Long range order in atomistic models for solids

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Mini-course – Lecture 2

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Particles, Fluids and Patterns:
Analytical and Computational Challenges

Outline

1. Mermin's no-crystallization theorem in $d = 2$
2. The harmonic approximation
3. The Ariza-Ortiz model and main results

We intend to exclude that particles interacting with a stable and tempered 2-body potential in $d = 2$ can form a crystal associated with a Bravais lattice with basis $\mathbf{a}_1, \mathbf{a}_2$ at $\beta > 0$. Setting:

- Torus Λ_L with sides $L\mathbf{a}_1, L\mathbf{a}_2$, and $N = L^2$
- Pair potential $V_\Lambda(\mathbf{Q}^{(N)}) = \sum_{i<j} v_{\Lambda_L}(\mathbf{q}_i - \mathbf{q}_j) \equiv \sum_{i<j} v_{ij}$
- Potential $W_\Lambda(\mathbf{Q}^{(N)}) = \sum_i w_{\Lambda_L}(\mathbf{q}_i) \equiv \sum_i w_i$ pinning particles at $\mathbb{L} = \cup_{\mathbf{n}\in\mathbb{Z}^2}\{n_1\mathbf{a}_1 + n_2\mathbf{a}_2\}$
- Expectation $\langle\cdot\rangle_{\beta,\Lambda_L,\epsilon} \equiv \langle\cdot\rangle$ w.r.t. Gibbs distrib. $\propto d\mathbf{Q}^{(N)} e^{-\beta\Phi_{\Lambda_L}}$ with $\Phi_\Lambda = V_\Lambda + \epsilon W_\Lambda$
- Reciprocal vectors: $\mathbf{G}_1, \mathbf{G}_2$ s.t. $\mathbf{a}_i \cdot \mathbf{G}_j = 2\pi\delta_{i,j}$. Reciprocal lattice: $\mathbb{L}^* := \cup_{\mathbf{n}\in\mathbb{Z}^2}\{n_1\mathbf{G}_1 + n_2\mathbf{G}_2\}$
- First Brillouin zone: $\mathcal{B} := \{\xi_1\mathbf{G}_1 + \xi_2\mathbf{G}_2 : \xi_1, \xi_2 \in [0,1)\}$ (at finite L: $\mathcal{B}_L := \{n_1\mathbf{G}_1/L + n_2\mathbf{G}_2/L : 0 \le n_1, n_2 < L\}$)
- For $\mathbf{k} \in \mathcal{B}_L$, let $\hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{k}) := \frac{1}{N}\langle\sum_i e^{-i\mathbf{k}\cdot\mathbf{q}_i}\rangle$.

Crystallization criterion:

1. $\hat{\rho}_\epsilon(\mathbf{G}) := \lim_{L\to\infty} \hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{G})$ is non-zero and s.t. $\lim_{\epsilon\to 0^+} |\hat{\rho}_\epsilon(\mathbf{G})| > 0$ for at least one non-zero $\mathbf{G} \in \mathbb{L}^*$.
2. For any bounded $\gamma : \mathcal{B} \to \mathbb{R}$ and $p = 1, 2$:

$$\lim_{L\to\infty} L^{-2} \sum_{\substack{\mathbf{k}\in\mathcal{B}_L:\\ \mathbf{k}\neq\mathbf{0}}} \gamma(\mathbf{k}) |\hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{k})|^p = 0$$

The two conditions cannot simultaneously hold, as a consequence of Bogoliubov's inequality:

$$\langle \Big| \sum_i \psi_i \Big|^2 \rangle \geq \frac{|\langle \varphi_i \boldsymbol{\nabla} \psi_i \rangle|^2}{\langle \frac{\beta}{2} \sum_{i,j} \Delta v_{ij} |\varphi_i - \varphi_j|^2 + \epsilon\beta \sum_i \Delta w_i |\varphi_i|^2 + \sum_i |\boldsymbol{\nabla}\varphi_i|^2 \rangle},$$

valid for any pair of smooth functions ψ, φ from Λ_L to $\mathbb{C}$ (here $\psi_i = \psi(\mathbf{q}_i)$ and $\varphi_i = \varphi(\mathbf{q}_i)$).

If we now choose $\psi(\mathbf{q}) = e^{-i(\mathbf{k}+\mathbf{G})\cdot\mathbf{q}}$ and $\varphi(\mathbf{q}) = \sin(\mathbf{k}\cdot\mathbf{q})$ for two non-zero vectors $\mathbf{G} \in \mathbb{L}^*$ and $\mathbf{k} \in \mathbb{B}_L$, Bogoliubov's inequality reads:

$$\langle \Big| \sum_i e^{-i(\mathbf{k}+\mathbf{G})\cdot\mathbf{q}_i} \Big|^2 \rangle \geq \frac{\frac{|\mathbf{k}+\mathbf{G}|^2}{4} \big| \langle \sum_i (e^{-i\mathbf{G}\cdot\mathbf{q_i}} - e^{-i(\mathbf{G}+2\mathbf{k}_i)\cdot\mathbf{q_i}}) \rangle \big|^2}{(A)+(B)+(C)}, \quad \text{where:}$$

$$(A) = \frac{\beta}{2} \sum_{i,j} \langle \Delta v_{i,j} |\sin(\mathbf{k}\cdot\mathbf{q}_i) - \sin(\mathbf{k}\cdot\mathbf{q}_j)|^2 \rangle \leq \frac{\beta}{2} |\mathbf{k}|^2 \sum_{i,j} \langle \Delta v_{i,j} |\mathbf{q}_i - \mathbf{q}_j|^2 \rangle$$

$$(B) = \epsilon\beta \sum_i \langle \Delta w_i |\sin(\mathbf{k}\cdot\mathbf{q})|^2 \rangle \leq \epsilon\beta \sum_i \langle \Delta w_i \rangle$$

$$(C) = |\mathbf{k}|^2 \sum_i \langle (\cos(\mathbf{k}\cdot\mathbf{q}))^2 \rangle \leq N|\mathbf{k}|^2$$

Recalling that $\hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{p}) = \frac{1}{N}\sum_i \langle e^{-i\mathbf{p}\cdot\mathbf{q}_i} \rangle$, dividing both sides by N:

$$\frac{1}{N} \langle \Big| \sum_i e^{-i(\mathbf{k}+\mathbf{G})\cdot\mathbf{q}_i} \Big|^2 \rangle \geq \frac{|\mathbf{k}+\mathbf{G}|^2 \big| \hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{G}) - \hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{G}+2\mathbf{k}) \big|^2}{C_1|\mathbf{k}|^2 + C_2}$$

where $C_1 = 4 + 2\frac{\beta}{N}\sum_{i,j} \langle \Delta v_{i,j} |\mathbf{q}_i - \mathbf{q}_j|^2 \rangle$, $C_2 = 4\frac{\beta}{N}\sum_i \langle \Delta w_i \rangle$.

Let $\gamma : \mathcal{B} \to \mathbb{R}$ be a smooth non-negative function supported on the ball of radius $|\mathbf{G}*|/4$ (where $|\mathbf{G}^*|$ is the minimum length of a non-zero vector in $\mathbb{L}^*$) of total integral 1. If we multiply both sides of the previous inequality by $\gamma(\mathbf{k})$ and sum over $\mathbf{k} \in \mathbb{B}_L \setminus \mathbf{0}$ we get:

$$\frac{1}{L^2}\sum_{\mathbf{k}\neq\mathbf{0}}\gamma(\mathbf{k})\big(1+\frac{1}{N}\sum_{i\neq j}\langle e^{i(\mathbf{G}+\mathbf{k})\cdot(\mathbf{q}_i-\mathbf{q}_j)}\rangle\big) \geq$$

$$\geq \frac{1}{L^2}\sum_{\mathbf{k}\neq\mathbf{0}}\gamma(\mathbf{k})\frac{|\mathbf{k}+\mathbf{G}|^2\big|\hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{G})-\hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{G}+2\mathbf{k})\big|^2}{C_1|\mathbf{k}|^2+C_2}$$

We now let $L \to \infty$. If hypothesis (2) on $\hat{\rho}_{\Lambda_L,\epsilon}$ holds, then all the terms in the RHS involving $\hat{\rho}_{\Lambda_L,\epsilon}(\mathbf{G}+2\mathbf{k})$ vanish as $L \to \infty$.

Suppose also that $\exists\ \alpha_0, \alpha_1, \alpha_2$ independent of ϵ s.t., letting $\Gamma(\mathbf{q}) := \frac{1}{L^2} \sum_{\mathbf{k}\neq\mathbf{0}} \gamma(\mathbf{k}) e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{q}}$:

$$\begin{aligned} &\lim_{L\to\infty} \frac{1}{N} \sum_{i\neq j} \langle \Gamma(\mathbf{q}_i - \mathbf{q}_j)\rangle \leq \alpha_0 \\ &\lim_{L\to\infty} C_1 \leq \alpha_1, \qquad \lim_{L\to\infty} C_2 \leq \alpha_2 \end{aligned} \tag{*}$$

then

$$1 + \alpha_0 \geq |\hat{\rho}_\epsilon(\mathbf{G})|^2 (3|\mathbf{G}^*|/4)^2 \int_{\mathcal{B}} \frac{d\mathbf{k}}{|\mathcal{B}|} \frac{\gamma(\mathbf{k})}{\alpha_1|\mathbf{k}|^2 + \epsilon\alpha_2}$$

The integral in the RHS diverges $\propto \log(1/\epsilon)$ as $\epsilon \to 0^+$: therefore $\lim_{\epsilon\to 0^+} |\hat{\rho}_\epsilon(\mathbf{G})| = 0$, as announced.

It remains to prove assumption (*). For this purpose, consider:

$$Z_{\Lambda_L}(\epsilon, \lambda, \eta, \rho) := \frac{1}{N!} \int d\mathbf{q}_1 \cdots d\mathbf{q}_N e^{-\beta\Psi_{\Lambda_L}(\mathbf{Q}^{(N)})}, \qquad \text{where:}$$

$$\Psi_{\Lambda_L}(\mathbf{Q}^{(N)}) = (V_{\Lambda_L} + \epsilon W_{\Lambda_L})(\mathbf{Q}^{(N)}) + \lambda \sum_{i<j} \Delta v_{ij} |\mathbf{q}_i - \mathbf{q}_j|^2 + \eta \sum_i \Delta w_i + \rho \sum_{i<j} \Gamma_{ij}$$

Ψ_{Λ_L} is a stable and tempered potential, so that Fisher's theorem on the existence of the thermodynamic limit holds. Therefore

$$\lim_{N=L^2\to\infty} \frac{1}{N} \log Z_{\Lambda_L}(\epsilon,\lambda,\eta,\rho) = f(\epsilon,\lambda,\eta,\rho)$$

exists, it is finite for $\epsilon,\lambda,\eta,\rho$ sufficiently small and convex in λ,η,ρ. Note that:

$$\frac{1}{N}\partial_\lambda \log Z_{\Lambda_L}(\epsilon,\lambda,\eta,\rho)\big|_{\lambda=\eta=\rho=0} = \frac{1}{N}\sum_{i<j}\langle \Delta v_{ij}|\mathbf{q}_i-\mathbf{q}_j|^2\rangle$$

$$\frac{1}{N}\partial_\eta \log Z_{\Lambda_L}(\epsilon,\lambda,\eta,\rho)\big|_{\lambda=\eta=\rho=0} = \frac{1}{N}\sum_{i}\langle \Delta w_i\rangle$$

$$\frac{1}{N}\partial_\rho \log Z_{\Lambda_L}(\epsilon,\lambda,\eta,\rho)\big|_{\lambda=\eta=\rho=0} = \frac{1}{N}\sum_{i<j}\langle \Gamma(\mathbf{q}_i-\mathbf{q}_j\rangle$$

By convexity, the (possibly subsequential) limits of these quantities are bounded as $N\to\infty$ (because the derivative of a convex function $f: I\to\mathbb{R}$ in an internal point $x_0\in I$ can be bounded by $\frac{2\max_{x\in I}|f(x)|}{\mathrm{dist}(x_0,\partial I)}$)

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Back to the "real" model

Classical particles interacting via pair potential $v(\mathbf{q}) = \varphi(|\mathbf{q}|)$, with minimum deep and narrow at $\ell_0 \equiv 1$:

$$H(\mathbf{Q}^{(N)}) = \sum_{i<j} V(|\mathbf{q}_i - \mathbf{q}_j|).$$

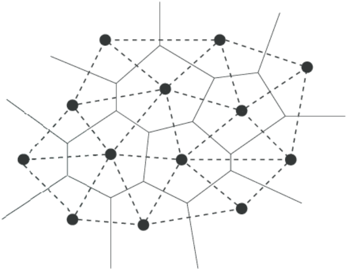
In 2D $\mathrm{argmin}_q H(q) =$ triangular lattice (Radin 1981, Theil 2006).

In 3D, min expected to be FCC (Flatley-Theil 2015).

Consider, e.g., $d = 2$.
Energy well approximated by

$$H_{nn}(\mathbf{Q}^{(N)}) = \sum_{\langle \xi,\eta\rangle \in \mathcal{E}(\mathbf{Q}^{(N)})} V(|\mathbf{q}(\xi) - \mathbf{q}(\eta)|)$$

where $\mathcal{E}(\mathbf{Q}^{(N)})$ is the edge set of the Delaunay triangulation $DT(\mathbf{Q}^{(N)})$.



The harmonic approximation

Take $DT(\mathbf{Q}^{(N)})$ to be (a portion $\mathbb{T}_L$ of) the triangular lattice $\mathbb{T}$. Write $\mathbf{q}(\mathbf{x}_i) = \mathbf{x}_i + \mathbf{u}(\mathbf{x}_i)$ with $\mathbf{x}_i \in \mathbb{T}$. Expanding we get:

$$H_{nn}(\mathbf{Q}^N) \simeq E_0 + H_{harm}(\mathbf{Q}^{(N)}), \qquad \text{with:}$$

$$H_{harm}(\mathbf{U}^{(N)}) = \tfrac{\varphi''(1)}{2} \sum_{\langle \mathbf{x},\mathbf{y}\rangle \in \mathbb{T}_L} [(\mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{y})) \cdot (\mathbf{x} - \mathbf{y})]^2$$

A similar formal derivation can be repeated in $d = 3$, with $\mathbb{T}$ replaced by the FCC lattice $\mathbb{F}$, a Bravais lattice with basis vectors

$$\mathbf{a}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \qquad \mathbf{a}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \qquad \mathbf{a}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

Harmonic model: exactly solvable statistical mechanics model with formal Gibbs measure $\propto \prod_{x \in \mathcal{L}} d\mathbf{u}(\mathbf{x}) e^{-\beta H_{harm}(\mathbf{U})}$ where $\mathcal{L} = \mathbb{T}, \mathbb{F}$, depending on whether $d = 2, 3$.

Positional LRO in the harmonic model, I

Take finite L and let $\mathcal{L}_L$ be the discrete torus obtained by taking a portion of $\mathcal{L}$ of sides $L\mathbf{a}_1, \ldots, L\mathbf{a}_d$ with periodic boundary conditions. Let $\langle\cdot\rangle_{\beta,L,\epsilon}$ be the expectation w.r.t. Gibbs distribution

$$\propto \prod_{\mathbf{x}\in\mathcal{L}_L} d\mathbf{u}(\mathbf{x}) e^{-\beta(H_{harm}(\mathbf{U}^{(N)})+\epsilon\|\mathbf{U}^{(N)}\|^2)}$$

with $N = L^d$. We say that the system exhibits positional Long Range Order (LRO) if

$$\lim_{\epsilon\to 0^+}\lim_{L\to\infty}\langle|\mathbf{u}(\mathbf{0})|^2\rangle_{\beta,L,\epsilon} = c_1(\beta)$$
$$\liminf_{|\mathbf{x}-\mathbf{y}|\to\infty}\lim_{\epsilon\to 0^+}\lim_{L\to\infty}\langle|\mathbf{u}(\mathbf{x})-\mathbf{u}(\mathbf{y})|^2\rangle_{\beta,L,\epsilon} = c_2(\beta)$$

with $c_1(\beta), c_2(\beta)$ two positive functions, tending to 0 as $\beta\to\infty$.

Positional LRO in the harmonic model, II

Let us focus, e.g., on the first condition. Let

$$\mathbf{u}(\mathbf{x}) = \tfrac{1}{L^d} \sum_{\mathbf{k}\in\mathcal{B}_L} e^{-i\mathbf{k}\cdot\mathbf{x}}\hat{\mathbf{u}}(\mathbf{k}) \quad \Leftrightarrow \quad \hat{\mathbf{u}}(\mathbf{k}) = \sum_{\mathbf{x}\in\mathcal{L}_L} e^{i\mathbf{k}\cdot\mathbf{x}}\mathbf{u}(\mathbf{x})$$

so that

$$\begin{aligned} H_{harm}(\mathbf{U}^N) &= \frac{1}{L^d} \sum_{\mathbf{k}\in\mathcal{B}_L} \sum_i |\hat{\mathbf{u}}(\mathbf{k})\cdot\mathbf{a}_i|^2 2(1-\cos(\mathbf{k}\cdot\mathbf{a}_i)) \\ &\equiv \frac{1}{L^d} \sum_{\mathbf{k}\in\mathcal{B}_L} \hat{u}(-\mathbf{k})\cdot\hat{A}(\mathbf{k})\hat{u}(\mathbf{k}), \end{aligned}$$

where $\hat{A}(\mathbf{k}) = \sum_i 2(1-\cos(\mathbf{k}\cdot\mathbf{a}_i))\,\mathbf{a}_i\otimes\mathbf{a}_i$, and the sum over i runs over $\{1,2,3\}$ if $d=2$ and over $\{1,\dots,6\}$ if $d=3$.

[In $d=2$, we can choose

$$\mathbf{a}_1 = \begin{pmatrix}1\\0\end{pmatrix}, \qquad \mathbf{a}_2 = \begin{pmatrix}-1/2\\ \sqrt{3}/2\end{pmatrix}, \qquad \mathbf{a}_3 = \begin{pmatrix}-1/2\\ -\sqrt{3}/2\end{pmatrix}.$$

In $d=3$ we can choose $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ as the basis vectors of $\mathbb{F}$, and $\mathbf{a}_4 = \mathbf{a}_3 - \mathbf{a}_2$, $\mathbf{a}_5 = \mathbf{a}_1 - \mathbf{a}_3$, $\mathbf{a}_6 = \mathbf{a}_2 - \mathbf{a}_1$.]

Positional LRO in the harmonic model, III

For small $\mathbf{k}$, $\hat{A}(\mathbf{k}) = \hat{A}_0(\mathbf{k}) + O(|\mathbf{k}|^4)$, where

$$\hat{A}_0(\mathbf{k}) = \sum_i (\mathbf{k}\cdot\mathbf{a}_i)^2 \mathbf{a}_i \otimes \mathbf{a}_i,$$

whose eigenvalues are all of order $|\mathbf{k}|^2$ as $\mathbf{k} \to \mathbf{0}$. In $d = 2$, this is particularly easy to check:

$$\hat{A}_0(\mathbf{k}) = \begin{pmatrix} \frac{9}{8}k_1^2 + \frac{3}{8}k_2^2 & \frac{3}{4}k_1 k_2 \\ \frac{3}{4}k_1 k_2 & \frac{3}{8}k_1^2 + \frac{9}{8}k_2^2 \end{pmatrix} \equiv \frac{3}{8}|\mathbf{k}|^2 + \frac{3}{4}\mathbf{k}\otimes\mathbf{k},$$

whose eigenvalues are $\frac{3}{8}|\mathbf{k}|^2$, $\frac{9}{8}|\mathbf{k}|^2$.

We thus find:

$$\langle|\mathbf{u}(\mathbf{0})|^2\rangle_{\beta,L,\epsilon} = \frac{1}{L^d}\sum_{\mathbf{k}\in\mathcal{B}_L}\langle|\mathbf{u}(\mathbf{k})|^2\rangle_{\beta,L,\epsilon} = \frac{1}{\beta}\frac{1}{L^d}\sum_{\mathbf{k}\in\mathcal{B}_L}\mathrm{Tr}\big[\hat{A}(\mathbf{k}) + \epsilon\mathbb{1}\big]^{-1}$$

Positional LRO in the harmonic model, IV

Taking $L \to \infty$ we find:

$$\lim_{L\to\infty} \langle |\mathbf{u}(\mathbf{0})|^2 \rangle_{\beta,L,\epsilon} = \int_{\mathcal{B}} \frac{d\mathbf{k}}{|\mathcal{B}|} \mathrm{Tr}\big[\hat{A}(\mathbf{k}) + \epsilon \mathbb{1}\big]^{-1}$$

which is:

- positive and of order $1/\beta$ uniformly in ϵ as $\epsilon \to 0^+$ if $d = 3$
- positive and $\sim$ (const.)$\frac{1}{\beta} \log(\epsilon^{-1})$ as $\epsilon \to 0^+$ if $d = 2$

In other words, the harmonic model predicts positional LRO in $d = 3$ and no positional LRO in $d = 2$.

Orientational LRO in the harmonic model

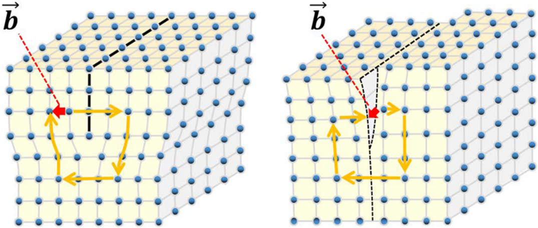
The same computation shows that:

$$\begin{aligned}\lim_{L\to\infty}\langle|\mathbf{u}(\mathbf{0})-\mathbf{u}(\mathbf{a}_i)|^2\rangle_{\beta,L,\epsilon} &= \lim_{L\to\infty}|1-e^{-i\mathbf{k}\cdot\mathbf{a}_i}|^2\langle|\hat{\mathbf{u}}(\mathbf{k})|^2\rangle_{\beta,L,\epsilon}\\ &= \int_{\mathcal{B}}\frac{d\mathbf{k}}{|\mathcal{B}|}2(1-\cos(\mathbf{k}\cdot\mathbf{a}_i))\mathrm{Tr}\big[\hat{A}(\mathbf{k})+\epsilon\mathbb{1}\big]^{-1}\end{aligned}$$

which is positive and of order $1/\beta$ uniformly in ϵ as $\epsilon\to 0^+$ both in $d=2$ and in $d=3$.

The KTHNY model

The harmonic model neglects dislocations



In their famous paper on XY, Kosterlitz-Thouless 1973 studied also 2D crystals; they proposed to add a pair interaction among dislocations with Burgers vectors $\{b_i\}$ located at $\{r_i\}$ of the form (letting $r_{ij} = r_i - r_j$):

$$H_{dis}(b) = K \sum_{i<j} \left[b_i \cdot b_j \log |r_{ij}| - \frac{(b_i \cdot r_{ij})(b_j \cdot r_{ij})}{|r_{ij}|^2} + \frac{1}{2} b_i \cdot b_j \right]$$

In addition to this interaction energy, dislocations come with finite self-energy. Similar formula in 3D with $\log |r_{ij}| \rightsquigarrow 1/|r_{ij}|$.

2D melting

KT model investigated further in Nelson-Halperin, Young 1979.

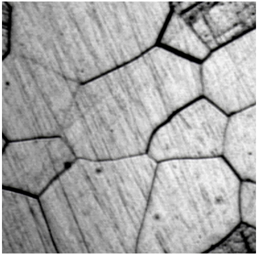
Predictions in $d = 2$:

- $T < T_m$: algebraic decay of positional correlations & orientational LRO
- $T_m < T < T_i$: exponential decay of positional correlations & algebraic decay of orientational correlations
- $T > T_i$: exponential decay of all correlations

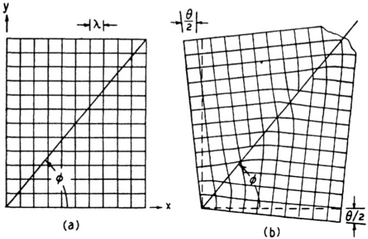
Model intrinsically mesoscopic, BUT unclear whether it supports grains

Grains and grain boundaries

Typical configurations consist of grains with ‘constant’ orientations θ_i



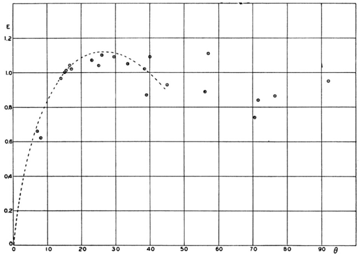
On the grain boundaries: finite density of defects.

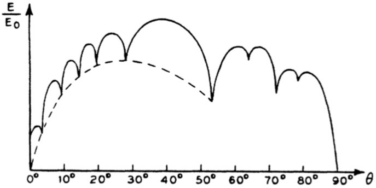


A mesoscopic model of grains

Grains have finite surface tension. Read-Shockley law:

$$\tau(\Delta\theta) \underset{\Delta\theta\to 0}{\sim} \Delta\theta(A - \log(\Delta\theta))$$





Effective model: $E(\theta) = \sum_{i<j} v(\theta_i - \theta_j)$

with $v(\theta) \geq 0$ e $v(\theta) \sim -\theta \log \theta$ per $\theta \to 0^+$. Notwithstanding this singular behavior, MW holds (Ioffe-Schlosman-Velenik 2005) $\Rightarrow$ this suggests no orientational LRO in $d = 2$.

To order or not to order?

How to explain this contradiction?

Vague answer: neighboring grains never display arbitrarily small $\Delta\theta_{ij}$: these are pinned to discrete set of magic angles $\Rightarrow$ at mesoscopic level the system behaves like a clock model rather than like XY $\Rightarrow$ orientational LRO possible in 2D

It would be desirable to identify a treatable microscopic model of a crystal, supporting dislocations and grains, in which prove or disprove existence of 2D orientational LRO (as well as characterize the typical low T configurations: do they correspond to grains with discrete relative orientations?)

The Ariza-Ortiz model is a good candidate: it is a sort of vectorial analogue of the Villain model. Our main results on LRO concern the 'easy' case of $d = 3$, which we started to study as a preparation to $d = 2$.

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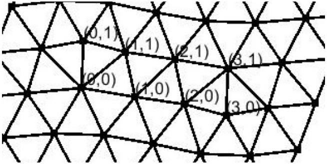
Heuristic derivation from the "real" model

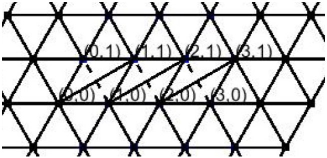
Start from $$H_{nn}(q) = \sum_{\langle \xi,\eta\rangle \in \mathcal{B}(q)} V(|q(\xi) - q(\eta)|).$$

Re-express sum to be over bonds $\mathcal{B}$ of reference lattice:

$$\begin{aligned} H_{nn}(q) &= \sum_{\langle x,y\rangle \in \mathcal{B}} V(|q(\varphi(x,y)) - q(\psi(x,y))|) \\ &= \sum_{\langle x,y\rangle \in \mathcal{B}} V(|x - y + u(\varphi(x,y)) - u(\psi(x,y)) + \sigma(x,y)|), \end{aligned}$$

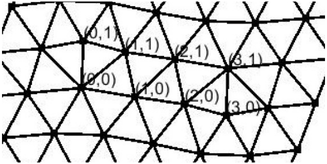
where $\quad q(x) \equiv x + u(x), \qquad \varphi(x,y) - \psi(x,y) \equiv x - y + \sigma(x,y).$

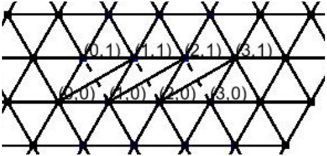




Relabelling edges around dislocation

In this example, letting the positively oriented edges be $(x, x + \delta_i)$ with $\delta_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\delta_2 = \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix}$, $\delta_3 = \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix}$,





On positively oriented edges: $\varphi(x, y) \equiv x$. Moreover, $\psi(x, y) = y$ unless:

- $x = (1,0), (2,0), (3,0)$ & $y = x + \delta_2 \Rightarrow \psi(x, y) = y + \delta_1$
- $x = (1,1), (2,1), (3,1)$ & $y = x + \delta_3 \Rightarrow \psi(x, y) = x - \delta_1$

$\sigma(x, y) = \mp\delta_1$ only along edges for which $\psi(x, y) = y \pm \delta_1$.

Further approximations

We expect that, typically,

$$u(\varphi(x,y)) - u(\psi(x,y)) + \sigma(x,y) \ll 1$$

which motivates the harmonic approx:

$$H_{nn}(q) \rightsquigarrow \frac{V''(1)}{2} \sum_{\langle x,y\rangle \in \mathcal{B}} [(u(\varphi(x,y)) - u(\psi(x,y)) + \sigma(x,y)) \cdot (x-y)]^2.$$

Finally, we'll make the linearized plasticity approx:

$$u(\varphi(x,y)) - u(\psi(x,y)) \approx u(x) - u(y)$$

which leads us to the AO Hamiltonian:

$$H_{AO}(u,\sigma) = \frac{1}{2} \sum_{\langle x,y\rangle \in \mathcal{B}} [(u(x) - u(y) + \sigma(x,y)) \cdot (x-y)]^2.$$

Symmetries

The Ariza-Ortiz Hamiltonian is invariant under following symmetries:

1. Translations: $u(x) \mapsto u(x) + \tau$ for any $\tau \in \mathbb{R}^d$
2. Linearized rotations: $u(x) \mapsto u(x) + Sx$ for any $d \times d$ skew-symmetric matrix S.
3. Gauge invariance:

$$(u(x), \sigma(x, y)) \mapsto (u(x) + v(x), \sigma(x, y) + v(y) - v(x))$$

for any $v : \mathcal{L} \to \mathcal{L}$

Linearized rotations: approximation of invariance under rotations: $u(x) \mapsto R(x + u(x)) - x$ for all $R \in SO(d)$. Distinctive feature of microscopic models of elasticity.

Statistical mechanics

Take $\Lambda \subset \mathcal{L}$, let $\mathcal{B}_\Lambda$ restriction of $\mathcal{B}$ to edges touching Λ, and

$$\mathcal{C}^0_\Lambda = \{u : \mathcal{L} \to \mathbb{R}^d : u\big|_{\Lambda^c} = 0\}, \quad \mathcal{C}^1_{\mathcal{L},\Lambda} = \{\sigma : \mathcal{B} \to \mathcal{L} : \sigma\big|_{\mathcal{B}^c_\Lambda = 0}\}$$

be the sets of functions on Λ and $\mathcal{B}_\Lambda$ with Dirichlet b.c.

Let $\phi(u, \sigma) = \varphi(\mathrm{d}u - \sigma)$ be a gauge-invariant observable:

$$\langle \phi \rangle_{\beta,\Lambda} = \frac{1}{Z_{\beta,\Lambda}} \sum_{\sigma \in \mathcal{C}^1_{\mathcal{L},\Lambda}/\text{gauge}} \int_{\mathcal{C}^0_\Lambda} du \, e^{-\beta(H_{AO}(u,\sigma) - W(\mathrm{d}\sigma))} \varphi(\mathrm{d}u - \sigma),$$

with $W(q) = \sum_f w_0 |q(f)|^2$.

Main result

Theorem (G., Theil JEMS 2022)

Let $\mathcal{L}$ be the 3D FCC lattice and $k_0 \in \mathcal{L}^*$.

There exists C, β_0, r_0 s.t., for $\beta \geq \beta_0$, $|x-y| \geq r_0$,

$$\liminf_{\Lambda \nearrow \mathcal{L}} \langle e^{ik_0 \cdot (u(x)-u(y))} \rangle_{\beta,\Lambda} \geq e^{-C/\beta}.$$

Open questions

1. Existence of thermodynamic limit (in $d = 2, 3$)?
2. Exponential decay at small β (in $d = 2, 3$)?
3. For $\mathcal{L}$ the 2D triangular lattice:
    - algebraic decay at large β?
    - orientational LRO? (for which gauge-invariant correlation?)

Related result: Bauerschmidt-Conache-Heydenreich-Merkl-Rolles 2019