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QUANTUM SINE-GORDON THERMODYNAMICS

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Resume - En utilisant la méthode du théorème de Bethe, nous analysons les propriétés thermiques du modèle sine-Gordon quantique. Nous présentons un système d'équations intégrales nonlinéaires pour la distribution thermique des diverses excitations, que l'on résout numériquement. La chaleur spécifique que nous obtenons ainsi est en bon accord avec les expériences récentes dans les matériaux unidimensionnels magnétiques CsNiF₃ et TMMC, ce qui indique que les effets quantiques sont importants.

Abstract - Using the Bethe ansatz method we analyze the thermodynamics of the quantum sine-Gordon model. We present a finite set of coupled nonlinear integral equations for the thermodynamic equilibrium densities of the various excitations, which we solve numerically. We calculate the specific heat and we compare our results with recent experiments on CsNiF₃ and TMMC. The good accord obtained indicates the importance of quantum effects.

One dimensional magnetic materials have recently attracted a lot of interest as possible candidates for the observation of nonlinear modes. In particular CsNiF₃ and TMMC are described by quantum Hamiltonians which, in a certain regime of temperature and magnetic field, were shown to be approximated by the sine-Gordon (SG) Hamiltonian /1/. These are chains of planar spins coupled ferromagnetically (antiferromagnetically) in the presence of a magnetic field in the easy plane, where the soliton corresponds to a 2π-twist (π-twist) of the spins. Experimental evidence for magnetic soliton contribution has been obtained /2,3/ by neutron scattering experiments, the results analyzed in terms of classical sine-Gordon dynamics. This interpretation however is controversial as multiple linear excitations and quantum effects are important and the mapping of the spin Hamiltonian to the SG model ambiguous. Furthermore in recent specific heat experiments /4,5/ a magnetic field dependent peak was observed in qualitative agreement with classical SG thermodynamics. Thus it is essential to analyze the quantum SG model in order to conclude about the importance of quantum effects and clarify the validity of the SG mapping /6/.

The SG model is known to be completely integrable in its classical version and diagonalizable in its quantum version using the Bethe ansatz method. To develop the thermodynamics we use the equivalence between three models: the XYZ spin 1/2 chain, the massive Thirring model (MTM) and the quantum SG model. It is established in the literature that the basic excitations of the MTM (a relativistic fermion model) are holes in the Dirac sea and strings (in momentum space) of particles forming bound states corresponding to the solitons and quantized breathers respectively. The excitation spectrum is given by the DHN expression $E_j = 2E_s \sin \left( 3\pi (j-\nu) \right)$ where $E_s$ is the soliton energy and $\nu$ the MTM coupling ($\nu$ is related to the SG coupling $g^2$ by: $\nu = -g^2 / \beta$). The thermodynamics of the XYZ model was analyzed by Takahashi and Suzuki; by taking the appropriate continuum limit to the MTM we recover the thermodynamics of the quantum SG model. This analysis /7/ leads to a set of coupled nonlinear integral equations describing the thermodynamic equilibrium densities of the various
excitations. For particular values of the coupling \( \mu \) of the form \( \mu = n - \frac{1}{2} \), \( n \) an integer, this set is finite:

\[
h_j = \ln \left( 1 + \exp \left( -\frac{E_j}{T + \sum_{k \neq j} B_{jk} h_k} \right) \right) \quad j = 1, \ldots, n-2
\]

\[
h_{n-1} = \ln \left( 1 + \exp \left( -\frac{E_{n-1}}{T + \sum_{k < n-1} B_{n-1,k} h_k} \right) \right)
\]

where * denotes convolutions, \( B_{jk} \) are known dressed phase shifts between excitations of order \( j \) and \( k \) and \( h_j \) describe the equilibrium densities. Solving these equations numerically by iteration, we obtain the densities \( h_j \) and then the free energy is given by:

\[
F = -T \sum_j E_j h_j d(n) \sum_j \frac{h_j}{2^j}
\]

The theoretical analysis is expressed in terms of two dimensionless parameters, the coupling \( g^2 \) and the temperature to soliton mass ratio \( T/E_s \).

The theoretical curve is related to experiment by a proportionality factor:

\[
C_{\text{exp}} \frac{1}{\hbar} = \frac{E_s a}{\hbar c} C_{\text{BA}} (g^2 T/E_s)
\]

where \( a \) is the lattice spacing and \( C_s \) the velocity in the SG system. The classical soliton energy \( E^* \) is proportional to \( \sqrt{g^2} \) for \( \text{CsNiF}_3 \) and to \( H \) for TMMC and related to \( E_s \) by a quantum renormalization factor, \( E_s = r E^* \). So plotting the experimental results as \( C_{\text{exp}} \frac{1}{\hbar} = \frac{E_s a}{E_s} \) for the different magnetic field values (corresponding to different soliton energies) as a function of \( T/E_s \), all points should scale on a universal curve \( C_{\text{BA}} \) depending on \( g^2 \). The value of \( g^2(0.19 \text{ for } \text{CsNiF}_3 \text{ and } 3.19 \text{ for } \text{TMMC}) \) is known from the spin hamiltonians so the only arbitrary parameter entering the comparison is the renormalization factor \( r \).

Furthermore Ramirez and Wolf present the specific heat difference with and without magnetic field. As the simplest approximation to the zero magnetic field specific heat we subtract a term linearly dependent on temperature, corresponding to a phonon gas. For TMMC, Borsa et al/8/ further subtract the specific heat due to linear spin waves. In this case we consider appropriate to subtract the specific heat of a massive phonon gas of mass \( m = 2 \sin \left( \pi (n - \frac{1}{2}) \right) \) corresponding to the quantum SG phonons. The results are presented in Figures 1. and 2.

Figure 1. \text{CsNiF}_3 specific heat. The solid curve is the Bethe ansatz result for \( n = 28 \).
For CsNiF, we use a renormalization factor $r=0.7$ as suggested in reference/4/. The results for field values between 4 and 10 kGauss scale well, the amplitude and position of the peak in accord with the BA curve. Quantitatively the agreement is greatly improved, an indication of the importance of quantum effects. The cause of the deviations observed might be the crude approximation for the zero field specific heat, experimental uncertainties or corrections due to imperfect mapping to the SG model.

![TMMC specific heat](image)

**Figure 2.** TMMC specific heat. The solid curve is the Bethe ansatz result for $n=8$.

For TMMC the SG approximation is expected to be valid/9/ at low fields, $H<5$ Tesla, where the out of plane fluctuations are small. At present we have only one set of data in this regime so we cannot check the scaling property (we confirm however that the higher field data, $H=7.6$, 10 Tesla don't scale properly). We vary the renormalization factor $r$ and we obtain an optimal fit for $r=0.54$. This value is not in accord with the one given in reference/3/ ($r=0.79$). To clarify this discrepancy an analysis of the neutron scattering results in terms of the quantum SG dynamics seems necessary, keeping in mind the ambiguities present in the comparison with the specific heat experiment.

In conclusion these preliminary results indicate the importance of quantum effects; further experiments and theoretical work is necessary to arrive at definite conclusions.

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