# Are atomistic equilibrium distributions ordered?

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# Structure

1. Models without reference configuration
2. Screening assumption
3. Atomistic dislocation models

# Equilibrium models for crystals without underlying lattice

Joint work with Luke Williams

Box $\Lambda \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, torus, periodic boundary conditions

Configurations: $Y \subset \Lambda$, $\#Y = |\Lambda| = n$

Interaction potential: $v(r)$, e.g. $v(r) = r^{-12} - r^{-6}$

Hamiltonian: $H[Y] = \sum_{y,y' \in Y} v(|y - y'|)$

Boltzmann-Gibbs distribution (canonical ensemble, density = 1):

$$\mathbb{P}_{\theta,\Lambda}(Y) = e^{-\beta\,(H[Y] - n\,f_\Lambda(\theta))},$$

inverse temperature $\beta$, free energy

$$f_\Lambda(\beta) = -\frac{1}{n\,\beta} \log \int_{\Lambda^n} \mathrm{e}^{-\beta\,H[Y]}.$$

**Problem:** Characterization of $\min_{\#Y=n} H[Y]$ can be hard.

# Decomposition into cells

Reference cell: $\boxtimes \subset \mathbb{R}^2$, eg $\boxtimes = \{(0,0),(0,1),(1,0),(1,1)\}$.

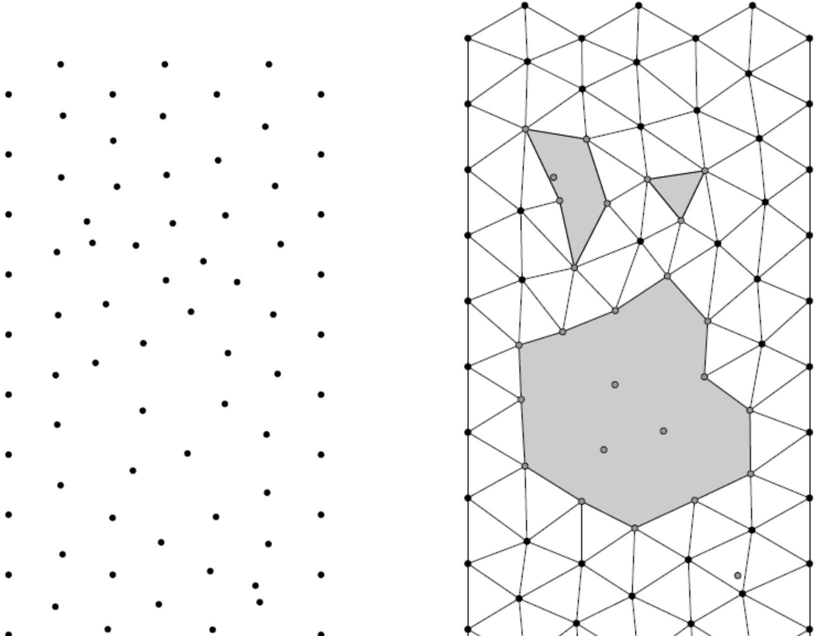
**Definition:** $\square \in \mathcal{T}$ if

- $\square \subset Y$,
- $\min_{R \in SO(2), t \in \mathbb{R}^2} \max_{y \in \square} \min_{y' \in Y} |Ry + t - y'| < \varepsilon = 0.1$
- $\mathrm{int}(\mathrm{conv}(\square)) \cap Y = \emptyset$.

**Admissible configurations** $Y$:

- $\mathcal{T}$ is unique.
- $\mathrm{meas}(\mathrm{conv}(\square) \cap \mathrm{conv}(\square')) = 0$ if $\square \neq \square'$
- Simply connected cells can be mapped to simply connected lattice points.

# Illustration



# Local Hamiltonian

Local model: $H_{\mathrm{loc}}[Y] = \sum_{\Box \in \mathcal{T}} v(\Box)$.

Cell energy: $v(\Box) \in \mathbb{R}$, $\min v = v(\boxtimes) = -\sigma < 0$.

Euclidean invariance: $v(R\Box + t) = v(\Box)$ for all $R \in SO(d),\ t \in \mathbb{R}^d$.

If

- $\min v < 0$,
- $\boxtimes$ is unit-cell of lattice $\mathcal{L}$
- periodic boundary conditions

then $H$ is minimized by lattice configurations.

# Continuum interpolation

- $u_\square : \mathrm{conv}(\square) \to \mathrm{conv}(\boxtimes)$ piecewise affine, $\boxtimes = u_\square(\square)$,
- $V_\square = \nabla u_\square$ (piecewise constant)
- $D = \Lambda \setminus \cup_{\square \in \mathcal{T}} \mathrm{conv}(\square)$.
- Choose reasonable interpolation in $D$.
- $\mathrm{supp}\, \mathrm{curl}(V) \subset D$
- $W(V) := (v(\square) + \tau) \det V^{-1}$ so that $\int_{\mathrm{conv}(\square)} W(V) = v(\square) + \tau$.

Integral representation of the energy:

$$E[Y] = -\tau|\Lambda| + \int_{\Lambda\setminus D} W(V(x))\, \mathrm{d}x + \tau\, |D|$$

Properties of $W$:

- Euclidean invariance: $W(R\,F) = W(F) \quad \forall R \in SO(d)$.
- $W(F) \geq c\, \mathrm{dist}(F, SO(d))^2$

# Orientational order

**Order parameter:** $\mathrm{supp}(\varphi) \subset \mathbb{R}^d$ compact, $\int_{SO(d)} \mathrm{d}R\, \varphi(R\,\cdot\,) = 0$.

$$\begin{aligned} a &= n^{-1} \max_{R \in SO(d)} \sum_{y \neq y' \in Y} (\varphi(R(y-y')), \\ A_\beta &= \lim_{n\to\infty} \mathbb{E}_\beta(a). \end{aligned}$$

**Orientational symmetry breaking:** There exists $\beta_{\mathrm{crit}}$ such that

$$A_\beta \begin{cases} = 0 & \text{if } \beta < \beta_{\mathrm{crit}}, \\ > 0 & \text{if } \beta > \beta_{\mathrm{crit}}. \end{cases}$$

Only results on inequality!

# Translational symmetry breaking

Bravais lattice $\mathcal{L} \subset \mathbb{R}^d$.
**Order parameter**: $\varphi \in C(\mathbb{R}^d)$ $\mathcal{L}$-periodic, $\int_{\mathbb{R}^d/\mathcal{L}} \mathrm{d}x\, \varphi(x) = 0$,

$$\begin{aligned} a &= n^{-2} \max_{R \in SO(d)} \sum_{y \neq y' \in Y} \varphi(R(y-y')), \\ A &= \lim_{n \to \infty} \mathbb{E}_\theta(a). \end{aligned}$$

**Long-range order transition:** There exists $\mathcal{L}(\theta)$, $\theta_{\mathrm{crit}}$ such that

$$A \begin{cases} = 0 & \text{if } \theta < \theta_{\mathrm{crit}} \\ > 0 & \text{if } \theta > \theta_{\mathrm{crit}} \end{cases}$$

**Theorem.** (Mermin-Wagner 1966): No long-range order if $d < 3$.

# Main result

$d = 2$
$\mathrm{curl}\, V \in L^2(\Lambda)$ $\alpha$-neutral if

- $\mathrm{supp}\,\mathrm{curl}\, V \subset \cup_i B_\alpha(x_i)$, $\int_{B_\alpha(x_i)} \mathrm{curl}\, V = 0$,
- $\min_{i \neq j} |x_i - x_j| > 2\alpha + 1$.

Enforce neutrality:

$$H[Y] = \sum_{\square \in \mathcal{T}} v(\square) + \chi_{\alpha-\text{neutral}}.$$

**Theorem (T.-Williams '17)**

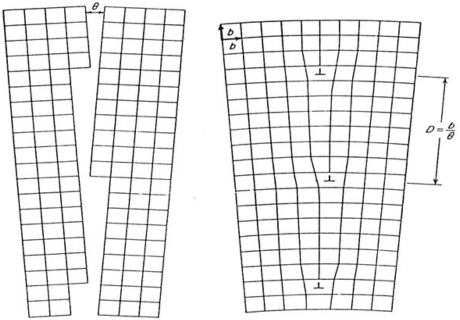
$\rho = 1$. *If* $\sigma / \log \alpha$ *sufficiently large, then* $\lim_{\beta \to \infty} A_\beta = 0$.

We expect that $\mathbb{E}(|D|) \sim \exp(\beta\, v_0)\, n$.

Aumann '15: $v_0 \sim -n$ ( $\Rightarrow D = \emptyset$ almost surely).

Aim: Remove neutrality assumption.

# Grain boundaries




- Grain boundaries can be seen as walls of edge dislocations with the **same** sign.
- Excluded by neutrality assumption.
- Configurations with grains are orientationally **disordered**.

# Orientational order in $L^2$

Recall order parameter:

$$A(\beta) = \lim_{|\Lambda|\to\infty} \mathbb{E}_\beta \left( |\Lambda|^{-1} \min_{R\in SO(2)} \|V - R\|_{L^2}^2 \right).$$

**Structure of proof**

Step 1 (deterministic)

$$\min_{R\in SO(d)} \|V - R\|_{L^2(\Lambda)}^2 \leq C\,(H[Y] - \min H).$$

NB: $C$ is random with large maximum.

Step 2 (standard)

$$\lim_{\beta\to\infty} \lim_{n\to\infty} \frac{1}{n} \mathbb{E}_{\beta,n}(H_\Lambda - \min H_\Lambda) = 0.$$

# Rigidity estimates

**Theorem (Friesecke, Müller, Scardia, Zeppieri, Aumann)**

$V \in W^{1,p}(\Lambda)$, $\Lambda \subset \mathbb{R}^2$ **simply** *connected. Then*

$$\min_{R \in SO(2)} \|V - R\|_{L^2} \leq C \,\|\mathrm{dist}(V, SO(2))\|_{L^2} + C_p \,\|\mathrm{curl} V\|_{L^p},$$

*where*

$$C_p(r\Lambda) = r^{2-\frac{2}{p}}\, C_p(\Lambda).$$

Need: $p = 2$ (energy scaling), $C_p = O(1)$ as $|\Lambda| \to \infty$ (Thermodynamic limit).

**Theorem (T.-Williams'18)**

*If $V$ is $\alpha$-neutral and admissible, then* $C_2(r\Lambda) = C_2(\Lambda) = \log \alpha$.

# Proof of Step 1

If

- $C\,\|\mathrm{dist}(F, SO(d))\|^2_{L^2(\square)} \leq W(F)$ (modelling assumption)
- $C\,\|\mathrm{dist}(V, SO(d))\|^2_{L^2(\Lambda)} + C\,\|\mathrm{curl}\, V\|^2_{L^2(\Lambda)} \geq \min_{R\in SO(2)} \|V - R\|^2_{L^2(\Lambda)}$ (rigidity estimate)

then

$$\begin{aligned} H[Y] - \min H &= \int_{\Lambda\setminus D} W(V) + \tau\,|D| \\ &\geq C\,\|\mathrm{dist}(V, SO(d))\|^2_{L^2(\Lambda)} + C\,\|\mathrm{curl}\, V\|^2_{L^2(\Lambda)} \\ &\geq \min_{R\in SO(2)} \|V - R\|^2_{L^2(\Lambda)}. \end{aligned}$$

# Examples

$d = 2$, $|\Lambda| = n$

$$V(x) = \begin{cases} \mathrm{Id} & \text{if } \mathrm{dist}(x, D) \geq 1, \\ \text{interpolation} & \text{if } 0 < \mathrm{dist}(x, D) < 1, \\ R & \text{else.} \end{cases}$$

$|\partial D| \sim n^{\frac{1}{2}}$, $|D| \sim n$ (No orientational ordering).

MSZ sharp: $\|V - R\|_2 \sim n^{\frac{1}{2}}$, $\|\mathrm{dist}(V, SO(2))\|_2 \sim n^{\frac{1}{4}}$, $\|\mathrm{curl} V\|_1 \sim n^{\frac{1}{2}}$.
Need: $|\partial D| = |D| = \varepsilon\, n$
MSZ: $\|V - R\|_2 = (\varepsilon\, n)^{\frac{1}{2}} \leq \varepsilon\, n = \|\mathrm{curl} V\|_1$ too weak.

Dilute, paired dislocations, $p = 2$.
$\|V - R\|_2, \|\mathrm{dist}(V, SO(2)\|_2 \sim \varepsilon^{\frac{1}{2}}\, n^{\frac{1}{2}}$, $\|\mathrm{curl} V\|_2 = \varepsilon^{\frac{1}{p}}\, n^{\frac{1}{p}}$, $C_2^{TW} = \log \alpha$
($C_2^{Aumann} = n^{\frac{1}{2}}$ not sharp!).

# Atomistic models with dislocations

Jointly with Alessandro Giuliani

**Observation: $\alpha$-neutrality constitutes an obstruction to disorder.**

Are unconstrained samples $\alpha$-neutral with high probability?

- Order is not a consequence of energy considerations
- Need proper statistical treatment

# Models with edge dislocations: Ariza-Ortiz 2005

2-dimensional system: $x \in \mathcal{L} \subset \mathbb{R}^2$ are lattice points.

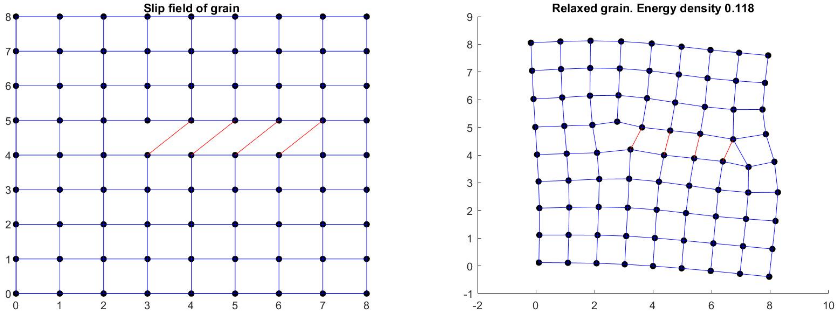
$$H_{\mathrm{AO}}(u, \sigma) = \sum_{e \in \text{edges}} \frac{1}{2}[(\mathrm{d}u(e) - \sigma(e)) \cdot \mathrm{d}x(e)]^2 + \tau \sum_{f \in \text{faces}} |\mathrm{d}\sigma(f)|,$$

where $\tau$ is the core energy,

$$\begin{aligned} \text{edge } e &= (x, x'), \\ \mathrm{d}u(e) &= u(x) - u(x'), \\ \text{displacement } u &: \text{vertices} \to \mathbb{R}^2 \text{ (vectorial)}, \\ \text{slip } \sigma &: \text{edges} \to \text{vertices}, \\ \mathrm{d}\sigma &: \text{faces} \to \mathcal{L}. \end{aligned}$$

Nonlinear model is also possible.

# Illustration of the Ariza-Ortiz model




Undeformed and relaxed configuration for Ariza-Ortiz model. Slipped bonds are red.

# Statistical mechanics

The probability factorizes because of linearity:

$$\begin{aligned}
\mathbb{P}_\beta(u,\sigma) &= \frac{1}{Z(\beta)} \mathrm{e}^{-\beta H_{\mathrm{AO}}(u,\sigma)} \\
&= \underbrace{\frac{1}{Z_1(\beta)}\, \mathrm{e}^{-\beta H_{\mathrm{AO}}(u-L_1\sigma,0)}}_{\text{elastic part}}\ \underbrace{\frac{1}{Z_2(\beta)} \mathrm{e}^{-\beta H_{\mathrm{AO}}(0,L_2 \mathrm{d}\sigma)}}_{\text{dislocation interactions}},
\end{aligned}$$

where $L_1$ and $L_2$ are linear operators and

$$\begin{aligned}
Z_1(\beta) &= \int_{\mathbb{R}^{2\times\text{vertices}}} \mathrm{e}^{-\beta H_{\mathrm{AO}}(u,0)}\, \mathrm{d}u, \\
Z_2(\beta) &= \sum_{q\in\mathcal{L}^{\text{faces}}} \mathrm{e}^{-\beta H_{\mathrm{AO}}(0,L_2 q)}.
\end{aligned}$$

Order parameter: Angle-angle correlation

$$f(\beta) = \langle |L_2\, \mathrm{d}\sigma|^2 \rangle \geq 0.$$

Perfect order: $f(\beta) = 0$. Elastic contributions can be computed explicitly (Gaussian integral).

# Screw dislocations

Simpler version:
Villain model, vertices $X = \mathcal{L} \cap \Lambda$, local excitation $u(x) \in [0,1]$.

$$
\begin{aligned}
Z &= \int_{[0,1]^X} \mathrm{d}u \prod_{x \sim x'} \sum_{\sigma(x,x') \in \mathbb{Z}} \exp(-\tfrac{\beta}{2} \left(u(x) - u(x') - \sigma(x,x')\right)^2) \\
&= \sum_{q \in \mathbb{Z}^X} \int_{\mathbb{R}^X} \mathrm{d}u \prod_{x' \sim x'} \exp(-\tfrac{\beta}{2}(u(x) - u(x') + \mathrm{d}^* \Delta^{-1} q)^2) \\
&= \int_{\mathbb{R}^X} \mathrm{d}u \prod_{\text{edges } e} \exp(-\tfrac{\beta}{2}(\mathrm{d}u(e))^2) \times \sum_{q \in \mathbb{Z}^X} \exp(\tfrac{\beta}{2} q \Delta^{-1} q)
\end{aligned}
$$

Analysis of vortex-charge contribution: Fröhlich-Spencer 1981.

# Does the model allow for disorder?

Read-Shockley law: $\gamma_s = \gamma_0(A - \log\theta)\theta$ if $|\theta| \ll 1$.

**Theorem**

Let

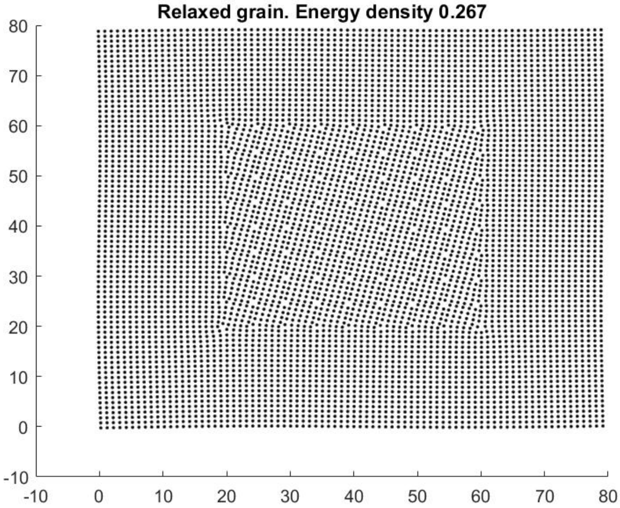
$$E_{\mathrm{gb}}(m) = \lim_{M\to\infty} \frac{1}{M} \min_u H_{\mathrm{AO}}\left(u, \sum_{j=0}^{M-1} (\delta(x - jv) - \delta(x - mb - jv))b\right),$$

with $n$ wall spacing, $b \in \mathcal{L}$ (Burgers vector) and $v \in \mathbb{R}^2$ (wall direction).
If $v \cdot b = 0$,

$$E_{\mathrm{gb}}(m) = \frac{8\pi}{3}\log|v| + O\left(1 + e^{-m/|v|}\log|v|\right), \quad m, |v| \gg 1.$$

Proof: Riemann sum in Fourier space.
Previous results: Luckhaus-Lauteri 2017.

# Relaxed grain boundary with free boundary conditions




Grain boundaries are not ordered and are expected to be unlikely!

# Large dislocation core energy

$$f(\beta) = \langle |L_2 \,\mathrm{d}\sigma|^2 \rangle_q = \frac{1}{Z} \sum_q |L_2 q|^2 \Big[ \prod_{f \in \text{faces}} \lambda(q(f)) \Big] e^{-\frac{\beta}{2}(q, Gq)},$$

with $G$ Green's function, activity

$$\lambda(q) = \begin{cases} 1 & \text{if} \quad q = 0, \\ z & \text{if} \quad q \in \mathcal{L} \text{ and } |q| = 1, \\ 0 & \text{otherwise,} \end{cases}$$

$z^{-1}$ = core energy. Aim: Expand $f(\beta)$ in $z$.
Sine-Gordon transform:

$$e^{-\frac{\beta}{2}(q, Gq)} = \int \mathrm{d}\phi \; e^{-\frac{1}{2\beta}(\phi, G^{-1}\phi)} e^{i(\phi, q)}$$

provides a nice way to compute the expansion in $z$ (exponent is small).

# Future work: Renormalization group

Rewrite partition function using Sine-Gordon:

$$Z = \int \mathrm{d}\phi \; e^{-\frac{1}{2\beta}(\phi, G^{-1}\phi)} \Big[ \prod_f \big(1 + 2z \sum_{i=1}^{3} \cos(\phi(f) \cdot b_i)\big) \Big] \, .$$

First term:

$$\langle | L_2 \, \mathrm{d}\sigma |^2 \rangle_q = C_1 z^2 \mathrm{e}^{-C_2 \beta} + O(z^4), \quad 0 < z \ll 1.$$

Fröhlich-Spencer: Renormalization group provides control of higher order terms in simpler setting.

**Work in progress**

# Summary

- No periodicity but order at finite temperature
- Translational vs orientational order
- Only orientational order in 2 dim
- Orientational order for 2-dim models with screened dislocations
- First results for the Ariza-Ortiz model