Elastic Theory Has Zero Radius of Convergence

Alex Buchel and James P. Sethna
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501
(Received 18 April 1996)

In nonlinear elastic theory, the inverse bulk modulus K, for example, depends on the compression P: $1/K(P) = c_0 + c_1P + c_2P^2 + \cdots + c_nP^n + \cdots$. Elastic materials that allow cracks are unstable at finite temperature with respect to fracture under a stretching load. As a result, the above power series has zero radius of convergence: it is an asymptotic series. For a two-dimensional isotropic elastic medium allowing cracks we compute the asymptotic form $c_{n+1}/c_n \to Cn^{1/2}$ as $n \to \infty$. We present an explicit formula for C as a function of temperature and material properties. [S0031-9007(96)00920-9]

PACS numbers: 62.20.Mk, 46.30.Nz, 62.20.Dc, 64.60.Qb

Hooke's law, $F = kx$, representing the elastic response of a body to an external stress, is only the first term in a Taylor's series. This Letter addresses the convergence properties of this expansion. We argue generally that the radius of convergence of elastic theory is zero, and for two-dimensional isotropic elastic theory allowing for brittle fracture, we can calculate the asymptotic behavior of the coefficients.

For simplicity, let us consider the bulk modulus $K(P)$,

$$\frac{1}{K(P)} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = c_0 + c_1P + c_2P^2 + \cdots + c_nP^n + \cdots . \quad (1)$$

Under stretching ($P < 0$), the true ground state is fractured into pieces (relieving the strain energy). As a result, $P = 0$ cannot be a point of analyticity for $K(P)$, and thus (1) has zero radius of convergence.

Similar arguments were used by Dyson [1] in 1952, where he argued that calculations in quantum electrodynamics, expressed as a power series in the fine structure constant $e^2/\hbar c \approx 1/137$, have zero radius of convergence (because negative values of e^2 lead to unstable theories). This did not prevent these calculations from being useful (indeed, they represent the best quantitative agreement between theory and experiment known to science). The community believes these expansions are asymptotic in the same sense as is Stirling's approximation $\Gamma(n) = (n-1)! \sim e^{-n}n^n(2\pi/n)^{1/2}(1 + 1/12n + 1/288n^2 + \cdots)$: at any fixed n no matter how large, Stirling's series in $1/n$ eventually diverges, but the difference between the function and the Mth approximation goes to zero faster than $1/n^M$ as $n \to \infty$.

Since Dyson's work, field theoretic methods have been developed [2–5] to relate the instabilities in the theories at small negative couplings to the high-order terms in perturbation theory. Here we apply these methods to a particular case, using the statistical mechanics of thermally nucleated cracks to calculate the high-order terms c_n in the inverse bulk modulus (1). Statistical and thermodynamic approaches to crack nucleation and fracture have an established history [6]. However, most work in this area is concentrated on failure at rather high stresses, near the threshold for instability (the spinodal point). The high-order terms in the perturbative expansion of the inverse bulk modulus are governed by the elastic response of the material to infinitesimally small tension (see below), so we are far away from the spinodal point and linear elastic theory is an adequate description.

Consider an infinite two-dimensional isotropic elastic material subject to uniform compression P at infinity. Creation of a cut of length ℓ will increase the energy by $2\alpha\ell$, where α is the surface tension (the energy per unit length of edge), with a factor of 2 because of the two free surfaces. On the other hand, for negative P (uniform tension) the cut will open up because of elastic relaxation. Calculating this relaxation energy we find the total energy E of a crack of length ℓ:

$$E(\ell) = 2\alpha\ell - \frac{\pi P^2(1-\sigma^2)\ell^2}{4Y}, \quad (2)$$

where σ is the Poisson ratio and Y is Young's modulus of the linear elastic material (ignoring crack fluctuations). Introducing

$$\ell_c = \frac{4Y\alpha}{\pi P^2(1-\sigma^2)} \quad (3)$$

we can rewrite the energy of the crack as

$$E(\ell) = 2\alpha\ell - \alpha\frac{\ell^2}{\ell_c}. \quad (4)$$

It follows that cracks with $\ell > \ell_c$ will grow, giving rise to the fracture of the material, while those with $\ell < \ell_c$ will heal—a result first obtained by Griffith [7]. This is the instability that is responsible for the breakdown of elastic perturbation theory. Because the energy $E(\ell_c) = \alpha\ell_c$ grows as $1/P^2$ as $P \to 0$, interactions between thermally nucleated cracks are unimportant at small P and low temperatures (allowing us to use the "dilute gas approximation").

The thermodynamic properties of a macroscopic system can be obtained from its partition function Z:

$$Z = \sum_{N=0}^{\infty}\sum_n \exp(-\beta E_{nN}), \quad (5)$$

 0031-9007/96/77(8)/1520(4)$10.00

where the summation N is over all possible numbers of particles (cracks in our case) and the summation n is over all states of the system with N cracks. Once a perturbative expansion for the free energy is known, one can calculate the power series expansion for the inverse bulk modulus using

$$\frac{1}{K(P)} = -\frac{1}{PA}\left(\frac{\partial F}{\partial P}\right)_T. \tag{6}$$

For $P < 0$, our model is in a metastable state, and direct computation of the partition function should yield a divergent result. A similar problem for the three-dimensional Ising model was solved by Langer [8]: one has to compute the partition function in a stable state $P > 0$, and then do an analytical continuation in parameter space to the state of interest. The free energy develops an imaginary part in the unstable state, related to the decay rate for fracture [9]: the situation is similar to that of barrier tunneling in quantum mechanics [10], where the imaginary part in the energy gives the decay rate of a resonance. The calculation of the imaginary part of the partition function is dominated by a saddle point, that in our case is a straight cut of length ℓ_c. The straight cut is the saddle point because it gains the most elastic relaxation energy for a given number of broken bonds.

We will show now how this procedure is implemented for a simplified model that does not include the quadratic fluctuations around the saddle point. Following the general prescription, we put our material under uniform compression P. In this case the opening of a thermally nucleated cut does not relieve the energy of the elastic deformation, but rather increases it. We cannot use (2) directly for the calculation of the material partition function: the latter assumes the equilibrium opening of the cut under tension $-P$, which for the case of compression corresponds to the unphysical overlap of the elastic material. To overcome this obstacle we introduce another collective coordinate v describing the elliptical opening of a cut. More specifically, if the cut is parametrized as $x(\theta) = (\ell/2)\cos\theta$, $\theta \in [0, 2\pi)$, this opening is $y(\theta) = v\sin\theta$. (The choice for this collective coordinate is motivated by the fact that for the material under tension the equilibrium crack shape is exactly of this form.) A cut of length ℓ in equilibrium under pressure P with an elliptical opening of height $2v$ increases the elastic energy of the material by

$$E(\ell, v, P) = 2\alpha\ell + \frac{\pi Y}{4(1-\sigma^2)}v^2 + \frac{\pi P\ell}{2}v, \tag{7}$$

where the first term is the energy to create the cut, the second term is due to the increase in the elastic deformation energy introduced in the surrounding material by the crack opening, and the third term is the work against the external pressure. [Note that minimizing (7) with respect to v for $P < 0$ gives Eq. (2).] The partition function for the material with a single cut $Z_{\rm cut}$ can be calculated directly

$$\begin{aligned} Z_{\rm cut} &= Z_0\left(2\pi\frac{A}{\lambda^2}\right)\int_0^\infty \frac{d\ell}{\lambda}\int_0^\infty \frac{dv}{\lambda}\exp[-\beta E(\ell, v, P)] \\ &= Z_0\left(2\pi\frac{A}{\lambda^2}\right)\int_0^\infty \frac{d\ell}{\lambda}\int_0^\infty \frac{dv}{\lambda} \\ &\quad\times \exp\left\{-\beta\left(2\alpha\ell + \frac{\pi Y}{4(1-\sigma^2)}v^2 + \frac{\pi P\ell}{2}v\right)\right\}, \end{aligned} \tag{8}$$

where the factor $2\pi A/\lambda^2$ comes from the zero modes for rotating and translating the cut, λ is the ultraviolet cutoff of the theory (roughly, the interatomic distance), and Z_0 is the partition function for the uncracked material (unity for the present calculation without quadratic fluctuations). From (8) it follows that $Z_{\rm cut}$ is holomorphic in the complex P plane except for a branch cut $P \in (-\infty, 0)$. The analytical continuation to the upper branch cut $-P + i0$ is now straightforward. Using [11] $\lim_{\epsilon\to+0}\int f(x)\,dx/(x + i\epsilon) = \text{P.V.}\int f(x)\,dx/x - i\pi f(0)$ we find

$$\begin{aligned} Z_{\rm cut}(-P) &= \lim_{\epsilon\to+0} Z_{\rm cut}(-P + i\epsilon) \\ &= \lim_{\epsilon\to+0} Z_0\left(2\pi\frac{A}{\lambda^2}\right)\int_0^\infty \frac{d\ell}{\lambda}\int_0^\infty \frac{dv}{\lambda}\exp\left[-\beta\left(2\alpha\ell + \frac{\pi Y}{4(1-\sigma^2)}v^2 + \frac{\pi\ell(-P+i\epsilon)}{2}v\right)\right] \\ &= Z_0\frac{2}{\beta}\left(2\pi\frac{A}{\lambda^2}\right)\text{P.V.}\int_0^\infty \frac{dv}{\lambda}\,\frac{\exp[-(\beta\pi Y v^2)/4(1-\sigma^2)]}{4\alpha\lambda - \pi P\lambda v} - Z_0\frac{2i}{\beta P\lambda^2}\left(2\pi\frac{A}{\lambda^2}\right)\exp\left\{-\frac{4\beta Y\alpha^2}{\pi P^2(1-\sigma^2)}\right\}. \end{aligned} \tag{9}$$

In a dilute gas approximation the partition function for the material with N cuts Z_N is given by

$$Z_N = Z_0\frac{(Z_{\rm cut}/Z_0)^N}{N!}, \tag{10}$$

which from (5) determines the material free energy $F = -(1/\beta)\ln Z$,

$$F = -\frac{1}{\beta}\ln\sum_{N=0}^{\infty} Z_N = -\frac{1}{\beta}\ln Z_0 - \frac{1}{\beta}\frac{Z_{\rm cut}}{Z_0}. \tag{11}$$

Following (9) and (11) we find the imaginary part of the free energy for negative pressure (stretching)

$$\text{Im } F(-P) = \frac{2}{\beta^2 P\lambda^2}\left(2\pi\frac{A}{\lambda^2}\right)\exp\left\{-\frac{4\beta Y\alpha^2}{\pi P^2(1-\sigma^2)}\right\}. \tag{12}$$

The analytical properties of the partition function $Z_{\rm cut}$ in the complex P plane allows a Cauchy representation

[3,5] for the free energy

$$F(P) = \frac{1}{\pi}\int_{-\infty}^{0} \frac{\mathrm{Im}\ F(P')}{P' - P}\, dP'. \tag{13}$$

As was first established for similar problems in field theory [2–4], this relation determines the high-order terms in the expansion of the free energy $F(P) = \sum_n f_n P^n$,

$$f_n = \frac{1}{\pi}\int_{-\infty}^{0} \frac{\mathrm{Im}\ F(P')}{P'^{n+1}}\, dP'. \tag{14}$$

Because the saddle-point calculation becomes more and more accurate as $P \to 0$, and because the integrals in Eq. (14) are dominated by small P as $n \to \infty$, using the saddle-point form for the imaginary part of the free energy yields the correct $n \to \infty$ asymptotic behavior of the high-order coefficients f_n in the free energy. For the present (simplified) calculation (12)

$$f_n = (-1)^{n+1}\Gamma\left(\frac{n+1}{2}\right)\left(\frac{\pi(1-\sigma^2)}{4\beta Y\alpha^2}\right)^{n/2} \times \left(2\pi\frac{A}{\lambda^2}\right)\frac{(1-\sigma^2)^{1/2}}{2\pi^{1/2}\beta^{5/2}\alpha\lambda^2 Y^{1/2}}\,. \tag{15}$$

We can then use the thermodynamic relation (6) to show $c_n = -(n+2)f_{n+2}/A$, and thus calculate the asymptotic behavior of the expansion of the bulk modulus:

$$\frac{c_{n+1}}{c_n} \longrightarrow -n^{1/2}\left(\frac{\pi(1-\sigma^2)}{8\beta Y\alpha^2}\right)^{1/2} \quad \text{as } n \longrightarrow \infty, \tag{16}$$

which indicates that the high-order terms c_n in the perturbative expansion for the inverse bulk modulus roughly grow as $(n/2)!$ [In principle one could obtain the asymptotic coefficients of the expansion (15) and (16) directly from the real part of the free energy (9) and (11) but this is not convenient when we incorporate quadratic fluctuations.]

In a companion, longer publication [12] we flesh out this simplified calculation into a complete asymptotic analysis, including quadratic fluctuations. There we calculate analytically the prefactors arising from the following two types of quadratic fluctuations: (i) *curvy cuts*—changes in the shape of the tear in the material: deviations of the broken bonds from a straight-line configuration, and (ii) *surface phonons*—thermal fluctuations of the free surface of the crack about its equilibrium opening shape. Here we mention only the results. (1) We find that fluctuation modes that do not open the cut decouple from the normal modes that have a displacement discontinuity along the cut, and therefore act the same as they did in the uncracked material, contributing to Z_0 in Eq. (8). (2) The collective coordinate v, describing one of the discontinuous normal modes, decouples from the rest of the discontinuous normal modes, and is the only mode coupled to external pressure. (3) The transformation from the functional space of the displacement fields $\vec{U}(x, y)$ to the vector space of the collective coordinates is orthogonal. So if we assume the measure to be Cartesian in the original functional space $DU_x DU_y$, it will remain Cartesian in the space of the collective coordinates [no Jacobians multiply $d\ell dv$ in Eq. (8)]. (4) The quadratic fluctuations renormalize the prefactor in (12) and the surface tension α develops temperature dependent corrections. (5) The precise form of the surface tension renormalization and the prefactor depends on the regularization prescription (exactly how the ultraviolet cutoff is introduced to the theory). (6) For the types we have tried (ξ function and cutoff regularization), the asymptotic ratio of the elastic coefficients (16) are *independent of regularization*, except for the temperature-dependent corrections to the surface tension α. For cracks in three dimensions, we expect the scaling $c_{n+1}/c_n \sim n^{1/4}$ as $n \to \infty$, using similar arguments.

We warn the reader to treat our results in the proper context. First, we do not expect this calculation to have experimental implications in the near future. Real fracture invariably occurs on inhomogeneities in the material: preexisting surface or bulk microcracks, dislocation tangles, or grain boundaries. Even for a perfect dislocation-free crystal with stabilized surfaces, the effects we describe will remain immensely small: the reason that incredibly tiny compression makes (relatively) large changes in volume (leading to large high-order terms in the power series) is because the compression suppresses the (already incredibly rare) opening of large thermally nucleated cracks. Measuring these effects would seem infeasible.

Second, our results can be viewed as a straightforward extension to the solid-gas sublimation point of Langer [8,9] and Fisher's [13] theory of the essential singularities at the liquid-gas transition. Indeed, if we allow for vapor pressure in our model, then our system will be in the gas phase at $P = 0$. The essential singularity we calculate shifts from $P = 0$ to the vapor pressure. If we measure the nonlinear bulk modulus as an expansion about (say) atmospheric pressure, it should converge—but the radius of convergence would be bounded by the difference between the point of expansion and the vapor pressure.

Third, we have forbidden dislocation nucleation and plastic flow in our model. Dislocation emission is crucial for ductile fracture, but by restricting ourselves to a brittle fracture of defect-free materials we have escaped many (lethal) complications. Dislocations are in principle important: the nucleation [14] barrier E_{dis} for two edge dislocations in an isotropic linear-elastic material under uniform tension P with equal and opposite Burger's vectors $\vec{b}$ is

$$E_{\mathrm{dis}} = \frac{Yb^2}{4\pi(1-\sigma^2)}\ln\frac{Y}{P} + E_0\,, \tag{17}$$

where E_0 is a P independent part that includes the dislocation core energy. The fact that E_{dis} grows like $1/\ln P$ as $P \to 0$ (much more slowly than the corresponding barrier for cracks) tells that in more realistic models dislocations and the resulting plastic flow [15] cannot be

ignored. While dislocations may not themselves lead to a catastrophic instability in the theory (and thus to an imaginary part in the free energy?), they will strongly affect the dynamics of crack nucleation (e.g., nucleation on grain boundaries and dislocation tangles).

Fourth, we ignore void formation. It would seem natural to associate the pressure P times the unit cell size with the chemical potential μ of a vacancy. At negative chemical potentials, the dominant fracture mechanism becomes the nucleation of vacancy clusters or voids (rather than Griffith-type microcracks), as noted by Golubović and collaborators [16]. For negative chemical potential μ, their vacancy clusters (up to constants) have energy $E_{\rm vac}(R) \sim \alpha R - |\mu| R^2$. If we identify μ with P, comparing with (2) we see that the vacancy cluster gains an energy linear in P (while the crack gain is only quadratic). This leads to a problem that maps onto Langer's calculation, yielding the asymptotic relation $c_{n+1}/c_n \sim n$, so the coefficients in this case would diverge more strongly: $c_n \sim n!$ However, the identification of μ with P demands a mechanism for relieving elastic tension by the creation of vacancies. The only bulk mechanism for vacancy formation is dislocation climb, which we have excluded from consideration; creation of vacancies at surfaces will not relieve forces applied to the lattice planes.

It is amazing to us how the extreme nonlinear terms in the response are determined from the linear elastic theory, and how little impact this has in practice.

We acknowledge the support of DOE Grant No. DE-FG02-88-ER45364. We thank Yakov Kanter, Eugene Kolomeisky, Paul Houle, Tony Ingraffea, Paul Wawrzynek, and Robb Thompson for useful conversations.

[1] F. J. Dyson, Phys. Rev. **85**, 631 (1952).
[2] C. M. Bender and T. T. Wu, Phys. Rev. **184**, 1231 (1969).
[3] E. Brézin, J. C. Le Guillou, and J. Zinn-Justin, Phys. Rev. D **15**, 1558 (1977).
[4] G. Parisi, Phys. Lett. **66B**, 167 (1977).
[5] E. B. Bogomolny, Phys. Lett. **67B**, 193 (1977).
[6] R. I. B. Selinger, Z. Wang, and W. M. Gelbart, Phys. Rev. A **43**, 4396 (1991), and references therein.
[7] A. A. Griffith, Philos. Trans. R. Soc. London A **221**, 163 (1920).
[8] J. S. Langer, Ann. Phys. (N.Y.) **41**, 108 (1967); see also N. J. Günther, D. A. Nicole, and D. J. Wallace, J. Phys. A **13**, 1755 (1980).
[9] J. S. Langer, Ann. Phys. (N.Y.) **54**, 258 (1969).
[10] I. Affleck, Phys. Rev. Lett. **46**, 388 (1981).
[11] J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (Addison-Wesley, Redwood City, CA, 1970), 2nd ed., p. 481.
[12] A. Buchel and J. P. Sethna (to be published).
[13] M. E. Fisher, Physics **3**, 255 (1967).
[14] D. R. Nelson, Phys. Rev. B **18**, 2318 (1978).
[15] Two-dimensional dislocation-mediated plastic flow is closely related to the problem of vortex nucleation and superflow decay in superfluid films: V. Ambegaokar, B. I. Halperin, D. R. Nelson, and E. D. Siggia, Phys. Rev. Lett. **40**, 783 (1978); V. Ambegaokar, B. I. Halperin, D. R. Nelson, and E. D. Siggia, Phys. Rev. B **21**, 1806 (1980); P. Minnhagen, O. Wetman, A. Jonsson, and P. Olsson, Phys. Rev. Lett. **74**, 3672 (1995).
[16] L. Golubović and A. Peredera, Phys. Rev. E **51**, 2799 (1995). They conclude with the interesting and apparently correct statement that voids smaller than the Griffith length can nonetheless grow and fracture the material.