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QUANTUM THERMODYNAMICS OF SINE-GORDON, $\varphi^4$ AND DOUBLE SINE-GORDON CHAINS

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Abstract — The quantum partition function of non-linear one dimensional Klein-Gordon fields is evaluated by an improved variational method yielding an effective potential to be inserted in a configurational integral which takes into account quantum effects. Results are presented for Sine-Gordon, $\varphi^4$ and Double Sine-Gordon discrete chains. The continuum limit can be easily obtained.

1. INTRODUCTION

Great interest was recently devoted to the statistical mechanics of one- dimensional models which admit soliton or solitary-wave solutions [1-3]. One important class of these systems is represented by the non-linear Klein-Gordon fields which can reproduce the behaviour of many nearly one-dimensional systems in condensed matter, in particular magnetic chains [4,5]. Their scalar field theories are described in the discrete version by the Lagrangian:

$$L = A a \sum_i \left[ \frac{1}{2} \dot{\Phi}_i^2 - \frac{1}{2} \Omega_0^2 (\Phi_i - \Phi_{i-1})^2 - \Omega_0^2 U(\Phi_i) \right] = \frac{A a}{2} \sum_i \dot{\Phi}_i^2 - V(\Phi)$$

(1.1)

where $\Phi = \{\Phi_i\}$ are scalar variables on a periodic chain with $N$ sites and spacing $a$, and $U(\Phi_i)$ is a local potential with unitary second derivative in its absolute minima.

The SG (Sine-Gordon), DSG (Double Sine-Gordon) and $\varphi^4$ theories are obtained for

SG : $U(\varphi) = 1 - \cos \varphi$

DSG : $U(\varphi) = \frac{1}{\cosh^2 \rho} (1 - \cos \varphi) + \frac{\tanh \rho}{4} (1 - \cos 2\varphi)$

$\varphi^4$ : $U(\varphi) = \frac{1}{8} (\varphi^2 - 1)^2$

(1.2)

The DSG potential contains the parameter $\rho \in [0, \infty]$, and for $\rho \to 0(\infty)$ it reduces to a $2\pi - (\pi -)$ SG model.

In the continuum limit ($a \to 0$, $\Omega_0 a = e_0 = 1$, $h = 1$), rescaling the field ($\Phi = g \Psi$ with $g = A^{-1/2}$) and defining the mass ($m = \Omega_1$), the Lagrangian reads:

$$L_0 = \int_{-\infty}^{+\infty} dx \left[ \frac{\dot{\Psi}^2}{2} - \frac{1}{2} \left( \frac{\partial \Psi}{\partial x} \right)^2 - \frac{m^2}{g^2} U(g \Psi) \right]$$

(1.3)

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In this limit the SG is integrable while $\varphi^4$ is not. However kink-like excitations are always available with a rest energy in the classical case: $E_K = \nu A c_0 \Omega_1$ (SG: $\nu = 8$; DSG: $\nu = 4(1 + 2\rho/\sinh 2\rho)$; $\varphi^4$: $\nu = 2/3$). The DSG kink resembles a pair of $\pi$-SG kinks at distance $2\rho$ [6,7].

The following dimensionless parameters are useful: $R \equiv \Omega_0/\Omega_1$, measures the kink length in lattice units, and $R \to \infty$ in the continuum limit. $Q \equiv h\Omega_1/E_K = h/(\nu A c_0)$, is the 'coupling constant' (the usual field theoretic definition is $g^2 h = \nu Q$). $t \equiv T/E_K$, is the reduced temperature.

The classical partition function of these fields can be always evaluated, at least numerically, by transfer matrix [8]. However this method cannot, in principle, share between the contributions coming from linear and non-linear excitations, so that the interpretation of the results requires other techniques [19].

The solitary-wave phenomenology permits this interpretation [9,10]. At the beginning it was limited to the dilute gas approximation (lowest temperatures), afterwards it has been extended at higher temperatures by accounting for interaction effects [11]. Recently, for integrable systems, action angle variables have been used after overcoming initial difficulties related with the boundary conditions [12].

The quantum partition function has been calculated exactly for the integrable systems like SG, using Bethe-Ansatz or quantum inverse scattering [13,14]. Apparently the calculations are easier for strong coupling, whereas more and more difficulties arise when the classical limit is approached [13], i.e. for $Q \leq 0.25$.

The semiclassical approach can be used for any systems [15,16], but the calculations are limited to the self consistent gaussian approximation, neglecting the soliton-soliton interaction, which turns out to be essential, for instance, in the explanation of the behaviour of the specific heat with temperature, even in the classical case [11].

Coherent state approach [17] and Wigner expansion [18] have been proposed, but in both cases the quantum character of each degree of freedom is treated at same level of $\hbar$ so that the convergency of the expansions is poor unless some uncontrolled rearrangements are done [19].

We think that the path integral approach can be an ideal tool to calculate the quantum effects starting from the classical partition function. Using the variational method [20], we can construct an effective potential to be inserted in a configurational integral, reducing quantum statistical mechanics calculations to the classical ones. The details of the method have been the subject of a set of papers [21], and applications to magnetic chains have been given [22]. We will give here some new results for the above Klein-Gordon fields, showing the validity of the approach at all temperatures for low coupling and its applicability to integrable and non integrable models.

2. THE EFFECTIVE POTENTIAL

The variational method [20,21] gives for the free-energy $F$:

$$e^{-\beta F} \simeq e^{-\beta F_0} = \left( \frac{Aa}{2\pi \hbar^2 \beta} \right)^{N/2} \int d\varphi \ e^{-\beta V_{\text{eff}}(\varphi)}$$  \hspace{1cm} (2.1)

where

$$V_{\text{eff}}(\varphi) = Aa \sum_i \left[ \frac{\Omega_0^2}{2} (\varphi_i - \varphi_{i-1})^2 + \Omega_1^2 \sum_{n=0}^{\infty} \frac{1-n}{n!} \left( \frac{D}{2} \right)^n L^{(2n)}(\varphi_i) \right] - \frac{1}{\beta} \sum_k \ln \frac{f_k}{\sinh f_k}$$  \hspace{1cm} (2.2)
Here \( f_k(\varphi) = \beta \hbar \omega_k(\varphi)/2 \) and the frequencies \( \omega_k(\varphi) \) are determined together with the orthogonal matrix \( U_{ki}(\varphi) \) by minimizing the Jensen inequality with respect to the trial action \([20,21]\). They are defined by the self-consistent secular equation

\[
\omega_k^2 \delta \varepsilon_k = \sum_{i,j} U_{ki} U_{ij} \left[ \Omega_k^2 \left( 2 \delta_{ij} - \delta_{i,j+1} - \delta_{i,j-1} \right) + \delta_{ij} \Omega_k^2 \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{D_i}{2} \right)^n U^{(2n+2)}(\varphi_i) \right] \tag{2.3}
\]

where

\[
D_i(\varphi) = \sum_k U_{ki}^2 \frac{\alpha_k}{2} = \sum_k U_{ki}^2 \frac{1}{2 A \omega_k} \left( \coth f_k - \frac{1}{f_k} \right) \tag{2.4}
\]

\( \alpha_k/2 \) is the difference between the total mean square fluctuation and the classical one of the \( k \)-component of the field, calculated in one loop approximation.

The apparently complicated implicit dependence on the field configuration makes it necessary to resort to approximation methods. It has been shown \([21]\) that, at lowest temperatures, the use of a self consistent steepest-descent method yields the known results of the semiclassical approximation \([15,16]\).

In the low-\( Q \) limit a very interesting expansion is obtained. Setting \( \Omega_k^2 = 4 \Omega^2_0 \sin^2(ka/2) + \Omega^2_1 \):

\[
\omega_k^2 = \Omega_k^2 + \delta \omega_k^2(\varphi) + O(Q^2)
\]

\[
\delta \omega_k^2(\varphi) = \Omega_k^2 \sum_i U_{ki}^2 \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{D_i}{2} \right)^n U^{(2n+2)}(\varphi_i) - 1 \tag{2.5}
\]

Hence, replacing (2.5) in the logarithmic term of \( V_{\text{eff}} \) one gets

\[
V_{\text{eff}}(\varphi) = A_0 \sum_i \left[ \frac{1}{2} \Omega_k^2 (\varphi_i - \varphi_{i-1})^2 + \Omega_k^2 U_{\text{eff}}(\varphi_i) \right] - \frac{1}{\beta} \sum_k \ln \frac{F_k}{\sinh F_k} + O(Q^2) \tag{2.7}
\]

\[
U_{\text{eff}}(\varphi_i) = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{D_i}{2} \right)^n U^{(2n)}(\varphi_i) - \frac{D_i}{2} \tag{2.8}
\]

where \( F_k = \beta \hbar \Omega_k/2 \) . The logarithmic term in (2.7) translates the free energy of classical oscillators to the corresponding quantum one, i.e. it accounts in fully quantum way for the linear excitations with the frequencies \( \Omega_k \). \( D(t) \) represents the quantum renormalization parameter and is consistently calculated by (2.4) using \( \Omega_k \) instead of \( \omega_k \), so that it is site- and configuration- independent and easily computable, since in this limit \( U_{ki} \) is an ordinary real Fourier transformation \([20]\). \( D(0) = (2\pi)^{-1} \nu Q \ln 8R + O(R^{-2}) \) coincides with that previously found in the semiclassical renormalization theory \([15]\).

The effective local potentials related to (1.2) are

SG : \( U_{\text{eff}}(\varphi) = e^{-D/2(1 - \cos \varphi)} + \frac{D^2}{8} \)

DSG : \( U_{\text{eff}}(\varphi) = \frac{1}{\cosh^2 \rho} e^{-D/2(1 - \cos \varphi)} + \frac{\tanh^2 \rho}{4} e^{-2D(1 - \cos 2\varphi)} + \frac{1 + 3 \tanh^2 \rho}{8} D^2 \tag{2.9} \)

\( \varphi^4 : \ U_{\text{eff}}(\varphi) = \frac{1}{8} (\varphi^2 - 1 + 3D)^2 - \frac{3}{4} D^2 \)

The expansion (2.7) for the effective potential is surely valid if the condition \( \beta \hbar \delta \omega_k^2/(4\Omega_1) \ll 1 \) is satisfied, which amounts to require

\[
Q \ll \frac{16}{\nu U^{(4)}(\varphi_{\text{min}})} ; \quad t \gg \frac{1}{8} U^{(4)}(\varphi_{\text{min}}) \tag{2.10} \]

where \( \nu = \frac{\beta}{2 \pi} \ln R \).
where $\varphi_{\text{min}}$ is an absolute minimum of $U(\varphi)$ ($\nu U^{(4)}(\varphi_{\text{min}}) = 8$ for SG, $1/4$ for $\varphi^4$). The latter condition can be estimated in the most unfavourable conditions replacing $D(t)$ with its maximum value $D(0)$, giving

$$t \gg \frac{\nu U^{(4)}(\varphi_{\text{min}})}{16 \pi} Q^2 \ln 8R$$

(2.11)

Notice that the Wigner expansion is valid for $\beta \hbar \Omega_0 / 2 \ll 1$, or $t \gg QR / 2$, so that (2.7) constitutes a very significant improvement.

The advantage of (2.7) is that the complicated implicit dependence on the field configuration is absent. Besides the logarithmic term, which accounts for the quantum character of the linear excitations and is $\varphi$-independent, we are left with an effective potential which usually resembles $V(\varphi)$, apart from the quantum renormalization of some parameters entering the single site potential. Therefore the configurational integral (2.1) can be calculated by any classical method, like temperature expansions [11] or numerical transfer matrix [8], and it accounts for the nonlinear contribution to the free energy.

3. RESULTS

In order to test the validity of eqs. (2.7) and (2.9) we have calculated, by numerical transfer matrix, some thermodynamic quantities, namely the nonlinear contribution to the specific heat per site $\delta c$, the nonlinear contribution to the internal energy per site $\delta u$, and — for SG and DSG — the magnetization $m = \langle \cos \varphi_t \rangle$. We have numerically verified that the classical nonlinear free energy per site multiplied by $R$ (which gives a linear density) is insensitive to $R$, at least on the scale of our figures, provided that $R \geq 4$.

For $\delta c$ in the SG case we have made a comparison with quantum Monte Carlo calculations [23], (figure 1). The SG magnetization is shown in figure 2: note the lack of saturation at $t = 0$ in the quantum case, which is due to the quantum vacuum fluctuations.

![Figure 1. SG chain: $\delta c$. Continuous line: classical. Dashed l. and (▲): $Q = 0.1$, $R = 2.9$. Dash-dotted l. and (■): $Q = 0.1$, $R = 10$. Symbols are quantum MC data from [23].](image1)

![Figure 2. SG chain: $m = \langle \cos \varphi_t \rangle$ for $R = 10$. Continuous line: classical. Dashed l.: quantum for $Q = 0.1$ and $Q = 0.2$.](image2)

In order to test the theory with the existing solutions for integrable system [13,14] we must perform the continuum limit. However for $R \to \infty$ $D$ is a divergent quantity and one must replace $\Omega_k$ with its zero-T renormalized counterpart in (2.5), and rederive (2.6-8). The effective potential turns out to look like (2.7),
apart from the overall appearance of the convergent renormalization parameter $D'(t) \equiv D(t) - D(0)$.

This has been shown in [21] for SG and $\varphi^4$. The comparison with the available Bethe-Ansatz data [13], as well as with the rescaled Monte Carlo simulations [23], is made in fig.3 for the non linear specific heat density $\delta C$. We notice that the coupling $Q = \pi/10$ is rather high, since it produces a further renormalization of the quantum kink energy by a factor $1 - Q/\pi = 0.9$, which is not accounted for in the low coupling theory. It follows that the agreement is fully satisfactory. Unfortunately exact data for lower coupling are not available, because of the difficulties mentioned in the introduction.

Figure 3. SG field: non linear specific heat density $\delta C$. $E^0_0$ is the zero-T renormalized soliton energy. Dashed line: Bethe-Ansatz results from [13]. Symbols: as in fig.1, with proper rescaling.

Figure 4. $\varphi^4$ chain: $\delta u$ for $R = 5$.

Figure 5. $\varphi^4$ chain: $\delta c$ for $R = 5$.

Figure 6. DSG chain: $\delta c$ for $R = 5$. Continuous lines: classical. Dashed lines: quantum for $Q = 0.1$.

Figure 7. DSG chain: $m = (\cos \varphi_1)$ for $R = 5$. Continuous lines: classical. Dashed lines: quantum for $Q = 0.1$. 
In the above figures we have also reported our results for the non integrable $\varphi^4$ and DSG chains, together with the corresponding classical results. Note that the $Q = 0$ results coincide with the classical ones, because from the classical point of view one can take $E_K = h\Omega_1/Q$ finite when letting $Q \to 0$, $h \to 0$.

The quantum effect on the excess specific heat of the $\varphi^4$ and the DSG chain does not differ significantly, as expected after the choice of the temperature scale and of the coupling parameter, both of which are weighted through the respective kink energy.

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