Mechanical Instabilities at Finite Temperature

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The Outline

• Review of thermal fluctuations and isostaticity
• Finite-T mechanical instability in an ordered lattice

Anton Souslov
(Georgia Tech)
Carlos Mendoza
(Universidad Nacional Autonoma de Mexico)
Tom Lubensky
(Penn)


• Finite-T mechanical instability in disordered lattices

Leyou Zhang
(University of Michigan)

• Zhang and Mao, in preparation.
Why Do We Care About Thermal Fluctuations?

- The simplest model for phase transitions: the Ising model

\[ H = -J \sum_{<i,j>} S_i \cdot S_j \]

- Mean-field theory:

\[ T_C = z J \]

with mean-field exponents near the transition

- Ferromagnetic \( m \neq 0 \) \( T_C \) Paramagnetic \( m = 0 \)

| Ordered, low symmetry | Disordered, high symmetry |

- Thermal fluctuations completely change what we know about this transition.
Why Do We Care About Thermal Fluctuations?

• The simplest model for phase transitions: the Ising model

\[ H = -J \sum_{<i,j>} S_i \cdot S_j \]

• Taking into account fluctuation effects

<table>
<thead>
<tr>
<th>( d &lt; d_L )</th>
<th>( d_L &lt; d &lt; d_U )</th>
<th>( d &gt; d_U )</th>
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<tbody>
<tr>
<td>( 0 )</td>
<td>( \infty )</td>
<td>The Wilson-Fisher fixed point</td>
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<tr>
<td>Fluctuations destroy ordered phase</td>
<td>Continuous transition Non-meanfield critical exponents</td>
<td>The Gaussian fixed point</td>
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<td>Continuous transition Gaussian critical exponents</td>
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• More complicated models: fluctuation could also change a transition that is continuous in MF level to **discontinuous**.
What About Mechanical Instability?

Isostatic point

# degrees of freedom = # of constraints

Packing fraction, or potential, or stress ...

Mechanically unstable (liquid) → Mechanically stable (solid)

Metallic glasses
Granular matter
Emulsions
Self-assembled open lattices
Colloids
Foams
Network glasses
Fiber networks
How Do Fluctuations Change This Scenario?

- Another way to ask the question: “What is the finite-T phase diagram of mechanical instability?”
- Do thermal fluctuations:
  - Favor certain phases over others?
  - Change the order of the transition?
  - Give new scaling laws?
- This is a very challenging question:
  - The $T = 0$ isostatic point is **NOT** a single universality class
  - No readily available field-theory at isostaticity: system specific

Diagram:

- $T$
- Isostatic point
- Packing fraction, or potential, or stress ...
- Mechanically unstable
- Mechanically stable
Central force system of $N$ particles in $d$ dimensions:

number of floppy modes

$N_0 = Nd - N_C + N_S$

Isostaticity:
0 internal floppy modes
Index theorem for topological phonons

states of self-stress

Example: $Nd = 6 \times 2 = 12$

$N_C = 8$
$N_S = 0$
$N_0 = 4 = 3 + 1$

$N_C = 9$
$N_S = 0$
$N_0 = 3 = 3 + 0$

$N_C = 9$
$N_S = 1$
$N_0 = 4 = 3 + 1$

Rigid-body translations
+rotations

Internal floppy mode

- J. C. Maxwell, Phil. Mag. 27, 598 (1864).
- C. L. Kane and T. C. Lubensky, Nat. Phys. 10, 39 (2014).
\[ N_0 = Nd - N_C + N_S \]

States of self-stress \( N_S \) depend on the architecture

“Simple” isostatic condition in periodic lattices: \( z = 2d \)

Kagome lattice

States of self-stress

Twisted kagome lattice

States of self-stress lifted
No floppy modes except for trivial translations

Two different universality classes!

“The \( T = 0 \) isostatic point is not a single universality class”

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Square Lattice Model

A simple lattice model with a controlled mechanical instability

• NN bond: harmonic spring
  \[ V_{NN} = \frac{k}{2} \Delta R^2 \]

• NNN bond: anharmonic spring
  - Harmonic \( \kappa \)
  - Quartic \( g \)
  \[ V = \frac{\kappa}{2} \Delta R^2 + \frac{g}{4!} \Delta R^4 \]
The $T = 0$ Mechanical Instability

Consider one plaquette:

- When $\kappa > 0$ 
  stable state $(T = 0)$: square

- When $\kappa < 0$ 
  stable state $(T = 0)$: rhombus
Questions:
1. Which “zig-zagging configuration” is more preferred?  
2. What is the stability boundary of the square phase?

Favored: order-by-disorder
2. What is the stability boundary of the square phase?

**Method:** Calculate fluctuation corrected shear rigidity (integrate out finite wavelength fluctuations)

What’s special: floppy modes living on a 1D manifold in $p$-space and give a divergent contribution to shear modulus $\rightarrow$ fluctuation driven first order transition (similar to Brazovskii ‘75 theory for finite wavelength instability)
Transitions near mechanical instability can become first-order if a large number of modes simultaneously become critical at the isostatic point (connection to glass transitions).

This is a mechanical transition in an ordered lattice, which can be seen as a special type of structural phase transition (crystal - crystal), what about liquid – (disordered) solid?
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Two Model Lattices

Rigidity percolation in a triangular lattice

\[ T = 0 \] transition

\[ p_c \approx \frac{2}{3}, \quad \xi \sim (p - p_c)^{-1.21} \]

Non-meanfield

Square lattice with random NNN bonds

\[ p_c = 0, \quad \xi \sim (p - p_c)^{-1} \]

Meanfield,
Agrees with Jamming


- Mao, Xu, & Lubensky, PRL 104, 085504 (2010)
Effective Medium Theory at $T = 0$ & $T > 0$

EMT: Map the disordered lattice into a regular lattice with force constant $k_m(p)$

\[
\frac{k_m}{k} = \frac{p - p_c}{1 - p_c} \quad \text{with} \quad p_c = \frac{2}{3}
\]

Turn on $T$ → Corrections to these EMT equations

\[
\frac{\kappa_m}{\kappa} = \frac{p - \sqrt{\kappa_m/k}}{1 - \sqrt{\kappa_m/k}}
\]

- Mao, Xu, & Lubensky, PRL, 104, 085504 (2010)
Finite-T EMT Phase Diagrams

Boundary: \( T \sim (p - p_c)^2 \)

Entropic \( G \sim T \)

Critical \( G \sim \sqrt{T} \)

Mechanical \( G \sim (p - p_c) \)

Boundary: \( T \sim p^3 \)

Critical \( G \sim T^{2/3} \)

Nonaffine Mechanical \( G \sim p^2 \)

Affine Mechanical \( G \sim p \)
Why Thermal Fluctuations Stabilize Under-Coordinated Systems?

- Through anharmonic terms – schematic picture as following
  - Hamiltonian $H \sim k u^2 + g u^4$ (u: some deformation field)
  - Rigidity of $u$ at $T = 0$ is: $k$
  - Rigidity of $u$ at $T > 0$ is: $\frac{\partial^2 F}{\partial u^2} \sim k + g \langle u^2 \rangle k + gT$
  
- In these simple lattice models
  - Fluctuations introduce effective tension on strings

- In more general cases, e.g., near jamming
  - Gaps at $T = 0$ below $\phi_c$
  - May be effectively filled at $T > 0$
Earlier works on lattices at finite $T$

- Plischke, Vernon, Joos, & Zhou PRE 60, 3129 (1999).
- Dennison, Sheinman, Storm, & Mackintosh, PRL 111, 095503 (2013).

Monte Carlo simulation on triangular lattice rigidity percolation:

Our **analytic** phase diagram:
What happens when thermal fluctuations are introduced near point J?

- Ikeda, Berthier, & Sollich, PRL 109, 018301 (2012).
- Parisi & Zamponi, RMP 82, 789 (2010).

A sketch of suggested phase diagram:
THANK YOU!