Basic Training Due Wed Feb 11

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Exercises

If you'd like to consult the text, it's available online at http://pages.physics.cornell.edu/sethna/StatMech/EntropyOrderParametersComplexity.pdf.

(N.1) **Fracture nucleation: elastic theory has zero radius of convergence.**[1] (Condensed matter) ③

In this exercise, we shall use methods from quantum field theory to tie together two topics which American science and engineering students study in their first year of college: Hooke's law and the convergence of infinite series.

Consider a large steel cube, stretched by a moderate strain $\epsilon = \Delta L/L$ (Figure N.1). You may assume $\epsilon \ll 0.1\%$, where we can ignore plastic deformation.

(a) *At non-zero temperature, what is the equilibrium ground state for the cube as $L \to \infty$ for fixed ϵ?* (Hints: Remember, or show, that the free energy per unit (undeformed) volume of the cube is $\frac{1}{2}Y\epsilon^2$. Notice figure N.2 as an alternative candidate for the ground state.) *For steel, with $Y = 2 \times 10^{11}\,\mathrm{N/m^2}$, $\gamma \approx 2.5\,\mathrm{J/m^2}$,*[2] *and density $\rho = 8000\,\mathrm{kg/m^3}$, how much can we stretch a beam of length $L = 10\,m$ before the equilibrium length is broken in two? How does this compare with the amount the beam stretches under a load equal to its own weight?*

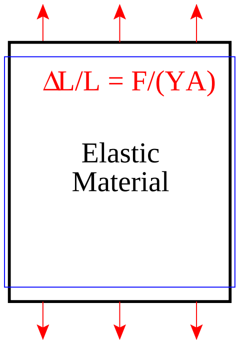

Fig. N.1 Stretched block of elastic material, length L and width W, elongated vertically by a force F per unit area A, with free side boundaries. The block will stretch a distance $\Delta L/L = F/YA$ vertically and shrink by $\Delta W/W = \sigma\,\Delta L/L$ in both horizontal directions, where Y is Young's modulus and σ is Poisson's ratio, linear elastic constants characteristic of the material. For an isotropic material, the other elastic constants can be written in terms of Y and σ; for example, the (linear) bulk modulus $\kappa_{\mathrm{lin}} = Y/3(1-2\sigma)$.

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[1] This exercise draws heavily on Alex Buchel's work [1, 2].

[2] This is the energy for a clean, flat [100] surface, a bit more than 1eV/surface atom [4]. The surface left by a real fracture in (ductile) steel will be rugged and severely distorted, with a much higher energy per unit area. This is why steel is much harder to break than glass, which breaks in a brittle fashion with much less energy left in the fracture surfaces.

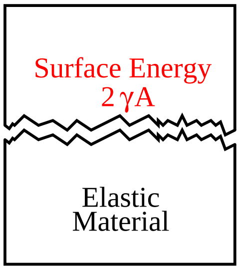

Fig. N.2 Fractured block of elastic material, as in figure N.1 but broken in two. The free energy here is $2\gamma A$, where γ is the free energy per unit area A of (undeformed) fracture surface.

Why don't bridges fall down? The beams in the bridge are in a *metastable state*. What is the barrier separating the stretched and fractured beam states? Consider a crack in the beam, of length ℓ. Your intuition may tell you that tiny cracks will be harmless, but a long crack will tend to grow at small external stress.

For convenient calculations, we will now switch problems from a stretched steel beam to a taut two-dimensional membrane under an isotropic tension, a negative pressure $P < 0$. That is, we are calculating the rate at which a balloon will spontaneously pop due to thermal fluctuations.

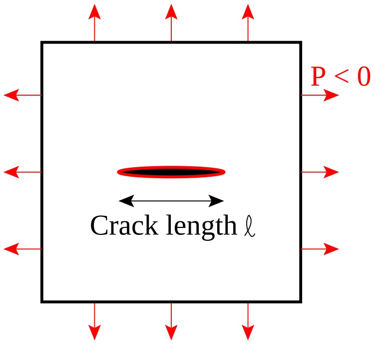

Fig. N.3 Critical crack of length ℓ, in a two-dimensional material under isotropic tension (negative hydrostatic pressure $P < 0$).

The crack costs a surface free energy $2\alpha\ell$, where α is the free energy per unit length of membrane perimeter. A detailed elastic theory calculation shows that a straight crack of length ℓ will release a (Gibbs free) energy $\pi P^2(1-\sigma^2)\ell^2/4Y$.

(b) *What is the critical length ℓ_c of the crack, at which it will spontaneously grow rather than heal? What is the barrier $B(P)$ to crack nucleation? Write the net free energy change in terms of ℓ, ℓ_c, and α. Graph the net free energy change ΔG due to the the crack, versus its length ℓ.*

The point at which the crack is energetically favored to grow is called the *Griffiths threshold*, of considerable importance in the study of brittle fracture.

The predicted fracture nucleation rate $R(P)$ per unit volume from homogeneous thermal nucleation of cracks is thus

$$R(P) = (\text{prefactors}) \exp(-B(P)/k_B T). \qquad (\text{N.1})$$

One should note that thermal nucleation of fracture in an otherwise undamaged, undisordered material will rarely be the dominant failure mode. The surface tension is of order an eV per bond ($> 10^3\,{}^\circ\text{K}/\text{Å}$), so thermal cracks of area larger than tens of bond lengths will have insurmountable barriers even at the melting point. Corrosion, flaws, and fatigue will ordinarily lead to structural failures long before thermal nucleation will arise.

Advanced topic: Elastic theory has zero radius of convergence.

Many perturbative expansions in physics have zero radius of convergence. The most precisely calculated quantity in physics is the gyromagnetic ratio of the electron [3]

$$\begin{aligned}(g-2)_{\text{theory}} = {} & \alpha/(2\pi) - 0.328478965\ldots(\alpha/\pi)^2 \\ & + 1.181241456\ldots(\alpha/\pi)^3 \\ & - 1.4092(384)(\alpha/\pi)^4 \\ & + 4.396(42)\times 10^{-12} \qquad (\text{N.2})\end{aligned}$$

a power series in the fine structure constant $\alpha = e^2/\hbar c = 1/137.035999\ldots$. (The last term is an α-independent correction due to other kinds of interactions.) Freeman Dyson gave a wonderful argument that this power-series expansion, and quantum electrodynamics as a whole, has zero radius of convergence. He noticed that the theory is sick (unstable) for any negative α (corresponding to a pure imaginary electron charge e). The series must have zero radius of convergence since any circle in the complex plane about $\alpha = 0$ includes part of the sick region.

How does Dyson's argument connect to fracture nucleation? Fracture at $P < 0$ is the kind of instability that Dyson was worried about for quantum electrodynamics for $\alpha < 0$. It has implications for the convergence of nonlinear elastic theory.

Hooke's law tells us that a spring stretches a distance proportional to the force applied: $x - x_0 = F/K$, defining the spring constant $1/K = dx/dF$. Under larger forces, the Hooke's law will have corrections with higher powers of F. We could define a 'nonlinear spring constant' $K(F)$ by

$$\frac{1}{K(F)} = \frac{x(F) - x(0)}{F} = k_0 + k_1 F + \dots \quad \text{(N.3)}$$

Instead of a spring constant, we'll calculate a nonlinear version of the bulk modulus $\kappa_{\mathrm{nl}}(P)$ giving the pressure needed for a given fractional change in volume, $\Delta P = -\kappa \Delta V/V$. The linear isothermal bulk modulus[3] is given by $1/\kappa_{\mathrm{lin}} = -(1/V)(\partial V/\partial P)|_T$; we can define a nonlinear generalization by

$$\begin{aligned}\frac{1}{\kappa_{\mathrm{nl}}(P)} &= -\frac{1}{V(0)}\frac{V(P) - V(0)}{P} \\ &= c_0 + c_1 P + c_2 P^2 + \dots + c_N P^N + \cdots\end{aligned} \quad \text{(N.4)}$$

This series can be viewed as higher and higher-order terms in a nonlinear elastic theory.

(c) *Given your argument in part (a) about the stability of materials under tension, would Dyson argue that the series in eqn N.4 has a zero or a non-zero radius of convergence?*

In Exercise 1.5 we saw the same argument holds for Stirling's formula for $N!$, when extended to a series in $1/N$; any circle in the complex $1/N$ plane contains points $1/(-N)$ from large negative integers, where we can show that $(-N)! = \infty$. These series are *asymptotic expansions.* Convergent expansions $\sum c_n x^n$ converge for fixed x as $n \to \infty$; asymptotic expansions need only converge to order $O(x^{n+1})$ as $x \to 0$ for fixed n. Hooke's law, Stirling's formula, and quantum electrodynamics are examples of how important, powerful, and useful asymptotic expansions can be.

Buchel [1, 2], using a clever trick from field theory [5, Chapter 40], was able to calculate the large-order terms in elastic theory, essentially by doing a Kramers–Krönig transformation on your formula for the decay rate (eqn N.1) in part (b). His logic works as follows.

- The Gibbs free energy density $\mathcal{G}$ of the metastable state is complex for negative P. The real and imaginary parts of the free energy for complex P form an analytic function (at least in our calculation) except along the negative P axis, where there is a branch cut.
- Our isothermal bulk modulus for $P > 0$ can be computed in terms of $\mathcal{G} = G/V(0)$. Since $\mathrm{d}G = -S\,\mathrm{d}T + V\,\mathrm{d}P + \mu\,\mathrm{d}N$, $V(P) = (\partial G/\partial P)|_T$ and hence[4]

$$\begin{aligned}\frac{1}{\kappa_{\mathrm{nl}}(P)} &= -\frac{1}{V(0)}\frac{(\partial G/\partial P)|_T - V(0)}{P} \\ &= -\frac{1}{P}\left(\left.\frac{\partial \mathcal{G}}{\partial P}\right|_T - 1\right).\end{aligned} \quad \text{(N.5)}$$

(d) *Write the coefficients c_n of eqn N.4 in terms of the coefficients g_m in the nonlinear expansion*

$$\mathcal{G}(P) = \sum g_m P^m. \quad \text{(N.6)}$$

- The decay rate $R(P)$ per unit volume is proportional to the imaginary part of the free energy $\mathrm{Im}[\mathcal{G}(P)]$, just as the decay rate Γ for a quantum state is related to the imaginary part $i\hbar\Gamma$ of the energy of the resonance. More specifically, for $P < 0$ the imaginary part of the free energy jumps as one crosses the real axis:

$$\mathrm{Im}[\mathcal{G}(P \pm \mathrm{i}\epsilon)] = \pm(\text{prefactors})R(P). \quad \text{(N.7)}$$

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[3] Warning: For many purposes (e.g. sound waves) one must use the *adiabatic* elastic constant $1/\kappa = -(1/V)(\partial V/\partial P)|_S$. For most solids and liquids these are nearly the same.

[4] Notice that this is not the (more standard) pressure-dependent linear bulk modulus, $\kappa_{\mathrm{lin}}(P)$ which is given by $1/\kappa_{\mathrm{lin}}(P) = -(1/V)(\partial V/\partial P)|_T = -(1/V)(\partial^2 \mathcal{G}/\partial P^2)|_T$. This would also have a Taylor series in P with zero radius of convergence at $P = 0$, but it has a different interpretation; $\kappa_{\mathrm{nl}}(P)$ is the nonlinear response at $P = 0$, while $\kappa_{\mathrm{lin}}(P)$ is the pressure-dependent linear response.

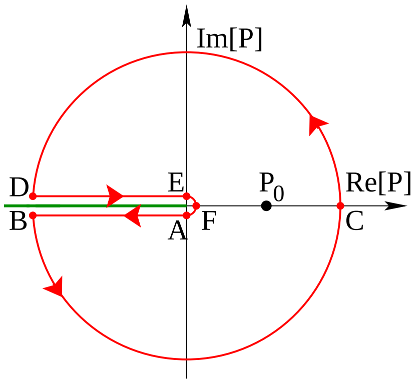

Fig. N.4 Contour integral in complex pressure. The free energy density $\mathcal{G}$ of the elastic membrane is analytic in the complex P plane except along the negative P axis. This allows one to evaluate $\mathcal{G}$ at positive pressure P_0 (where the membrane is stable and $\mathcal{G}$ is real) with a contour integral as shown.

- Buchel then used Cauchy's formula to evaluate the real part of $\mathcal{G}$ in terms of the imaginary part, and hence the decay rate R per unit volume:

$$\begin{aligned}\mathcal{G}(P_0) =& \frac{1}{2\pi \mathrm{i}} \oint_{ABCDEF} \frac{\mathcal{G}(P)}{P-P_0}\,\mathrm{d}P\\ =& \frac{1}{2\pi \mathrm{i}} \int_B^0 \frac{\mathcal{G}(P+\mathrm{i}\epsilon)-\mathcal{G}(P-\mathrm{i}\epsilon)}{P-P_0}\,\mathrm{d}P\\ &+ \int_{EFA} + \int_{BCD}\\ =& \frac{1}{\pi}\int_B^0 \frac{\mathrm{Im}[\mathcal{G}(P+\mathrm{i}\epsilon)]}{P-P_0}\,\mathrm{d}P\\ &+ (\text{unimportant})\end{aligned} \tag{N.8}$$

where the integral over the small semicircle vanishes as its radius $\epsilon \to 0$ and the integral over the large circle is convergent and hence unimportant to high-order terms in perturbation theory.

The decay rate (eqn N.1) for $P < 0$ should be of the form

$$R(P) \propto (\text{prefactors}) \exp(-D/P^2), \tag{N.9}$$

where D is some constant characteristic of the material. (You may use this to check your answer to part (b).)

(e) *Using eqns. N.7, N.8, and N.9, and assuming the prefactors combine into a constant A, write the free energy for $P_0 > 0$ as an integral involving the decay rate over $-\infty < P < 0$. Expanding $1/(P - P_0)$ in a Taylor series in powers of P_0, and assuming one may exchange sums and integration, find and evaluate the integral for g_m in terms of D and m. Calculate from g_m the coefficients c_n, and then use the ratio test to calculate the radius of convergence of the expansion for $1/\kappa_{\mathrm{nl}}(P)$, eqn N.4.* (Hints: Use a table of integrals, a computer algebra package, or change variable $P = -\sqrt{D/t}$ to make your integral into the Γ function,

$$\Gamma(z) = (z-1)! = \int_0^\infty t^{z-1} \exp(-t)\mathrm{d}t. \tag{N.10}$$

If you wish, you may use the ratio test on every second term, so the radius of convergence is the value $\lim_{n\to\infty} \sqrt{|c_n/c_{n+2}|}$.)

(Why is this approximate calculation trustworthy? Your formula for the decay rate is valid only up to prefactors that may depend on the pressure; this dependence (some power of P) won't change the asymptotic ratio of terms c_n. Your formula for the decay rate is an approximation, but one which becomes better and better for smaller values of P; the integral for the high-order terms g_m (and hance c_n) is concentrated at small P, so your approximation is asymptotically correct for the high order terms.)

Thus the decay rate of the metastable state can be used to calculate the high-order terms in perturbation theory in the stable phase! This is a general phenomena in theories of metastable states, both in statistical mechanics and in quantum physics.

References

[1] Buchel, A. and Sethna, J. P. (1996). Elastic theory has zero radius of convergence. *Physical Review Letters*, **77**, 1520.

[2] Buchel, A. and Sethna, J. P. (1997). Statistical mechanics of cracks: Thermodynamic limit, fluctuations, breakdown, and asymptotics of elastic theory. *Physical Review E*, **55**, 7669.

[3] Sethna, J. P. (1997). Quantum electrodynamics has zero radius of convergence. http://www.lassp.cornell.edu/sethna/Cracks/QED.html.

[4] Skriver, H. (2004). The hls metals database. http://http://databases.fysik.dtu.dk/hlsPT/.

[5] Zinn-Justin, J. (1996). *Quantum field theory and critical phenomena (3rd edition)*. Oxford University Press.