Crystallization in classical particle systems

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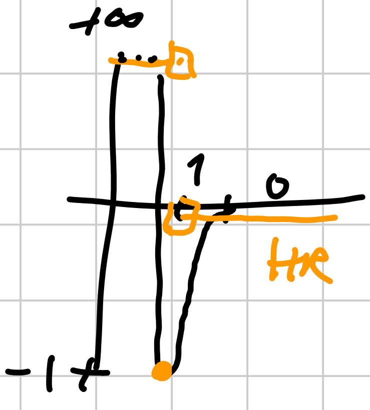
— lecture 3 —

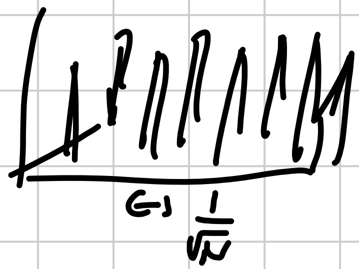
Summary so far on en. min., 2D

$$E(x_1, \dots, x_N) = \sum_{i \neq j} V(x_i - x_j), \quad V = \text{soft HR pot. or HR pot.}$$



$$E \simeq \underbrace{N \cdot e_\infty}_{\to \text{ governs crystalliz.}} + \underbrace{\int_{\partial''\Omega''} s/th..}_{\to \text{ shape}} + \text{l.o.t.}$$

Au Yeung, GF, Schmidt

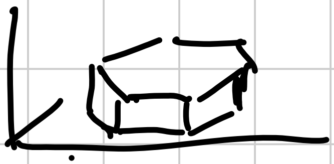


Ind. of shape $\mu_N = \frac{1}{N}\sum_{i=1}^{N} \delta_{\frac{x_i}{\sqrt{N}}} \xrightarrow{*} c_0 \chi_\Omega$, finite per.

(Minimizers up to $O(\sqrt{N})$)

Unique explicit shape (Minimizers)

$$\mu_N \xrightarrow{*} c_0 \chi_{\text{regular hexagon}}$$



Pf of explicit shape   Use

1) ground states of finite-N HR model have "global rigidity"
2) Γ-conv. result yielding a surf. en. (based on Alicandro Braides Cicalese 2006)
3) Unique min. of Γ-limit (Taylor; Fonseca/S. Müller)

1) **Theorem** (Heitmann, Radin 1981)

$S=\{x_1,\dots,x_N\}$ minimizer of 2D HR model

$\Rightarrow$ S subset of $R\mathcal{L}+a$, $\quad R\in SO(2)$, $a\in\mathbb{R}^2$, $\mathcal{L}$ = triang. lattice

$\mathcal{L}=\mathrm{Span}_{\mathbb{Z}}\left\{\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}\frac{1}{2}\\ \sqrt{3}/2\end{pmatrix}\right\}$ triang. latt.

Pf idea $\quad S$ = general N-particle config.

$N(x)=\{y\in S : |y-x|=1\}$ n. nbrs of x

$\partial S = \{x\in S ; \#N(x)<6\}$

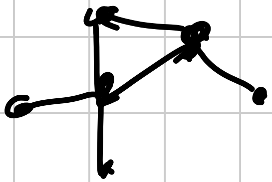
Key lemma $\quad S$ minimizer of E_N = N-particle en.

$\Rightarrow$ $S\setminus\partial S$ —"— $E_{N-\#\partial S}$

Key tool $\quad d=\sum_{x\in\partial S}\#N(x)$

More geometric interpretation (work in progress, GF + Lucia de Luca)

Config's in HR $\rightsquigarrow$ graph $\rightsquigarrow$ metric $\rightsquigarrow$ curvature (many notions)



(edge $\Leftrightarrow$ distance 1)

($d(x,y) =$ min. # of edges from x to y)

$$N(x) = S^1(x)$$

Euler curvature: $K(x) = 6 - \#\text{edges in } S^1(x)$

[$K(x) = 6 - \# S^1(x)$ Knill ..]

[$K(x) = 2\# S^1(x) - \# S^2(x)$ —//— ...]

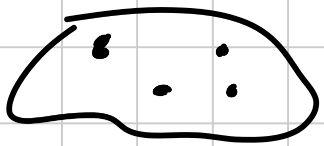
$K(x) = 0$ if x interior pt in triang. latt.,

$$\sum_{S} K(x) = \int_{\partial S} K(x) = 3|\partial S| + 6 \quad \text{for nice subsets of } \mathcal{L}$$

$$\Rightarrow \sum_{S} K(x) - 3|\partial S| = 6 \quad \text{—//—}$$

Philosophy: view defects as sources of discrete curvature

Inspiration: Garroni Leoni Ponsiglione $\min \int \mathbb{C}\beta \cdot \beta$ s/t $\operatorname{curl} \beta = \sum_i \delta_{x_i}$
in mesoscopic plasticity models



(Müller, Zeppieri, Scardia .. $\operatorname{dist}^2(\beta, SO(2))$ ...)

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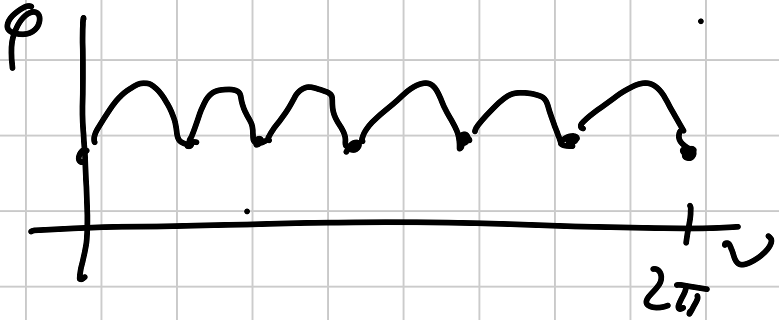
2) <u>Gamma limit</u>

$$I_N(\mu) = \begin{cases} \int_{\mathbb{R}^2 \times \mathbb{R}^2 \setminus \text{diag.}} N V(N^{1/2}|x-y|)\, d\mu(x)\, d\mu(y), & \mu = \frac{1}{N}\sum_{i=1}^{N} \delta_{\frac{x_i}{\sqrt{N}}} \\ +\infty & \text{else} \end{cases}$$

$$I_N(\mu) = \mathcal{E}(x_1, \dots, x_N) \qquad x_i \in \mathcal{L}.$$

<u>Thm</u> (Au Yeung, GF, Schmidt)

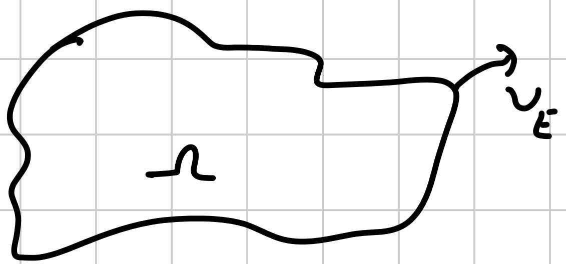
$$\frac{1}{\sqrt{N}}\left(I_N - N e_\infty\right) \xrightarrow[\text{weak* conv. of } \mu]{\Gamma} \begin{cases} \int_{\partial^* E} \varphi(\nu_E)\, d\mathcal{H}^1, & \mu = \frac{2}{\sqrt{3}}\chi_E, \ E \text{ finite per.}, \int \mu = 1, \\ +\infty & \text{else} \end{cases}$$



$$\varphi(\nu) = 2\left(\nu_2 - \frac{\nu_1}{\sqrt{5}}\right),$$

$$\nu = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}, \quad \theta \in \left[0, \frac{2\pi}{6}\right],$$

per.



Wulff-Herring-Gibbs en.

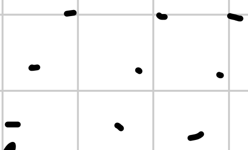
3) Minimizer unique, given by "Wulff construction".

$$E = \lambda \cdot \{ x \in \mathbb{R}^2 : x \cdot n \leq \varphi(n) \quad \forall n \in S^1 \}$$

Taylor; Fonseca/Müller.

Quasicrystals.

Recall $\mathcal{L}$ Bravais lattice in $\mathbb{R}^d$ $\Leftrightarrow$ $\mathcal{L} = A\mathbb{Z}^d$, $A \in M^{d\times d}$, invertible



Fourier transform $\hat{\rho}(\xi) = \int_{\mathbb{R}^d} e^{-i\xi\cdot x}\rho(x)\,dx$

$\rho \in \mathcal{S}'(\mathbb{R}^d)$ $\quad \langle \hat{\rho}, \varphi\rangle_{\mathcal{S}',\mathcal{S}} := \langle \rho, \hat{\varphi}\rangle \ \forall \varphi\in\mathcal{S}$

F.T. of empirical meas. of a Bravais lattice is well defined

$$\rho = \sum_{a\in\mathcal{L}} \delta_a =: \delta_{\mathcal{L}}$$

F.T. is in fact again the empir. meas. of a Br. lattice !!!

$$\hat{\delta}_{\mathcal{L}} = \frac{(2\pi)^d}{|\det A|}\,\delta_{\mathcal{L}'},$$ $\mathcal{L}'$ reciprocal lattice

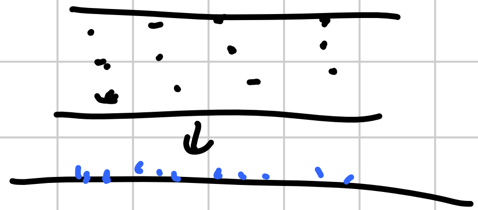
$\mathcal{L}' = \{\xi \in \mathbb{R}^d : \xi\cdot a \in 2\pi\mathbb{Z} \ \forall a \in \mathcal{L}\} = (2\pi)A^{-T}\mathbb{Z}^d$

$\mathcal{L}'' = \mathcal{L}$

Def. A topologically discrete subset $\mathcal{S}$ of $\mathbb{R}^d$ is called a <u>quasicrystal</u> if $\hat{\delta}_{\mathcal{S}}$ is a countable sum of Dirac masses with coefficients, $\sum_{j=1}^{\infty} a_j \delta_{\xi_j}$, & $\mathcal{S}$ is not periodic.

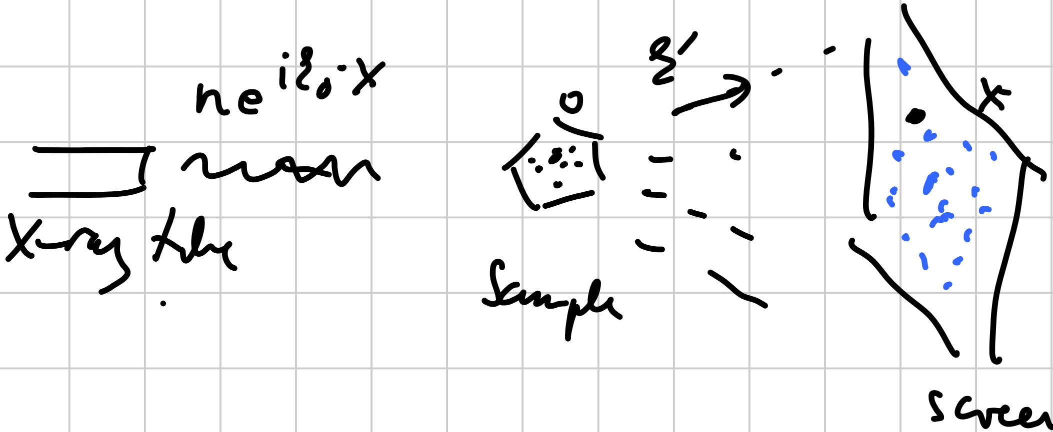
Q: Classify quasicrystals.

Ex's: Penrose tilings ; cut & project



Q: Find simple model en. s.th. GS is quasicrystalline.

Why Fourier tf? **A:** Because it governs X-ray diffraction patterns



$I(x)$ intensity of diffracted radiation

$$I(x) = \frac{\text{const}}{|x|^2} \left| n'(x)\, \hat{\varrho}\left(k'(x) - k_0\right) \right|^2$$

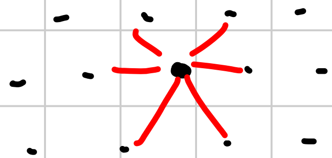
$$n'(x) = P_{k'(x)^\perp}\, n, \qquad k'(x) = |k_0| \frac{x}{|x|}$$

GF, James, Juestel, arXiv Tue 16.6.2015

3D.

HR model in 3D $\qquad E(x_1, \dots, x_N)$

Def. (GF, Au Yeung, unpublished)



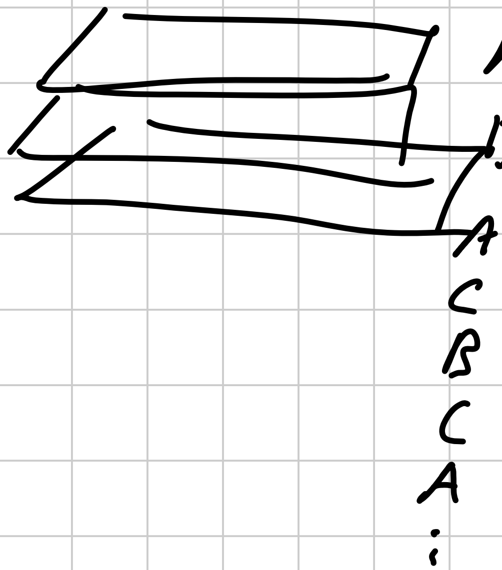
$$\mathcal{E}(\mathcal{S}) = \lim_{R\to\infty} \sum_{x \in B_R} \left(E(x, \mathcal{S}) - e_\infty \right)$$

$$E(A,B) = \sum_{x\in A} \sum_{y \in B} V(|x-y|)$$

$$e_\infty = \text{kissing no.} = \begin{cases} 6 & 2D \\ 12 & 3D \end{cases}$$

Fact: Unique min. of $\mathcal{E}$ in 2D is the triang. latt.,

Conj.: 3D: any stacking seq. of triang. lattice without repetition



3D vs 2D: no rigidity of 12 nbrs of a pt

open set