# Quantized Spin Waves in Antiferromagnetic Heisenberg Chains

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The quantized stationary spin wave modes in one-dimensional antiferromagnetic spin chains with easy axis on-site anisotropy have been studied by means of Landau-Lifshitz-Gilbert spin dynamics. We demonstrate that the confined antiferromagnetic chains show a unique behavior having no equivalent, neither in ferromagnetism nor in acoustics. The discrete energy dispersion is split into two interpenetrating $n$ and $n'$ levels caused by the existence of two sublattices. The oscillations of individual sublattices as well as the standing wave pattern strongly depend on the boundary conditions. Particularly, acoustical and optical antiferromagnetic spin waves in chains with boundaries fixed (pinned) on different sublattices can be found, while an asymmetry of oscillations appears if the two pinned ends belong to the same sublattice.

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The necessity to write bits of information on ever decreasing time scales requires more and more fast switching of magnetization in nanometer and micrometer sized elements. An important role for the speed of magnetization reversal is played by confined spin waves, which can promote or inhibit the switching depending on the spatial distribution of the nonlinear oscillations, their amplitude and temperature [1,2]. While the ferromagnetic spin waves have been broadly studied in confined systems, the investigations on magnetic excitation patterns in confined antiferromagnets are still very limited.

The majority of theoretical studies on standing spin waves are concerned with antiferromagnetic systems of infinite extension [3–5]. The increasing interest in nanosystems, however, drives the focus of experimental studies towards confined magnetic structures [6,7]. Thus far the antiferromagnetic spin waves have been observed only by means of neutron scattering [8,9] and antiferromagnetic resonance [10], which are unable to provide spatial resolution. However, new methods like Brillouin light scattering [11], time-resolved Kerr microscopy [12], and scanning thermal microwave resonance microscopy [13] give the unique possibility of visualizing standing spin waves on the nanometer scale. Therefore, the theoretical predictions on confined antiferromagnetic excitations are important from the point of view of fundamental physics as well as for future experiments.

Here we propose a promising direction for experiments on standing spin waves by means of a theoretical description of the spin dynamics in confined antiferromagnetically coupled chains with easy axis on-site anisotropy.

In the following we consider chains consisting of classical, antiferromagnetically coupled Heisenberg spins with energy contributions from exchange interaction, anisotropy, and external magnetic field. Such a spin model might be interpreted as the classical limit of a quantum mechanical, localized model with large spin.

The magnetic properties of the system are well described by the model Hamiltonian

$$\mathcal{H} = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - D_z\sum_i (S_i^z)^2 - \mu_s\sum_i[\mathbf{B}_{\rm OF}\cos(\omega t)\mathbf{S}_i + \mathbf{B}\mathbf{S}_i], \tag{1}$$

where $\mathbf{S}_i = \boldsymbol{\mu}_i/\mu_s$ is a three-dimensional magnetic moment of unit length. The first sum in Eq. (1) is the exchange interaction between nearest neighbors with the coupling constant $J > 0$. The second sum represents a uniaxial anisotropy, with the $z$ axis as the easy axis. For the sake of understanding we first study a low anisotropy limit of the Heisenberg model with $D_z \ll J$. The last sum is the coupling of the spins to a static external magnetic field $\mathbf{B} = B_z\mathbf{z}$ and to an oscillating field $\mathbf{B}_{\rm OF} \perp \mathbf{B}$ with the frequency $\omega$.

The underlying equation of motion for magnetic moments is the classical Landau-Lifshitz-Gilbert (LLG) equation [14]. To describe the quantized spin wave spectrum we have calculated the absorbed power $P$ at each lattice point $i$ as

$$P_i = \frac{\omega\mu_s B_{\rm OF}}{\mathcal{T}}\int_0^{\mathcal{T}} S_i^B(t)\sin(\omega t)dt, \tag{2}$$

where $S_i^B$ gives the projection of a magnetic moment on the axis of oscillating field [15]. Physically, $P$ reflects the amount of energy (power), which is transformed into spin wave excitations.

The finite chains of length up to $l = 100a$ lattice constants $a$ have been simulated by solving the LLG equation. The calculations were performed with fixed and opened chain ends. The simulations were started with a relaxed magnetic configuration, saturated in the $z$ direction. Then an oscillating magnetic field was applied and the absorbed power was calculated at each site [Eq. (2)]. The sign of $P_i$ reflects the phase of the excitation at site $i$. $P_i$ is positive when both $S_i^B(t)$ and $\sin(\omega t)$ have the same sign and negative for the case of opposite signs. This means that the maximum (minimum) describes oscillations in phase (antiphase) with the oscillating field and $P_i = 0$ means no or no arranged oscillation. The values of $P_i$ can be immediately plotted as a function of the distance vector and thus yield spatially resolved spin wave eigenmodes. The obtained patterns contain full information about the amplitude and the phase of an excitation. To observe the absorbed power $P$ as a function of frequency an averaging over the whole sample must be performed. For that the averaged signal $P_{\rm av}$ has been introduced:

$$P_{\rm av} = \frac{1}{N}\sum_{i=1}^{N} |P_i|. \tag{3}$$

With the help of Eq. (3) the power spectra, dispersion curves, and the field dependencies of normal modes can be easily calculated.

Figure 1 shows the spatially resolved signal $P_{\rm av}$ as a function of frequency for a one-dimensional antiferromagnetic chain with one fixed end, while the inset shows the corresponding dispersion relation.

Apart from the energy gap at zero wave vector $k$ one can recognize in Fig. 1 two groups of peaks, with larger and smaller peak height. All peaks lie on the same straight dispersion line predicted in [3] (see inset). In Ref. [3] the dispersion curve has been obtained in the framework of the mean field theory, where instead of anisotropy and exchange constants an effective field has been used. We have derived the dispersion relation using the exact Hamiltonian [Eq. (1)] for an infinite, one-dimensional antiferromagnet. The following relation has been found:

$$\frac{\hbar\omega}{J} = \sqrt{4\sin^2(ka) + 2\frac{D_z}{J}\left(2\frac{D_z}{J} + 4\right)} \pm 2\frac{\mu_B B_z}{J}. \tag{4}$$

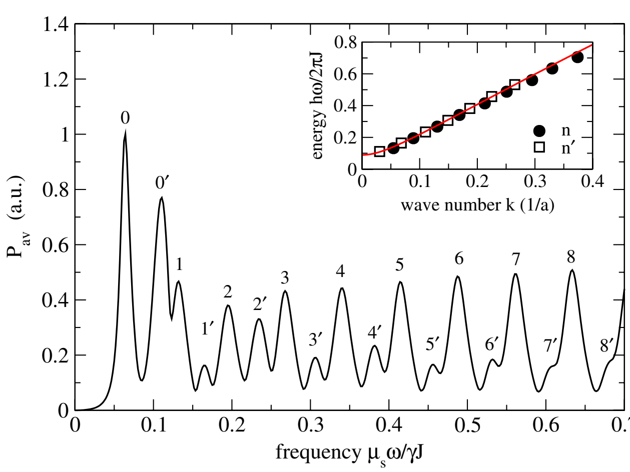


FIG. 1 (color online). Spatially resolved signal $P_{\rm av}$ and dispersion of standing spin waves in an antiferromagnetic spin chain with one fixed end and anisotropy ($D_z/J = 0.001$). A detailed description of the nomenclature is given in the text.

The main difference between the finite and the infinite system is the discrete character of $\hbar\omega = E(k)$ for finite antiferromagnets.

Mathematically, the two peak groups correspond to two solutions of the LLG equation. Physically, they correspond to two kinds of spin wave modes $n$ and $n'$. The modes are defined by the number of nodes of a standing wave. The first six spin wave modes ($n = 0, \ldots, 2$, $n' = 0, \ldots, 2$) for a chain with a fixed end at $x = 0$ are shown in Fig. 2 (left). The fast oscillations correspond to the two sublattices with opposite orientation of magnetization, which rotate in opposite directions, while the envelope describes the standing wave. In the case of one or two open ends the $n$ and $n'$ differ by the character of the oscillation of the open end(s). As can be seen from Fig. 2 (left) the $n$ modes finish before the maximum, while the $n'$ ones finish after the maximum.

This behavior is really unique and has no equivalent either in ferromagnetic systems nor in acoustics, where the open ends always show a maximal amplitude. In order to understand this interesting phenomenon we have analyzed the phases of $n$ and $n'$ modes. An example for chains with two open ends is given in Fig. 2 (right). One can see that an $n'$ ($n$) mode can always be continued in an $n$ ($n'$) mode. The physical reason is the following: because of the existence of two sublattices two *different* solutions of the LLG equation are required. The two solutions may have identical energy. The identical energy for both sublattices (two possible solutions of the LLG) requires identical periodicity and phase of the sublattice standing waves, which is not allowed because of the orthonormality of two solutions. In order to relieve the degeneracy, two modes of identical periodicity but shifted in phase are formed. The average energy of these modes is equal to the energy of a conventional mode $E_{\rm c}$ ending at maximal amplitude $(E_n + E_{n'})/2 = E_{\rm c}$ [see Fig. 2 (right)]. By that means the system reaches a minimal possible energy and, at the same time, assures two different solutions for the dynamics of staggered magnetization. Thus, the energy splitting is a compromise between the energy minimization and the complexity of the antiferromagnetic structure.

While the two energy levels lie on the same dispersion curve at zero external static magnetic field, they can be separated when an external field is switched on. Figure 3 gives an example of this band splitting as follows from Eq. (4) for zero anisotropy. For finite anisotropy the two bands are additionally shifted to higher energies corresponding to the value of anisotropy. The error bars in Fig. 3 come from the fact that the wave numbers have been determined statistically. We conclude from our analysis that the spin wave modes in applied field are not sinusoidal any more. This seems to be a direct consequence of the fact that $n'$ modes shift to higher frequencies with increasing magnetic field, whereas $n$ modes shift in the opposite direction (see inset of Fig. 3).

The case of a chain with two fixed ends is especially interesting as it includes two different realizations of boundary conditions: (i) both ends belong to the same

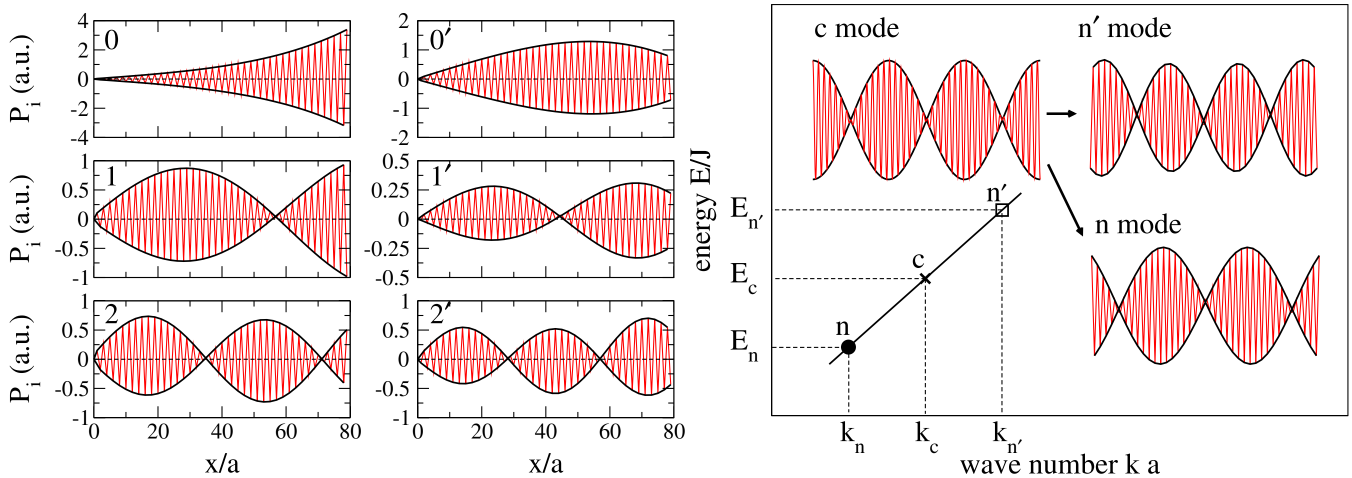

FIG. 2 (color online). Left: First six spin wave modes of a chain with one fixed end and the anisotropy ($D_z/J = 0.001$). Right: Splitting of a conventional $c$ mode into $n$ and $n'$ modes in antiferromagnetic chains with open ends.

sublattice, (ii) the ends belong to different sublattices. First we discuss possibility (i). The chains belonging to case (i) can be constructed only from an odd number of atomic sites. This fact determines a number of interesting properties of such chains. The dispersion curve and an example of a standing wave for antiferromagnetic chains of case (i) are shown in Fig. 4. The first remarkable feature of the standing wave is its asymmetry. Second, the dispersion curve does not show an energy splitting characteristic for chains with open ends; it means that $n'$ nodes are extinct. Third, the edges pinned at the same sublattice cause a degeneracy of the two solutions: no odd modes can be found anymore (see Fig. 4).

The reason for the asymmetry of the standing wave described above can be understood on the basis of the following symmetry considerations. Each lobe of the standing wave (the black envelope function in Fig. 4) contains the higher-frequency oscillations of the sublattices [gray (red) sinusoidal curve in Fig. 4]. The number of these oscillations depends on the position of the node of the envelope function. From the point of view of the kinetic energy, the nodes should be preferentially positioned between atomic sites. This effect is similar to Peierl's instability for spin density waves where the doubling of the period of the wave vector leads to an envelope wave, having nodes between the atomic sites. The positioning of the nodes of the standing wave between atomic sites is easy for a chain with one or two open ends. This possibility, however, becomes forbidden if both fixed chain ends belong to the same sublattice. The prohibition is caused by the fact that the positioning of the nodes between atomic sites will lead to the different number of oscillations between neighboring nodes of the standing wave, which is incompatible with the periodicity requirements. Therefore, the nodes $n$ lie on atomic sites. This configuration leads to

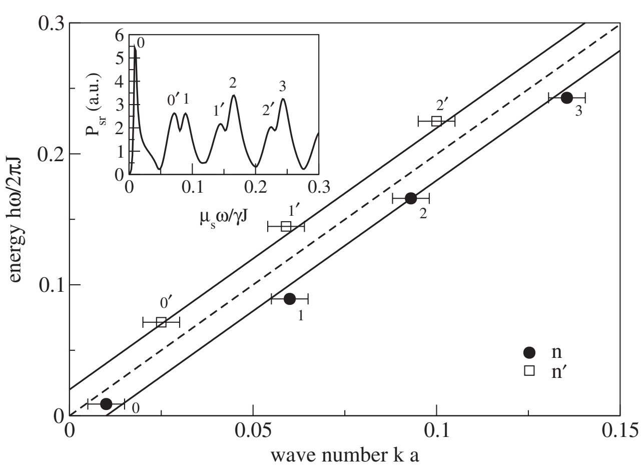

FIG. 3. Band splitting of the dispersion curve at an external field of $\mu_s B_z/J = 0.01$. The straight lines and the dashed line correspond to the analytical predictions given by Eq. (4) with and without external field, respectively ($D_z/J = 0$).

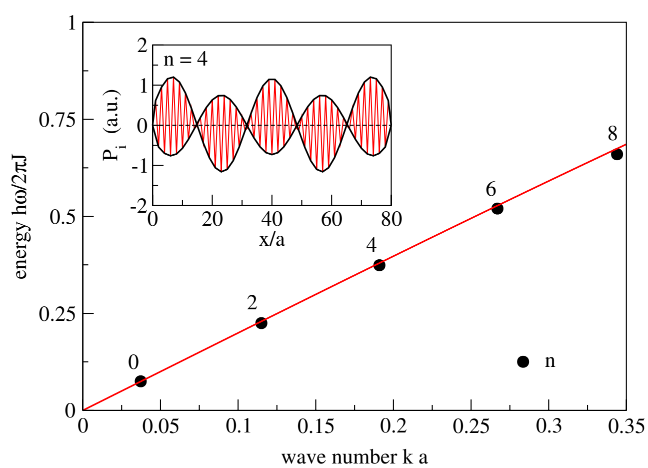

FIG. 4 (color online). Dispersion relation and standing spin wave of a chain with ends fixed at the same sublattice [case (i), $l = 78a$, i.e., 79 lattice sites]. The solid line represents the analytical prediction.

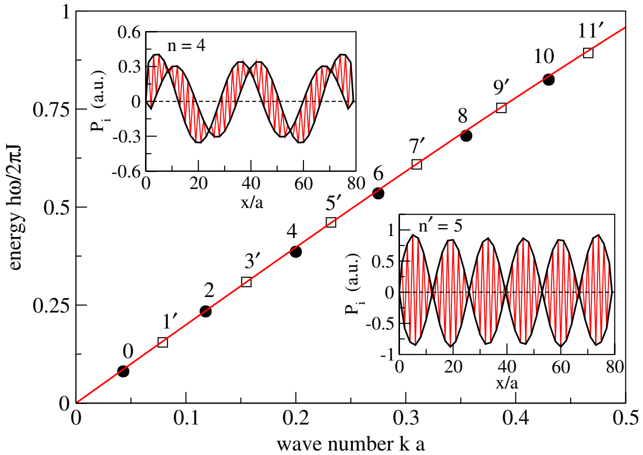


FIG. 5 (color online). Acoustic (even $n$, filled circles) and optical (odd $n$, open squares) standing antiferromagnetic spin waves in chains with ends fixed at different sublattices [case (ii), $l = 79a$, i.e., 80 lattice sites]. The straight line corresponds to the analytical solution.

several important consequences. First, only an even number of nodes is possible. This explains the absence of odd $n$'s. Second, the on-site placement of $n$ assures the periodicity of the whole pattern; i.e., each lobe of the wave pattern contains an identical number of smaller oscillations. However, the number of positive and negative oscillations in each lobe differs by one. Thereby the number of negative oscillations in a lobe $j$ is equal to the number of positive ones in the neighboring lobe $j \pm 1$. This peculiarity leads to the asymmetry of the whole pattern.

Chains of type (ii) may only have an even number of atomic sites. For chains of type (ii) the nodes of the standing wave can easily form between two atomic sites. Therefore, both $n$ and $n'$ modes can be found (see Fig. 5). Interestingly, no odd $n$ modes and no even $n'$ modes have been found in the simulations. The existing $n$ modes of odd parity (see bottom inset in Fig. 5) are very similar to those of even $n$ modes of case (i); i.e., the sublattices oscillate in antiphase. The oscillations do not show any asymmetry as the number of positive and negative oscillation is equal in each lobe of the envelope function. The even $n$ modes (see upper inset in Fig. 5) are very unusual. Both sublattices are oscillating in phase with the applied field, but the corresponding standing waves are shifted with respect to each other by 4–5 interatomic distances. Additionally, an asymmetry of two standing waves can be observed. These two regimes can be regarded as antiferromagnetic acoustical and optical standing spin waves and can be visualized as a superposition of two ferromagnetic standing spin waves for different sublattices.

In summary, we have demonstrated that quantized spin waves do exist in antiferromagnets. The characteristics of the antiferromagnetic standing waves have no equivalents in either acoustics nor in ferromagnetic samples. Particularly, the discrete energy dispersion is split into $n$ and $n'$ modes because of the existence of two sublattices. The splitting of the dispersion curve, the configuration of oscillations, as well as the symmetry of standing waves, strongly depend on the boundary conditions. In chains with open boundaries we find spin wave modes of odd and even parity in $n$ as well as in $n'$ energy levels. The phases of oscillations in $n$ and $n'$ bands are shifted by one eighth of the wave vector, while the average energy of both oscillations is equal to the energy of a conventional, unshifted mode. The chains with pinned ends can be subdivided into two main cases: the ones with both ends belonging to the same sublattice and that have the ends at different sublattices. In the first case the energy splitting does not appear and the $n'$ modes of odd parity do not exist. A very particular asymmetry of the envelope function has been observed for this geometry. In the second case the energy splitting is recovered. Very peculiar acoustical and optical antiferromagnetic spin waves have been found if the two ends belong to the same sublattice. The unusual behavior is explained on the basis of symmetry considerations.

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