Thermal Nucleation of Kink-Antikink Pairs

Mark Alford,[1] Hume Feldman,[2] and Marcelo Gleiser[3]
[1] *Institute for Theoretical Physics, University of California, Santa Barbara, California 93106*
[2] *Department of Physics, University of Michigan, Ann Arbor, Michigan 48109*
[3] *Department of Physics and Astronomy, Dartmouth College, Hanover, New Hampshire 03755*
(Received 11 October 1991)

We numerically study the thermal nucleation of kink-antikink pairs in (1+1)-dimensional classical field theory coupled to a heat bath. We study the dependence of the kink lifetime and number density on temperature *and* on the coupling to the heat bath (viscosity). We qualitatively confirm Kramers's prediction of the viscosity dependence, and find a slight reduction in the effective kink mass compared with its zero-temperature value. We find no suppression of kink production beyond the Boltzmann factor, and we confirm a recent prediction of the renormalization of the barrier at high viscosity.

PACS numbers: 11.10.Lm

The study of thermally induced transitions over energy barriers in systems with a finite or infinite number of degrees of freedom is of great importance in many areas of physics, from condensed matter and nonlinear optics to particle physics and cosmology. For example, coherent thermal excitations over potential barriers appear in connection with dislocation theory [1], Josephson transmission lines [2], and cosmological phase transitions [3]. Interest in the dynamics of such systems has been steadily increasing due to recent claims that thermal effects may play a fundamental role in the cosmological generation of the baryon number excess during the electroweak phase transition [4], although some authors [5] have conjectured that the rate is entropically suppressed by the large number of degrees of freedom involved. Thermal nucleation of kink-antikink pairs has been studied in the recent literature [6,7], as well as simulations of the nonperturbative thermal effects responsible for baryon number violation at the electroweak scale [8], with interesting results. Given the relevance of the topic not only to our understanding of thermal processes that may have occurred in the early Universe, but also to other similar phenomena occurring in different physical systems, we decided to examine the thermal nucleation of kink-antikink pairs in some detail.

The system we chose to study is the real scalar field ϕ in 1+1 dimensions, with a double-well potential $V=(\lambda/4)(\phi^2-a^2)^2$. It is well known that this system exhibits stable localized "kink" solutions, and at finite temperature we expect the spontaneous nucleation of kink-antikink pairs. As mentioned above, there have been two previous works on this topic. Grigoriev and Rubakov [6] examined the nucleation of kink-antikink pairs in a microcanonical approach, by following the deterministic evolution of the field ϕ at fixed energy. Bochkarev and de Forcrand [7] studied the stochastic dynamics of ϕ by coupling it to a heat bath and solving the Langevin equation (1) in the high viscosity limit, which then reduces to a first-order equation in time [9]. However, their results are difficult to interpret because the high viscosity approximation requires $\tilde{\eta}\gg 1$ (see below), while they considered only $\tilde{\eta}=1$, where $\tilde{\eta}$ is the dimensionless viscosity coefficient. In neither study was the measured kink lifetime compared with any theoretical predictions.

In this Letter we study the kink density and lifetime for a wide range of viscosities and temperatures, using the full second-order equation of motion (1), with a longer simulation time for increased accuracy. We discuss the theoretical predictions for these quantities, and compare them with the numerical results, finding good agreement in most cases.

Description of the system.—The classical dynamics of the (1+1)-dimensional scalar field theory in contact with a heat bath may be modeled by the stochastic Langevin equation,

$$\frac{\partial^2\phi}{\partial t^2}=\frac{\partial^2\phi}{\partial x^2}-\eta\frac{\partial\phi}{\partial t}-\lambda\phi(\phi^2-a^2)+\xi(x,t)\,, \qquad (1)$$

where η is the viscosity coefficient, and ξ is the Gaussian stochastic force with vanishing mean, related to η by the fluctuation-dissipation theorem, $\langle\xi(z)\xi(z')\rangle=2\eta T\delta^2(z-z')$, where $z=(x,t)$ and T is the temperature of the heat bath. In writing Eq. (1) we implicitly assumed that the system is Markovian: The correlation time scale for the noise is much smaller than the typical relaxation time for the system, which is the inverse of the oscillation frequency around stable equilibrium points, $\omega=a\sqrt{2\lambda}$. The explicit kink solution is $\phi_K(x)=a\tanh(a\sqrt{\lambda/2}x)$ [10]. The size of a kink is $R\simeq 1/(a\sqrt{\lambda/2})=2/\omega$, and its mass is $M_K=\sqrt{8\lambda/9}a^3$. In the associated quantum theory the low-energy excitations would be mesons of mass $m=\hbar\omega$. Our analysis will be purely classical, being valid only for energies much greater than m, when the typical field configurations contain many quanta. This means we must study temperatures $T\gg m$, and take the weak coupling limit ($a^2\gg\hbar$) so that $M_K\gg m$. In order for the predictions of the next section to be valid we must have a dilute gas of well-defined kinks, so $T\ll M_K$.

To simplify the analysis we first introduce dimensionless variables $\tilde{\phi}=\phi/a$, $\tilde{x}=a\sqrt{\lambda}x$, $\tilde{t}=a\sqrt{\lambda}t$, in terms of which the Langevin equation becomes

$$\frac{\partial^2\tilde{\phi}}{\partial\tilde{t}^2}=\frac{\partial^2\tilde{\phi}}{\partial\tilde{x}^2}-\tilde{\eta}\frac{\partial\tilde{\phi}}{\partial\tilde{t}}-\tilde{\phi}(\tilde{\phi}^2-1)+\tilde{\xi}\,, \qquad (2)$$

where

$$\tilde{\eta}=\eta/a\sqrt{\lambda},\quad \tilde{\xi}=\xi/a^3\lambda\,,$$
$$\langle\tilde{\xi}(\tilde{x},\tilde{t})\tilde{\xi}(\tilde{x}',\tilde{t}')\rangle=2\tilde{\eta}\theta\delta(\tilde{t}-\tilde{t}')\delta(\tilde{x}-\tilde{x}')\,. \tag{3}$$

The system is now independent of a, λ, and $\hbar$: The kink mass is $\tilde{M}=\sqrt{8/9}$, and the dimensionless temperature is $\theta\equiv T/(\sqrt{\lambda}a^3)$, so $\tilde{M}/\theta=M_K/T$. The high viscosity approximation mentioned above involves ignoring the $\partial^2\tilde{\phi}/\partial\tilde{t}^2$ term, which is valid when $\tilde{\eta}\gg 1$.

Theoretical results.— The quantities measured were the density of kink-antikink pairs $\tilde{n}$, the kink lifetime $\tilde{\tau}_0$, and their dependence on viscosity and temperature. By standard arguments [e.g., Eq. (18) of Ref. [11]] the equilibrium kink density is

$$\tilde{n}=\frac{dN}{d\tilde{x}}(\theta)\propto\frac{1}{\sqrt{\theta}}\exp(-\tilde{M}_{\text{eff}}/\theta)\,, \tag{4}$$

where we expect $\tilde{M}_{\text{eff}}=\tilde{M}$.

The other quantity we measured was the equilibrium kink lifetime, or kink pair correlation time $\tilde{\tau}_0$, defined by

$$G(\tilde{\tau})=\langle\tilde{n}(\tilde{t}+\tilde{\tau})\tilde{n}(\tilde{t})\rangle_{\tilde{t}}-\langle\tilde{n}(\tilde{t})\rangle_{\tilde{t}}^2=A\exp(-\tilde{\tau}/\tilde{\tau}_0)\,, \tag{5}$$

where $\langle\cdots\rangle_{\tilde{t}}$ denotes an average over a large interval of time $\tilde{t}$. It can be written in terms of the pair nucleation rate per unit length $\tilde{\Gamma}$ and the kink density $\tilde{n}$ [11]:

$$\tilde{\tau}_0^{-1}\propto\tilde{\Gamma}/\tilde{n}\,. \tag{6}$$

The pair nucleation rate per unit length has been calculated for classical field theories without friction [12] and for multidimensional particle systems in the large and small viscosity regimes [13,14]. At large viscosity the rate is suppressed by overdamping. As the viscosity drops the rate rises, until we reach small viscosity where we again expect suppression since it is harder for the heat bath to feed energy into the system. However, at very small viscosity the rate should go to a constant, since even in the absence of noise there will still be some kink production [6,12]:

$$\tilde{\Gamma}\propto f(\tilde{\eta})(1/\sqrt{\theta})\exp(-\tilde{B}_{\text{eff}}/\theta)\,,$$
$$f(\tilde{\eta})=\begin{cases}(\tilde{\eta}^2/4+\tilde{\omega}_b^2)^{1/2}-\tilde{\eta}/2 & (\tilde{\eta}\gtrsim 1),\\ a+b\tilde{\eta} & (\tilde{\eta}\ll 1).\end{cases} \tag{7}$$

Here $\tilde{\omega}_b$ is a frequency associated with the curvature of the top of the barrier, of order 1, and a and b are constants that depend on the barrier and also, potentially, on the temperature [13]. Naively one would expect the effective barrier to be $\tilde{B}_{\text{eff}}=2\tilde{M}$, since kinks are nucleated in pairs. However, in the high viscosity limit the motion of a kink will be diffusive, so that its mean square displacement is $\langle\Delta\tilde{x}^2(\tilde{t})\rangle=2D\tilde{t}$ (with diffusion coefficient $D=\theta/\tilde{\eta}$). Since the lifetime $\tilde{\tau}_0$ is the time taken for a kink and antikink to meet and annihilate, it follows that $\langle\Delta\tilde{x}^2(\tilde{\tau}_0)\rangle\propto 1/\tilde{n}^2$ [11], so from (4), (6), and (7) we can write

$$\tilde{\tau}_0\propto[1/f(\tilde{\eta})]\exp(\tilde{U}_{\text{eff}}/\theta)\,,$$
$$\tilde{U}_{\text{eff}}\equiv\tilde{B}_{\text{eff}}-\tilde{M}_{\text{eff}}=\begin{cases}2\tilde{M}_{\text{eff}} & \text{(high viscosity)},\\ 2\tilde{M}-\tilde{M}_{\text{eff}} & \text{(naive)}.\end{cases} \tag{8}$$

Note that the high viscosity result corresponds to a nucleation barrier $\tilde{B}_{\text{eff}}=3\tilde{M}_{\text{eff}}$, which deviates from the naive estimate because of the effects of friction on the nucleation process.

Numerical analysis.— We study the thermal production of kink-antikink pairs by numerically solving the Langevin equation with periodic boundary conditions on a spatial lattice of length $L=200$ and lattice spacing $l=0.5$, with time step $\varepsilon=0.02$. The lattice field $\Phi_i(n)$ is the average of $\tilde{\phi}$ over the ith cell at time $\tilde{t}=n\varepsilon$, and $\Pi_i(n)$ is the average of $\partial\tilde{\phi}/\partial\tilde{t}$ at $\tilde{t}=(n-\frac{1}{2})\varepsilon$. We propagated them by the leapfrog algorithm:

$$\Pi_i(n+1)=\Pi_i(n)+\varepsilon\{[\Phi_{i-1}(n)+\Phi_{i+1}(n)-2\Phi_i(n)]/l^2-\tilde{\eta}\Pi_i(n)-\Phi_i(n)[\Phi_i^2(n)-1]+\Xi_i(n)\}\,,$$
$$\Phi_i(n+1)=\Phi_i(n)+\varepsilon\Pi_i(n+1)\,, \tag{9}$$

where the Gaussian noise $\Xi_i(n)$ obeys $\langle\Xi_i(n)\rangle=0$ and $\langle\Xi_i(n)\Xi_j(m)\rangle=(2\tilde{\eta}\theta/l)\delta_{ij}\delta_{mn}$.

For each value of viscosity and temperature we propagated the Langevin equation through 9×10^6 iterations, corresponding to a final time of $t_f=1.8\times10^5$ in dimensionless units. We chose homogeneous initial conditions, $\Phi_i(0)=-1$ and $\Pi_i(0)=0$. The noise and viscosity thermalized the system quickly, and caused the formation of kink-antikink pairs. A typical snapshot in time is given in Fig. 1. To count the number of kinks and antikinks while ignoring thermal noise we first calculated a smoothed field by averaging Φ over blocks of dimensionless length of $\Delta L=5$, which is roughly the size of two kinks. We then counted one kink (or antikink) whenever the smoothed field went through zero. This criterion has the advantage of being symmetric under $\Phi\to-\Phi$, so it is equally easy to create a pair starting from a fluctuation around $\Phi=1$ or $\Phi=-1$. In order to obtain the dimensionless kink lifetime $\tilde{\tau}_0$ we evaluated the correlation function [Eq. (5)] and fitted with an exponential. When errors are quoted on measured values of τ_0 they will delimit the range of values that gave a reasonable fit by eye.

We checked the dependence of our results on the lattice length, the lattice spacing, the time step, the final time, the random number generator, and the random

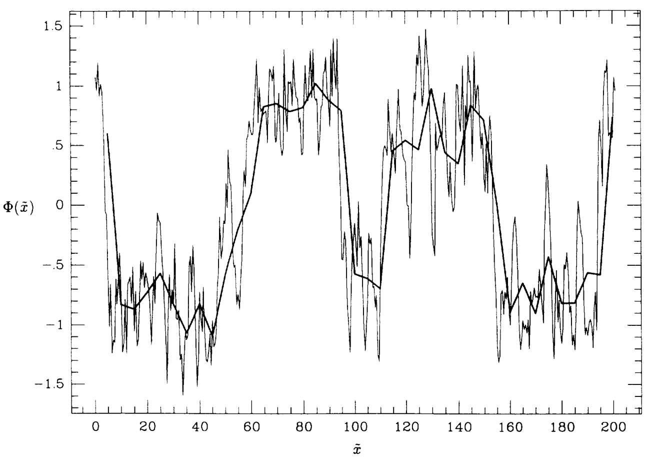

FIG. 1. A sample field configuration at temperature $\theta=0.24$, and its smoothed version in which thermal noise is greatly reduced.

number seed. Within the limits of numerical accuracy, no dependence was found, implying that the lattice calculation correctly approximates the continuum classical field theory.

Numerical results.— (1) Kink density $\tilde{n}$. As one would expect for an equilibrium quantity, $\tilde{n}$ turns out to be independent of $\tilde{\eta}$. In Fig. 2 we give the temperature dependence, which shows an excellent fit by the Boltzmann law [Eq. (4)] although the effective mass is

$$\tilde{M}_{\rm eff}=(0.75\pm0.05)\tilde{M}\quad(\text{measured})\,. \tag{10}$$

Compared with the result $\tilde{M}_{\rm eff}=0.55\tilde{M}$ found in Ref. [7], this is closer to the expected value $\tilde{M}_{\rm eff}=\tilde{M}$, but still shows a significant reduction. Marchesoni [15] points out that this may arise from the finite size of the solitons, finite length of the lattice, or phonon dressing effects due to the lattice discretization. It is also interesting to note that the data favor higher $\tilde{M}_{\rm eff}$ at lower temperatures, suggesting that we may be seeing the effects of thermal noise, which swamps the tails of the kink configuration

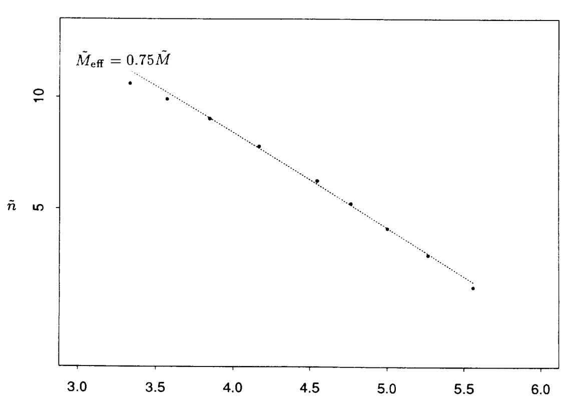

FIG. 2. Soliton pair density (logarithmic scale) as a function of inverse temperature. The errors were less than 1%. The fitted curve for $\tilde{M}_{\rm eff}=0.75\tilde{M}$ is shown [see Eq. (4)].

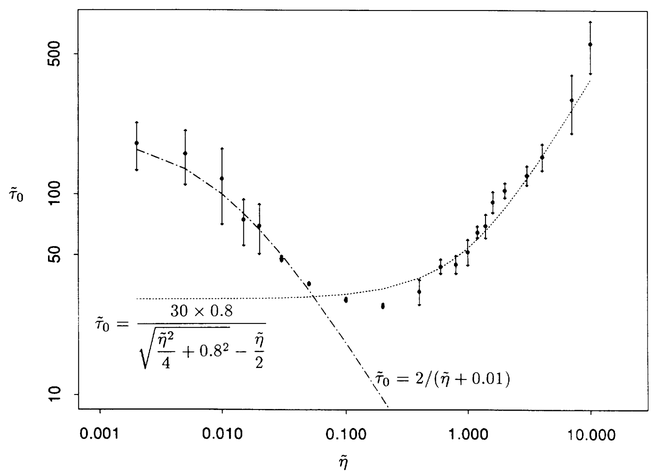

FIG. 3. Kink lifetime as a function of viscosity, at temperature $\theta=0.24$. Fits with the high and low viscosity predictions [Eq. (7)] are shown.

(see Fig. 1).

(2) Kink lifetime $\tilde{\tau}_0$ versus viscosity at temperature $\theta=0.24$ is shown in Fig. 3 for $\tilde{\eta}=0.002$ to 10.0. For viscosities outside this range it became hard to fit $G(\tilde{\tau})$ by an exponential: The increasing size of the error bars at the ends of the range reflects the onset of this problem. We see a good fit with the predicted behavior [Eqs. (7) and (8)]. The high viscosity fit used $\tilde{\omega}_b=0.8$, which is of order 1 as expected. To the best of our knowledge this is the first qualitative confirmation of Kramers's prediction for systems with an infinite number of degrees of freedom.

(3) Kink lifetime versus temperature. In Fig. 4 we have given $\tilde{\tau}_0$ as a function of θ at three different viscosi-

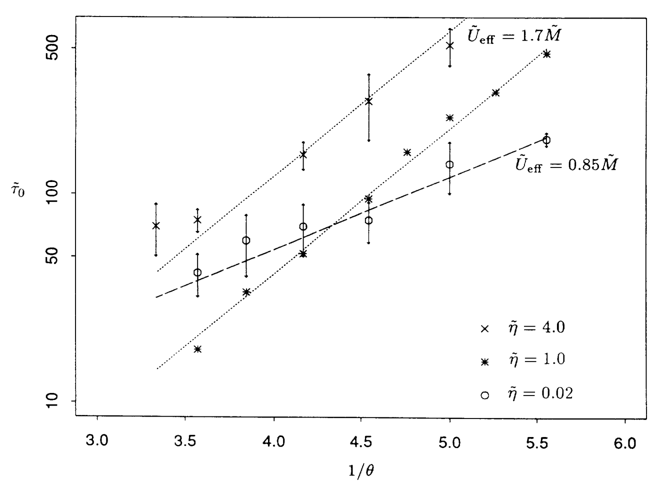

FIG. 4. Kink lifetime as a function of inverse temperature for three different viscosities $\tilde{\eta}=0.02$, 1.0 and 4.0. The error bars on the $\tilde{\eta}=1$ observations have been omitted for clarity; they would be a little larger than the plotting symbols. Fits with the expected exponential dependence [Eq. (8)] are shown. For $\tilde{\eta}=4.0$ we used the slope that fitted $\tilde{\eta}=1.0$.

ties: $\tilde{\eta}=0.02$, 1.0, and 4.0. For $\tilde{\eta}=1$ we see $\tilde{U}_{\rm eff}=(1.7\pm0.2)\tilde{M}$, which also gives a reasonable fit for $\tilde{\eta}=4$. By (10) this is equal to $(2.3\pm0.4)\tilde{M}_{\rm eff}$, consistent with the prediction [Eq. (8)] that $\tilde{U}_{\rm eff}$ should be twice the effective mass, and verifies the prediction of Hänggi that the barrier height $\tilde{B}_{\rm eff}$ would be renormalized at high viscosity. At the lowest viscosity we measure $\tilde{U}_{\rm eff}=(0.85\pm0.15)\tilde{M}=(1.1\pm0.2)\tilde{M}_{\rm eff}$, which is not consistent with the naive estimate [Eq. (8)] which would predict $\tilde{U}_{\rm eff}=(1.25\pm0.05)\tilde{M}$. This is probably due to the temperature dependence of the low viscosity prefactor, which is known to occur in multidimensional systems (Ref. [13], Sec. 2.5).

Our analysis shows no extra temperature suppression of the nucleation rate of nonperturbative field configurations. However, we have confirmed the high viscosity barrier renormalization result of Ref. [11]. This fact has important consequences in most physical systems in which thermal nucleation plays an important role, for example, in the creation of monopoles in the early Universe. Related questions arise in the study of cosmological phase transitions. A first-order transition may generate an out-of-equilibrium phase of false vacuum which decays by nucleation of bubbles of true vacuum. This is assumed in most inflationary models, baryogenesis at both the grand unification and the electroweak scale, and the formation of quark nuggets at the quark-hadron phase transition [3]. However, this picture may be wrong, since if a system cools slowly enough then it could remain in equilibrium. Recently, it has been suggested by Gleiser, Kolb, and Watkins [3] that nonperturbative effects play a crucial role in the equilibration properties of these systems. Clearly, the Langevin approach is ideally suited to study this question. Another application is baryon number generation in the electroweak phase transition. As our results indicate, knowledge of η (which is related to the coupling constants in the model) will ultimately determine if enough baryon number excess can be generated [16]. We intend to investigate these questions in the near future.

M.G.A. and M.G. were supported by NSF Grant No. PHY89-04035. We thank the National Center for Supercomputing Applications (NCSA), Urbana, Illinois.

[1] A. Seeger and P. Schiller, in *Physical Acoustics*, edited by W. P. Mason (Academic, New York/London, 1966), Vol. IIIA, p. 361.

[2] R. K. Dodd, J. C. Eilbeck, J. D. Gibbon, and H. C. Morris, *Solitons and Nonlinear Wave Equations* (Academic, London, 1982).

[3] E. W. Kolb and M. S. Turner, *The Early Universe* (Addison-Wesley, Reading, MA, 1990); A. D. Linde, *Particle Physics and Inflationary Cosmology* (Harwood Academic, New York, 1990); see also, M. Gleiser, E. W. Kolb, and R. Watkins, Nucl. Phys. **B364**, 411 (1991), and references therein.

[4] V. A. Kuzmin, V. A. Rubakov, and M. E. Shaposhnikov, Phys. Lett. **155B**, 36 (1985); M. E. Shaposhnikov, Nucl. Phys. **B287**, 757 (1987); **B299**, 797 (1988); P. Arnold and L. McLerran, Phys. Rev. D **36**, 581 (1987); N. Turok and J. Zadrozny, Phys. Rev. Lett. **65**, 2331 (1990); A. Cohen, D. Kaplan, and A. Nelson, Phys. Lett. B **245**, 561 (1990).

[5] J. Ellis, R. Flores, S. Rudaz, and D. Seckel, Phys. Lett. B **194**, 241 (1987).

[6] D. Yu. Grigoriev and V. A. Rubakov, Nucl. Phys. **B299**, 67 (1988).

[7] A. I. Bochkarev and Ph. de Forcrand, Phys. Rev. Lett. **63**, 2337 (1989); **64**, 2213 (1990).

[8] J. Ambjorn, M. Laursen, and M. E. Shaposhnikov, Phys. Lett. B **197**, 49 (1987); Nucl. Phys. **B299**, 483 (1989); J. Ambjorn, T. Askgaard, H. Porter, and M. E. Shaposhnikov, Phys. Lett. B **244**, 479 (1990).

[9] G. Parisi, *Statistical Field Theory* (Addison-Wesley, Reading, MA, 1988).

[10] R. Rajaraman, *Solitons and Instantons* (North-Holland, Amsterdam, 1982).

[11] P. Hänggi, F. Marchesoni, and P. Sodano, Phys. Rev. Lett. **60**, 2563 (1988).

[12] M. Dine, O. Lechtenfeld, B. Sakita, W. Fischler, and J. Polchinski, Nucl. Phys. **B342**, 381 (1990).

[13] P. Hänggi, J. Stat. Phys. **42**, 105 (1986).

[14] H. A. Kramers, Physica (Utrecht) **7**, 284 (1940).

[15] F. Marchesoni, Phys. Rev. Lett. **64**, 2212 (1990).

[16] A. Ringwald, Phys. Lett. B **201**, 510 (1988).