Master 2 Matière Condensée et Nanophysique: Internship projects

Eigenmodes of percolating ideal spring clusters

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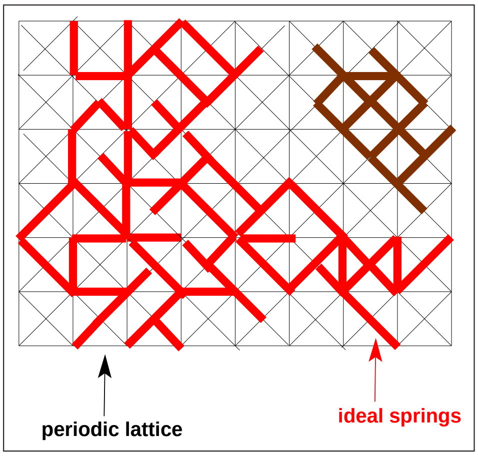
Research context:

Our research group is interested in the statistical physics of soft matter and the rheology of complex fluids with a particular emphasis on systems involving polymers [1]. Using simple coarse-grained models many fundamental and generic aspects of such systems can be investigated by means of Monte Carlo (MC) or molecular dynamics simulations [2,3]. One current research theme focuses on the linear elastic response of transient self-assembled polymer gels [1,4] and microemulsions bridged by so-called telechelic polymers [5,6].

Project description:

A very simple model for such gel-like polymer systems is provided by two-dimensional networks of harmonic springs (bold lines) randomly placed on a period lattice and permanently connected (if possible) with other springs. It is assumed that all forces vanish at zero temperature. At low densities the system behaves as a gas of spring clusters with a vanishing shear modulus G. Above a critical density ρ_{p} a *percolating* cluster is formed spanning the system [4], i.e. the spring network behaves as a solid with a finite shear modulus G. One objectif of the proposed study is the numerical determination of $G(\rho)$ as a function of the spring density ρ [7,8].



Required tasks and workflow:

1. Generalization of existing MC code allowing
   - the comparison of different lattice types,
   - tunable repulsive interactions between the bonds and/or the spring end groups,
   - annealed thermalized configurations where springs are broken and recombined using a Monte Carlo Metropolis scheme at finite temperatures T [2,3].
2. Sampling of configuration ensembles with increasingly large system sizes;
3. Characterization of percolating and non-percolating clusters (critical exponents) [4];
4. Diagonalization of the "dynamical matrix" (a $dN \times dN$ matrix characterizing the system Hamiltonian of a zero-temperature configuration) for the lowest eigenvalues using Lanczos (recursion) method for sparse matrices [3];
5. Determination of $G(\rho)$ and other elastic moduli using the degenerated lowest eigenfrequencies [7] and comparison with theoretical predictions [8];

6. Optional: Detailed analysis of the eigenmodes (some corresponding to localized modes, some to propagating plane wavesion relation) and the density of states ("*phonons*" $\Leftrightarrow$ "*fractons*") [9] as a function of the spring density;

7. Optional: Molecular dynamics simulations [2] of one permanently fixed network at low T and test of the obtained elastic moduli using the stress fluctuation formalism [6,7];

8. Preparation of internship report and talk.

References:

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[9] S. Alexander and R. Orbach, *Density of states on fractals: "fractons"*, Phys. Rev. Lett. **43**, L625 (1982).