Statistical mechanics of nonlinear elasticity for a hard-disk system

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Principles of nonlinear elasticity

Minimize \[ \int_{\Omega} \sum_{i,j} \frac{\partial t_{ij}}{\partial x_j} \, d^3x \]

"deformation matrix"

"stored energy function"

Euler-Lagrange \[ \sum_j \frac{\partial t_{ij}}{\partial x_j} = 0 \]

Stress tensor \[ t_{ij} = \frac{\partial f}{\partial (\partial u_i / \partial x_j)} \]

Constitutive relation \[ f = f(\ldots, \partial u_i / \partial x_j, \ldots) \]

Quasi-convexity (a desirable property of \( f \))

"if \( \nabla u = A = \text{const on } \partial \Omega \)
then the minimizer has \( \nabla u = A \) within \( \Omega \)"

Morrison's Theorem (1952):

QC + continuity \( \Rightarrow \) variational problem is soluble
The "unconstrained" partition function

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

Hamiltonian \quad \text{temperature} \quad \text{potential energy}

\[ = \frac{(2\pi mkT)^N}{N!} \int \cdots \int e^{-\frac{W}{kT}} \, dq_1 \cdots dq_{2N} \]

Configurational integral

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

\[ = \frac{1}{N!} \int \cdots \int X_{hc}(q_1, \ldots, q_N) X_{wall}(q_1, \ldots, q_N) \, dq_1 \cdots dq_N \]

\[ X_{hc} := \begin{cases} 1 & \text{if disks overlap} \\ 0 & \text{otherwise} \end{cases} \]

\[ X_{wall} := \begin{cases} 1 & \text{if all disks are inside container} \\ 0 & \text{otherwise} \end{cases} \]
The model: hard disks of diameter 1

Denote the set of possible labels (a triangular lattice with spacing 1) by

\[ \Lambda := \{ i \mathbf{e}_1 - j \mathbf{e}_2 : (i, j) \in \mathbb{Z} \} \]

The particle whose label is \( k \in \Lambda \) has position \( \mathbf{x}_k \).

Hard-core constraint

\[ |\mathbf{x}_k - \mathbf{x}_l| \geq 1 \quad \text{if} \quad k \neq l \]
The model: hard disks of diameter 1

Denote the set of possible labels (a triangular lattice with spacing 1) by \( \Lambda := \{ ie_1 - j e_2 \mid i, j \in \mathbb{Z} \} \)

\( e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \)
\( e_2 = \begin{bmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix} \)

The particle whose label is \( k \in \Lambda \) has position \( x_k \)

Hard-core constraint
\( |x_k - x_l| \geq 1 \) if \( k \neq l \)

Netscape constraint
\( |x_k - x_l| \leq \sqrt{2} \) if \( |k - l| = 1 \)
The constrained configurational integral

\[ K \] any convex finite set in \( \Delta \)

\[ A \] any matrix in \( \mathbb{A} \)

the set of "allowed" deformation matrices, ie those with:

\[ 1 \leq |A e_i| \leq \sqrt{2} \quad (i = 1, 2, 3) \]

\[ \delta \] any small positive number.

There are two types of constrained C.I.

\[ Q^a_\delta (K; A) := \int_{R^{2N}} d^{2N} X \chi_{hc} (X) \chi_{net} (X) \chi^{(a)}_{anc} (X) \]

\[ \chi_{hc} := 1 \text{ if } |x_k - x_\ell| \geq 1 \text{ whenever } k \neq \ell, \text{ else } 0 \]

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

\[ \chi^{(tight)}_{anc} := 1 \text{ if } |x_k - A k| \leq \delta \text{ whenever } k \in \delta K, \text{ else } 0 \]

\[ \chi^{(loose)}_{anc} := 1 \text{ if } |x_k - A k| \geq 1 + \delta \text{ whenever } k \in \delta K \]

AND \( |x_k - A k| \leq \sqrt{2} - \delta \) whenever \( k \in \delta K \) and \( |k - 2| = 1 \)

else \( 0 \)
Tight Anchoring

The anchored particle
Stay inside circle of
radius

anchor points
Ak: kεDK
Loose Anchoring

The anchored particles stay inside circles of radius $\sqrt{2} - \delta$ and outside circles of radius $1 + \delta$. 
The anchored partiles
Stay inside circle and outside radius 1 + 9
Anchor points: KEJK

Loose Anchoring

Tight Anchoring
Theorem 2: thermodynamic limit for equilateral triangle

\[ \Delta_3 = \ldots \]

\[
\lim_{p \to \infty} \frac{\ln Q^0_\theta(\Delta_{2p-1}, A)}{|\Delta_{2p-1}|} = \frac{\ln Q^0_\theta(\Delta_{2p-2}, A)}{|\Delta_{2p-2}|} = : \psi(A)
\]

exists and is independent of \( \theta \)

Thermodynamic interpretation

Free energy per particle ("stored energy")

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

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

\[ = -kT \psi(A) + \text{kinetic energy term} \]

\[ \text{log of free volume per particle} \quad \text{independent of } A \quad \text{can be ignored} \]
Theorem 2

\[ [Q^t_\delta(\Delta_2)]^3 Q^l_\delta(\Delta_1) \leq Q^t_\delta(\Delta_5) \]

\[ 3 \log Q^t_\delta(\Delta_{2p-1}) + \log Q^l_\delta(\Delta_{2p-2}) \leq \log Q^t_\delta(\Delta_{2p+1}) \]

\[ \frac{3}{4} \Psi^t_\delta(p) + \frac{1}{4} \Psi^l_\delta(p) \leq \Psi^t_\delta(p+1) \]

Also,

\[ 2^{-2p} \log Q^t_\delta(\Delta_{2p-2}) \]

The sequence \( \Psi^t_\delta(p) + \Psi^l_\delta(p) \) \( p = 1, 2, \ldots \)

is bounded and increasing \( \Rightarrow \) limit.
Theorem 3 (Triangulation inequality)

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

$n$ a positive integer

$\psi(\cdot)$ a homeomorphism (continuous & invertible)

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

$\nabla u = \text{const}$ on each sub-triangle

Then

$$\sum_{\text{sub-triangles } k} \psi(\nabla u(k)) \leq n^2 \psi(A)$$
Theorem 4. The function $\Psi(\cdot)$ is Lipschitz continuous on any compact convex subset of $\mathcal{A}$.

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

$$|\Psi(A_1) - \Psi(A_2)| \leq K(B) \|A_1 - A_2\|$$
Theorem 5: "Quasi Convexity" of $-\Psi$

\[ \Omega \xrightarrow{\nabla} \Omega \]

\[ A \text{ is an allowed } 2 \times 2 \text{ matrix} \]

\[ u(x) = Ax \quad \text{for } x \notin \Omega \]

\[ \nabla u(x) \in \mathcal{A} \quad \text{for } x \in \Omega \]

\[ u(\cdot) \text{ is Lipschitz continuous} \]

\[ \text{and so is its inverse} \]

\[ i.e. \ (1 + \delta) |x - x'| < |u(x) - u(x')| < (1 - \delta) |x - x'| \]

\[ \int_{\Omega} \overline{\Psi}(\nabla u(x)) \, d^2x \geq \overline{\Psi}(A) \int_{\Omega} d^2x \]

where \( \overline{\Psi} = -\Psi = \frac{1}{kT} \text{ free energy per particle} \)

\[ + \text{k.e. term} \]