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Exact Thermodynamics of the Double sinh-Gordon Theory in 1 + 1 Dimensions

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We study the classical thermodynamics of a (1 + 1)-dimensional double-well sinh-Gordon theory. Remarkably, the Schrödinger-like equation resulting from the transfer integral method is quasi-exactly solvable at several temperatures. This allows exact calculation of the partition function and some correlation functions above and below the short-range order ("kink") transition, in striking agreement with high resolution Langevin simulations. Interesting connections with the Landau-Ginzburg and double sine-Gordon models are also established. [S0031-9007(97)04557-2]

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The statistical mechanics of nonlinear coherent structures in low dimensions has long attracted theoretical attention, both for the intrinsic interest in such fundamental problems as kink nucleation and dynamics, as well as in diverse applications, e.g., in conducting polymer physics [1] and DNA denaturation [2]. Both analytic and numerical techniques have been applied to these problems: Well known among them are the (analytic) transfer integral method and the (numerical) Langevin method. The transfer integral technique converts the problem of finding the classical partition function Z_{cl} to an eigenvalue problem for a Schrödinger-like equation to which familiar approximation methods such as WKB can then be applied [3]. The advantage of Langevin methods is that (unlike Monte Carlo) real time quantities such as temporal correlation functions can be computed, and kinks and/or antikinks tracked both in space and time.

In the past, applications of these methods have yielded comparisons of approximate analytic results with numerical data to only rather low levels of accuracy, of order of tens of percent [4]. In this Letter we report substantial progress on both fronts. We discuss a nonintegrable (1 + 1)-dimensional field theory for which thermodynamic quantities can be computed exactly at several temperatures using techniques from quasi-exactly solvable (QES) potentials [5] in quantum mechanics. This theory is in the same class as the more familiar Landau-Ginzburg model and also admits exactly known kink solutions [6]. We have carried out very high resolution Langevin simulations and find excellent agreement with the exact results at the checkpoint temperatures. The high accuracy of the Langevin simulations allows the use of the probability distribution function (PDF) to directly compute thermodynamic quantities [7] thus providing an alternative to conventional methods based on fluctuations.

In order to calculate Z_{cl} exactly at various temperatures, one has to solve a Schrödinger equation with a temperature dependent mass. While completely solvable potentials are rare, in the last few years several double-well QES models have been discovered for which the exact classical partition function can be found at one given temperature. The drawback has been that the exact eigenstates are known only for a given set of couplings, and as a result, it has not been possible to obtain the exact Z_{cl} at more temperatures. In this Letter we show that for the double sinh-Gordon (DSHG) QES problem, if the ground state energy is known for n different values of coupling constants, then Z_{cl} can be evaluated for any of these theories (with a given set of coupling constants) at n different temperatures. This is also true for the triple well ϕ^6 and the double sine-Gordon (DSG) models, results for which will be reported elsewhere [8]. We conjecture that this result holds for a large class of QES problems.

The double-well ϕ^4 model in $1 + 1$ dimensions has been extensively studied. However, in this case the Schrödinger equation does not possess known exact solutions. To overcome this problem we turn to the DSHG potential:

$$V_{\mathrm{DSHG}}(\phi) = (\zeta \cosh 2\phi - n)^2, \qquad (1)$$

where ζ is a positive parameter. In order to have a double-well potential, $n > \zeta$, in which case the two minima are located at $\cosh 2\phi_0 = n/\zeta$. Moreover, for the system to be QES, n has to be a positive integer. This potential is the hyperbolic analog of the double sine-Gordon system. Similar potentials arise in the context of the quantum theory of molecules (e.g., a homonuclear diatomic molecule), wave motion describing the normal modes of vibration of a stretched membrane of variable density, and as the solution of a Fokker-Planck equation [9]. The hyperbolic analog of the sine-Gordon equation is a single-well potential (sinh-Gordon) and thus uninteresting from the soliton statistical mechanics perspective.

The DSHG potential written in the form (1) has all the generic features of a double-well potential such as Landau-Ginzburg, but allows for much greater analytic progress. Below we find exact solutions for (1) a kink, (2) phonon dispersion, (3) a kink lattice, and (4) the first few eigenvalues and eigenfunctions of the transfer operator at certain temperatures, allowing thereby analytic calculation of the PDF and correlation functions in the thermodynamic limit.

We exhibit below the exact kink and kink lattice solutions for the DSHG theory (details will be given in Ref. [8]). A kink is a time independent solution resulting from the minimization of the total energy density $\varepsilon(x) = V_{\mathrm{DSHG}}(\phi) + (g/2)\phi_x^2$ with the boundary conditions $\phi \to \pm\phi_0$ as $x \to \pm\infty$. The constant g is often introduced in condensed matter treatments as a phenomenological parameter and controls the kink size. In a field theoretic context, however, $g = 1$, and this is the value we choose here. (All the solutions given below can be written for arbitrary g.)

The kink-antikink solution located at x_0 is $(n > \zeta)$

$$\phi(x) = \pm \tanh^{-1}\left[\tanh \phi_0 \tanh\left(\frac{x - x_0}{\xi}\right)\right], \qquad (2)$$

where $\tanh \phi_0 = \sqrt{(n - \zeta)/(n + \zeta)}$, $\xi = [2(n^2 - \zeta^2)]^{-1/2}$. The kink has topological charge $Q = \int_{-\infty}^{\infty} \frac{\partial \phi}{\partial x}\, dx = 2\phi_0$. Traveling kink solutions are obtained by boosting to velocity v via $x \to (1 - v^2)^{-1/2}(x - vt)$. The statistical mechanics of kinks is governed largely by the kink energy (or rest mass):

$$E_s = 4\xi n\sqrt{n^2 - \zeta^2} \tanh^{-1}\left(\sqrt{\frac{n - \zeta}{n + \zeta}}\right) - 2\xi(n^2 - \zeta^2).$$

The phonon dispersion around the minima $\pm\phi_0$ for this model is $\omega_q^2 = q^2 + 8(n^2 - \zeta^2) = q^2 + (2/\xi)^2$ and the phonon contribution to the free energy per unit length is

$$F_{\mathrm{vib}} = \frac{1}{2\pi\delta} \ln\left(\frac{2\pi}{\delta\beta}\right) + \frac{1}{\beta}\sqrt{2(n^2 - \zeta^2)}, \qquad (3)$$

with δ being the lattice constant and $\beta \equiv 1/k_B T$.

In order to understand kink-antikink interactions, it is very useful to construct kink lattice solutions (a kink-antikink chain). For the DSHG theory, this solution is

$$\begin{aligned} \phi_L(x) &= \pm \tanh^{-1}\left[\tanh \phi_1 \,\mathrm{sn}\left(\frac{x - x_0}{\xi_L}, k\right)\right], \\ k &= \frac{\tanh \phi_1}{\tanh \phi_2}; \qquad (4) \\ \xi_L &= \frac{k}{2\sqrt{2}\,\zeta \sinh \phi_1 \cosh \phi_2}; \qquad d = 4K\xi_L, \end{aligned}$$

where d is the periodicity of the kink lattice, $K(k)$ is the complete elliptic integral of the first kind with modulus k, $\mathrm{sn}(x, k)$ is the Jacobi elliptic function, and with $0 < V_0 < V(\phi = 0) = (n - \zeta)^2$,

$$\begin{aligned} \cosh 2\phi_{1,2} &= \frac{n}{\zeta} \mp \frac{\sqrt{V_0}}{\zeta}; \\ k^2 &= \frac{n^2 - (\sqrt{V_0} + \zeta)^2}{n^2 - (\sqrt{V_0} - \zeta)^2}. \end{aligned} \qquad (5)$$

The topological charge (per period) in the lattice problem $Q_L = 2\phi_L(K) = 2\phi_1$ is smaller than the single kink case. The kink size in the kink lattice ξ_L is also smaller than the free kink size ξ.

The energy of the kink lattice per period (i.e., energy per kink-antikink pair plus the interaction energy) is

$$E_L = 4\xi_L\left[(n + \zeta)^2 K + \frac{\xi^2}{\xi_L^2}(n^2 - \zeta^2)(K - E) - 4n\zeta\Pi\right],$$

where $E(k)$ and $\Pi(\tanh^2 \phi_1, k)$ are complete elliptic integrals of second and third kind, respectively. In the dilute limit $(k \to 1, d \to \infty)$ the divergences in $K(k)$ and $\Pi(\tanh^2 \phi_1, k)$ exactly cancel out and we recover the single kink result E_s. The interaction energy as a function of separation (i.e., k or d) is given by $E_{\mathrm{in}} = E_L - 2E_s$.

Turning now to the computation of Z_{cl}, we note that this calculation can be divided into two parts: a trivial Gaussian integration over the field momentum, and a computation of the configurational partition function, which via the transfer integral method becomes equivalent to solving a Schrödinger-like equation [3]. The Hamiltonian for the DSHG theory is

$$H = \int dx\left[\frac{1}{2}\pi^2 + \frac{1}{2}(\partial_x\phi)^2 + V_{\mathrm{DSHG}}(\phi)\right] \qquad (6)$$

and this leads to the Schrödinger equation for the eigenvalues and eigenfunctions of the transfer operator

$$-\frac{1}{2\beta^2}\frac{\partial^2}{\partial\phi^2}\Psi_k + (\zeta\ \cosh\ 2\phi - n)^2\Psi_k = E_k\Psi_k\,. \tag{7}$$

Remarkably, this equation is an example of a QES system. Using results for a related potential from Ref. [5], at $2\beta^2 = 1$ the eigenstates of the first n levels can be found for $n = 1, 2, 3, 4$. (We have extended this to the cases $n = 5, 6$.) However, what one really wants is to consider a given fixed-n theory and obtain eigenstates at *different* temperatures. It is easy to see from Eq. (7), by simple rescaling, that solutions of a fixed-n theory at certain values of β are the same as the solutions of *another* theory (different n and ζ) at $2\beta^2 = 1$. Depending on the chosen value of n, exact solutions are available at different fixed values of β. Here, we restrict ourselves to one such family ($n = 2$) which allows the exact computation of the first few eigenstates at $8\beta^2 = m^2$ ($m = 1, \ldots, 6$). For illustration, two examples of the (unnormalized) ground states are given below (see also Fig. 1). The first (high temperature, $\beta^2 = 1/8$) has an eigenfunction with a single peak, while the second (lower temperature, $\beta^2 = 1/2$) has a double peak:

$$\begin{aligned}\Psi_0(\phi)|_{\beta^2=\frac{1}{8}} &= \exp\left(-\frac{1}{4}\zeta\ \cosh\ 2\phi\right),\\ \Psi_0(\phi)|_{\beta^2=\frac{1}{2}} &= \cosh\ \phi\ \exp\left(-\frac{1}{2}\zeta\ \cosh\ 2\phi\right),\end{aligned} \tag{8}$$

with corresponding ground state energies, $E_0 = 4 + \zeta^2$, $E_0 = \zeta^2 - 2\zeta + 3$. The PDF for the field is the square of the normalized ground state eigenfunctions. Solutions at higher energies and other values of β are given in Ref. [8].

Once the eigenvalues of the transfer operator are known, they can be used to compute the correlation functions $C_1(x) = \langle\phi(0)\phi(x)\rangle$ and $C_2 = \langle\delta\phi^2(0)\delta\phi^2(x)\rangle$, using

$$C_1(x) = \sum_k |\langle\Psi_k|\phi|\Psi_0\rangle|^2\ \exp[-\beta|x|(E_k - E_0)]\,, \tag{9}$$

$$C_2(x) = \sum_k |\langle\Psi_k|\delta\phi^2|\Psi_0\rangle|^2\ \exp[-\beta|x|(E_k - E_0)]\,. \tag{10}$$

It is apparent that at large distances, C_1 and C_2 are dominated by the lowest state with nonvanishing matrix elements: the first excited state in the case of C_1 and the second excited state in the case of C_2. Since E_0, E_1, and E_2 are known at certain temperatures, the large distance behavior of these correlation functions can be found exactly and compared with the results from simulations. Static structure factors may also be calculated in much the same way.

At this point, it is important to mention the connection between the "quantum" calculations and kink physics. In the context of kink statistical mechanics, it is usual to introduce a phenomenological description of kinks as particles in a grand canonical ensemble. However, this is unnecessary, and all such thermodynamical information can be extracted directly from the Schrödinger description of the transfer operator. For example, the kink density has been obtained in this way in Ref. [10]. Simpler quantities like C_1 and C_2 have obvious natural interpretations in terms of kinks. The C_1 correlation length is related to the kink-antikink spacing and increases monotonically as β increases (Fig. 2).

The behavior of the C_2 correlation length requires a little explanation, since C_2 is not directly sensitive to domain size. At both high temperatures (no kinks) and low temperatures (number of kinks exponentially suppressed), the correlation length is essentially that set by thermal phonons, and is therefore small. However, at temperatures close to the kink transition, nonlinear fluctuations on

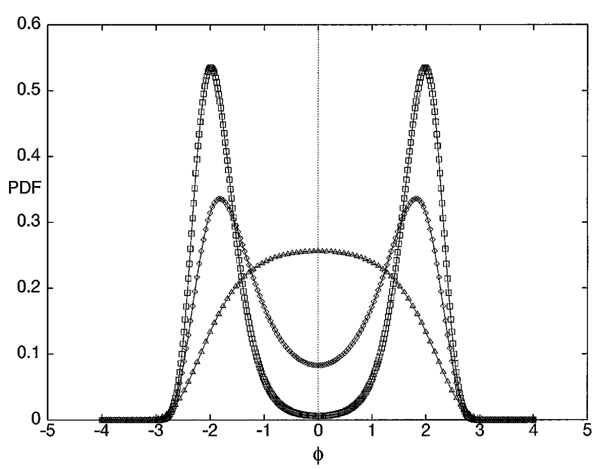

FIG. 1. The numerically evaluated PDFs at three values of β^2: 1/8 (triangles), 1/2 (diamonds), and 9/8 (squares). The corresponding continuum exact solutions are the solid lines.

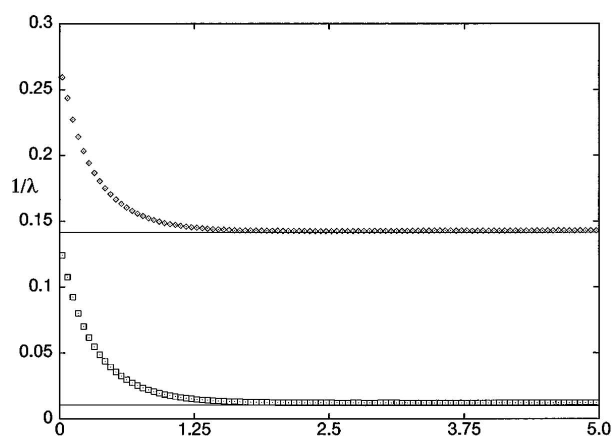

FIG. 2. The numerically obtained inverse correlation lengths from $C_1(x)$ for β^2: 1/2 (diamonds), and 9/8 (squares). The large $|x|$ continuum exact results are the solid lines.

the kink length scale become important and can dominate C_2. At these intermediate temperatures, one expects the C_2 correlation length to rise to a maximum value, on the order of the kink size, and this is indeed what we observe numerically (Fig. 3). The Schottky anomaly in the specific heat [10] arises for the very same reason.

The exact results described above can be compared against those obtained from Langevin methods. The additive noise Langevin equation for the DSHG theory is

$$\partial_{tt}^2 \phi = \partial_{xx}^2 \phi - \eta \partial_t \phi - 4\zeta(\zeta \cosh 2\phi - 2) \sinh 2\phi + F(x,t),$$

where $F(x,t)$ is a stochastic (Gaussian, white) external force which satisfies the fluctuation-dissipation relation linking the noise strength to the viscosity η,

$$\langle F(x,t)F(x',t')\rangle = 2\eta\beta^{-1}\delta(x - x')\delta(t - t'). \quad (11)$$

This stochastic PDE can be solved by standard methods [11] which we implemented on massively parallel computers. Typical choices for the lattice constant are often dictated by memory limitations rather than by accuracy. Comparisons with the exact results have led us to conclude that errors up to 30% may be expected if lattice discretization is done as coarsely, as has been the norm so far in numerical calculations. The existence of nontrivial exact continuum results has proven to be essential in carefully estimating error and convergence in field theoretic Langevin simulations [12]. Our present simulations were typically performed on 5×10^5 site lattices with a lattice constant $\delta = 0.025$ and time step $\epsilon = 0.005$.

Figure 1 shows the striking agreement between the numerically obtained and the exact continuum PDFs at three temperatures: The worst case departure is at the level of parts per thousand. The comparisons for the

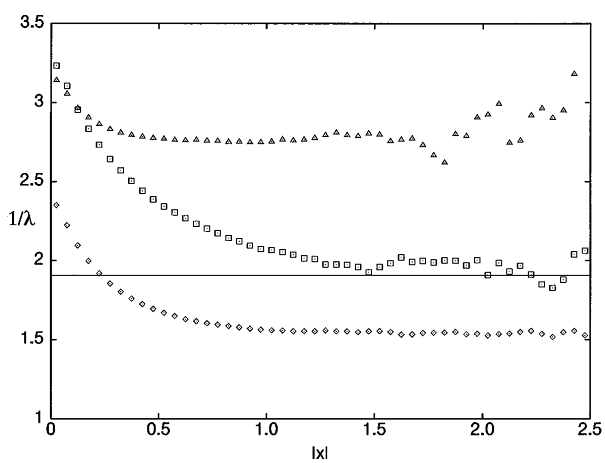

FIG. 3. The numerically obtained inverse correlation lengths from $C_2(x)$ for the same three temperatures and symbol conventions as in Fig. 1. The solid line is the large $|x|$ continuum exact result for $\beta^2 = 9/8$. The largest correlation length is at the intermediate value of β (diamonds).

inverse correlation lengths are given in Figs. 2 and 3. DSHG system parameters are $n = 2$, $\zeta = 0.05$. For C_1, the numerical values are $1/\lambda = 0.1425$ ($\beta^2 = 1/2$) and $1/\lambda = 0.012$ ($\beta^2 = 9/8$) as compared to the exact values in the continuum theory of 0.14142 and 0.0105, respectively. The small offset between the continuum and lattice calculations is due to the finite value of the lattice constant and is consistent with estimates from higher-order contributions to the transfer integral [12].

The high quality of these numerical simulations implies that the PDF can now be used directly to compute thermodynamic quantities at *any* temperature. Since the PDF is just the square of the ground state wave function of the Schrödinger equation (7), one can use it to compute the ground state energy E_0 numerically, from which the internal energy ($U = \partial E_0/\partial\beta$), the free energy ($F = E_0/\beta$), and the entropy ($S = \beta\partial E_0/\partial\beta - E_0$) can all be computed in a straightforward way [8]. The specific heat involves two β derivatives and is difficult to obtain with good accuracy, but in this case, the standard energy fluctuation method is quite effective. The use of the PDF complements traditional techniques utilizing energy fluctuations in Langevin simulations which are not suited to free energy and entropy calculations.

The QES nature of the DSHG theory allows not only the exact computations of E_0 at several temperatures, but also of $\partial E_0/\partial\beta$, using first order perturbation theory: $\partial E_0/\partial\beta|_{\beta=\beta_0} = (\Psi_0, \partial^2\Psi_0/\partial\phi^2)$ where β_0 is one of the special temperatures, e.g., Eq. (8). Thus the internal energy U and the entropy S can also be found exactly at these temperatures [8]. Once again, these quantities can be used to validate numerical work over a broad range of temperatures.

As a final point, we consider the relationship of the DSHG theory to the more familiar Landau-Ginzburg model. Scrutiny of Eqs. (1)–(5) reveals the following important connection between the kink (and kink lattice) solutions of the ϕ^4 model and the double sine-Gordon (DSG) and DSHG models. Consider the ϕ^4 potential $V_4(u) = [(n + \zeta)u^2 - (n - \zeta)]^2$. The substitution $u = \tanh\ \phi$ takes the (static) equations of motion over to the DSHG equations. The alternative substitution $u = \tan\ \phi$ leads to the DSG model. This means that *all* known solutions of the ϕ^4 theory can be directly taken over to the DSHG and DSG theories (and vice versa). As one use of this interesting relationship, the DSG kink lattice solution (not known heretofore in the literature) can be written down directly for $V_{\mathrm{DSG}} = (\zeta \cos 2\phi - n)^2$:

$$\phi_L = \pm \tan^{-1}\left[\tan\ \phi_1 \operatorname{sn}\left(\frac{x - x_0}{\xi_L}, k\right)\right], \quad (12)$$

simply by using the substitution tanh → tan in Eq. (4).

This connection enables us to write down by inspection not just the kink solutions, but their total energy as well, which is often a very tedious task. Moreover, since we know that the DSHG model is an example of a QES system, and considering the very similar way in which the DSG and DSHG models are related to ϕ^4, it is logical to conjecture that the DSG model must also be a QES system. Indeed, this is the case, and we have found several exact eigenvalues and eigenfunctions for many temperatures. The exact statistical mechanical results for the DSG model, similar to the DSHG results presented here, will be reported later [8].

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