

TWO DIMENSIONAL SOLITON ENERGY AND ESR IN AFM

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The energy $E' \equiv E/(JS^2) = 4\pi + \epsilon = 12.6 + \epsilon$ for static 2-d solitons in classical Heisenberg magnets ($JS_i \cdot S_k$) with weak easy-axis anisotropy (DS_z^2) is calculated. It agrees with $E' = 12.7 \pm 1.2$ found by reinterpreting ESR line broadening in antiferromagnets according to the Arrhenius law.

1. Introduction

Solitons as localized excitations are well established for one-dimensional (1-d) problems. Theoretically, 1-d spin chains with Heisenberg exchange and easy-axis anisotropy can be mapped onto the 1-d Sine-Gordon equation (SGE) for the classical and continuous limit. The SGE has the static soliton solution $\tan(\vartheta/2) = \exp(x/x_0)$. Experimentally, as an example [1], such excitations were found to broaden Mössbauer lines in 1-d antiferromagnets (AFM) according to the Arrhenius law proposed by Bloembergen et al. [2] for NMR relaxation and by Mikeska [3] for line broadening in AFM.

For 2-d magnets, the situation is different. Although the 2-d XY-magnet with its vortices is a well treated subject, not much is known for the 2-d Heisenberg magnet with easy-axis anisotropy, which can be mapped onto the 2-d SGE. According to a proof by Derrick [4], this 2-d SGE has no localized static solutions, stable or unstable. However, this proof applies only to the one-parameter SGE (polar angle ϑ , constant azimuthal angle ϕ of the spins). Enz [5] treated a round excitation with a vortex-like structure (variable ϕ). He added a further term to the Hamiltonian in order to stabilize this static excitation. Without that term, Kosevich et al. [6] found no static solution in their continuous treatment.

It is surprising that a static solution for 2-d solitons in the isotropic Heisenberg magnet in the classical and continuous limit is seldom cited in the soliton literature. It was used by Skyrme [7] and was derived in an elegant way by Belavin et al. [8] and corresponds to the well known conformal mapping of a plane onto a unit sphere ("stereographic projection" for geographical maps) $\tan(\vartheta/2) = r/r_0$. For $J = 1, S = 1$, the energy density on the surface of the unit sphere is constant and unity, hence the energy of this static excitation is 4π independent of r_0 .

It is the aim of this contribution [9] to calculate the shape and the energy of a static soliton for the 2-d magnet with Heisenberg exchange J and weak easy-axis anisotropy D and to compare its energy with experiment.

2. Evaluation of static solitons in a 2-d lattice

Here, the procedure of the evaluation of 2-d solitons will be sketched. Assume the following Hamiltonian for classical spins S

$$H = -J \sum (S_i \cdot S_k - S^2) - D \sum (S_{iz}^2 - 1), \quad (1)$$

with isotropic exchange (constant J) between nearest neighbors and uniaxial (easy axis) single spin anisotropy (constant D). The spins S are at positions (m, n) in a discrete square lattice with lattice constant a . Assume a "round" excitation with an "up" spin at the center position $(0, 0)$, with a vortex-like structure such that each spin is tilted away from the up direction towards the direction of the radius-vector. Select a spin i at the

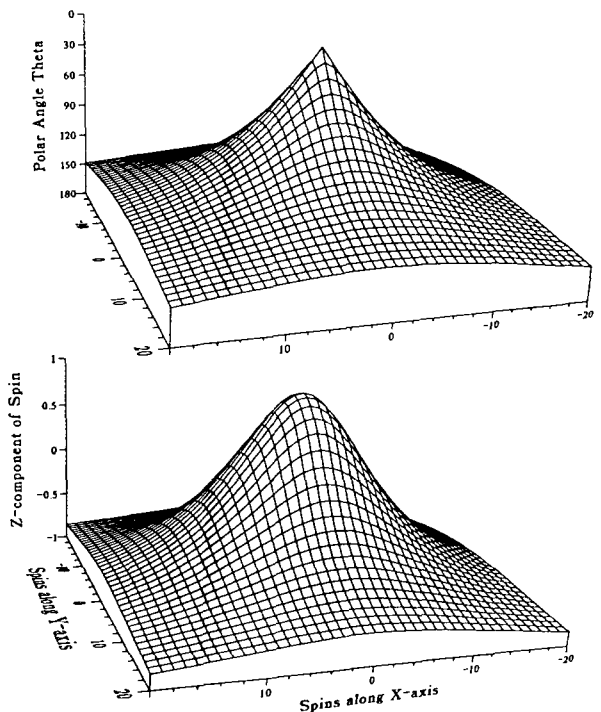


Fig. 1. Illustration of static 2-d soliton for $2D' = 10^{-4}$.

x -axis $(m, 0)$. It interacts with its four neighbors denoted $i-1$ $(m-1, 0)$, $i+1$ $(m+1, 0)$, $+k$ $(m, +1)$, and $-k$ $(m, -1)$, respectively, with polar angle $\vartheta_k \equiv \vartheta_{+k} = \vartheta_{-k}$. The energy E_i can be written as

$$E_i/(JS^2) = -\cos(\vartheta_{i-1} - \vartheta_i) - \cos(\vartheta_i - \vartheta_{i+1}) - 2 \sin \vartheta_k \sin \vartheta_i \cos \alpha - 2 \cos \vartheta_k \cos \vartheta_i - [D/(JS^2)](\cos^2 \vartheta_i - 1), \quad (2)$$

with $\cos \alpha = m/(m^2 + 1)^{1/2}$. An approximation for ϑ_k

$$\vartheta_k \approx \vartheta_i + (\vartheta_{i+1} - \vartheta_{i-1})[(m^2 + 1)^{1/2} - m], \quad (3)$$

connects ϑ_k with ϑ_i and ϑ_{i-1} . Therefore, the equilibrium condition for spin i $\partial E_i / \partial \vartheta_i = 0$ gives a recursion formula connecting ϑ_{i+1} with ϑ_i and ϑ_{i-1} :

$$\vartheta_{i+1} = \vartheta_i + \sin^{-1} \left\{ \sin(\vartheta_i - \vartheta_{i-1}) - 2 \sin \vartheta_k \cos \vartheta_i \cos \alpha + 2 \cos \vartheta_k \sin \vartheta_i + [2D/(JS^2)] \sin \vartheta_i \cos \vartheta_i \right\}. \quad (4)$$

Localized solutions of eq. (3) iteratively combined with eq. (4) are calculated by starting with $\vartheta(0, 0) = 0$ and varying $\vartheta(1, 0)$ till the spins approach the "down" direction for large distances. For weak anisotropies $D \ll J$, the shape deviates little from $\tan(\vartheta/2) = r/r_0$. A heuristic description of the computed functions is found if r/r_0 is replaced by $(1/g)\text{sh}(gr/r_0)$ with $ga/r_0 \approx [D/(JS^2)]^{1/2}$. The radius r_0/a for $\vartheta = 90^\circ$ increases strongly for decreasing anisotropy, and diverges for $D \rightarrow 0$, which was tested also analytically. Therefore, the solutions of ref. [8] diverge in any discrete 2-d lattice, similar to a Bloch wall for $D \rightarrow 0$ in a 1-d linear chain of discrete spins. However, in contrast to 1-d, the normalized energy $E' \equiv E/(JS^2)$ is nearly independent of D as long as $D \ll J$ and is only slightly greater than $4\pi = 12.57$. As examples, the radii r_0/a are 2.3, 10.7, 44, 183, and the corresponding normalized energies E' are 13.5, 12.9, 12.64, 12.58 for the normalized anisotropies $2D' \equiv 2D/(JS^2) = 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}$, re-

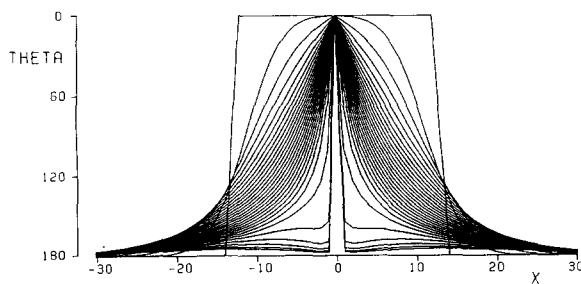


Fig. 2. Polar angle ϑ (degrees) versus x -axis (spin numbers) of a decaying excitation, see text, plotted after equal time intervals; $2D' = 10^{-2}$. (The final state would be highly unstable for small symmetry-breaking fields.)

spectively. Fig. 1 illustrates the shape of such an excitation.

3. Dynamical simulations: type of instability

In order to study the instability of the localized excitations, the spin dynamics were simulated using the equations of motion with Landau–Lifshitz damping for 40×40 spins. A round "island" of "up" spins in a large domain of "down" spins decays rapidly to a shape of about $\tan(\vartheta/2) = r/r_1$, then r_1 decays slowly till r_1 is about r_0 . Then, the excitation collapses rapidly, see fig. 2. The corresponding energy E'_1 has a similar time dependence with $E'_1 \approx E'$ as the limit between slow and rapid decay. Therefore, although the static solutions mentioned above are unstable, they are the limit of a band of long living localized excitations, and their lifetime diverges for $D \rightarrow 0$.

4. Comparison with experiment: ESR line broadening

A recent alternate interpretation [10] of ESR line broadening in layered 2-d AFM according to an Arrhenius law [2,3] yielded normalized energies $E' = 12.7 \pm 1.2$ for four different compounds with small easy-axis anisotropies, probably a fortuitous agreement with the above values, since the interpretation of these data in terms of critical exponents is well established, see references in ref. [10]. The strongest argument against the alternate interpretation is that thermal activation is doubtful for such high ratios of $E/(kT)$. However, excitations with larger ratios $E/(kT)$ seem to broaden NMR lines [11] according to [2].

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