Rice's ansatz for overdamped ϕ^4 kinks at finite temperature

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The dynamics of a kink driven by noise is analyzed using the two collective variables of the Rice ansatz: position and width. Starting from a stochastic partial differential equation, with the ϕ^4 potential in the overdamped limit, the pair of stochastic differential equations for the collective variables are derived without approximation other than the ansatz itself. From the steady state probability density of the kink width, the diffusivity of a kink is calculated.

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Extended nonlinear systems often exhibit localized structures, such as moving domain walls, that move about under the influence of perturbations [1–4]. The ϕ^4 equation studied in this work can be used to model such structures in multiple dimensions, but we restrict ourselves to one space dimension, where they are known as kinks [3]. The one-dimensional equation, as well as serving as a general model for a chain of coupled double-well oscillators [5], has been used to model specific physical systems such as the polymer polyacetalene [6], charge-density-wave condensates [7], and Josephson-junction transmission lines [8].

Analytical progress towards understanding the dynamics of kinks can be made using a known exact solution, $\Phi(x)$, of the unperturbed equation that determines the characteristic shape of the structure. An approximate formula or "ansatz" for the configuration at time t is $\phi(x,t)=\Phi(x-X(t))$, where $X(t)$, the position of the center of the structure at time t, is considered as a dynamical variable or "collective coordinate" [9,10].

Although kinks behave like point particles in many circumstances [4,11], it is possible to find signatures of the internal mode of a kink [12] by, for example, adding a periodic perturbation and looking for resonances [13]. The frequency associated with the interval mode has a different physical origin from that associated with the localized periodic modes known as breathers found in some systems [14]. The latter is a bound state of a kink and antikink, whereas the internal mode is present in a single isolated kink.

A simple analytical model for the dynamics of a single kink including the internal mode of a kink is obtained via Rice's ansatz, where the solution is assumed to be of the form $\Phi((x-X(t))/G(t))$ [15]. That is, both the kink width $G(t)$ and position $X(t)$ are collective coordinates.

Rice considered the underdamped, noiseless dynamics of a ϕ^4 field. He derived reduced equations for the kink width and position, and found solutions in which the kink width oscillates [15]. While the solutions he found do not correspond to exact solutions of the partial differential equation, the characteristic frequency found for the oscillations of the kink width is very close to that found in a formal expansion of the solution of the partial differential equation [16]. The latter frequency corresponds to the eigenvalue of the "shape mode" eigenfunction obtained on linearising about a single kink solution [3]. Quantitative predictions, obtained using the Rice ansatz, of resonances in the response of a ϕ^4 field to periodic driving have been confirmed by numerical solutions of the partial differential equation [13,17].

We shall study the overdamped, noisy dynamics governed by the stochastic partial differential equation (SPDE) for a field whose value at position x and time t is denoted by $\boldsymbol{\phi}_t(x)$:

$$\frac{\partial}{\partial t}\boldsymbol{\phi}_t(x)=\boldsymbol{\phi}_t(x)-\boldsymbol{\phi}_t^3(x)+\frac{\partial^2}{\partial x^2}\boldsymbol{\phi}_t(x)+(2kT)^{\frac{1}{2}}\boldsymbol{\eta}_t(x). \tag{1}$$

The last term in Eq. (1) is space-time white noise: $\langle \boldsymbol{\eta}_t(x)\boldsymbol{\eta}_{t'}(x')\rangle=\delta(x-x')\delta(t-t')$; the amplitude of the noise is $(2kT)^{1/2}$, where T has the interpretation of temperature and k of Boltzmann's constant.

The function $\Phi(x)$ is a stationary solution of the unperturbed equation. That is, $\Phi(x)$ satisfies

$$\Phi(x)-\Phi^3(x)+\frac{\partial^2}{\partial x^2}\Phi(x)=0, \tag{2}$$

with the boundary conditions $\Phi(x)\to\pm 1$ as $x\to\pm\infty$. In the case of the ϕ^4 equation, the stationary solution is $\Phi(y)=\tanh(y/\sqrt{2})$. Because the perturbations we consider are stochastic, we implement Rice's ansatz as follows:

$$\boldsymbol{\phi}_t(x)=\Phi\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t}\right). \tag{3}$$

The kink position and width are now stochastic processes whose values at time t are denoted by $\mathbf{X}_t$ and $\mathbf{G}_t$. We shall derive the corresponding pair of coupled stochastic differential equations. The resulting steady state distribution of $\mathbf{G}_t$ and the diffusivity, $D_{\mathrm{r}}=\frac{1}{2}\lim_{t\to\infty}\langle\mathbf{X}_t^2\rangle/t$, will be calculated exactly. The pair of coupled stochastic differential equations (SDEs) for $\mathbf{X}_t$ and $\mathbf{G}_t$ have the form

$$d\mathbf{X}_t=a(\mathbf{X}_t,\mathbf{G}_t)dt+\sigma(\mathbf{X}_t,\mathbf{G}_t)d\mathbf{W}_t^{(\mathrm{x})}, \tag{4}$$

$$d\mathbf{G}_t = b(\mathbf{X}_t, \mathbf{G}_t)dt + \rho(\mathbf{X}_t, \mathbf{G}_t)d\mathbf{W}_t^{(g)}, \tag{5}$$

where $\langle d\mathbf{W}_t^{(x)} d\mathbf{W}_t^{(x)} \rangle = \langle d\mathbf{W}_t^{(g)} d\mathbf{W}_t^{(g)} \rangle = \delta(t-t')dt$. The functions $a(x,g)$, $b(x,g)$, $\sigma(x,g)$ and $\rho(x,g)$, and possible correlations between the Wiener processes $\mathbf{W}_t^{(x)}$ and $\mathbf{W}_t^{(g)}$ are to be determined. We use the Ito convention to perform changes of variables; exactly equivalent results can be obtained using the Stratonovich convention.

In order to carry out the reduction of the SPDE (1), we write, using the notation of stochastic differentials, the SDE for the evolution of the field at a point x:

$$d\boldsymbol{\phi}_t(x) = \left(\boldsymbol{\phi}_t(x) - \boldsymbol{\phi}_t^3(x) + \frac{\partial^2}{\partial x^2}\boldsymbol{\phi}_t(x) \right) dt + (2kT)^{1/2} d\mathbf{B}_t(x), \tag{6}$$

where $\langle d\mathbf{B}_t(x) d\mathbf{B}_{t'}(x') \rangle = \delta(x-x')\,\delta(t-t')dt$. In particular, for a square integrable function $f(x)$,

$$\int_{-\infty}^{\infty} [f(x) d\mathbf{B}_t(x)]dx = \left(\int_{-\infty}^{\infty} f^2(x)dx \right)^{1/2} d\mathbf{W}_t. \tag{7}$$

Because the function $\Phi(y)$ satisfies Eq. (2) and

$$\frac{\partial^2}{\partial x^2}\boldsymbol{\phi}_t(x) = \mathbf{G}_t^{-2}\Phi''\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right), \tag{8}$$

we can rewrite Eq. (6) as

$$d\boldsymbol{\phi}_t(x) = (-1+\mathbf{G}_t^{-2})\Phi''\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right) dt + (2kT)^{1/2} d\mathbf{B}_t(x). \tag{9}$$

We proceed to rewrite the left-hand side of Eq. (9) using ansatz (3), general form (4) and (5) and the Ito formula for change of variables:

$$\begin{aligned} d\boldsymbol{\phi}_t(x) = & -\mathbf{G}_t^{-1}\Phi'\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right) d\mathbf{X}_t \\ & + \frac{1}{2}\mathbf{G}_t^{-2}\Phi''\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right) \sigma^2(\mathbf{X}_t, \mathbf{G}_t)dt \\ & - (x-\mathbf{X}_t)\mathbf{G}_t^{-2}\Phi'\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right) d\mathbf{G}_t \\ & + \frac{1}{2}\Bigg[(x-\mathbf{X}_t)^2\mathbf{G}_t^{-4}\Phi''\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right) \\ & + 2(x-\mathbf{X}_t)\mathbf{G}_t^{-3}\Phi'\left(\frac{x-\mathbf{X}_t}{\mathbf{G}_t} \right) \Bigg] \rho^2(\mathbf{X}_t, \mathbf{G}_t)dt. \end{aligned} \tag{10}$$

Equating Eqs. (9) and (10) gives a differential relation at each space point x. To find an equation for the evolution of the stochastic collective variable $\mathbf{X}_t$, we multiply each equation by $\Phi'[(x-\mathbf{X}_t)/\mathbf{G}_t]$ and integrate over x. Because $\Phi'(y)$ is an even function of y, we obtain

$$d\mathbf{X}_t = \left(\frac{2kT}{E_k}\mathbf{G}_t \right)^{1/2} d\mathbf{W}_t^{(x)}, \tag{11}$$

where

$$E_k = \int_{-\infty}^{\infty} [\Phi'(u)]^2 du = \left(\frac{8}{9} \right)^{1/2}. \tag{12}$$

Comparing with Eq. (4), we find that $a(x,g)=0$ and $\sigma(x,g) = [(2kT/E_k)g]^{1/2}$.

To find the SDE for $\mathbf{G}_t$, we multiply (9) and Eqs. (10) by $(x-\mathbf{X}_t)\Phi'((x-\mathbf{X}_t)/\mathbf{G}_t)$ (an odd function of $x-\mathbf{X}_t$) and integrate over x

$$\begin{aligned} & -\alpha_r E_k \mathbf{G}_t d\mathbf{G}_t - \frac{1}{4}E_k\sigma^2(\mathbf{X}_t, \mathbf{G}_t)dt \\ & \quad + (-\tfrac{3}{4}\alpha_r E_k + \alpha_r E_k)\rho^2(\mathbf{X}_t, \mathbf{G}_t)dt \\ & \quad = -\frac{1}{2}E_k\mathbf{G}_t^2(-1+\mathbf{G}_t^{-2}) + \mathbf{G}_t(2kT\alpha_r E_k \mathbf{G}_t)^{1/2} d\mathbf{W}_t^{(g)}, \end{aligned}$$

where $\langle d\mathbf{W}_t^{(x)} d\mathbf{W}_t^{(g)} \rangle = 0$ and

$$\alpha_r E_k = \int_{-\infty}^{\infty} x^2\Phi'(x)^2 dx = \sqrt{\frac{8}{9}}\left(\frac{\pi^2}{6} - 1 \right) = 0.608\cdots. \tag{13}$$

Thus

$$\begin{aligned} d\mathbf{G}_t = & -\frac{1}{2}\alpha_r^{-1}(\mathbf{G}_t - \mathbf{G}_t^{-1})dt + \frac{1}{4}\mathbf{G}_t^{-1}(-\alpha_r^{-1}\sigma^2(\mathbf{X}_t, \mathbf{G}_t) \\ & + \rho^2(\mathbf{X}_t, \mathbf{G}_t))dt + \left(\frac{2kT}{\alpha_r E_k}\mathbf{G}_t \right)^{1/2} d\mathbf{W}_t^{(g)}. \end{aligned} \tag{14}$$

Inserting

$$\sigma^2(\mathbf{X}_t, \mathbf{G}_t) = \frac{2kT}{E_k}\mathbf{G}_t$$

and

$$\rho^2(\mathbf{X}_t, \mathbf{G}_t) = \frac{2kT}{\alpha_r E_k}\mathbf{G}_t,$$

we obtain

$$d\mathbf{G}_t = -\frac{1}{2}\alpha_r^{-1}(\mathbf{G}_t - \mathbf{G}_t^{-1})dt + \left(\frac{2KT}{\alpha_r E_k}\mathbf{G}_t \right)^{1/2} d\mathbf{W}_t^{(g)}. \tag{15}$$

The pair of SDEs (11) and (15) are the required equations of motion. Note that $d\mathbf{X}_t$ and $d\mathbf{G}_t$ are independent of the kink position at time t, which is a mean zero, Gaussian random variable. To obtain the diffusivity of a kink, we find from Eq. (11),

$$D_r = \frac{1}{2}\lim_{t\to\infty}\frac{\langle \mathbf{X}_t^2 \rangle}{t} = \frac{kT}{E_k}\lim_{t\to\infty}\langle \mathbf{G}_t \rangle. \tag{16}$$

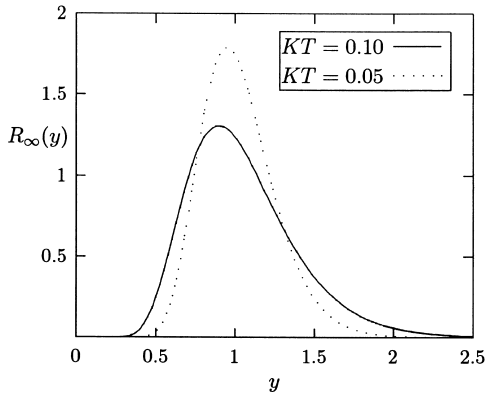

FIG. 1. The steady state density of the kink width $\mathbf{G}_t$ is shown for two values of kT.

The SDE (15) cannot be solved analytically, but we can obtain the statistics of $\mathbf{G}_t$ as $t\to\infty$, which is all that is required to evaluate Eq. (16). Let $R_t(y)$ be the probability density of $\mathbf{G}_t$:

$$R_t(y)=\frac{d}{dy}\mathcal{P}[\mathbf{G}_t<y]. \tag{17}$$

Then, from Eq. (15), the steady state density of $\mathbf{G}_t$ is given by [18]

$$\lim_{t\to\infty} R_t(y)=N^{-1}y^{-1}\exp\left[-\frac{E_k}{2kT}\left(y+\frac{1}{y}\right)\right], \tag{18}$$

where

$$N=\int_0^\infty y^{-1}\exp\left[-\frac{E_k}{2KT}\left(y+\frac{1}{y}\right)\right]dy=2K_0\left(\frac{E_k}{KT}\right). \tag{19}$$

The function K_0 is the modified Bessel function of the second kind of order zero. Note that the constant α_{r} determines the time scale of the evolution of $\mathbf{G}_t$, but does not appear in the steady state density.

The steady state density (18) is peaked close to $\mathbf{G}_t=1$, but is asymmetrical. See Fig. 1. As $t\to\infty$, the mean value for $\mathbf{G}_t$ is given by

$$\begin{aligned}\lim_{t\to\infty}\langle\mathbf{G}_t\rangle&=N^{-1}\int_0^\infty \exp\left[-\frac{E_k}{2kT}\left(y+\frac{1}{y}\right)\right]dy\\&=\frac{K_1\left(\frac{E_k}{kT}\right)}{K_0\left(\frac{E_k}{kT}\right)}\\&=1+\frac{1}{2}\frac{kT}{E_k}-\frac{11}{128}\left(\frac{kT}{E_k}\right)^2+\cdots.\end{aligned} \tag{20}$$

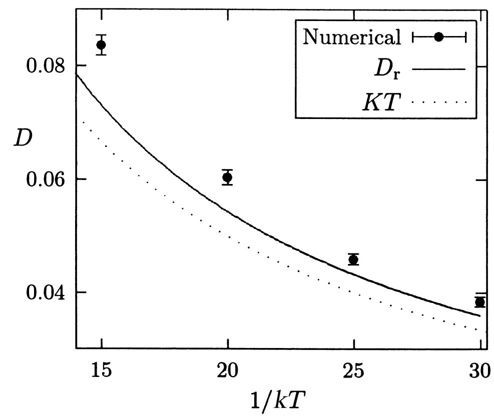

FIG. 2. The diffusivity of a kink under the Rice ansatz (solid line). The dotted line is $1/kT$. Also shown are numerical results, from solution of SPDE (1) with $L=200$.

The mean value of $\mathbf{G}_t$ in the steady state is seen to be larger, by terms in powers of (kT/E_k), than the simplest approximation which is $\mathbf{G}_t=1$. The kink diffusivity under the Rice ansatz is given by

$$\begin{aligned}D_{\mathrm{r}}&=\frac{1}{2}\lim_{t\to\infty}\frac{\langle\mathbf{X}_t^2\rangle}{t}\\&=\frac{kT}{E_{\mathrm{k}}}\lim_{t\to\infty}\langle\mathbf{G}_t\rangle\\&=\frac{kT}{E_k}\frac{K_1\left(\frac{E_k}{KT}\right)}{K_0\left(\frac{E_k}{kT}\right)}\end{aligned} \tag{21}$$

$$=\frac{kT}{E_k}\left(1+\frac{1}{2}\frac{kT}{E_k}-\frac{11}{128}\left(\frac{kT}{E_k}\right)^2+\cdots\right). \tag{22}$$

The kink diffusivity calculated under the simpler "fixed shape" ansatz $\boldsymbol{\phi}_t(x)=\Phi(x-\mathbf{X}_t)$ is found to be $D_{\mathrm{f}}=(kT/E_{\mathrm{k}})$ [19–26]. We see that taking the shape mode into account produces terms of higher order in (KT/E_{k}).

In Fig. 2 we plot diffusivity (22) that results from the Rice ansatz as a function of KT. We also display kink diffusivities estimated numerically from direct numerical simulations of SPDE (1). We solved the equation of motion with periodic boundary conditions, starting with a kink and antikink with separation $L/2$ on a ring of perimeter L. With these initial conditions, we measured the mean time to collision of kink-antikink pairs. Under the assumption that kinks and antikinks perform independent Brownian motion with diffusivity D, the mean collision time $\langle\tau\rangle$ of two kinks initially separated by $L/2$ on a ring with circumference L is given by

$$\langle\tau\rangle=\frac{L^2}{8D}. \tag{23}$$

The Rice ansatz explicitly takes into account the shape mode and gives contributions, at higher than linear order in (kT/E_{k}), to the kink diffusivity calculated from the fixed shape ansatz. However, it does not explicitly take into account the influence of extended ''phonon'' modes [3]. It may be expected that, once phonon modes are included in analytical calculations, the predicted diffusivity of a kink will be still closer to the numerical results of Fig. 2, with larger coefficients in the nonleading terms in Eq. (22). Indications are that there is indeed a positive contribution from phonon modes [27–29], although the calculations are much lengthier than those that result from the Rice ansatz.

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