Statistical Physics of Athermal Systems
Lecture 3

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1 From Gaussian fields to elasticity

In Lecture 2 we saw that a quadratic theory is controlled by a single kernel. The response is obtained by inverting this kernel, and the Gaussian correlation function is obtained from the same inverse. For a static Gaussian field,

$$H[\phi] = \frac{1}{2}\int \mathrm{d}^d r\, \mathrm{d}^d r'\, \phi(\mathbf{r})\, \Gamma(\mathbf{r}-\mathbf{r}')\, \phi(\mathbf{r}') - \int \mathrm{d}^d r\, h(\mathbf{r})\phi(\mathbf{r}), \tag{1}$$

we have

$$\chi = \Gamma^{-1}, \qquad G = k_{\mathrm{B}}T\, \Gamma^{-1} = k_{\mathrm{B}}T\, \chi. \tag{2}$$

For the simple translationally invariant model,

$$H[\phi] = \int \mathrm{d}^d r \left[\frac{K}{2}(\nabla\phi)^2 + \frac{t}{2}\phi^2 - h\phi\right], \tag{3}$$

It is useful to do the Fourier transform explicitly. Write

$$\phi(\mathbf{r}) = \int_{\mathbf{k}} \phi_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad h(\mathbf{r}) = \int_{\mathbf{k}} h_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}},$$
$$\nabla\phi(\mathbf{r}) = \int_{\mathbf{k}} i\mathbf{k}\, \phi_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}.$$

Using translational invariance,

$$\int \mathrm{d}^d r\, \phi^2 = \int_{\mathbf{k}} \phi_{\mathbf{k}}\phi_{-\mathbf{k}},$$
$$\int \mathrm{d}^d r\, (\nabla\phi)^2 = \int_{\mathbf{k}} k^2 \phi_{\mathbf{k}}\phi_{-\mathbf{k}},$$
$$\int \mathrm{d}^d r\, h\phi = \int_{\mathbf{k}} h_{-\mathbf{k}}\phi_{\mathbf{k}}.$$

Therefore

$$H = \frac{1}{2}\int_{\mathbf{k}} (Kk^2 + t)\phi_{\mathbf{k}}\phi_{-\mathbf{k}} - \int_{\mathbf{k}} h_{-\mathbf{k}}\phi_{\mathbf{k}}.$$

The coefficient multiplying the quadratic field is the Fourier-space stiffness kernel,

$$\Gamma(\mathbf{k}) = Kk^2 + t, \qquad G(\mathbf{k}) = \frac{k_{\mathrm{B}}T}{Kk^2 + t}. \tag{4}$$

To see the second relation directly, set the source to zero and use

$$P[\phi] \propto \exp\left[-\frac{1}{2k_{\mathrm{B}}T}\int_{\mathbf{k}}(Kk^2+t)\phi_{\mathbf{k}}\phi_{-\mathbf{k}}\right].$$

Each Fourier mode is a Gaussian variable with variance $k_{\mathrm{B}}T/(Kk^2+t)$.

We therefore have (completing the squares, as previously done)

$$\langle\phi_{\mathbf{k}}\rangle = \frac{h_{\mathbf{k}}}{Kk^2+t}, \tag{5}$$

so the same kernel controls both the response and the Gaussian correlation.

We now replace the scalar field by the displacement field of a solid. The same quadratic kernel now becomes the elastic stiffness matrix. Its eigenmodes become phonons in a crystal or vibrational modes in an amorphous solid.

2 Elasticity of a crystal

We first do the calculation for a crystal. Translation symmetry lets us diagonalize the problem in plane waves. The same Hessian construction can also be used for a disordered contact network, but in that case the plane waves are not the correct basis for diagonalization.

2.1 One-dimensional chain

Consider a one-dimensional chain of identical particles of mass m, equilibrium spacing a, and nearest-neighbour spring constant k. Let u_i be the displacement of particle i from its equilibrium position. The harmonic energy is

$$U = \frac{k}{2}\sum_i (u_{i+1}-u_i)^2. \tag{6}$$

The force on particle i is

$$m\ddot{u}_i = -\frac{\partial U}{\partial u_i} = k(u_{i+1}-2u_i+u_{i-1}). \tag{7}$$

For wavelengths much longer than a, write $u_i = u(x_i)$ with $x_i = ia$. Taylor expansion gives

$$u_{i+1}-2u_i+u_{i-1} = a^2\partial_x^2 u + O(a^4). \tag{8}$$

Therefore

$$m\partial_t^2 u = ka^2\partial_x^2 u. \tag{9}$$

If the chain has cross-sectional area A, the mass density is $\rho = m/(aA)$, and the continuum equation becomes

$$\rho\,\partial_t^2 u = E\,\partial_x^2 u, \qquad E = \frac{ka}{A}. \tag{10}$$

Thus the elastic wave speed is

$$c^2 = \frac{E}{\rho} = \frac{ka^2}{m}. \tag{11}$$

We can obtain the same result directly from the energy. Since

$$u_{i+1}-u_i \simeq a\partial_x u, \tag{12}$$

we have

$$U \simeq \frac{k}{2}\sum_i a^2(\partial_x u)^2 = \frac{ka}{2}\int \mathrm{d}x\,(\partial_x u)^2. \tag{13}$$

Dividing by A gives the elastic energy

$$F = \frac{1}{2}\int \mathrm{d}x\, E\,\epsilon^2, \qquad \epsilon = \partial_x u. \tag{14}$$

The stress is therefore

$$\sigma = \frac{\partial f}{\partial \epsilon} = E\epsilon. \tag{15}$$

Hooke's law is thus the continuum form of the microscopic harmonic energy.

The same calculation also shows where "prestress" enters. A strictly one-dimensional chain has no transverse degree of freedom, so its quadratic energy contains only the longitudinal spring stiffness. To expose the prestress term, consider the same nearest-neighbour chain embedded in two dimensions and let the equilibrium bond carry a compressive force $f_0 > 0$. For a central potential, $V'(a) = -f_0$. If

$$\delta\mathbf{u}_i = \mathbf{u}_{i+1} - \mathbf{u}_i \tag{16}$$

is the relative displacement of one bond, then

$$\delta^2 V_i = \frac{1}{2}V''(a)\left(\delta u_i^{\parallel}\right)^2 - \frac{f_0}{2a}\left|\delta\mathbf{u}_i^{\perp}\right|^2, \tag{17}$$

where

$$\delta u_i^{\parallel} = \hat{\mathbf{n}}\cdot\delta\mathbf{u}_i, \qquad \delta\mathbf{u}_i^{\perp} = \delta\mathbf{u}_i - \hat{\mathbf{n}}\delta u_i^{\parallel}. \tag{18}$$

The first term is the usual longitudinal stiffness. The second term is negative for a compressed bond. Thus a prestressed chain becomes softer to transverse distortions even though the bare spring constant $V''(a)$ has not changed. This is the simple version of the prestress contribution that becomes important in a jammed contact network.

2.2 Three-dimensional elasticity

In d dimensions, the displacement is a vector field

$$\mathbf{r} \to \mathbf{r} + \mathbf{u}(\mathbf{r}). \tag{19}$$

The linearized strain tensor is the symmetric part of the displacement gradient,

$$\epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i). \tag{20}$$

The antisymmetric part corresponds to an infinitesimal rigid rotation and does not cost elastic energy in an isotropic solid.

For a crystal with a general lattice symmetry, the harmonic elastic energy has the form

$$F = \frac{1}{2}\int \mathrm{d}^d r\, C_{ijkl}\epsilon_{ij}\epsilon_{kl}. \tag{21}$$

The elastic tensor satisfies the major and minor symmetries

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}, \tag{22}$$

leaving a symmetry-dependent number of independent elastic constants.

The stress tensor follows from variation with respect to strain,

$$\sigma_{ij} = \frac{\partial f}{\partial \epsilon_{ij}} = C_{ijkl}\epsilon_{kl}. \tag{23}$$

Mechanical equilibrium is

$$\partial_i \sigma_{ij} = 0 \tag{24}$$

in the absence of body forces.

For an isotropic solid the tensor reduces to two Lamé coefficients,

$$C_{ijkl} = \lambda \delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{25}$$

and the free energy density is

$$f = \frac{\lambda}{2}(\nabla \cdot \mathbf{u})^2 + \mu\, \epsilon_{ij}\epsilon_{ij}. \tag{26}$$

In two dimensions this can be written explicitly in terms of the three independent strain components. Since

$$\nabla \cdot \mathbf{u} = \epsilon_{xx} + \epsilon_{yy}, \qquad \epsilon_{ij}\epsilon_{ij} = \epsilon_{xx}^2 + \epsilon_{yy}^2 + 2\epsilon_{xy}^2,$$

we obtain

$$f = \frac{1}{2}(\lambda + 2\mu)\epsilon_{xx}^2 + \frac{1}{2}(\lambda + 2\mu)\epsilon_{yy}^2 + \lambda \epsilon_{xx}\epsilon_{yy} + 2\mu\epsilon_{xy}^2.$$

Introduce the engineering strain vector

$$\boldsymbol{e} = \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ 2\epsilon_{xy} \end{pmatrix}.$$

Then

$$f = \frac{1}{2}\boldsymbol{e}^{\mathsf{T}} \begin{pmatrix} \lambda + 2\mu & \lambda & 0 \\ \lambda & \lambda + 2\mu & 0 \\ 0 & 0 & \mu \end{pmatrix} \boldsymbol{e}.$$

This is the two-dimensional stiffness matrix. Differentiating with respect to strain gives

$$\begin{aligned} \sigma_{xx} &= (\lambda + 2\mu)\epsilon_{xx} + \lambda\epsilon_{yy}, \\ \sigma_{yy} &= \lambda\epsilon_{xx} + (\lambda + 2\mu)\epsilon_{yy}, \\ \sigma_{xy} &= 2\mu\epsilon_{xy}. \end{aligned}$$

For uniform isotropic compression in two dimensions, $\epsilon_{xx} = \epsilon_{yy} = \epsilon$ and $K = \lambda + \mu$. A pure area preserving shear measures μ. The stress–strain relation is

$$\sigma_{ij} = \lambda \delta_{ij}\epsilon_{kk} + 2\mu\epsilon_{ij}. \tag{27}$$

Here μ is the shear modulus. In d dimensions the bulk modulus is

$$K = \lambda + \frac{2\mu}{d}. \tag{28}$$

2.3 Longitudinal and transverse phonons

The equations of motion are

$$\rho\,\partial_t^2 u_i = \partial_j \sigma_{ij}. \tag{29}$$

For an isotropic solid this becomes

$$\rho\,\partial_t^2 \mathbf{u} = (\lambda+\mu)\nabla(\nabla\cdot\mathbf{u}) + \mu\nabla^2\mathbf{u}. \tag{30}$$

Take a plane wave

$$\mathbf{u}(\mathbf{r},t) = \mathbf{u}_0 \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \tag{31}$$

Decompose the polarization into longitudinal and transverse parts:

$$\mathbf{u} = \mathbf{u}_L + \mathbf{u}_T, \qquad \mathbf{k}\times\mathbf{u}_L = 0, \qquad \mathbf{k}\cdot\mathbf{u}_T = 0. \tag{32}$$

We obtain

$$\omega_L^2 = \frac{\lambda+2\mu}{\rho}k^2, \tag{33}$$

$$\omega_T^2 = \frac{\mu}{\rho}k^2. \tag{34}$$

Thus

$$c_L = \sqrt{\frac{\lambda+2\mu}{\rho}}, \qquad c_T = \sqrt{\frac{\mu}{\rho}}. \tag{35}$$

In a conventional crystal, $\omega \sim ck$ at small k, so counting wavevectors gives the Debye law

$$D_{\mathrm{Debye}}(\omega) \sim \omega^{d-1}. \tag{36}$$

In three dimensions, $D(\omega) \sim \omega^2$ at low frequency. The low-frequency modes are extended plane waves, and their stiffness is controlled by the macroscopic elastic constants.

3 Hessian analysis

The same elasticity can be obtained without introducing continuum fields at the outset. Let $\mathbf{R}_i$ be a mechanically stable crystal configuration and write

$$\mathbf{r}_i = \mathbf{R}_i + \mathbf{u}_i. \tag{37}$$

Expand the microscopic potential energy:

$$U = U_0 + \sum_{i\alpha}\left.\frac{\partial U}{\partial r_{i\alpha}}\right|_0 u_{i\alpha} + \frac{1}{2}\sum_{i\alpha,j\beta}\left.\frac{\partial^2 U}{\partial r_{i\alpha}\partial r_{j\beta}}\right|_0 u_{i\alpha}u_{j\beta} + \mathcal{O}(u^3) \tag{38}$$

Mechanical equilibrium makes the linear term vanish,

$$\left.\frac{\partial U}{\partial r_{i\alpha}}\right|_0 = 0, \tag{39}$$

so the energy can be expanded as

$$U = U_0 + \frac{1}{2}\mathbf{u}^{\mathsf{T}} H \mathbf{u} + O(u^3). \tag{40}$$

The Hessian is the microscopic stiffness matrix. Its eigenvectors satisfy

$$H\mathbf{e}_\alpha = \lambda_\alpha \mathbf{e}_\alpha, \tag{41}$$

and for equal particle masses

$$\omega_\alpha^2 = \frac{\lambda_\alpha}{m}. \tag{42}$$

For a periodic crystal, translational invariance means that the Hessian can be diagonalized in Fourier space. The resulting dynamical matrix has eigenvalues $m\omega_\alpha^2(\mathbf{k})$, and the elastic constants are encoded in the small-k expansion. This is the microscopic origin of continuum elasticity in a crystal.

4 A basic elastic field theory

We now return to the field-theory language of Lecture 2, but replace the scalar field ϕ by the displacement field u_i.

For an isotropic elastic solid,

$$H[\mathbf{u}] = \frac{1}{2}\int \mathrm{d}^d r \left[\lambda(\nabla\cdot\mathbf{u})^2 + 2\mu\,\epsilon_{ij}\epsilon_{ij}\right]. \tag{43}$$

Using Fourier components $u_i(\mathbf{r}) = \int_{\mathbf{k}} u_i(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}$, where $\int_{\mathbf{k}} \equiv \int \mathrm{d}^d k/(2\pi)^d$, the quadratic energy can be written

$$H = \frac{1}{2}\int_{\mathbf{k}} u_i(-\mathbf{k})\,\Gamma_{ij}(\mathbf{k})\,u_j(\mathbf{k}), \tag{44}$$

We can derive this as follows. In Fourier space,

$$\epsilon_{ij}(\mathbf{k}) = \frac{i}{2}(k_i u_j + k_j u_i). \tag{45}$$

The compression term in the elastic energy contributes

$$\frac{\lambda}{2}\int_{\mathbf{k}} k_i u_i(-\mathbf{k}) k_j u_j(\mathbf{k}), \tag{46}$$

and the shear term contributes

$$\mu\int_{\mathbf{k}} \epsilon_{ij}(-\mathbf{k})\epsilon_{ij}(\mathbf{k}) = \frac{\mu}{2}\int_{\mathbf{k}} \left[k^2 u_i(-\mathbf{k})u_i(\mathbf{k}) + k_i u_i(-\mathbf{k}) k_j u_j(\mathbf{k})\right]. \tag{47}$$

Adding these two pieces and collecting the coefficient of $u_i(-\mathbf{k})u_j(\mathbf{k})$ gives

$$\Gamma_{ij}(\mathbf{k}) = \mu k^2 \delta_{ij} + (\lambda+\mu) k_i k_j. \tag{48}$$

In two dimensions this matrix is explicitly

$$\Gamma(\mathbf{k}) = \begin{pmatrix} (\lambda+2\mu)k_x^2 + \mu k_y^2 & (\lambda+\mu)k_x k_y \\ (\lambda+\mu)k_x k_y & \mu k_x^2 + (\lambda+2\mu)k_y^2 \end{pmatrix}.$$

In order to make progress, the useful variables are the longitudinal and transverse projectors,

$$P_{ij}^L(\mathbf{k}) = \frac{k_i k_j}{k^2}, \tag{49}$$

$$P^T_{ij}(\mathbf{k}) = \delta_{ij} - \frac{k_i k_j}{k^2}. \tag{50}$$

They obey $P^L + P^T = I$. The orthogonality and idempotence relations can be written as

$$P^L P^L = P^L, \qquad P^T P^T = P^T, \qquad P^L P^T = 0. \tag{51}$$

Since $k_i k_j = k^2 P^L_{ij}$ and $\delta_{ij} = P^L_{ij} + P^T_{ij}$, we can rewrite the stiffness matrix as

$$\Gamma_{ij}(\mathbf{k}) = k^2 \left[(\lambda + 2\mu) P^L_{ij} + \mu P^T_{ij} \right]. \tag{52}$$

Therefore $\frac{1}{(\lambda+2\mu)k^2}$ controls longitudinal fluctuations, whereas $\frac{1}{\mu k^2}$ controls transverse fluctuations, as we saw in the dispersion relations in Section 2.3. So as $\mu \to 0$, the transverse response and transverse fluctuations become large. That is seen near jamming where the small shear modulus has a dramatic effect.

Now, since the sectors are orthogonal, the longitudinal and transverse sectors are independent. The inverse therefore follows by inverting the coefficient in each sector,

$$\Gamma^{-1}_{ij}(\mathbf{k}) = \frac{P^L_{ij}}{(\lambda + 2\mu)k^2} + \frac{P^T_{ij}}{\mu k^2}. \tag{53}$$

Therefore we can use this to compute the displacement correlations, as was done for the correlations in the scalar field computation.

To see how this kernel enters the mechanical response, add a body force through

$$H_{\text{source}} = -\int_{\mathbf{k}} f_i(-\mathbf{k}) u_i(\mathbf{k}). \tag{54}$$

The stationarity condition is

$$\frac{\delta H}{\delta u_i(-\mathbf{k})} = 0 \tag{55}$$

Leading to

$$\Gamma_{ij}(\mathbf{k}) u_j(\mathbf{k}) = f_i(\mathbf{k}). \tag{56}$$

Hence

$$u_i(\mathbf{k}) = \Gamma^{-1}_{ij}(\mathbf{k}) f_j(\mathbf{k}). \tag{57}$$

The transverse part of the response scales as $1/\mu$, so the response becomes large as the shear modulus becomes small.

For a thermal elastic solid, the same quadratic form gives the Gaussian covariance

$$\langle u_i(\mathbf{k}) u_j(-\mathbf{k}) \rangle = k_{\mathrm{B}} T \left[\frac{P^L_{ij}}{(\lambda + 2\mu)k^2} + \frac{P^T_{ij}}{\mu k^2} \right]. \tag{58}$$

We can also define the static susceptibility by

$$\chi_{ij}(\mathbf{k}) = \frac{\delta u_i(\mathbf{k})}{\delta f_j(\mathbf{k})} = \Gamma^{-1}_{ij}(\mathbf{k}). \tag{59}$$

The covariance can therefore be written as

$$G_{ij}(\mathbf{k}) = k_{\mathrm{B}} T \, \chi_{ij}(\mathbf{k}). \tag{60}$$

For the athermal systems considered in this course, the last relation is not used as a fluctuation relation: the mechanical response of a fixed configuration is still governed by the inverse stiffness, but the statistical measure over distinct packings must be specified separately, as we will see in the next Lecture.