

Statistical Mechanics of Kinks in 1 + 1 Dimensions

Francis J. Alexander^{1,*} and Salman Habib^{2,†}

¹Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

²T-6, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

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We investigate the thermal equilibrium properties of kinks in a classical ϕ^4 field theory in 1 + 1 dimensions. The distribution function, kink density, and correlation function are determined from large scale simulations. A dilute gas description of kinks is shown to be valid below a characteristic temperature. A double Gaussian approximation to evaluate the eigenvalues of the transfer operator enables us to extend the theoretical analysis to higher temperatures where the dilute gas approximation fails. This approach accurately predicts the temperature at which the kink description breaks down.

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The statistical mechanics of coherent structures such as solitons and solitary waves in nonlinear systems has been a subject of study for some time [1]. Recent interest has been fueled by new applications not only in condensed matter physics [2,3], but also by potential applications in particle physics (sphalerons) [4] and cosmology (domain walls, baryogenesis) [5]. In this paper we focus on the classical equilibrium statistical mechanics of solitary wave solutions ("kinks") of a tachyonic mass ϕ^4 field theory in 1 + 1 spacetime dimensions with Lagrangian

$$L = \frac{1}{2} (\partial_t \Phi)^2 - \frac{1}{2} (\partial_x \Phi)^2 + \frac{1}{2} m^2 \Phi^2 - \frac{1}{4} \lambda \Phi^4. \quad (1)$$

For our simulations we use the dimensionless form of this theory, given by the transformations $\Phi \rightarrow a\phi$, $x \rightarrow x/m$, and $t \rightarrow t/m$, where $a^2 = m^2/\lambda$. The equation of motion then becomes

$$\partial_{tt}^2 \phi = \partial_{xx}^2 \phi - \phi(\phi^2 - 1). \quad (2)$$

What makes this model so useful is that its behavior is representative of a large class of soliton-bearing systems. Moreover, it is amenable to both theoretical analysis and numerical simulation.

The statistical mechanics of kinks in this system has been studied by two approaches. In the first, and phenomenological, approach one assumes that the kinks and the fluctuations ("phonons") about the asymptotic field minima may be treated as weakly interacting elementary excitations. The canonical partition function can then be found by standard methods [1,6,7]. Alternatively, as shown by Krumhansl and Schrieffer (KS) [6], building on earlier work of Scalapino, Sears, and Ferrell [8], it is possible to calculate the partition function, in principle exactly, by exploiting a transfer operator technique. KS showed that in the low temperature ("dilute gas") limit the partition function factorizes into a contribution from a harmonic term and from a tunneling term which they were able to identify with the phonon and kink contributions, respectively, in the phenomenological theory. The ideas of KS were further refined and extended to a wider class of systems by Currie, Krumhansl, Bishop, and Trulinger [7]. In particular, interactions of kinks with linear-

ized phonons were considered, leading to substantial corrections to the results of KS.

A key result of these efforts is the prediction that the spatial density of kinks

$$n_k \propto \sqrt{E_k \beta} \exp(-E_k \beta), \quad (3)$$

where $E_k = \sqrt{8/9} m^3/\lambda$ ($E_k = \sqrt{8/9}$ for the dimensionless form of the theory) is the kink energy, and β the inverse temperature (for the dimensionless case, $\beta \rightarrow \beta/a^3 \sqrt{\lambda}$). A related prediction is that at low temperatures the field correlation length λ defined by

$$\langle \phi(0)\phi(x) \rangle \sim \exp(-x/\lambda) \quad (4)$$

has an exponential temperature dependence [7],

$$\lambda = \frac{1}{4} \left(\frac{\pi}{3} \right)^{1/2} \frac{1}{\sqrt{E_k \beta}} \exp(E_k \beta). \quad (5)$$

Computer simulations to verify these results date back to Ref. [9] where only a qualitative agreement was found. Recent work [10-12] has led to more detailed comparisons; however, significant discrepancies have been reported. This has led to theoretical speculation [13,14] regarding possible corrections to the dilute gas theory of kinks. It has been suggested that these discrepancies are due to finite size effects and phonon dressing of the bare kink energy (breather contributions to the free energy may also be significant [15]). As we show in this Letter, the earlier simulations were not carried out at low enough temperatures: Nevertheless, the authors interpreted their results in terms of WKB formulas that are simply not a valid description over the range of temperatures studied. In this intermediate temperature regime, there is no unique characterization of what constitutes a kink and how to differentiate it from a nonlinear phonon. By going to low enough temperatures where the dilute gas results are valid, we are also able to rule out an earlier claim of substantial phonon dressing even at these temperatures [9].

We have studied the equilibrium statistical mechanics of kinks in the ϕ^4 model (1) by implementing a Langevin

code on a massively parallel computer. The key idea is to supplement the equation of motion (2) with noise and viscosity terms obeying an appropriate fluctuation-dissipation theorem so that the system is driven to thermal equilibrium at the desired temperature [16]. To understand our results in the high and intermediate temperature regions not susceptible to a dilute gas analysis, we have used a double Gaussian wave function approximation for the quantum mechanical problem which results from applying the transfer operator method. Not only is this method accurate but it also suggests a natural decomposition of nonlinear phonon and kink degrees of freedom in the intermediate temperature regime (details will be reported elsewhere [17]). Our results are (1) the dilute gas predictions for the kink density and the correlation length are in good agreement with the simulations below a certain (theoretically estimable) temperature, (2) above this temperature the double Gaussian results for the kink number and the correlation length agree with the simulations, (3) kinks are found to disappear above a characteristic temperature, in good agreement with our theoretical prediction, and (4) our Gaussian approximation accurately describes the classical single point field distribution function at high and intermediate temperatures where the dilute gas (WKB) approximation breaks down.

The canonical partition function for the Lagrangian (1) is given by the functional integral

$$Z = \int D\phi D\pi \exp[-\beta H(\phi, \pi)], \quad (6)$$

where π is the canonical momentum of the field and H the field Hamiltonian. The transfer operator technique [8] reduces the calculation of the partition function in the thermodynamic limit to simply finding the ground state energy of the double well quantum Hamiltonian (here written for the dimensionless case),

$$H_Q = \frac{1}{2} p^2 - \frac{1}{2\beta^2} \bar{\phi}^2 + \frac{1}{4\beta^4} \bar{\phi}^4, \quad (7)$$

where $\bar{\phi} = \beta\phi$. At low temperatures the two wells are widely separated and the ground state energy is given by the oscillator ground state energy for one of the wells minus the tunnel-splitting term, usually calculated by WKB methods. The dilute gas or WKB approximation for the kink number is valid when the tunnel splitting is small enough such that only the first two energy eigenstates are necessary to estimate the ground state energy of the Hamiltonian (7) [18]. At higher temperatures where kinks still exist, higher energy states cannot be ignored. Since kinks are associated with tunneling, we expect them to vanish when the ground state energy is higher than the classical barrier height: This intuition is confirmed by our simulations.

One can compare the simulations of the kink system with numerical solutions for the energy eigenvalues of the Hamiltonian H_Q . Instead, we take a different approach

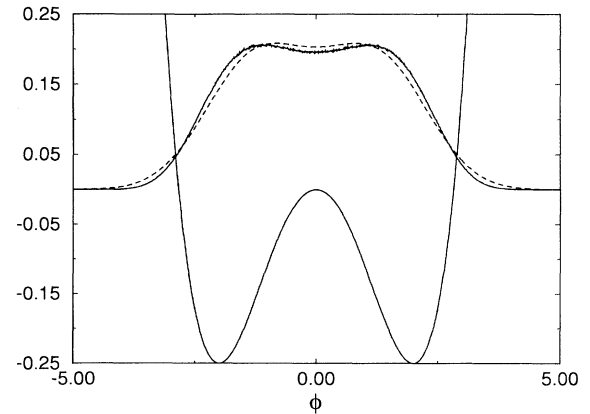


FIG. 1. The classical distribution function $P[\phi]$ given by the simulation (solid line) and the distribution Ψ_0^2 from the double Gaussian approximation (dashed line) plotted against $\bar{\phi}$ for $\beta=2$. The potential $V = -(1 - \bar{\phi}^2/2\beta^2)\bar{\phi}^2/2\beta^2$ of the equivalent quantum problem (7) is also shown.

by implementing a double Gaussian variational method which is an order of magnitude more accurate than the simple Gaussian approximation [19] for this problem and correctly accounts for the reduction of energy due to overlap terms in the wave functions of the two wells, at least for moderate to large overlaps. Three qualitatively different regimes exist: (1) All the energy eigenvalues lie above the classical barrier, (2) the ground state energy lies below the classical barrier height, and (3) the energy difference between the ground and first excited state becomes negligible in comparison with the energy difference between the ground and the second excited state (this occurs for $\beta > 6$). Our simulations confirm the theoretical expectations that there are no kinks in region (1), that there are kinks, but that the dilute gas approximation is invalid in region (2), and finally, that the dilute gas approximation is accurate in region (3) (a regime unexplored in detail by previous simulations).

We measure the classical single point field distribution function $P[\phi]$ directly in our simulations. For the analogous quantum mechanical problem this is just the square of the ground state wave function Ψ_0 . Results from the simulations and our theory are compared in Fig. 1 and are in reasonable agreement. The presence of kinks implies a double peak in $P[\phi]$ [20] (the converse is false) while a single peak at the origin means that kinks and thermal phonons can no longer be distinguished. From the simulations such a transition occurs at $\beta \approx 1.7$, in agreement with the theoretical calculation of when Ψ_0^2 goes over from a double to single peaked distribution. As expected, this is also the temperature ($\beta = 1.734$) where the ground state energy crosses the classical barrier height (a discussion of various methods to determine the characteristic temperature is given in Ref. [21]). The double peaks in the distribution function move inward from the classical minimum as the temperature increases

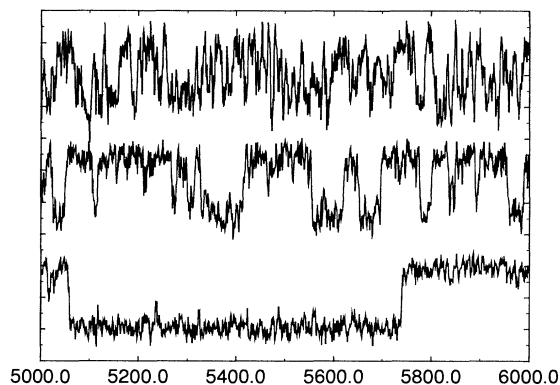


FIG. 2. Field configurations, from top to bottom, at $\beta=2$, $\beta=4$, and $\beta=8$. Only a 1000 lattice unit sample of the total lattice size of 16 384 is shown.

(this is clearly seen in Fig. 1). Physically this can be understood as nonlinear phonon corrections due to the fact that near each minimum, the potential is not symmetric under reflection around the minimum.

The Langevin equation for the dimensionless theory is

$$\partial_t^2 \phi = \partial_{xx}^2 \phi - \eta \partial_t \phi + \phi(1 - \phi^2) + F(x, t). \quad (8)$$

To guarantee an approach to equilibrium, the Gaussian, white noise F , and the viscosity η are related via the fluctuation-dissipation theorem:

$$\langle F(x, t) F(x', t') \rangle = 2\eta\beta^{-1} \delta(x - x') \delta(t - t'). \quad (9)$$

We carried out numerical simulations on lattices with 16 384 sites and solved the Langevin equation using a standard Euler algorithm. The time step was $\Delta t = 0.02$ and the lattice spacing was $\Delta x = 0.5$. For all the simulation results reported here we used a viscosity of $\eta = 1.0$.

Our system size is 1 to 2 orders of magnitude larger than that in most previous simulations. Large system sizes are necessary to get acceptable statistics at low temperatures. Systems were evolved from a random initial condition to equilibrium. The length of time necessary to ensure equilibrium increased with inverse temperature. For $\beta=8$ the time required was approximately 10^7 time steps, and for the highest temperatures, less than 10^5 steps.

Two quantities of interest reported here are the kink number and the field correlation length. To compute the kink number, we need an operational way to identify kinks, although there is an exact kink solution available theoretically. As a result we examine several possible definitions, all of which rely on a knowledge of the kink size. From the classical solution for a kink centered at x_0 , $\phi = \tanh[(x - x_0)/\sqrt{2}]$, the kink scale L_k is approximately 8 lattice units. Raw kink configurations are shown in Fig. 2. At low temperatures ($\beta > 5$), kinks may be identified easily; however, at higher temperatures this is clearly not the case.

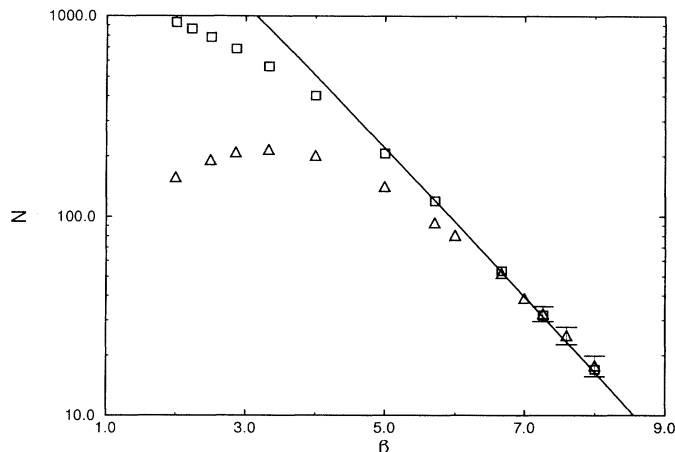


FIG. 3. Total number of kinks and antikinks as a function of β . Squares denote counts with a smoothed field (smoothing scale of 8 lattice units) definition of kinks, triangles for the zero-crossing count method explained in the text, and the solid line is a fit by (3). Where not shown, error bars are of the order of the sizes of the symbols. The smoothed field result is in agreement with the results of Ref. [12] for $\beta < 5$.

The simplest thing to do is to count the number of zero crossings of the field, since one may argue that these are the “tunneling events” which correspond to kinks. However, at higher temperatures there are zero crossings due to thermal noise, and counting all zero crossings would lead to a gross overestimation of the number of kinks. A possible solution is to use a smoothed field by either averaging or block spinning the actual field configuration over a length of the order of the kink scale. The latter approach was taken in previous simulations [10–12]. This solution is not without flaws either, as rapid fluctuations can still appear as kinks. We prefer to count kinks in the following way: At a particular time we first find all zero crossings. To test the legitimacy of a given zero crossing we check for zero crossings one kink scale (8 lattice units) to its right and to its left. If no zero crossings are found, we count it as a kink; otherwise not.

The number of kinks is plotted against β in Fig. 3. Above $\beta \sim 6$, the averaged field method and our method for counting kinks agree. Moreover, in this (low temperature) range, the dilute gas expression for the kink number (3) is in excellent agreement with the data. At elevated temperatures, there is a clear disagreement between the two methods of counting kinks. The average field technique has the number of kinks monotonically increasing with temperature, whereas, in accord with intuition and the behavior of $P[\phi]$, the second technique clearly shows a reduction in the kink number at higher temperatures. Moreover, in this temperature regime the number of kinks computed with the smoothing method depends strongly on the smoothing scale. We conclude that for $\beta < 6$ the number of kinks cannot be extracted

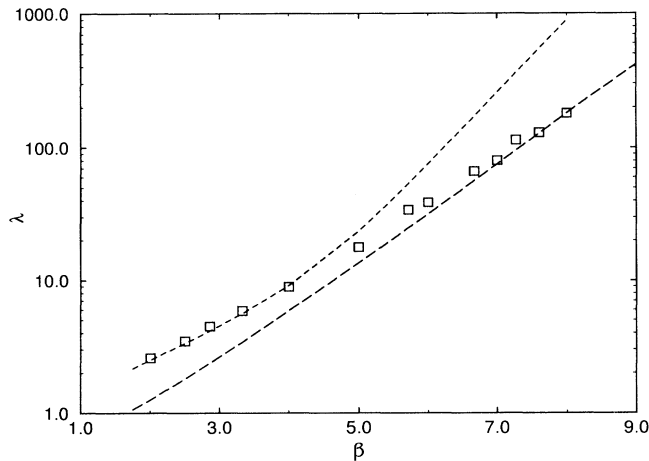


FIG. 4. Field correlation length λ as a function of β . The short-dashed line is the Gaussian prediction, whereas the long-dashed line is the WKB result (5).

with any confidence from the smoothing method. Unfortunately, this is precisely the temperature regime explored in previous simulations. (The problem with defining a kink number at intermediate temperatures has also been noted recently by Krasnitz and Potting [22].)

The correlation length λ is plotted against β in Fig. 4. For $\beta > 6$, the WKB prediction (4) holds, whereas for $\beta < 5$, where the wave function overlaps are not negligible, the double Gaussian approximation is valid. Fortunately, there are no ambiguities here with regard to measurements at higher temperatures.

As a consequence of the above results, we conclude that the dilute gas or WKB approximation is excellent for $\beta > 6$ with no further phonon dressing of the bare kink energy beyond that already included in (3) and (5) at these low temperatures. At higher temperatures, the WKB analysis fails, though theoretical progress is possible with the double Gaussian technique.

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*Electronic address: fja@goshawk.lanl.gov

†Electronic address: habib@eagle.lanl.gov

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