Non-Linear Excitations in Antiferromagnetic Chains

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Recent theoretical and experimental results on non-linear excitations in one dimensional classical antiferromagnetic chains are reviewed with a particular emphasis on dynamic properties. The main investigated substance is TMMC which can be regarded as a quasi-one-dimensional antiferromagnet with easy plane anisotropy. A discussion of Haldane's conjecture that there is an excitation gap for integer, but not half-integer spin is given. The open questions and possible investigation for the future are discussed.

I. Introduction

The methods of theoretical physics, with few xexceptions, have been dominated by linear equations, linear vector spaces, and linear methods (Fourier transforms, perturbation theory and linear response theory). Although the importance of non-linearity was recognized a long time ago, it was at that time hardly possible to treat the effects of non-linearity, except as a perturbation to the basis solution of the linearized theory. During the last two decades, however, it has become more widely recognized in many areas that non-linearity can result in qualitatively new phenomena which cannot be constructed via perturbation theory starting from linearized equations. Moreover, the common characteristics of non-linear phenomena in very distinct fields have allowed progress in one discipline to transfer rapidly to others. Although we do not have an entirely systematic approach to non-linear problems, we do, however, have an increasing number of well-defined paradigms that both reflect typical qualitative features and permit qualitative analysís of a wide range of non-linear systems. One of these paradigms that we will be concerned with in this review paper is the soliton, which is an essential part of non-linear science. To define a soliton precisely, we consider the motion of a wave described by an equation that, in general, will be non-linear. A traveling wave solution to such an equation is one that depends on the space x and time t variables only through the combination $s = x - ut$, where u is the constant velocity of the wave. If the traveling wave is a localized single pulse moving through space without changing its shape and, in particular, without spreading out or dispersing, it is a solitary wave or a ***kink.*** A solitary wave, with the additional property that it preserves its form exactly when it interacts with other solitary waves,was called by Zabusky and Kruskal[1] by the name of ***soliton.***

For good reviews of soliton theories see Scott et al.[2] and Barone et al.[3]. For application of solitons in Condensed Matter, see refs. 4-8, and, in particular[9], for an excellent review paper dealing with statistical mechanics of solitons.

Solitons are best realized in one dimensional (1D) models where theory and experiments are well developed and, to date, topological solitons have been clearly experimentally identified only in these models. It is well known that in magnetic -1D models the regime of strong correlation without long-range order (LRO) is present all the time because LRO is suppressed in ideal 1D systems: we have only short-range order (SRO) characterized by the correlation length ξ. In one dimension, the spin system is never static but always dynamic and therefore large-amplitude fluctuations are important.

The first theoretical description of solitons in magnetic systerns was proposed by Villain in 1975 for a one-dimensional antiferromagnetic (AF) Ising Hamiltonian[10]. In 1978 Mikeska[11] showed that the dynamics of a quasi-1D ferromagnet (F) with easy-plane anisotropy, subjected to an externa1 field in the anisotropic plane, reduces to the sine-Gordon equation which has a soliton solution describing localized 2π-rotations of spins lying in the easy plane. In the same year, Kjems and Steiner[12] presented the first experimental evidence for the existence, in the quasi-1D ferromagnet $CsNiF_3$, of the soliton predicted by Mikeska being sooner after contested by Reiter[13] who showed that two-magnon scattering should also give rise to a central peak with a similar dependence of its width on the transfered momentum. A lot of research followed then (see [14] for references) and even today some problems still remain[15].

In 1980, Boucher et al.[16-22], in a study on the compound $(CH_3)_4NMnCl_3$ (TMMC), were the first to show that soliton excitations also existed in planar antiferromagnetic chains in a field, resulting in a particularly intense central peak. Theoretical studies done also in 1980, by Mikeska[23], Leung et al.[24], and Maki[25] showed that a 1D-classical easy-plane antiferromagnetic Harniltonian could be reduced to a sine-Gordon Hamiltonian. Corrections to the sine-Gordon model with allowance for fluctuations which bring the spins out of the easy plane were done later by Harada et al.[26], Fluggen and Mikeska, Etrich and Mikeska[27], Costa and Pires[28], Gouvêa and Pires[29], and Wysin et al.[30,31]. The role of quantum effects for a chain with finite spin values were considered by Maki[32], Wright et al.[33], and Pires et al.[34], while the role of the lattice discrete structure was studied by Talim and Pires [35].

Soliton effects in an AF-quantum Ising like chain have also been measured[36-38] and Villain's theory[10] was used to interpret the experimental data. There is a good review paper by Izyumov[14] about solitons in ferromagnetic materials; the AF-chain is analysed briefly. We will, in this paper, be interested in the study of dynamical fluctuations induced by solitons in the antiferromagnetic chain. Here we will be interested mostly in theoretical aspects since Boucher [39] has recently reviewed how non-linear excitations can be observed experimentally in antiferromagnets. The experimental results in 1D-AF rely mostly on data obtained on three different compounds: $(CH_3)_4\ NMnCl_3$ $(TMMC)_3$, $CsCoCl_3$ and $Ni(C_2H_6\ N_2)_2\ ND_2\ (ClO_4)$ [NENP].

Solitons in 1D-antiferromagnets are of interest for several reasons:

1. In most 1D-magnetic salts the exchange coupling is anti- ferromagnetic [40];
2. Solitons in ferromagnets and antiferromagnets have very different properties. For instance, much larger magnetic fields are required to drive the antiferromagnet into the regime where the soliton rest energy is large compared to k_BT and solitons form a dilute gas of noninteracting e4lementary excitations [21];
3. Solitons are best observed in antiferromagnets where the contribution to the central peak is large compared tc two-magnon processes, whereas in ferromagnets both processes are of the same order. Besides, experiments and numerical simulations which have been made hitherto upon the ferromagnetic chain seem still to leave some degree of uncertainty with regard to soliton influence[15].
4. In the last years new basic questions have been raised concerning the properties of low dimensional anti-ferromagnetic systems. The discovery of the high T_c superconductors has renewed the interest in two dimensions and Haldane's conjecture which predicts a non-magnetic ground state for integer spin antiferromagnetic chains has developed new theoretical approaches [41].
5. From a fundamental point of view the antiferromagnet is also more interesting since its Hamiltonian can be niapped to the Hamiltonian of the dynamical non-linear σ model, a well studied model in quantum field theory[42,43].

We should also note that domain walls in three- dimensional crystals with characteristics similar to solitons in the 1D-model have been largely investigated by several authors[44-50] but these are macroscopic structures which cannot make an intrinsic contribution to dynamics.

II. Classical Models

Tetramethyl ammonium manganese trichloride (TMMC) is one of the most studied one dimensional antiferromagnets. Due to the large spin value ($S = 5/2$) of the Mn ions, a classical description can be used to describe the spin dynamics in this compound. The (quasi) one dimensional character of TMMC is due to the physical separation imposed by the large $[CH_3]_4N^+$ groups resulting in Mn-chains magnetically isolated from one another: the ratio of interchain to intrachain exchange interactions is roughly 10^{-4}. The three dimensional ordering temperature T_N (which is a function of the magnetic field) is about two orders of magnitude below intrachain exchange energy. TMMC has an anisotropy of dipolar origin $\delta S_n^z S_{n+1}^z$ leading the system to a crossover to the XY model at low temperatures[51], and a single-ion anisotropy in the easy-plane[52]. At low temperature and for small anisotropy, $[S_n^z]^2$ has the same effect as[53] $-S_n^z S_{n+1}^z$ so that we can start with a Hamiltonian given by:

$$\mathcal{H} = 2J\sum_n \left[\vec{S}_n \cdot \vec{S}_{n+1} + \delta\,(S_n^z)^2 + b\,(S_n^x)^2\right] - \gamma H_x \sum_n S_n^x - \gamma H_z \sum_n S_n^z \tag{2.1}$$

where $\gamma = g\mu_B$. For $J > 0$, $\delta > 0$ and $b > 0$ the ground state is along the y-direction. Although there is no long-range magnetic order in the one-dimensional model (2.1), a strong correlation is observed and this correlation creates an antiparallel alignment of the neighboring spins, so that at $T = 0$ we can speak of two antiparallel sublattices which are oriented at almost right-angles to the applied field with a slight bending along the magnetic field because of the smallness of $\gamma H/JS$. We will always consider δ and $b << 1$ which is the case in real quasi-1D antiferromagnets: it has been found that (2.1) can describe the experimental findings in TMMC if we assume $J/k_B = 6.5K$, $\delta = 0.008$, and $b = 2.6 \times 10^{-4}$.

After obtaining the equations of motion by using

$$i\dot{\vec{S}} = [\vec{S}, \mathcal{H}], \tag{2.2}$$

we treat the spin components as classical vectors with spherical components[11],

$$\vec{S}_n^A = S(\sin\theta_n^A \cos\phi_n^A, \sin\theta_n^A \sin\phi_n^A, \cos\theta_n^A)$$

$$\vec{S}_n^B = S(\sin\theta_n^B \cos\phi_n^B, \sin\theta_n^B \sin\phi_n^B, \cos\theta_n^B) \tag{2.3}$$

where A and B refer to each sublattice. However, for small magnetic fields ($\gamma H << $ JS) and at low temperatures, the spins are almost antiparallel and it is more convenient to rewrite Eq. (2.3) using the angle variables introduced by Mikeska[23],

$$\begin{aligned}\vec{S}_n &= (-1)^n S\{\sin[\theta_n + (-1)^n\nu_n] \\ &\quad \cos[\phi_n + (-1)^n\alpha_n], \\ &\quad \sin[\theta_n + (-1)^n\nu_n]\sin[\phi_n + (-1)^n\alpha_n], \\ &\quad \cos[\theta_n + (-1)^n\nu_n]\}.\end{aligned} \tag{2.4}$$

Of course both parametrizations are equivalent to one another. 8, and ϕ_n are slowly varying angle fields, and since ν_n and a, describe deviations from perfect antialignment, they can be assumed to be small at low temperatures. The variables on neighboring sites can be expressed through an expansion about $z =$ na, where a is the lattice parameter and z is the coordinate along the chain. Going over to the continuum limit amounts to substitute all angle fields as θ_n by $\theta(z)$ and to neglect the terms in order higher than a^2. Full non-linearity in the angle fields 8 and ϕ must be maintained, but the equations of motion can be approximated by an expansion up to quadratic order in v, a and $\partial/\partial z$. Notice that if we write,

$$\vec{\ell} = \frac{\vec{S}_A - \vec{S}_B}{2S} \quad , \quad \vec{m} = \frac{\vec{S}_A + \vec{S}_B}{2S} \tag{2.5}$$

we have,

$$\begin{aligned}\vec{\ell} &= (\sin 8\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta), && (2.6.a)\\ \vec{m} &= (-\alpha\sin\theta\sin\phi + \nu\cos\theta\cos\phi, \alpha\sin\theta\cos\phi \\ &\quad + \nu\cos\theta\sin\phi,\ -\nu\sin\theta), && (2.6.b)\end{aligned}$$

which gives

$$m^2 = \mathrm{v}^2 + \alpha^2\sin^2 8. \tag{2.6c}$$

The equations of motion for the angle variables are then given by,

$$\frac{1}{4JS}\frac{\partial\theta}{\partial t} = 2\alpha\sin\theta + h,\ \sin 4, \tag{2.7}$$

$$\frac{1}{4JS}\frac{\partial\phi}{\partial t} = -\frac{2\nu}{\sin\theta} + \mathrm{h,}\ \cos\phi\cot 6 - \mathrm{h,,} \tag{2.8}$$

$$\begin{aligned}\frac{1}{4JS}\frac{\partial\nu}{\partial t} &= -\frac{a^2}{2}\sin\theta\frac{\partial^2\phi}{\partial z^2} - a^2\cos\theta\frac{\partial\theta}{\partial z}\frac{\partial\phi}{\partial z} - \\ &2\nu\alpha\cos 0 - \frac{\mathrm{b}}{2}\sin 0\sin 24 + h_x\alpha\cos\phi,\end{aligned} \tag{2.9}$$

$$\begin{aligned}\frac{1}{4\mathrm{JS}}\frac{\partial\alpha}{\partial t} &= \frac{\mathrm{a}^2}{2\sin\theta}\frac{\partial^2\theta}{\partial z^2} - \frac{2\nu^2\cos\theta}{\sin^2\theta} \\ &-\cos\theta\left[\frac{a^2}{2}\left(\frac{\partial\phi}{\partial z}\right)^2 + 2\alpha^2\right] + \delta\cos\theta \\ &-b\cos\theta\cos^2\phi - h_x\left(\alpha\sin\phi\cot\theta + \nu\frac{\cos\phi}{\sin^2\theta}\right)\end{aligned} \tag{2.10}$$

where h, $= \gamma H_\alpha/4JS$. After eliminating the small angles v and a, we find

$$\begin{aligned}&\frac{\partial^2\theta}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\theta}{\partial t^2} = \\ &\sin\mathrm{e}\cos\theta\left[\left(\frac{\partial\phi}{\partial z}\right)^2 - \frac{\mathrm{i}}{c^2}\left(\frac{\partial\phi^2}{\partial t}\right)^2\right] + \\ &(2\mathrm{b} + h_x^2)\sin 0\cos 0\cos^2\phi - \\ &(26 + h_z^2)\sin 0\cos 0 - \mathrm{h,\ h,}\ \cos\phi\sin^2\theta - \\ &\frac{h_x}{2JS}\left(\frac{\partial\phi}{\partial t}\right)\cos\phi\sin^2\theta - \frac{h_z}{2JS}\left(\frac{\partial\phi}{\partial t}\right)\cos\theta\sin\theta,\end{aligned} \tag{2.11}$$

and

$$\begin{aligned}&\frac{\partial^2\phi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = \\ &-2\cot\theta\left[\left(\frac{\partial\theta}{\partial z}\right)\left(\frac{\partial\phi}{\partial z}\right) - \frac{1}{c^2}\left(\frac{\partial\theta}{\partial t}\right)\left(\frac{\partial\phi}{\partial t}\right)\right] \\ &-(2b + h_x^2)\sin\phi\cos\phi - \mathrm{h,\ h,}\ \sin\phi\cot\theta \\ &+\frac{h_x}{2JS}\left(\frac{\partial\theta}{\partial t}\right)\cos\phi + \frac{h_z}{2JS}\left(\frac{\partial\theta}{\partial t}\right)\cot\theta,\end{aligned} \tag{2.12}$$

where c = $4JSa$. On the other hand using the classical and continuum approximations directly on Eq. (2.1) we get

$$\begin{aligned}\mathcal{H} &= \text{constant} + JS^2\int\frac{dz}{a}\left\{\left(\frac{\partial\theta}{\partial z}\right)^2 + \right. \\ &4\nu^2 + \sin^2\theta\left[4\alpha^2 + \left(\frac{\partial\phi}{\partial z}\right)^2\right] + 2\delta\cos^2\theta + \\ &2\mathrm{b}\sin^2 6\cos^2 4 - 4\mathrm{h,}\ (\mathrm{v}\cos 0\cos 4 - \\ &\left.-\alpha\sin 6\sin\phi) - 4h_z\nu\sin 8\right).\end{aligned} \tag{2.13}$$

Using Eqs.(2.7) - (2.10) to eliminate the variables v and a in (2.13) and taking h, = 0 for simplicity we obtain,

$$\begin{aligned}\mathcal{H} &= \text{constant} + JS^2\int\frac{dz}{a}\left\{\left(\frac{\partial\theta}{\partial z}\right)^2 + \right. \\ &\sin^2\theta\left(\frac{\partial\phi}{\partial z}\right)^2 + \frac{1}{c^2}\left[\left(\frac{\partial\theta}{\partial t}\right)^2 + \right.\end{aligned}$$

$$+\sin^2\theta\left(\frac{\partial\phi}{\partial t}\right)^2\Bigg]+$$
$$+2\delta\cos^2\theta+(2b+h_x^2)\sin^2\theta\cos^2\phi\Big\}. \tag{2.14}$$

To treat (2.14) as a classical Hamiltonian we have to write $\mathcal{H}$ in terms of θ, ϕ, $\partial\theta/\partial z$, $\partial\phi/\partial z$ and the momenta p_θ and p_ϕ. Taking,

$$\begin{aligned} p_\theta &= \frac{1}{8J}\frac{\partial\theta}{\partial t}+\frac{Sh_x}{2}\sin\phi\,; \\ p_\phi &= \frac{1}{8J}\sin^2\theta\frac{\partial\phi}{\partial t}-\frac{Sh_x}{2}\cos\theta\sin\theta\cos\phi, \end{aligned} \tag{2.15}$$

we can rewrite (2.14) as,

$$\mathcal{H}=JS^2\int dz\,h+\text{constant}; \tag{2.16}$$

with,

$$\begin{aligned} h=&\left(\frac{\partial\theta}{\partial z}\right)^2+\sin^2\theta\left(\frac{\partial\phi}{\partial z}\right)^2+\frac{4}{S^2}p_\theta^2 \\ &+\frac{4p_\phi^2}{S^2\sin^2\theta}-\frac{4h_x}{S}\sin\phi\, p_\theta+ \\ &+\frac{4h_x}{S}\cot\theta\cos\phi\, p_\phi+2\delta\cos^2\theta+2b\sin^2\theta\cos^2\phi \end{aligned} \tag{2.17}$$

Using now Hamilton's equations for a continuum system,

$$\dot q=\frac{\partial h}{\partial p_q}\qquad \dot p_q=-\frac{\partial h}{\partial q}+\frac{d}{dz}\left(\frac{\partial h}{\partial q_z}\right) \tag{2.18}$$

with $q=\theta$, ϕ and $q_z=dq/dz$ we obtain Eqs.(2.11), (2.12) with $h_x=0$ showing that (2.16) is indeed the correct classical Hamiltonian. We remark that it is not straightforward to write a classical Hamiltonian starting from a quantum Hamiltonian when spin variables are involved. For instance, the quantum Hamiltonian for a spin $\vec{S}$ in a magnetic field $\vec{H}$ is $\mathcal{H}=-\gamma\vec{S}\cdot\vec{H}$ whereas the classical counterpart is not $\mathcal{H}_c=-\gamma SH\cos\theta$ since the kinetic energy term is missing. In fact, in taking the classical limit directly from the quantum Hamiltonian for the ferromagnet we obtain an incomplete classical Hamiltonian and to obtain the correct equations of motion an extra term would have to be added (see, for instance, refs. [54] and [55]). For the antiferromagnet we get the correct result because the, at first indetermined, variables v and α provide the extra degrees of freedom which transform into the *kinetic energy* terms when we go to the classical limit.

If the solutions of (2.11) and (2.12) are constrained to make only small excursions about the ground state $\theta=\pi/2$, $\phi=\pi/2$, we write: $\phi=\pi/2-\varepsilon\tilde\phi$, $\theta=\pi/2-\varepsilon\tilde\theta$, and obtain, in the small-angle limit, taking $h_x=0$,

$$\begin{aligned} &\tilde\theta_{zz}-\frac{1}{c^2}\tilde\theta_{tt}-2\delta\tilde\theta=-\varepsilon^2\tilde\theta\left(\tilde\phi_z^2-\frac{1}{c^2}\tilde\phi_t^2\right) \\ &-(2b+h_x^2)\varepsilon^2\tilde\theta\tilde\phi^2-\frac{4}{3}\varepsilon^2\delta\tilde\theta^3 \\ &-\frac{\varepsilon h_x}{2JS}\left(\frac{\partial\tilde\phi}{\partial t}\right)\tilde\phi. \end{aligned} \tag{2.19}$$

and

$$\begin{aligned} &\tilde\phi_{zz}-\frac{1}{c^2}\tilde\phi_{tt}-(2b+h_x^2)\tilde\phi= \\ &-\frac{2}{3}\varepsilon^2(2b+h_x^2)\tilde\phi^3+2\varepsilon^2\tilde\theta\Big(\tilde\theta_z\tilde\phi_z- \\ &\frac{1}{c^2}\tilde\theta_t\tilde\phi_t\Big)+\frac{\varepsilon}{2JS}h_x\tilde\theta_t\tilde\phi, \end{aligned} \tag{2.20}$$

with subscripts t and z implying differentiation with respect to t or z. To lowest order (we take $\varepsilon=0$ in the above equations) the solutions are,

$$\tilde\theta_1=A\exp[i(\omega_1 t-qz)],$$

and

$$\tilde\phi_1=B\exp[i(\omega_2 t-qz)]. \tag{2.21}$$

This is, we have two magnon branches with energy,

$$\begin{aligned} \omega_1^2(q) &= (2\delta+q^2)c^2, \\ \omega_2^2(q) &= (2b+h_x^2+q^2)c^2, \end{aligned} \tag{2.22}$$

here q is measured in units of the lattice constant along the chain, and the zone center is at $Q=\pi$, with q being $q=\pi-Q$. Physically, one of the modes, 1-magnon, represents the spin fluctuations out of the easy plane (out-of-plane mode) while the other mode, 2-magnon, is the fluctuation in the easy plane (in plane mode) against the magnetic field.

For the discrete lattice the magnon energy is given by

$$\left.\begin{matrix}\omega_1^2(q)\\ \omega_2^2(q)\end{matrix}\right\}=c^2[1+\delta\pm\cos q]$$
$$\left[1+b\pm\left(1-\frac{h_x^2}{2}\right)\cos q\right], \tag{2.23}$$

which for small q reduces to (2.22). Note that the division of the system into sublattices splits the $[0,\pi]$ range into two ranges: $[0,\pi/2]$ which gives the 1-magnon; and the range $[\pi/2,\pi]$ (mapped into $[0,\pi/2]$), which gives the 2-magnon.

To obtain higher-order solutions for (2.19) and (2.20), the term proportional to ε must be retained. This term, for $h_x \neq 0$, introduces a coupling between the lowest-order solutions $\tilde{\phi}_1$ and $\tilde{\theta}_1$ and is responsible for the appearance of double magnon-modes. These modes have in fact been observed by Boucher et al.[56] in TMMC using inelastic neutron scattering combined with neutron-polarization analysis.

Let us now discuss the full non-linear equations (2.11) and (2.12): their static limit agrees with the corresponding limit for the equations of motion for a ferromagnet with two anisotropies $(b+h_x^2/2)$ and $(\delta+h_z^2/2)$. The field-anisotropy equivalence was discussed in [29] where it was shown that, for the calculation of some properties, an antiferromagnet with a field h_α applied along an a-direction is entirely equivalent to a ferromagnet with anisotropy $B_\alpha = h_\alpha^2/2$. The dynamics, however, is quite different for both models. We note also that for $h_\alpha = 0$ Eqs. (2.11) and (2.12) exhibit Lorentz invariance. It means that, in this case, all effects of soliton dynamics are reduced to Lorentz contraction of its thickness, and, therefore, if a soliton is stable for zero velocity ($u = 0$), then it remains stable for all velocities $u < c$.

Let us consider here the case $h_\alpha = 0$, leaving the more general case to the next Section. Since for this case $\theta = \pi/2$ and $\phi = \pi/2$ satisfy Eqs.(2.11) and (2.12), complete dynamical solutions are obtained from

$$\theta = \pi/2 \ , \quad \frac{\partial^2\phi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = -2b\cos\phi\sin\phi \qquad (2.24.a)$$

with

$$a = 0 \quad \text{and} \quad \nu = -\frac{1}{2c}\frac{\partial\phi}{dt}, \qquad (2.24.b)$$

and

$$\phi = \pi/2 \ , \quad \frac{\partial^2\theta}{\partial z^2} - \frac{1}{c^2}\frac{a^2 e}{\partial t^2} = -2\delta\cos\theta\sin\theta \qquad (2.25.a)$$

with

$$\nu = 0, \quad \text{and} \quad \alpha = \frac{1}{2c\sin\theta}\frac{\partial\theta}{\partial t}. \qquad (2.25.b)$$

Eqs. (2.24) and (2.25) are the well known sine-Gordon (SG) equations in the variables 24 and 2θ, respectively. The SG equation,

$$\frac{\partial^2\Psi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\Psi}{\partial t^2} = m^2\sin\Psi \qquad (2.26)$$

is completely integrable[57] with the result that only three mode types are required to specify the solution of an arbitrary initial value problem. These modes are:
a) small amplitude solutions (in our case, magnons), i.e. extended periodic harmonic waves with dispersion relation

$$\omega^2(q) = (m^2 + q^2)c^2,$$

b) traveling waves of permanent profile, described by,

$$\Psi(z,t) = 4\tan^{-1}\{\exp[\pm\gamma m(z-ut-z_0]\} \qquad (2.27)$$

where $\gamma = (1-u^2/c^2)^{-1/2}$, and the plus (+) and minus (-) signs correspond to solitons and antisolitons, respectively.

The soliton (or antisoliton) describes a localized change in the phase of two physically equivalent values: $\Psi = 0$ and $\Psi = 2\pi$. In the antiferromagnet, this implies rotation of the spin vector $\vec{S}$ in the plane by an angle π in an interval ξ of the order $1/m\gamma$. Apart from the simplest solution (2.27), the SG equation also has n-soliton solutions which can be regarded as a set of n separate solitons, each one with its own parameters u_n and z_{0n} representing the velocity and coordinate of the soliton-center. This n-soliton solution satisfies the principle of asymptotic superposition implying that individual solitons recover their profile after collisions. Thus the only result of a collision between solitons is a phase change or better, after a collision with other soliton with velocity u', the position of a soliton with velocity u is displaced by an amount,

$$\Delta_S(u,u') = 2m^{-1}ln(2/|u-u'|). \qquad (2.28)$$

It is this circumstance that allows us to treat the n-soliton solution, when the soliton density is small, as a superposition of independent quasiparticles.
c) breathers, which are large amplitude solutions given by,

$$\Psi_B(z,t;\omega_b) = 4\tan^{-1}\left\{\frac{(\omega_0^2/\omega_B^2-1)^{1/2}\sin\gamma\omega_B[(t-uz/c_0^2)]}{\cosh[\gamma m(z-ut)(1-\omega_B^2/\omega_0^2)^{1/2}]}\right\}, \qquad (2.29)$$

where the oscillation frequency ω_B lies in the range $0 < \omega_B < \omega_0$ with $\omega_0 = mc$. Breathers can be viewed as coherent anharmonic (i.e. non linear) magnons. Indeed, in quantized theory, breathers are multimagnon bound states[42]. Because breather's effects can be analysed in terms of perturbation theory (anharmonic magnons)[58], we will not consider that mode in this paper. For a discussion about breather's effects see, for instance, refs. [59-62].

Thus, the soliton solution of Eq. (2.24) is,

$$\phi = \pi/2 + 2\tan^{-1}\left[e^{\pm\gamma\sqrt{2b}(z-ut)}\right] \qquad (2.30)$$

or

$$\sin\phi = \tanh[\gamma\sqrt{2b}(z-ut)] \qquad (2.31)$$

A similar solution ($b \to 5$) exists for the θ variable in Eq. (2.25). Inserting these solutions in the continuum Hamiltonian (2.13), we obtain the soliton energies

$$E_{xy} = 4JS^2\gamma\sqrt{2b}, \quad E_{yz} = 4JS^2\gamma\sqrt{2\delta}, \qquad (2.32)$$

where xy refers to the soliton in the xy plane and yz to the one in the yz plane. The soliton stability will be studied in Section III, where it will be shown that only the lowest energy soliton is stable. We can also write the soliton energy (say for the xy soliton) as,

$$E(p) = [(E^0_{xy})^2 + p^2]^{1/2}, \tag{2.33}$$

where $E^0_{xy} = 4JS^2\sqrt{2b}$ and p is the soliton momentum. It is possible then to interpret a soliton as a *relativistic* particle of rest energy E^0_{xy}, and mass $m = E^0_{xy}/c^2$, moving with a velocity u and localized at a point z_0. The limiting velocity c represents the magnon velocity. In the non relativistic limit (u << c), we have for the soliton energy

$$E(p) \approx E^0_{xy} + \frac{p^2}{2m}. \tag{2.34}$$

III. Discussion of Solutions to the Equations of Motion

The general solutions to Eqs. (2.11) and (2.12) are very difficult to obtain and, for this reason, we will consider here some special cases only. First, let us insert $\phi = \pi/2$ into those equations obtaining,

$$\frac{\partial^2\theta}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\theta}{\partial t^2} = -(2\delta + h_z^2)\sin\theta\cos\theta, \tag{3.1}$$

$$-h_x h_z \cot\theta + \frac{h_z}{2JS}\left(\frac{\partial\theta}{\partial t}\right)\cot\theta = 0. \tag{3.2}$$

Eq. (3.2) is satisfied for h, = 0 and in this case, from (3.1) we have a dynamical soliton solution (SG solution - as given by Eqs. (2.30) and (2.31)) in the yz plane. If h, ≠ 0 and h, = 0, then (3.2) implies in $\partial\theta/\partial t = 0$, and we have a static soliton in the yz plane.

Of course, we have a similar situation for the xy case ($\theta = \pi/2$): a dynamical xy soliton exists only if h, = 0. For h, ≠ 0 and h, = 0, we have a static soliton in the xy plane with energy

$$E^0_{xy} = 4JS^2 h_x. \tag{3.3}$$

In (3.3) we have taken b = 0 for the sake of simplicity and because in most materials this anisotropy is very small (in TMMC, b ≈ 10^{-4}). Thus if $h,$ < $h,$ = $\sqrt{2\delta}$, the xy soliton has energy lower than the yz soliton. However, for h, # 0 (which implies v ≠ 0 - see Eq. (2.27)), there is no analytic solution. More generally, we can treat the additional terms in (2.11) and (2.12) as small perturbations expanding the out of plane deviation $\theta(s)$, where s = $z - $ ut, around the static solution $\theta = \pi/2$. Keeping terms up to first order,

$$\phi(s) \approx \phi_{sg}(s) \quad , \quad \theta(s) \approx \frac{\pi}{2} + \tilde{\theta}, \tag{3.4}$$

where $\phi_{sg}(s)$ is the dynamical sine-Gordon soliton (Eq(2.30)),we obtain the formal solution[27,63],

$$\tilde{\theta}(s) = \pm\frac{u}{\lambda}\left\{sech^2(h_x s) - \frac{1}{4}\int d\xi \right.$$
$$[\exp(ih_x s\xi)]\frac{\xi^2(\xi + i\tanh(h_x s))}{\xi^2 + 1 + \lambda}$$
$$\left.\text{cosech}\left(\frac{\pi\xi}{2}\right)\right\} - \frac{r}{\lambda}sech(h_x s), \tag{3.5}$$

where

$$\lambda = \frac{26}{h_x^2} - 1 \quad \text{and} \quad r = \frac{h_z}{h_x}.$$

For h, << 2δ and h, << h,, the soliton energy is given by [63],

$$E_{,,} \approx E^0_{xy}\left[1 + \frac{u^2}{c^2}\left(\frac{1}{2} + \frac{4}{3\lambda}\right) + \frac{r}{\lambda}\left(\pm\frac{3\pi}{8}u - \frac{r}{2}\right)\right], \tag{3.6}$$

where S/A represents Soliton/Antisoliton. We see that for h, ≠ 0 (r ≠ 0) we have a nonvanishing out-of-plane amplitude even for zero velocity, u = 0. This additional out-of-plane component due to h,, for a soliton moving in the $h,$ direction, is opposed to the out-of-plane component due to soliton motion.

For h, = 0 and $h_x \to$ h, the energy is given by[27],

$$E \simeq E^0_{xy}\left[1 + \frac{u^2}{c^2}\left(\frac{\pi^2}{8\lambda} + \frac{1}{2}\right)\right]. \tag{3.7}$$

The curvature of the xy soliton dispersion (3.7) changes sign at h, = h,, which means that for h, > h, the xy soliton is unstable against spontaneous motion.

A more detailed numerical calculation, for the case b = 0 and h, = 0, has been carried out by Costa and pires[2"] and Wysin et al.[30]. A continuum limit ansatz and direct numerical simulations on the discrete lattice performed by Wysin et al.[30] show that the xy and yz solitons belong to a single continuously connected energy dispersion branch, this is, the xy and yz branches are continuously connected. They also show that for h < h,, where static yz solitons are unstable, there can be stable moving yz solitons. From the numerical integration, it was found that the xy solitons are stable above and below the critica1 field h,, at least for 6 = 0.08 (the value for TMMC), 0.08 ≤ h ≤ 0.6 and $|u/c| < 1$. Even for h > h, they show no tendency to decay to lower energy yz solitons. At the critica1 field h_c(h_c = 0.4 for TMMC) there is a continuum of xy solitons all with the same energy and velocity. For small velocities u << c, the sine-Gordon theory adequately describes the yz branch. Static yz solitons are stable only if h > h,, while dynamic yz solitons require a minimum applied field to be stable. This minimum field decreases with the increase of velocity. For h < h, the static yz soliton decays towards a configuration involving a lower energy xy soliton. In Figure 1 we show the soliton energy for the general solution as a function, of the soliton velocity u for field values h < h,, h = h, and h > h,.

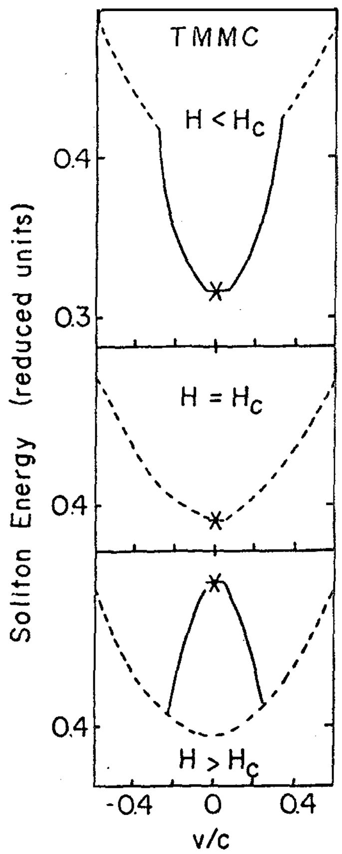

Figure 1: Soliton energy as a function of velocity in case of TMMC (from [90]). The full line corresponds to xy solitons; for h = h, this branch collapses in one point: all the solitons become static. The dashed lines describe the yz soliton.

A numerical investigation of collisions of soliton- antisoliton pairs in the model discussed above has also been done by Wysin and Bishop[64], the results being: for low- velocity xy solitons and low fields $h < 0.2h_c$ there is sine Gordon like transmission. At higher fields but still with h < h,, the low-velocity pairs annihilate to spin waves, or possibly form breathers, and the higher-velocity xy solitons undergo SG-like transmission. For h > h, the negative-effective mass xy solitons reflect. Most of the cases tested for yz soliton- antisoliton pairs resulted in transmission consistent with their nearness to SG behaviour. The exceptions included some cases at small velocity for h > h,, where annihilation occurs. Then in the strict sense of the word, in general, the xy and yt solitons are not solitons and should better be called by the name of kinks.

The Hamiltonian (2.1) with fourth-order anisotropic terms $(S_n^z)^4$, $(S_n^x)^4$ and $(S_n^x S_n^z)^4$ (but without a magnetic field) has been studied by Pires[65]. Dynamical solitons in a 1D antiferromagnet with both an easy axis (Ising-like) and an applied magnetic field along the easy axis have been studied theoretically by Kimura and de Jonge[66] (for more details, see Section XII). A classical one dimensional Heisenberg antiferromagnet with a single-ion anisotropy and a Dzyaloshinskii-Moriya term has been investigated by Pandit et al.[67] in order to explain experimental data on the polymer $\{Co[(C_4H_9)_2PO_2]_2\}_x$. They showed that, in certain ranges of coupling constants, solitons in such antiferromagnet can be approximated by sine-Gordon or double-sine-Gordon solitons.

The parametrization (2.4) is not suítable when the applied magnetic field is very large, because the spin-flop angle will also be large destroying the antialignment implicit in (2.4). In this case, parametrization (2.3) is more indicated and we will have two topologically distinct π solitons in the xy plane. In the first type soliton one sublattice experiences a phase jump of 2α, where a = $\cos^{-1}(h_x/2)$ is the spin-flop angle while the other sublattice rotates by $2(\pi-\alpha)$. For small magnetic fields, this type of soliton is the one which corresponds to the sine-Gordon soliton. For large fields this soliton has a more complicated structure. In the second type soliton, the two sublattices interchange their directions by rotating through $\pm 2\alpha$ angles. For more details see [34] and [68].

Talim and Pires[35] have used perturbation theory to study corrections to the xy and yt solitons arising from the influence of lattice discreteness. They have shown that for TMMC, at the temperatures where most experiments have been done, these corrections are so small that can be neglected.

We have based our theory of solitons, even in [35], entirely on a continuum approximation to the lattice model. One of the qualitative differences between a lattice model and a continuum model is that a soliton in the former model is somehow ***pinned*** to a lattice site whereas a soliton in the latter model is free to slide without any extra cost of energy. The pinning energy is the minimum energy required to move the soliton from one lattice site to another. However Sasaki[69] has shown that, for TMMC, very large magnetic fields, as compared to h,, would be needed in order to have appreciable values for the pinning energy. Therefore it is impossible to observe the effects of soliton pinning in this material.

Numerical sirnulations carried out directly on the discretized sine-Gordon model and ferromagnetic chains have revealed, besides the pinning effect, decrease of velocity, distortion of the profile, damping and decay of solitons into small amplitude oscillations (spin-wave modes). The narrower soliton (half width of 2 lattice spacings) becomes unstable and decays at a relatively early evolution stage than the wider one (see [70] and references cited therein). Possibly the same would be true for the AF chain. A qualitative measure of discreteness importance is the ratio of the lattice constant α to the characteristic width ξ of the soliton solution to the unperturbed sine-Gordon equation. The lattice discreteness effect is negligible for static solitons if $a/\xi << 1$. We have seen that for u = 0, a/ξ = h for the xy soliton and $a/\xi = \sqrt{2\delta}$ for the yz soliton. In TMMC, 6 = 0.01 and the highest magnetic field used in experiments corresponds to h = 0.19, showing that the discreteness effect can be expected to be quite small. Note also that, for h > h, $= \sqrt{2\delta}$ the important soliton is the yz soliton whose width independs on h.

IV. Phenomenoilogical Calculation of the Soliton Density

In this section we will discuss a phenomenological calculation for the soliton density in the antiferromagnetic chain, and, in doing so, we will study the soliton stability. For h < h, the xy soliton is the lowest energy soliton and we will treat only this case (a similar treatment can be done for h > h,). For a phenomenological theory we need the spectrum and phase shift of spin waves in the presence of solitons[71]. The behavior of small oscillations in the presence of a single static soliton $\phi_0(z)$ is determined by solutions to (2.11) and (2.12) (with h, = 0) of the form,

$$\phi(z,t) = \phi_0(z) + \xi(z,t)$$

$$\theta(z,t) = \pi/2 + \tilde{\theta}(z,t) + \eta(z,t) \qquad (4.1)$$

where $\tilde{\theta}$ is the out-of-plane deviation given by Eq.(3.5). Substitution of (4.1) into (2.11) and (2.12), linearization in ξ and η, and writing

$$\begin{aligned} \xi(z,t) &= r(z)e^{i\omega t} \\ \eta(z,t) &= s(z)e^{i\omega t} \end{aligned} \qquad (4.2)$$

lead to the following eigenvalue equations:

$$\frac{d^2r}{dz^2} + \frac{\omega^2}{c^2}r = m^2(1 - 2\mathrm{sech}^2 mr)r + i\frac{2h_x}{c}ws \quad \mathrm{sech}\, mz \qquad (4.3)$$

$$\frac{d^2s}{dz^2} + \frac{\tilde{\omega}^2}{c^2}s = m^2(1 - 2\mathrm{sech}^2 mr)s - i\frac{2h_x}{c}wr \quad \mathrm{sech}\, mz \qquad (4.4)$$

where $m^2 = h_x^2 + 2b$ and $\tilde{\omega}^2 = w^2 - (26 - m^2)c^2$.

Far from the soliton center we find

$$\omega_1^2(q) = (2\delta + q^2)c^2 \quad , \quad \omega_2^2(q) = (m^2 + q^2)c^2 \qquad (4.5)$$

in agreement with Eqs.(2.22).

Let us consider just the case h, = 0. For this case the problem can be solved exactly. Eq.(4.3) possesses a bound state solution with $\omega_{1b} = 0$, as in the SG problem, describing translational invariance of the soliton center[71]. Eq.(4.4) has the same form, only now $\tilde{\omega}$ = 0 gives a bound state with frequency

$$\omega_{2b}^2 = 2(\delta - b)c^2. \qquad (4.6)$$

As we see ω_{2b}^2 has to be positive for the out-of-plane motion (fluctuations in the z direction), this means b < δ. The bound state becomes soft at the crossover anisotropy b = 6, i.e., the static xy soliton becomes unstable. Both (4.3) and (4.4) for h, = 0 have the same phase shift $\Delta(q)$ for the continuum states. We have [71,72]

$$\Delta(q) = 2\tan^{-1}(\sqrt{2b}/q). \qquad (4.7)$$

For h, $\neq$ 0 the calculations are more complicated and only recently have been performed by Costa[73] using the Born approximation, which for this reason just misses the points specifically of interest for a real antiferromagnetic chain in an externa1 magnetic field.

The soliton density for Hamitonian (2.1) (with b = 0, and h, = 0, for simplicity) can be easily calculated. According to Currie et al.[71] the average number of both solitons and antisolitons is given by

$$n = -\beta F = \frac{2}{L}\ln\int\frac{dz}{2\pi}dp\exp[-\beta(E(p) + S)], \quad (4.8)$$

where F is the free energy per unit length, L is the system size, z is the position of soliton (or antisoliton), $\beta = 1/k_BT$ and $E(p)$ is the energy-dispersion of solitons. S is the self-energy given by

$$\beta S = \int\frac{dq}{2\pi}\frac{d\Delta(q)}{dq}\ln[\beta^2(\omega_1(q)\omega_2)q))] + \sum_i \ln(\beta\omega_{ib}), \qquad (4.9)$$

where $\omega_1(q)$, $\omega_2(q)$, and $\Delta(q)$ are the frequencies and asymptotic phase shift of the linear scattering solutions to the equations of motion [Eq.(4.5) and Eq.(4.7) multiplied by 2] and ω_{ib} are the frequencies of the bound states.

For h, << 26 the essential contribution to the free energy F comes from the lower branch of the spectrum, (i.e. the xy soliton), then we can neglect effects of the yr branch. Inserting (4.5), (4.7) (multiplied by 2), (4.8) and (4.9) into (4.12) we obtain

$$\exp(-\beta S) = \frac{2\beta c h_x(1 + h_x/\sqrt{2\delta})}{(1 - h_x^2/2\delta)^{1/2}}. \qquad (4.10)$$

Using the expression for E(p) given by (2.33) we can write

$$E(p) \simeq E_{xy}^0 + p^2/2\tilde{M}, \qquad (4.11)$$

where $\mathrm{M} = M(1 + 8/3\lambda)$, $M = E_{xy}^0/c^2$.

Inserting *(4.13)* and *(4.14)* into *(4.11)* we finaily find

$$n = n_s(1 + h_x/\sqrt{2\delta})\left[\frac{1 + 8/3\lambda}{(1 - h_x^2/2\delta)}\right]^{1/2} \qquad (4.12)$$

where n_s is the soliton density for the SG model given by

$$n_s = 4\sqrt{\frac{2}{\pi}} J^{1/2} S h_x \left(\frac{h_x}{T}\right)^{1/2} \exp(-4JS^2 h_x/T). \tag{4.13}$$

As we can see, for low temperature and small magnetic fields, the leading correction to the SG result comes from spin fluctuations out of the easy plane, i.e. the out-of-plane magnon mode not present in the pure SG model.

For $h_x << \sqrt{2\delta}$, we see from the above calculations that we can use the decoupled model. Thus, we neglect the last term on the right hand sides of (4.3) and (4.4) and replace the magnetic field by an effective anisotropy[74] $b = h_x^2/2$. This agrees with the well known fact that the thermodynamical properties of the Hamiltonian (2.1) are equivalent to those of a ferromagnetic Heisenberg model with two single-site anisotropic terms[75,76].

V. Dynamics Structure Factors: Transverse Correlation Function for the xy Soliton

We start by studying the transverse spin-correlation function in the xy plane given by

$$\begin{aligned}&< S^y(z,t)S^y(0,0) >= (-1)^n S^2 \times \\ &< \sin\phi(z,t)\sin\phi(0,0)\sin\theta(z,t)\sin\theta(0,0) >,\end{aligned} \tag{5.1}$$

where $z = na$. In antiferromagnetic chains, the soliton regime gives rise to a very special feature: each time a soliton passes by there is a flipping of the spins associated with the two sublattices, i.e., the spin components perpendicular to the field change its orientation from $\pm S_n^y$ to $\mp S_n^y$ destroying the long range correlation that would exist in the absence of solitons. In this manner, the S^y spin components can be correlated only within a distance comparable to the distance between 2 solitons. In an approximate description on a length scale large compared to the soliton extension, we can write (5.1) as[23]

$$\begin{aligned}&< S^y(z,t)S^y(0,0) >= \\ &= (-1)^n < (S_n^y)^2 >< \sigma(z,t)\sigma(0,0) >,\end{aligned} \tag{5.2}$$

where $\sigma(z,t) = \pm 1$ is a quantity of the Ising type. We have [77] $\sigma(z,t)\sigma(0,0) = (-1)^m$, where m is the number of solitons in the space-time interval between the points (0,0) and (z,t). Since for a soliton gas with N particles the probability $p(m)$ of finding m solitons obeys the Poisson distribution, $p(m) = (N^m/m!)e^{-N}$, we have

$$\begin{aligned}&< \sigma(z,t)\sigma(0,0) >=< (-1)^m > \\ &= \sum p(m)(-1)^m = e^{-2N(z,t)}.\end{aligned} \tag{5.3}$$

$N(z,t)$ is the average number of solitons (and antisolitons) at $t = 0$, consisting of two contributions: (i) the number of solitons between 0 and z, which will not pass z in the time interval between 0 and t; (ii) the number of solitons outside the range from 0 to z, which will pass z in the time interval between 0 and t. The number of solitons and antisolitons with velocity u is given by

$$N(u) = 2n_s P(u), \tag{5.4}$$

where $P(u)$, the probability of finding a soliton with velocity u is, within Boltzmann statistics, expressed as

$$P(u) = \frac{1}{\sqrt{\pi}u_\theta} \exp\left[-\left(\frac{u}{u_\theta}\right)^2\right], \tag{5.5}$$

where $u_\theta = c(2\beta hJS^2)^{-1/2}$ is the thermal velocity. We find then for $N(z,t)$

$$\begin{aligned}N(z,t) \ = \ &\left(\int_{-\infty}^{0} du \int_{0}^{z-vt} dz_0 + \int_{0}^{z/t} du \int_{0}^{z-vt} dz_0 \right. \\ &\left. + \int_{z/t}^{\infty} du \int_{z-vt}^{0} dz_0 \right) N(u)\end{aligned} \tag{5.6}$$

or

$$N(z,t) = 2n_s u_\theta |t| f[z/(u_\theta|t|)] \tag{5.7}$$

with

$$f(y) = \pi^{-1/2}\left[e^{-y^2} + 2y\int_0^y e^{-x^2}dx\right]. \tag{5.8}$$

For $t \to 0$, we have $f(y) \sim y$ leading to

$$< S^y(z,0)S^y(0,0) >=< (S_n^y)^2 > (-1)^n e^{-4n_s z}. \tag{5.9}$$

Thus if ξ^{-1} is the inverse correlation length for the transverse correlation function we have

$$\xi^{-1} = \Gamma_q = 4n_s. \tag{5.10}$$

ξ characterizes the average size of an antiferromagnetic region between two solitons. Note that the calculation above, although performed in the xy limit, does not depend on the form of the soliton and therefore is quite general.

For $y >> 1$ or $y << 1$, we can approximate $f(y)$ by the function $\pi^{-1/2}(1+\sqrt{\pi}y)$ obtaining[23],

$$S^{yy}(q,\omega) =< (S_n^y)^2 > \frac{1}{\pi^2}\frac{\Gamma_\omega}{\omega^2+\Gamma_\omega^2}\frac{\Gamma_q}{\Gamma_q^2+q^2} \tag{5.11}$$

with

$$\Gamma_\omega = 4n_s u_\theta/\pi^{1/2}. \tag{5.12}$$

A different approximation of $f(y)$ by $\pi^{-1/2}(1+\pi y^2)^{-1/2}$ gives the expression[25]

$$S^{yy}(q,\omega) =< (S_n^y)^2 > \frac{1}{2\pi}\frac{\Gamma_\omega^2/\Gamma_q}{[\Gamma_\omega^2(1+q^2/\Gamma_q^2)+\omega^2]^{3/2}}. \tag{5.13}$$

These two different approximations lead to essentialy the same result: the transverse fluctuations give rise to an intense central peak around q = 0 and w = 0. However, (5.11) predicts the energy width to be independent of q, $\Delta\omega = 2\Gamma_\omega$, while (5.13) yields $\Delta\omega$ = 1.533 $\Gamma_\omega(1+q^2/\Gamma_q^2)^{1/2}$.

We can see from (5.11) and (5.12) that the transverse correlation function for an antiferromagnet is of a different nature than for the xx or zz correlation functions (see Sections VI and VII). This difference is related to the fact that the S^x and S^z spin components behave differently in respect to solitons: they do not suffer the flipping experienced by S_n^y when a soliton passes. In particular the widths of $S^{yy}(q,\omega)$ along q and w are proportional to the soliton density, indicating that interference effects occur in the scattering process, so that the central peak is not associated with the scattering by a single soliton. Neutrons are scattered coherently by the region in a chain between two solitons.

We also remark that the characteristic properties of the antiferromagnetic chain from a physical point of view are quite distinct from the ferromagnetic chain, in particular the antiferromagnetic central peak is a δ-function when no solitons are present whereas in the ferromagnet the external magnetic field induces long range order, which is not destroyed by solitons.

Using the equivalence between Hamiltonian (2.1) (with $h_x = 0$) and a ferromagnet with 2 anisotropies, ξ can be calculated via the transfer matrix method[29,78]. In the limits $h << h_c$, $h \simeq h_c$, $h >> h_c$, the results agree with the phenomenological calculations performed in Section IV (see [29] for these limits). Since it is almost impossible to perform an analytical phenomenological calculation of n_s for all values of h, we can use the result obtained from transfer matrix calculation for ξ in order to have n_s. However, it would be very interesting to have numerical calculations of n_s for an antiferromagnetic chain for all values of h, in the line of Gaulin[79] and Gerling[80] in order to compare with the result from the transfer matrix method.

Equations (5.11) and (5.13) were derived ignoring interference between solitons and magnons. For a study of the influence of soliton-magnon interferences on the zero-order magnon and soliton peaks, we consider a linear superposition of 2N (anti) solitons and the real part of a general magnon solution. We consider also the small-amplitude fluctuations v and α neglected in Eq (5.1). Calculations performed in the sine-Gordon limit, for the xy soliton contribution, give the following result for the soliton peak (flipping mode)[81] ,

$$S_{sol}^{yy}(q,\omega) = \left\{1 - \frac{1}{2\pi\tilde{\beta}h}\left[1 + \frac{h}{\sqrt{2\delta}} - \frac{2n_s}{h} + \frac{1}{2}\right.\right.$$
$$\left.\left.\left(-1 + \frac{3n_s}{h} + 4\pi h^2\right)\frac{< \sin^2\phi\cos^2\phi >}{< \cos^2\phi >}\right]\right\} S^{yy}(q,\omega) \tag{5.14}$$

where $\tilde{\beta} = 2JS^2/k_BT$, and $S^{yy}(q,\omega)$ is given by (5.11) or (5.13). As we can see from (5.14) the soliton-induced central peak is reduced in intensity if soliton-magnon interferences are taken into account. Also, the small amplitude v diminishes the intensity: the contribution due to v leads to the term $4\pi h^2$ in (5.14). Besides the soliton peak, the calculation furnishes a magnon peak, which is absent when soliton-magnon interaction is neglected, and two magnon process. The extra contribution to the central peak from multi-magnon processes is very small compared to the flipping mode and can therefore be neglected.

VI. Longitudinal Correlation Function in the SG Limit

For $h << h_c$ the $S^{xx}(q,\omega)$ correlation function is given by

$$S^{xx}(q,\omega) = \frac{1}{(2\pi)^2}\int dzdt(-1)^n S^2$$
$$< \cos\phi(z,t)\cos\phi(0,0) > e^{i(qz-\omega t)}. \tag{6.1}$$

The average in (6.1) can be calculated initially by considering that only one soliton is excited thermally in a chain. In this case this average implies in integration with respect to all possible soliton positions and velocities[23], i.e.

$$< \cos\phi(z,t)\cos\phi(0,0) >=$$
$$\int N(u)\cos\phi(z,t)\cos\phi(0,0)dz_0du, \tag{6.2}$$

where $N(u)$ is given by (5.4). In the non - relativistic sine-Gordon limit we have (see section 2)

$$\cos\phi(z,t) = sech[h(z-z_0-ut)]. \tag{6.3}$$

From (6.1), (6.2) and (6.3) we obtain

$$S^{xx}(q,\omega) = \frac{1}{(2\pi)^2}\frac{2n_sS^2}{\sqrt{\pi}u_\theta}\int e^{iqz}e^{-i\omega t}e^{-au^2}\times$$
$$sech[h(z-z_0-ut)]sech(hz_0)dudtdz_0dz, \tag{6.4}$$

where q is measured from π, and $a = u_\theta^{-2}$. Defining $y = z - z_0 - ut$, and using

$$\int_{-\infty}^{\infty} e^{iqy} sech\, hydy = \frac{\pi}{h} sech\left(\frac{q\pi}{2h}\right),$$

and

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(qu-\omega)t}dt = \delta(qu-\omega),$$

we find

$$S^{xx}(q,\omega) = S^2(n_s\pi^{1/2}/h^2u_\theta q)$$
$$\exp[-\omega^2/(u_\theta q)^2]sech^2(\pi q/2h). \tag{6.5}$$

Eq (6.5) gives a central peak superimposed on the flipping mode. It becomes narrower as $q \to 0$ with a diverging intensity. However when the instrumental resolution is taken into account, the resulting peak becomes much smaller than the $S^{yy}(q,w)$ peak[18]. In fact, the contribution from $S^{zz}(q,w)$ is comparable to the contribution from multimagnon processes to the central peak [13]. The different nature of the transverse and longitudinal correlations in an antiferromagnetic chain is manifested by different temperature dependences of the intensity of the central peak. For the longitudinal correlations this dependence shows an increase with T as the soliton density is increased, whereas in the case of the transverse correlation there is a reduction inversely proportional to the soliton density.

The longitudinal correlations in an antiferromagnet are entirely due to the structure factor of one soliton and behave similarly to a ferromagnet. Therefore, in the range of the parameters where the intensity of the transverse correlation is high, the corresponding intensity for the longitudinal correlation should be low.

If we now take into account the soliton-magnon interaction and the small amplitude fluctuations v and α, we obtain[81]

$$S^{xx}_{sol}(q,\omega) = [1-\Delta_1(q,\omega)-\Delta_2(q,\omega)]S^{xx}(q,\omega) \quad (6.6)$$

where

$$\Delta_1(q,\omega) = \frac{1}{2\pi\tilde{\beta}h}\left[1+\frac{h}{\sqrt{2\delta}}-\frac{2n_s}{h}-\frac{1}{2}\left(1-\frac{3n_s}{h}\right)\frac{h^2+q^2}{2h^2}\right], \quad (6.7)$$

$$\Delta_2(q,\omega) = \frac{1}{2}\frac{\omega^2}{q^2}\left(\frac{h}{4JS}\right)^2\left(\frac{h^2+q^2}{h^2}\right), \quad (6.8)$$

and $S^{xx}(q,\omega)$ is given by (6.5). The contribution $\Delta_2(q,\omega)$ comes from the small amplitude v. This term gives rise to a peak in $S^{xx}_{\rm sol}(q,\omega)$ at a frequency $\omega_p = u_\theta q$. The soliton-induced central peak is reduced in its intensity by a factor that differs from the one in the longitudinal case due to the different way of calculations of the averages in the sine and cosine terms. For the contributions to the magnon peak, see ref [82]. This peak, which is sharp as long as only harmonic inagnons are taken into account, acquires a width due to the soliton-magnon interaction.

We must point out that in this section we have considered only the case of extremely high anisotropy so that spins are confined to the easy plane. When the anisotropy parameter is finite, we should obtain important corrections that would alter the above results. The classical SG model can be regarded only as a first approximation which provides a qualitative understanding of the non linear dynamics. A quantitative theory requires allowance for the out-of-plane motion.

Despite of the theoretical calculations presented here and in the latter section the influence of the solitons on the magnons has not been unambiguously measured by experiment. Also solitons and non linear coupling between single-and higher-order spin waves can be described theoretically quite well, however a coherent theory describing both on the basis of the same Ansatz does not exist at present.

VII. The Out-of-Plane Structure Factor

In this section we will calculate the out-of-plane correlation function in the limit of low temperatures. For $h_x^2 << 2\delta$ $(b = 0)$, the spins are mainly restricted to the xy plane and the out-of-plane spin component S_n^z, described by θ_n and v (cf.eq.(2.4)), is very small. The expressions for θ_n and ν_n corresponding to a soliton in that plane were derived in Section III (eq.(3.5)) and are given by

$$\begin{aligned}\theta_n &\simeq \pi/2 + u(R/2JS)sech^2[h_x(z-ut)],\\ \nu_n &\simeq -u(h_x/4JS)sech[h_x(z-ut)]\end{aligned} \quad (7.1)$$

where $z = na$ and $R = h_x^2/2\delta$. Because θ_n and ν_n are both small quantities we will not start here by considering initially the sole effect of one soliton in the chain - as we did in the calculation of $S^{zz}(q,w)$. Here it is more convenient to include solitons and magnons from the very beginning. Then we describe S_n^z as a superposition of a soliton and the real part of a general magnon solution, i.e.,

$$\begin{aligned}S_n^z &= (-1)^n S\sin[(\theta_n+(-1)^n\nu_n + Re\sum\gamma_q\tilde{\theta}_q(z,t)]\\ &\simeq (-1)^n[\theta_n+(-1)^n\nu_n+Re\sum\gamma_q\tilde{\theta}_q(z,t)]\end{aligned} \quad (7.2)$$

Up to lowest order in soliton density there is no soliton magnon interference. Isolating the soliton contribution to $S^{zz}(q,\omega)$ we obtain

$$\begin{aligned}S^{zz}_{\rm sol}(q,\omega) = \frac{S^2}{4\pi^2}\int\int dtdz e^{i(qz-\omega t)}\\ \{<\theta(r,t)\theta(0,0)> + <\nu(r,t)\nu(0,0)> +\\ + <\theta(r,t)\nu(0,0)> + <\nu(r,t)\theta(0,0)>\}\end{aligned} \quad (7.3)$$

Obviously this equation refers to the part of $S^{zz}(q,\omega)$ due to the structure factor of the out-of-plane component of one soliton and we remark here that, as will be shown below (eq.(7.4)), it is more complex than the corresponding quantity for a ferromagnet because of the contribution from v. Inserting eqs.(7.1) into (7.3) and integrating in respect to all soliton positions and velocities, we obtain

$$S^{zz}_{\rm sol}(q,\omega) = \frac{n_s\sqrt{\pi}}{(2JS)^2u_\theta}\frac{\omega^2}{q^3}\exp\{-\omega^2/(u_\theta q)^2\}$$

$$\left\{\left(\frac{q}{2\delta}\right)^2 csch^2(\pi q/2h_x) - \right.$$
$$- \left(\frac{q}{2\delta}\right) sech(\pi q/2h_x) csch(\pi q/2h_x) +$$
$$\left.\frac{1}{4} sech^2(\pi q/2h_x)\right\} \qquad (7.4)$$

where the contribution to the Bragg peak was neglected. We note that $S^{zz}_{sol}(q,\omega)$ vanishes at w = 0, but has peaks ai. $\omega = \pm u_\theta q$. This component is difficult to be observed experimentally. However, if observed, it will consist of a direct observation of the soliton, in the sense that what will be obtained will be the scattering from the solitons themselves, and not from domains between solitons - this is also true for the longitudinal ccrrelation function. However, comparing (7.4) with $S^{xx}(q,\omega)$ we see that whereas the temperature dependente is the sanie in both cases, the ω and q dependentes are different.

The calculation of the averages appearing in (7.3) led to the soliton density n_s [in (7.4)] which refers to the SG result. However, we must remark that for consistency, we should have used the soliton density calculated in Section IV since we are strictly handling quantities, as the out-of-plane component, related to deviations from the SG model.

We also emphasize that calculations performed in this section are valid only for small magnetic fields h_x. For large fields, a more complex structure would be obtained.

Besides the central peak we have also, similarly to what happens in S^{xx}, magnon peaks. We remark that for the out-of-plane correlation function, the magnon bound states discussed in Section IV will cause additional magnon peitks. However, up to the present moment, these modes have not been observed experimentally.

Dynamical effects of soliton-soliton and soliton-magnon collisions in the sine-Gordon limit have been discussed in refs.[83-87].

VIII. Quantum Corrections

Let us consider quantum corrections at T = 0. For simplicity we will consider Hamiltonian [2.1] with $h_y = h_z = 0$. The effect of the magnetic field h_x will be taken into account via an effective anisotropy[34]. In the absence of solitons, the energy of the vacuum comes only from continuiim states (magnon modes). When the soliton is introduced, the first two continuum states disappear to beconie bound states with w = 0 and ω_b. The first state (q = 0) of $\omega_1(q)$ becomes the bound state $\omega = 0$ (translation mode) and the first state (q = 0) of $\omega_2(q)$ becomes the bound state w = ω_b. The contribution of these two states to the energy of the soliton will then be

$$E_b = \frac{1}{2}(0 - m_1 c) + \frac{1}{2}(\omega_b - m_2 c), \qquad (8.1)$$

where $m_1^2 = 2b$, $m_2^2 = 2\delta$. The contribution from other states, which remain in the continuum in the presence of the kink, will be

$$E_{\text{cont}} = \frac{1}{2}\left[\sum_{n=1}(\omega_1(q_n) - \omega_1(k_n)) + \sum_{n=1}(\omega_2(q_n) - \omega_2(k_n))\right], \qquad (8.2)$$

where q_n is the wave number of the n-th mode in the continuum in the presence of the kink, and k_n the wave number in the vacuum. Since we have used a periodic box of length L, q_n and k_n are related by the periodic boundary condition

$$Lq_n + \Delta(q_n) = 2n\pi = k_n L, \qquad (8.3)$$

where $\Delta(q)$ is given by Eq. (4.7). From (8.3) we obtain

$$\omega(q) \simeq \omega(k) - \Delta(k)\frac{\partial\omega}{\partial k}. \qquad (8.4)$$

In the limit L $\to \infty$ the discrete sum (8.2) becomes an integral

$$E_{\text{cont}} = -\frac{1}{2\pi}\int_0^\lambda \Delta(k)\frac{\partial\omega_1}{\partial k}dk - \frac{1}{2\pi}\int_0^\lambda \Delta(k)\frac{\partial\omega_2}{\partial k}dk, \qquad (8.5)$$

where λ is the ultraviolet cut-off, given by the lattice spacing. Integrating (8.5) by parts, adding (8.1) and doing a few manipulations we find

$$E_b + E_{\text{cont}} = -\frac{2\omega_1(0)}{\pi} + \frac{1}{2}\omega_b - \frac{m_1 c}{\pi}\left[\int_0^\lambda \frac{dk}{\sqrt{m_1^2+k^2}} + \int_0^\lambda \frac{dk}{\sqrt{m_2^2+k^2}} + \int_0^\lambda \frac{(m_2^2 - m_1^2)dk}{(k^2+m_1^2)\sqrt{k^2+m_2^2}}\right]. \qquad (8.6)$$

Although we have a discrete chain (finite λ), one loop correction to the magnons mass[33] is equivalent to normal ordering of the Hamiltonian. This contributes with terms

$$\int_0^\lambda dk(m_1^2+k^2)^{1/2}.$$

These terms renormalize the magnon masses, i.e. they are responsible for the renormalization of the parameters of the Hamiltonian[33]. Thus if we use renormalized values for the anisotropy parameters δ and b, as obtained from experimental data for instance, or calculating them following the procedure presented in [33], these terms have already been taken into account and we do not need to write them here. Collecting all terrns we arrive finally to the static soliton energy, at zero temperature

$$E_s^0 = E_{xy}^0\left\{1-\frac{2}{\pi S}+\frac{1}{2S}\left(\frac{m_2^2}{m_1^2}-1\right)^{1/2}\right.$$
$$\left.\left(1-\frac{2}{\pi}\tan^{-1}\sqrt{\frac{m_2^2}{m_1^2}-1}\right)\right\}. \tag{8.7}$$

In the sine Gordon limit, this is, for $m_1 >> m_2$ we obtain the well known result[42]

$$E_s^0=(1-1/\pi S)E_{xy}^0.$$

At finite temperature the soliton energy is given by[34]

$$E_s = E_s^0+\omega_b(e^{\beta\omega_b}-1)^{-1}-2m_1c^2(F_1^0+F_2^0)-$$
$$2m_1c^2\omega_b^2\int_0^\infty dk[\pi\omega_1^2(k)\omega_2^2(k)(e^{\beta\omega_b}-1)]^{-1}, \tag{8.8}$$

where

$$F_i^0=\frac{1}{\pi}\int_0^\infty\frac{dk}{\omega_i(k)}\frac{1}{[\exp(\beta\omega_i(k)-1)]}. \tag{8.9}$$

We must bear in mind, however, that there are certain difficulties in reducing the dynamics of a quantum Heisenberg chain to the quantum SG equation. Therefore, at present there is no self-consistent quantum theory of a quasi-one-dimensional antiferromagnet (or ferromagnet) of the type of TMMC.

IX. Results in TMMC

As we have already discussed, the externa1 field H, $= H(H_z = 0)$ plays the role of a magnetic anisotropy which competes with the dipolar interaction 6. The two types of solitons, xy and yz, studied in section II and III result from this competition. The corresponding soliton phase diagram has been established experimentally[22] and is shown in figure 2.

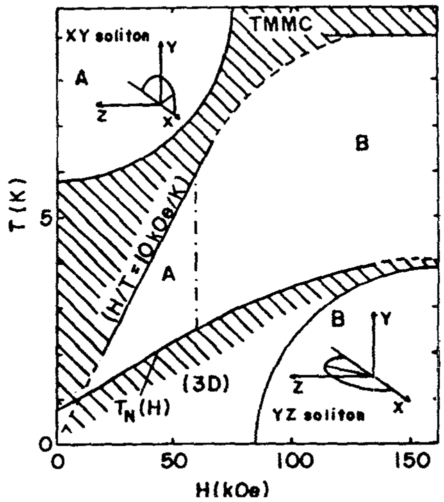

Figure 2: Soliton phase diagram in TMMC. The curve T_{3D} represents the three dimensional ordering temperature and the curve $H/T = 10kOe/K$ the limit where $\Delta N_s/N_s \leq 0.3$ (AN, = number of spins inside one soliton, and N_d = number of spins between solitons) (from [22]).

The transverse function $S^{yy}(q,\text{w})$ has been experimentally investigated by using inelastic neutron scattering and NMR methods[22-28]. In order to properly analyse the experimental data, the quantities we must keep on mind are the soliton energy E, and the widths Γ_q and Γ_ω which in the (xy) sine-Gordon limit are given by equations (5.10) and (5.12), respectively. We have seen in section III that for h << h, the sine-Gordon soliton energy E_{xy}^0 increases proportionally to the field H, i.e, $E_{xy}^0 = g\mu_B SH = \alpha_{SG}H$ which, for TMMC, gives $\alpha_{SG} = 0.336$K kOe^{-1}. However, for T = 2.5K and H = 36 kOe, the experimental value obtained[22] for a was (0.269±0.03) KkOe^{-1}, much lower than α_{SG}. This discrepancy can be explained by 'the discussion done in section III: the out-of-plane fluctuations are crucial and must be considered whenever dynamical problems are being studied. Due to out-of-plane fluctuations, the xy-soliton deviates from the sine-Gordon behavior, i.e. the sine Gordon limit does not describe correctly the real anti ferromagnetic chain. We can incorporate the effects of the fluctuations on the soliton energy by writing $E_{xy} = \alpha H$, with $a = \alpha_{SG} - \alpha_{OP}$, where α_{OP} is related to the out-of-plane fluctuations. As the magnetic field increases up to H $\geq$ H, (H, $= 4JSh_c/\gamma$), the soliton energy must show a crossover behavior because now the yt-sine-Gordon soliton is the one with lower energy and this energy independs on H. In order to put all these facts together and to analyse the experimental data, we define a function E, which will be called the soliton energy. This function must be defined such that it reduces to E_{xy}^0 and E_{yz}^0 energies in the limits H << H_c and H >> H,, respectively. We define

$$E_s=-T\ln\left[\left(\frac{\pi}{2}\right)^{1/2}\frac{JS^2T^{1/2}}{(\gamma HS)^{3/2}}\Gamma_q\right], \tag{9.1}$$

and

$$\alpha=-\frac{\partial}{\partial u}\ln\left[\frac{\Gamma_q}{k_p}u^{-3/2}\right], \tag{9.2}$$

where u = H/T and k_p = T/4JS^2. These definitions arise naturally from equations (5.10) and (4.16) if we substitute 4JS^{2}h, $= E_{xy}^0$ by E, (arguing that there is a renormalization on the soliton energy) and impose E, $= \alpha H$. Equations (9.1) and (9.2) can be used to calculate E, and α if we know how to calculate Γ_q for any value of T and H. Now using the fact that from the thermodynamical point of view the easy plane antiferromagnetic chain in an external magnetic field is equivalent to the feriomagnetic chain with two anisotropic terrns, and that for this latter model transfer matrix results for Γ_q are available at low temperature we can calculate E, and a so that no sine-Gordon approximation is involved[2]". Computing Γ_q (see eq.(3.33) of [29]) for T = 2.5K and H = 36kOe and using (9.2) we obtain a = 0.28K kOe, in close agreement with the experimental value[20]. In figure 3 we present $\Gamma_q[H(H/T)^{1/2}]^{-1}$ as a function of H/T for T = 2.5K on a semilog scale. The experimental data were taken from[18] and the agreement is very good. The data shown in Figure 3 correspond to H < $H_c(H_c \approx 69$ kOe), the region where the xy soliton is the relevant one. In figure 4 we show $\Gamma_q T$ as a function of T^{-1} for an applied magnetic field of H = 83kOe and the agreement is quite good. Notice that the theoretical calculation[88] does not make use of any adjustable parameter.

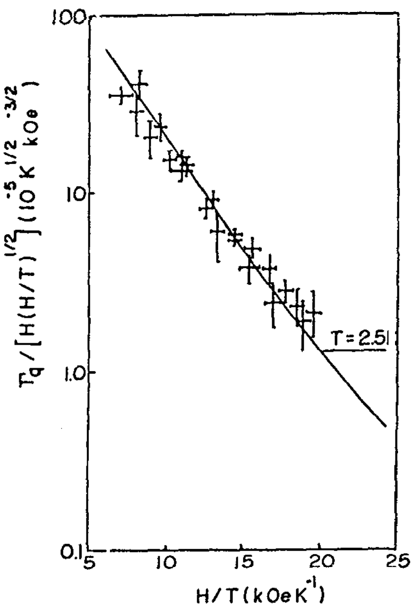

Figure 3: Comparison between theory (solid line, from [29]) and experimental data (from [18]) for Γ_q as a function of H/T (Γ_q is given in reciprocal lattice units).

In figure 5, we show the soliton energy calculated from (9.1) as function of H, for T = 2.4K. The experimental data were taken from [22]. We have used the renormalized values for the parameters of the Hamiltonian as discussed in ref. [33]. We remark that in [29] only the renormalization of the anisotropic term was included whereas here we consider the renormalization in the magnetic field term also[33] and this leads to a slight better agreement with the experimental data.

If in Eq.(8.7) we take $m_1 = h$, i.e. we use an equivalent anisotropy foi*the magnetic field, use for m_1 and m_2 the same renorrnalized values for TMMC as we did above and calculate E_s^0 numerically we find that for H < 60kOe the calculated values can be fitted by the

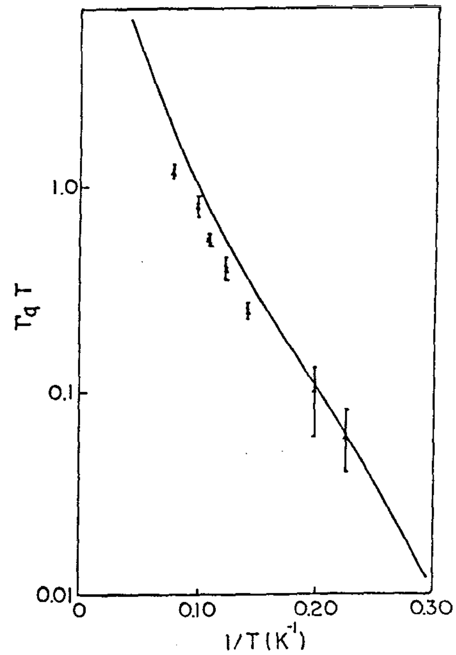

Figure 4: $\Gamma_q T$ as a function of T^{-1} for an applied magnetic field of H = 89kOe. The solid line was calculated as explained in the text. The experimental data are from [18].

expression $E_s^0 = \alpha H$ with a = 0.28 (the same value obtained above). The calculation for E at finite temperature performed in [34] is valid only for small magnetic fields (H << 60 KOe) and therefore can not be used here. In the classical calculations, at finite temperature, of Fig.3, 4 and 5 the spins moved out of the xy plane (since no SG approximations was used). Thus if we believe that the quantum result at T = 0 is correct for TMMC then it seems likely that quantum fluctuations at finite T restrict the spin motions more strongly than expected to the easy plane, thereby reducing the out-of-plane motion. Experiments that probe $S^{yy}(q,w)$ show evidence for nonlinear excitations but they do not provide information about the structure (form factors) of the solitons.

However, analysing data obtained for $S^{xx}(q,w)$ by using inelastic polarised neutron scattering experiments, Boucher and coworkers" were able to observe directly the soliton excitations in TMMC. In order to reach the desired soliton regime, the field value was fixed at H = 45kOe and the temperature was varied between 2K $\leq$ T $\leq$ 15K. $S^{xx}(q,w)$ was obtained from the measured cross section after subtracting the residual contribution from $S^{yy}(q,w)$. The experimental values of the frequency width obtained from $S^{xx}(q,w)$ (from [84]) are shown in Figure 6. At $q = 0$ the width has a non-null value, in contradiction with the non interacting soliton gas model (Eq. (6.5)) but consistent with the theory discussed in Ref. [83]. The full line in Figure 6 was calculated theoretically by Boucher et al.[84]

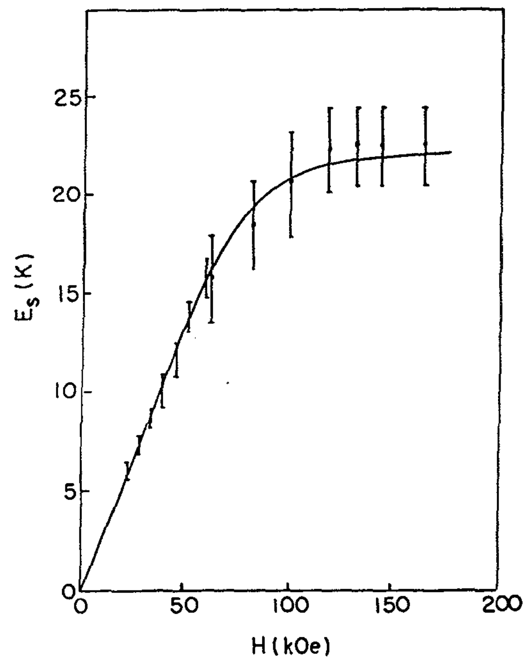

Figure 5: Soliton energy E, as a function of the magnetic field. The solid line is calculated theoretically for 2.4K. The experimental data are from [22].

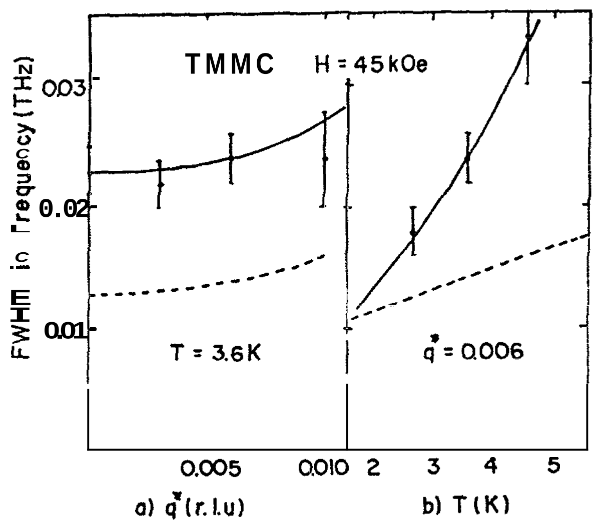

Figure 6: Energy width (FWHM) as observed for the soliton mode $S^{xx}(q,\omega)$ a) as a function of wavevector q, and b) as a function of temperature. The dashed lines correspond to the noninteracting soliton gas model and the full lines account for the dynamical damping (from [84]).

by taking into account the collision effects discussed in Ref.[83].

It should be mentioned that the agreement between theory and experiment for $S^{xx}(q,w)$ is remarkable if we recall that the theoretical calculation was performed using the SG limit. The SG theory appears however to be a useful starting point and we would expect a gradual change over from SG to some other description. It is therefore not too surprising that the experiments show sine- Gordon-like features.

Effects due to the three-dimensional ordering temperature T_N have been discussed in Refs. [89-91].

X. Thermodynamics of a One-Dimensional Magnetic chain

From transfer matrix calculations we have the free energy for hamiltonian (2.1) in the limit h << h, [92]

$$F = T\ln\frac{2JS}{T} + T(\sqrt{\delta}+\sqrt{b}) - \frac{T^2}{4JS^2} + \dots$$
$$-16JS^2b\sqrt{\frac{2}{\pi}}\left(\frac{T}{E^0_{xy}}\right)^{1/2}\left[1-\frac{7}{8}\left(\frac{T}{E^0_{xy}}\right)\right.$$
$$\left.-\frac{59}{128}\left(\frac{T}{E^0_{xy}}\right)^2 - \dots\right] - e^{E^0_{xy}/T}$$
$$-\frac{256JS^2\delta}{\pi}\left\{\ln\left(\frac{4\gamma_e E^0_{xy}}{T}\right) - \frac{5}{4}\left(\frac{T}{E^0_{xy}}\right)\right.$$
$$\left.\left[1+\ln\left(\frac{4\gamma_e E^0_{xy}}{T}\right)+\dots\right]e^{-2E^0_{xy}/T}\right\} \tag{10.1}$$

The first three terms are contributions from spin waves: The first two are linear spin wave contributions from the in plane magnons $\sqrt{b}$ and from out of plane magnons $\sqrt{\delta}$ as can be obtained directly by an harmonic treatment of the Hamiltonian. The T^2 and higher-order terms are contributions of non-linear spin waves: interaction between magnons, multi- magnons states, breathers, and so on. The last two terms in (10.1) are interpreted as the free energy of kinks (F_k). The leading term is equal to the free energy of an ideal gas of kinks with thermally renormalized creation energy. This renormalization arises from *phase shift* interactions between magnons and kinks. There are three possible sources to the finite temperature correction to F_k. In the sine- Gordon limit they are given by:

i) *relativistic* dependence of the bare kink energy on the momentum p, $E(p) = ((E^0_{xy}) + p^2)^{1/2}$.
ii) momentum dependence of the renormalization, and
iii) anharmonic magnon contribution to the renormalization.

The first and second corrections can be included in the phenomenological treatment using the correct expression for the soliton energy instead of taking the non-relativistic result. This gives a correction of the form $1-(5/8)(T/E^0_{xy})$. The third correction appears due to the contribution of anharmonic magnons to the renormalization of the soliton energy via a phase shift. Theodorakopoulos[93] using the relativistic energy and including all contributions to the relevant phase shifts (even magnon-magnon scattering) has obtained the correct factor $1-(7/8)(T/E_{xy})$. The last term in (10.1), $e^{-2E^0_{xy}/T}$, is due to two-soliton interaction[94].

For the contribution of non-linear excitations to the specific heat of TMMC see [92, 95-99]. However, as pointed out by Steiner and Bishop[7], thermodynamic measurements have the drawback that they are not selective but pick up the contributions from all excitations and therefore the unambiguous identification of one contribution s difficult.

We close this section mentioning some others relevant works in one-dimensional classical AF chains. Buys et al.[100] measured the magnetic field dependence of the thermal conductivity of TMMC and DMMC between 1.5 and 7 K and in fields up to 90 kOe. They found that, in the paramagnetic phase, the data could be very well interpreted by soliton-phonon scattering.

De Jongh and de Groot[91] have argued that the field induced transitions in a weakly anisotropic quasi-one-dimensional Heisenberg antiferromagnet were examples of soliton-mediated phase transitions. Agreement with data on TMMC and K_2FeF_4 was found. Those authors extended their analysis to below the 3D transition temperature in order to interpret experimental results of Mossbauer effect in the compound K_2FeF_5. They showed that to explain the field dependence of the average angle $<\phi>$ (in the ideal soliton gas approximation, $<\phi>=2n_s\int_{-\infty}^{\infty}\phi_s(z)dz$) between the hyperfine field and the AF axis in the spin-flopping configuration it is necessary to assume that the static $\pi-$ SG solitons should be exc ted in pairs with an energy equal to $2E_{SG}$. Thiel et al.[101] studied the contribution to the Mossbauer lineividth in quasi-one-dimensional antiferromagnets with easy axis anisotropy due to thermal excitations of inoving kinks. Experimental data on $Fe(N_2H_5)_2(SO_4)_2$, $RbFeCl_32H_2O$ and $CsFeCl_32H_20$ confirm the predicted exponential temperature dependente of the linewidth.

Gaullin and Col ins[102] reported evidence for the presence of solitons in $CsMnBr_3$ at 15K by neutron scattering experimer ts.

Sasaki[103] calculated soliton contributions to the dynamical structure factors of the easy-plane antiferromagnetic chain in the sine-Gordon approximation for $q\simeq\pi(Q\simeq 0)$. He obtained soliton modes similar to Eq. (6.8) but with a much smaller intensity.

Riseborough and Reiter[104] calculated multi spin-wave contributions to the central peak in TMMC. They found, however, that the theoretical results were not in agreement with the experimental data, which required the additional solitons contribution to describe them.

Holyst[105] has stutlied the dynamical properties of a quasi-one-dimensiona antiferromagnet in the presence of the magnetic field below the Néel temperature, T_N, of such a model. By the use of an interchain mean field approach the equations of motion were reduced to the double-sine-Gordon equation which has as special solutions moving $2\pi-$solitons having a form of pairs of weakly coupled n-solitons. He found that, on the contrary of what happens above T_N , the transverse correlation function $S_\perp(q,w)$ had a Gaussian form instead of a Lorentz-like distribution, and that the intensity of this peak increased with temperature but decreased with the strength of the magnetic field. Such behavior reflects the fact that above T_N, $S_\perp(q,w)$ is determined by the regions between the n-solitons while below T_N it depends on the spin distribution inside the solitons. A qualitative agreement with data for TMMC was found. Before that however Rettori[106] had performed a more consistent analysis of the soliton excitation taking into account explicitly, via mean field approximation, the interchain interaction.

XI - Easy Axis Model

In this section we will consider the easy-axis antiferromagnetic model described by the Hamiltonian

$$\mathcal{H}=2J\sum_n[\vec{S}_n\cdot\vec{S}_{n+1}-\delta(S^z_n)^2]. \tag{11.1}$$

Classically we have a doubly degenerate ground state with aligned Néel order along the z axis. The study of this model has become important in connection with the so called Haldane's conjecture[41], as we will see in this and in the next section.

Using the results given in section (II) we can readly write the equations of motion, in the continuum limit, for Hamiltonian (11.1)

$$\begin{aligned}\frac{\partial^2\theta}{\partial z^2}\quad\frac{1}{c^2}\frac{\partial^2\theta}{\partial t^2}\quad\sin 0\cos 0&\left[\left(\frac{\partial\phi}{\partial z}\right)^2\right.\\ &\left.-\frac{1}{c^2}\left(\frac{\partial\phi}{\partial t}\right)+2\delta\right]=0,\end{aligned} \tag{11.2}$$

$$c^2\frac{\partial}{\partial z}\left(\sin^2\theta\frac{\partial\phi}{\partial z}\right)-\frac{\partial}{\partial t}\left(\sin^2\theta\frac{\partial\phi}{\partial t}\right)=0. \tag{11.3}$$

We also have

$$\begin{aligned}\mathcal{H}&=\text{const}+JS^2\int dz\left\{\left(\frac{\partial\theta}{\partial z}\right)^2+\sin^2\theta\left(\frac{\partial\phi}{\partial z}\right)^2\right.\\&\left.+\frac{1}{c^2}\left[\left(\frac{\partial\theta}{\partial t}\right)^2+\sin^2\theta\left(\frac{\partial\phi}{\partial t}\right)^2\right]+2\delta\sin^2\theta\right\}\end{aligned} \tag{11.4}$$

Eqs.(11.2) and (11.3) have small-amplitude spin-wave solutions,

$$\theta=\theta_0<<1\qquad\phi=\omega(k)t-kz, \tag{11.5}$$

where

$$\omega^2(k) = \omega_0^2 + k^2c^2, \quad \text{with} \quad \omega_0^2 = 2\delta c^2. \qquad (11.6)$$

The stationary soliton solution can be sought in the form[41,107]

$$\theta = \theta(z) \ , \ \phi = \omega t. \qquad (11.7)$$

Lorentz invariance allows the moving solution to be obtained by a boost of the static soliton. Taking (11.7) into (11.2) and (11.3) we find

$$\frac{d^2\theta}{dz^2} = \frac{(\omega_0^2 - \omega^2)}{c^2} \sin\theta\cos\theta. \qquad (11.8)$$

As boundary condition for the function $\theta(z)$ we choose the condition

$$\theta \to 0, \ \pi, \ \frac{\partial \theta}{\partial z} \to 0 \quad \text{when} \quad |z| \to \infty, \qquad (11.9)$$

which corresponds to localization of magnetization in the soliton. For $w^2 < \omega_0^2$ Eq.(11.7) has, as we saw in section II, the soliton solution

$$\cos\theta = \tanh[(z - z_0)/r], \qquad (11.10)$$

where $r^2 = c^2(\omega_0^2 - \omega^2)^{-1}$. This solution describes a 180° domain wall of the antiferromagnet with $\theta(-\infty) = \pi$, $\theta(+\infty) = 0$, and $\theta = \pi/2$ at the center of the soliton.

Since the anisotropy term does not depend on ϕ, there exists one integral of motion - the z component of the total magnetization $\vec{M} = \vec{S}_n + \vec{S}_{n+1}$. We shall represent this integral in the form, using Eqs.(2.6b) and (2.8),

$$\begin{aligned}\frac{M_z}{2S} &= \int_{-\infty}^{\infty} \frac{(S_n^z + S_{n+1}^z)}{2S} dz = -\frac{1}{4JS}\int_{-\infty}^{\infty} \sin^2\theta \frac{\partial\phi}{\partial t} dz \\ &= -\frac{\omega}{c}\int_{-\infty}^{\infty} \sin^2\theta dz = -\frac{\omega}{c}\int_{-\infty}^{\infty}(1-\cos^2\theta)dz.\end{aligned} \qquad (11.11)$$

The total azimuthal spin carried by the soliton can be interpreted as given by

$$\frac{S^z}{S} = \frac{\omega}{c}\int_{-\infty}^{\infty}\cos^2\theta dz = \frac{\omega}{c}r, \qquad (11.12)$$

where we have used (11.10) to integrate (11.12). Thus,

$$S^z = S\omega(\omega_0^2 - \omega^2)^{-1/2}. \qquad (11.13)$$

The field momentum of the magnetization field

$$P = \int dz \left(P_\theta \frac{\partial\theta}{\partial z} + P_\phi \frac{\partial\phi}{\partial z}\right) \qquad (11.14)$$

is also a conserved quantity. Using Eq.(2.15) we obtain,

$$P = \int \frac{dz}{8J}\left(\frac{\partial\theta}{\partial t}\frac{\partial\theta}{\partial z} + \sin^2\theta \frac{\partial\phi}{\partial t}\frac{\partial\phi}{\partial z}\right) \qquad (11.15)$$

or

$$P = \frac{vJS^2}{(c^2 - v^2)^{1/2}}\int dz\left[\left(\frac{\partial\theta}{\partial z}\right)^2 + \frac{\omega^2}{c^2}\sin^2\theta\right]. \qquad (11.16)$$

From (11.4) and (11.16) we obtain the soliton energy- momentum relation,

$$E_m(P) = \left[[(S^z)^2 + S^2]\omega_0^2 + c^2P^2\right]^{1/2}. \qquad (11.17)$$

Now we introduce the semiclassical quantization of the allowed values of the internal precession frequency of the soliton [41]. This simply means that S^z is quantized in integer steps S^z = m (taking $\hbar = 1$). Eq.(11.17) becomes then

$$E_m(P) = [(m^2 + S^2]\omega_0^2 + c^2P^2]^{1/2}, \qquad (11.18)$$

and the parameter w is given by $\omega = \omega_0 m(m^2+S^2)^{-1/2}$. We have now an extra degree of freedom, as compared to the xy (or yz) soliton studied in Section III, since there we kept, let us say, ϕ = constant, where here we have ϕ = wt. This extra degree of freedom leads to the term $m^2\omega_0^2$, representing internal modes, in the soliton energy (11.18).

Comparing (11.18) with (11.6) we see that in the semi-classical limit (i.e. S large) the soliton energy gap is always much larger than that of the elementary magnon. For $|m| << S$ we have $E_m(0) \simeq S\omega_0 + m^2w_0/2S$. For $|m| >> S$, $w \to \omega_0$, $E_m(0) \simeq m\omega_0$ and the rest energy can be interpreted in terms of $|m|$ magnons weakly bounded. In (11.18) the allowed discrete values of m were not specified, only their integer spacing. However, as Haldane has pointed out[41], we know that the spin wave functions are eigenstates of $\bar{T}$ (where $\bar{T}$ is the time-reversal operator) with $\bar{T}^2 \equiv (-1)^{2m} = (-1)^{2s} = \pm 1$. The soliton extended structure involves an odd number of spins of the underlying magnetic chain: thus its wave function must also have the eigenvalue $\bar{T}^2 = (-1)^{2s}$. The allowed values of the soliton spin m are then integers if the underlying spin chain has integer spin, and half integers if S is half integer. However, as we will see below, the two cases have distinct behavior.

In Fig.(7) we show the result for half integer spins. In the classical case the energy of the soliton is larger than the energy of the magnon. Due to the internal precession it is also decomposed in several states. The lowest energy state is characterized by the magnetic quantum number m = $\pm 1/2$. The application of an externa1 field will split these soliton states allowing, in principle, the observation of the internal precessions[39]. We remark here that for the quantum AF Ising-like chain with S = 1/2 the lowest excited states are states with one wall centered at a site n. A spin-wave state with just one spin Aipped has a higher energy value (see Fig. 8). Then the magnon has a higher energy than the soliton. Note however that a propagating domain wall in this case can only be called a soliton in the sense that it moves with a constant velocity and shape and connects two degenerate ground states. It is not a sine Gordon soliton as the one in the classical model[108]. However for the classical or quantum model the gap vanishes in the isotropic limit.

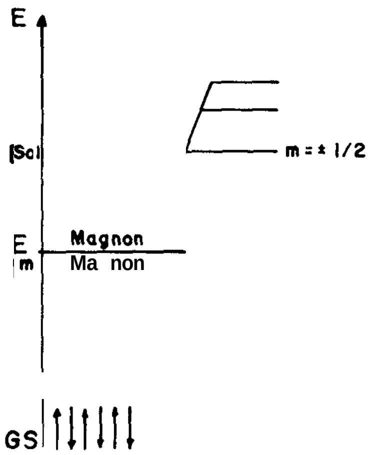

Figure 7: Energy of the excited states in AF-Ising-like chain for the half integer spins.

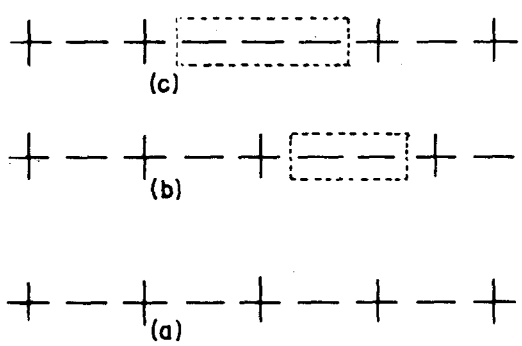

Figure 8: Excited states in AF-Ising-chains for s = 1/2. a) Néel ground state. b) soliton, and c) one spin flipped (magnon).

In the case of integer spin, Figure 9, the semiclassical picture of the soliton and magnon described above will only be valid for weak but finite anisotropy. What happens is that the magnon excitation for the isotropic Hamiltonian in the harmonic approximation is gapless. However, as we will see in the next section, the nonlinear vacuum fluctuations dynamically break this symmetry and the collrctive mode develops a finite rest energy E_0 for integer spins. This nonlinear mechanism will only be suppressed by the anisotropy if $\omega_0 >> E_0$. As the isotropic limit $\omega_0 \rightarrow 0$ is approached, these nonlinear effects mean that the renormalized soliton rest energy will eventually become lower than the renormalized magnon rest energy. The lowest-energy excitation is then the principal $m = 0$ soliton (see Fig.(9)). As pointed out by Haldane[41] the eventual disappearance of Néel order in the ground state as the isotropic limit is approached will be signaled by an instability against pairs of the order- destroying topological soliton excitation; i.e. if E_0 is comparable to the energy associated with non-linear quantum fluctuation we have the creation of pairs of soliton - antisoliton and the ordering will be destroyed (similarly to the Kosterlitz - Thouless transition in the 2D-XY model[109].) Also, it is the thermal excitation of solitons, not the thermal excitations of magnons, that disorders the system at any finite temperature.

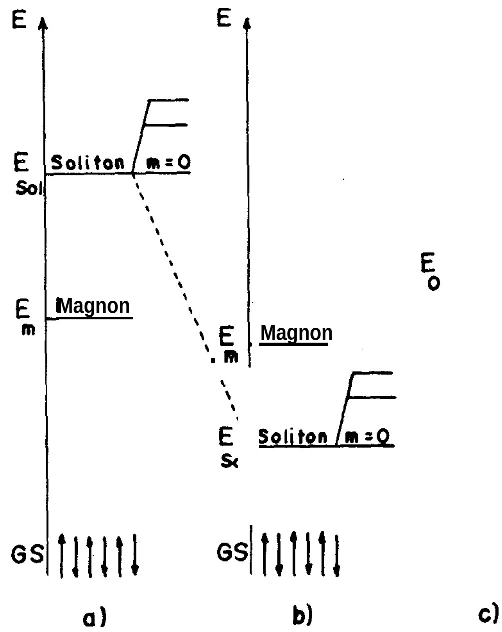

Figure 9: Energy of the excited states in AF-Ising-like chains for classical integer spins. For a decreasing anisotropy (a)→ (b) (Ising → Heisenberg) the energy for the non magnetic soliton ($m = 0$) is renormalized and becomes smaller than the magnon energy. Finally, in the isotropic limit (c), a non magnetic ground state is reached with a first excited state at the energy E_Q.

XII - The Haldane Gap

In this section we will present some arguments for the origin of the gap for an AF with integer spin. First we will discuss a field theoretical argument in the line of Haldane[41] and Affleck[110,111]. In order to do so we will rederive the continuum limit for Hamiltonian (11.1), taking only the exchange term since the anisotropic term will not be affected by the following procedure. Here we will define variables $\vec{\psi}$ and h?, combining each spin on an even site, 2i, with the spin to its right, at

$(2i+1)$ as in refs. [110, 111],

$$\begin{aligned}\vec{\psi}(2i+1/2) &= (\vec{S}_{2i+1}-\vec{S}_{2i})/2S \\ \vec{M}(2i+1/2) &= (\vec{S}_{2i+1}+\vec{S}_{2i})/2\end{aligned} \tag{12.1}$$

$\vec{\psi}$ and $\vec{M}$ obey the constraints $\vec{\psi}\cdot\vec{M}=0$ and

$$\vec{\psi}^2 = 1+1/S-M^2/S^2 \to 1.$$

Assuming that $\vec{\psi}$ and $\vec{M}$ are slowly varying on the lattice scale we can write the Hamiltonian $H_0 = 2J\sum \vec{S}_n \,.\, \vec{S}_{n+1}$ using a gradient expansion. Keeping terrns up to $O(\vec{\psi}^2)$ and $O(\vec{M}^2)$ only, since $\vec{M}$ effectively contains a time derivative, and using

$$\begin{aligned}&\vec{S}_{2i}\,.\,\vec{S}_{2i+1} = 2\vec{M}(2i+1/2)^2 + \text{constant}\\ &\vec{S}_{2i}\,.\,\vec{S}_{2i-1} = -S^2\vec{\psi}(2i+1/2)\,.\,\vec{\psi}(2i-3/2)\\ &+S[\vec{M}(2i-3/2)\cdot\vec{\psi}(2i+1/2)\\ &-\vec{\psi}(2i-3/2)\cdot\vec{M}(2i+1/2)]\\ &+\vec{M}(2i+1/2)\cdot\vec{M}(2i-3/2)\\ &\sim 2S^2\left(\frac{\partial\vec{\psi}}{\partial z}\right)^2 - S\left(\vec{M}\cdot\frac{\partial\vec{\psi}}{\partial z}+\frac{\partial\vec{\psi}}{\partial z}\cdot\vec{M}\right)+2\vec{M}^2,\end{aligned} \tag{12.2}$$

we can write

$$\begin{aligned}\mathcal{H}_0 &= J\int dz\left\{4\vec{M}^2+2S^2\left(\frac{\partial\vec{\psi}}{\partial z}\right)^2\right.\\ &\left.-S\left(\vec{M}\cdot\frac{\partial\vec{\psi}}{\partial z}+\frac{\partial\vec{\psi}}{\partial z}\cdot\vec{M}\right)\right\}.\end{aligned} \tag{12.3}$$

In terms of the angle parametrization given by Eq.(2.4) the last term on the right hand side of Eq.(12.3) can be written as dF/dz, a total derivative of a function F, and it has no effect on the classical equations of motion. Therefore this term has been neglected in the study we have done before.

Classically we can take the integral of this term as a constant, and since $M^2 = S^2(\nu^2+\alpha^2 sin^2\theta)$ we obtain the exchange part of Eq.(2.13). However, following Affleck[110,111] we rewrite (12.3)

$$\begin{aligned}\mathcal{H}_0 &= \frac{cS}{4}\int\left\{g^2\left[\vec{M}-\frac{\theta}{4\pi}\frac{\partial\vec{\psi}}{\partial z}\right]^2\right.\\ &\left.+\frac{1}{g^2}\left(\frac{\partial\vec{\psi}}{\partial z}\right)^2\right\}dz\end{aligned} \tag{12.4}$$

where $g = 2/S$ and $\theta = 2\pi S$. Writting $\mathcal{H}_0 = (cS/4)\int hdz$, we observe that h follows from the Lagrangian density

$$\begin{aligned}\mathcal{L} &= (1/2g)\partial_u\vec{\psi}\cdot\partial^u\vec{\psi}\\ &+(\theta/8\pi)\epsilon^{u\nu}\vec{\psi}\cdot(\partial_u\vec{\psi}\times\partial_n u\vec{\psi})\end{aligned} \tag{12.5}$$

with constraint $\vec{\psi}^2=1$ and where $\varepsilon^{u\nu}$ is the Levi-Civita antisymmetric symbol. To understand the meaning of 0 we note that on the compactified Euclidean space (i.e $\vec{\psi}(\vec{x}) \to$ constant at $|\vec{x}|\to\infty$) both $\vec{\psi}$ and $\vec{x}$ can be represented by points on a sphere S^2 and the integral

$$Q = (1/8\pi)\int d^2\vec{x}\epsilon^{u\nu}\vec{\psi}\cdot(\partial_u\vec{\psi}\times\partial_\nu\vec{\psi}) \tag{12.6}$$

measures the winding number of the sphere onto the sphere[42]. It is the Jacobian for the change of variables from polar coordinates in $\vec{x}$ - space (with $\vec{x}$ the spatial coordinate on a sphere) to polar coordinate in $\vec{\psi}$- space. Q is an integer for any smooth (finite - action) field configuration. Since the action is given by

$$S = \int \mathcal{L}dt$$

we obtain[112] from Eq.(12.5)

$$S = S_0 + i\theta Q. \tag{12.7}$$

Since Q in an integer-valued topological charge, e^{-S} is a periodic function of 6 for any smooth field configuration. Thus we expect all physical properties of the model, which in Feynman's formulation of quantum mechanics can be derived from the path integral $\int d\vec{\psi}e^{-iS/\hbar}$, to be periodic in 8. Thus we see that for integer-S chains we effectivelly have $0 = 0$. The action is then real and corresponds to a classical two-dimensional ferromagnet at finite temperature[112], $T = g$. On the other hand, for half-integer S we have $\theta = \pi$. The action is now complex and there is no correspondence to a standard classical two-dimensional problem.

The generation of a mass, for $0 = 0$, can be seen using the large n-limit of the $0(n)$ non linear a model as follows[110]. This model is defined by the Lagrangian,

$$\mathcal{L} = \frac{n}{2g}\partial_u\vec{\psi}\cdot\partial^u\vec{\psi}, \quad \vec{\psi}^2 = 1 \tag{12.8}$$

with $\vec{\psi}$ a n-component vector. It is convenient to include the constraint in the Lagrangian writing

$$\mathcal{L} = \frac{n}{2g}\left[\left(\partial_u\vec{\psi}\right)^2 + i\lambda(\vec{\psi}^2 - i)\right]. \tag{12.9}$$

Hence $\vec{\psi}$ is then no longer constrained. The path integral becomes then

$$Z = \int d\vec{\psi}d\lambda\exp\left(\frac{i}{\hbar}S\right) \tag{12.10}$$

where here $S = \int d^2\vec{x}\mathcal{L}$. Thus

$$\begin{aligned}Z &= \int d\vec{\psi}d\lambda\exp\left[\frac{i}{\hbar}\int d^2\vec{x}\left\{\left(\frac{n}{2g}\right)[(\partial_u\vec{\psi})^2\right.\right.\\ &\left.\left.+i\lambda(\vec{x})(\vec{\psi}^2-1)\right\}\right]\end{aligned} \tag{12.11}$$

Integrating over the $\vec{\psi}$ field, using,

$$\int_{-\infty}^{\infty} e^{-bz^2} dz = e^{-1/2 \ln b} e^{\ln \sqrt{\pi}}$$

we obtain

$$Z = \int d\lambda \exp\left[\frac{i}{\hbar}\frac{n}{2}\left\{-\frac{i\lambda}{g} + \mathrm{tr}\ln(-\partial^2 + i\lambda)\right\}\right] \tag{12.12}$$

up to an irrelevant constant factor. We have thus an effective action

$$S_{eff}(A) = \frac{n}{2}\left(-\int d^2P\left[\frac{i\lambda}{g} + \mathrm{tr}\ln(-\partial^2 + i\lambda)\right]\right). \tag{12.13}$$

Because there is a factor of n in S_{eff} we may ignore the fluctuations of λ and evaluate Z using the method of steepest descent at the lowest action saddle point. This method[113] is applicable, in general, to integrals of the form

$$I(\alpha) = \int e^{\alpha f(z)} dz. \tag{12.14}$$

The saddle point is given by $\frac{df}{dz}|_{z_0} = 0$ The integral is then approximated by

$$I(\alpha) \simeq \sqrt{\frac{2\pi}{\alpha\beta}} e^{\alpha f(z_0)} e^{i\phi}, \tag{12.15}$$

where β and ϕ are defined in Ref. [113]. In our case

$$f(r) = \int d^2\vec{x}\left\{\frac{i\lambda}{g} + \mathrm{tr}\ln(-\partial^2 + i\lambda)\right\}. \tag{12.16}$$

Let us write the saddle point λ_0 as $i\lambda_0 = m^2$, then $\frac{df}{d\lambda}|_{\lambda_0} = 0$ gives

$$-\frac{i}{g}\int d^2\vec{x} + i\int \frac{d^2\vec{x}}{(-\partial^2 + m^2)} = 0. \tag{12.17}$$

Fourier transforming Eq.(12.17) we find,

$$\frac{1}{g} = \int \frac{d^2\vec{k}}{(2\pi)^2}\frac{1}{k^2 + m^2} = \frac{1}{2\pi}\ln(\lambda/m). \tag{12.18}$$

where we have iotroduced an ultraviolet cut-off λ (λ^{-1} = a, the lattice spacing). The mass parameter **m** is then given by,

$$m = \lambda e^{-2\pi/g}, \tag{12.19}$$

leading to the gap energy for the collective modes

$$\epsilon_0 = mc = (c/a)e^{-\pi S}, \tag{12.20}$$

and to the correlation length (in units of a) at T = 0

$$\xi = m^{-1} = e^{\pi S}. \tag{12.21}$$

The mapping performed above, between the 1D antiferromagnetic system and the non linear sigma model, shows that all integer-spin models will be massive, at least for large enough spin where the mapping works. The mapping may not be very accurate at S = 1, but should be at least qualitatively correct, providing a useful phenomenological model. However the study of exactly solvable models[114], quantum Monte Carlo calculation[115], finite size calculation[116] and finite size scaling[117] supports the existence of a finite gap for S = 1 isotropic-Heisenberg AF system. Recently this gap have been calculated by Sakai and Takahashi[118] using the Lanczos algorithm and by Rezende[119] using a modified spin-wave theory. In Rezende's calculation it is easy to see that the antiferromagnetic ground state is quantum disordered and therefore the gap in the spin-wave spectrum has a simple interpretation: it costs energy to create an infinite- wavelength magnon in the disordered ground state. The spin-wave theory is however unable to predict the absence of a gap in half-odd-integer spin systems.

Experimental evidence for the Haldane gap has been sought-intensively by inelastic neutron scattering, because this is the only method of investigating the magnetic excitations over the whole Brillouin zone. So far three systems have been studied: NENP[120], $AgVP_2S_6$ [121] and $CsNiCl_3$ [122–125].

The first evidence came from experiments on the S = 1 system $CsNiCl_3$, which is highly isotropic in its couplings[122]. In the organic, S = 1 AF chain system $Ni(C_2H_6N_2)_2NO_2(ClO_4)$ (NENP), Ni ions are the magnetic ions and the system does not order three dimensionally down to 1.2K. The magnetic properties of this compound are well described by the Hamiltonian

$$\mathcal{H} = 2J\sum_n \vec{S}_n \cdot \vec{S}_{n+1} + 2D\sum_n (S_n^z)^2. \tag{12.22}$$

with J = 24K, D $\simeq$ 6K and $S = 1$. Magnetic excitations have been observed by neutron inelastic scattering measurements, showing two energy gaps $\varepsilon_0^{\parallel} \simeq$ 30K and $\varepsilon_0^{\perp} \simeq$ 14K ($\parallel$ and $\perp$, with respect to the chain axis). The average value $(\varepsilon_0^{\perp} + \varepsilon^{\parallel})/2 \simeq 0.4(2J)$ is in agreement with the value for the isotropic chain[120]. A time of flight inelastic neutron scattering experiment on the powder sample of $AgVP_2S_6$ [121] has also indicated an energy gap. But because of the powder averaging the available information is rather limited. Apart from zero-field neutron scattering, a number of other measurements have been made in nonzero applied magnetic fields. These include susceptibility[120], NMR[39], high-field magnetization[128–129], and neutron scattering in a finite field[126]. In all these measurement the Haldane gap is quite evident.

To conclude this section let us consider the half-integer spin models. Haldane[41] has conjectured that the isotropic model is massless. One reason is that the spin-1/2 chain, solvable by the Bethe ansatz is massless as is the spin - 3/2 chain studied numerically by Schulz and Ziman[116]. Recently Shankar and Read[130] have shown that the nonlinear O(3) sigma model in 1+1 dimensions with topological parameter θ = a is indeed massless for all values of the coupling g. A search for a physical understanding of the difference between the half-integer and integer case has also been initiated[110-131] invoking the 'zero-spin-defect' picture. Gomez Santos[131] has presented a simple model to study the behavior of the spin-1 chain in the antiferromagnetic regime, identifying domain walls as the relevant excitations, and constructing a variational Hamiltonian as follows: keeping in mind the interest in the antiferromagnetically dorninated regime, he has discarded all the states with nearest-neighbor parallel spins. Thus, the only sources of AF disorder are sites with $S_z = 0$ (spin-O defects, SZD). The two spins at the left and right of a single SZD should be antiparallel. A typical example of a state within this restricted set could have the following form

$$\ldots \downarrow\uparrow\downarrow\ 0\uparrow\ 0\,0\ \downarrow\uparrow\ ..$$

where arrows mean $S_z = \pm 1$ and circles mean $S_z = 0$. The Hamiltonian has been then approximately solved, and its critical properties fully analyzed, obtaining complete agreement with Haldane's proposal.

XIII - Conclusion

In the present review we have shown that antiferromagnetic chains offer good examples of soliton excitations, and that the soliton picture is consistent with experimental observations. Some points however deserve a further study. The ballistic-diffusive crossover observed in TMMC for broad solitons is not completely understood and a clear understanding of the impurity-induced diffusion process is needed. Also the questions of the soliton mode damping (if it is due to collisions or not) must be considered. The theory for these collision effects is pratically phenomenological and more work is necessary for a proper understanding.

Concerning the Haldane gap problem, recent polarized neutron inelastic scattering in $CsNiCl_3$ with applied magnetic field[125] showed that neither the classical spin wave theory nor more elaborated theory[132,133] fully accounts for the experimentally observed dispersion relation in the 3D ordered phase. The experimental information available about the ground state of the quasi-1D AF $CsNiCl_3$ cannot be explained without .a thorough theoretical treatment of the influence of a magnetic field on the ground state and the excitations of a Haldane system[134].

It seems to us that low-dimensional magnetic materials will continue to develop as accessible models in which to investigate fundamental nonlinear processes.

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