l'}|) \right) \, dx_1 \ldots dx_N. \]

Summary

• Rigorous lower bound for pair energy

\[ E(\{y\}) = \sum_{x \neq x'}^{N} V(|y(x) - y(x')|) \geq CN \]

• \( C = \min_r V^*(r) \) binding energy per particle

• Ground state is a dilated copy of \( A_2 \).