Solution of Kramers' problem for a moderately to heavily damped elastic string

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We obtain the nucleation rate of critical droplets for an elastic string moving in a double-well potential and subject to noise and damping forces. We obtain this rate for a class of potentials that includes both the asymmetric ϕ^4 and the ϕ^6 potentials. The frequencies of small oscillations about the critical droplet are obtained from a Heun equation. We solve the Fokker-Planck equation for the phase-space probability density by projecting onto the eigenfunction basis. We present a comparison with simulations for the case of the asymmetric ϕ^4 potential.

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The calculation of the thermal decay rate for a system in a metastable state, separated by high-energy barriers from neighboring lower-energy stable states, has a long history [1] but remains active today [2]. The decay process is described by the nucleation of droplets of the stable phase appearing in the surrounding background of the metastable phase. In a celebrated early paper [3], Kramers calculated this rate for a system described by a single (reaction) coordinate; this quantity was needed to understand thermal dissociation rates of molecules. The same problem, generalized to higher-dimensional phase spaces, has subsequently arisen in many different fields, including condensation of liquid from supersaturated vapor [4], cosmological phase transitions [5], and protein folding [6]. Langer gave a general formulation of the theory [7] and major reviews [8,9] were written to commemorate the 50th anniversary of Kramers' paper.

A specific application and line of development of nucleation theory has been to the motion of dislocations in crystals. This work was initiated by Seeger and collaborators [10] and by Hirth and Lothe [11] with important contributions from others, e.g., [12–14]. The dislocation is modeled as a one-dimensional continuum elastic string, which is under tension, moving in an asymmetric local potential, and subject to damping and noise forces arising from contact with a heat bath. The dislocation moves through the crystal by nucleation of bound soliton-antisoliton pairs in its displacement field $u(x,t)$.

In the present paper, we give a nearly exact calculation of this soliton-antisoliton nucleation rate, for moderate to large damping, and for a *class* of local potentials that includes those most used in theories of first-order phase transitions. We do this by relating the problem to a solution of a Heun equation [15–18], and by using the eigenvalues and eigenfunctions from the Heun equation to solve the appropriate Fokker-Planck equation (FPE).

Our equation of motion for the transverse displacement $u(x,t)$ of a one-dimensional string is the stochastic partial differential equation (PDE) (subscripts denote partial derivatives, primes denote differentiation with respect to the argument, all quantities are dimensionless [19]),

$$u_{tt}-c_0^2u_{xx}+V_1'(u)=-\gamma u_t+\zeta(x,t). \tag{1}$$

The damping and noise forces are from a heat bath at temperature T. c_0 is a characteristic velocity, $\gamma>0$ is a damping constant, and $\zeta(x,t)$ is a random force density with zero-mean, Gaussian distribution, and δ-function correlations in both space and time proportional to $T\gamma$. [We also use the deterministic equation of motion (DEOM), which is Eq. (1) with zero on the right.] We give the rate calculation for a class of local potentials indexed by a parameter $K>0$,

$$V_1(u)=\frac{1}{2}au^2-\frac{1}{3}u^{K+2}+\frac{1}{4}u^{2K+2}. \tag{2}$$

This class includes both the asymmetric ϕ^4 ($K=1$) and ϕ^6 ($K=2$) potentials; both of these have been extensively used, e.g., in Landau-Ginzburg theories, to describe first-order phase transitions. The "shape parameter" a lies in the interval $0<a<2/9$ for all K. For these values of a, $V_1(u)$ has a metastable minimum at $u=0$ separated by a local maximum from a stable minimum at a value $u_{\min}>0$. At $a=\frac{2}{9}$, all the minima of $V_1(u)$ are degenerate. Previous calculations of the nucleation rate have only been for $K=1$ and have been further restricted either to small asymmetry ($a\approx\frac{2}{9}$) and/or to large damping ($\gamma\to\infty$). Our method is not subject to these restrictions.

The critical droplet extremizes the static energy and so is a solution of the equation

$$\frac{\delta}{\delta u(x)}\int_{-\infty}^{\infty}dx\left[\frac{1}{2}c_0^2u_x^2+V_1(u)\right]=-c_0^2u_{xx}+V_1'(u)=0, \tag{3}$$

which is the static limit of the DEOM. In addition, the critical droplet satisfies boundary conditions of being nearly everywhere equal to the uniform metastable solution, $u(x)\equiv 0$, but with a single localized fluctuation over the maximum and into the stable well of $V_1(u)$. The solution is

$$u_b(x)=\left\{\sqrt{\frac{a}{2}}[\tanh(X_+)-\tanh(X_-)]\right\}^{1/K}, \tag{4}$$

where $X_\pm=\sqrt{a}(x\pm x_0)/(2c_0)$. This "bounce" [20] solution is a soliton and an antisoliton separated by $2x_0(a)=c_0/(\sqrt{a})\ln\{[(\sqrt{2}/3)+\sqrt{a}]/[(\sqrt{2}/3)-\sqrt{a}]\}$, which ap-

proaches infinity as $a \to 2/9$. The energy of the bounce E_b is obtained by using Eq. (4) to evaluate the energy integral in Eq. (3) [21]. There is a family of degenerate solutions of Eq. (3) obtained by translating Eq. (4).

We demonstrate that $u_b(x)$ is a saddle point on the energy surface over the phase space of solutions of the DEOM and then calculate the nucleation rate from the spectrum of small oscillations about it. To investigate the stability of the bounce, we substitute $u(x,t)=u_b(x)+\phi(x)e^{i\omega t}$ into the DEOM and linearize with respect to ϕ. We obtain a Schrödinger equation,

$$\phi''+[4\lambda(a)-v(y)]\phi=0, \tag{5}$$

where $y=[K\sqrt{a}/(2c_0)]x$, the eigenvalue in terms of the frequency is $4\lambda(a)=4(\omega^2/a-1)/K^2$,

$$v(y)=-\frac{2(K+1)(K+2)(\nu+1)\operatorname{sech}^2 y}{K^2(\nu-\tanh^2 y)} + \frac{4(K+1)(2K+1)\nu \operatorname{sech}^4 y}{K^2(\nu-\tanh^2 y)^2}, \tag{6}$$

and $\nu(a)=[1+\sqrt{1-9a/2}]/[1-\sqrt{1-9a/2}]$. Depending on a, the "potential energy" in Eq. (6) has one or two attractive wells and is asymptotic to zero at large $|y|$, so the spectrum has discrete bound states with negative eigenvalues $\lambda(a)$ [or $\omega^2<a$] and a continuum of positive eigenvalues [or $\omega^2>a$]. Since the DEOM is a nonlinear Klein-Gordon equation, the derivative of the bounce is a solution of Eq. (5) with $\omega^2(a)=0$ [or $\lambda(a)=-1$] (the "translation mode") [22]. The bounce has even parity, its derivative has odd parity, and consequently the translation mode is not the ground state of Eq. (5). There must be a solution with $\omega^2(a)<0$, which implies that the bounce is unstable [23].

To solve Eq. (5) we change the independent variable to $z=\tanh^2(y)$ ($0<z<1$ for $-\infty<y<\infty$) and obtain a Heun ODE with regular singular points at 0, 1, ∞, and $\nu(a)$. For $0<a<2/9$, $\infty>\nu(a)>1$, so $\nu(a)$ is outside the physical domain of z. We change the dependent variable to $A(z)=z^{\xi}(z-1)^{\mu}(z-\nu)^{\kappa}\phi(z)$ and then find that to put the resulting equation into "normal form" for the Heun equation [17,18] we must choose certain values for the exponents: $\xi=0$ or $-1/2$, $\kappa=(1+1/K)$ or $-(2+1/K)$, and $\mu^2=-\lambda(a)$. The result is

$$\frac{d^2A}{dz^2}+\left(\frac{1/2-2\xi}{z}+\frac{1-2\mu}{z-1}-\frac{2\kappa}{z-\nu}\right)\frac{dA}{dz}+\left\{\left[2\mu\kappa-\frac{3}{2}\kappa +2\kappa\xi+2\mu\xi-\frac{\mu}{2}-\xi+\left(1+\frac{1}{K}\right)\left(2+\frac{1}{K}\right)-\lambda\right]z-2\kappa\xi +\frac{\kappa}{2}-\frac{3}{2}\left(1+\frac{1}{K}\right)+\nu\left[-2\mu\xi+\frac{\mu}{2}+\xi+\lambda+\frac{1}{2}\left(1+\frac{1}{K}\right) \times\left(1+\frac{2}{K}\right)\right]\right\}\frac{A}{z(z-1)(z-\nu)}=0. \tag{7}$$

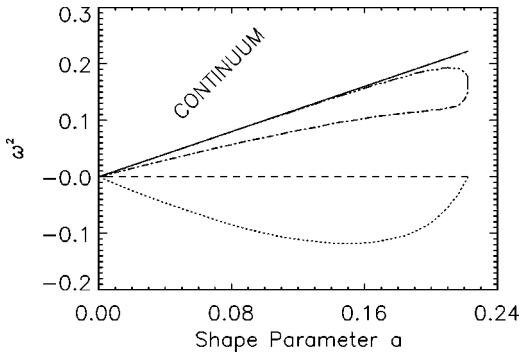

FIG. 1. Squares of small oscillation frequencies for the discrete spectrum for the case $K=1$. The solid line is the $\omega^2=a$ lower limit to the continuum.

We use power series to solve Eq. (7) and obtain a three-term recursion relation, which we convert to a continued fraction and analyze using methods described by Erdelyi [25]. The requirement to obtain a convergent series to a function that approaches zero at large $|y|$ for the bound states determines μ as a function of $\nu(a)$, which then gives values of $\omega^2(a)$ for the bound-state eigenvalues. At this point we specialize to the case $K=1$, because numerical methods must be used to obtain solutions of the continued fraction and because simulation results for nucleation rates are available for this case [26]. The values of $\omega^2(a)$ for the bound-state eigenvalues are shown in Fig. 1. For a general value of a, there are the unstable mode with $\omega_0^2<0$, the translation mode with $\omega_1^2=0$, and two other bound states with $\omega_2^2,\omega_3^2>0$. In addition, there is a continuous spectrum for $\omega^2>a$ [27].

We now use these results to obtain the thermal nucleation rate for the formation of stable phase droplets, adapting techniques described by Langer [7] and by Büttiker and Landauer [28] but not restricted to the overdamped limit. The method is applicable for all $K>0$, but the final results we show are for $K=1$, since we use the eigenvalues shown in Fig. 1. The stochastic PDE in Eq. (1) is equivalent to a functional Fokker-Planck equation (FPE) for the phase-space probability distribution function (PDF) $\rho(\{u,\pi\},t)$ (a functional of the fields), where $\pi(x)$ is the momentum density function,

$$\frac{\partial\rho}{\partial t}=-\int_{-\infty}^{\infty}dx\left\{\frac{\delta}{\delta u(x)}\left[\frac{\delta H}{\delta\pi(x)}\rho+T\frac{\delta\rho}{\delta\pi(x)}\right] +\frac{\delta}{\delta\pi(x)}\left[\left(-\frac{\delta H}{\delta u(x)}-\gamma\frac{\delta H}{\delta\pi(x)}\right)\rho -\gamma T\frac{\delta\rho}{\delta\pi(x)}-T\frac{\delta\rho}{\delta u(x)}\right]\right\}. \tag{8}$$

Here H is the Hamiltonian, which is the kinetic energy $\int dx\,\pi^2/2$ added to the potential energy shown in Eq. (3). Since Eq. (8) is a continuity equation in phase space, at each x there is a displacement $J_{u,x}(\{u,\pi\})$ and a momentum density $J_{\pi,x}(\{u,\pi\})$ component of the probability current, which can be read from the right-hand side.

We solve Eq. (8) subject to the same boundary conditions used by previous authors [8]. Namely, we obtain a steady-state problem ($\partial\rho/\partial t=0$) by imagining that probability is fed back into the metastable well as it flows over the barrier into the stable well. This is accomplished by taking the PDF to approach the equilibrium distribution $\exp(-H/T)$ at the metastable region and to approach zero at the stable region. The restriction that the PDF approach the equilibrium distribution in the metastable well precludes applying our solution to the underdamped case. However, since we solve the FPE on the whole phase space rather than contracting it to just configuration space, our solution is not restricted only to the overdamped limit. We write $\rho=B(\{u,\pi\})\exp(-H/T)$ and rewrite the FPE in terms of B. Next we expand the fluctuations of the displacement and momentum density fields away from the bounce solution in terms of the complete set of eigenfunctions obtained from Eq. (5),

$$u(x,t)=u_b(x)+\sum_n \zeta_n(t)\phi_n(x), \tag{9}$$

$$\pi(x,t)=0+\sum_n \xi_n(t)\phi_n(x). \tag{10}$$

Near the bounce solution in phase space, the Hamiltonian has the diagonalized small oscillation form

$$H[u,\pi]\approx E_b+\frac{1}{2}\sum_n \xi_n^2+\frac{1}{2}\sum_n \omega_n^2\zeta_n^2 \tag{11}$$

in terms of the small oscillation frequencies obtained from the eigenvalues of Eq. (5). We rewrite the divergence in Eq. (8) in terms of components and derivatives along the eigenfunction directions ζ_n, ξ_n, and evaluate H from Eq. (11). In these coordinates the stationary FPE (8) is

$$\sum_n (\partial_{\zeta_n} J_{u,n}+\partial_{\xi_n} J_{\pi,n})=0, \tag{12}$$

and is an infinite-dimensional PDE for B. Next we utilize Kramers' method [3] to collapse this PDE to an ODE, by assuming that B is a function of only the single variable

$$y=\sum_n (R_n\zeta_n+S_n\xi_n). \tag{13}$$

To obtain a normalizable B, it comes out that only R_0 and S_0 can be nonzero. Then B is proportional to an error function normalized by the partition function $Z_{\rm ms}$ for the metastable well in phase space [7]. Correspondingly, the only two nonzero components of the probability current are $J_{u,0}$ and $J_{\pi,0}$. We integrate the current over a surface passing through the saddle point, including an integration over the translation mode, to get the total flux. Our result for the nucleation rate per unit length is

$$\frac{I}{L}=\frac{1}{2(2\pi)^{3/2}}\frac{\gamma}{c_0\sqrt{|\omega_0^2|}\omega_2\omega_3}\times\left[\sqrt{1+\frac{4|\omega_0^2|}{\gamma^2}}-1\right]\cdot\sqrt{\frac{E_b}{T}}e^{-E_b/T}\times\left[\frac{\prod_{n=0}^{\infty}\omega_{ms,n}}{\prod_{n=4}^{\infty}\omega_n}\right]. \tag{14}$$

It is easy to show that the bounce energy E_b is proportional to c_0. Therefore, for each a and γ the results for the nucleation rate fall on a single curve when $c_0 I/L$ is plotted versus c_0/T.

In Eq. (14), the $\omega_{{\rm ms},n}$ are the frequencies of small oscillation about the metastable minimum of the local potential; these enter through the evaluation of $Z_{\rm ms}$ and are obtained from a Klein-Gordon equation. The infinite products go over the continuum spectra for both the bounce and the metastable configurations. We evaluate this ratio by taking its logarithm, then writing ω in terms of the eigenvalue λ introduced earlier, and introducing the densities of states (DOS) $g(\lambda)$ and $g_{\rm ms}(\lambda)$ to convert the resulting sums into integrals, so that

$$\frac{\prod_{n=0}^{\infty}\omega_{{\rm ms},n}}{\prod_{n=4}^{\infty}\omega_n}=a^2 e^{1/2\int_0^\infty d\lambda[g_{ms}(\lambda)-g(\lambda)]\ln(1+\lambda)}. \tag{15}$$

Finally, we evaluate the DOS for the bounce by a WKB technique similar to that used by Büttiker and Landauer [28].

There are two restrictions on the parameters for this theory to be valid. One requires $T\ll E_b$ or $c_0/E_b\ll c_0/T$ so that a critical droplet is distinguishable from thermal motion. Secondly, the boundary condition that the PDF describe thermal equilibrium in the metastable well requires the damping to be greater than a certain minimum magnitude. The restriction is $\gamma>\sqrt{|\omega_0^2|}$ [8].

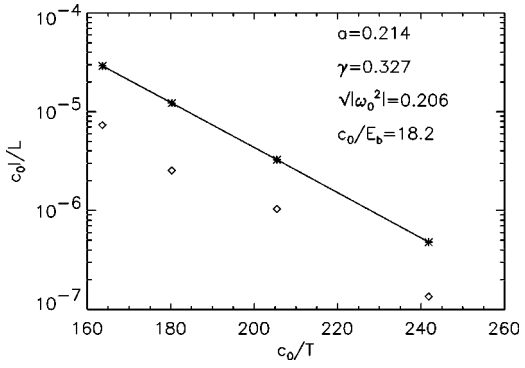

FIG. 2. Comparison of Eq. (14) (asterisks) with rates obtained from computer simulations in [26] (diamonds) for $K=1$ and $a=0.214$. The solid line is to guide the eye.

Simulations of the system described by Eqs. (1) and (2) with $K=1$ have been carried out by Alford, Feldman, and Gleiser [26]. They present results for five different parameter sets for the shape parameter a and damping γ, but only one of their γ values satisfies the restriction given above. [The values of $\omega_0^2(a)$ were not known when [26] was written.] The comparison between our values from Eq. (14) and the simulation results for this one case is shown in Fig. 2. Our results are larger than the simulation values by factors ranging from about 3.2 to 4.8. We suggest two possible sources for the discrepancy. One is our use of an approximate DOS in Eq. (15). If the logarithm factor is omitted from the integral in Eq. (15), the resulting integral of the difference of the DOS's should have the value 4, according to Levinson's theorem. At $a=0.214$, using our approximate DOS the integral is 4.12, which overestimates Levinson's theorem sum rule by a factor of 1.03. The overestimate could be larger for the integral in Eq. (15), because of the logarithmic factor. A second source of differences between our theory and the simulation could be the same reasons that caused differences between theory and simulation for the symmetric ϕ^4 system for the energy dependence of the nucleation rate. These differences were resolved by performing long simulations on large systems [29].

Over the temperature range from the simulations shown in Fig. 2, the exponential factor in Eq. (14) dominates the temperature dependence. In a subsequent paper [19], we will present results for other parameter values and over larger ranges, including the ϕ^6 potential $(K=2)$.

In summary, we have presented a calculation of the nucleation rate for critical droplets of a continuum one-dimensional elastic system moving in a double-well potential. We have shown that the evaluation of the fluctuation spectrum can be related to solving the Heun equation for a class of potentials that includes the ϕ^4 and ϕ^6 functions used for essentially all descriptions of first-order phase transitions. We then solved the functional phase-space Fokker-Planck equation for our system by using the eigenfunctions and eigenvalues from the Heun equation. Our results are exact except for the calculation of the DOS for the continuum spectrum by the WKB method. We have proposed two possible reasons for the differences between our theory and the simulations.

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