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DOUBLE SINE-GORDON MODEL FOR THE CLASSICAL AND QUANTUM THERMODYNAMICS OF MAGNETIC CHAINS

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Abstract. – The Double Sine-Gordon (DSG) model has been often used for describing anisotropic spin chains. We firstly present classical transfer matrix calculations of thermodynamic quantities. Secondly, the effects of the quantum fluctuations are taken into account by means of an effective potential, which was successfully used for SG models.

1. Introduction

One-dimensional non-linear field models have been extensively implemented for describing the magnetic chains [1]. Thermodynamics of some compounds were explained in terms of linear and non-linear excitations of classical integrable models like Sine-Gordon (SG) and non-linear Schroedinger equation [2]. The necessity to take into account quantum effects was later recognized. However kink excitations are also present in non integrable fields like discrete SG and φ^4 so that a variational method was introduced [3] which can be successfully applied for both cases.

In this paper we present classical and quantum thermodynamics of the Double Sine-Gordon (DSG) model. This non integrable field [4] can map many condensed matter systems. For magnetic chains it has been used to study the linear magnetic optical birefringence of anisotropic spin chains (like CoBP, CDC, ...) [5]. Another interesting application of DSG regards the coupling of SG solitons induced by interchain interactions in quasi one-dimensional systems [6]. The vanishing of the magnetization can be explained in terms of the crossover between DSG and SG.

2. The DSG model

The discrete DSG model is described by the following lagrangian

$$L = Aa \sum_i \left[\frac{1}{2}\dot{\varphi}_i^2 - \frac{1}{2}\Omega_0^2 (\varphi_i - \varphi_{i-1})^2 - \Omega_1^2 \mathcal{U}(\varphi_i) \right] \equiv \equiv \frac{Aa}{2} \sum_i \dot{\varphi}_i^2 - V(\varphi) \quad (1)$$

where $\varphi = \{\varphi_i\}$ are dimensionless scalars on a periodic chain with N sites and spacing a. The potential $V(\varphi)$ contains a bilinear nearest-neighbour exchange term and a nonlinear single-site potential

$$\mathcal{U}(\phi) = \frac{1}{\cosh^2 \rho}(1 - \cos\phi) + \frac{\tanh^2 \rho}{4}(1 - \cos 2\phi) \quad (2)$$

which satisfies $\mathcal{U}''(\phi_{\min}) = 0$ in its absolute minima $\phi_{\min} = 0, \pm 2\pi, \ldots$ The parameter ρ, ranging from 0 to $+\infty$, drives continuously the system from a 2π – SG to a π-SG model.

In the continuum limit ($a \to 0$, $\Omega_0 a = c_0 = \text{const.}$, $x = (ai)\,\Omega_1/c_0$) the potential reads

$$V(\varphi(x)) = Ac_0\Omega_1 \int_{-\infty}^{+\infty} \mathrm{d}x \left[\frac{1}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 + \mathcal{U}(\varphi(x)) \right] \quad (3)$$

and it is known to admit, besides the absolute minima $\varphi_0(x) = 0, \pm 2\pi, \ldots$, local minimum configurations like

$$\varphi_K(x) = \psi(x+\rho) + \psi(x-\rho), \quad \psi(x) \equiv 2\tan^{-1} \mathrm{e}^x \quad (4)$$

with energy $E_K(\rho) = \nu_\rho A c_0 \Omega_1$, $\nu_\rho 4(1 + 2\rho/\sinh 2\rho)$, i.e. the classical static DSG kink. It is apparent that this kink resembles a pair of π-SG kinks at distance 2ρ.

We find it useful to introduce the following dimensionless parameters: $t \equiv T/E_K$, is the reduced temperature; $R \equiv \Omega_0/\Omega_1$, which is the π-SG kink length in lattice units, so that the length of the DSG kink is $R.(1 + 2\rho)$. In the continuum limit $R \to \infty$. $Q \equiv \hbar\Omega_1/E_K$, is the "coupling constant" , and measures the degree of nonlinearity of the system.

3. Quantum thermodynamics by effective potential

By use of the variational principle we have been able to derive an effective potential [3], to be inserted in the classical configurational integral, which yields a very good approximation for the quantum partition function in the low-Q regime. It reads

$$V_{\text{eff}}(\varphi) = Aa \sum_i \left[\frac{1}{2}\Omega_0^2 (\varphi_i - \varphi_{i-1})^2 + \Omega_1^2 \mathcal{U}_{\text{eff}}(\varphi_i) \right] - -\frac{1}{\beta} \sum_k \ln \frac{F_k}{\sinh F_k} \quad (5)$$

where $F_k = \beta\hbar\Omega_k/2$, $\Omega_k^2 = 4\Omega_0^2 \sin^2(ka/2) + \Omega_1^2$ is the dispersion relation for the harmonic chain (k belongs to the first Brillouin zone), and

$$\mathcal{U}_{\text{eff}}(\varphi) = \frac{1}{\cosh^2 \rho} \mathrm{e}^{-D/2}(1 - \cos\varphi) + + \frac{\tanh^2 \rho}{4} \mathrm{e}^{-2D}(1 - \cos 2\varphi) + \frac{1 + 3\tanh^2 \rho}{8} D^2. \quad (6)$$

This effective local potential contains the temperature dependent renormalization parameter

$$D(t) = \frac{\nu_\rho Q}{2\pi} \int_0^\pi \mathrm{d}k \frac{\Omega_0}{\Omega_k} \left(\coth F_k - \frac{1}{F_k} \right) \qquad (7)$$

which is the difference between the total mean square fluctuation of φ_i and the corresponding classical one, calculated in the Gaussian approximation.

The effective potential (5) has been previously used for the SG case [7], and the results have been successfully compared with Quantum Monte Carlo data for the specific heat, as well as with exact Bethe Ansatz calculations in the continuum limit.

4. Results and discussion

We have set up a numerical procedure for evaluating the free energy by means of the exact Transfer Matrix method.

CLASSICAL DSG. – The nonlinear specific heat per site δc turns out to be most sensitive to the features of the DSG potential, and indeed it shows an interesting dependence on the parameter ρ (Fig. 1). Note that the curves for $\rho = 0$ and $\rho = \infty$ represent the respective SG limits. The $\rho = \infty$ curve appears to be shifted because of the choice of the temperature scale: E_K ($\rho = \infty$) is twice the energy of the π-SG kink. For ρ raising from zero the peak value δc_M shows an interesting behaviour. Since $E_K(\rho)$ has its relevant variation for $0.5 \leq \rho \leq 2.5$, we attribute to the lowering energy cost of creating kinks the increase of δc_M in the same range; for $0 \leq \rho \leq 0.5$ the increasing size of the kinks gives rise to additional excluded volume, which lowers the kink density and hence δc_M; finally, for ρ decreasing from ∞, the π-SG kinks couple in pairs with decreasing distance, yielding a higher density.

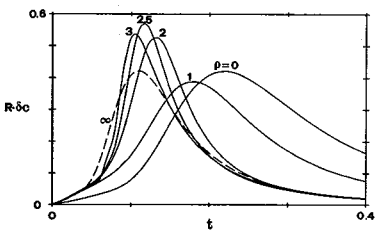

Fig. 1. – Classical nonlinear specific heat per site δc for $R = 5$.

In figure 2 we report results for the magnetization $m = \langle \cos(\varphi_i) \rangle$. In the π-SG limit $\rho = \infty$, m is identically vanishing by symmetry reasons. For finite ρ we can observe a crossover between a low-temperature behaviour, where no kinks are excited and the system fluctuates around its absolute minima, and the temperature region where kink excitations do occur and cause a decrease in the magnetization which is larger for larger ρ, i.e. when a larger portion of the kink resides about the relative minimum $\varphi_i = \pi$ of $\mathcal{U}(\varphi_i)$.

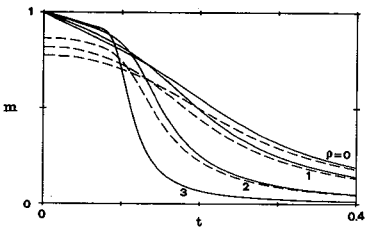

Fig. 2. – Magnetization $m = \langle \cos(\varphi_i) \rangle$ for $R = 5$. Continuous lines: classical. Dashed lines: quantum for $Q = 0.1$.

QUANTUM DSG. – In figure 3 we report the quantum corrected δc, in the cases $\rho = 1, 2$. The reduction of δc appears to be more relevant with respect to the SG case [7].

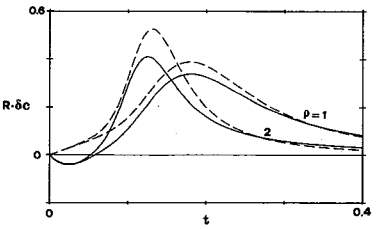

Fig. 3. – Quantum corrected nonlinear specific heat per site δc, for $Q = 0.1$ and $R = 5$. Dashed lines: corresponding classical result.

In figure 2 we also report the quantum magnetization. Its most relevant feature is the lack of saturation at $T = 0$, which is due to the quantum vacuum fluctuations: by the definition of $D(t)$ we have indeed $m(t = 0) = \mathrm{e}^{-D(0)/2}$

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