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Identification of an intrinsic localized spin-wave resonance in antiferromagnetic chains with single-ion easy-plane anisotropy

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We find that a stationary intrinsic localized spin-wave resonance can exist and is long lived within the linear spin-wave spectrum for a perfect one-dimensional antiferromagnetic chain of classical spins with single-ion easy-plane anisotropy. Numerical simulation studies demonstrate that the excitation is stable with regard to a noise perturbation. The resonance is infrared active and its frequency decreases with increasing maximum spin deviation. [S0163-1829(97)52418-0]

It has been realized for decades that spatially localized modes can occur in purely harmonic lattices only when disorder is introduced so that the translational invariance of the underlying lattice is broken.[1] In recent years it has been noted that some vibrations in perfectly periodic lattices containing both nonlinearity and discreteness[2–5] appear to localize and the study of this *intrinsic localization* in various nonlinear periodic lattices is proving quite fruitful.[6–15] These intrinsic localized modes have somewhat the character of previously studied force constant defects, but they may appear anywhere in the homogeneous lattice and are mobile. Recently, it has been shown that intrinsic localized spin-wave modes (ILSMs) can occur in both classical ferromagnetic chains with on-site easy-plane anisotropy[16,17] and antiferromagnetic chains with on-site easy-axis anisotropy.[18] Like their vibrational counterpart, the ILSMs extend over only a few lattice sites and have amplitude-dependent frequencies outside the linear spin-wave bands. A large number of antiferromagnets actually are characterized by easy-plane anisotropy and an unanswered question is whether such ILSMs can exist in easy-plane antiferromagnetic chains.

In this paper we have investigated stationary ILSMs in chains of classical spins coupled antiferromagnetically through nearest-neighbor exchange interactions with on-site uniaxial easy-plane anisotropy. Although no ILSMs are found above the top of the linear spin-wave spectrum which, in this case, is gapless, a symmetric single-peaked intrinsic localized spin-wave resonance (ILSR) can exist with frequency lower than the $q=0$ frequency of the upper branch of the linear spin-wave spectrum. This numerical study demonstrates that intrinsic in-band resonant modes can be stable.

We consider a one-dimensional antiferromagnetic chain of N spins (N even) which is described by the Hamiltonian

$$H=2J\sum_n \mathbf{S}_n\cdot\mathbf{S}_{n+1}+D\sum_n (S_n^z)^2, \tag{1}$$

where both the nearest-neighbor exchange constant J and the single-ion anisotropy constant D are positive. The z axis is therefore a hard axis. The anisotropy that is used in Eq. (1) is an effective anisotropy which may arise from either the interaction of the magnetic moments with their neighboring ions via spin-orbit coupling or the long-range dipolar interaction between the magnetic moments. It has been pointed out[17] that some magnetic superlattices can also be described by an energy functional similar to Eq. (1).[19] In this case the spins are truly classical since each spin is the total spin moment of a magnetic layer.

We assume that the chain is magnetically ordered along the x axis at low temperatures with spins pointing alternatively parallel or antiparallel to the x axis. The equations of motion for the x, y, and z components become

$$\frac{\hbar}{2JS}\frac{ds_n^x}{dt}=[(s_{n-1}^z+s_{n+1}^z)s_n^y-(s_{n-1}^y+s_{n+1}^y)s_n^z]-As_n^y s_n^z, \tag{2a}$$

$$\frac{\hbar}{2JS}\frac{ds_n^y}{dt}=[(s_{n-1}^z+s_{n+1}^z)s_n^x-(s_{n-1}^x+s_{n+1}^x)s_n^z]+As_n^x s_n^z, \tag{2b}$$

$$\frac{\hbar}{2JS}\frac{ds_n^z}{dt}=(s_{n-1}^x+s_{n+1}^x)s_n^y-(s_{n-1}^y+s_{n+1}^y)s_n^x. \tag{2c}$$

Here we have introduced dimensionless variables $A=D/J$ and $\mathbf{s}_n=\mathbf{S}_n/S$ where S is the magnitude of spin. Thereafter we shall treat $\mathbf{s}_n$ as a classical vector of unit length.

To obtain the two linear spin-wave dispersion relations s_n^x is approximated as $s_n^x=(-1)^n$ in Eqs. (2b) and (2c). With cyclic boundary conditions applied the eigenfrequencies are

$$\Omega_\pm^2(q)=4\sin^2 qa+2A(1\pm\cos qa), \tag{3}$$

where a is the lattice spacing between two adjacent spins and the dimensionless frequency $\Omega_\pm(q)=\hbar\omega_\pm(q)/2JS$. These standard dispersion curves are plotted in Fig. 1 for the case of $A=1.0$. Since the ground state possesses rotational symmetry about the hard axis, i.e., the z-axis, the lower branch of linear spin-wave excitations, $\Omega_-(q)$, is gapless as shown in Fig. 1, while the upper branch, $\Omega_+(q)$, exhibits a ''gap'' below $\Omega_+(0)=2\sqrt{A}$. The two branches are degenerate at the Brillouin zone boundary.

Can an intrinsic localized spin-wave mode exist at the zone boundary of the plane-wave spectrum? A necessary condition is that the substitution of $q=\pi/2a+i\kappa$ into Eq. (3) gives a real localized mode frequency; however, since a complex frequency is found this possibility is excluded. In a strict sense there is no gap for the spin-wave excitations

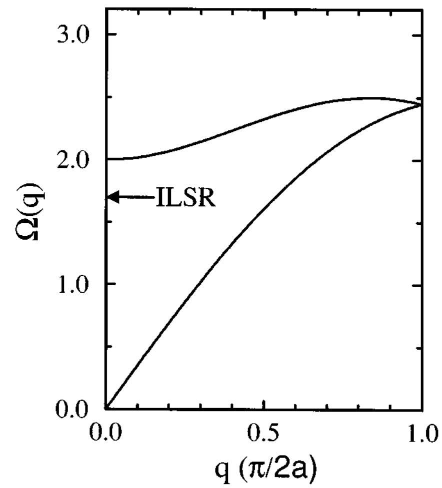

FIG. 1. Linear spin-wave spectrum for an antiferromagnetic chain with easy-plane anisotropy. The anisotropy parameter is $A=1.0$. The ILSR arrow identifies the frequency of the intrinsic localized spin-wave resonance described in the text.

shown in Fig. 1, even though the upper and lower branches do have different polarizations, so we now investigate the possibility that a nonlinear localized resonance may oscillate at a frequency below $\Omega_+(0)$. Since the linear spin waves are elliptically polarized we anticipate that the nonlinear resonant spin-wave excitation would also be elliptically polarized. To find the eigenvector of a stationary ILSR we use the ansatz

$$s_n^y(t)=s_n^y\cos\omega_r t,\quad s_n^z(t)=s_n^z\sin\omega_r t$$

and (4)

$$s_n^x(t)=(-1)^n\{1-(s_n^y)^2\cos^2\omega_r t-(s_n^z)^2\sin^2\omega_r t\}^{1/2}.$$

Here the squared terms in s_n^y and s_n^z cannot be neglected. Substituting Eq. (4) into Eqs. (2b) and (2c) we obtain, in the rotating wave approximation (RWA) where higher harmonics are ignored, the following coupled time-independent nonlinear equations:

$$\begin{aligned}(-1)^{n+1}\Omega_r s_n^y&=f(s_n^z,s_n^y)[s_{n-1}^z+s_{n+1}^z+As_n^z]\\&\quad+[f(s_{n-1}^z,s_{n-1}^y)+f(s_{n+1}^z,s_{n+1}^y)]s_n^z,\\(-1)^{n+1}\Omega_r s_n^z&=[f(s_{n-1}^y,s_{n-1}^z)+f(s_{n+1}^y,s_{n+1}^z)]s_n^y\\&\quad+f(s_n^y,s_n^z)[s_{n-1}^y+s_{n+1}^y],\end{aligned}\tag{5}$$

where

$$f(a,b)=(1-a^2)^{1/2}F\left(-\frac{1}{2},\frac{1}{2},2,\frac{b^2-a^2}{1-a^2}\right),\tag{6}$$

and F is the hypergeometric function.[20] Since a stationary localized resonance, if it exists, should bifurcate from the spatially uniform $q=0$ mode of the upper branch in Fig. 1 which has the eigenvector

$$\{s_{2n}^y,s_{2n}^z,s_{2n+1}^y,s_{2n+1}^z\}\propto\{\sqrt{A}/2,-1,\sqrt{A}/2,1\},$$

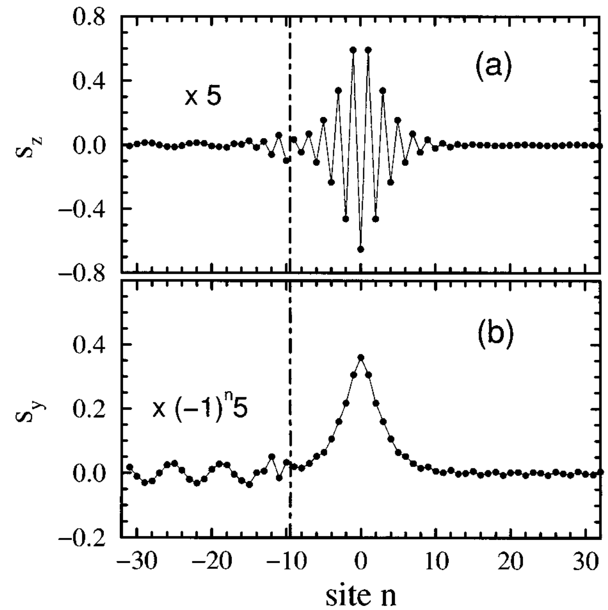

FIG. 2. Shape of a stationary intrinsic localized spin-wave resonance with the maximum spin deviation $s_0^z=-0.65$ and the anisotropy parameter $A=1.0$. (a) The spin deviation s_n^z versus lattice site index n. The left side shows a factor 5 expansion of the ordinate to display the plane-wave character in the wings. (b) The spin deviation s_n^y versus site index n. The left side shows the same factor 5 expansion and a sign alternation to illustrate the resonant mode plane-wave character.

we seek the symmetric single-peaked localized solution with the same pattern of sign alternation near the center of the resonance. Far away from the mode center the localized solution would be mixed with the spatially uniform plane-wave solution from the lower branch. To explore this possibility in detail we numerically solve the set of coupled nonlinear equations given by Eq. (5) for a chain of 64 spins with periodic boundary conditions using the globally convergent Newton method. We find that the intrinsic localized resonance does exist for a range of anisotropy parameters.

As an illustration the spin deviation versus site index of an ILSR is plotted in Fig. 2 as filled circles for the parameters $s_0^z=-0.65$ and $A=1.0$. The frequency of this ILSR is found to be $\Omega_r=0.9301\Omega_+(0)$ within the RWA. As expected, near the center of the resonance the sign of the z component of the spin deviation alternates from one spin to the next while the sign of the y component does not change. Hence the time-periodic and spatially localized ILSR has an oscillating net magnetic moment in the y direction. Unlike the intrinsic localized gap modes found before in antiferromagnetic chains[18] with easy-axis anisotropy, the spin deviations do not disappear with increasing distance from the center. Instead the localized excitation evolves into a weak plane-wave pattern, as expected for a resonance, which has the eigenvector character of the lower branch. The seemingly irregular off-center region of s_n^y far from the center exhibits a smooth plane-wave pattern under the transformation $s_n^y\rightarrow(-1)^n s_n^y$. This sign alternation of s_n^y is a characteristic feature of the lower branch. The wave number q associated with the small amplitude off-center plane wave can be obtained from the Fourier transform of s_n^z in q space. For the

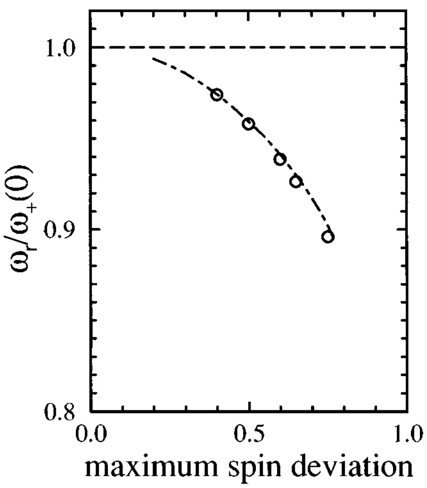

FIG. 3. Comparison between the rotating wave approximation (RWA) frequency and the MD simulation frequency for a stationary ILSR versus spin deviation. The anisotropy parameter $A=1.0$. The dot-dashed curve is obtained using the RWA, and the open circles are results calculated from the first $820T_+(0)$ MD simulation points of the net magnetic moment $M^y(t)$.

ILSR shown in Fig. 2, $q=0.6(\pi/2a)$, corresponding to a frequency of $0.9277\Omega_+(0)$ in the lower branch, which is in good agreement with the ILSR frequency given the fact that the small size of the lattice limits the wave-number accuracy.

The dot-dashed curve in Fig. 3 shows the ILSR frequency found in the RWA as a function of the maximum spin deviation s_0^z. The frequency drops further into the lower spin-wave band as s_0^z increases. Later these RWA frequencies will be compared to molecular-dynamics (MD) simulation frequencies.

Since the RWA has been used to obtain the ILSR eigenvector the mode stability needs to be checked by means of MD simulations. In MD simulations the numerically determined eigenvector is used as the initial condition, i.e., $\mathbf{s}_n=((-1)^n\sqrt{1-(s_n^z)^2},0,s_n^z)$, and the discrete equations of motion for the x-y-z spin components are integrated numerically by using the fourth-order Runge-Kutta method with a time step of $T_+(0)/200$ where $T_+(0)=\pi\hbar/JS\Omega_+(0)$. At each step conservation of energy and spin length (to 1 part in 10^5) serve as checks on the numerical accuracy.

These molecular-dynamics simulations show that the ILSR with modest spin deviations can last many hundreds of periods without apparent decay. For example, the time evolution of the ILSR energy density $e(n)=J\mathbf{S}_n\cdot(\mathbf{S}_{n-1}+\mathbf{S}_{n+1})+D(S_n^z)^2$ averaged over one period is plotted in Fig. 4. The parameters are the same as those in Fig. 2. No decay can be seen after $800T_+(0)$. When a noise perturbation ($<0.1\%$) is added, the ILSR in Fig. 4 remains fixed for about $800T_+(0)$ and then moves while still localized. It is found that as the maximum spin deviation is increased, the amplitude of the plane-wave component in both wings of this excitation increases. As a consequence the ILSR can become unstable and delocalize after sufficient time as might be expected for a localized excitation which is ''on speaking terms'' with the plane-wave spectrum.

Since the ILSR is a collective excitation, the calculation of power spectrum of the total magnetic moment, $\mathbf{M}(t)=\Sigma_n\mathbf{s}_n(t)$, is a useful method with which to identify the relative strength of the different frequency components of the excitation as well as to check the accuracy of the RWA. In the uniaxial case M^z commutes with the Hamiltonian, and is therefore a constant of motion. Figure 5 shows the log power spectrum of $M^y(t)$ for the ILSR plotted in Fig. 2. This power spectrum is calculated from the first $820T_+(0)$ MD data values. A strong peak appears at $\Omega_r=0.9265\Omega_+(0)$, which should be compared to $0.9301\Omega_+(0)$ found in the RWA. Since the eigenvector is not an exact eigenvector due to the RWA, linear spin waves are also excited. However, the strength of the power spectrum peak at $\Omega_+(0)$ is more than three orders of magnitude weaker than the resonance peak. Peaks at the third and fifth harmonics are also present in the power spectrum (not shown), but their strengths are at least four orders of magnitude weaker than the peak corresponding to the fundamental ILSR frequency indicating that the RWA is a good approximation for this Hamiltonian.

The MD simulation frequency versus spin deviation is plotted in Fig. 3 as open circles and these values compare well with the RWA frequencies represented by the dashed

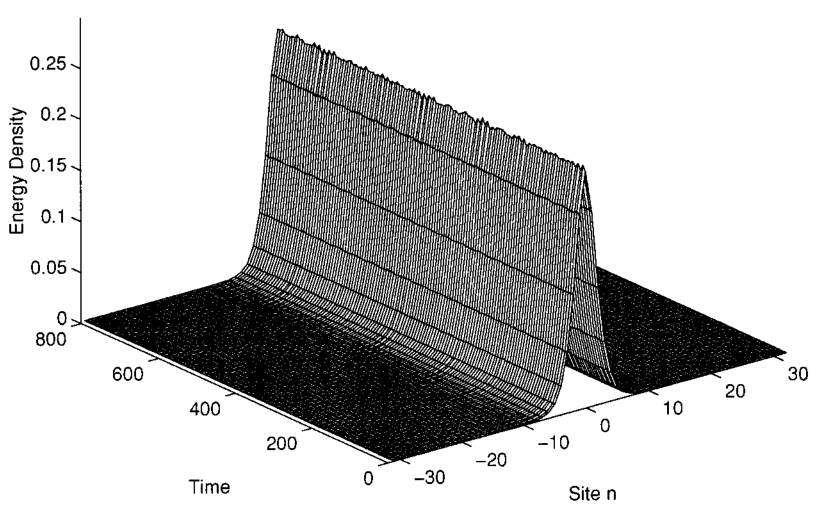

FIG. 4. Time evolution of the energy density of the ILSR shown in Fig. 2. The energy density shown here is measured from the ground-state energy and averaged over one period. The time is measured in units of $T_+(0)$.

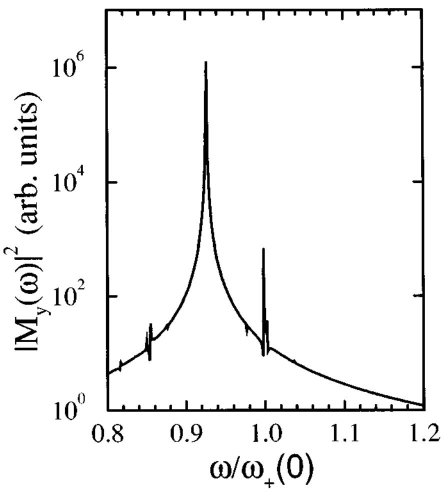

FIG. 5. Power spectrum of the net magnetic moment $M^y(t)$ of the stationary ILSR shown in Fig. 2. Besides the strong peak at $0.9265\omega_+(0)$ corresponding to the ILSR a much weaker peak appears in the power spectrum at $\omega_+(0)$, indicating that linear spin waves are also excited due to the inaccuracy in the eigenvector resulting from the rotating wave approximation.

line. The MD simulation frequency is slightly lower than the corresponding RWA frequency and the difference between the two becomes larger as the maximum spin deviation increases. The difference grows because more and more energy goes into higher harmonics, but even so the overall agreement is quite good over the entire range.

In summary we have shown that an intrinsic localized spin-wave resonance can exist in one-dimensional antiferromagnetic chains with on-site uniaxial easy-plane anisotropy. Since the ILSR has a nonzero total magnetic moment oscillating along the y axis, it can couple to infrared radiation. Although from analytical work lattice dynamics resonance modes already have been proposed to be a natural consequence of intrinsic localization,[21] our MD study successfully demonstrates that in-band nonlinear localized excitations in a discrete lattice can be stable. The key feature in this nonlinear dynamics problem is the polarization difference between the two plane-wave branches. In our numerical simulations the smaller the frequency of the $q=0$ mode in the upper branch, the less strongly coupled the resulting ILSR is to the other branch of the plane-wave spectrum. The analogy between the spin-wave and vibrational problems is clear. Because of the polarization difference between the optic and acoustic phonon branches in a one-dimensional anharmonic diatomic chain, a similar uncoupling of an opticlike intrinsic resonance mode from the acoustic plane-wave spectrum would be expected to occur.

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