Stability and jamming transition in hard granular materials: Algebraic graph theory

Nicolas Rivier

IPCMS, Université Louis Pasteur, 67084 Strasbourg Cedex, France

GDR CHANT 21/11/07

Within this workshop

- Modelisation of (hard) granular materials (as a graph, generic)
- Changes of scale (jamming transition is a scaling phase transition)

Aims

- Model for dry, hard (stiffness/load >> 1) granular materials, generic

To explain

- (Dry) liquid
- (Fragile) solid (held together by frustration)
- Jamming transition (scaling, 2nd order)

The problem

- Hard **granular** material: Highly nonlinear
- But nonlinearity in constraints that are either geometric or naïve # theory:
- **Edge**: Boolean, cst.length if exists
- **Circuits**: odd circuits are non-trivial
- Dynamics reduces to **linear algebra of graph**

Granular material as a graph

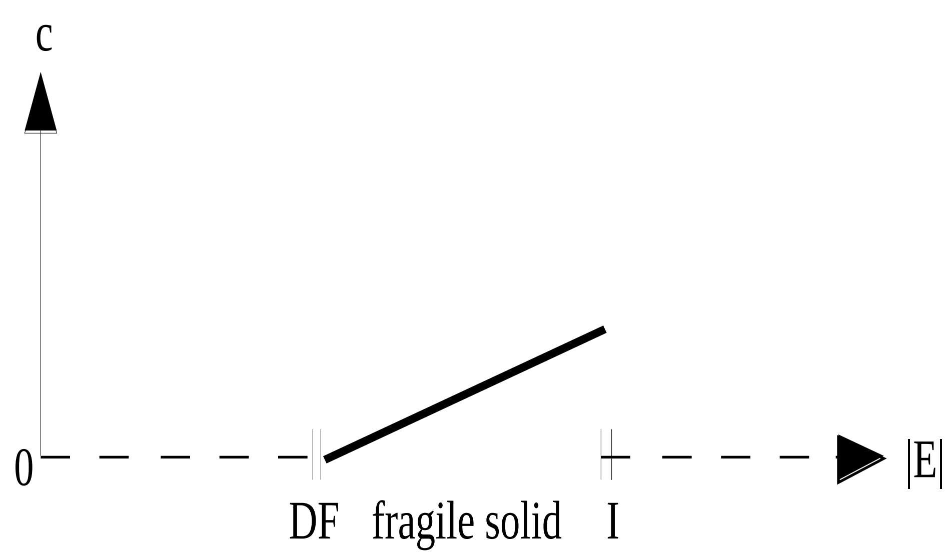
- Hard, dry granular (stiffness/load >> 1)
- Force = contact, <u>repulsive</u> (same sign), boolean, scalar (∞ tangential friction). Nonlinearity <u>in</u> geometrical constraints
- <u>Graph</u>: (*n*) vertex = grain, edge = contact (boolean), circuits odd/even. <u>Discrete</u> (no defect-free continuum limit).
- <u>Linear</u> algebra <u>on</u> <u>graphs</u>: normal modes. Eigenvectors, eigenvalues $\{\lambda\}$, DOS $D(\lambda)$ (Bloch waves, graviton)

Granular matter

- ***Isostatic*** (neither overconstrained, nor floppy when stiffness/load >> 1)
- 1. ***Dry fluid*** (ball-bearing). No odd circuits
- Fragile, ***jammed solid*** stabilized by ***odd circuits*** (≠ close packing in crystallisation)
- 3. Odd vorticity form (R-) loops, large in ***disordered*** granular solids
- 4. Scaling: jamming transition is a (RG, fixed point, etc) true phase transition in ***disordered*** granular solids
- Essential importance of ***disorder*** and ***grains*** (ie. (odd) numbers).

Phase diagram of a hard granular material

DF = dry fluid   I = isostatic packing
|E| = # edges   c = # odd circuits



Circuits

- No odd circuits: dry <u>liquid</u> (ball bearing) (non-slip rotation of grains) (M-B,H,R'04)
- (c) **odd circuits**: fragile **<u>solid</u>** (stability: non-slip rotation frustrated). No defect-free continuum description.
- Odd vorticity form loop (R-loop) (R'79). [Order: small R-loops (O(a)).] **Disorder**: large R-loops (O(L)). Frustration $0 < \lambda_1 < 4c/n \sim 1/L$ (R'06)
- c/4 lowest modes (Bloch waves). DOS $D(\lambda) \sim L^{\mathbf{0}}$, independent of dim, or L (W,N,W'05, R'07)

1. Even circuits only

- No odd circuits: dry <u>liquid</u> (ball bearing) (non-slip rotation of grains)
- Pure gauge connection

Local frame (**t**,**n**,**k**)

- Replace now vertices and edges by spherical grains in contact. The edge linking grains i and i+1 is represented by the vector $\mathbf{R}_{i,i+1} = (R_i+R_{i+1})\mathbf{t}_{i.i+1}$, with fixed length R_i+R_{i+1} and unitary directional vector $\mathbf{t}_{i,i+1}$. With time t, it can rotate at a rate $\phi_{i,i+1}$ around the axis $\mathbf{k}_{i,i+1}$, thus

$$d\mathbf{R}_{i,i+1}/dt = \phi_{i,i+1}(R_i+R_{i+1})\mathbf{n}_{i,i+1},$$

thereby defining a local orthonormal frame (**t**,**n**,**k**) for each edge (i,i+1), with $(\mathbf{k}\Lambda\mathbf{t}) = \mathbf{n}$, etc. Thus,

$$d\mathbf{t}/dt = \phi(\mathbf{k}\Lambda\mathbf{t}) = \phi\mathbf{n}, \qquad d\mathbf{n}/dt = \phi(\mathbf{k}\Lambda\mathbf{n}) = -\phi\mathbf{t}.$$

(The local frame is not Frenet's because it is defined through time derivative on a discrete polygonal curve, rather than as derivative along the curve).

Closure relations (polygons in **t**, **n**, or **k**)

- A circuit of s edges is the skew polygonal curve in the **t**'s,

  $\sum \mathbf{R}_{i,i+1} = \sum (R_i + R_{i+1})\mathbf{t}_{i,i+1} = 0$ (1)

($\sum$ from $i = 1$ to s ($s+1 \equiv 1$)). Also,

$\sum d\mathbf{R}_{i,i+1}/dt = \sum \phi_{i,i+1}(R_i + R_{i+1})\mathbf{n}_{i.i+1} = 0$

is an orthogonal, skew polygon in the **n**'s. Higher time derivatives contain combinations of **t** and **n**.

There is a third polygon in the **k**'s,

$\sum \mathbf{h}_{\,i,i+1} = \sum (-1)^i \phi_{i,i+1}(R_i + R_{i+1})\mathbf{k}_{i.i+1} = 0$ (for s even)

Rolling without slip. Connection

- Rolling without slip : the two grains have the same velocity at the point of contact

$$\mathbf{v}_1 + \omega_1 \Lambda (R_1 \mathbf{t}_{12}) = \mathbf{v}_2 + \omega_2 \Lambda (-R_2 \mathbf{t}_{12}),$$

with the velocities of the centers of the two grains related by $\mathbf{v}_2 = \mathbf{v}_1 + d\mathbf{R}_{12}/dt$. Non-slip condition is a relation (connection) between the angular rotation velocity vectors ω of the two spheres in contact:

$$(R_1 \omega_1 + R_2 \omega_2) \Lambda \mathbf{t}_{12} = d\mathbf{R}_{12}/dt.$$

In the local frame, $R_1\omega_1 + R_2\omega_2 = -\alpha_{12}\mathbf{t}_{12} - \beta_{12}\mathbf{n}_{12} - \gamma_{12}\mathbf{k}_{12}$, components $\beta = 0$, $-\gamma_{12} = \phi_{12}(R_1 + R_2)$, but α is an arbitrary coefficient of connection between ω_1 and ω_2.

Circuits (=arches, chain of forces)

- No odd circuits: dry liquid (ball bearing) (non-slip rotation of grains) $\lambda_1 = 0$
- (c) **odd circuits**: fragile **solid** (stability: non-slip rotation frustrated). No defect-free continuum description.
- Odd vorticity form **loop** (R-loop) (R'79). [Order: small R-loops (O(a).] **Disorder**: large R-loops (O(L)). Frustration $0 < \lambda_1 < 4c/n \sim 1/L$
- c/4 lowest modes (Bloch waves). DOS $D(\lambda) \sim L^{\mathbf{0}}$, independent of dim, or L

Bearing 2D

centers of the grains are at rest ($\phi = 0$), on a plane

- In 2D (planar polygons of cogwheels), $R_1\omega_1 = -R_2\omega_2$ ($\alpha = 0$), the axes of rotation are collinear, the angular velocities have opposite signs (different colors) and a necessary and sufficient condition for non-slip rotation is that all circuits are even.

Bearing 3D

- In 3D, where neither are the centers of the grains coplanar nor the axes of rotation collinear, the same condition holds, but it is only sufficient [2]. The non-slip condition, $R_1\omega_1 + R_2\omega_2 = -\alpha_{12}\mathbf{t}_{12}$ defines a *connection* α between two spheres in contact that gives $R_2\omega_2$ in terms of $R_1\omega_1$, then $R_3\omega_3$ in terms of $R_2\omega_2$, etc. Around a circuit with s edges, $s+1\equiv 1$,

$$-R_1\omega_1 + (-1)^s R_1\omega_1 = -\sum(-1)^i\alpha_{i,i+1}\mathbf{t}_{i,i+1}.$$

- If s is even, one obtains a sum rule on the connections,

$$\sum(-1)^i\alpha_{i,i+1}\mathbf{t}_{i,i+1} = 0.$$

- The connection α is carried from one sphere to the next, and, around a circuit, back to the initial sphere. The *pure gauge* connection

$$\alpha_{i,i+1} = K(-1)^i (R_i+R_{i+1})$$

reduces the sum rule to the geometric condition (1) for closure of the polygonal circuit.

Pure gauge connection

- The *pure gauge* connection

$$\alpha_{i,i+1} = K(-1)^i\,(R_i+R_{i+1})$$

reduces the sum rule to the geometric condition (1) for closure of the polygonal circuit. (Mahmoodi-Baram et al. 2004)

It is consistent ("pure gauge")

- for an even circuit, regardless of the starting sphere.

- for all contact paths between any two spheres in the absence of odd circuits.

- K is a constant for the whole packing ($K = 0$ implies that the axes of rotation of all the grains are collinear).

Dry fluid. Grain centers move

- If grain centers move, two grains in non-slip contact are connected by the relation

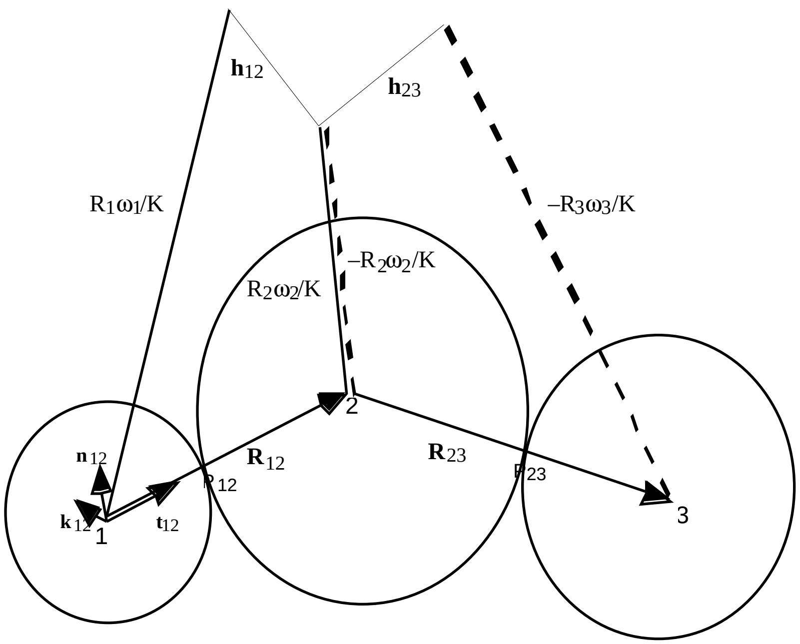
$$R_1\omega_1 + R_2\omega_2 = -\alpha_{12}\mathbf{t}_{12} + \phi_{12}(R_1+R_2)\mathbf{k}_{12};$$

and the **n**-components $R_1\omega_1.\mathbf{n}_{12} = -R_2\omega_2.\mathbf{n}_{12}$ have opposite signs (different colors). With the vector **h** defined as $K\mathbf{h}_{i,i+1} = (-1)^i\phi_{i,i+1}(R_i+R_{i+1})\mathbf{k}_{i,i+1}$, the there is a consistency relation that is a sum rule for any even circuit,

$$\sum\mathbf{h}_{i,i+1} = \sum(-1)^i\phi_{i,i+1}(R_i+R_{i+1})\mathbf{k}_{i.i+1} = 0 \qquad (s \text{ even}),$$

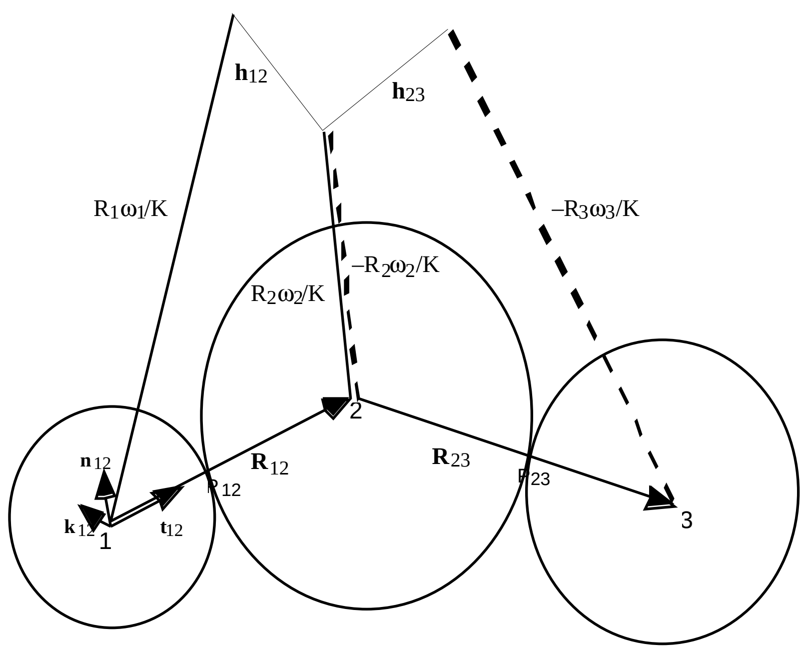
a closure relation on the **k**'s (R 2005).

Hinges for even circuit



- For spherical grains, the non-slip condition with the pure gauge connection $[R_1\omega_1+R_2\omega_2]/K$ + $\mathbf{R}_{12}$ + $\mathbf{h}_{12}$ = 0 defines a non-planar tetragon. An even circuit is a flexible cylinder with polygonal bases $\sum \mathbf{R}_{i,i+1} = 0$ and $\sum \mathbf{h}_{i,i+1} = 0$.

Spherical grains rolling without slip:



The axis of rotation of grain 2, ω_2 serves as the *hinge* between object 1[grain 1 rolling on grain 2, = non-planar tetragon (lines)

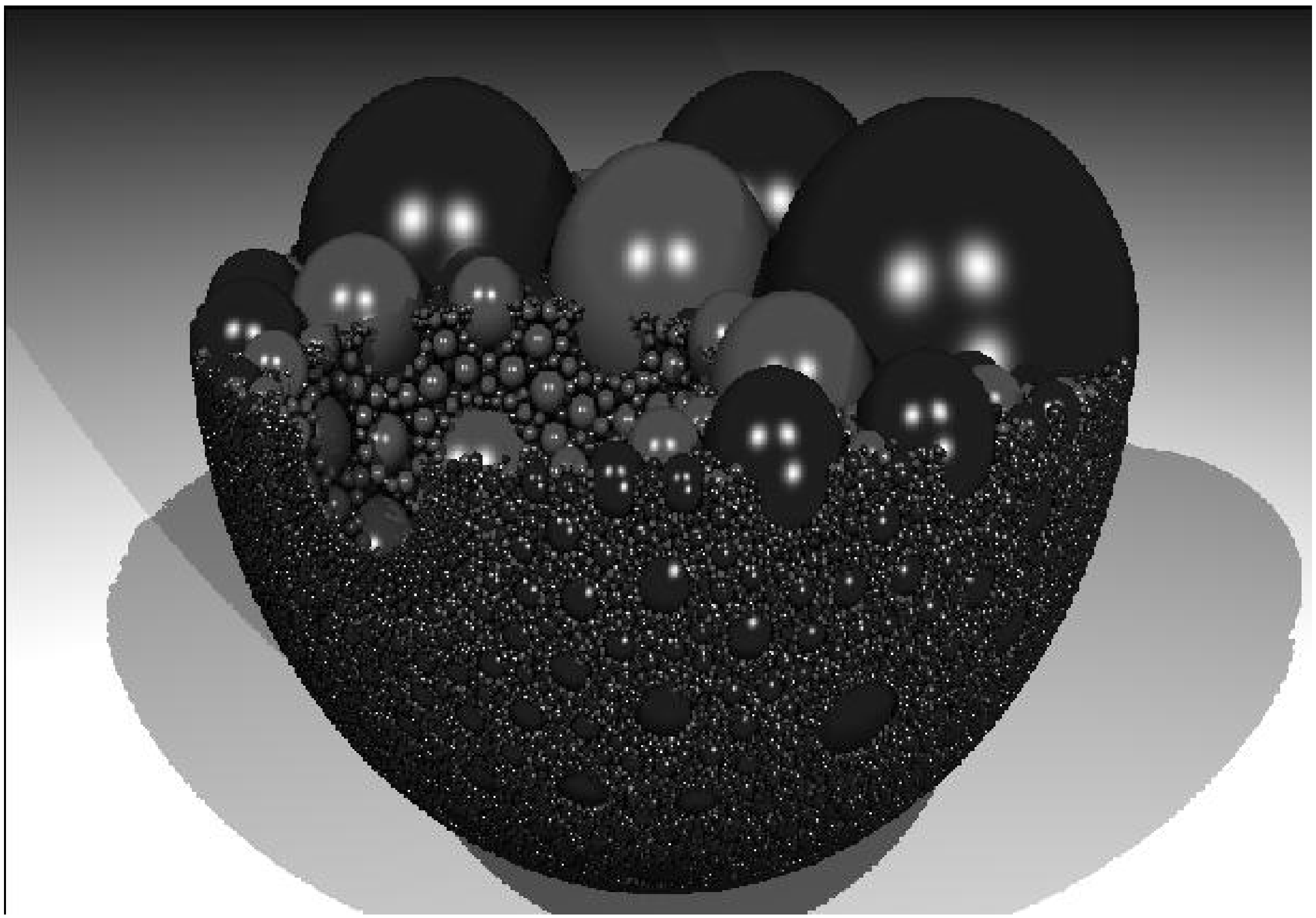
$\{\mathbf{R}_{12}, R_1\omega_1/K, R_2\omega_2/K, \mathbf{h}_{12}\}]$

and object 2 [grain 2 rolling on grain 3, = non-planar tetragon (dotted lines)

$\{\mathbf{R}_{23}, -R_2\omega_2/K, -R_3\omega_3/K, \mathbf{h}_{23}\}]$

Bichromatic packing = dry fluid

(Mahmoodi-Baram, Herrmann (‘04)



- This is a 3D bearing

2. Algebraic graph theory: Adjacency matrix and dynamical matrix

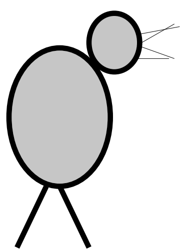
- Graph Γ
- Adjacency matrix $A_{ij} = 1$ if i,j in contact

$\forall$ $\Delta_{ij} = z_i\delta_{ij}$, $z_i = \Sigma_j A_{ij}$ valency (degree) of vertex i

- **D** incidence matrix
- $\mathbf{Q} = \mathbf{DD^t} = \mathbf{\Delta - A}$
- $\mathbf{adjQ} = \kappa\, \mathbf{J}$
- Complexity $\kappa(\Gamma)$ = # spanning trees

Woodstock's matrix J

$$\begin{bmatrix} 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1&1&1&1&1&1&1&1 \end{bmatrix}$$



matrice de Woodstock
(le copain de Snoopy)

Dynamical matrix

- The matrix **Q** is the *dynamical matrix* of a physical system on the graph Γ, where the vertices are particles of the same mass, and the edges are springs with the same stiffness. The interaction between two vertices connected by an edge can have either sign.

- By contrast, the dynamical matrix of a hard granular system, where the vertices are grains with the same momentum of inertia, and the edges are struts, representing the non-slip rotation of the grains on each other, is $\mathbf{K} = \Delta + \mathbf{A} = 2\Delta - \mathbf{Q}$. Interaction has one sign.

Importance of sign constraint

- Because of the sign difference, corresponding to the signs of the interactions, the spectrum of eigenvalues of **Q** and **K**, and their respective eigenvectors, are essentially different, and this difference is associated with *odd circuits*. If there are only even circuits, **K** is changed into $\mathbf{OKO}^{-1} = \Delta - \mathbf{A} = \mathbf{Q}$ by an unitary transformation **O** that changes the sign of odd rows and columns.

Dynamics of a graph (edges = springs)

[NB: topological dynamics only:
ground state, where frustrating stress lies, strain (= eigenvector)
Recall: force is a scalar]

Potential energy of the graph is

$$V = (1/2)\, k \sum_{(ij)} (x_i - x_j)^2$$

(sum over edges). Two vertices connected by a spring have equal stress-free translations $(x_i – x_j) = 0$, and the force can have either sign].

Euler-Lagrange equations of motion

$$[-\lambda \mathbf{1} + (\Delta - \mathbf{A})]\, \mathbf{x} = \mathbf{0},$$

where the eigenvalues $\lambda = m\omega^2/k$ of the dynamical matrix $\mathbf{Q} = \Delta - \mathbf{A}$ are related to the frequencies ω of the normal modes of oscillation.

Lowest ev. $\lambda_1 = 0$, $|\mathbf{1}\rangle = \mathbf{j} = (1,1,1,1\ldots,1)^t$ (Woodstock).

Why granular matter is different

- Granular matter is represented by a graph, but its dynamics is different because :
  - (i) The forces betwen grains in contact are repulsive (they have a sign constraint) and the granular packing is isostatic if grains can roll on each other without slip.
  - (ii) The stability of a granular packing is caused by the presence of odd circuits.

Dynamics of a graph (edges = struts)

[NB: topological dynamics only:
ground state, where frustrating stress lies, strain (= eigenvector)
Recall: force is a scalar]

- Potential energy of the graph is

$$V = (1/2)\ k \sum_{(ij)} (\theta_i+\theta_j)^2.$$

Two grains in contact have opposite stress-free rotations $(\theta_i+\theta_j) = 0$, and the force is always repulsive. Because of the + sign, the dynamical matrix of the granular network is now $\mathbf{K} = \Delta+\mathbf{A} = 2\Delta-\mathbf{Q}$, where $\mathbf{Q} = \Delta-\mathbf{A}$ is the usual dynamical matrix for a network of unit masses connected by springs of unit stiffness.

Details: No odd circuits: from K to Q

- Consider first a connected bichromatic graph, without odd circuits. Let $(-1)^i$ be the color of vertex i. The adjacency matrix has a non-zero entry $A_{ij} = 1$ only if i and j have opposite colors. The unitary transformation $O_{ij} = (-1)^i\delta_{ij}$ changes the sign of odd rows and columns, $A'_{ij} = (-1)^i A_{ij} (-1)^j$ and transforms the dynamical matrix $\mathbf{K} = \Delta+\mathbf{A}$ into $\mathbf{K'} = \mathbf{OKO}^{-1} = \Delta-\mathbf{A} = \mathbf{Q}$ that is the dynamical matrix for an elastic network.
- Now, the lowest eigenvalue of **Q** is zero with the corresponding Woodstock eigenvector **j**. It is nondegenerate since (rank**Q**) = n–1 for a connectd graph. Transforming back, the lowest eigenvalue of the dynamical matrix **K** of the bichromatic packing is zero, one soft mode with the alternating eigenvector **a** $= (1,-1,1,-1,...)^t = \mathbf{Oj}$. A granular material without odd circuit is bearing of grains rotating without slip on each other.

Lowest ev. $\lambda_1 = 0$, $|\mathbf{a}\rangle = \mathbf{Oj} = (1,-1,1,-1\ldots,-1)^t$.

Graph with odd circuits

- $\mathbf{A} = \mathbf{A}^0 + \mathbf{A}^*$. $\mathbf{A}^0$ spanning. $\mathbf{A}^*$ sparse matrix, one edge per odd circuit between two vertices of same color.
- Under unitary transformation **O**, $\mathbf{A}^{0\prime} = -\mathbf{A}^0$ changes sign, whereas $\mathbf{A}^{*\prime} = \mathbf{A}^*$ remains unchanged because it connects vertices with the same color. Thus, $\mathbf{K} = (\Delta^0 + \mathbf{A}^0) + (\mathbf{1}^* + \mathbf{A}^*)$, is transformed into

$$\mathbf{K}' = (\Delta^0 - \mathbf{A}^0) + (\mathbf{1}^* + \mathbf{A}^*) = \mathbf{Q}^0 + \mathbf{J}^*,$$

where $(\mathbf{1}^* + \mathbf{A}^*) = \mathbf{J}^*$ is a **very sparse** matrix with $\neq 0$ entries only for one pair of separated vertices a, b with the same color in every odd circuit. $\mathbf{J}^*$ is the direct sum over all odd circuits of the matrix whose entries $J^*_{ij} = 1$ if i,j = a,b, and zero elsewhere. The lowest eigenvalue of $\mathbf{Q}^0$ is zero, with eigenvector $\mathbf{j}$.

Thus: Rayleigh-Ritz on $\mathbf{K}' = \mathbf{Q}^0 + \mathbf{J}^*$, $\mathbf{Q}^0 |\mathbf{j}\rangle = 0$

Lowest eigenvalue of K

- The Rayleigh-Ritz variational principle yields an upper bound for the lowest eigenvalue of K,

  $$0 < \lambda_1 \leq \langle \mathbf{j}|\mathbf{K'}|\mathbf{j}\rangle / \langle \mathbf{j}|\mathbf{j}\rangle = \langle \mathbf{a}|\mathbf{K}|\mathbf{a}\rangle / \langle \mathbf{a}|\mathbf{a}\rangle$$

  $$= \langle \mathbf{j}|\mathbf{J^*}|\mathbf{j}\rangle / \langle \mathbf{j}|\mathbf{j}\rangle = \sum_{\text{odd circuits}}(4/n) = 4c/n,$$

  where c is the number of odd circuits and n the number of vertices in the graph.

  Thus, $\lambda_1 \approx 4c/n$ is a measure of the **frustration** generated by the odd circuits, and diluted into the whole connected network. The granular material is rigid, but fragile (stress concentrate on paths – odd circuits – that form a sparse network and can be locally disconnected).

  The corresponding eigenvector is alternating, nearly homogeneously.

3. Odd vorticity forms loops

- Theorem [R'79] Odd vorticity close as loops (R-loop), or terminate at the surface of the material, without passing through any irreducible even circuit.
- [Ordered granular: small R-loops (O(a))]
- **Disorder**: largest R-loop (O(L)). Scaling.
- Frustration $0 < \lambda_1 < 4c/n \sim 1/L$. Area of film = $c \sim L^{\mathrm{D}-1}$
- Unjamming: break contacts on film attached to largest R-loop:
- Unjamming transition as $L \sim \infty$.

4. Near jamming

- Disordered granular: largest R-loop ~ L. Break one edge/odd circuit to unjam. Broken edges on film bounded by R-loop.
- # odd circuits = c = # broken edges ~ L^{D-1} = (D–1)-area of the film bounded by R-loop.
- Frustration: $0 < \lambda_1 < 4c/n \sim 1/L$
- Large number ($c/4 \sim L^{D-1}$) of low-energy modes (Bloch-like) (W,N,W'05, R'07)
- DOS: $D(\lambda)$ = #modes/en^{y}./vol. ~ $L^{D-1} / L^{D} /(1/L) \sim L^{0}$ independent of dim, or size L (W,N,W'05, R'07)

Eigenvectors: Bloch waves of blobs Q^{00} connected by broken edges

- Q^{00} block diagonal, with, on the diagonal, c conventional $d_k x d_k$ dynamical matrices $Q^{00}{}_k$, each of rank d_k –1 and zero-eigenvalue eigenvector $(\exp[-i\ldots_k])\mathbf{j}_k$

- Zero-eigenvalue eigenvector $Q^{00}|e_\alpha\rangle = 0$:

  $|e_\alpha\rangle = (\exp[i\ldots^1{}_\alpha],\ldots,\exp[i\ldots^1{}_\alpha];\exp[i\ldots^2{}_\alpha],\ldots, \exp[i\ldots^2{}_\alpha];$

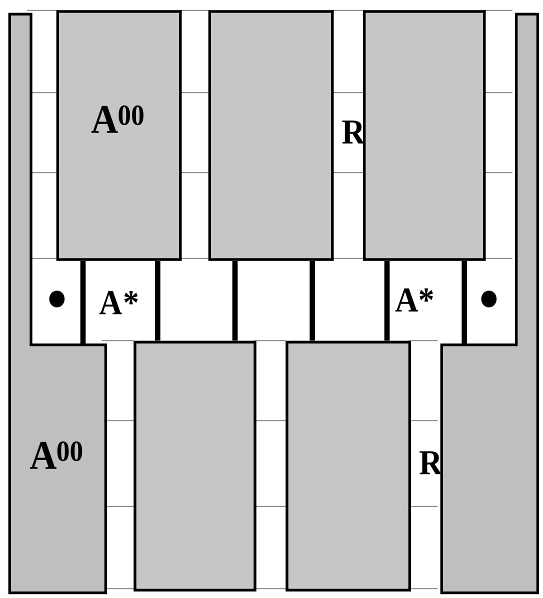
  $\ldots;\exp[i\ldots^c{}_\alpha],\ldots,\exp[i\ldots^c{}_\alpha])^+$

  with $\langle e_\alpha|e_\alpha\rangle = \sum d_k = n$

  and $\langle e_\alpha|e_\beta\rangle = \sum d_k \exp[i(\mu^k{}_\alpha - \ldots^k{}_\beta)] = 0, \quad \alpha \neq \beta$

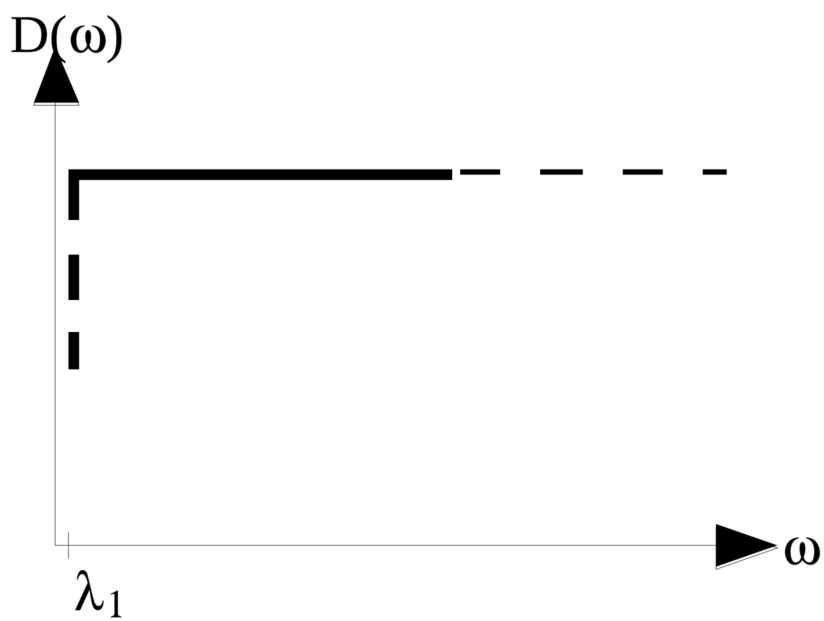
Construction of the Bloch function. Chain of blobs (2D)

one R-line (˚…˚ in 2D) of size ~L



DOS near jamming (schematic)

Simulations of O'Hearn, Nagel et al.(2005)



Flat DOS near jamming

- DOS: D(λ) ~ $L^{D-1}/L^D/(1/L) \sim L^0$
- Universal, **plateau** (Alexander'98, Nagel et al.'02,'03) for $\lambda > \lambda_1 < 4c/n \sim 1/L$, indep. of size of material L, of space dim. D
- Large specific heat ~T in « weakly connected amorphous solids ». No need for 2LS or tunnelling modes. Large entropy available to decrease free energy upon jamming (hard repulsion: no energy sink available)

Conclusions = keywords

- Discrete: odd circuits
- Disorder: large R-loops
- Scaling with *L*
- Interaction repulsive only ($\theta_i + \theta_j$)
- Apply shear: break odd circuits:

    Dry quicksand (Lohse et al., R-Suarez et al.)

    Silent earthquakes/soil liquefaction

    Dilatancy

    Sliding tectonic plates (San Andreas fault)