Nonperturbative evaluation of the diffusion rate in field theory at high temperatures

Alexander Bochkarev*
Institut für Theoretische Physik, Universität Bern, CH-3012 Bern, Switzerland

Philippe de Forcrand
IPS, Eidgenössische Technische Hochschule Zurich, CH-8092 Zurich, Switzerland
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The Kramers approach to the rate of thermally activated escape from a metastable state is extended to field theory. The diffusion rate in the (1+1)-dimensional sine-Gordon model as a function of temperature and friction coefficient is evaluated numerically by solving the Langevin equation in real time. A clear crossover from the semiclassical to the high-temperature domain is observed. The temperature behavior of the diffusion rate allows one to determine the kink mass which is found equal to the corresponding classical value. The Kramers predictions for the dependence on viscosity are qualitatively valid in this multidimensional case. In the limit of vanishing friction the diffusion rate is shown to coincide with the one obtained from direct measurements of the conventional classical real-time Green's function at finite temperature.

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I. INTRODUCTION

Statistical systems with finite energy barriers separating different domains of the phase space may exhibit metastable states. Evaluation of the rate of escape from those states is an important dynamical problem. The simple example of a statistical system where one degree of freedom is exposed to the potential illustrated by Fig. 1 was first considered by Kramers [1]. At temperatures

$$\omega_0 \ll T \ll E_S, \tag{1.1}$$

where we take $\hbar = k = 1$, ω_0 is the scale of quantum fluctuations and E_S is the barrier height, the classical thermodynamical fluctuations contribute to the escape rate $\Gamma \sim \exp(-E_S/T)$ of the system initially localized in the well. Kramers [1] suggested determining the escape rate by means of the classical Langevin equation:

$$\dot{\phi} = p/M, \quad \dot{p} = -\frac{\partial U}{\partial \phi} - \gamma p + \eta(t), \tag{1.2}$$

$$\langle \eta(t)\,\eta(0)\rangle = 2T\gamma M\delta(t), \tag{1.3}$$

where γ is a friction coefficient, introduced as an input parameter in this phenomenological description and M corresponds to the mass of the would be Brownian particle. γ determines how strong the coupling of the system to the heat bath is, represented by the white noise η, and therefore how fast the system reaches equilibrium. The normalization of the random force (1.3) (the Einstein relation) comes from the fluctuation-dissipation theorem. In the case of one degree of freedom the escape rate $\Gamma(T,\gamma)$ has been obtained analytically [9] in the domain of very small γ and for moderate-to-large friction $\gamma \gg \omega_-$, where ω_- is the negative eigenmode of the fluctuations near the stationary point $\phi = \phi_s$. In quantum field theory one often deals with an analogous problem of penetration through some energy barrier. One very important example is anomalous fermion- (or axial charge) number violation in gauge theories with nontrivial structure of the ground state [2]. Here the static energy barrier separates different classical vacua with definite integer Chern-Simons numbers [3]. Penetration through this energy barrier leads to the dissipation of the fermionic number. The system at high temperature is expected to exhibit thermal activation behavior of the rate of anomalous fermion number nonconservation [4]. The problem specific for the field theory is that the energy barrier — the analogue of U in Eq. (1.2) — is not known explic-

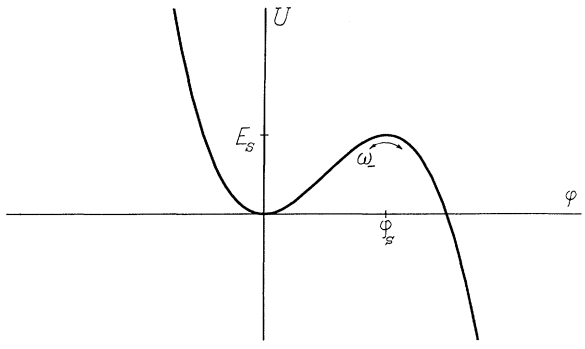

FIG. 1. Typical potential creating a metastable state at finite temperature.

*On leave of absence from INR, Russian Academy of Science, Moscow 117312, Russia.

itly. This energy barrier is in the multidimensional configurational space. Only the static field configuration, corresponding to the top of that barrier, is known from topological considerations [5] or explicitly in some models [6].

In previous works [7,8] we suggested following Kramers in studying the energy barrier in field theory. In [8] we introduced the microscopical classical Langevin equation in real time in the $(1+1)$-dimensional Abelian-Higgs theory and observed the Brownian motion of the Chern-Simons variable between topologically distinct classical vacua. Our measurements of the diffusion rate revealed its thermal activation dependence on the temperature in the domain (1.1). Although this approach is applicable in the interesting domain of high temperatures, where the semiclassical approximation is not valid, it was difficult to get data there, because it required rather big lattices. Meanwhile, it was argued in [12] that our results were difficult to interpret, since they were based on the first-order Langevin equation, derived normally for large friction coefficients, while, in fact, $\gamma = 1$ had been used.

In the present paper we deal with a simpler model, the sine-Gordon field theory in $1+1$ dimensions, which allows one to obtain not only accurate quantitative results but also to check qualitative conclusions valid beyond this particular model. In fact, this model is very similar to the Abelian-Higgs theory. On the classical level the sine-Gordon theory has an infinite number of degenerate vacua with a finite energy barrier separating them. At nonzero temperatures one observes a random walk between those vacua. At temperatures (1.1) this random process goes through the formation of kink-antikink pairs, so the rate of the process (diffusion rate) is sensitive to the density of kinks. The sine-Gordon model is also important in solid state physics, since it describes the Josephson junction transmission lines [9]. The dilute gas of kinks has been analytically studied before [10] by means of the effective macroscopical Langevin equation. Previous numerical calculations of the density of kink gas as a function of temperature in the $(1+1)$-dimensional scalar field theory with the double well potential has revealed an intriguing fact: the thermal activation behavior of the density of kinks $n \sim \exp(-E_K^{\rm eff}/T)$ involved an effective kink mass $E_K^{\rm eff}$, which was found to be 20–30 % smaller than the classical value $E_K^{\rm cl}$ [7, 11, 12]. One source of uncertainties in measuring the density of kinks was the *ad hoc* criterion (suggested in [15]) for counting the number of kinks in a given field configuration. The very notion of a kink is ambiguous at finite temperature. The advantage of the sine-Gordon model is a possibility to avoid this criterion problem. The quantity we measure is very well defined: it is the diffusion parameter of the average field. We measure the diffusion rate in the semiclassical domain (1.1) of temperatures and beyond. The measurements allow us to extract the value of the kink mass $E_K^{\rm eff}$, which we find to coincide with the classical kink mass $E_K^{\rm cl}$. We therefore conclude that the previously observed discrepancy was an artifact of the criterion used.

We also measure the viscosity dependence of the rate by means of the second-order Langevin equation. We find a remarkable coincidence of this dependence with the one predicted by the first-order Langevin equation down to very small values of the friction coefficient. This implies that one can use the first-order Langevin approach in field theory, in particular, for $\gamma \sim 1$.

In the limit of vanishing friction we find a nonzero diffusion rate. Since in this limit the Langevin equations (1.2) become the Hamiltonian ones, we perform a direct numerical measurement of the classical real-time two-point Green's function, which describes the diffusion, as a Gibbs' average. These ensemble averages give the same thermal activation behavior of the rate as obtained in the Langevin measurements and, what is less trivial, they prove to be equal in magnitude to the Langevin measurements in the limit of vanishing friction. This establishes an important equivalence between the Gibbs ensemble measurements of the real-time classical Green's functions at finite temperature and the corresponding Langevin measurements done in the asymptotic domain of very small friction.

In the next section we explain the relevance of simulations of the classical field theories to the behavior of quantum field theories at high temperatures. We emphasize a particular relation between the lattice spacing of the classical systems under consideration and the temperature. In Sec. III we briefly introduce the $(1+1)$-dimensional sine-Gordon model at finite temperature. Then we describe the first- and second-order Langevin equations. Sections IV and V contain the results of our numerical simulations.

II. CLASSICAL SYSTEMS—FOR QUANTUM THEORIES

It is well known that the partition function of a $(D+1)$-dimensional quantum field theory in the limit of high temperature may be obtained by means of the corresponding D-dimensional classical field theory. To see how this emerges consider, for instance, a scalar field theory in $D+1$ dimensions, defined by the action of the general form

$$S = \int d^{D+1}x \left(\frac{1}{2}(\partial\phi)^2 + \frac{m^2}{2}\phi^2 + \lambda U_{\rm int}\right). \quad (2.1)$$

The partition function of the corresponding statistical system is given by functional integral with the following Matsubara action:

$$S_M = \int_0^\beta dx_4 \int d^D x \left[\frac{1}{2}\left(\frac{1}{\hbar}\partial_4\phi\right)^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{m^2}{2}\phi^2 + \lambda U_{\rm int}\right], \quad (2.2)$$

where $\beta = 1/T$ is the inverse temperature, $\hbar$ is Planck's constant, and periodic boundary conditions are imposed on the field in the imaginary-time direction. Equation (2.2) implies that in any of the limits

$$\hbar \to 0 \quad \text{or} \quad T \to \infty \quad (2.3)$$

the static x_4-independent field configurations dominate in the functional integral. If one ignores for a moment ultraviolet divergences and performs the limit (2.3) formally, the contribution of the static modes is determined by the action

$$S_{\rm eff} = \beta \int d^D x \left(\frac{1}{2}(\nabla\phi)^2 + \frac{m^2}{2}\phi^2 + \lambda U_{\rm int} \right). \quad (2.4)$$

This action does not mention Planck's constant. The functional integral with the action (2.4) determines the partition function of the corresponding classical system. To be more accurate, one should keep in mind that nonstatic modes do not decouple in the ultraviolet-divergent diagrams, which means that the action (2.4) involves renormalized Largangian parameters—running coupling constants, normalized on the temperature. The renormalization effects are the memory about the quantum nature of the original theory (2.2). To obtain the effective action (2.4) is, in general, a separate problem [13]. In some simple cases in low dimensions the action (2.4) is simply a static Hamiltonian.

Let us see explicitly how the reduction takes place, for example, in the case of a weak interaction ($\lambda \ll 1$). The free energy of a gas of particles of mass m, corresponding to (2.1), in the one-loop approximation reads

$$F = TV \sum_n \int \frac{dk^D}{(2\pi)^D} \frac{1}{2} \ln\left(\omega_n^2 + \omega_k^2\right), \quad (2.5)$$

where $\omega_n = 2\pi n T$, $n = 0, \pm 1, \pm 2, \ldots$ are Matsubara frequencies, $\omega_k = \sqrt{m^2 + k^2}$, and V is a D-dimensional volume. The temperature-dependent part

$$F = TV \int \frac{dk^D}{(2\pi)^D} \ln\left[1 - \exp\left(-\beta\omega_k\right)\right] \quad (2.6)$$

becomes, in the limit $T \gg m$,

$$F = -TV \int \frac{dk^D}{(2\pi)^D} \beta k\, n_B(\beta k), \quad (2.7)$$

where n_B is the Bose distribution so that

$$F = -\kappa V T^{D+1} \quad (2.8)$$

with

$$\kappa = \frac{\Omega}{(2\pi)^D} \Gamma(D+1)\, \zeta(D+1), \quad (2.9)$$

where $\Omega = 2\pi^{D/2} / \Gamma(D/2)$ is a surface of the D-dimensional sphere [14].

If we want to obtain the same expression by means of the effective theory (2.4) we have to perform the limit $\beta \to 0$ in the integrand of Eq. (2.7), which gives the divergent factor

$$F = -TV \int \frac{dk^D}{(2\pi)^D}. \quad (2.10)$$

This divergent integral counts the number of degrees of freedom of the classical field theory (the Rayleigh-Jeans divergence). Thus the partition function of the classical field theory is something which needs to be defined. Regularization is necessary for this end.

The vacuum energy of the effective theory (2.4),

$$F = -TV \int \frac{dk^D}{(2\pi)^D} \frac{1}{2} \ln G_\Lambda, \quad (2.11)$$

is determined by the regularized propagator

$$G_\Lambda = 1 / \left(\omega_k^2 + \omega_k^4/\Lambda^2\right). \quad (2.12)$$

For the temperature-dependent cutoff,

$$\Lambda = cT, \quad c \propto 1, \quad (2.13)$$

one recovers the result (2.8) with c determined by κ.

This simple exercise illustrates one general and important statement. The effective D-dimensional classical field theory (2.4), which serves for the calculation of the high-temperature limit of the corresponding $(D+1)$-dimensional quantum field theory, has a physical cutoff, given by Eq. (2.13). If we assume lattice regularization for the original theory (2.2), we conclude that the continuum limit is performed simultaneously with the limit (2.3). One should perform the thermodynamical limit in the functional integral with the effective action (2.4), but not the continuum one. It is essential that the lattice spacing $a^{-1} \propto \Lambda$ here is the physical cutoff, unambiguously fixed by the temperature

$$a^{-1} \propto T/\hbar. \quad (2.14)$$

In this sense the original quantum field theory may be studied at high temperatures by simulating the classical functional integral with the regularized action (2.4) and a temperature-dependent cutoff (2.14) [15]. As soon as nontrivial lattice spacing dependence is observed in a study of the classical systems at high temperatures the relation (2.14) is to be taken into account.

III. KRAMERS' APPROACH IN FIELD THEORY

We consider the sine-Gordon model in 1+1 dimensions defined by the action:

$$S = \int d^2x \left(\frac{1}{2}(\partial\tilde{\phi})^2 - \frac{m^2}{\lambda}\{1 - \cos[\sqrt{\lambda}\tilde{\phi}(x)]\} \right). \quad (3.1)$$

On the classical level the theory has an infinite number of degenerate vacua with $\phi = 2\pi n$, $n = 0, \pm 1, \pm 2, \ldots$. In the quantum theory the mass m determines the scale of quantum fluctuations and the self-coupling constant λ is bounded [16]: $\lambda < 8\pi$. The well-known static solution to the classical equations of motion interpolating between different classical vacua $\tilde{\phi}_k = \frac{4}{\sqrt{\lambda}} \arctan\left(e^{mx}\right)$ has energy

$$E_k = 8m/\lambda \quad (3.2)$$

which is parametrically large, in the sense that λ is a parameter of the semiclassical (loop) expansion. If m is chosen as a unit of measure, the Lagrangian in Eq. (3.1) may be rescaled to the one which has no free parameters:

$$S = \frac{1}{\lambda} \int d^2x \left(\frac{1}{2}(\partial\phi)^2 - \{1 - \cos[\phi(x)]\} \right). \quad (3.3)$$

The sine-Gordon model provides one with a good opportunity to study thermal activation phenomena in field theory. The potential energy is completely bounded at infinity for the zero mode $\bar{\varphi} = \frac{1}{L}\int_0^L dx\,\varphi(x)$, which allows for the Brownian motion of $\bar{\varphi}$ at finite temperature. Any initial state localized around one classical vacuum is far from equilibrium. In the case of periodic boundary conditions fluctuations of the field between different vacua proceed via formation of a pair of kink and antikink and their separation from each other. Creation and annihilation of kink-antikink pairs is essentially a random walk between different classical vacua. Thus the diffusion rate Γ of $\bar{\varphi}$ is sensitive to the kink mass, which determines the height of the static energy barrier between different vacua. For periodic boundary conditions kinks and antikinks appear in pairs, so one expects in the semiclassical domain of temperatures $m \ll T \ll E_k$:

$$\Gamma_{\mathrm{PBC}} \sim \exp(-2E_k/T). \tag{3.4}$$

In the case of free boundary conditions a configuration with a single kink may appear as a result of the thermal fluctuations. The kink's motion through space brings the system from the neighborhood of one classical vacuum to the vicinity of another vacuum. Therefore for free boundary conditions we expect

$$\Gamma_{\mathrm{FBC}} \sim \exp(-E_k/T). \tag{3.5}$$

Following Kramers, we describe evolution of some initial nonequilibrium state localized around one classical vacuum by solving the real-time Langevin equations.

Let us discretize the system of size $L = Na$, where a is lattice spacing. The Hamiltonian, corresponding to Eq. (3.3) is

$$\tilde{H} = \tilde{K} + \tilde{U}, \tag{3.6}$$

$$\tilde{K} = \sum_{n=1}^{N} \frac{1}{2}\frac{\lambda}{a^D}(\tilde{p}_n)^2, \tag{3.7}$$

$$\tilde{U} = \sum_{n=1}^{N} \frac{a^D}{\lambda}\left\{\frac{1}{2}(\phi_{n+1}-\phi_n)^2/a^2 + 1 - \cos[\phi_n]\right\}, \tag{3.8}$$

where D is dimensionality of space, $D = 1$ in our case. To generate a system with the density matrix $\hat{\rho} = \exp(-\tilde{H}/T)$, one naturally employs the second-order Langevin equations of the form

$$\dot{\phi}_n = \frac{\lambda}{a^D}\tilde{p}_n(i), \tag{3.9}$$

$$\dot{\tilde{p}}_n = \frac{a^D}{\lambda}\{(\phi_{n-1}+\phi_{n+1}-2\phi_n)/a^2 - \sin(\phi_n)\} - \gamma\tilde{p}_n + \acute{\eta}_n, \tag{3.10}$$

which is a straightforward generalization of Eqs. (1.2) and (1.3) to the case of many degrees of freedom. Equations (3.6)–(3.10) indicate that formally we deal with a classical gas of particles of mass

$$M = a^D/\lambda \tag{3.11}$$

from which one concludes that the normalization of the random force, fixed by the Einstein relation [see Eq. (1.3)], is $\langle \acute{\eta}_n(t)\,\acute{\eta}_m(0)\rangle = 2T\gamma a^D \delta(t)\,\delta_{nm}/\lambda$. The average kinetic energy is independent of the effective mass M according to the usual formulas of quantum statistics $\langle\tilde{K}\rangle = NT/2$.

The form of the rescaled action Eq. (3.3) implies that the classical dynamics does not depend on λ. To see it explicitly rescale the momentum: $\tilde{p} = \lambda p$. Then the density matrix looks like

$$\hat{\rho} = \exp(-H_{\mathrm{eff}}/\theta_{\mathrm{eff}}), \tag{3.12}$$

$$\theta_{\mathrm{eff}} = \frac{\lambda T}{a^D}, \tag{3.13}$$

$$H_{\mathrm{eff}} = \sum_{n=1}^{N}\left\{\frac{1}{2}(p_n)^2 + \frac{1}{2}(\phi_{n+1}-\phi_n)^2/a^2 + 1 - \cos[\phi_n]\right\}. \tag{3.14}$$

The corresponding Langevin equations indeed do not contain the parameter of the semiclassical expansion λ explicitly:

$$[\phi_n(i+1) - \phi_n(i)]/\varepsilon = p_n(i), \tag{3.15}$$

$$[p_n(i+1) - p_n(i)]/\varepsilon = (\phi_{n-1}+\phi_{n+1}-2\phi_n)/a^2 - \sin(\phi_n) - \gamma p_n + \eta_n(i), \tag{3.16}$$

where

$$\langle\eta_n(i)\,\eta_m(j)\rangle = \frac{2\gamma\theta_{\mathrm{eff}}}{\varepsilon}\delta_{nm}\,\delta_{ij} \tag{3.17}$$

and we have discretized Langevin time by the amount of ε. Physical quantities are obtained in the limit $\varepsilon \to 0$. Notice that the normalization of the white noise (3.17) is different from that in [12].

Equations (3.12)–(3.14) define the effective classical system we are going to simulate. It incorporates the lattice spacing a as an input parameter, determined in the underlying quantum theory by Eq. (2.14). The kinetic energy of the effective system (3.12)–(3.14) averaged over the evolution (3.16) may be evaluated to check the effective temperature θ_{eff}:

$$\langle K_{\mathrm{eff}}\rangle = \frac{1}{2}N\theta_{\mathrm{eff}}. \tag{3.18}$$

In the Lagrangian formalism, both sets of equations, (3.9) and (3.10) and (3.15) and (3.16), are equivalent to the following second-order Langevin equation for the field ϕ:

$$\ddot{\phi}_n + \gamma\dot{\phi}_n = -\frac{\partial H_{\mathrm{eff}}}{\partial\phi_n} + \eta_n. \tag{3.19}$$

The second term on the left-hand side (LHS) of Eq. (3.19) is the damping force. It dominates over the first one at large friction or large times $t > \gamma^{-1}$. Then neglecting the first term in the LHS of Eq. (3.19) one obtains the first-order Langevin equation:

$$\phi_n(i+1) - \phi_n(i) = -\frac{\varepsilon}{\gamma}\frac{\partial H_{\rm eff}}{\partial \phi_n} + \sqrt{\frac{2\theta\varepsilon}{\gamma a^D}}\,\xi_n, \tag{3.20}$$

where $\theta = \lambda T$ and ξ is a random variable with Gauss' distribution of variance 1. θ is the only parameter of the classical model (apart from the lattice spacing). To fix the physical temperature one needs to know λ. Since λ is a parameter of the semiclassical expansion according to Eq. (3.3), it is fixed only in the underlying quantum theory.

The RHS of Eq. (3.20) depends on the ratio ε/γ, not separately on ε and γ. This implies a simple friction dependence of, say, the diffusion rate determined by means of the first-order Langevin equation: the diffusion rate must be inversely proportional to the friction coefficient $\Gamma(T,\gamma) \sim 1/\gamma$. Thus within the first-order Langevin treatment the absolute value of the diffusion rate is fixed in a simple way by the friction coefficient γ, which is a dimensional quantity. The second-order Langevin equation, valid for arbitrary friction, predicts nontrivial friction dependence, which has been evaluated explicitly by Kramers [1] in the case of one degree of freedom coupled to the heat bath. In the limit of large γ that friction dependence of the escape rate, of course, reduces to the one we just derived from the first-order Langevin equation. The question we would like to clarify is how large the friction coefficient must be in the case of field theory to allow one to use the first-order Langevin equation instead of the second-order one. Our numerical data proves to be helpful for this end.

IV. NUMERICAL SIMULATIONS

We have solved the second-order Langevin equations (3.15)–(3.17) numerically for the system of size $L = 50, a = 1$. This volume is sufficient to accommodate a few kinks (which size is 1 in our units) at low temperatures. The diffusion parameter $\Delta(t)$ has been measured, defined following [8] as

$$\langle\Delta(t)\rangle = \frac{1}{t_0}\int_0^{t_0} dt'\,\{\bar\varphi(t'+t) - \bar\varphi(t')\}^2. \tag{4.1}$$

From $\langle\Delta(t)\rangle$ we extract the diffusion rate $\Gamma \equiv \lim_{t\to\infty}\langle\Delta(t)\rangle/t$. Although Γ is proportional to the kink density at low temperature, it is defined for all temperatures, independently of the notion of kink, and without need to identify kinks at finite temperature. The system was observed over 5×10^7 to 2×10^8 iterations (i.e., a time $t_0 \sim 10^6$). The longer runs were necessary to reduce statistical errors at the lower temperatures where the diffusion rate is smaller. The time step was typically $\varepsilon = 0.02$. The Brownian motion of $\bar\varphi$ has been unambiguously observed. Figure 2 demonstrates the diffusion

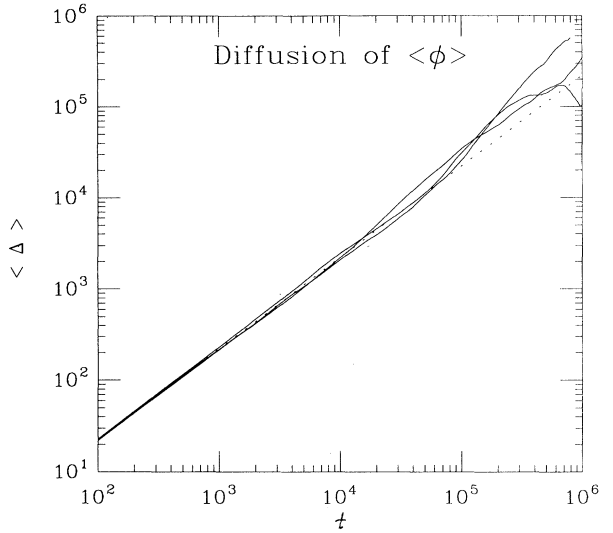

FIG. 2. Time dependence of the diffusion parameter (4.1) obtained from the second-order Langevin equation. Measurements were performed every 100 iterations. The parameters are $T = 6$, $L = 50$, $\varepsilon = 0.02$. Three solid lines correspond to different lattice spacings: $a = \{1, 0.5, 0.25\}$; the dashed line is a fit with slope 1.

at temperature $T = 6$ for three different values of the lattice spacing. The rate is obviously insensitive to the lattice spacing and the relatively large value $a = 1$ may be used to obtain physical results. Large values of a are preferable to save computer time.

Periodic as well as free boundary conditions[1] were studied. In both cases we measured the diffusion rate in the range of temperatures $\theta \cong 1.33$–18. The semiclassical domain corresponds to $\theta \ll 8$ in accordance with (3.2). Figure 3 shows the temperature dependence of the diffusion rate on a logarithmic scale. In the case of free boundary conditions all the data points starting from $T \cong 3$ downwards lie on a straight line. This implies the expected thermal activation behavior (3.5). The slope of the straight line is seen to be 8, which is exactly the classical value of the kink mass (3.2). In the case of periodic boundary conditions, a somewhat more interesting phenomenon is observed: starting around $T = 2$ the slope of the straight line changes from 8 to 16, which corresponds to the classical energy of a kink-antikink pair. This is again in accordance with the expectations (3.4) for periodic boundary conditions. The sensitivity to the boundary conditions appears in the lowest-temperature domain. Figure 4 shows that at higher temperatures

[1] In that case, the discrete Hamiltonian Eq. (3.14) is

$$H_{\rm eff} = \sum_{n=1}^{N}\left\{\frac{1}{2}(p_n)^2 + 1 - \cos[\phi_n]\right\} + \sum_{n=1}^{N-1}\left\{\frac{1}{2}(\phi_{n+1}-\phi_n)^2/a^2\right\}. \tag{4.2}$$

there is no dependence on the boundary conditions. The crossover temperature below which the kink-antikink pair energy is observed in (3.4) depends on the system size L. The larger the volume L the smaller that crossover temperature.

The diffusion rate can also be measured in the high-temperature domain $\theta \geq 8$, where the semiclassical approximation is not valid. Our numerical results are shown in Fig. 5 for both types of boundary conditions. The diffusion rate does not depend on the choice of boundary conditions as it is not associated with the production of kink-antikink pairs any more.

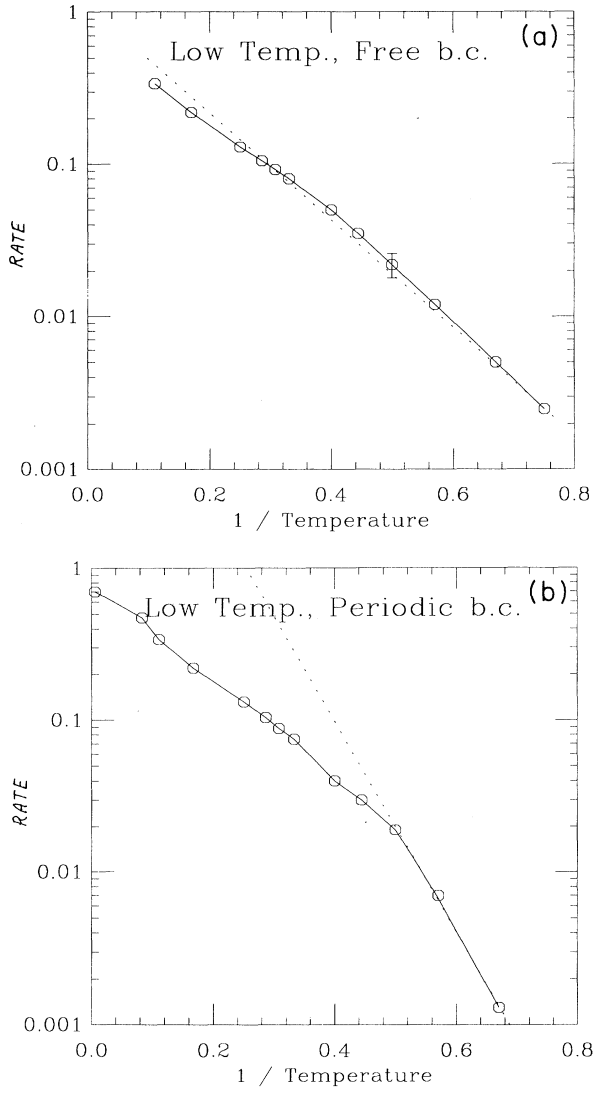

FIG. 3. Temperature dependence of the diffusion rate on a logarithmic scale for (a) free and (b) periodic boundary conditions. $L = 50$, $a = 1$. A typical uncertainty is shown for $T = 2$. The dashed lines correspond to the Boltzmann exponent with slope given by the classical value of the kink mass $M_k = 8$ in (a) and the energy of the kink-antikink pair $2M_k = 16$ in (b).

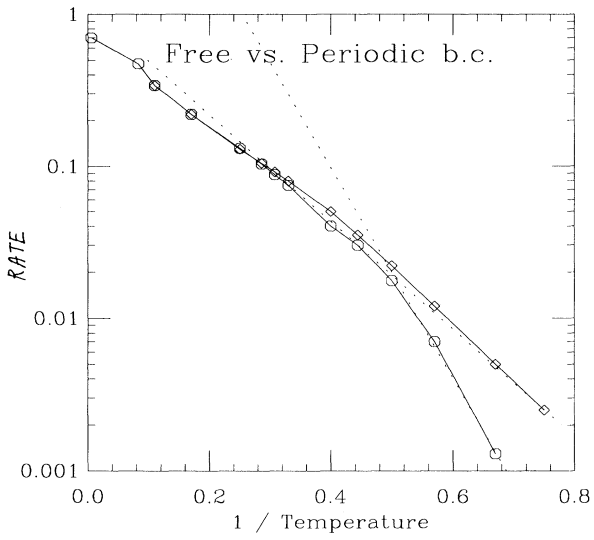

FIG. 4. Temperature dependence for free vs periodic boundary conditions at both high and low temperatures.

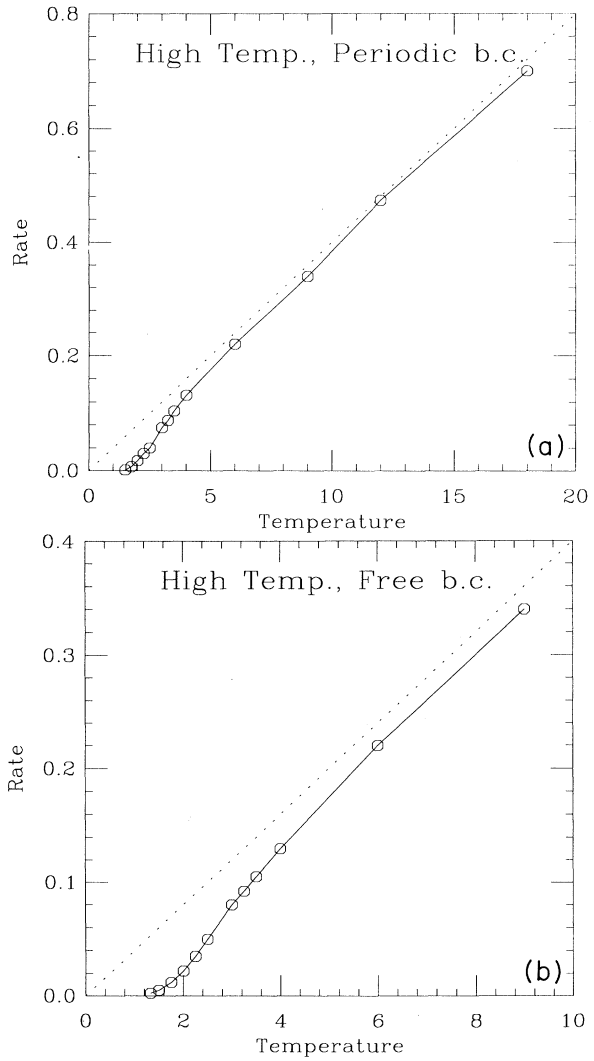

FIG. 5. Temperature dependence of the diffusion rate at high temperatures. The dashed line is a prediction from the corresponding first-order free Langevin equation.

At high temperatures the Langevin equation (3.20) can be integrated explicitly, because the noise term, whose contribution is proportional to $\sqrt{T}$, dominates over the regular force. Then the analytical predition for the rate is

$$\Gamma = \frac{2T}{\gamma L}. \tag{4.3}$$

The numerical measurements are in perfect agreement with Eq. (4.3).

The crossover temperature from the semiclassical to the high-temperature domain is seen to be around $T = 3$. Perhaps surprisingly it is less than the kink energy (3.2). To determine it more accurately we have measured the probability distribution of the averaged field $\bar{\varphi}$, whose logarithm determines the effective potential $V(\bar{\varphi}, T)$. One can see in Fig. 6 that at $T = 2$ there is a deep parabolic well at the origin, so that most of the time the field oscillates around $\bar{\varphi} = 0$. Beyond the parabolic well the potential is flat. This implies the free motion between the different vacuum sectors, which proceeds via the formation of kink-antikink pairs, seen as the modulation of the high frequency oscillations corresponding to the parabolic well. The deeper the well the better the very notion of the kink configuration is at $T \neq 0$. At temperature $T = 3$ the parabolic well is rather shallow, so the low frequency modulations usually interpreted as kinks become hard to identify. The effective potential is almost entirely flat, which means that the transitions between different classical vacua do not require smooth low frequency configurations any more. This is obviously the boundary of the semiclassical domain of temperatures. At temperature $T = 6$ there is no sign of the confining parabolic well.

Thus we have found that the effective potential $V(\bar{\varphi}, T)$ of the diffusing variable is flat in the high-temperature domain, starting from $T \simeq 3$. This result is interesting in the context of the baryogenesis within the standard electroweak theory [17,18]. In the standard model there is a variable, which is expected to diffuse at finite temperature. It is the Chern-Simons variable $N_{\rm CS}$. Diffusion of $N_{\rm CS}$ leads to the dissipation of the baryonic number. This effect could be responsible for the production of the baryon asymmetry in the expanding Universe. In [19] a scenario for baryogenesis within the standard model was suggested, in which the crucial assumption was the flat effective potential $V(N_{\rm CS})$ in the high-temperature domain. While to measure properly $V(N_{\rm CS})$ in the electroweak theory is not easy, our data in the sine-Gordon model indicate that the flat effective potential $V(N_{\rm CS})$ is a rather plausible assumption. We would like to emphasize again the similarity between the sine-Gordon model and Abelian-Higgs theory in 1+1 dimensions. The zero mode $\bar{\varphi}$ of the sine-Gordon theory plays the role of the Chern-Simons variable in the Abelian-Higgs model. One can decompose $\varphi \to \bar{\varphi} + \delta\varphi$, to demonstrate that the effective potential $V(\bar{\varphi}, T)$ is a bounded periodic function, allowing for the Brownian motion.

We now turn to the dependence on the friction coefficient. The friction coefficient γ is a dimensional input

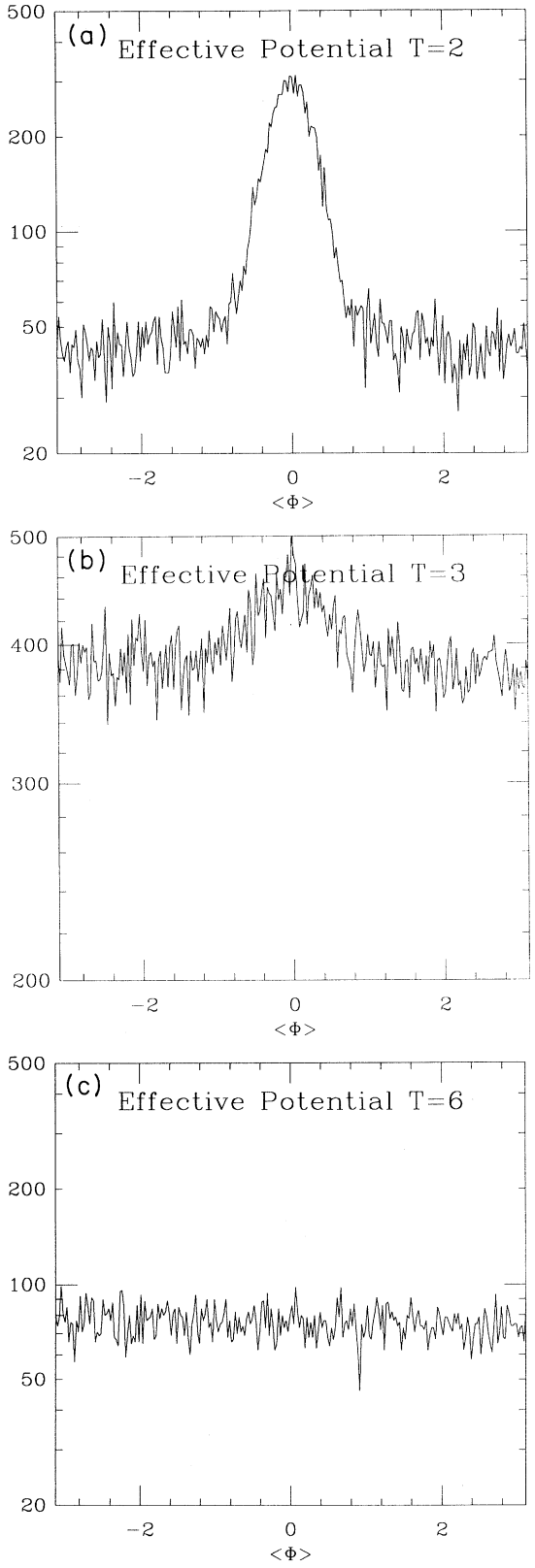

FIG. 6. Logarithm of the probability distribution (effective potential) of $\bar{\varphi}$ at different temperatures indicated on the plots.

parameter in the Langevin equation (3.19). It determines the scale as it is seen, for instance, from formula (4.3), derived for large γ. Although the friction dependence of the escape rate has been obtained analytically in [1] in the case of one degree of freedom exposed to the heat bath, it is a less trivial task in the field theory. We have measured the friction dependence of the diffusion rate numerically by solving Eqs. (3.15) and (3.16) for the two temperatures $T = 2, 6$ and for various friction coefficients. The results are shown in Figs. 7 and 8. In both the semiclassical and high-temperature domains we find the same behavior of the rate. The inverse rate varies linearly with the friction coefficient from large $\gamma > 1$ down to very small $\gamma \sim 10^{-2}$: $\Gamma^{-1} \propto (\gamma + \text{const})$. This simple friction dependence coincides with the one predicted by the first-order Langevin equation. Therefore we obtain experimental evidence that the first-order Langevin equation may be used to explore the large-time behavior of the correlators not only for large, but also for small friction coefficients, in particular, for $\gamma \sim 1$.

One can see from Fig. 8 that the rate does not diverge in the limit $\gamma \to 0$. It approaches some finite asymptotic value. Meanwhile the original Langevin equations become the conventional Hamiltonian ones in the limit $\gamma \to 0$. Therefore we expect the rate extracted from the second-order Langevin simulations in the limit of vanishing friction to coincide with the one obtained by means of microcanonical simulations. To verify this conjecture we first of all notice that the microcanonical simulations of classical systems in real time [15] naturally correspond to some fixed energy, not temperature. To obtain the time-dependent Gibbs averages, one has to average the result of the microcanonical measurement over the initial field configuration with the Gibbs weight:

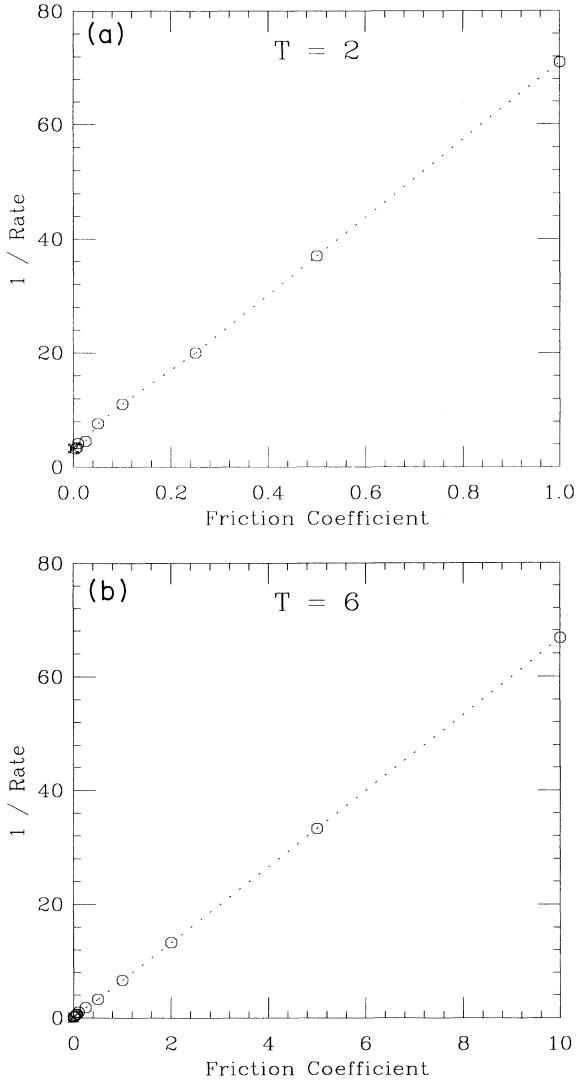

FIG. 7. Friction dependence of the rate in the (a) low and (b) high temperature domains obtained from the second-order Langevin equation. $L = 50$, $a = 1$. The dashed straight line is a prediction from the first-order Langevin equation, derived normally for large friction $\gamma > 1$ or large times.

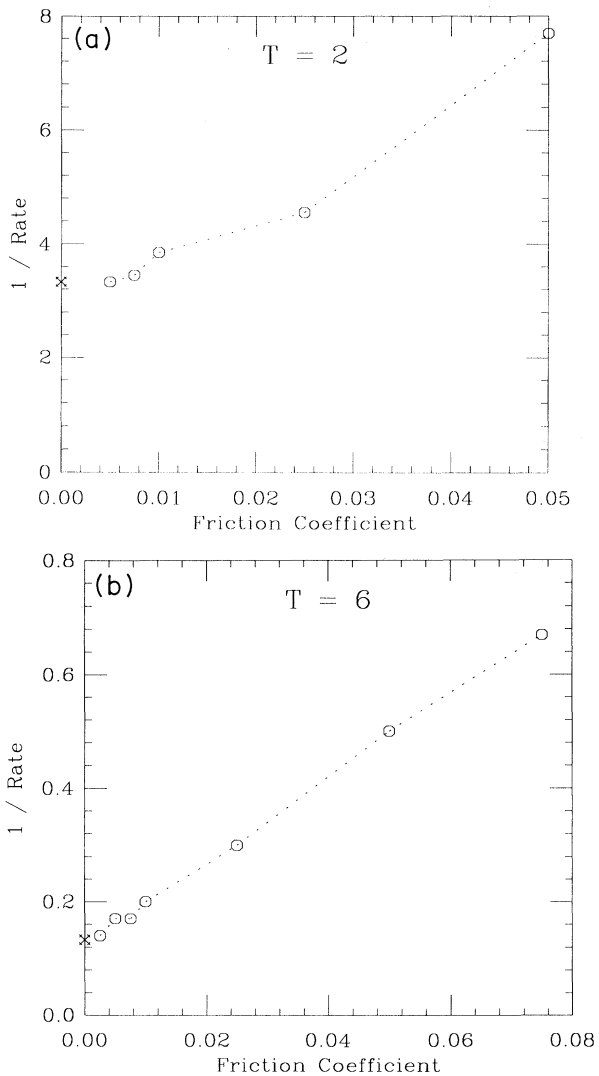

FIG. 8. Same as in Fig. 7, but only the points corresponding to very small values of the friction coefficient are shown. The cross points on the y axis are the extrapolations.

$$\langle \Delta(t) \rangle = \frac{\int \mathcal{D}\varphi_0 \mathcal{D}p_0 \exp[-H(\varphi_0, p_0)/T] \{\bar{\varphi}(t, \varphi_0, p_0) - \bar{\varphi}(0)\}^2}{\int \mathcal{D}\varphi_0 \mathcal{D}p_0 \exp[-H(\varphi_0, p_0)/T]}. \quad (4.4)$$

The problem here is that the value of the diffusion parameter Δ at time t, obtained as a result of the Hamiltonian evolution, is a functional of the initial field configuration $\{\varphi_0, p_0\} = \{\varphi(t=0), p(t=0)\}$. This functional is not known explicitly. However, following the suggestion by Smit [20] we evaluate this functional numerically. This means that to measure the Gibbs averaged diffusion parameter directly we calculate numerically $[\varphi(t) - \varphi(0)]^2$ from the Hamiltonian evolution for a given starting configuration $\{\varphi_0, p_0\}$, then update this starting configuration by means of the Metropolis procedure, corresponding to some temperature T, then do microcanonical evolution again and so perform the Gibbs average.

In this way the diffusion parameter (4.4) has been measured. The function $\langle \Delta(t) \rangle$ is shown in Fig. 9. One can see a crossover between two domains of time. At short times $t \lesssim 10^2$ the deterministic behavior is observed $\langle \Delta(t) \rangle \sim t^2$, while at $t \gtrsim 10^2$ the Brownian motion sets in $\langle \Delta(t) \rangle \sim t$. The corresponding diffusion rate as a function of temperature is shown in Fig. 10. The thermal activation behavior is clearly seen at low temperatures. As a result we observe a remarkable coincidence between the data from the second-order Langevin simulations in the limit of vanishing friction and the direct Gibbs averages. One obtains $\Gamma(T=2) \simeq 0.3$ and $\Gamma(T=6) \simeq 8$ from both Fig. 8 and Fig. 10. This result answers the question of how to relate the Langevin measurements to the direct calculations of the Gibbs average (4.4).

V. COMMENTS ON THE ERRORS

As mentioned above, all the runs, the results of which are presented, were long enough to make statistical errors negligible. The two main sources of systematic errors are the finite lattice spacing a and the time step ε. The insensitivity to the lattice spacing was discussed before (see Fig. 2). Here we would like to address the artifacts of the discretization of the Langevin time.

It is known [21] that the finite time step in Langevin simulations makes the temperature of the simulated system T_{eff} larger than the input one T: $\Delta T \equiv T_{\text{eff}} - T = O(\varepsilon)$. To check the effective temperature we measure the diffusion parameter at rather small times, as shown on Fig. 11. The Brownian diffusion is clearly observed at short times, but it has nothing to do with the motion of the system between topologically different vacua. At short times the white noise always dominates over the regular force in the Langevin equation. Therefore the short-time behavior of $\langle \Delta(t) \rangle$ is, in fact, controlled by the free Langevin equation, which immediately implies diffusion of $\bar{\varphi}$. This short-time diffusion is already sensitive to the discretization effects. Its diffusion rate is given by T_{eff}, which has been measured numerically and is shown in Fig. 12. One can see that the effective tem-

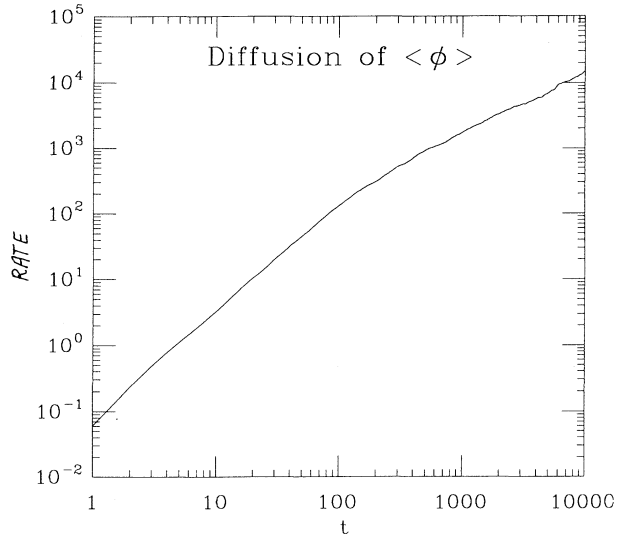

FIG. 9. Time dependence of the diffusion parameter (4.1) obtained from direct measurements of the Gibbs average (4.4) for periodic boundary conditions. The temperature is $T = 1.5$. The initial field configuration was updated by means of the Metropolis procedure 100 times and each time 10^6 leapfrog iterations of the microcanonical evolution were performed. $L = 50$, $a = 1$, $\varepsilon = 0.1$

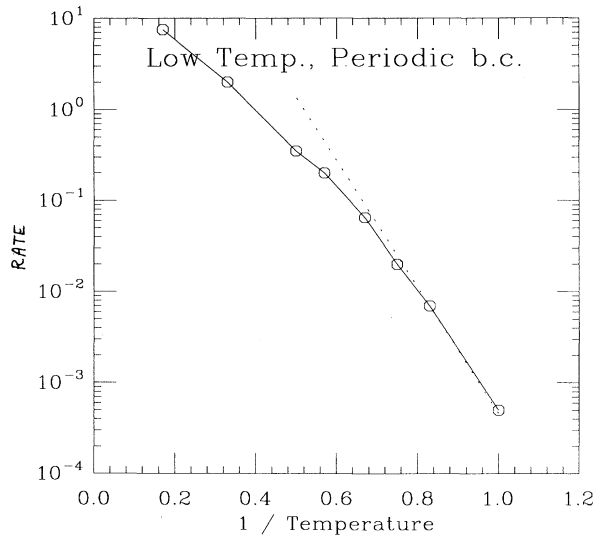

FIG. 10. Temperature dependence of the diffusion rate obtained from direct measurements of the Gibbs average (4.4). The dashed line corresponds to the Boltzmann factor with the energy of the kink-antikink pair. The parameters of the measurements are as in Fig. 9.

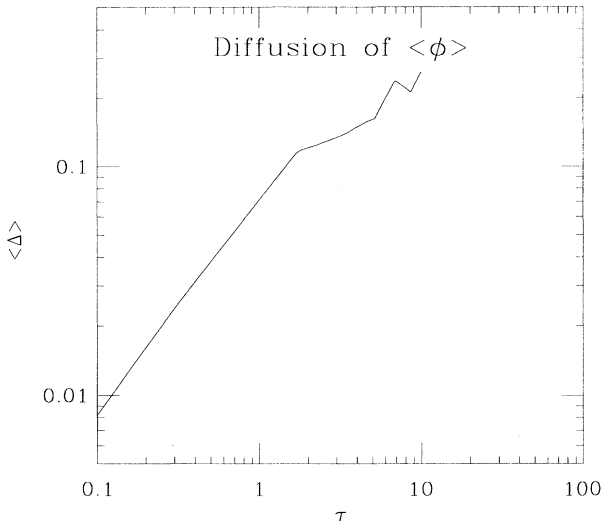

FIG. 11. The typical diffusion at short times, controlled by the free Langevin equation.

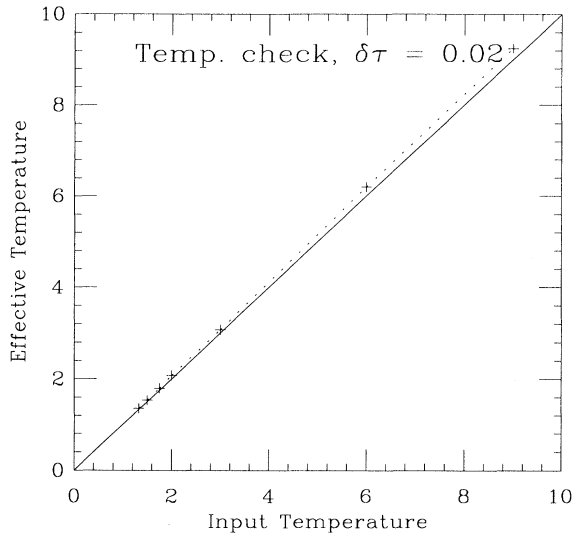

FIG. 12. The effective temperature of the simulated system obtained from the short-time diffusion. The dashed line is a fit. The solid line corresponds to the input temperature. The deviation is proportional to the time step ε.

perature of the simulated system follows the input one with fairly high accuracy. Since these measurements are obtained from very short runs, the computer time needed is quite small. So we have also checked that $\Delta T = c\varepsilon$, with $c = 1.5 \pm 0.5$.

Another alternative to checking the effective temperature of the simulated system is measuring the Langevin average of the canonical momentum squared over the whole run: $\langle p^2 \rangle = T_{\text{eff}}$. This way is not easily generalizable for theories where there is a coupling between the canonical momenta and coordinates in the Hamiltonian, as in gauge theories.

VI. CONCLUSIONS

The study of the sine-Gordon field theory in 1+1 dimensions shows that the classical Langevin simulations in real time prove to be efficient in obtaining valuable information about the nonperturbative effects in field theory at high temperatures. In the semiclassical domain of temperatures, kinks are seen as smooth modulations of the high frequency oscillations of the field. The diffusion between different classical vacua is due to random process of production and free motion of kink-antikink pairs during the Langevin evolution. This is very well confirmed by the measured temperature dependence of the diffusion rate, which exhibits thermal activation behavior with the classical value of the kink mass in the Boltzmann exponent.

Crossover is observed between the semiclassical and high-temperature domain, where the semiclassical approximation is not valid. The effective potential of the diffusing variable is found flat at high temperatures. In the high-temperature domain at moderate friction the diffusion rate follows the prediction of the free Langevin equation.

The dependence of the diffusion rate on the friction coefficient is found to be identical to the prediction of the first-order Langevin equation down to rather small friction coefficients $\gamma \sim 10^{-2}$. This justifies the use of the first-order Langevin equation in the calculations of correlation functions at large real times.

We also measure the diffusion parameter directly as the Gibbs ensemble average by means of the Metropolis procedure and microcanonical evolution. The corresponding diffusion rate is found to coincide with the smooth extrapolation of Langevin measurements in the limit of vanishing friction coefficient.

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