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Kink solitons in an antiferromagnetic chain with orthorhombic symmetry

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ABSTRACT

The essentials of a Sine-Gordon gas are briefly indicated. The mapping of an antiferromagnetic chain with orthorhombic symmetry on the Sine-Gordon system is analyzed in detail. The Sine-Gordon profile for the static domain wall is found to linearly stable. In this analysis it became clear that the hard axis switching has to be treated carefully. The agreement between experimental data on the spin-spin correlation function, the specific heat and the thermal conductivity is discussed.

INTRODUCTION

In this review we will discuss the occurrence and the stability of domain walls in quasi-one-dimensional antiferromagnetic insulators and some related physical properties. The domain walls will be described as Solitons. These are then considered as nonltnear excitation of a system in thermal equilibrium. Special attention will be given to the theoretical aspect, which are essential for the interpretation of the experimental data in terms of solitons.

The statistical mechanics of a Sine-Gordon [6] and [1] system will be indicated very briefly only those quantities which are needed for further discussion will be introduced without any deviation.

Then we will show how dimensional antiferromagnetic chain can be mapped on a Sine-Gordon system. This mapping [17],[16] and [18] will be given in detail because it is very instructive. The range or system parameters where the magnetic chain behaves as a Sine-Gordon system is related to the approximations, made in this mapping.

When the correspondence between both systems is established it remains to prove that the Solitons are stable entities in the magnetic system.

THEORETICAL CONSIDERATIONS AND CALCULATIONS

The Sine-Gordon system is described by the following

Hamiltonian:

$$H= \Sigma \tfrac{1}{2} \pi_n\pi_n + \tfrac{1}{2} c^2 (Y_{n+1} – Y)^2 + \omega^2c^2 (1 – \cos Y_n), \qquad (1)$$

where c is the velocity of the linear excitations of the system, ω is the frequency of the linear excitations and π_n is the momentum canonically adjoint to the position Y_n.

The particles on a one-dimensional array feel locally a cosine potential and interact with each other harmonically.[11] The system allows linear excitations, which we will call magnons for further inference. It allows solitons and anti-solitons and there are also the so-called breathers, much are bound states of a soliton and an anti-soliton.

The shape of a soliton in the continuum approximation is given by

$$Y(x - vt) = 4\tan^{-1}(\exp\pm \omega g(x - x_o - vt)), \qquad (2)$$

where v denotes the velocity of the soliton, g is the Lorenz factor and x_o is the center of the soliton. The cosine of Y(x-vt) differs only substantially from zero in the vicinity of the soliton center. The sine of half Y(x-vt) changes from most 1 to almost -1 in the same region.[2]

The partition function Ƶ of the system described by the Hamiltonian can be calculated using the transfer matrix formalism. On the other hand a phenomenological theory of a non-interacting soliton gas can be constructed. The comparison of the Phenomenological free energy with the classical exact free energy leads to an expression for the solitons density in terms of the system parameter ω and the soliton energy divided by kT.[10] The soliton density is given by:

$$n = \left(\frac{2}{\pi}\right)^{1/2} \omega \left(\frac{E_{sol}}{K_T}\right)^{1/2} \exp -\left(\frac{E_{sol}}{\cdot K_T}\right) \qquad (3)$$

This is one of the basic quantities which is used to estimate the number of solitons present in the magnetic system provided one knows the relation between the parameters of the magnetic system and the Sine-Gordon parameters ω and E_{sol}. it is clear that from the free energy the specific heat can be obtained in function of the temperature. The static correlation function can also be obtained using the transfer matrix formalism [14] and [7].

The dynamic correlation functions require additional approximations. In the phenomenological gas approach the correlations between the cosine of Y(x) at one space time point and another space time point are obtained by averaging over the velocity distribution of the solitons. The Sine of half Y(x) can be approximated by a step-function that changes from 1 to -1 at the soliton center.

The one-dimensional magnetic system which we will consider has an isotropic exchange integral J, a single ion-anisotropy A, along the z-axis and is subjected to a magnetic field in the x-direction which together with a single ion anisotropy D, breaks the isotropy of the X – Y plane.[9] Taking only next neighbour interaction into account the Hamiltonian for this chain is given by

$$H = \Sigma\, JS_{n+1}S_n + A(S_n^{\,2})^2 - D(S_n^{\,x})^2 - g\mu_B HS_j^{\,x}, \qquad (4)$$

where S_j^x means that x -component of the spin on the j^{th} position in the chain. For J and A positive it represents an antiferromagnetic chain with an easy plane. For relatively low magnetic fields it is the X – Y plane, for a high magnetic field strength the easy plane becomes the Y – Z plane.

The classical equations of motion can be obtained via the quantal commutation relations and taking then the classical limit [17] and or via Poisson brackets which exploit the fact that spin and angular momentum are analogous.

There are several methods to map Hamiltonian on the Sine- Gordon Hamiltonian.[3] In all of them some approximations are involved and the algebra of the mapping is tedious and even not always straight forward. Therefore another variation, which tries to combine the advantage of the other methods, will be given. It should be remarked that the Hamiltonian is bilinear in the spin variables. The nonlinearity in the equations of motion arises from the rotation symmetry of the generous S^x, S^y, S^z, For reasons of convenience it is preferred to have the non-linearity in the Hamiltonian, while the generators of the equation of motion behave linear.

The villain transformation [12] represents the spin commutation relations by operator functions of canonically adjoint local operators. These operators are very similar to the well-known position and momentum operators of a quantum particle. If one does not bother about the domain of the operators, the classical equivalent is straightforward, this results is replacing by h [S(S+1) ½] by S, the spin-length and obtaining the following representation of the spin- algebra

$$S^z{}_j = S_{sj} \tag{5}$$

$$\left.\begin{aligned} S^+{}_j &= S^I \exp Y_j (1 - S^2{}_j)^{½} \\ S^-{}_j &= S (1 - S^2{}_j)^{½} \exp^{-iYj} \end{aligned}\right\} \tag{6}$$

Where S_j and Y_j are canonically adjoint. Denoting the square root by ω_j the following expression for the Hamiltonian [16] is obtained in the new variables.

$$H = JS^2 (h_{exchange} + h_{anisotropy} + h_{Zeeman}) \tag{7}$$

$$h_{exchange} = \Sigma_j (S_j +_1S_j +_1\omega_j +_1\omega_j \cos(Y_{J+1} - Y_j)) \tag{8}$$

$$h_{anisotropy} = \Sigma_j \frac{A}{S_j{}^2} - \frac{D}{J}\omega_j{}^2 \cos^2 Y_j \tag{9}$$

$$h_{Zeeman} = \Sigma_j \frac{g\mu_B HS_j}{(JS)} \omega_j \cos Y_j \tag{10}$$

The equations of motion are then obtained using the Poisson- bracket: [13]

$$(S_j , Y_j) = \delta_{ij} \tag{11}$$

$$(A, B) = \Sigma \frac{\delta A}{\delta S_j} \cdot \frac{\delta B}{\delta Y_j} - \frac{\delta A}{\delta Y_j} \cdot \frac{\delta B}{\delta S_j}$$

(12)

The equation for S_j is then

$$D_t S_j = (S_j, H) = \frac{\delta H}{\delta Y_j} \tag{13}$$

$$\frac{\delta H}{\delta Y_j} = JS^2 \left[\omega_{j+1}\, \omega_j \sin (Y_{j+1} - Y_j) - \omega_j - {}_i\omega_j \sin(Y_j - Y_{j-1}) + \frac{g\mu_B HS_j}{(JS)} \omega_j \sin Y_j + \frac{D}{\delta\omega_j} \omega_j \sin^2 Y_j \right] \tag{14}$$

The equation for Y_j is then:

$$D_t Y = \frac{\delta H}{\delta S_j} = - JS^2 \left[\frac{\delta\omega_j}{\delta S_j} (\omega_{j+1} \cos(Y_{j+1} - Y_j) + \omega_{j-1} \cos(Y_j - Y_{j-1})) + S_{j+1} + S_{j-1} + \frac{2A}{JS_j} + \frac{2D}{JS_j} \cos^2 Y_j - g\mu_B \cdot \frac{\delta\omega_j}{\delta S_j} \right] \tag{15}$$

where

$$\frac{\delta\omega_j}{\delta S_j} = - \frac{S_j}{\omega_j} \tag{16}$$

It is clear that $S_j = S_{j+1} = 0$ for all j is a solution of equation (15) that expresses that Y_j is time independent

$$D_t Y_j = 0 \tag{17}$$

The static solution for Y_j can then be obtained from the following equation.

$$\sin(Y_{j+1} - Y_j) - \sin(Y_j - Y_{j-1}) + \frac{D}{J}\sin 2Y_j + g\mu_B \frac{H}{JS}\sin Y_j = 0 \tag{18}$$

This equation determines the orientation of the spins in the plane given by equation (17), which indicates that we are looking for solutions without out-of-plane components.

Now we will define new variables as

$$Y_{2j} = \frac{\pi}{2} + \theta_j + \frac{1}{2\theta_j} \tag{19}$$

$$Y_{2j+1} = -\frac{\pi}{2} + \theta_j - \frac{1}{2\theta_j} \tag{20}$$

For the j cell θ_j measures the average of the angles Y_{2j} and Y_{2j+1}, θ_j measures the deviation from π to their difference for a relatively large exchange j the adjacent spins will be almost antiparallel, this implies that θ is small. In order to derive from equation (18) tractable expressions we substitute θ_j and $\theta_{j,}$ and linearize with respect to θ_j, $\theta_{j+1} - \theta_{j-1}$ and $\theta_{j+1} + \theta_{j-1} - 2\theta_j$. The result of this calculation is the following set of coupled equations which are non-linear in $\theta_{j,}$ the variable that describes the absolute orientation of the spins in the j^{th} cell:

$$2\theta_j\theta_{j+1} - \theta_{j-1}{}^{-½}(\theta_{j+1} - \theta_{j-1}) - 2\frac{D}{J}\sin 2\theta_j - g\mu_B\frac{H}{JS}\theta_j \sin\theta_j = 0 \tag{21}$$

$$4\theta_j + (\theta_{j+1} - \theta_{j-1}) + ½\,(\theta_{j-1} + \theta_{j+1} - 2\theta_j - 2\frac{D}{J}\theta_{j-1}\cos 2\theta_j + 2\,g\mu_B \frac{H}{JS}\cos\theta_j = 0 \tag{22}$$

In the continuum limit these equation becomes

$$a^2\theta + a\theta + 2\frac{D}{J}\sin 2\theta + g\mu_B\frac{H}{JS}\sin\theta = 0 \tag{23}$$

$$4\theta + 2a\theta + a^2\theta - 2\frac{D}{J}\theta\cos 2\theta + 2g\mu_B\frac{H}{JS}\cos\theta = 0 \tag{24}$$

where a the spacing between the particles. The coupled equations require two additional approximations afore we arrive at a Sine- Gordon profile for the static domain wall. [4]

The underlined term in equation (24) is at least order smaller than the other terms provided that the exchange integral j is large quantity, indeed the proportion $\frac{D}{J}$ is then small and also, θ. This term is neglected completely in all mapping procedures, this omission limits the validity range of the mapping to chains where the neighbouring spins are strongly coupled via the exchange interaction and to chain where the local spin intersect weakly with an anisotropic

perturbation coming from the single ion anisotropic and the magnetic field. If we follow Mikeska, we neglect all derivatives of θ and the first order derivative of θ, this leads to:

$$c^2\theta - ((g\mu_B H)^2 - BJS^2D)\sin 2\theta = 0 \qquad (25)$$

where $c^2 = (2_j Sa)^2$

If we follow (Ieung et al), we will neglect the second derivative of θ and then we obtain

$$c^2\theta - ((g\mu_B H)^2 - 8JS^2D)\sin 2\theta = 0 \qquad (26)$$

where $c^2 = \frac{c^2}{2}$

Theoretically, this is amazing result. For comparison with experiment, it is no problem because in both cases c or c is the limiting group velocity of the magnon. It should be noted that depending on the sign of $(g\mu_B H)^2 - 8JS^2D)$, we have to add $\frac{\pi}{2}$tan θ in order to obtain the same shape as equation (2). The Sine Gordon parameter is then:

$$\omega^2 c^2 = \left|(g\mu_B H)^2 - 8JS^2D)\right| \qquad (27)$$

Treating the spins as classical vectors and introducing the angle variables of Mikeska the compounds of the spin in the ith position on the chain are given by:

$$S_i^x = (-1)^i\ S \sin(\theta_i + (-1)^i\ \theta_j) \cos (\theta_i + (-1)^i\ \theta_i) \quad (28)$$

$$S_i^y = (-1)^i\ S \sin(\theta_i + (-1)^i\ \theta_j) \cos (\theta_i + (-1)^i\ \theta_j) \quad (29)$$

$$S_i^z = (-1)^i\ S \cos(\theta_i + (-1)^i\ \theta_j) \quad (30)$$

If we make the continuum approximation, assume that θ_i and θ_j are small compared with θ_i and θ_y the following Hamiltonian density is obtained:

$$H = \tfrac{1}{2} js^2 \int {}^{dz}/_{\theta}\ (h_{exchange} + h_{anisotropy} + h_{zeeman} \quad (31)$$

$$h_{exchange} = \theta^2\phi^2 + 4\theta^2 + [\theta^2\phi^2 + 4\Psi^2] \sin 2\theta \quad (32)$$

$$h_{anisotropy} = {}^{2A}/_{J} \cos^2\theta - {}^{2D}/_{J} \cos^2\phi\sin^2\theta \quad (33)$$

$$h_{zeeman} = {}^{-2g\mu BH}/_{JS}\ (\theta\cos\phi \cos\phi - \Psi\sin\theta \sin\phi) \quad (34)$$

The equation of motion for the angle variables are then given by

$$D_t\theta = 4JS\Psi \sin\theta + 2g\mu_B H \sin \theta \quad (35)$$

$$D_t\phi = {}^{4JS\theta}/_{(\sin\theta)} + g\mu_B H \cos\phi \cot\phi \quad (36)$$

$$D_t\theta = -JS\theta^2\phi \sin\theta - JS\cos[2\theta^2\phi\Phi + 4\theta\Psi] + DS \sin\theta \sin2\phi + g\mu_B H\Psi \cos \theta \quad (37)$$

$$D_t\Psi = \frac{\dfrac{JS\theta^2\phi \sin\phi}{\sin\theta + 4\ JS\theta^2 \cos\theta}}{\dfrac{(\sin^2) - [JS\theta^2\phi^2 + 4\ JS\Psi^2] + 2AS \cos\theta + 2\ Ds \cos\theta \cos^2\Phi - g\mu_B H\ \theta\cos\phi}{(\sin^2\theta)}} \quad (38)$$

RESULTS AND DISCUSSION

The ideal gas soliton theory gives the following expression for the magnetic part of the specific heat

$$C_H = \frac{K}{a} - \frac{E_{soL}}{KT} - \frac{1}{2}^{2} - \frac{1}{2} 2n, \tag{39}$$

where n is given by equation (3) and 2n represents the total soliton and anti-soliton density. If the proportionality factor between E_{soi} and the magnetic field is used as a parameter which can be fitted the agreement with the data is reasonable certainly from the qualitative viewpoint. This is used as an argument in favour of the Soliton description of propagative domain waits. However, one should bare in mind that equation (39) is the specific heat of a system described by Hamiltonian (1). Using numerical transfer matrix methods the thermodynamical quantities generated by Hamiltonian (4) can also be calculated in the classical approach. It is found that there is a serious discrepancy between the ideal soliton gas and the transfer operator results for the complete system. It is believed that the good agreement of the experimental results with the sollton gas theory is accidental in the sense that contributions arising from out-of-plane degrees of freedom of the spins are somewhat compensated by the quantum corrections.[8]

The neutron scattering and NMR experiment measure spin-spin correlation function. This dynamic correlation function has been calculated classically on the basis that soutons act independently and that their density is low, indeed Poisson statistics can then be used. The theoretical parameter, which controls the Poisson distribution, is the mean number of solitons on a given interval and during a given lapse of time. The mean number of solitons is like the density controlled by E_{soi}: This energy is used again as a fitting parameter. [5]

Heat conductivity experiments on TMMC and DMMC [$(CH_3)_2$ NH_2MnCl_3] show in the magnetic field dependence a reduction which could be caused by the presence of domain walls. Using a model which allows resonant scattering between phonons and solitons, it is possible to fit the experimental data quite well. The soliton parameters here have the same 20% reduction as those of the neutron scattering experiments. This reduction is found with respect to be theoretical calculated parameters, obtained from measurements of the magnon dispersion for example.

CONCLUSION

The interpretation of experimental results on propagative domain walls in quasi one dimensional antiferromagnetic chain relies on the ideal soliton gas picture as far as the dynamic spin-spin correlation functions are concerned.[15] The key quantity in this analysis is the soliton-energy-the formulation energy of a domain wall-measured via the soliton density. The energy can be obtained from theory within 20%.

There are however difficulties with the specific heat in the sense that an approximative calculation (the ideal soliton gas) gives apparently a better agreement with experiment than a classical but numerical exact calculation of the same quantity via the transfer matrix method for the antiferromagnetic chain

Also the heat conductivity gives an indication that there are domain walls involved. The interaction mechanisms which are proposed is still speculative, with the merit however that the data are fitted well.

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