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Brownian motion of a sine-Gordon kink

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We prove that the center of mass of a sine-Gordon kink in contact with a thermal reservoir approaches equilibrium by undergoing a Brownian motion in the limit that $k_BT \ll E_k$ where E_k is the rest energy of the kink. Our method consists of introducing a collective variable Hamiltonian for the kink system in which the center of mass of the kink is a canonical variable. Next we use standard projection-operator techniques to derive the equation of motion of the distribution function of the center of mass of the kink. Then we show that in the limit $k_BT \ll E_k$ the distribution function satisfies the Fokker-Planck equation of Brownian motion.

There have been many studies[1-3] recently of the statistical mechanics of systems which have nonlinear kink solutions as "particle"-like. Most of the studies deal with equilibrium properties, such as proving that in the appropriate limit the nonlinear system behaves as a dilute gas of kinks and that their interactions can be treated by a generalized virial expansion. In the case of nonequilibrium properties there have been computer simulations and some theoretical studies[4-7] which have investigated the possibility that a kink undergoes some kind of Brownian motion as it approaches equilibrium by interchange of momenta with phonons.

In this Rapid Communication we show that a sine-Gordon (SG) kink in contact with a thermal bath undergoes Brownian motion in the limit that k_BT/E_k is small where E_k is the rest energy of the kink. Specifically we consider the SG system without kinks in contact with a thermal bath and let the SG system come to equilibrium at temperature T below the temperature E_k/k_B. At $t=0$ we create a kink and show that kink center-of-mass momentum approaches equilibrium undergoing a Brownian motion. The physical cause of the Brownian motion is the nonlinear interaction of the thermal phonons with the center of mass of the kink. The many fast small momentum transfers to the Brownian particle by the thermal phonons are responsible for the Markovian behavior of the kink. The fundamental starting point of our derivation is the use of our collective variable formalism[8,9] whereby the center-of-mass variable of the kink $X(t)$ is introduced as a canonical variable which allows us to describe the kink, SG phonons, and interactions by fully canonical equations of motion. Consequently, we can carry out the derivation of the Fokker-Planck equation (FPE) for the kink in exactly the same manner as for present rigorous derivations of the Brownian motion for a heavy-mass particle.

The Lagrangian for a class of kink models is

$$\bar{L} = (m/2)\sum \dot{y}_n^2 - (\eta/2)\sum (y_{n+1}-y_n)^2 - (W/2)\sum V(y_n/a) \; , \tag{1}$$

where an overhead dot indicates a time derivative, a and $W/2$ are the period and amplitude of the underlying potential V, respectively, η is the force constant of the springs, m is the mass of the particle, and y_n is the displacement of the nth particle from the nth trough of the underlying potential. When we introduce dimensionless variables in Eq. (1) we obtain

$$L \equiv (a^2\eta)^{-1}\bar{L} = \tfrac{1}{2}\sum \dot{Q}_n^2 - \tfrac{1}{2}\sum (Q_{n+1}-Q_n)^2 - \left[\frac{1}{4l_0^2}\right]\sum V(Q_n) \; , \tag{2}$$

where $Q_n \equiv y_n/a$, the dimensionless time is $\tau \equiv \frac{1}{2}(\omega_m t)$, the square of the frequency ω_m is $\omega_m^2 \equiv 4\eta/m$, and l_0 is the dimensionless coupling constant, which is defined as $l_0 = (\pi\omega_m/2\omega_s)$ where $\omega_s^2 = 2\pi^2 W/a^2 m$. A large value of l_0 corresponds to the case where the harmonic forces between the particles are larger than the force due to the underlying potential.

When we take the continuum limit of Eq. (2) we obtain

$$(2\pi)^{-2}L = \int dx\, \mathcal{L} = \int dx [\tfrac{1}{2}\dot{\phi}^2 - \tfrac{1}{2}(\partial\phi/\partial x)^2 - (\pi/l_0)^2 V(\phi)] \; , \tag{3}$$

where $2\pi Q_n \leftrightarrow \phi$, $n \leftrightarrow x$, and $V(\phi)$ is the potential energy. In this paper we use the SG potential $V(\phi) = 1 - \cos\phi$.

Next we express ϕ in terms of the static kink solution of the SG, σ, plus a radiation field χ such that $\phi(x,t) = \sigma(x - X(t)) + \chi(x,t)$ where $\sigma(x) = 4\tan^{-1}\exp(\pi x/l_0)$. In order to render the transformation from ϕ variables to the χ and X variables canonical (for a full discussion see Refs. 8 and 9), we are required to impose the constraints

$$C_1 = \int dx (\partial\sigma/\partial X)\chi(x,t) = 0$$

and

$$C_2 = \int dx (\partial\sigma/\partial X)\pi(x,t) = 0 \; , \tag{4}$$

where

$$\pi(x,t) \equiv \partial\mathcal{L}/\partial\chi = \dot{\chi}(x,t)$$

and

$$\partial\sigma/\partial X=(2\pi/l_0)\operatorname{sech}\{\pi/[x-X(t)]l_0\} .$$

When we transform the Lagrangean equation (3) to the Hamiltonian, introduce the canonical variables X, P, χ, and π, impose the constraints C_1 and C_2, and derive Hamilton's equations of motion we obtain

$$M_X\ddot{X}(t)=F(X,\chi)\equiv\int dx'(\partial\sigma/\partial X)\{\partial^2\chi(x',t)/\partial x'^2+\partial V[\sigma(x'-X(t))]/\partial\sigma-\partial V[\sigma(x'-X(t))+\chi(x',t)]/\partial\sigma\} , \tag{5}$$

$$\ddot{\chi}(x,t)=f(X,\chi)\equiv(1-\mathbf{P}_X)[\partial^2\chi/\partial x^2+\partial V(\sigma)/\partial\sigma-\partial V(\sigma+\chi)/\partial\sigma] , \tag{6}$$

where the mass $M_X\equiv\int(\partial\sigma/\partial X)^2dx=2\pi/l_0$ and

$$\mathbf{P}_XO(x)\equiv[\partial\sigma(x)/\partial X](1/M_X)\int dx'[\partial\sigma(x')/\partial X]O(x') . \tag{7}$$

Equations (5)-(7) constitute a complete closed set of equations for the field χ coupled to the center-of-mass motion X.

The linearized equation for χ is

$$\ddot{\chi}=(1-\mathbf{P}_X)\{\partial^2\chi/\partial x^2-[\partial^2V(\sigma)/\partial\sigma^2]\chi\}=\{\partial^2\chi/\partial x^2-[\partial^2V(\sigma)/\partial\sigma^2]\chi\}\equiv\Lambda\chi(x,t) . \tag{8}$$

The linear SG operator Λ is Hermitian and has the static solution $\Lambda\partial\sigma/\partial X\equiv0$, which follows from the translational invariance of the operator Λ. Consequently, $\mathbf{P}_X\Lambda=0$ and $\mathbf{P}_X$ has no effect in the linearized equation for χ. The eigenfunctions and eigenvalues of Λ are

$$\psi_k(x)=[2\pi\omega(k)]^{-1/2}[ik-(\pi/l_0)\tanh(\pi x/l_0)]e^{-ikx} ,$$
$$\omega(k)^2=k^2+(\pi/l_0)^2 . \tag{9}$$

We use the complete orthonormal set of functions (9) as a basis for the expansion of $\chi(x,t)$, i.e.,

$$\chi(x,t)=\sum\alpha_k\psi_k(x)e^{i\omega(k)t} .$$

The Hamiltonian of the SG system in the collective canonical coordinates is

$$H=P_X^2/2M_X+\tfrac{1}{2}\int dx\pi(x)^2+\int dx\{\tfrac{1}{2}[\chi'(x)+\sigma'(x)]^2-(\pi/l_0)^2[1-\cos(\sigma+\chi)]\} . \tag{10}$$

When we retain up to only quadratic terms in χ, $H\approx H_K+H_{\text{phonon}}$, where

$$H_{\text{phonon}}\equiv\tfrac{1}{2}\int\pi(x)^2dx+\tfrac{1}{2}\int dx[\chi'(x)^2+(\pi/l_0)^2\chi(x)^2\cos\sigma(x)] , \tag{11}$$

the kink rest energy is

$$E_K\equiv\int dx\{\tfrac{1}{2}\sigma'(x)^2+(\pi/l_0)^2[1-\cos\sigma(x)]\}=8\pi/l_0$$

and

$$H_k=P^2/2M_X+E_k .$$

Next we project out the phonon degrees of freedom by assuming that the phonon modes are distributed according to a canonical ensemble-phonon-bath hypothesis. For this purpose we shall have recourse to the Zwanzig projection technique.[10]

From the equations of motion (5) and (6) we go to the corresponding Liouville equation

$$\partial W/\partial t=(\Gamma_0+\Gamma_I)W , \tag{12}$$

where

$$\Gamma_0=-\pi\partial/\partial\chi-f(X,\chi)\partial/\partial\pi ,$$
$$\Gamma_I=-(P/M_X)\partial/\partial X-F(X,\chi)\partial/\partial P , \tag{13}$$

and $W(X,P,\chi,\pi;t)$ is the probability distribution function for the kink-phonon system. Zwanzig's method consists in separating the Liouvillian operator into an unperturbed, Γ_0, and a perturbation part Γ_I. Accordingly, the distribution W is factorized by introducing a projection operator $\mathbf{P}$ as follows

$$\mathbf{P}W(X,P,\chi,\pi;t)\equiv W_I(X,P;t)W_0(X,\chi,\pi)\equiv W_0(X,\chi,\pi)\int d\chi\,d\pi W(X,P,\chi,\pi;t) , \tag{14}$$

where $\Gamma_0W_0=0$ defines the equilibrium phonon-bath distribution, i.e.,

$$W_0(X,\chi,\pi)=Z^{-1}e^{-H_{\text{phonon}}/k_BT} , \tag{15}$$

and where Z is the relevant partition function. W_0 depends on the variable X because the phonon described by χ and π are the SG phonons in the presence of the kink with center of mass at X.

Following Zwanzig's method the FPE for $\mathbf{P}W$ has the form

$$\partial\mathbf{P}W(t)/\partial t=\mathbf{P}\Gamma_I(t)\mathbf{P}W(t)+\int_0^t d\tau\Gamma_I(t)\exp\left[\int_\tau^t ds\mathbf{Q}\Gamma_I(s)\right]\mathbf{Q}\Gamma_I(\tau)\mathbf{P}W(\tau) , \tag{16}$$

where

$$W(t)=e^{-\Gamma_0t}W(X,P,\chi,\pi;t);\ \Gamma_I(t)=e^{-\Gamma_0t}\Gamma_Ie^{\Gamma_0t} , \tag{17}$$

and $\mathbf{Q}=\mathbf{1}-\mathbf{P}$. The phonons are assumed to be at equilibrium for $t=0$ in order to make the inhomogeneous terms vanish. A rigorous expansion technique of the Liouvillian equation (16) has been developed by several authors.[11] For the sake of brevity we report here only the leading terms of such an expansion which are relevant to our analysis of the kink dynamics. It is understood that the reliability of the whole procedure rests on the possibility of defining a (small) perturbation parameter that justifies the truncation of the expansion at some step. We come back to this point later on. It suffices to say here that we verified explicitly that proceeding to further steps in the expansion of the Liouvillian equation (16) only produces higher-order terms in the parameter k_BT/E_k.

The first-order term in the expansion of the FPE (16) can be written in a simplified form:

$$\partial W_l/\partial t=-(P/M_X)\partial W_l/\partial X+\int_0^t \langle \Gamma_l(t)\Gamma_l(\tau)\rangle W_l(\tau)d\tau \ . \tag{18}$$

Here $\langle \cdots \rangle$ denotes the average taken over the phonon-bath variables in the presence of the kink [note that $\langle F(X,\chi)\rangle=0$]. The integrand on the right-hand side of Eq. (18) can be simplified further. The first perturbation operator Γ_l reduces to $-F(X,\chi)\partial/\partial P$, because the average $\langle \cdots \rangle$ of an X derivative is identically zero. The second operator Γ_l acts directly on the distribution function W_l, whence

$$\Gamma_l(\tau)W_l(\tau)=-(P/Mk_BT+\partial/\partial P)F_0(\tau)W_l(\tau) \ .$$

Here, F_0 denotes the time evolution of the force (5) driven by the unperturbed operator Γ_0. Equation (18) can be finally reduced to

$$\partial W_l/\partial t=-(P/M_X)\partial W_l/\partial X +\gamma_1\partial/\partial P(P+M_Xk_BT\partial/\partial P)W_l \ , \tag{19}$$

$$\gamma_1=(M_Xk_BT)^{-1}\int_0^\infty \langle F_0(\tau)F_0(0)\rangle d\tau \ , \tag{20}$$

where k_BT is the dimensionless temperature measured in our energy units ηa^2. γ_1 is positive definite and plays the role of the friction coefficient for the Brownian particle.

Our determination of γ_1 has been obtained under the following assumptions.

(i) *The Markovian limit*: The upper integration limit in Eq. (18) is made to tend to infinity. Such an approximation is justified by the assumption that the initial condition memory gets lost during the many interactions of short duration that occur in a time $1/\gamma_1$.

(ii) *Small phonon fluctuation*: It is assumed that the perturbation regime is characterized by relatively small phonon amplitudes. In spite of this simplification, however, the intrinsic nonlinear nature of $F(X,\chi)$ is preserved. In the power expansion

$$F(X,\chi)=\int dx'[\partial\sigma(x)/\partial X][(\chi''-V_\sigma^{(2)}\chi)-\tfrac{1}{2}V_\sigma^{(3)}\chi^2 -\tfrac{1}{6}V_\sigma^{(4)}\chi^3+\cdots] \ , \tag{21}$$

the term linear in χ is identically zero, while the quadratic term in χ does not contribute to γ_1 because of frequency condition and parity. The notation $O_\alpha^{(n)}$ is the nth order derivative with respect to the α variable. Since $(\partial\sigma/\partial X)V_\sigma^{(4)}=V_\sigma^{(3)}=\sigma_X^{(3)}$, the force dependence on χ is then strongly nonlinear:

$$F(t)\approx-\tfrac{1}{6}\int dx'\sigma_X^{(3)}[x'-X(t)]\chi^3(x',t) \ . \tag{22}$$

The unperturbed time dependence of the force is then reproducible by expanding $\chi(x,t)$ in the eigenfunction basis $\psi_k(x)$ and, consequently, expressing W_0 in terms of a_k and a_k^* as follows:

$$W_0=N\exp[-(2k_BT)^{-1}\textstyle\sum_k \omega(k)^2a_k^*a_k] \ , \tag{23}$$

where N is the normalization. The expression for γ_1 thus obtained involves time, space, and wavelength integrations. We are able to analytically perform the time and space integrations, but we have to carry out the k integrations numerically. We use the following facts to carry out the time and space integrals and reduce the three k integrations to two k integrations.

(a) The time integration produces δ functions of the type $\delta(\omega(k)-\omega(k')-\omega(k''))$, where $\omega(k)$, $\omega(k')$, and $\omega(k'')$ are positive definite; (b) $\chi(x,t)=\chi^*(x,t)$ and, therefore, $a_{-k}=a_k^*$; (c) the unperturbed phonon-mode averages are Gaussian and given by $\langle a_ka_{k'}^*\rangle=\delta_{kk'}$ and $\langle a_ka_{k'}\rangle=\langle a_k^*a_{k'}^*\rangle=0$; (d) $\sigma_X^{(3)}=(\pi/l_0)^3\operatorname{sech}[\pi(x-X)/l_0]\times[1-2\operatorname{sech}^2\pi(x-X)/l_0]$ is even in x.

In view of these properties the number of terms of the normal-mode expansion of Eq. (22) contributing to γ_1 can be reduced greatly. After some lengthy calculations we arrived at the following expression:

$$\gamma_1=(k_BT)^2/M_XI=(l_0/2\pi)I(k_BT)^2 \ , \tag{24}$$

where

$$I=\left(\frac{1}{30}\right)^2\int_{-\infty}^{+\infty}dk'\int_{-\infty}^{+\infty}dk''\frac{K^2[-30Kkk'k''+2K^4-K^2(5+20\kappa)+(10\kappa-3)]^2}{\cosh^2(\pi K/2)\omega^4(k)\omega^4(k')\omega^4(k'')[\partial\omega(k)/\partial k]} \ , \tag{25}$$

with $K=k-k'-k''$, $\kappa\equiv kk'+kk''-k'k''$, and $\omega^2(k)=[\omega(k')+\omega(k'')]^2$. The integrations over k and k' in I must be performed numerically. Our final result for the dimensionless inverse relaxation time in units of the frequency at the bottom of the continuum $\omega_c=\pi/l_0$ is

$$\gamma_1/\omega_c=3.95(k_BT/E_k)^2 \ , \tag{26}$$

where we have used the fact that $I=0.0125$. From Eq. (19) the dimensionless diffusion coefficient in momentum space is $D_P\equiv\gamma_1M_Xk_BT=I(k_BT)^3$, which goes at the third power of the temperature, and the dimensionless spatial diffusion coefficient is $D_X\equiv[I(8\pi/l_0)(k_BT/E_k)]^{-1}$ and is inversely proportional to the first power of the temperature.

In order to obtain the FPE we require the time scale for the bath variables (phonons in our case) to be fast compared with the time scale of the variables $X(t)$ and $P(t)$, so that we can extend the limit of the integral in Eq. (20) to infinity and at the same time use the noninteracting propagator in the force correlation function. We can look at this requirement on time scales from two different but essentially equivalent points of view. The first point of view is to see that the above approximations are just those of the first Born-Markov approximation which is justified if $\epsilon \equiv \tau_i/\tau_f \ll 1$, where τ_i is the interaction time and τ_f is the relaxation time. In the present case τ_i is the correlation time of the SG phonons whose magnitude is $\approx l_0/\pi$ and the relaxation time τ_f is $1/\gamma_1$. Consequently, $\epsilon = \gamma l_0/\pi$, which is equal to $\frac{1}{2} l_0^2 (k_B T)^2 I = 0.4 (k_B T/E_k)^2$. When Eq. (18) is expanded to higher order in χ each succeeding term in the expansion is down from the preceding term by a factor of $k_B T/E_k$, which demonstrates that our solution is an expansion in $k_B T/E_k$. Thus our deviation for the Brownian motion for the SG kink requires that the temperature be much less than the energy to create a kink. An alternative point of view on our requirement for the validity of the FPE is to observe that with the velocity variable scaled with the thermal velocity the relaxation time $1/\gamma_1$ is inversely proportional to the mass of the Brownian particle just as in conventional Brownian motion theory where the dimensionless parameter $M^{-1} \ll 1$. The only difference is that because the soliton is an extended object and not a "point particle" the interaction time is proportional to l_0 so that the dimensionless parameter $\epsilon = \gamma_1 \tau_i \approx M^{-2}$ instead of M^{-1}.

In a series of papers, Ogata and Wada[6] studied the momentum transfer between a kink and a phonon, the viscosity, and the Brownian-like motion of a one-dimensional ϕ^4 kink system. Even though the SG system and the ϕ^4 system are different and our respective approaches are different we still find many results which are qualitatively the same. Although the above authors do not directly evaluate the force correlation function (20) in their approach, they do calculate quantities that are essentially the same. In both the ϕ^4 and the SG problems the first nonvanishing contribution to the force correlation function is proportional to the sixth order in the phonon amplitude and thus to $(k_B T)^3$ because the quadratic term in χ vanishes due to the translational invariance and the quartic term in χ also vanishes in both cases. In conclusion the only difference between the relaxation time $1/\gamma_1$ in the center-of-mass Brownian motion of the ϕ^4 and SG systems is the value of the dimensionless integrals I which reflect the difference in the shape functions and eigenfunctions of the respective linearized equations of the two theories.

In Ref. 6 there is a statement to the effect that completely integrable systems such as the SG system cannot undergo Brownian motion. We have proven in this paper that the SG system does undergo Brownian motion due to collision with thermal phonons in the limit $k_B T/E_k \rightarrow 0$. The reason the SG kink undergoes Brownian motion is the same as in ordinary Brownian motion, namely, that although the kink plus phonon interactions conserve momentum and energy, the bath erases this information by the bath keeping the phonons in a thermal distribution.

In conclusion, we have shown that the single SG soliton in interaction with a thermal bath undergoes Brownian motion in the limit $k_B T/E_k$ goes to zero in exactly the same manner as does a massive Brownian particle. Our derivation of Brownian motion for the center of mass applies also to the double SG system as well as to the SG and ϕ^4 systems. In a future publication we will show that we can use the overall approach of the present paper to show that the internal modes of the double SG and ϕ^4 systems also undergo a generalized Brownian motion, and that in addition the internal modes are coupled to the stochastic motion of the center of mass.

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[1] J. P. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).
[2] K. Sasaki, Phys. Rev. B **33**, 2214 (1986).
[3] T. Miyashita and K. Maki, Phys. Rev. B **31**, 1836 (1985); F. Marchesoni, Phys. Lett. **115A**, 29 (1986).
[4] Y. Wada and J. R. Schrieffer, Phys. Rev. B **18**, 3897 (1978).
[5] N. Theodorakopoulos, Z. Phys. B **33**, 395 (1979).
[6] M. Ogata and Y. Wada, J. Phys. Soc. Jpn. **55**, 1252 (1986), and references contained therein.
[7] J. A. Combs and S. Yip, Phys. Rev. B **28**, 6873 (1983).
[8] C. R. Willis, M. El Batanouny, and P. Stancioff, Phys. Rev. B **33**, 1904 (1986).
[9] C. R. Willis, M. El Batanouny, S. Burdick, R. Boesch, and P. Sodano, Phys. Rev. B **35**, 3496 (1987).
[10] R. Zwanzig, Phys. Rev. **124**, 983 (1961); N. Nordholm and R. Zwanzig, J. Stat. Phys. **13**, 347 (1975).
[11] See, e.g., P. Grigolini and F. Marchesoni, Adv. Chem. Phys. **62**, 29 (1985), and references contained therein.