Statistical mechanics of cracks: Fluctuations, breakdown, and asymptotics of elastic theory

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We study a class of models for brittle fracture: elastic theory models that allow for cracks but not for plastic flow. We show that these models exhibit, at all finite temperatures, a transition to fracture under applied load similar to the first-order liquid-gas transition. We study this transition at low temperature for small tension. Using the complex variable method in a two-dimensional elastic theory, we prove that the energy release in an isotropically stretched material due to the creation of an arbitrary curvy cut is the same to cubic order as the energy release for the straight cut with the same end points. We find the energy spectrum for crack shape fluctuations and for crack surface phonons, under a uniform isotropic tension. For small uniform isotropic tension in two dimensions, we calculate the essential singularity associated with fracturing the material in a saddle point approximation including quadratic fluctuations. This singularity determines the lifetime of the material (half-life for fracture), and also determines the asymptotic divergence of the high-order corrections to the zero temperature elastic coefficients. We calculate the asymptotic ratio of the high-order elastic coefficients of the inverse bulk modulus, and argue that the result is unchanged by nonlinearities—the ratio of the high-order nonlinear terms are determined solely by the linear theory. [S1063-651X(97)02706-2]

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I. INTRODUCTION

Early in the theory of fracture, Griffith [1] used Inglis' stress analysis [2] of an elliptical flaw in a linear elastic material to predict the critical stress under which a crack irreversibly grows, causing the material to fracture. Conversely, for a stressed solid the Griffith criterion determines the crack nucleation barrier: if the material has microcracks due to disorder or (less commonly) thermal fluctuations, how long does a microcrack have to be to cause failure under a given load? In a sense, a solid under stretching is similar to a supercooled gas: the point of zero external stress plays the role of the liquid-gas condensation point. Fisher's [3] theory of the condensation point predicts that the free energy of the system develops an essential singularity at the transition point. In this paper we develop a framework for the field-theoretical calculations of the thermodynamics of linear elastic theory with cracks (voids) that naturally incorporates the quadratic fluctuations, and we calculate the analog of Fisher's essential singularity. Following Langer [4], the imaginary part of the essential singularity can be used to determine the lifetime to fracture. This is similar to a resonance problem in quantum mechanics, where the imaginary part of the energy determines the decay rate of the resonance.

There is much work on thermal fluctuations leading to failure at rather high tensions, near the threshold for instability (the spinodal point) [5]; there is also work on the role of disorder in nucleating cracks at low tensions [6]. We are primarily interested in the thermal statistical mechanics of cracks under *small* tension. We must admit and emphasize that, practically speaking, there are no thermal crack fluctuations under small tension—our calculations are of no practical significance. Why are we studying thermal cracks in this formal limit? First, for sufficiently small tension, the bulk of the material (excluding regions near the crack tips) obeys linear elastic theory, thus making analytical analysis of the fracture thermodynamics tractable. Second, the *real* part of our essential singularity implies that nonlinear elastic theory is not convergent. Just as in quantum electrodynamics [7] and other field theories [8], for all finite temperatures, nonlinear elastic theory is an asymptotic expansion, with zero radius of convergence at zero pressure. We will calculate the high-order terms in the perturbation expansion governing the response of a system to infinitesimal tension. We find it intriguing that Hooke's law is actually a first term in a divergent asymptotic series.

The paper is organized as follows. In Sec. II, using the complex variable method in a two-dimensional elastic theory, we calculate the energy release due to the equilibrium opening of an arbitrary curvy crack to quadratic order in kink angles. In Sec. III we find the spectrum of the boundary fluctuations (surface phonons) of a straight cut under uniform isotropic tension at infinity. Section IV is devoted to the calculation of the imaginary part of the free energy. The calculation of the contribution of thermal fluctuations depends on the ''molecular structure'' of our material at short length scales — in field theory language, it is *regularization-dependent*. We calculate the imaginary part of the free energy both for the ζ function and a particular lattice regularization, and determine the temperature-dependent renormalization of the surface tension. Earlier we showed [9] that the thermal instability of an elastic material with respect to fracture results in a nonanalytical behavior of the elastic constants (e.g., the bulk modulus) at zero applied stress. In Sec. V we extend the calculation [9] of the high-order expansion of the inverse bulk modulus by including quadratic fluctuations. We show there that the asymptotic ratio of the high-order elastic coefficients, written in terms of the renormalized surface tension, is *independent* of regularization (for the cases we studied), and we argue also that they are independent of nonlinear effects near the crack tips. (The asymptotic *nonlinear* coefficients depend only on the *linear* elastic moduli.) In Sec. VI we perform the simplified calculation (without fluctuations) in several more general contexts: anisotropic strain (nonlinear Young's modulus), cluster nucleation and dislocation nucleation, and three-dimensional brittle fracture. We also discuss the effects of vapor pressure—nonperturbative effects when bits detach from the crack. Finally, we summarize our results in Sec. VII.

II. ENERGY RELEASE OF ''SLIGHTLY'' CURVY CUTS

Elastic materials under a stretching load can relieve deformation energy through the formation of cracks and voids. The famous Griffith criteria [1] for crack propagation is based on the balance between the strain energy release and the increase in the material surface energy due to extending the crack: only long cracks release enough strain energy to pay for the new surfaces. In the course of thermal fluctuations a crack can originate from the successive breaking of atomic bonds. The line of the broken bonds need not be straight, and thus the contribution of curvy cuts must be included in the material free energy. As we explain in Sec. IV, we have to know only the energy release due to the *equilibrium* opening of a curvy cut; moreover, for the quadratic analysis of the essential singularity of the free energy it is sufficient to consider only a small (quadratic) deviation of the broken bonds from the straight line configuration. In this section we calculate the energy release due to the equilibrium opening of a ''slightly'' curvy cut in a two-dimensional, isotropic, linear elastic infinite medium subject to a uniform isotropic tension T at infinity.

Perturbation methods based on the Muskhelishvili's [10] methods for the straight cut have been used previously for the determination of the stress intensity factors of ''slightly'' curvy or kinked cracks [11,12]. A particularly elegant approach was developed by Cotterell and Rice [12]. They calculated the stress intensity factors of a slightly curvy crack subject to a generic opening traction at the surface to the first order in the deviation of the cut from the straight line. Their result, when applied in the case of a uniform isotropic tension at infinity predicts that the energy release of a curvy cut coincides with the energy release of the straight cut (with the same endpoints) to the first order in the deviation. (This also follows from the symmetry arguments that we present later in the section.) In this section we will use their techniques to obtain a stronger result: the energy release of a curvy cut opened by a uniform isotropic tension at infinity coincides to *cubic* order with the energy release of the straight cut with the same end points.

An elastic state is completely defined once displacements (u,v) are known everywhere, where the deformed position of a point (x,y) is $\{x+u(x,y),y+v(x,y)\}$. Rather than considering these two functions, Muskhelishvili [10] introduces two complex functions $\phi(z)$ and $\psi(z)$ that in equilibrium should be the functions of only one complex variable z (i.e., they do not depend $\overline{z}$). Moreover, in our case (a uniform isotropic tension at infinity), $\phi(z)$ decomposes as

$$\phi(z)=\tfrac{1}{2}Tz+\phi_0(z). \tag{1}$$

The functions $\phi_0(z)$ and $\psi(z)$ are holomorphic in the complex z plane including infinity but excluding the cut contour. This description associates the components of stress $(\sigma_{xx},\sigma_{yy},\sigma_{xy})$ and displacement (u,v) to (ϕ,ψ) by the following relations:

$$\begin{aligned}\sigma_{xx}+\sigma_{yy}&=2(\phi'(z)+\overline{\phi'(z)}),\\ \sigma_{yy}-\sigma_{xx}+2i\sigma_{xy}&=2(\overline{z}\phi''(z)+\psi'(x)),\\ 2\mu(u+iv)&=\chi\phi(z)-z\overline{\phi'(z)}-\overline{\psi(z)}.\end{aligned} \tag{2}$$

[The detailed discussion of the change of ''variables'' $(u,v)\rightarrow(\phi,\psi)$ along with the derivation of Eqs. (1) and (2) can be found in [10].] The change of variable is especially convenient for the investigation of the crack energetics. In the new variables the energy release due to the equilibrium opening of the cut is given by [13]

$$E_{\text{release}}=-\frac{\pi T}{4\mu}(1+\chi)\mathrm{Re}[y_1], \tag{3}$$

with y_1 being the residue of $\psi(z)$ at infinity. The material elastic constants μ and χ can be expressed through its Young's modulus Y and Poisson ratio σ as follows:

$$\begin{aligned}\mu&=\frac{Y}{2(1+\sigma)},\\ \chi&=\frac{3-\sigma}{1+\sigma}.\end{aligned} \tag{4}$$

(The given value for χ corresponds to a plain stress in a three-dimensional elastic theory; for a plain strain one should use $\chi=3-4\sigma$.)

Before proceeding with the actual calculation of the energy release, we briefly discuss the standard lore concerning the determination of the energy release for the infinite-size system. The proper determination is extremely important for a correct description of the essential singularity in the free energy, which arises only in the thermodynamic limit [14]. For a finite-size system the energy release is a well-defined quantity that depends on the shape of the material boundary. The situation becomes more subtle in case of an infinite elastic medium. In principle one can calculate the energy release analyzing stress fields near the crack tips, and thus avoid the necessity of worrying about infinite-sized medium. This method, developed by Irwin in the 1950s, is known as the stress intensity approach [15]. Alternatively, the energy release can be calculated considering the system as a whole. In this approach, to compute the energy release one has to evaluate the work done by external forces and the change in the energy of elastic deformation. The change in the energy of the elastic deformation involves the difference between two infinitely large quantities for an infinite material; the latter thus requires some sort of infinite-volume limit. Extending Bueckner's analyses [16], Rice [17] showed that two methods give identical results if one carefully accounts for the boundary relaxation before taking the infinite-size limit. He presented the expression for the energy release in terms of stresses and strains local to the crack. The latter does not ''feel'' the shape of the boundary in the infinite-volume limit. In fact, expression (3) strongly relies on this conclusion.

To illustrate the correspondence between the energy release of a curvy cut and the straight one with the same end points, let us consider a rare example where it is possible to

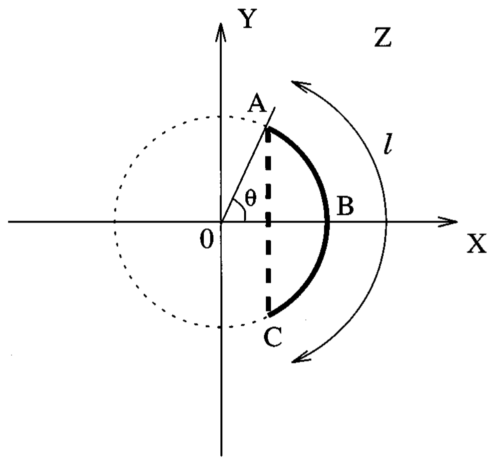

FIG. 1. The ''smile''-like cut ABC and the straight cut AC result in the same energy release to cubic order in θ.

find an exact analytical solution. Suppose a material with a ''smile'' cut—an arc of a circle ABC—of total arc length ℓ (Fig. 1) is subject to a uniform isotropic stretching T at infinity. Expanding the exact answer in [10] about $z=\infty$, we find

$$\psi_{ABC}(z)=-\frac{T\ell^2}{8z}\frac{8\sin^2\theta/2}{\theta^2(3-\cos\theta)}+O\left(\frac{1}{z^2}\right), \tag{5}$$

which, according to Eq. (3), gives the energy release E_{ABC}

$$E_{ABC}=\frac{\pi T^2\ell^2}{32\mu}(1+\chi)\frac{8\sin^2\theta/2}{\theta^2(3-\cos\theta)}. \tag{6}$$

On the other hand, for a straight cut AC of length $(\ell/\theta)\sin\theta$, the holomorphic function $\psi_{AC}(z)$ has an asymptotic behavior [10]

$$\psi_{AC}(z)=-\frac{T\ell^2}{8z}\frac{\sin^2\theta}{\theta^2}+O\left(\frac{1}{z^2}\right) \tag{7}$$

resulting in the energy release E_{AC},

$$E_{AC}=\frac{\pi T^2\ell^2}{32\mu}(1+\chi)\frac{\sin^2\theta}{\theta^2}. \tag{8}$$

For small θ we find, from Eqs. (6) and (8), the advertised result: the energy release of ABC coincides with that of AC to cubic order in θ, but not to quartic order,

$$\begin{aligned} E_{ABC}&=\frac{\pi T^2\ell^2}{32\mu}(1+\chi)\left(1-\frac{\theta^2}{3}+\frac{77\theta^4}{720}+O(\theta^6)\right),\\ E_{AC}&=\frac{\pi T^2\ell^2}{32\mu}(1+\chi)\left(1-\frac{\theta^2}{3}+\frac{2\theta^4}{45}+O(\theta^6)\right). \end{aligned} \tag{9}$$

We now proceed with the general proof. First, an arbitrary cut is approximated by a finite number of line segments, parametrized by kink angles α_i—the angles between consecutive kinks. The exact shape of the cut is then restored as the length of each link goes to zero (as their number goes to infinity). The energy release is evaluated to cubic order in the kink angles, e.g., for the n-kink regularization, the energy release $E_n(\{\alpha_i\})$ for a curvy cut with a fixed separation ℓ_p between the end points is approximated as

$$\begin{aligned} E_n(\{\alpha_i\})=&E^{(0)}+\sum_{i=1}^{n}E_i^{(1)}\alpha_i+\sum_{i=1}^{n}\sum_{j=1}^{n}E_{ij}^{(2)}\alpha_i\alpha_j\\ &+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{m=1}^{n}E_{ijm}^{(3)}\alpha_i\alpha_j\alpha_m+O(\alpha_i^4), \end{aligned} \tag{10}$$

where E^0 is the energy release for a straight cut of length ℓ_p and the coefficients $E_i^{(1)}$, $E_{ij}^{(2)}$, and $E_{ijm}^{(3)}$ depend only on the positions of the kinks along the cut. We claim that all coefficients up to cubic order are zero, and thus the energy of a curvy cut and the straight one with the same end points can differ only at $O(\alpha_i^4)$.

That $E_i^{(1)}$ and $E_{ijm}^{(3)}$ (in fact, all terms odd in the kink angles) are zero follows from a symmetry argument: cuts (having the same number of segments with the corresponding segments being of the same length) with kink angles $\{\alpha_i\}$ and $\{-\alpha_i\}$, respectively, are mirror images of each other with respect to the first link. The boundary condition for our problem (a uniform tension at infinity) is reflection invariant, so

$$E_n(\{\alpha_i\})=E_n(\{-\alpha_i\}), \tag{11}$$

which requires that all energy release terms odd in the kink angles vanish. To calculate $E_{ij}^{(2)}$ for a given pair of indexes, we can put all kink angles to zero except for α_i and α_j, reducing the n-kink problem to a two-kink one. From now on we will consider only the two-kink problem to quadratic order in the kink angles.

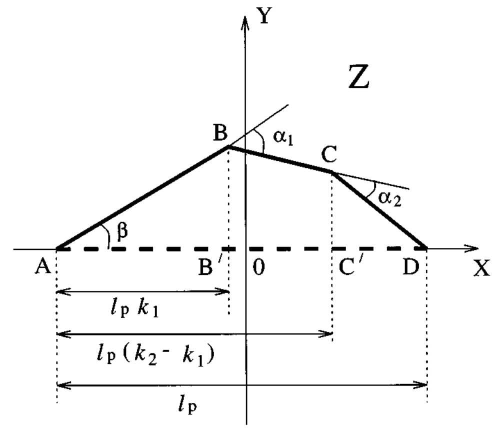

FIG. 2. The two-kink cut $ABCD$ can be considered as a *deformation* of a straight cut AD.

We choose the coordinate system XY in the complex z plane in such a way that the ends of the two-kink cut are on the X axis, symmetric with respect to the Y axis (Fig. 2). Assuming a uniform isotropic tension T at infinity we rewrite Eq. (3), explicitly indicating the dependence of the energy release on the kink angles,

$$E_2(\alpha_1,\alpha_2)=-\frac{\pi T}{4\mu}(1+\chi)\mathrm{Re}[y_1(\alpha_1,\alpha_2)], \tag{12}$$

where $y_1(\alpha_1,\alpha_2)$ is $1/z$ coefficient in the expansion of the function $\psi(z)$ at infinity. As discussed earlier in the section, $\psi(z)$ is a holomorphic function in the complex z plane including infinity (the extended complex plane) but excluding the two-kink cut. The other function $\phi(z)$ that is necessary for the specification of the equilibrium elastic state satisfies Eq. (1), with $\phi_0(z)$ holomorphic in the same region as $\psi(z)$. The analytical functions $\phi(z)$ and $\psi(z)$ must provide a stress-free cut boundary, which, following [10], can be expressed as

$$if(\phi,\psi)=[\phi(z)+z\overline{\phi'(z)}+\overline{\psi(z)}]|_W^X=0, \tag{13}$$

where $f=F_x+iF_y$ is the complex analog of the force acting on the portion of the cut boundary between points W and X.

It is important to note that any two pairs of functions $(\phi_0^1(z),\psi^1(z))$ and $(\phi_0^2(z),\psi^2(z))$ that are holomorphic in the extended z plane excluding the same curvy cut, and which provide the stress-free cut boundaries to $O(\alpha^3)$, Eq. (13), can differ only by $O(\alpha^3)$ everywhere:

$$\begin{aligned}\delta\phi(z)&=\phi_0^1(z)-\phi_0^2(z)=O(\alpha^3),\\ \delta\psi(z)&=\psi^1(z)-\psi^2(z)=O(\alpha^3).\end{aligned} \tag{14}$$

This follows explicitly from Cauchy's theorem, but also follows from the elastic theory. Each pair $(\phi_0^1(z)+Tz/2,\psi^1(z))$ or $(\phi_0^2(z)+Tz/2,\psi^2(z))$ defines the equilibrium elastic state with stresses of order $O(\alpha^3)$ along the cut boundary and uniform isotropic stretching T at infinity. So, $(\delta\phi(z),\delta\psi(z))$ corresponds to the equilibrium state with the specified stresses of order $O(\alpha^3)$ along the cut boundary and zero tension at infinity. Thus Eq. (14) follows, because the response to this force within linear elastic theory must be linear. The above argument guarantees that once we find $\phi_0(z)$ and $\psi(z)$ that satisfy the discussed constraints to $O(\alpha^3)$, we can use them to calculate the energy release of the curvy cut to quadratic order.

Let functions $\phi^s(z)$ and $\psi^s(z)$ define the equilibrium elastic state of a material with a straight cut AD subject to a uniform tension T at infinity. $\phi_0^s(z)=\phi^s(z)-Tz/2$ and $\psi^s(z)$ should then be holomorphic in the extended complex z plane excluding the straight cut, and should provide stress-free boundaries along AD. Muskhelishvili finds [10]

$$\begin{aligned}\frac{d\phi^s(z)}{dz}&=\frac{T}{2}\frac{z}{\sqrt{z^2-\ell_p{}^2/4}},\\ \frac{d\psi^s(z)}{dz}&=\frac{T}{8}\frac{z\ell_p{}^2}{(z^2-\ell_p{}^2/4)\sqrt{z^2-\ell_p{}^2/4}}.\end{aligned} \tag{15}$$

[To obtain $\phi^s(z)$ and $\psi^s(z)$, we integrate Eq. (15); the arbitrariness in the integration constants reflect the ambiguity in the displacements up to a rigid motion of the material as a whole.] Note that $\phi_0^s(z)$ and $\psi^s(z)$ can be ''made'' holomorphic everywhere in the complex z plane excluding the two-kink cut $ABCD$, and thus can serve as a good starting point for the construction of $\phi_0(z)$ and $\psi(z)$. The process of an analytical continuation is demonstrated by Fig. 3. $\phi_0^s(z)$ [or equivalently $\psi^s(z)$] is holomorphic in the z plane excluding the straight cut AD, Eq. (4a). Removing the region $ABCDA$, Eq. (4b), we make it holomorphic in the complex plane excluding $ABCDA$. Now we analytically continue $\phi_0^s(z)$ from the link AD, Eq. (4c), into the removed region [the continuation is possible explicitly using Eq. (15)]. The obtained function becomes holomorphic everywhere in the complex z plane excluding the two-kink cut $ABCD$, Eq. (4d), moreover the original function and the one obtained through the analytical continuation coincide outside $ABCDA$.

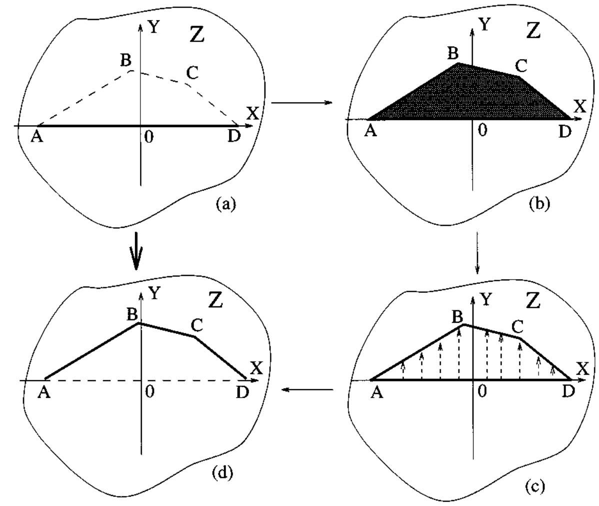

FIG. 3. Functions $\phi_0^s(z)$ and $\psi^s(z)$ holomorphic in the complex z plane excluding the straight cut AD (a), can be ''made'' holomorphic in the complex z plane excluding the two-kink cut $ABCD$ (d).

The idea of constructing the holomorphic functions $\phi_0(z)$ and $\psi(z)$ is simple: we start with the functions $\phi_0^s(z)$ and $\psi^s(z)$ and calculate to quadratic order the stresses along the two-kink cut boundary $ABCD$ under the analytical continuation as described by Fig. 3. The stresses along the curvy cut boundary (Fig. 4) are then compensated for up to quadratic order in the kink angles by introducing counter forces along the original (straight) cut, leading to corrected functions $\delta\phi^c(z)$ and $\delta\psi^c(z)$, where $\phi(z)=\phi^s(z)+\delta\phi^c(z)+O(\alpha^3)$ and $\psi(z)=\psi^s(z)+\delta\psi^c(z)+O(\alpha^3)$. For the calculation of the energy release (12), we need the real part of the residue of $\psi(z)$ at infinity: we will show that the residue of $\delta\psi^c(z)$ at infinity is zero and thus the residues of $\psi(z)$ and $\psi^s(z)$ at $z=\infty$ are the same—which means that the energy release for the curvy cut $ABCD$ is the same as that for the straight cut AD.

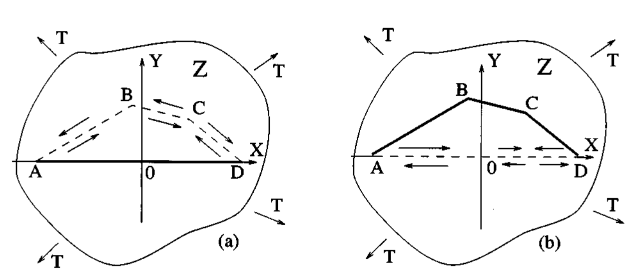

FIG. 4. The stress free boundary of a two-kink $ABCD$ cut (b) can be mimicked by applying the tangential force to the previously unstressed (a) straight cut boundary AD.

Let us assume that points W and X are on the upper boundary of the link AB. From Fig. 2, $z=t+i\beta(t+\ell_p/2)+O(\alpha^3)$, where $t\in AB'$ and $\beta=(1-k_1)\alpha_1+(1-k_2)\alpha_2+O(\alpha^3)$. Using Eq. (13), we find

$$\begin{aligned} if(\phi_0^s,\psi^s)=&[\phi^s(t)^+ + t\overline{\phi^s(t)'^+}+\overline{\psi^s(t)^+}]|_W^X + i\beta(t+\ell_p/2)\\ &\times(\phi^s(t)'^+ + \overline{\phi^s(t)'^+} - t\overline{\phi^s(t)''^+} - \overline{\psi^s(t)'^+})|_W^X\\ &-\frac{\beta^2(t+\ell_p/2)^2}{2}(\phi^s(t)''^+ + t\overline{\phi^s(t)'''^+}\\ &-2\overline{\phi^s(t)''^+}+\overline{\psi^s(t)''^+})|_W^X+O(\alpha^3)\\ =&2\beta^2(t+\ell_p/2)^2\phi^s(t)''^+|_W^X+O(\alpha^3), \end{aligned} \tag{16}$$

where t runs along AB'; the + superscript means that the values of $\phi_0^s(t)$ and $\psi(t)$ should be taken at the upper boundary of the straight cut. To obtain the second expression in Eq. (16), one can plug in the explicit form (15), or—more elegantly—note that for $t\in AB'$, $\phi^s(t)$ is pure imaginary and $\psi^s(z)'=-z\phi^s(z)''$. Either way, it follows that the functions $\delta\phi^c(z)$ and $\delta\psi^c(z)$ satisfy

$$\begin{aligned} i\delta f=&[\delta\phi^c(t)^+ + t\overline{\delta\phi^c(t)'^+}+\overline{\delta\psi^c(t)^+}]|_W^X\\ =&-2\beta^2(t+\ell_p/2)^2\phi^s(t)''^+|_W^X. \end{aligned} \tag{17}$$

This is the force we need to add along the straight cut just below segment AB to cancel the stress along the curvy cut. Similar expressions can be found for the forces needed below BC and CD. To find $\delta\phi^c(z)$ and $\delta\psi^c(z)$ we have to solve the elasticity problem for the material with the straight cut AD, subject to these applied forces $i\delta f$ along the cut boundary. Fortunately, this problem allows a closed analytical solution [10]. Expanding the exact expression for $\delta\psi^c(z)$ in [10], we find

$$\delta\psi^c(z)=\frac{\ell_p}{4\pi i z}\oint_\gamma \mathrm{Re}[i\delta f(x(\sigma))]d\sigma+O\left(\frac{1}{z^2}\right), \tag{18}$$

where the integration is along the unit circle γ in the complex plane, and $i\delta f$ is a function of a variable point $x(\sigma)=\ell_p(\sigma+1/\sigma)/4$ along the straight cut boundary AD. Notice from Eq. (17) that $i\delta f$ is pure imaginary evaluated on the upper boundary of the link AB: in this case $|t|<\ell_p/2$, and so the argument of the square root in Eq. (15) is negative, resulting in pure imaginary $\phi^s(t)'$, thus $\phi^s(t)''$ is also pure imaginary. In fact, as it can be checked explicitly, $\mathrm{Re}[i\delta f]=0$ for arbitrary W and X along the cut boundary. So we conclude from Eq. (18) that the residue of $\delta\psi^c(z)$ at infinity is zero, and thus the energy release for the curvy cut $ABCD$ is the same as for the straight cut AD. The underlying physical reason for this seemingly remarkable coincidence is that to imitate the stress free curvy cut to quadratic order in the kink angles we have to apply only tangential force along the straight cut (pure imaginary $i\delta f$ means $F_y=0$), which does not work because a straight cut under a uniform isotropic tension at infinity opens up but does not shrink [10].

We find that the energy release $E(\ell_p)$ of the curvy cut with projected distance ℓ_p between the end points is the same to quadratic order in the kink angles as the energy release of the straight cut of length ℓ_p. The latter one is given by the second formula in Eq. (9) with $\theta=0$ (it also coincides with Griffith's result),

$$E(\ell_p)=\frac{\pi T^2\ell_p^2}{32\mu}(1+\chi). \tag{19}$$

The natural variables to describe the curvy cut are its total length ℓ and its curvature $k(x)$, $x\in[0,\ell]$. In what follows we express Eq. (19) in these variables, and find the normal modes of the curvature that diagonalize the energy release.

For the two-kink cut $ABCD$ (Fig. 2) of total length ℓ, one can find

$$\begin{aligned} \ell_p=\ell\Bigg(&1-\frac{x_1(\ell-x_1)}{2\ell^2}\alpha_1^2-\frac{x_1(\ell-x_2)}{\ell^2}\alpha_1\alpha_2\\ &-\frac{x_2(\ell-x_2)}{2\ell^2}\alpha_2^2\Bigg)+O(\alpha^3), \end{aligned} \tag{20}$$

where x_1 and x_2 parametrize the kink positions: the length of the link AB is assumed to be x_1 and the length of the segment ABC equals x_2. Similarly, for the n-kink cut of total length ℓ with the kink angles $\{\alpha_i\}$ parametrized by their distance $\{x_i\}$ from the cut end,

$$\ell_p=\ell\left(1-\tfrac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j\left[-\frac{x_ix_j}{\ell^2}+\frac{\min(x_i,x_j)}{\ell}\right]\right)+O(\alpha^3). \tag{21}$$

Expressing the kink angles through the local curvature of the curve, $\alpha_i=k(x_i)\Delta x_i/\lambda$, we find the continuous limit of Eq. (21),

$$\ell_p=\ell\left(1-\tfrac{1}{2}\int_0^\ell\int_0^\ell\frac{dx\,dy}{\lambda^2}k(x)M(x,y)k(y)\right)+O(k(x)^3), \tag{22}$$

with

$$M(x,y)=-\frac{xy}{\ell^2}+\frac{\min(x,y)}{\ell}, \tag{23}$$

and the scale λ is introduced to make the curvature dimensionless (λ can be associated with the ultraviolet cutoff of the theory—roughly the interatomic distance). Substituting Eq. (23) into Eq. (19), we find the energy release $E(\ell,k(x))=E(\ell_p)$ of the curvy cut in its intrinsic variables

$$\begin{aligned} E(\ell,k(x))=&\frac{\pi T^2\ell^2}{32\mu}(1+\chi)\\ &\times\left(1-\int_0^\ell\int_0^\ell\frac{dx\,dy}{\lambda^2}k(x)M(x,y)k(y)\right)\\ &+O(k(x)^3). \end{aligned} \tag{24}$$

To find the normal modes of the curvature we have to find the eigenvalues and eigenvectors of the operator $M(x,y)$. If $k_n(x)$ is an eigenvector of $M(x,y)$ with eigenvalue λ_n, then

$$\lambda_n k_n(x)=\int_0^{\ell}\frac{dy}{\lambda}M(x,y)k_n(y). \qquad (25)$$

From Eq. (23), $M(0,y)=0$ and $M(\ell,y)=0$ for arbitrary $y\in[0,\ell]$, so from Eq. (25) the eigenvectors of $M(x,y)$ must be zero at $x=0$ and $x=\ell$: $k_n(0)=k_n(\ell)=0$. An arbitrary function $k_n(x)$ with this property is given by the Fourier series

$$k_n(x)=\sum_{m=1}^{\infty}c_m\left(\frac{2\lambda}{\ell}\right)^{1/2}\sin\frac{\pi m x}{\ell}, \qquad (26)$$

where the overall constant $\sqrt{2\lambda/\ell}$ is introduced to normalize the Fourier modes with the integration measure dx/λ over $x\in[0,\ell]$. One can explicitly check from Eq. (25) that each Fourier mode $\sqrt{2\lambda/\ell}\sin(\pi m x/\ell)$ is in fact an eigenvector of $M(x,y)$ with the eigenvalue $\lambda_m=\ell/(\pi^2m^2\lambda)$. In terms of the amplitudes of the normal modes $\{c_n\}$, Eq. (24) is rewritten as

$$E(\ell,\{c_n\})=\frac{\pi T^2\ell^2}{32\mu}(1+\chi)\left(1-\sum_{n=1}^{\infty}\frac{\ell}{\pi^2n^2\lambda}c_n^2\right)+O(c_n^3). \qquad (27)$$

Equation (27) is the main result of the section: we have calculated the energy release of an arbitrary curvy cut in its intrinsic variables—the total length ℓ and the curvature $k(x)$, $x\in[0,\ell]$—to quadratic order in $k(x)$, and found the normal modes of the curvature that diagonalize the energy release.

Finally, we mention that the measure in the kink angle space is Cartesian—$\Pi_i d\alpha_i$—[and thus the functional measure $Dk(x)\equiv D\alpha(x)$ is Cartesian], so the measure in the vector space of the amplitudes of the normal modes $\{c_n\}$ is also Cartesian—$\Pi_{n=1}^{\infty}dc_n$, because the Fourier transformation $\{k(x)\}\rightarrow\{c_n\}$ is orthonormal. This will be important in Sec. IV, where we will be integrating over crack shapes.

III. SURFACE PHONONS

In the previous sections we extensively discussed the calculation of the energy release due to the equilibrium opening of a cut in an elastic material. Since our goal is to deal with cracks as thermal fluctuations, we must also deal with the more traditional elastic fluctuations—phonons or sound. We find here that the bulk fluctuations decouple from the new surface phonon modes introduced by the cut. We discuss the quadratic fluctuations for linear elastic material with a straight cut of length ℓ subject to a uniform isotropic tension T at infinity; more specifically, we calculate the energy release for the material with an arbitrary opening of the straight cut, and we find collective coordinates that diagonalize the change in the energy.

An elastic state of the fluctuating material can be defined through the specification of its displacements $\vec{U}=(u,v)$ at every point (x,y). For the material with a cut, the fields $u(x,y)$ and $v(x,y)$ can in principle have a discontinuity along the cut: assuming that the cut is an interval $(x,y)=([-\ell/2,\ell/2],0)$,

$$2g_x(x)=u(x,0+)-u(x,0-) \quad \text{for } x\in[-\ell/2,\ell/2] \qquad (28)$$

and

$$2g_y(x)=v(x,0+)-v(x,0-) \quad \text{for } x\in[-\ell/2,\ell/2] \qquad (29)$$

may be nonzero. It is clear that the arbitrary state $\vec{U}$ can be decomposed into a superposition of two states $\vec{U}_g=(u_g,v_g)$ and $\vec{U}_c=(u_c,v_c)$: $\vec{U}_g$ is the equilibrium elastic state that maximizes the energy release for given displacement discontinuity (g_x,g_y) at the cut boundaries (28) and (29) and tension T at infinity, and $\vec{U}_c$ is given by $(u_c,v_c)=(u-u_g,v-v_g)$, and is a continuous displacement field everywhere. The state $\vec{U}$ describing the actual fluctuation of the elastic material should provide zero traction at the cut boundaries. This is not, however, a requirement for states $\vec{U}_g$ and $\vec{U}_c$ separately. In fact, for the state $\vec{U}_g$ to be an equilibrium one one needs to apply forces along the cut boundaries to insure the displacement discontinuity (g_x,g_y). For any physical fluctuation $\vec{U}$ (satisfying the traction-free boundary condition at the cut), the corresponding continuous state $\vec{U}_c$ will also have forces at the seam where the cut is stitched together: these forces from above and below are equal and opposite at each point of the (former) cut.

The energy release is the sum of the work done by the external forces and the work done by the internal forces. We define the energy release E for the elastic state $\vec{U}$ with respect to the equilibrium state of the material $\vec{U}_0=(u_0,v_0)$ without the cut under the same loading at infinity, as a limit of this difference for finite size samples with boundary Γ_b and enclosed area A. We find

$$E=\oint_{\Gamma_b}T\vec{n}\cdot(\vec{U}-\vec{U}_0)d\ell+\tfrac{1}{2}\int\int_A(\sigma_{ij}^0e_{ij}^0-\sigma_{ij}e_{ij})dA, \qquad (30)$$

where σ_{ij}^0 and e_{ij}^0 are the stresses and strains of the equilibrium elastic state of the uncracked material $\vec{U}_0$; σ_{ij} and e_{ij} are the stresses and strains of the elastic state of material with the straight cut and displacement field $\vec{U}$; and $\vec{n}$ is a unit normal pointing outwards from the regularization boundary Γ_b. The first integral in Eq. (30) describes the work of the external traction and the second one accounts for the change in the elastic deformation energy. We rewrite the energy release (30) making use of the decomposition $\vec{U}=\vec{U}_g+\vec{U}_c$ to obtain

$$\begin{aligned}E=&\oint_{\Gamma_b}T\vec{n}\cdot(\vec{U}_g-\vec{U}_0)d\ell+\tfrac{1}{2}\int\int_A(\sigma_{ij}^0e_{ij}^0-\sigma_{ij}^ge_{ij}^g)dA\\&-\tfrac{1}{2}\int\int_A\sigma_{ij}^ce_{ij}^cdA+\oint_{\Gamma_b}T\vec{n}\cdot\vec{U}_cd\ell\\&-\tfrac{1}{2}\int\int_A(\sigma_{ij}^ge_{ij}^c+\sigma_{ij}^ce_{ij}^q)dA. \qquad (31)\end{aligned}$$

The first two integrals in Eq. (31) give the energy release for the elastic state $\vec{U}_g$. According to our decomposition this energy release is maximum for given $g_x(x)$ and $g_y(x)$, and thus can not increase linearly by tuning $\vec{U}_c$. The latter is true only if the last two integrals on the right-hand side of Eq. (31)—linear in $\vec{U}_c$—cancel each other. This decoupling can be verified explicitly: integrating by parts and using the fact that $\vec{U}_g$ is an equilibrium state, we find

$$\oint_{\Gamma_b} T\vec{n}\cdot\vec{U}_c d\ell - \tfrac{1}{2}\int\int_A (\sigma^g_{ij}e^c_{ij}+\sigma^c_{ij}e^g_{ij})dA = -\tfrac{1}{2}\oint_{\Gamma_h}\vec{F}_h\cdot\vec{U}_c \tag{32}$$

where the integration on the right-hand side of Eq. (32) is over the cut contour. The force $\vec{F}_h$ applied at the cut boundary of the state $\vec{U}_g$ must be antisymmetric (to have an antisymmetric displacement discontinuity), while by definition, the displacements at the cut for the state $\vec{U}_c$ are symmetric. The latter means that the right-hand side of Eq. (32) vanishes identically. From Eqs. (31) and (32),

$$\begin{aligned} E = &\oint_{\Gamma_b} T\vec{n}\cdot(\vec{U}_g-\vec{U}_0)d\ell \\ &+\tfrac{1}{2}\int\int_A (\sigma^0_{ij}e^0_{ij}-\sigma^g_{ij}e^g_{ij})dA \\ &-\tfrac{1}{2}\int\int_A \sigma^c_{ij}e^c_{ij}dA, \end{aligned} \tag{33}$$

the energy factors, and the last term representing the continuous degrees of freedom, do not ‘‘feel’’ the presence of the cut and thus will have exactly the same spectrum as that of the uncracked material.

This decoupling is more subtle than we are pretending here, and depends upon how one describes the continuous medium on a microscopic scale—the regularization. We will discuss this in Sec. IV, where we will show that decoupling is perfect in the ‘‘split atom’’ lattice regularization.

From Clapeyron’s theorem [18], the elastic energy of the uncracked material is given by

$$\tfrac{1}{2}\int\int_A \sigma^0_{ij}e^0_{ij}dA = \tfrac{1}{2}\oint_{\Gamma_b} T\vec{n}\cdot\vec{U}_0 d\ell. \tag{34}$$

The elastic energy of the material with the cut is determined by

$$\tfrac{1}{2}\int\int_A \sigma^g_{ij}e^g_{ij}dA = \tfrac{1}{2}\oint_{\Gamma_b} T\vec{n}\cdot\vec{U}_g d\ell + \tfrac{1}{2}\oint_{\Gamma_h}\vec{F}_h\cdot\vec{U}_g d\ell. \tag{35}$$

Following Eqs. (33)–(35), we find the energy release E_g,

$$E_g = \tfrac{1}{2}\oint_{\Gamma_b} T\vec{n}\cdot(\vec{U}_g-\vec{U}_0)d\ell - \delta E, \tag{36}$$

where

$$\delta E = \tfrac{1}{2}\oint_{\Gamma_h}\vec{F}_h\cdot\vec{U}_g d\ell. \tag{37}$$

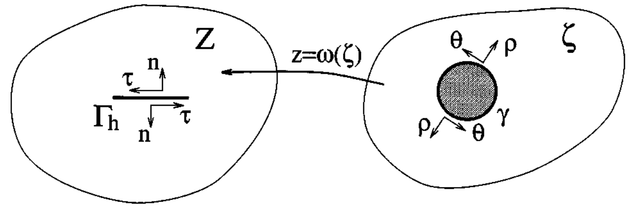

FIG. 5. The determination of the holomorphic functions describing the equilibrium elastic state of the material with a straight cut is simplified in the conformal plane ζ, where the unit circle γ corresponds to cut boundary Γ_h in the original z plane.

In the spirit of Sec. II, the equilibrium elastic state $\vec{U}_g$ can be described by the analytical functions $\phi(z)$ and $\psi(z)$; $\phi_0(z)=\phi(z)-Tz/2$ and $\psi(z)$ are holomorphic in the extended complex z plane excluding the straight cut, and are constrained to provide the displacement discontinuity (g_x, g_y). In [13] the integral in Eq. (36) has been identified in Muskhelishvili’s variables with Eq. (3). The energy release E_g is then smaller than the one given by Eq. (3) by δE,

$$E_g = -\frac{\pi T}{4\mu}(1+\chi)\mathrm{Re}[y^g_1] - \delta E, \tag{38}$$

where y^g_1 is the $1/z$ coefficient in the expansion of $\psi(z)$ at infinity.

To determine the functions $\phi_0(z)$ and $\psi(z)$ we conformally map the complex z plane with the cut to the outside of the unit circle γ (Fig. 5),

$$z=\omega(\zeta)=\frac{\ell}{4}\left(\zeta+\frac{1}{\zeta}\right), \tag{39}$$

so that the unit circle in the ζ plane is mapped to the straight cut boundary Γ_h in the original plane, $\Gamma_h=\omega(\gamma)$.

The elasticity problem is reformulated in the conformal plane as follows: we have to find analytical functions $\phi_g(\zeta)=\phi(\omega(\zeta))$ and $\psi_g(\zeta)=\psi(\omega(\zeta))$, such that $\phi_{g0}(\zeta)=\phi_g(\zeta)-\ell\zeta/4$ and $\psi_g(\zeta)$ are holomorphic in the extended complex ζ plane outside the unit circle and give the maximum energy release with displacement discontinuity (g_x, g_y) at the cut boundary. We introduce

$$g(\sigma)=u_g+iv_g|_\gamma, \tag{40}$$

where $\sigma=\exp(i\alpha)$, $\alpha\in[0,2\pi)$, is a parametrization of the unit circle γ. Since σ and $1/\sigma$ represent opposite points across the cut, Eqs. (28) and (29) require

$$g(\sigma)-g(1/\sigma)=2[g_x(\omega(\sigma))+ig_y(\omega(\sigma))], \quad \alpha\in[0,\pi). \tag{41}$$

It is important to note that the equilibrium elastic state that maximizes the energy release for given displacement discontinuity (g_x, g_y) is unique; on the other hand, Eq. (41) determines only the asymmetric modes $g^{\mathrm{asym}}(\sigma)$ of the crack opening displacement for this state,

$$\begin{aligned} 2g^{\mathrm{asym}}(\sigma) &= [u_g(\sigma)+iv_g(\sigma)]-[u_g(1/\sigma)+iv_g(1/\sigma)] \\ &= 2[g_x(\omega(\sigma))+ig_y(\omega(\sigma))]. \end{aligned} \tag{42}$$

The symmetric modes $g^{\text{sym}}(\sigma)$

$$2g^{\text{sym}}(\sigma)=[u_g(\sigma)+iv_g(\sigma)]+[u_g(1/\sigma)+iv_g(1/\sigma)], \quad (43)$$

left unconstrained by Eq. (41), should then be relaxed to provide the maximum energy release for given $g^{\text{asym}}(\sigma)$. Thus, to calculate the energy release E_g of the elastic state $\vec{U}_g$ we first find the energy release $E(g)=E(g^{\text{asym}}+g^{\text{sym}})$ for the equilibrium state with an arbitrary displacement along the cut boundary $g(\sigma)$, and then maximize the result with respect to g^{sym}

$$E_g=\max_{g^{\text{sym}}}E(g^{\text{asym}}+g^{\text{sym}}). \quad (44)$$

In what follows we will use $\phi_\zeta(\zeta)$ and $\psi_\zeta(\zeta)$ to describe the equilibrium elastic state with an arbitrary displacement $g(\sigma)$ along the cut boundary and tension T at infinity. [The energy release for arbitrary $g(\sigma)$ is still given by Eqs. (37) and (38).] Making the change of variables $z\to w(\zeta)$ in Eq. (2) and putting $\zeta=\sigma$, we obtain a constraint on $\phi_\zeta(\zeta)$ and $\psi_\zeta(\zeta)$ that guarantees the displacements along γ to be $g(\sigma)$,

$$\chi\phi_\zeta(\sigma)-\frac{\omega(\sigma)}{\overline{\omega'(\sigma)}}\overline{\phi'_\zeta(\sigma)}-\overline{\psi_\zeta(\sigma)}=2\mu g(\sigma). \quad (45)$$

Once the solution (ϕ_ζ,ψ_ζ) of the elasticity problem is found, we can compute correction (37) to the energy release. Introducing the polar coordinates (ρ,θ) (Fig. 5) in the complex ζ plane, $\vec{F}_h=F_\rho\vec{\rho}+F_\theta\vec{\theta}$ and $\vec{U}_g=v_\rho\vec{\rho}+v_\theta\vec{\theta}$, and, using $d\ell=|\omega'(\sigma)||d\sigma|$, we find

$$\begin{aligned}\delta E&=\tfrac{1}{2}\oint_\gamma(F_\rho v_\rho+F_\theta v_\theta)|\omega'(\sigma)||d\sigma|,\\ &=\tfrac{1}{2}\oint_\gamma(\sigma_{\rho\rho}v_\rho+\sigma_{\rho\theta}v_\theta)|\omega'(\sigma)||d\sigma|,\end{aligned} \quad (46)$$

where in the second equality we express the force through the stress tensor components: $F_\rho=\sigma_{\rho\rho}$ and $F_\theta=\sigma_{\rho\theta}$. The stress tensor components $\sigma_{\rho\rho}$ and $\sigma_{\rho\theta}$ are given in terms of the $\phi_\zeta(\zeta)$ and $\psi_\zeta(\zeta)$ functions that, as we already mentioned, completely determine the equilibrium elastic state. Muskhelishvili finds [10]

$$\begin{aligned}\sigma_{\rho\rho}-i\sigma_{\rho\theta}=&\frac{\phi'_\zeta(\zeta)}{\omega'(\zeta)}+\frac{\overline{\phi'_\zeta(\zeta)}}{\overline{\omega'(\zeta)}}-\frac{\zeta^2}{\rho^2\overline{\omega'(\zeta)}}\Bigg\{\frac{\overline{\omega(\zeta)}}{\omega'(\zeta)}\phi''_\zeta(\zeta)\\ &-\frac{\overline{\omega(\zeta)}\omega''(\zeta)}{\omega'(\zeta)^2}\phi'_\zeta(\zeta)+\psi'_\zeta(\zeta)\Bigg\}.\end{aligned} \quad (47)$$

Noting that the transformation of the displacements along the unit circle in the Cartesian coordinates (u_g,v_g), $g=u_g+iv_g$, to the polar coordinates (v_ρ,v_θ), is [10]

$$v_\rho+iv_\theta=\frac{1}{\sigma}\frac{\overline{\omega'(\sigma)}}{|\omega'(\sigma)|}(u_g+iv_g)=\frac{1}{\sigma}\frac{\overline{\omega'(\sigma)}}{|\omega'(\sigma)|}g(\sigma), \quad (48)$$

we conclude, from Eq. (46), that

$$\begin{aligned}\delta E&=\tfrac{1}{2}\text{Re}\oint_\gamma(\sigma_{\rho\rho}-i\sigma_{\rho\theta})(v_\rho+iv_\theta)|\omega'(\sigma)||d\sigma|\\ &=\tfrac{1}{2}\text{Re}\oint_\gamma(\sigma_{\rho\rho}-i\sigma_{\rho\theta})\frac{\overline{\omega'(\sigma)}}{\sigma}g(\sigma)\frac{d\sigma}{i\sigma},\end{aligned} \quad (49)$$

where $\sigma_{\rho\rho}-i\sigma_{\rho\theta}$ is given by Eq. (47) with $\zeta\to\sigma$ $(\rho\to1)$. From Eqs. (38) and (49) we find the energy release $E(g)$,

$$\begin{aligned}E(g)=&-\frac{\pi T}{4\mu}(1+\chi)\text{Re}[y_1(g)]\\ &-\tfrac{1}{2}\text{Re}\oint_\gamma(\sigma_{\rho\rho}-i\sigma_{\rho\theta})\frac{\overline{\omega'(\sigma)}}{\sigma}g(\sigma)\frac{d\sigma}{i\sigma},\end{aligned} \quad (50)$$

where $y_1(g)$ is the $1/z$ coefficient in the expansion of $\psi_\zeta(\omega^{-1}(z))$ at $z=\infty$.

The equilibrium elastic problem for material with the straight cut allows a closed analytical solution for the arbitrary specified displacement $g(\sigma)$ along the unit circle in the conformal plane ζ. Using the fact that $\phi_{\zeta_0}(\zeta)$ and $\psi_\zeta(\zeta)$ are holomorphic functions outside the unit circle that satisfy Eq. (45), Muskhelishvili finds [10]

$$\begin{aligned}\phi_\zeta(\zeta)=&\frac{T\ell\zeta}{8}-\frac{2\mu}{\chi}\frac{1}{2\pi i}\oint_\gamma\frac{g(\sigma)d\sigma}{\sigma-\zeta}+\frac{T\ell}{8\chi\zeta},\\ \psi_\zeta(\zeta)=&\frac{\mu}{\pi i}\oint_\gamma\frac{\overline{g(\sigma)}d\sigma}{\sigma-\zeta}+\frac{T\ell}{8}\left(\frac{\chi}{\zeta}-\frac{2\zeta}{\zeta^2-1}\right)\\ &-\zeta\frac{1+\zeta^2}{\zeta^2-1}\left(\phi'_\zeta(\zeta)-\frac{T\ell}{8}\right)-\frac{\mu}{\pi i}\oint_\gamma\frac{\overline{g(\sigma)}d\sigma}{\sigma}.\end{aligned} \quad (51)$$

Assuming that $g(\sigma)$ is smooth, we represent it by a convergent Fourier series

$$g(\sigma)=\sum_{-\infty}^{+\infty}(a_n+ib_n)\sigma^n. \quad (52)$$

Using representation (52) for $g(\sigma)$ we find, from Eq. (50), the energy release E,

$$\begin{aligned}E(g)=&\frac{\pi T\ell(1+\chi)}{4\chi}(a_{-1}+\chi a_1)-2\pi\mu\sum_{n=1}^{+\infty}n\Bigg(a_n^2+b_n^2\\ &+\frac{a_{-n}^2+b_{-n}^2}{\chi}\Bigg)-\frac{\pi T^2\ell^2(1+\chi)}{128\mu}\left(\chi-2+\frac{1}{\chi}\right).\end{aligned} \quad (53)$$

The computations are tedious, but straightforward: first we substitute Eq. (52) into Eq. (51) to find the solution of the elasticity problem in terms of the Fourier amplitudes $\{a_n,b_n\}$, then we calculate the stress tensor components at the unit circle using Eq. (47), and, finally, plugging the result into Eq. (50) we obtain Eq. (53). The next step is to relax the symmetric modes in the crack opening displacement given by $g(\sigma)$. From Eqs. (52) and (40) we find

$$u_g=\sum_{n=1}^{+\infty}(a_n+a_{-n})\cos n\alpha+(b_{-n}-b_n)\sin n\alpha,$$
$$v_g=\sum_{n=1}^{+\infty}(b_n+b_{-n})\cos n\alpha+(a_n-a_{-n})\sin n\alpha, \tag{54}$$

which, with the change of variables

$$u_n=b_{-n}-b_n,$$
$$v_n=a_n-a_{-n},$$
$$\tilde{u}_n=b_n+b_{-n},$$
$$\tilde{v}_n=a_n+a_{-n}, \tag{55}$$

is rewritten as

$$u_g=\sum_{n=1}^{+\infty}\tilde{v}_n\cos n\alpha+u_n\sin n\alpha,$$
$$v_g=\sum_{n=1}^{+\infty}\tilde{u}_n\cos n\alpha+v_n\sin n\alpha. \tag{56}$$

It is clear now that the asymmetric modes of the crack opening displacement are described by $\{u_n,v_n\}$, while the symmetric ones are specified by $\{\tilde{u}_n,\tilde{v}_n\}$. [Recall that points parametrized by σ and $1/\sigma$ (or equivalently α and $-\alpha$) are opposite from one another across the cut.] The amplitudes $\{u_n,v_n\}$ are uniquely determined for the given (g_x,g_y). From Eqs. (42) and (56),

$$g_x(\ell\cos\alpha/2)+ig_y(\ell\cos\alpha/2)=\sum_{n=1}^{\infty}(u_n+iv_n)\sin n\alpha, \tag{57}$$

where $\alpha\in[0,\pi]$. Using the transformation inverse to Eq. (55), we can express the energy release (53) in terms of $\{u_n,v_n,\tilde{u}_n,\tilde{v}_n\}$. The obtained expression is maximum for

$$\tilde{u}_n=u_n\frac{\chi-1}{1+\chi},$$
$$\tilde{v}_n=v_n\frac{1-\chi}{1+\chi},\quad n\neq 1,$$
$$\tilde{v}_1=v_1\frac{1-\chi}{1+\chi}+\frac{T\ell(\chi-1)}{8\mu}, \tag{58}$$

and gives the energy release E_g,

$$E_g=\frac{T\ell\pi}{2}v_1-\frac{2\pi\mu}{\chi+1}\sum_{n=1}^{+\infty}n(u_n^2+v_n^2). \tag{59}$$

Finally, the maximum of Eq. (59) is achieved for

$$u_n^{\max}=0,$$
$$v_n^{\max}=0,\quad n\neq 1,$$
$$v_1^{\max}=\frac{\pi T\ell(1+\chi)}{8\mu} \tag{60}$$

and

$$E_g^{\max}=\frac{\pi T^2\ell^2(1+\chi)}{32\mu}, \tag{61}$$

which, as one might expect, corresponds to the equilibrium opening of the cut [10] and the energy release associated with this opening, Eq. (19). Expanding Eq. (59) about $\{u_n^{\max},v_n^{\max}\}$, $\{u_n,v_n\}\to\{u_n^{\max}+u_n,v_n^{\max}+v_n\}$, we find

$$E_g=\frac{\pi T^2\ell^2(1+\chi)}{32\mu}-\frac{2\pi\mu}{1+\chi}\sum_{n=1}^{+\infty}n(u_n^2+v_n^2). \tag{62}$$

Expression (62) is the desired result: we find that the crack opening displacements (specified on the unit circle in the conformal plane)

$$\{u,v\}=\left\{v_n\frac{1-\chi}{1+\chi}\cos n\alpha+u_n\sin n\alpha,u_n\frac{\chi-1}{1+\chi}\cos n\alpha+v_n\sin n\alpha\right\} \tag{63}$$

imposed on the saddle point cut opening

$$\{u^{\max},v^{\max}\}=\left\{0,\frac{\pi T\ell(1+\chi)}{8\mu}\sin\alpha\right\} \tag{64}$$

diagonalize the energy release, and thus are the normal modes; with the excitation of the nth normal mode with the amplitude $\{u_n,v_n\}$ the energy release decreases by $2\pi\mu n(u_n^2+v_n^2)/(1+\chi)$.

Although Eq. (59) has been derived for the material under uniform isotropic stretching at infinity, it can be reinterpreted to describe the minimum increase in the energy ΔE of the material under a uniform isotropic compression (pressure) P at infinity, due to the opening of the straight cut with a specified displacement discontinuity along its boundary. For the displacement discontinuity given by Eq. (57), we find, similar to Eq. (59),

$$\Delta E=\frac{P\ell\pi}{2}v_1+\frac{2\pi\mu}{\chi+1}\sum_{n=1}^{+\infty}n(u_n^2+v_n^2). \tag{65}$$

One can use the same arguments that lead to Eq. (33) to show that the crack opening normal modes (63) decouple from all continuous modes (that are present in the uncracked material) and thus leave their spectrum unchanged. The saddle point is, however, unphysical in this case: as follows from Eq. (64) [T in Eq. (64) should be replaced with $-P$], it corresponds to a configuration where the material overlaps itself.

IV. IMAGINARY PART OF THE PARTITION FUNCTION

Elastic materials at finite temperature undergo a phase transition to fracture at zero applied stress, similar to the first-order phase transition in spin systems below the critical temperature at zero magnetic field. The free energy of an elastic material under a stretching load develops an imaginary part which determines the material lifetime with respect to fracture. The imaginary part of the free energy has an essential singularity at zero applied stress. In this section we calculate this singularity at low temperatures in a saddle point approximation, including quadratic fluctuations.

Consider an infinite two-dimensional elastic material subject to a uniform isotropic stretching T at infinity. Creation of a straight 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, the cut will open up because of elastic relaxation. Using Eq. (61) for the energy release, we find the total energy $E(\ell)$ of the straight cut in equilibrium under stretching tension T,

$$E(\ell)=2\alpha\ell-\frac{\pi T^2\ell^2(1+\chi)}{32\mu}. \tag{66}$$

Introducing

$$\ell_c=\frac{32\mu\alpha}{\pi T^2(1+\chi)}, \tag{67}$$

we can rewrite the energy of the crack as

$$E(\ell)=2\alpha\ell-\alpha\frac{\ell^2}{\ell_c}. \tag{68}$$

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 [1]. At finite temperature a crack of any size can appear as a thermal fluctuation, which means that for arbitrary small stretching T the true ground state of the system is fractured into pieces, and so the free energy of the material cannot be analytical at $T=0$. Because the energy $E(\ell_c)=\alpha\ell_c$ grows as $1/T^2$ as $T\to 0$, interactions between thermally nucleated cracks are unimportant at small T 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,

$$Z=\sum_{N=0}^{\infty}\sum_{n}\exp(-\beta E_{nN}), \tag{69}$$

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.

To begin with, let us consider the partition function of the material with one cut Z_1,

$$Z_1=\sum_E \exp(-\beta E), \tag{70}$$

where the summation is over all energy states of the material with a single cut. 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 explicitly show in Sec. II that curving a cut reduces the energy release). For now we neglect all fluctuations of the critical droplet (the cut of length ℓ_c) except for its uniform contraction or expansion—fluctuations in the length of the straight cut. Introducing the deviation $\Delta\ell$ in the cut length from the critical length ℓ_c, $\Delta\ell=\ell-\ell_c$, we find, from Eq. (68),

$$E=\alpha\ell_c-\alpha\frac{\Delta\ell^2}{\ell_c}. \tag{71}$$

The fact that this degree of freedom has a negative eigenvalue means that direct computation of the partition function yields a divergent result. A similar problem for the three-dimensional Ising model was solved by Langer [19]: one has to compute the partition function in a stable state $P=-T$ (compression), 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 [4]: the situation is similar to that of barrier tunneling in quantum mechanics [20], where the imaginary part in the energy gives the decay rate of a resonance. We have explicitly implemented this prescription for the simplified calculation of the imaginary part of the free energy [9]: for the elastic material under a uniform isotropic compression at infinity, allowing for the nucleation of straight cuts of an arbitrary length with an arbitrary elliptical opening [mode v_1 in Eq. (65)], we calculated the free energy in a dilute gas approximation. We carefully performed the analytical continuation to the metastable state describing the elastic material under the uniform isotropic stretching T at infinity, and found the imaginary part of the free energy,

$$\mathrm{Im}F^{\mathrm{simple}}(T)=\frac{2}{\beta^2 T\lambda^2}\left(\pi\frac{A}{\lambda^2}\right)\exp\left\{\frac{-32\beta\mu\alpha^2}{\pi T^2(\chi+1)}\right\}, \tag{72}$$

where A is the area of the material and λ is the ultraviolet cutoff of the theory. [The version of Eq. (72), as derived in [9], overcounts the contribution from zero-restoring-force modes ($2\pi A/\lambda^2$) by factor 2. Because cracks tilted by θ and $\pi+\theta$ are identical, the proper contribution from rotations must be π, rather than 2π.]

The alternative to this analytical continuation approach is to deform the integration contour over the amplitude of the unstable (negative eigenvalue) mode from the saddle point $\Delta\ell=0$ along the path of the steepest descent [19]. More precisely, we regularize the direct expression for the partition function

$$Z_1=Z_0\left(\pi\frac{A}{\lambda^2}\right)\int_{-\ell_c}^{\infty}\frac{d\Delta\ell}{\lambda}\exp\left\{-\beta\left(\alpha\ell_c-\alpha\frac{\Delta\ell^2}{\ell_c}\right)\right\} \tag{73}$$

(which diverges at big $\Delta\ell$) by bending the $\Delta\ell$ integration contour from the saddle into the complex plane:

$$Z_1 = Z_0\left(\pi\frac{A}{\lambda^2}\right)\int_{-\ell_c}^{0}\frac{d\Delta\ell}{\lambda}\exp\left\{-\beta\left(\alpha\ell_c - \alpha\frac{\Delta\ell^2}{\ell_c}\right)\right\} + Z_0\left(\pi\frac{A}{\lambda^2}\right)\exp(-\beta\alpha\ell_c)\int_{0}^{\pm i\infty}\frac{d\Delta\ell}{\lambda}\exp\left\{\beta\alpha\frac{\Delta\ell^2}{\ell_c}\right\}. \quad (74)$$

In Eqs. (73) and (74) the factor $(\pi A/\lambda^2)$ comes from the zero-restoring-force modes for rotating and translating the cut, and Z_0 is the partition function for the uncracked material (unity for the present simplified calculation). The second integral in Eq. (74) generates the imaginary part of the partition function

$$\mathrm{Im}Z_1 = \pm\tfrac{1}{2}Z_0\left(\pi\frac{A}{\lambda^2}\right)\exp(-\beta\alpha\ell_c)\left(\frac{\pi\ell_c}{\beta\alpha\lambda^2}\right)^{1/2}, \quad (75)$$

with the $\pm$ sign corresponding to the analytical continuation to either side of the branch cut of the partition function. [We showed in [9] that the partition function, at least for the system without fluctuations, is an analytical function in complex T with a branch cut along the line $T\in[0,+\infty)$.] In a dilute gas approximation the partition function for the material with N cuts Z_N is given by

$$Z_N = Z_0\frac{(Z_1/Z_0)^N}{N!}, \quad (76)$$

which from Eq. (69) determines the material free energy

$$F = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\ln\sum_{N=0}^{\infty}Z_N = -\frac{1}{\beta}\ln Z_0 - \frac{1}{\beta}\frac{Z_1}{Z_0}. \quad (77)$$

Following Eqs. (75) and (77) we find the imaginary part of the free energy,

$$\mathrm{Im}F^{\mathrm{simple}}(T) = \pm\frac{2}{\beta^2 T\lambda^2}\left(\frac{2\beta\mu\lambda^2}{\chi+1}\right)^{1/2}\left(\pi\frac{A}{\lambda^2}\right)\times\exp\left\{\frac{-32\beta\mu\alpha^2}{\pi T^2(\chi+1)}\right\}. \quad (78)$$

Equation (78) differs from Eq. (72) only because for the calculation of the imaginary part of the free energy in [9] we used two degrees of freedom: the length of the cut and its elliptical opening, while in the current calculation there is only one degree of freedom. One can immediately restore Eq. (72) by adding the v_1 mode of Eq. (62) to the energy of the elastic material (71) and integrating it out. From Eq. (62), the v_1 mode generates an additional multiplicative contribution Z_{v_1} to the partition function for a single crack Z_1, and thus from Eq. (77) changes the imaginary part of the free energy for multiple cracks F^{simple}, $\mathrm{Im}F^{\mathrm{simple}}\to Z_{v_1}\mathrm{Im}F^{\mathrm{simple}}$,

$$Z_{v_1} = \int_{-\infty}^{+\infty}\frac{dv_1}{\lambda}\exp\left\{-\frac{2\pi\mu\beta}{1+\chi}v_1^2\right\} = \left(\frac{1+\chi}{2\mu\beta\lambda^2}\right)^{1/2}, \quad (79)$$

which cures the discrepancy between Eqs. (78) and (72). Although the analytical continuation method is theoretically more appealing, the calculation of the imaginary part through the deformation of the integration contour of the unstable mode is more convenient once we include the quadratic fluctuations. It is clear that both methods (properly implemented) must give the same results.

We have already emphasized that the above calculation ignores the quadratic fluctuations about the saddle point (except for the uniform contraction or extension of the critical droplet), which may change the prefactor in expression (78) for the imaginary part of the free energy, and may renormalize the surface tension α. There are three kinds of quadratic fluctuations we have to deal with. (I) *Curvy cuts*—changes in the shape of the tear in the material: deviations of the broken bonds from a straight-line configuration. (II) *Surface phonons*—fluctuations of the free surface of the crack about its equilibrium opening. (III) *Bulk phonons*—fluctuations of the elastic medium that are continuous at the cut boundary. Just as for the surface phonon coordinate v_1 above, we integrate over these fluctuations about the saddle point critical crack, keeping terms in the energy difference to quadratic order. We trace over all shapes and deformations in three steps: we trace over bulk modes, fixing the shape of the tear (the ''curvy crack'' of broken bonds) and fixing the shape of the crack surface (the ''surface phonons''), we then trace over the surface phonons, and finally we trace over the shapes of the tear, the location of the crack, and superpositions of many cracks.

In all cases the answer will depend upon the microscopic lattice-scale structure of the material. In field-theory language, our theory needs regularization: we must decide exactly how to introduce the ultraviolet cutoff λ. Here we discuss the lattice regularization, where the cutoff is explicitly introduced by the interatomic distance, and ζ-function regularization, common in field theory. We find that the precise form of the surface tension renormalization and the prefactor in the imaginary part of the free energy depends on the regularization prescription, but certain important quantities appear regularization independent.

The partition function of the elastic material, with one cut Z_1 in the saddle point approximation (74), will develop a multiplicative factor Z_f upon inclusion of the quadratic fluctuations $Z_1\to Z_f Z_1$ with

$$Z_f = \sum_{\Delta E}\exp(-\beta\Delta E). \quad (80)$$

A deviation ΔE from the saddle point energy is decomposed into three parts, with each part describing fluctuations of one of the above-mentioned three types,

$$\Delta E = \frac{\alpha\ell_c^2}{\pi^2\lambda}\sum_{n=1}^{\infty}\frac{1}{n^2}c_n^2 + \frac{2\pi\mu}{1+\chi}\sum_{n=1}^{\infty}n(u_n^2+v_n^2) + \Delta E_{\mathrm{continuous}}. \quad (81)$$

The first term in Eq. (81) accounts for the decrease in the energy release due to the curving of the saddle point cut of length ℓ_c with the curvature

$$k(x)=\sum_{n=1}^{\infty} c_n\left(\frac{2\lambda}{\ell_c}\right)^{1/2}\sin\frac{\pi n x}{\ell_c}, \quad x\in[0,\ell_c]. \tag{82}$$

The first term in Eq. (81) follows from Eq. (27) with $l=l_c$ given by Eq. (67). The second term in Eq. (81) describes the asymmetric modes in the fluctuations of the free surface of the saddle point crack about its equilibrium opening shape

$$u^{\text{asym}}(t)+iv^{\text{asym}}(t)=\sum_{n=1}^{\infty}(u_n+iv_n)\sin n\vartheta, \quad \vartheta\in[-\pi,\pi), \tag{83}$$

where a point at the cut boundary is parametrized by its distance $t=\ell_c(1+\cos\vartheta)/2$ from the cut end; $\vartheta\in[-\pi,0)$ parametrize the lower boundary displacements and $\vartheta\in[0,\pi)$ parametrize the displacements of the upper boundary points. The symmetric modes of the crack opening about its equilibrium opening shape are assumed to relax providing the minimum increase in the elastic energy for a given $\{u_n,v_n\}$. The latter guarantees that all additional modes with the continuous displacement at the cut boundary [the ones which give $\Delta E_{\text{continuous}}$—the last term in Eq. (81) describing the bulk phonons], decouple from $\{c_n,u_n,v_n\}$ and are the same as the ones for the uncracked material. Since the curvature modes $\{c_n\}$ give the equilibrium energy of the curvy cut, the response of the surface phonons to such a curving is already incorporated, so the quadratic fluctuations $\{c_n\}$ can be calculated independently from the quadratic fluctuations $\{u_n,v_n\}$. The latter means that there is no coupling between $\{c_n\}$ and $\{u_n,v_n\}$ modes in Eq. (81), and the spectrum of $\{u_n,v_n\}$ modes is the same as that for the straight cut of length ℓ_c, Eq. (62).

Strictly speaking, this decoupling is not trivial: perfect decoupling depends on the microscopic (lattice size) description of the elastic medium—i.e., the regularization we choose for the crack surface. To see this consider a regularization where an elastic medium is represented by a two-dimensional network of springs. The introduction of the cut can be viewed as splitting atoms (the split atom regularization) or splitting springs (the split spring regularization). In the first case the splitting introduces new degrees of freedom, and, after the antisymmetric surface phonons are removed, one is left with the same number of the bulk degrees of freedom as for the system before splitting. Moreover, it is clear that, in this regularization, the bulk modes are identical to those for the material without the cut: no springs were cut and the atoms are glued back together. This also provides a microscopic interpretation of the ''traction forces at the seam'' discussed in Sec. III: they become internal forces exerted by each of the half atoms onto its partner. The alternative of splitting springs definitely changes the spectrum of the bulk phonons: the bulk modes have fewer degrees of freedom in this regularization than the medium before introducing the cut. In this paper we consider the split atom regularization, which is technically easier to implement. Splitting springs instead of atoms is a more physical regularization, but one imagines that it will simply renormalize (shift) the surface tension and leave our results otherwise unchanged. (This shift is exactly what happens for the split atom and ζ-function regularizations we consider here.)

The last thing we have to settle before the calculation of Z_f is the proper integration measure for the surface phonon modes $\{u_n,v_n\}$. (We argued in the conclusion of Sec. II that the integration measure for the modes c_n is Cartesian—$\Pi_{n=1}^{\infty}dc_n$.) Here we show that because the functional measure in the displacement fields $(u(x,y),v(x,y))$ defined at each point of the material (x,y) is naturally Cartesian—$D[u(x,y)/\lambda]D[v(x,y)/\lambda]$—the integration measure for the modes $\{u_n,v_n\}$ must be of the form $\Pi_{n=1}^{\infty}(1/2\pi)du_ndv_n/\lambda^2$.

An arbitrary elastic displacement field for the material with a curvy cut is defined by specifying its bulk part $(u_{\text{bulk}}(x,y),v_{\text{bulk}}(x,y))$ [point (x,y) can be anywhere except at the cut boundary] and the cut part $(u^+_{\text{cut}}(t),u^-_{\text{cut}}(t),v^+_{\text{cut}}(t),v^-_{\text{cut}}(t))$ [the cut displacements are defined along the cut and are parametrized by the distance $t=\ell_c(1+\cos\vartheta)/2$, $\vartheta\in[0,\pi)$ from the cut end; the $+$ and $-$ superscripts are correspondingly the displacements at the upper and lower boundaries of the cut]. It is helpful to visualize the introduction of the cut into the material as splitting in half each of the atoms of the material along the cut boundary. Then, the bulk part of the displacement field combines degrees of freedom of all atoms left untouched by splitting, and the cut part describes the displacements of the split ones. The original measure is naturally

$$D[u_{\text{bulk}}(x,y)/\lambda]D[v_{\text{bulk}}(x,y)/\lambda]D[u_{\text{cut}}(t)^+u_{\text{cut}}(t)^-/\lambda^2]\times D[v_{\text{cut}}(t)^+v_{\text{cut}}(t)^-/\lambda^2].$$

First we separate the symmetric and asymmetric parts in the crack opening displacement

$$\begin{aligned}u^{\text{asym}}(t)&=\tfrac{1}{2}(u^+_{\text{cut}}(t)-u^-_{\text{cut}}(t)),\\ v^{\text{asym}}(t)&=\tfrac{1}{2}(v^+_{\text{cut}}(t)-v^-_{\text{cut}}(t)),\\ u^{\text{sym}}(t)&=\tfrac{1}{2}(u^+_{\text{cut}}(t)+u^-_{\text{cut}}(t)),\\ v^{\text{sym}}(t)&=\tfrac{1}{2}(v^+_{\text{cut}}(t)+v^-_{\text{cut}}(t)).\end{aligned} \tag{84}$$

Because the Jacobian of the transformation

$$(u_{\text{cut}}(t)^+,u_{\text{cut}}(t)^-,v_{\text{cut}}(t)^+,v_{\text{cut}}(t)^-)\rightarrow(u^{\text{asym}}(t),v^{\text{asym}}(t),u^{\text{sym}}(t),v^{\text{sym}}(t))$$

is constant,

$$\left|\frac{\partial(u_{\text{cut}}(t)^+,u_{\text{cut}}(t)^-,v_{\text{cut}}(t)^+,v_{\text{cut}}(t)^-)}{\partial(u^{\text{asym}}(t),v^{\text{asym}}(t),u^{\text{sym}}(t),v^{\text{sym}}(t))}\right|=\frac{1}{4}, \tag{85}$$

the integration measure remains Cartesian:

$$D[u_{\text{bulk}}(x,y)/\lambda]D[v_{\text{bulk}}(x,y)/\lambda]D[u^{\text{sym}}(t)v^{\text{sym}}(t)/\lambda^2]\times D[u^{\text{asym}}(t)v^{\text{asym}}(t)/4\lambda^2].$$

Now we can combine the bulk and symmetric cut parts of the measure by introducing the continuous displacement fields $(u_c(x,y),v_c(x,y))$ everywhere, including the cut boundary. The integration measure becomes

$$D[u_c(x,y)/\lambda]D[v_c(x,y)/\lambda]D[u^{\text{asym}}(t)v^{\text{asym}}(t)/4\lambda^2].$$

According to our decomposition, we specify the asymmetric cut opening, and find the equilibrium displacement fields that minimize the increase in the elastic energy. In other words, $(u^{\rm asym}(t),v^{\rm asym}(t))$ determine $(u_c^{\rm min}(u^{\rm asym},v^{\rm asym}), v_c^{\rm min}(u^{\rm asym},v^{\rm asym}))$. The transformations

$$\begin{aligned} u_c(x,y) &= u_c^{\rm min}(u^{\rm asym},v^{\rm asym})+\tilde{u}_c(x,y),\\ v_c(x,y) &= v_c^{\rm min}(u^{\rm asym},v^{\rm asym})+\tilde{v}_c(x,y), \end{aligned} \tag{86}$$

then completely decouple the surface phonon modes and the continuous modes that contribute to $\Delta E_{\rm continuous}$ in Eq. (81). The Jacobian of the transformation

$$\begin{aligned} &(u_c(x,y),v_c(x,y),u^{\rm asym}(t),v^{\rm asym}(t))\\ &\quad\to(\tilde{u}_c(x,y),\tilde{v}_c(x,y),u^{\rm asym}(t),v^{\rm asym}(t)) \end{aligned}$$

is unity (the transformation is just a functional shift) and so the measure remains unchanged,

$$D[\tilde{u}_c(x,y)/\lambda]D[\tilde{v}_c(x,y)/\lambda]D[u^{\rm asym}(t)v^{\rm asym}(t)/4\lambda^2].$$

The Fourier transformation (83) is orthogonal, but the Fourier modes are not normalized:

$$\int_0^{\pi} d\vartheta \sin^2 n\vartheta = \frac{\pi}{2}. \tag{87}$$

The latter means that at the final stage of the change of variables $(u^{\rm asym}(t),v^{\rm asym}(t))\to\{u_n,v_n\}$ there appear the Jacobian $\Pi_{n=1}^{\infty}(2/\pi)$, and so we end up with the integration measure $\Pi_{n=1}^{\infty}(1/2\pi)du_n dv_n/\lambda^2$.

From Eqs. (80) and (81), with the proper integration measure over the surface phonon modes, we find

$$\begin{aligned} Z_f &= \prod_{n=1}^{\infty}\int_{-\infty}^{+\infty} dc_n\\ &\quad\times\exp\left\{-\beta\frac{\alpha\ell_c^2}{\pi^2\lambda n^2}c_n^2\right\}\prod_{n=1}^{\infty}\int\int_{-\infty}^{+\infty}\frac{1}{2\pi}\frac{du_n dv_n}{\lambda^2}\\ &\quad\times\exp\left\{-\beta\frac{2\pi\mu n}{1+\chi}(u_n^2+v_n^2)\right\}Z_{\rm continuous}\\ &= \prod_{n=1}^{\infty}\left(\frac{\pi^3\lambda n^2}{\beta\alpha\ell_c^2}\right)^{1/2}\prod_{n=1}^{\infty}\frac{1+\chi}{4\pi\beta\mu\lambda^2 n}Z_{\rm continuous}, \end{aligned} \tag{88}$$

where

$$Z_{\rm continuous}=\sum_{\Delta E_{\rm continuous}}\exp(-\beta\Delta E_{\rm continuous}). \tag{89}$$

Because $\Delta E_{\rm continuous}$ corresponds to the degrees of freedom of the uncracked material (with the same energy spectrum), $Z_{\rm continuous}$ contributes to the partition function Z_0 of the material without the crack, which according to Eq. (77) drops out from the calculation of the imaginary part of the free energy. All the products over n in these expressions diverge: we need a prescription for cutting off the modes at short wavelengths (an ultraviolet cutoff).

First we will consider the ζ-function regularization. In this regularization prescription [21], the infinite product of the type $D=\Pi_{n=1}^{\infty}\lambda_n$ is evaluated by introducing the function $D_\zeta(s)$,

$$D_\zeta(s)=\sum_{n=1}^{\infty}\frac{1}{\lambda_n^s}, \tag{90}$$

so that

$$D=\exp(-D'_\zeta(0)). \tag{91}$$

It is assumed that sum (90) is convergent in some region of the complex s plane, and that it is possible to analytically continue $D_\zeta(s)$ from that region to $s=0$. From Eq. (88) we find

$$Z_f=D_1 D_2 Z_{\rm continuous}, \tag{92}$$

where D_1 and D_2 are obtained, following Eq. (91), from the corresponding ζ functions $D_{1\zeta}(s)$ and $D_{2\zeta}(s)$:

$$\begin{aligned} D_{1\zeta}(s) &= \left(\frac{\beta\alpha\ell_c^2}{\pi^3\lambda}\right)^{s/2}\sum_{n=1}^{\infty}\frac{1}{n^s}=\left(\frac{\beta\alpha\ell_c^2}{\pi^3\lambda}\right)^{s/2}\zeta_R(s),\\ D_{2\zeta}(s) &= \left(\frac{4\pi\beta\mu\lambda^2}{1+\chi}\right)^{s}\sum_{n=1}^{\infty}n^s=\left(\frac{4\pi\beta\mu\lambda^2}{1+\chi}\right)^{s}\zeta_R(-s). \end{aligned} \tag{93}$$

$\zeta_R(s)$ in Eqs. (93) is the standard Riemann ζ function, holomorphic everywhere in the complex s plane except at $s=1$. Noting that $\zeta(0)=-\frac{1}{2}$ and $\zeta'(0)=-(\ln 2\pi)/2$, we find, from Eqs. (91)–(93),

$$Z_f=\left(\frac{4\beta\alpha\ell_c^2}{\pi\lambda}\right)^{1/4}\left(\frac{2\beta\mu\lambda^2}{1+\chi}\right)^{1/2}Z_{\rm continuous}. \tag{94}$$

From Eqs. (77) and (88) we find the imaginary part of the free energy in the ζ-function regularization,

$$\mathrm{Im}F^{\zeta}=\left(\frac{16\beta^3\alpha\mu^2\lambda^5}{\pi(1+\chi)^2}\right)^{1/4}\left(\frac{\ell_c}{\lambda}\right)^{1/2}\mathrm{Im}F^{\rm simple} \tag{95}$$

where $\mathrm{Im}F^{\rm simple}$ is given by Eq. (78).

Second, we consider lattice regularization, which is more elaborate. We represent a curvy cut by $N+1=\ell_c/\lambda$ segments of equal length parametrized by the kink angles $\{\alpha_i\}$, $i\in[1,N]$. With our conventional parametrization of the cut $t=\ell_c(1+\cos\vartheta)/2, \vartheta[-\pi,\pi)$, the asymmetric modes of the crack opening displacements $\{u^{\rm asym}(t),v^{\rm asym}(t)\}$ are linear piecewise approximations for given asymmetric displacements of the "split" kink atoms $\{u_i^{\rm asym},v_i^{\rm asym}\}$, $i\in[1,N]$. More precisely, if t_i and t_{i+1} parametrize the adjacent kinks, we assume

$$\begin{aligned} u^{\rm asym}(t) &= u_i^{\rm asym}+\frac{u_{i+1}^{\rm asym}-u_i^{\rm asym}}{t_{i+1}-t_i}(t-t_i),\\ v^{\rm asym}(t) &= v_i^{\rm asym}+\frac{v_{i+1}^{\rm asym}-v_i^{\rm asym}}{t_{i+1}-t_i}(t-t_i) \end{aligned} \tag{96}$$

for $t\in[t_i,t_{i+1}]$. From the integration measure arguments for the ζ-function regularization, it is clear that the integration measure in this case must be $\Pi_{i=1}^{N}d\alpha_i\Pi_{i=1}^{N}du_i^{\rm asym}dv_i^{\rm asym}/4\lambda^2$. Now we have to write down the lattice regularization of the quadratic deviation ΔE from the saddle point energy (81). From Eqs. (19) and (21), the curving of the critical cut ℓ_c will reduce the energy release by ΔE_c,

$$\Delta E_c=\frac{T^2\pi(1+\chi)\ell_c^2}{32\mu}\sum_{i,j=1}^{N}\alpha_i\alpha_jM_{ij}^c=\alpha\ell_c\sum_{i,j=1}^{N}\alpha_i\alpha_jM_{ij}^c, \tag{97}$$

where

$$M_{ij}^c=-\frac{ij}{(N+1)^2}+\frac{\min(i,j)}{N+1}. \tag{98}$$

From Eq. (81) the surface phonon contribution to ΔE is given by

$$\Delta E_p=\frac{2\pi\mu}{1+\chi}\sum_{n=1}^{+\infty}n(u_n^2+v_n^2), \tag{99}$$

where, from Eq. (83),

$$u_n=\frac{2}{\pi}\int_0^{\pi}d\vartheta u^{\rm asym}(t(\vartheta))\sin n\vartheta,$$
$$v_n=\frac{2}{\pi}\int_0^{\pi}d\vartheta v^{\rm asym}(t(\vartheta))\sin n\vartheta. \tag{100}$$

In principle, for a given piecewise approximation of the asymmetric modes, Eq. (96), determined by $\{u_i^{\rm asym},v_i^{\rm asym}\}$, $i\in[1,N]$, one could calculate the Fourier amplitudes according to Eq. (100), and then plug the result into Eq. (99) to obtain ΔE_p in terms of $\{u_i^{\rm asym},v_i^{\rm asym}\}$. We will use another approach. Using $u^{\rm asym}(0)=u^{\rm asym}(\ell_c)=0$ [with the same equalities for $v^{\rm asym}(t)$], we integrate Eq. (100) by parts to obtain

$$u_n=\frac{2}{\pi}\int_0^{\pi}d\vartheta\frac{du^{\rm asym}(t(\vartheta))}{d\vartheta}\frac{\cos n\vartheta}{n},$$
$$v_n=\frac{2}{\pi}\int_0^{\pi}d\vartheta\frac{dv^{\rm asym}(t(\vartheta))}{d\vartheta}\frac{\cos n\vartheta}{n}. \tag{101}$$

Substituting Eq. (101) into Eq. (99), we find

$$\Delta E_p=\frac{8\mu}{\pi(1+\chi)}\int_0^{\pi}\int_0^{\pi}d\vartheta_1 d\vartheta_2\left[\frac{du^{\rm asym}(\vartheta_1)}{d\vartheta_1}\frac{du^{\rm asym}(\vartheta_2)}{d\vartheta_2}+\frac{dv^{\rm asym}(\vartheta_1)}{d\vartheta_1}\frac{dv^{\rm asym}(\vartheta_2)}{d\vartheta_2}\right]K(\vartheta_1,\vartheta_2), \tag{102}$$

where

$$K(\vartheta_1,\vartheta_2)=\sum_{n=1}^{\infty}\frac{\cos n\vartheta_1\cos n\vartheta_2}{n}. \tag{103}$$

Following [22]

$$\sum_{k=1}^{\infty}\frac{\cos kx}{k}=\frac{1}{2}\ln\frac{1}{2(1-\cos x)}, \tag{104}$$

we find an analytical expression for the kernel, Eq. (103),

$$K(\vartheta_1,\vartheta_2)=-\tfrac{1}{2}\ln 2-\tfrac{1}{2}\ln|\cos\vartheta_1-\cos\vartheta_2|. \tag{105}$$

Finally, introducing M_{ij}^p from

$$\sum_{i,j=1}^{N}(u_i^{\rm asym}u_j^{\rm asym}+v_i^{\rm asym}v_j^{\rm asym})M_{ij}^p=\int_0^{\pi}\int_0^{\pi}d\vartheta_1 d\vartheta_2\left[\frac{du^{\rm asym}(\vartheta_1)}{d\vartheta_1}\frac{du^{\rm asym}(\vartheta_2)}{d\vartheta_2}+\frac{dv^{\rm asym}(\vartheta_1)}{d\vartheta_1}\frac{dv^{\rm asym}(\vartheta_2)}{d\vartheta_2}\right]K(\vartheta_1,\vartheta_2), \tag{106}$$

we obtain

$$\Delta E_p=\frac{8\mu}{\pi(1+\chi)}\sum_{i,j=1}^{N}(u_i^{\rm asym}u_j^{\rm asym}+v_i^{\rm asym}v_j^{\rm asym})M_{ij}^p. \tag{107}$$

To calculate M_{ij}^p we substitute Eq. (96) directly into the right-hand side of Eq. (106), and read off the corresponding coefficient, given by the following three equations:

$$M_{ij}^p=f_2(i,j)+f_2(i+1,j+1)-f_2(i+1,j)-f_2(i,j+1)$$
$$f_2(i,j)=\frac{3}{4}+\frac{1}{(\cos\vartheta_{i-1}-\cos\vartheta_i)(\cos\vartheta_{j-1}-\cos\vartheta_j)}\times[f_1(i,j)+f_1(i-1,j-1)-f_1(i-1,j)-f_1(i,j-1)], \tag{108}$$
$$f_1(i,j)=\begin{cases}\dfrac{(\cos\vartheta_i-\cos\vartheta_j)^2}{4}\ln\left|\sin\dfrac{\vartheta_i-\vartheta_j}{2}\sin\dfrac{\vartheta_i+\vartheta_j}{2}\right|, & \text{if } i\neq j\\ 0 & \text{otherwise,}\end{cases}$$

where $\vartheta_0=0$, $\vartheta_{N+1}=\pi$, and ϑ_i parametrizes the ith kink (kinks are equally spaced in real space)

$$\vartheta_i=\arccos\left(1-\frac{2i}{N+1}\right),\quad i\in[1,N]. \tag{109}$$

From Eqs. (97) and (107) we find the quadratic deviation from the saddle point energy

$$\Delta E=\Delta E_c+\Delta E_p+\Delta E_{\rm continuous}=\alpha\ell_c\sum_{i,j=1}^{N}\alpha_i\alpha_jM_{ij}^c+\frac{8\mu}{\pi(1+\chi)}\sum_{i,j=1}^{N}(u_i^{\rm asym}u_j^{\rm asym}+v_i^{\rm asym}v_j^{\rm asym})M_{ij}^p+\Delta E_{\rm continuous}. \tag{110}$$

Thus the multiplicative factor Z_f to the partition function of the elastic material with one cut in the lattice regularization is given by

$$Z_f=\prod_{n=1}^{N}\int_{-\infty}^{+\infty}d\alpha_n\exp\left\{-\beta\alpha\ell_c\sum_{i,j=1}^{N}\alpha_i\alpha_jM_{ij}^c\right\}\prod_{n=1}^{N}\int\int_{-\infty}^{+\infty}\frac{du_n^{\text{asym}}dv_n^{\text{asym}}}{4\lambda^2}$$
$$\times\exp\left\{-\beta\frac{8\mu}{\pi(1+\chi)}\sum_{i,j=1}^{N}(u_i^{\text{asym}}u_j^{\text{asym}}+v_i^{\text{asym}}v_j^{\text{asym}})M_{ij}^p\right\}Z_{\text{continuous}}$$
$$=\left(\frac{\pi}{\beta\alpha\ell_c}\right)^{N/2}\det{}^{-1/2}M_{ij}^c\left(\frac{\pi^2(1+\chi)}{32\beta\mu\lambda^2}\right)^N\det{}^{-1}M_{ij}^pZ_{\text{continuous}},\qquad(111)$$

where $Z_{\text{continuous}}$ is given by Eq. (89).

The determinant coming from the curvy cuts M_{ij}^c can be calculated analytically. In Sec. II we showed that $\sin\pi nx/\ell$ are eigenvectors of operator (23), the continuous analog of M_{ij}^c. One can explicitly check that for $n\in[1,N]$, vectors $\vec{m}_n=\{\sin\pi ni/(N+1)\}$ are in fact eigenvectors of M_{ij}^c with eigenvalues

$$\lambda_n=\frac{1}{4(N+1)}\sin^{-2}\frac{\pi n}{2(N+1)},\qquad(112)$$

and so

$$\det M_{ij}^c=\prod_{n=1}^{N}\lambda_n=(N+1)^{-(N+1)}.\qquad(113)$$

To obtain Eq. (113), we take the limit $x\to0$ of

$$\sin2(N+1)x=2^{2N+1}\prod_{k=0}^{2N+1}\sin\left(x+\frac{k\pi}{2(N+1)}\right)\qquad(114)$$

[22], to obtain

$$N+1=4^N\prod_{k=1}^{2N+1}\sin\frac{k\pi}{2(N+1)}=4^N\prod_{k=1}^{N}\sin^2\frac{k\pi}{2(N+1)}.\qquad(115)$$

With Eq. (115), the calculation in Eq. (113) becomes straightforward. Recalling that $N+1=\ell_c/\lambda$, we can rewrite Eq. (111) making use of Eq. (113),

$$Z_f=\left(\frac{\beta\alpha\lambda}{\pi}\right)^{1/2}\left(\frac{\pi}{\beta\alpha\lambda}\right)^{\ell_c/2\lambda}\left(\frac{\ell_c}{\lambda}\right)^{1/2}\left(\frac{32\beta\mu\lambda^2}{\pi^2(1+\chi)}\right)^{1/2}$$
$$\times\left(\frac{\pi^2(1+\chi)}{32\beta\mu\lambda^2}\right)^{\ell_c/2\lambda}\det{}^{-1}M_{ij}^pZ_{\text{continuous}}.\qquad(116)$$

Note that the first three factors on the right-hand side of Eq. (116) (coming from the curvy cut fluctuations) have the asymptotic form, $N\to\infty$,

$$\left(\frac{\beta\alpha\lambda}{\pi}\right)^{1/2}\left(\frac{\pi}{\beta\alpha\lambda}\right)^{\ell_c/2\lambda}\left(\frac{\ell_c}{\lambda}\right)^{1/2}\approx N^{c_2}\exp\{c_0+c_1N\},\qquad(117)$$

with $c_0=0$, $c_1=\ln(\pi/\beta\alpha\lambda)/2$ and $c_2=1/2$.

We were unable to obtain an analytical expression for the surface phonon determinant $\det M_{ij}^p$. For $N=2,\ldots,100$ kinks we calculate the determinant numerically and fit its logarithm with $f(N)=p_0+p_1N+p_2\ln N$ (Fig. 6),

$$\det M_{ij}^p=N^{p_2}\exp\{p_0+p_1N\}.\qquad(118)$$

We find $p_0=0.09\pm0.02$, $p_1=0.166\pm0.002$, and $p_2=0.24\pm0.05$. [We expect that the surface phonon fluctuations contribute to Z_f similar to the curvy cut fluctuations (117)—hence the form of the fitting curve for $\det M_{ij}^p$.] From Eqs. (116)–(118),

$$Z_f=\exp\{p_1-p_0\}\left(\frac{32\beta^2\mu\alpha\lambda^3}{\pi^3(1+\chi)}\right)^{1/2}\left(\frac{\ell_c}{\lambda}\right)^{-p_2+1/2}$$
$$\times\left(\frac{\pi^3(1+\chi)\exp\{-2p_1\}}{32\beta^2\mu\alpha\lambda^3}\right)^{\ell_c/2\lambda}Z_{\text{continuous}},\qquad(119)$$

which, following, Eq. (77), gives the imaginary part of the free energy in the lattice regularization

$$\text{Im}F^{\text{lattice}}=\exp\{p_1-p_0\}\left(\frac{32\beta^2\mu\alpha\lambda^3}{\pi^3(1+\chi)}\right)^{1/2}\left(\frac{\ell_c}{\lambda}\right)^{-p_2+1/2}$$
$$\times\left(\frac{\pi^3(1+\chi)\exp\{-2p_1\}}{32\beta^2\mu\alpha\lambda^3}\right)^{\ell_c/2\lambda}\text{Im}F^{\text{simple}},\qquad(120)$$

with $\text{Im}F^{\text{simple}}$ from Eq. (78).

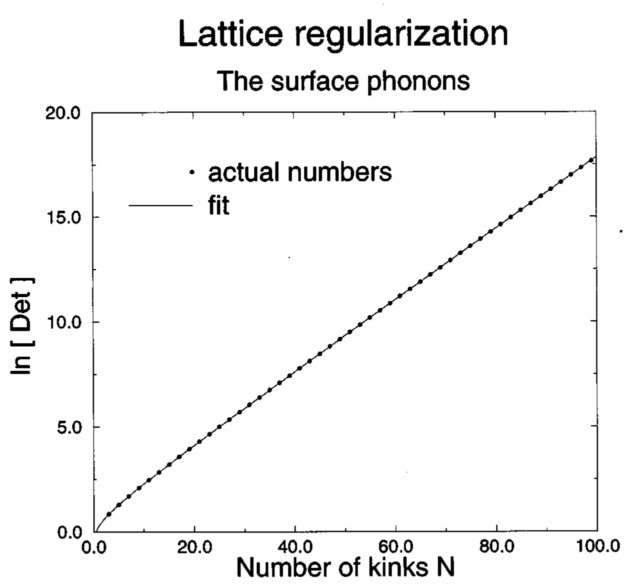

FIG. 6. We numerically calculate the logarithm of the surface phonon determinant $\det M_{ij}^p$, for $N=2,\ldots,100$ kinks, and fit the result with $f(N)=p_0+p_1N+p_2\ln N$.

Throughout the calculation we ignored the kinetic term in the energy of the elastic material: their behavior is rather trivial, as momenta and positions decouple. Because we introduce new degrees of freedom with our ''splitting atoms'' model for the crack, we discuss the effects of the corresponding new momenta. Before ''splitting,'' $(\ell_c/\lambda-1)$ atoms along the cut contribute

$$Z^u_{\text{kinetic}}=\prod_{i=1}^{\ell_c/\lambda-1}\int\int dp_{i_x}dp_{i_y}\left(\frac{\lambda}{2\pi\hbar}\right)^2 \times\exp\left\{-\beta\sum_{j=1}^{\ell_c/\lambda-1}\frac{p_{j_x}^2+p_{j_y}^2}{2m}\right\} \tag{121}$$

to the partition function of the uncracked material Z_0. [We do not consider the contribution to the partition function from the bulk atoms—they contribute in a same way to Z_0 as they do to Z_1, and thus drop out from the calculation of the imaginary part Eq. (77).] The configuration space integration measure for a classical statistical system is $dxdp/2\pi\hbar$; because we integrated out the displacements with the weight $1/\lambda$ to make them dimensionless, the momentum integrals have measure $dp\lambda/2\pi\hbar$, Eq. (121). The formation of the cut increases the number of the kinetic degrees of freedom by $(\ell_c/\lambda-1)$ (the number of split atoms). The split atoms contribute

$$Z^s_{\text{kinetic}}=\prod_{i=1}^{2(\ell_c/\lambda-1)}\int\int dp_{i_x}dp_{i_y}\left(\frac{\lambda}{2\pi\hbar}\right)^2 \times\exp\left\{-\beta\sum_{j=1}^{2(\ell_c/\lambda-1)}\frac{p_{j_x}^2+p_{j_y}^2}{m}\right\} \tag{122}$$

to the partition function of the material with the cut. From Eqs. (77), (121), and (122) the kinetic energy of the elastic material modify the imaginary part of the free energy by a factor Z_k:

$$\text{Im}F^{\text{lattice}}\to Z_k\text{Im}F^{\text{lattice}}, \tag{123}$$

with

$$Z_k=\frac{Z^s_{\text{kinetic}}}{Z^u_{\text{kinetic}}}=\left(\frac{m\lambda^2}{8\pi\beta\hbar^2}\right)^{\ell_c/\lambda-1}. \tag{124}$$

One might notice that for both (ζ function and lattice) regularizations the effect of the quadratic fluctuations can be absorbed into the renormalization of the prefactor of the imaginary part of the free energy calculated in a simplified model (without the quadratic fluctuations), Eq. (78), and the material surface tension α: the multiplicative factor to the imaginary part of the free energy has a generic form

$$\text{Im}F^{\text{simple}}\to n_0\left(\frac{\ell_c}{\lambda}\right)^{n_1}\exp\left\{n_2\frac{\ell_c}{\lambda}\right\}\text{Im}F^{\text{simple}}, \tag{125}$$

where the first two terms renormalize the prefactor of $\text{Im}F^{\text{simple}}$ and the other one can be absorbed into $\text{Im}F^{\text{simple}}$ through the effective renormalization of the surface tension

$$\alpha\to\alpha_r=\alpha+\frac{1}{2\beta\lambda}n_2. \tag{126}$$

From Eqs. (123) and (124) it follows that, in the case of the lattice regularization, the inclusion of the kinetic energy of the elastic material shifts the constants n_0 and n_2, thus preserving Eq. (125):

$$n_0\to n_0\left(\frac{8\pi\beta\hbar^2}{m\lambda^2}\right), \qquad n_2\to n_2+\ln\frac{m\lambda^2}{8\pi\beta\hbar^2}. \tag{127}$$

The calculation of the kinetic terms in the ζ-function regularization is more complicated. However, we have no reason to believe that it will change form (125).

V. ASYMPTOTIC BEHAVIOR OF THE INVERSE BULK MODULUS

In our earlier work [9], we discussed how the thermal instability of elastic materials with respect to fracture under an infinitesimal stretching load determines the asymptotic behavior of the high-order elastic coefficients. Specifically, for the inverse bulk modulus $K(P)$ in two dimensions (material under compression),

$$\frac{1}{K(P)}=-\frac{1}{A}\left(\frac{\partial A}{\partial P}\right)_\beta=c_0+c_1P+\cdots+c_nP^n+\cdots, \tag{128}$$

we found, within linear elasticity and ignoring the quadratic fluctuations,

$$\frac{c_{n+1}}{c_n}\to-n^{1/2}\left(\frac{\pi(\chi+1)}{64\beta\mu\alpha^2}\right)^{1/2} \quad \text{as } n\to\infty, \tag{129}$$

which indicates that the high-order terms c_n roughly grow as $(n/2)!$, and so the perturbative expansion for the inverse bulk modulus is an asymptotic one.

In this section we show that, except for the temperature-dependent renormalization of the surface tension $\alpha\to\alpha_r=\alpha+O(1/\beta)$, Eq. (129) remains true even if we include the quadratic fluctuations around the saddle point (the critical crack); moreover, we argue that Eq. (129) is also unchanged by the nonlinear corrections to the linear elastic theory near the crack tips.

We review how one can calculate the high-order coefficients of the inverse bulk modulus [9]. The free energy $F(T)$ of the elastic material is presumably analytical in the complex T plane function for small T except for a branch cut $T\in[0,+\infty)$—the axis of stretching. (We show this explicitly in the calculation within linear elastic theory without the quadratic fluctuations [9].) It is assumed here that neither nonlinear effects near the crack tips nor the quadratic fluctuations change the analyticity domain of the free energy for reasonably small T (i.e., $T\leqslant Y$). One can then use Cauchy's theorem to express the free energy of the material under compression $F(-P)$ (Fig. 7):

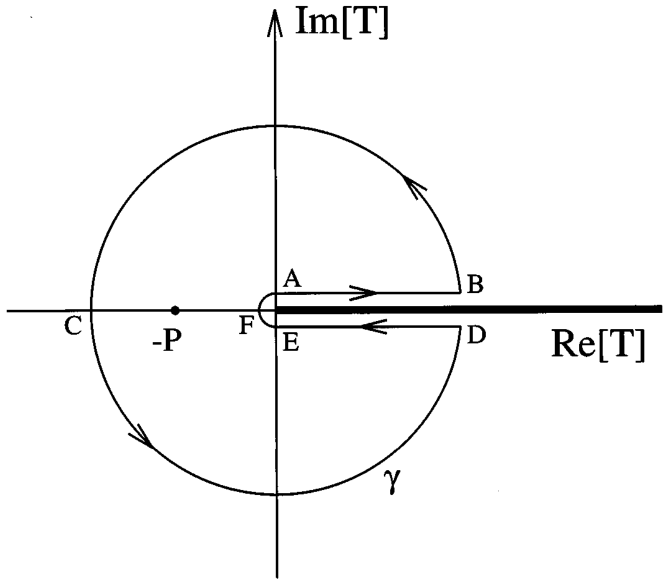

FIG. 7. The free energy of the elastic material $F(T)$ is analytical in the complex T plane except for a branch cut $T\in[0,+\infty)$. This allows a Cauchy representation for the free energy $F(-P)$ of the material under compression.

$$F(-P)=\frac{1}{2\pi i}\oint_\gamma \frac{F(T)}{T+P}dT. \tag{130}$$

The contribution to Eq. (130) from the arc EFA goes to zero as the latter shrinks to a point. In this limit we have

$$\begin{aligned}F(-P)&=\frac{1}{2\pi i}\int_0^B \frac{F(T+i0)-F(T-i0)}{T+P}dT\\&\quad+\frac{1}{2\pi i}\oint_{BCD}\frac{F(T)}{T+P}dT\\&=\frac{1}{\pi}\int_0^B\frac{\mathrm{Im}F(T)}{T+P}dT+\frac{1}{2\pi i}\oint_{BCD}\frac{F(T)}{T+P}dT.\end{aligned} \tag{131}$$

As was first established for similar problems in field theory [23–25], Eq. (131) determines the high-order terms in the expansion of the free energy $F(-P)=\Sigma_n f_n P^n$

$$f_n=\frac{(-1)^n}{\pi}\int_0^B\frac{\mathrm{Im}F(T)}{T^{n+1}}dT+\frac{(-1)^n}{2\pi i}\oint_{BCD}\frac{F(T)}{T^{n+1}}dT. \tag{132}$$

The second integral on the right-hand side of Eq. (132) produces a convergent series; and is hence unimportant to the asymptotics: the radius of convergence by the ratio test is of the order the radius of the circle BCD (i.e., larger than P by construction). The first integral generates the asymptotic divergence of the inverse bulk modulus expansion:

$$f_n\to\frac{(-1)^n}{\pi}\int_0^B\frac{\mathrm{Im}F(T)}{T^{n+1}}dT \quad \text{as} \quad n\to\infty. \tag{133}$$

Once a perturbative expansion for the free energy is known, one can calculate the power series expansion for the inverse bulk modulus using the thermodynamic relation

$$\frac{1}{K(P)}=\frac{1}{PA}\left(\frac{\partial F(-P)}{\partial P}\right)_\beta, \tag{134}$$

so that

$$\frac{c_{n+1}}{c_n}=\frac{(n+3)f_{n+3}}{(n+2)f_{n+2}}. \tag{135}$$

Note that because the saddle point calculation becomes more and more accurate as $T\to 0$, and because the integrals in Eq. (133) are dominated by small T 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. Following Eqs. (78) and (125) the imaginary part of the free energy including the quadratic fluctuations is given by

$$\begin{aligned}\mathrm{Im}F(T)=&\frac{2n_0}{\beta^2T\lambda^2}\left(1-\frac{n_1n_2}{2\beta\lambda\alpha_r}\right)\\&\times\left(\frac{2\beta\mu\lambda^2}{\chi+1}\right)^{1/2}\left(\frac{32\mu\alpha_r}{\pi T^2(\chi+1)\lambda}\right)^{n_1}\left(\pi\frac{A}{\lambda^2}\right)\\&\times\exp\left\{\frac{-32\beta\mu\alpha_r^2}{\pi T^2(\chi+1)}\right\},\end{aligned} \tag{136}$$

where α_r is given by Eq. (126). Note that n_0, n_1, n_2, and α_r in Eq. (136) are regularization dependent coefficients, by our calculations in Sec. IV. From Eqs. (133) and (135) we find

$$\frac{c_{n+1}}{c_n}\to-\left(\frac{\pi(\chi+1)}{32\beta\mu\alpha_r^2}\right)^{1/2}\frac{(n+3)\Gamma(n/2+n_1+2)}{(n+2)\Gamma(n/2+n_1+3/2)}. \tag{137}$$

In the limit $n\to\infty$, Eq. (137) is independent of B in Eq. (133). Using

$$\frac{\Gamma(n/2+n_1+2)}{\Gamma(n/2+n_1+3/2)}\to\left(\frac{n}{2}\right)^{1/2} \quad \text{as} \quad = n\to\infty, \tag{138}$$

we conclude from Eq. (137) that

$$\frac{c_{n+1}}{c_n}\to -n^{1/2}\left(\frac{\pi(\chi+1)}{64\beta\mu\alpha_r^2}\right)^{1/2} \quad \text{as} \quad n\to\infty. \tag{139}$$

Equation (139) is a very powerful result: it shows that apart from the temperature dependent (regularization dependent) correction to the surface tension (126), the asymptotic ratio of the high-order coefficient of the inverse bulk modulus is unchanged by the inclusion of the quadratic fluctuations (at least for the regularizations we have tried). One would definitely expect the surface tension to be regularization dependent: the energy to break an atomic bond explicitly depends on the ultraviolet (short scale) physics, which is excluded in the thermodynamic description of the system. This has analogies with calculations in field theory, where physical quantities calculated in different regularizations give the same answer when expressed in terms of the renormalized masses and charges of the particles [8]. Here only some physical quantities appear regularization independent.

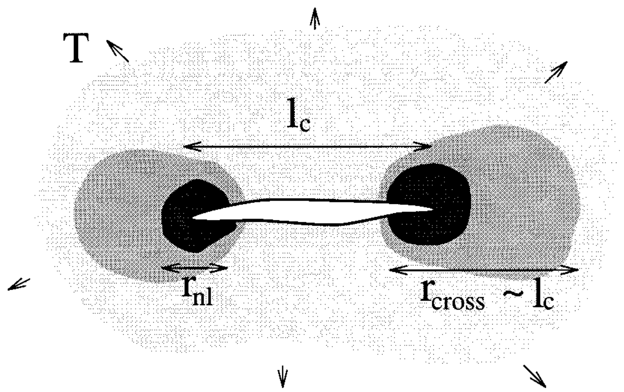

FIG. 8. In the crack system there are two well-defined zones: the outer zone, consisting of exclusively linear elastic material, and the inner, crack tip zone where the nonlinear processes take place. Such separation introduces two length scales: the first (r_{nl}) determines the size of the nonlinear zone, and the second (r_{cross}) gives the scale where the elastic fields near the crack tip deviate from the ones predicted by the SSY approximation to comply with the outer zone boundary conditions.

The analysis that leads to Eq. (139) is based on linear elastic theory that is known to predict unphysical singularities near the crack tips. From [10], the stress tensor component σ_{yy}, for example, has a square root divergence

$$\sigma_{yy} \sim T\left(\frac{\ell_c}{4r}\right)^{1/2} \quad \text{as} \quad r \to 0 \tag{140}$$

as one approaches the crack tip. One might expect that the proper nonlinear description of the crack tips changes the asymptotic behavior of the high-order elastic coefficients. We argue here that linear analysis gives, however, the correct asymptotic ration (139): the *linear* elastic behavior dominates the *nonlinear* asymptotics within our model.

It is clear that the vital question is how the energy release of the saddle point (critical) crack is changed by nonlinear processes (microcracking, emission of dislocations, etc.) in the vicinity of the crack tips as $T \to 0$. Following [26], in the crack system we distinguish two well-defined zones: the outer zone, consisting of exclusively linear elastic material, transmits the applied traction to the inner, crack tip zone where the nonlinear processes take place (Fig. 8). Such separation introduces two length scales to the problem: r_{nl} and r_{cross}. The first scale determines the size of the nonlinear process zone near the crack tips. It can be readily estimated from Eq. (140) by requiring the stresses at the boundary of the nonlinear zone to be of the order atomic ones $\sigma_{ij} \sim Y$:

$$r_{nl} \sim \ell_c\left(\frac{T}{Y}\right)^2 \sim \frac{\alpha}{Y}. \tag{141}$$

The second length scale is a crossover length r_{cross}, where the elastic fields near a crack tip deviate from the inner zone $\sqrt{r}$ strain asymptotics to depend on the outer-zone boundary conditions (i.e., the length of the crack in our case). Normally, r_{cross} is only a few times smaller than the crack length [15,27]—for the present calculation we assume $r_{cross} \sim \ell_c \sim Y\alpha/T^2$, Eq. (67).

First, let us consider the energy in the nonlinear zone. The saddle point energy is $\alpha \ell_c$, and diverges as $1/T^2$ as $T \to 0$, while the elastic energy in the nonlinear zone E_{nl} is bounded by the linear value

$$E_{nl} \sim \int_0^{r_{nl}} dr\, r\, \sigma_{ij}^2(r)/Y \sim \alpha^2/Y. \tag{142}$$

Since E_{nl} is fixed as $T \to 0$, it renormalizes n_0 in Eq. (125), and hence does not affect the asymptotics, Eq. (139).

Second, we consider how the existence of the inner (nonlinear) zone changes the energy in the outer (linear) zone. The elastic equations around the crack tip allow many solutions [27]; in each, the stresses σ_{ij} have the form $C_b r^b f_b(\theta)$, $r_{nl} \ll r \ll r_{cross}$, in polar coordinates (r,θ) centered at the crack tip, where b is a half integer, the C_b are constants, and the f_b are known trigonometric functions. Linear fracture mechanics predicts $b = -\frac{1}{2}$ to be the most singular solution [compare with Eq. (140)] only because modes with $b < -\frac{1}{2}$ would give rise to singular displacements at the crack tip. Incorporation of the nonlinear zone $r < r_{nl}$, however, removes this constraint. In other words, the nonlinear zone introduces new boundary conditions for linear elasticity solutions, allowing them to be more singular. The dominance of $b = -\frac{1}{2}$ solution is known as the small scale yielding (SSY) approximation. Analyzing the mode III antiplane shear fracture, Hui and Ruina argued [28] that the SSY approximation becomes more and more accurate as $\epsilon = r_{nl}/r_{cross} \to 0$. (They expect that the same result can be extended for mode I fracture.) Clearly, in our case $\epsilon \to 0$ as $T \to 0$; thus the dominant contribution still comes from $b = -\frac{1}{2}$ solution. In fact, following [27] we expect

$$\sigma_{ij}\{C_n\} = T\left[C_{-1/2}\left(\frac{\ell_c}{r}\right)^{1/2} + \sum_{n=\{\ldots,-7/2,-5/2,-3/2\}} C_n\left(\frac{r}{r_{nl}}\right)^n + \sum_{n=\{1/2,3/2,5/2,\ldots\}} C_n\left(\frac{r}{\ell_c}\right)^n\right]. \tag{143}$$

The inelastic stresses at the outer boundary of the nonlinear zone $r \sim r_{nl}$ are of order Y, thus, from Eq. (143), for $n < -\frac{1}{2}$, $C_n = O(\epsilon^{-1/2})$ (recall that $\epsilon = r_{nl}/r_{cross} \sim (T/Y)^2$]. These more singular terms in turn generate corrections to C_n with $n \geq \frac{1}{2}$ of order $O(\epsilon)$. [One can see this from the fact that the dominant contribution from the more singular terms at $r \sim \ell_c$ is $C_{-3/2}(\ell_c/r_{nl})^{-3/2} \sim \epsilon$.] The dependence of C_n in Eq. (143) on the polar angle θ is implied.

There is a formal analogy between the arguments presented here for the stress fields in the crossover zone with the quantum mechanical problem of the bound states of the hydrogen atom. When we treat the hydrogen nucleus as a point charge, for each orbital quantum number, the electron wave function has two solutions near the origin (the position of the nucleus): one is finite as $r \to 0$, and the other one is divergent [29,30]. In a point charge problem one immediately discards the divergent solution because it cannot be normalized, and thus cannot represent a bound state. However, in a finite-size nucleus model one notices that the electron wave function outside the nucleus is a mixture of the finite and the divergent solutions of the point charge problem. The normalization is resolved because inside the nucleus the electron wave function satisfies a different equation and becomes finite. The radius of the nucleus serves as a short-distance cutoff similar to $r_{\rm nl}$ in the crack problem.

The change in the contribution to the saddle point energy from the outer zone as a result of the introduction of the nonlinear zone, $\delta E_{\rm outer}$, is given by

$$\delta E_{\rm outer} \sim \int_{r_{\rm nl}}^{\ell_c} dr\, r \frac{\sigma_{ij}^2\{C_n\} - \sigma_{ij}^2\{C_n^{\rm linear}\}}{Y}. \tag{144}$$

The dominant contribution to Eq. (144) comes from the cross term between $n=-\frac{1}{2}$ and $-\frac{3}{2}$ corrections in Eq. (143),

$$\delta E_{\rm outer} \sim \frac{\alpha^2}{Y} \ln \frac{T}{Y}; \tag{145}$$

the correction renormalizes the n_1 coefficient in the imaginary part of the free energy (136) (regularization dependent in a first place), leaving the asymptotic ratio (139) intact.

It is no surprise that the nonlinear effects do not change the generic form of the imaginary part (136). The detailed nonlinear description of the crack tips is a specification of the ultraviolet (short scale) physics, and thus is nothing but another choice of the regularization. From our experience with ζ-function and lattice regularizations, we naturally expect that this *nonlinear* regularization preserves the form of the imaginary part (136).

Finally, let us consider the enhanced nucleation of secondary cracks in the high-strain outer-zone region—a possible cause for breakdown of the ''dilute gas'' approximation. Inside the nonlinear zone of the saddle point crack, the critical crack length for a second crack is of the order α/Y [from Eq. (67) with $T \sim Y$], and thus such microcracks can be easily created. In fact, the nucleation of these microcracks may well be the dominant mechanism of the main crack propagation. Microcrack nucleation in the nonlinear zone will change the stress fields near the crack tips, but, as we discuss above, has little impact on the saddle point energy (as the total energy in the nonlinear zone is finite). We show now that such secondary crack nucleation is exponentially confined to the nonlinear zone of the main crack. The probability $W(r_0)$ of the second crack nucleated somewhere at $r > r_0 \sim r_{\rm nl}$ ($r=0$ corresponds to a crack tip) is given by

$$W(r_0) \sim \int_{r_0}^{+\infty} \frac{r\,dr}{\lambda^2} \exp\{-\beta\alpha\ell(r)\}, \tag{146}$$

where $\ell(r)$ is a critical crack length at distance r from the tip of the critical crack. From Eq. (67), with T replaced with the stress field near the crack tip given by Eq. (140), we find

$$\ell(r) \sim \frac{\alpha Y}{\sigma_{ij}(r)^2} \sim r. \tag{147}$$

Equation (146) with Eq. (147) gives

$$W(r_0) \sim \int_{r_0}^{+\infty} \frac{r\,dr}{\lambda^2} \exp\{-\beta\alpha r\} = \frac{1+\beta\alpha r_0}{(\beta\alpha\lambda)^2} \exp\{-\beta\alpha r_0\}. \tag{148}$$

The exponential dependence of $W(r_0)$ on the boundary of the nonlinear zone $r_0 \sim r_{nl}$ in Eq. (148) means that the nucleation of another crack (in addition to the saddle point one) is exponentially confined to the nonlinear zone, justifying the dilute gas approximation.

VI. OTHER GEOMETRIES, STRESSES, AND FRACTURE MECHANISMS

In this section we discuss generalizations of our model, more exactly its simplified version without the quadratic fluctuations. We will do five things. In Sec. VI A we calculate the imaginary part of the free energy for arbitrary uniform loading, and find high-order nonlinear corrections to Young's modulus. We discuss the effects of dislocations and vacancy clusters (voids) in Secs. VI B and VI C. Section VI D deals with three-dimensional fracture through the nucleation of penny-shaped cracks: we calculate the imaginary part of the free energy and the asymptotic ratio of the successive coefficients of the inverse bulk modulus. Finally, in Sec. VI E we consider a nonperturbative effect: the vapor pressure of a solid gas of bits fractured from the crack surfaces, and show how it affects the saddle point calculation.

A. Anisotropic uniform stress and high-order corrections to Young's modulus

We calculated the essential singularity of the free energy at zero tension only for uniform *isotropic* loads at infinity. Within the approximation of ignoring the quadratic fluctuations, we can easily generalize to any uniform loading. In general, consider an infinite elastic material subject to a uniform asymptotic tension with $\sigma_{\rm yy}=T$, $\sigma_{\rm xx}=\epsilon T$ $(0 \leqslant \epsilon < 1)$, and $\sigma_{\rm xy}=0$. Using the strain-stress analysis of [10] and following Eqs. (2) and (3), we find the energy $E_{\rm release}$, released from the creation of the straight cut of length ℓ tilted by angle θ from the x axis,

$$E_{\rm release} = \frac{\pi T^2 \ell^2 (1+\chi)}{64\mu}[(1+\epsilon)+(1-\epsilon)\cos 2\theta]. \tag{149}$$

The isotropic result (19) is restored for $\epsilon=1$. The important feature that comes into play is that the crack rotation ceases to be a zero-restoring-force mode. Treating the crack rotation to quadratic order in θ from the saddle point value $\theta=0$, we obtain the total energy of the crack $E(\Delta\ell,\theta)$, similar to Eqs. (66)–(68) and (71),

$$E(\Delta\ell,\theta) = \alpha\ell_c - \frac{\alpha\Delta\ell^2}{\ell_c} + \alpha\ell_c(1-\epsilon)\theta^2. \tag{150}$$

As before, $\Delta\ell$ is the deviation of the crack length from the saddle point value ℓ_c, still given by Eq. (67). Following Eqs. (73)–(77), the imaginary part of the free energy for a dilute gas of straight cuts, excluding all quadratic fluctuations except for the uniform contraction-expansion (mode $\Delta\ell$) and the rotation (mode θ) of the critical droplet, is given by

$$\mathrm{Im}F^{\mathrm{simple}}(T,\epsilon)=\pm\frac{\pi}{2\beta^2\alpha\lambda}\left(\frac{A}{\lambda^2}\right)\times\left(\frac{1}{1-\epsilon}\right)^{1/2}\exp\left\{\frac{-32\beta\mu\alpha^2}{\pi T^2(\chi+1)}\right\}. \tag{151}$$

One immediately notices an intriguing fact: the ϵ dependence of the imaginary part is only in the prefactor, which, as we already know is regularization dependent. In particular, the latter means that the inverse Young's modulus—the elastic coefficient corresponding to the transition with path $\epsilon=0$—will have the same asymptotic behavior as that of the inverse bulk modulus (139): the asymptotic ratio of the high-order elastic coefficients of the inverse Young's modulus $Y(P)$

$$\frac{1}{Y(P)}=-\frac{1}{A}\left(\frac{\partial A}{\partial P}\right)_\beta=Y_0+Y_1P+\cdots+Y_nP^n+\cdots \tag{152}$$

[P in Eq. (152) is a uniaxial compression] is given by

$$\frac{Y_{n+1}}{Y_n}\to-n^{1/2}\left(\frac{\pi(\chi+1)}{64\beta\mu\alpha^2}\right)^{1/2}\quad\text{as}\quad n\to\infty. \tag{153}$$

B. Dislocations

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 complications. Dislocations are in principle important: the nucleation [31] barrier E_{dis} for two edge dislocations in an isotropic linear-elastic material under a uniform tension T with equal and opposite Burger's vectors $\vec{b}$ is

$$E_{\mathrm{dis}}=\frac{Yb^2}{4\pi(1-\sigma^2)}\ln\frac{Y}{T}+E_0, \tag{154}$$

where E_0 is a T-independent part that includes the dislocation core energy. The fact that E_{dis} grows like $1/\ln T$ as $T\to 0$ (much more slowly than the corresponding barrier for cracks) tells us that in more realistic models dislocations and the resulting plastic flow [32] 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., crack nucleation on grain boundaries and dislocation tangles) [15,26].

C. Vacancy clusters

We ignore void formation. It would seem natural to associate the negative pressure (tension) $(-T)$ 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 Peredera [33]. If we identify the chemical potential of a vacancy with $-T$, we find the total energy of creation a circular vacancy of radius R, $E_{\mathrm{vac}}(R)$, to be

$$E_{\mathrm{vac}}(R)=2\pi R\alpha-T\pi R^2. \tag{155}$$

From Eq. (155) the radius of the critical vacancy is $R_c=\alpha/T$, and its energy is given by $E_{\mathrm{vac}}(R_c)=\pi\alpha^2/T$. A saddle point is a circular void because a circular void gains the most energy (~ area of the void) for a given perimeter length. In principle, the exact shape of the critical cluster is also affected by the elastic energy release. However,

$$E_{\mathrm{release}}(R_c)=\frac{\pi T^2R_c^2(3\chi+1)}{8\mu}=\frac{\pi\alpha^2(3\chi+1)}{8\mu} \tag{156}$$

is fixed as $T\to 0$, and thus the energy of the vacancy is dominated by $E_{\mathrm{vac}}(R_c)$ for small T. [To obtain Eq. (156) we used the strain-stress analysis of [10] and expression (3) for the energy release.] Using the framework developed for the crack nucleation, we find that, in the case of voids (again, ignoring the positive frequency quadratic fluctuations) the imaginary part of the free energy is given by

$$\mathrm{Im}F^{\mathrm{simple}}_{\mathrm{vacancy}}(T)=\pm\frac{1}{2\beta}\left(\frac{A}{\lambda^2}\right)\left(\frac{1}{\beta T\lambda^2}\right)^{1/2}\exp\left\{\frac{-\pi\beta\alpha^2}{T}\right\}. \tag{157}$$

The special feature of calculation (157) is that translations are the only zero modes: the rotation of a circular vacancy cluster does not represent a new state of the system. From Eq. (157) we obtain, following Eqs. (132) and (135), the asymptotic ratio of the high-order coefficients of the inverse bulk modulus,

$$\frac{c_{n+1}}{c_n}\to-\frac{n}{\pi\beta\alpha^2}. \tag{158}$$

The divergence of the inverse bulk modulus is much stronger in this case: the high-order coefficients grow as $c_n\sim n!$, rather than as $(n/2)!$ (for the fracture through the crack nucleation).

Whether (158) is a realistic result is an open question. Fracture through vacancy cluster nucleation is an unlikely mechanism for highly brittle materials: the identification of μ with $(-T)$ demands a mechanism for relieving elastic tension by the creation of vacancies. The only bulk mechanism for vacancy formation is dislocation climb, which must be excluded from consideration — the dislocations in highly brittle materials are immobile [26]. Vacancy clusters might be important for the fracture of ductile (nonbrittle) materials. However, the nucleation of vacancies must be considered parallel with the nucleation of dislocations. Because at small T dislocations are nucleated much more easily [Eq. (154)] than vacancy clusters at low stresses, the dominant bulk mode of failure is much more likely to be crack nucleation at a dislocation tangle or grain boundary—as indeed is observed in practice.

D. Three-dimensional fracture

Our theory can be extended to describe a three-dimensional fracture transition as well. Studying elliptical cuts, Sih and Liebowitz [13] found that a penny-shaped cut in a three-dimensional elastic medium subject to a uniform isotropic tension T relieves the most elastic energy for a given area of the cut. The energy to create a penny-shaped cut of radius R, $E_{\text{penny}}(R)$, is given by [13]

$$E_{\text{penny}}(R)=2\pi\alpha R^2-\frac{4(1-\sigma)R^3T^2}{3\mu}. \tag{159}$$

The zero modes contribute in this case a factor $2\pi V/\lambda^3$ — 2π coming from the distinct rotations of the cut, and V/λ^3 coming from the translations of the cut. Here we find the imaginary part of the free energy to be

$$\mathrm{Im}F^{\text{simple}}_{\text{penny}}(T)=\pm\frac{1}{2\beta}\left(2\pi\frac{V}{\lambda^3}\right)\left(\frac{1}{2\beta\alpha\lambda^2}\right)^{1/2}\times\exp\left\{\frac{-2\beta\mu^2\pi^3\alpha^2}{3(1-\sigma)^2T^4}\right\}, \tag{160}$$

and the asymptotic ratio of the high-order elastic coefficients of the inverse bulk modulus

$$\frac{c_{n+1}}{c_n}\to-\left(\frac{3(1-\sigma)^2}{2\beta\mu^2\pi^3\alpha^2}\right)^{1/4}\left(\frac{n}{4}\right)^{1/4}. \tag{161}$$

E. Vapor pressure

The approach we used to calculate the imaginary part of the free energy is a perturbative one. In a sense, nothing prohibits us from considering cubic, quartic, etc. deviations from the saddle point energy. In fact, it is possible to develop an analog of Feynman diagram technique (as in quantum electrodynamics [29] or quantum field theory [8]) and calculate the contribution to the imaginary part to any finite order. It is important to realize that, even if we do this, the result would still be incomplete: we would miss interesting and important physics coming from nonperturbative effects. Here we discuss one such nonperturbative effect, namely, the ''vapor'' pressure of a solid gas of bits fractured from the crack surface. We find that including the vapor pressure, the essential singularity shifts from $T=0$ to $T=-P_{\text{vapor}}$. Consider a dilute gas of straight cuts of arbitrary length with an elliptical opening [mode v_1 in Eq. (59)] and a solid gas of fractured bits from the crack surface. Following [9], the partition function of the material with one cut Z_1 under a uniform isotropic tension T is

$$Z_1=Z_0\left(\pi\frac{A}{\lambda^2}\right)\int_0^\infty\frac{d\ell}{\lambda}\int_0^\infty\frac{dv_1}{\lambda}\times\exp\left\{-\beta\left(2\alpha\ell+\frac{2\pi\mu}{\chi+1}v_1^2-\frac{\pi T\ell}{2}v_1\right)\right\}Z_{\text{gas}}(\ell,v_1), \tag{162}$$

where $Z_{\text{gas}}(\ell,v_1)$ is the partition function of the gas of fractured bits inside the crack of area $\pi\ell v_1/2$. It costs $2\alpha\lambda$ to fracture one bit of size $\lambda\times\lambda$ from a crack step, so, in an ideal gas approximation, the partition function of the gas is determined by

$$Z_{\text{gas}}(\ell,v_1)=\sum_{n=0}^{\infty}\exp(-2\beta\alpha\lambda N)\left(\frac{\pi\ell v_1}{2\lambda^2}\right)^N\frac{1}{N!}=\exp\left\{\frac{\pi\ell v_1}{2\lambda^2}\exp(-2\beta\alpha\lambda)\right\}. \tag{163}$$

From Eqs. (162) and (163), it follows that the partition function of the gas effectively increases the tension T by the vapor pressure P_{vapor}, $T\to T+P_{\text{vapor}}$, where

$$P_{\text{vapor}}=\frac{1}{\beta\lambda^2}\exp(-2\beta\alpha\lambda). \tag{164}$$

In particular, the essential singularity of the free energy shifts from zero tension to minus the ''vapor'' pressure. This shift is clearly a nonperturbative effect. We were able to describe it only by allowing topologically different excitations in the system: a state of the elastic material with a bit completely detached from the crack surface *may not* be obtained by the continuous deformation of the crack surface (surface phonons) or the cut shape (curvy cuts). At zero external pressure, our material is in the gas (fractured) phase—not until P_{vapor} is the solid stable.

VII. SUMMARY

In this paper we studied the stress-induced phase transition of elastic materials under external stress: an elastic ''phase'' under positive pressure goes to a fractured ''phase'' under tension. Under a stretching load the free energy develops an imaginary part with an essential singularity at vanishing tension. To calculate the essential singularity of the free energy including quadratic fluctuations, we determined the spectrum and normal modes of surface fluctuations of a straight cut, and proved that under uniform isotropic tension a curvy cut releases the same elastic energy (to cubic order) as a straight one with the same end points. The imaginary part of the free energy determines the asymptotic behavior of the high-order nonlinear correction to the inverse bulk modulus [9]. We find that although the prefactor and the renormalization of the surface tension are both regularization dependent (once we include the quadratic fluctuations), the asymptotic ratio of the high-order successive coefficients of the inverse bulk modulus apparently is a regularization-independent result.

Within our model, the asymptotic ratio is unchanged by the inclusion of nonlinear effects near the crack tips. We generalized the simplified model (without the quadratic fluctuations) to anisotropic uniform strain, and calculated the asymptotic behavior of the high-order nonlinear coefficients of the inverse Young's modulus. We computed the imaginary part of the free energy (and the corresponding divergence of the high-order coefficients of the inverse bulk modulus) for fracture via void nucleation (which dominates at small external pressures): we argue that it may not occur in brittle fracture and should be preempted by dislocation motion in ductile fracture. We find that the simplified model applied to three-dimensional fracture predicts a $(n/4)!$ divergence of the nonlinear coefficients of the inverse bulk modulus.

Our results can be viewed as a straightforward extension to the solid-gas sublimation point of Langer [19,4] and Fisher's [3] 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 $P=0$, as noted in Sec. VI E. 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.

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