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Statistical mechanics of nonlinear elasticity for a hard-disk system

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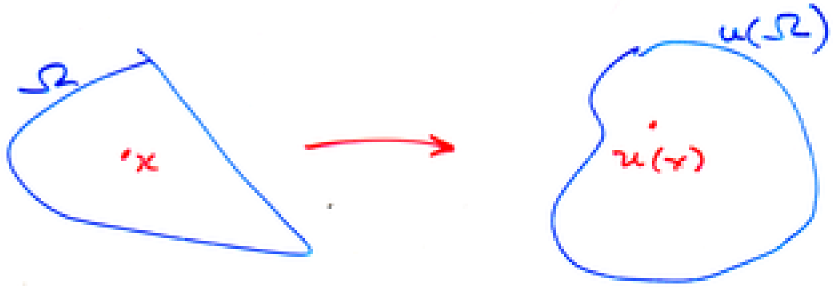
Principles of nonlinear elasticity



"deformation matrix"

Minimize $\displaystyle\int_{\Omega} f(\nabla u(x))\, d^3x$

"stored energy function"

Euler-Lagrange $\displaystyle\sum_j \frac{\partial t_{ij}}{\partial x_j} = 0$

Stress tensor $\displaystyle t_{ij} := \frac{\partial f}{\partial \left(\frac{\partial u_i}{\partial x_j}\right)}$

Constitutive relation

$$f = f\left(\dots, \frac{\partial u_i}{\partial x_j}, \dots\right)$$

Quasi - convexity (a desirable property of f)

"if $\nabla u = A =$ const on $\partial\Omega$

then the minimizer has $\nabla u = A$ within Ω"

Morrey's theorem (1952):

QC + continuity $\Rightarrow$ variational problem is soluble

The "unconstrained" partition function

partition function Hamiltonian temperature

$$Z := \frac{1}{N!}\int\cdots\int e^{-H/kT}\, dp_1\cdots dq_{2N}$$

potential energy

$$= \frac{(2\pi m kT)^N}{N!} \underbrace{\int\cdots\int e^{-W/kT}\, dq_1\cdots dq_{2N}}_{\text{configurational integral}}$$

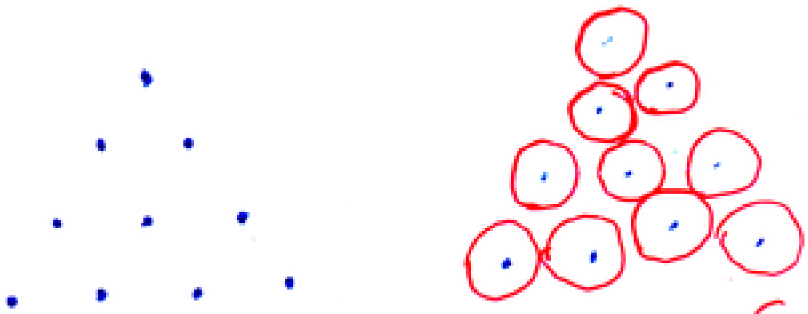
$$Q := \frac{1}{N!}\int\cdots\int e^{-W/kT}\, dq_1\cdots dq_N$$

$$= \frac{1}{N!}\int\cdots\int \chi_{hc}(q_1\cdots q_N)\,\chi_{wall}(q_1\cdots q_N)\,dq_1\cdots dq_N$$

$$\chi_{hc} := \begin{cases} 1 & \text{if no disks overlap} \\ 0 & \text{otherwise} \end{cases}$$

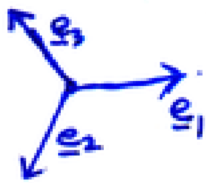
$$\chi_{wall} := \begin{cases} 1 & \text{if all disks are inside container} \\ 0 & \text{otherwise} \end{cases}$$

The model: hard disks of diameter 1



labels $\in \Lambda$ positions $\in \mathbb{R}^2$

Denote the set of possible labels (a triangular lattice with spacing 1) by $\Lambda := i\underline{e}_1 - j\underline{e}_2$ $(i,j \in \mathbb{Z})$



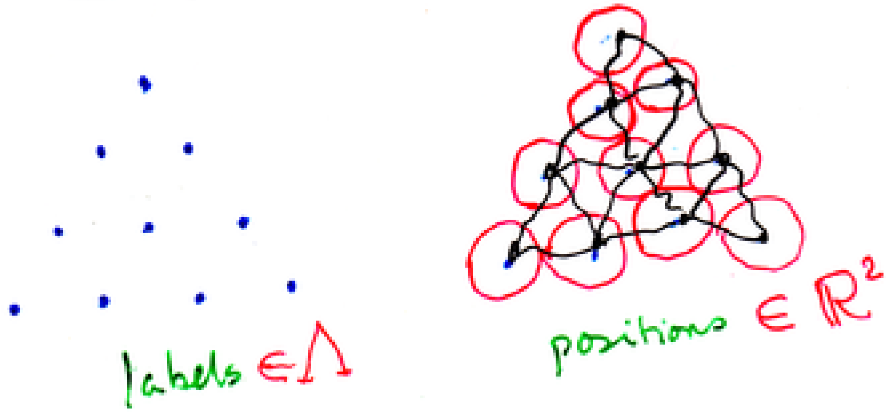
$\underline{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$\underline{e}_2 = \begin{bmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix}$

The particle whose label is $k \in \Lambda$ has position $\underline{x}_k$

Hard-core constraint
$$|\underline{x}_k - \underline{x}_l| \geq 1 \quad \text{if } k \neq l$$

The model: hard disks of diameter 1



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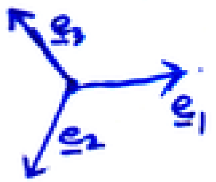

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Hard-core constraint

$$|\underline{x}_k - \underline{x}_\ell| \geq 1 \quad \text{if} \quad k \neq \ell$$

Network constraint

$$|\underline{x}_k - \underline{x}_\ell| \leq \sqrt{2} \quad \text{if} \quad |\underline{k} - \underline{\ell}| = 1$$

The constrained configurational integral

K any convex finite set in Λ

A any matrix in $\mathcal{A}$

the set of "allowed" deformation matrices ie those with

$1 < |A e_i| < \sqrt{2} \quad (i=1,2,3)$

δ any small positive number.

There are two types of constrained C. I.

$a \in \{loose, tight\}$

$$Q_\delta^{(a)}(K, \underline{\underline{A}}) := \int_{\mathbb{R}^{2N}} d^{2N}\underline{X}\, \chi_{hc}(\underline{X})\chi_{net}(\underline{X})\chi_{anc}^{(a)}(\underline{X})$$

$\underline{X} := \{\underline{x}_k : \underline{k} \in K\}$

$\chi_{hc} := 1$ if $|\underline{x}_k - \underline{x}_\ell| \geq 1$ whenever $k \neq \ell$, else 0

$\chi_{net} := 1$ if $|x_k - x_\ell| \leq \sqrt{2}$ whenever $|k-\ell| = 1$, else 0

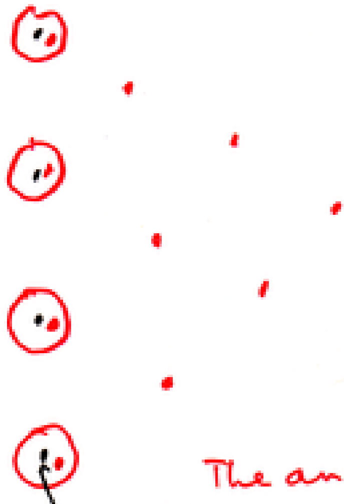
$\chi_{anc}^{(tight)} := 1$ if $|x_{\underline{k}} - A\underline{k}| \leq \delta$ whenever $\underline{k} \in \partial K$, else 0

$\chi_{anc}^{(loose)} := 1$ if $|x_{\underline{k}} - A\underline{\ell}| \geq 1+\delta$ whenever $\ell \in \partial K^c$

AND $|x_{\underline{k}} - A\ell| \leq \sqrt{2} - \delta$ whenever $\ell \in \partial K^c$ and $|\underline{k} - \ell| = 1$

else 0

Tight Anchoring

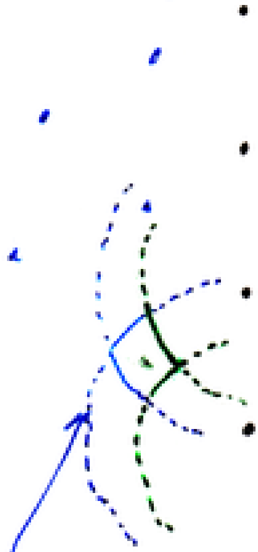


The anchored particles stay inside circle of radius δ

anchor points

$A_k : k \in \partial K$

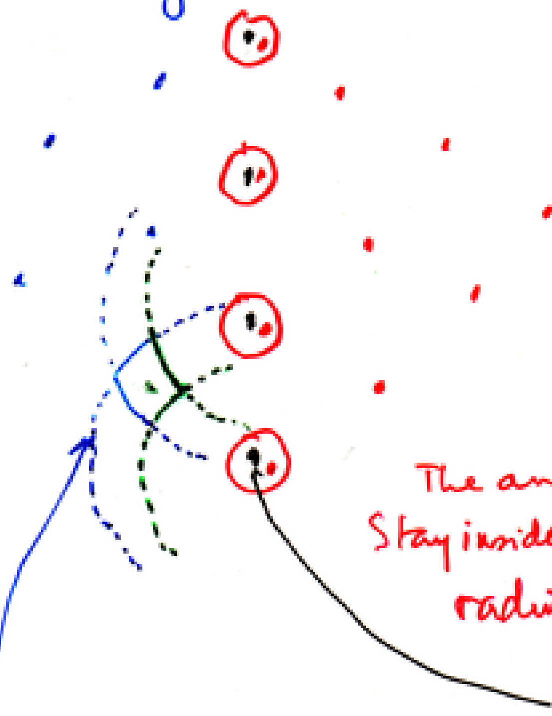
Loose Anchoring



The anchored particles stay inside circles of radius $\sqrt{2}-\delta$ and outside circles of radius $1+\delta$

Loose Anchoring

Tight Anchoring



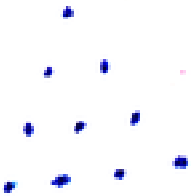
The anchored particles stay inside circle of radius δ

anchor points $A_k : k \in \partial K$

The anchored particles stay inside circles of radius $\sqrt{2}-\delta$ and outside circles of radius $1+\delta$

Theorem 2: thermodynamic limit for equilateral triangle

$\Delta_3 :=$



$$\lim_{p\to\infty} \frac{\ln Q_\delta^{(\ell)}(\Delta_{2p-1}, A)}{|\Delta_{2p-1}|} = \frac{\ln Q_\delta^{(t)}(\Delta_{2p-2}, A)}{|\Delta_{2p-2}|}$$

$$=: \psi(A)$$

exists and is independent of δ

Thermodynamic interpretation

Free energy per particle ("stored energy")

$$= -kT \lim_{N\to\infty} \frac{1}{N} \log(\text{partition function})$$

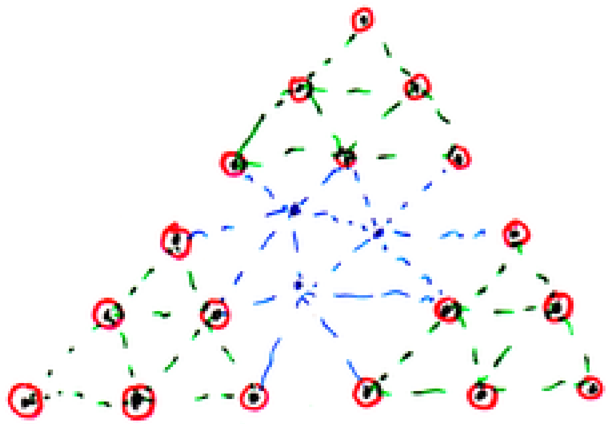
$$= kT\left(\log(2\pi mkT) - \psi(A)\right)$$

$$= -kT\,\psi(A) + \text{kinetic energy term}$$

log of free volume per particle

independent of A ∴ can be ignored

Idea behind proof of Theorem 2



$$\left[Q_\delta^t(\Delta_2)\right]^3 Q_\delta^\ell(\Delta_1) \le Q_\delta^t(\Delta_5)$$

$$3\log Q_\delta^t(\Delta_{2^p-1}) + \log Q_\delta^\ell(\Delta_{2^p-2}) \le \log Q_\delta^t(\Delta_{2^{p+1}-1})$$

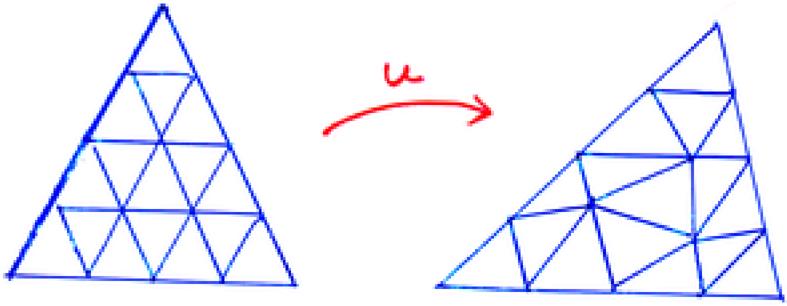
$$\frac{3}{4}\psi_\delta^t(p) + \frac{1}{4}\psi_\delta^\ell(p) \le \psi_\delta^t(p+1)$$

$$2^{-2p}\log Q^t(\Delta_{2^p-1}) \qquad 2^{-2p}\log Q^\ell(\Delta_{2^p-2})$$

Also $\frac{3}{4}\psi_\delta^\ell(p) + \frac{1}{4}\psi_\delta^t(p) \le \psi_\delta^\ell(p+1)$

The sequence $\psi_\delta^\ell(p) + \psi_\delta^t(p)$ $p = 1, 2, \ldots$ is bounded & increasing $\therefore \to$ limit.

Theorem 3 (Triangulation inequality)



If A a matrix in $\mathcal{D}$

n a positive integer

$\underline{u}(\cdot)$ a homeomorphism (continuous & invertible)

$\nabla u(x) = A$ for $x \notin \triangle$

∇u = const on each sub-triangle

Then

$$\sum_{\text{sub-triangles } \underline{k}} \psi\left(\nabla u(\underline{k})\right) \leq n^2 \psi(A)$$

Theorem 4 The function $\psi(\cdot)$ is Lipschitz continuous on any compact convex subset of $\mathcal{A}$

i.e. if $\mathcal{B}$ is the subset & $A_1, A_2 \in \mathcal{B}$ then

$$|\psi(A_1) - \psi(A_2)| \leq K(\mathcal{B}) \| A_1 - A_2 \|$$

Theorem 5 : "Quasi Convexity" of $-\psi$

$\underline{\underline{A}}$ is an allowed 2×2 matrix

$\underline{u}(x) = A\underline{x}$ for $\underline{x} \notin \Omega$

$\nabla \underline{u}(x) \in \mathcal{A}$ for $\underline{x} \in \Omega$

$\underline{u}(\cdot)$ is Lipschitz continuous & so is its inverse

i.e. $(1+\delta)|\underline{x}-\underline{x}'| < |u(\underline{x}) - u(\underline{x}')| < (\sqrt{2}-\delta)|\underline{x}-\underline{x}'|$

$$\int_\Omega \bar{\Psi}\left(\nabla \underline{u}(\underline{x})\right) d^2\underline{x} \geqslant \bar{\Psi}(\underline{A}) \int_\Omega d^2\underline{x}$$

where $\bar{\Psi} := -\psi = \frac{1}{kT} \times$ free energy per particle + k.e. term