Normal modes of vortices in easy-plane antiferromagnets: Exact results and Born approximation

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We investigate the spin-wave spectrum of two-dimensional easy-plane classical antiferromagnets in the presence of a planar vortex. The exact wave forms of spin waves are obtained and then compared with the Born approximation. Two modes in which the characteristic frequencies may be detected in resonance experiments are found. [S0163-1829(96)08133-7]

A large variety of layered magnetic insulators has been shown to exhibit the experimental characteristic of two-dimensional (2D) magnetism and has been useful in testing theories pertinent to 2D systems. In classical models for these quasi-two-dimensional magnetic materials, it has been found that nonlinear excitations play an active role in the static thermodynamic properties,[1] and are expected to be important in the spin dynamics.[2–6] Mobile vortices and solitons were considered by some authors[3–6] with the result that motion gives rise to a central peak in the frequency-dependent correlation function. But another mechanism that can affect the dynamics is the soliton-magnon (or vortex-magnon) interaction. Recently, the dynamic spin correlation function owing to a soliton-magnon interaction in the 2D isotropic classical antiferromagnet (described by the 2D nonlinear σ model) has been calculated by Zaspel *et al.*[7] They have shown, using the Born approximation, that magnons scattered by solitons result in an electron paramagnetic resonance (EPR) linewidth with a dominant $\exp(E_S/T)$ temperature dependence, where E_S is the soliton energy. Their calculations are in good agreement with EPR linewidth data on several previously measured spin-5/2 layered manganese compounds[8,9] and data on *n*-propylammonium tetrachloromanganate.[7]

Solitons interacting with magnons have been also considered, in the Born approximation, in quantization procedures for soliton states in the 2D nonlinear σ models (isotropic[10] and anisotropic[11]) and vortex states in the 2D anisotropic ferromagnets.[12] It has been found that the quantum corrections to the classical soliton, or vortex, energy, given by the zero-point energy of the spin waves measured with respect to the vacuum can change strongly the classical picture, introducing interactions between solitons[10] as well as an internal degree of freedom for solitons.[11]

The importance of the vortex-magnon interaction in discrete lattices has been studied in easy-plane ferromagnets by Wysin and Völkel[13] using numerical diagonalization on small systems. In particular, it has been shown how the spin-wave modes are related to the instability of vortices.[13,14]

Our purpose in this paper is to study the vortex-magnon interaction in 2D easy-plane antiferromagnets. Since the lowest-order effect of an inhomogeneous vortex is to produce an elastic scattering center for the magnons, we calculate the asymptotic phase-shifted cylindrical spin waves. In contrast to the ferromagnetic case[15] we find (besides the continuum states) two new internal motions of vortices whose characteristic frequencies can be detected in resonance or inelastic neutron scattering (INS) experiments. Next, the Born approximation (which is the standard procedure used by several authors[7,10–12,15]) is used to calculate the phase shift of the magnons and then compared with the exact result obtained here.

We begin with the Hamiltonian for a classical two-dimensional antiferromagnetic Heisenberg model with easy-plane symmetry:

$$H=J\sum_{\langle i,j\rangle}[\mathbf{S}_i\cdot\mathbf{S}_j+\lambda(S_i^z)^2], \tag{1}$$

where $J>0$ is the exchange constant, $\lambda>0$ is the anisotropy parameter, and $\mathbf{S}_i$ is the spin vector at site i of magnitude S. The continuum limit of this Hamiltonian can be obtained in the usual way[16] defining normalized vectors of magnetization $\mathbf{m}_n=(\mathbf{S}_{2n}+\mathbf{S}_{2n+1})/2S$ and the vectors of sublattice magnetization $\mathbf{l}_n=(\mathbf{S}_{2n}-\mathbf{S}_{2n+1})/2S$, where the subscripts refer to the different sublattices. Vectors $\mathbf{m}$ and $\mathbf{l}$ are related by $\mathbf{m}^2+\mathbf{l}^2=1$ and $\mathbf{m}\cdot\mathbf{l}=0$. In the critical fluctuation region the condition $|\mathbf{m}|<<|\mathbf{l}|\approx 1$ is satisfied and then the Hamiltonian can be expressed in terms of $\mathbf{l}$ only.[17] Using angular variables for $\mathbf{l}$, $\mathbf{l}=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$, the equation of motion can be written in the form[18]

$$\nabla^2\theta-\left(\frac{1}{c^2}\right)\left(\frac{\partial^2\theta}{\partial t^2}\right)=\sin\theta\cos\theta\left[(\nabla\phi)^2-\left(\frac{1}{c^2}\right)\left(\frac{\partial\phi}{\partial t}\right)^2\right]-2\lambda\sin\theta\cos\theta, \tag{2}$$

$$\nabla^2\phi-\left(\frac{1}{c^2}\right)\left(\frac{\partial^2\phi}{\partial t^2}\right)=-2\cot\theta\left[(\nabla\theta)\cdot(\nabla\phi)-\left(\frac{1}{c^2}\right)\left(\frac{\partial\theta}{\partial t}\right)\left(\frac{\partial\phi}{\partial t}\right)\right], \tag{3}$$

where $c=2JS$ is the spin-wave velocity. Nonlinear excitations can be obtained from these equations, but only for some special cases can the excitations be analytically obtained. For the case with $\lambda=0$ (isotropic Heisenberg model) general localized solutions have been obtained by Belavin and Polyakov.[19] The case of our interest ($\lambda > 0$) is the classical xy-like model with excitations being vortices easily obtained by integration of the equations of motion in a polar (r,φ) coordinate system. The static vortex solution is given by $\theta_v = \theta_v(\mathbf{r})$ and $\phi_v = \tan^{-1}(y/x)$. In particular, in models of three-component classical spins with easy-plane (xy) anisotropy, there are two possible types of vortices, known as ''in-plane'' and ''out-of-plane'' vortices, depending on whether the static vortex has zero or nonzero out-of-plane spin components, respectively. Völkel *et al.*[20] have shown numerically that for Hamiltonian (1), when λ is larger than a critical value ($\lambda_c \approx 0.5$) planar vortices are stable, but if λ is smaller than the critical value, out-of-plane vortices become stable where the central region of the vortex has spins not confined to the lattice plane. Other recent numerical simulations have also shown that a free vortex almost never travels more than one lattice constant.[21,22] For these reasons, i.e., since the planar vortex solution is exactly known $[\theta_v = \pi/2, \phi_v = \tan^{-1}(y/x)]$ and is stable for an appreciable range of anisotropy,[20] we will consider only a static planar vortex.

In order to determine the behavior of small oscillations in the presence of a static planar vortex, we assume that the spin polar and azimuthal angles can be expressed as $\theta(\mathbf{r},t) = \theta_v(\mathbf{r}) + \xi(\mathbf{r},t)$ and $\phi(\mathbf{r},t) = \phi_v(\mathbf{r}) + \eta(\mathbf{r},t)$. Here ξ and η are assumed to be small quantities which reduce to spin-wave solutions if no vortices are present. In the presence of a vortex, ξ and η give the change in the vortex configuration as a result of the vortex–spin-wave interaction. Recently, Ivanov *et al.*[23] studied the interaction between the ''out-of-plane'' vortex and magnons with the limitation that the form $\theta_v(\mathbf{r})$ was unknown, and so calculations had to be restricted by approximating $\theta_v(\mathbf{r})$ by its asymptotic form. Here, since the planar vortex solution is exactly known, we can obtain the exact wave forms of $\xi(\mathbf{r},t)$ and $\eta(\mathbf{r},t)$. To this end, to first order in small quantities, the equations for θ and ϕ become an uncoupled set of two partial differential equations to be solved for ξ and η. We get

$$\nabla^2 \xi - \left(\frac{1}{c^2}\right)\left(\frac{\partial^2 \xi}{\partial t^2}\right) - 2\lambda \xi = V(r)\xi, \tag{4}$$

$$\nabla^2 \eta - \left(\frac{1}{c^2}\right)\left(\frac{\partial^2 \eta}{\partial t^2}\right) = 0, \tag{5}$$

where $V(r) = -(\nabla \phi_v)^2 = -1/r^2$. Notice that the ''in-plane'' spin-wave oscillation $\eta(\mathbf{r},t)$ does not ''feel'' the presence of a planar vortex [see Eq. (5)], since we have a usual wave equation without any potential, resulting in free cylindrical waves solutions associated with the well-defined angular momentum (n) stationary states η_n of a free magnon. These solutions are written as

$$\eta_n(\mathbf{r},t) = J_n(qr) e^{in\varphi} e^{-i\omega_1 t} = \frac{1}{2}[H_n^{(1)}(qr) + H_n^{(2)}(qr)] e^{in\varphi} e^{-i\omega_1 t}, \tag{6}$$

where $\omega_1 = qc$ and $\mathbf{q}$ is the wave vector. At infinity, $\eta_n(\mathbf{r},t)$ results from the superposition of an incoming spin wave and an outgoing spin wave, whose amplitudes differ by a phase difference equal to $(n\pi + \pi/2)$.

In Eq. (4), when $V(r)$ is identically zero (absence of a vortex), the solution $\xi(\mathbf{r},t)$ reduces also to the plane wave $e^{i\mathbf{q}\cdot\mathbf{r}}$ and, as in the latter case, the partial waves become free cylindrical waves $\xi_n(\mathbf{r},t) = J_n(qr) e^{in\varphi} e^{-i\omega_2 t}$ with frequency $\omega_2 = (2\lambda + q^2)^{1/2} c$. Hence, it is easy to see that the lowest-order effect of a planar vortex introduced into the system $[V(r) = -1/r^2]$ is to produce an elastic scattering center for ''out-of-plane'' spin waves. The potential $V(r)$ associated with the vortex configuration is cylindrically symmetric, and then angular momentum is a good quantum number and the phase-shift matrix $\Delta_{nn'}(q)$ is diagonal.

Writing $\xi_n(\mathbf{r},t) = \xi_{0(n)}(r) e^{in\varphi} e^{-i\omega_2 t}$, Eq. (4) becomes

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\left(\frac{d}{dr}\right) + q^2 - \frac{(n^2-1)}{r^2}\right]\xi_{0(n)}(r) = 0, \tag{7}$$

with $\omega_2^2 - 2\lambda c^2 = \tilde{\omega}^2 = q^2 c^2$. For $|n| \geq 1$ the solutions of Eq. (7) are Bessel functions of order $\mu = \sqrt{n^2-1}$, i.e.,

$$\xi_{0(n)}(r) = J_\mu(qr) = \tfrac{1}{2}[H_\mu^{(1)}(qr) + H_\mu^{(2)}(qr)]. \tag{8}$$

For $n = 0$, we get the solution

$$\xi_{0(0)} = D e^{-iqr} r^i F(\tfrac{1}{2} + i|1+2i|2iqr) + E e^{-iqr} r^{-i} F(\tfrac{1}{2} - i|1-2i|2iqr), \tag{9}$$

where $F(a|b|c)$ are the confluent hypergeometric functions and D and E are constants of renormalization. The difference between $\xi_{0(n)} = J_\mu(qr)$ (solution in the presence of a vortex) and $J_n(qr)$ (solution in the absence of a vortex) is physically clear. As an incoming spin wave approaches the zone of influence of the potential, it is more and more perturbed by this potential. When, after turning back, it is transformed into an outgoing spin wave, it has accumulated a phase shift of $2\Delta_n(q)$ relative to the free outgoing spin wave that would have resulted if the potential $V(r)$ had been identically zero. In fact, the factor $e^{-2i\Delta_n(q)}$ summarizes the total effect of the potential on a magnon of angular momentum n, so that we can write

$$\xi_{0(n)} = \tfrac{1}{2}\{H_{|n|}^{(1)}(qr) + e^{-2i\Delta_n(q)} H_{|n|}^{(2)}(qr)\} \quad (r \to \infty). \tag{10}$$

By comparing the solution (10) (valid in $r \to \infty$) with the exact solution $\xi_{0(n)}$ of Eq. (7) at $r \to \infty$, we obtain the phase shifts

$$\Delta_0(q) = 2\pi,$$

$$\Delta_n(q) = (n - \sqrt{n^2-1})\pi/2 \quad \text{for } n \geq 1, \tag{11}$$

$$\Delta_n(q) = -(n + \sqrt{n^2-1})\pi/2 \quad \text{for } n \leq -1.$$

Notice that $\Delta_{|n|}(q) = \Delta_{-|n|}(q)$ and that the phase shift of the partial wave $\xi_{n,q}(r)$ does not depend on q, that is, on the energy.

Two modes are found in this antiferromagnetic system considering $\tilde{\omega} = 0$ with $n = 0$ and $n = 1$. We obtain two modes with a well-defined frequency determined by the strength of the easy-plane anisotropy, $\omega_b = \sqrt{2\lambda} c$, the wave forms of which are

$$\xi_{b_0}(r)=\beta_1\cos(\ln r)+\beta_2\sin(\ln r) \quad (r>0),$$
$$\xi_{b_1}(r)=\beta_3, \tag{12}$$

where β_1, β_2, and β_3 are constants of renormalization.

Equations (12) show that planar vortices possess two additional internal degrees of freedom, since l^z is described by oscillating functions with constant amplitudes. It is due to the fact that the spins can oscillate out of the plane $[l^z=\xi_{b_0}(r)e^{-i\omega_b t}$ or $l^z=\xi_{b_1}e^{i\varphi}e^{-i\omega_b t}]$ without any deviations η from the static in-plane angles. Characteristic frequencies of the internal motion can be detected in principle by EPR or INS. In our case, when λ is larger than a critical value λ_c ($\lambda_c\approx 0.5$ for the square lattice[20]), the frequency $\omega_b=\sqrt{2\lambda}c$ may be observed in experiments with quasi-two-dimensional antiferromagnets. In three dimensions, internal motion of domain walls in antiferromagnets was experimentally observed in thulium orthoferrite.[24].

A good candidate for a 2D easy-plane antiferromagnet is $B_aNi_2(PO_4)_2$, which can be described by the Hamiltonian (1) with $J=11$ K, $\lambda=0.66$, and $S=1$.[25] Of course, this antiferromagnet does not satisfy our conditions entirely since S is small. But with an approximation we expect that a characteristic frequency $\omega_b\approx\sqrt{2\lambda}c\approx 25.2$ K of the internal motion may be detected in this system by EPR or INS.

The scattering or continuum states can contribute to the correlation function. Vortex motion results in a central peak at zero frequency, which is far removed from EPR resonance. Hence, the time-dependent mechanism that can contribute to the EPR linewidth is the vortex-magnon interaction considered here. The EPR linewidth is the temporal integral of the four-spin correlation function,[26,27] and the determination of this function and its dependence on the vortex excitations will probably have to be done numerically and is beyond the scope of this paper. Zaspel *et al.*,[7] using the Born approximation, have shown that solitons interacting with magnons in classical 2D isotropic antiferromagnets results in an EPR linewidth $\exp(E_s/T)$. But one point to mention in their calculations is that they have only considered the s-wave ($n=0$) scattering, arguing that it is the main contribution to the soliton-magnon interaction. However, we have seen here that in the case of the vortex, all momentum angular channels seem to be important. To analyze it better we will calculate the phase shifts $\Delta_n(q)$ using the Born approximation and then compare the approximation with the exact result given by Eqs. (11). We can use our exact result to check the Born approximation and it may help to evaluate the calculations using this technique as in Refs. 7 and 10–12.

The first-order Born terms for the phase shifts are given, in general, by

$$\Delta_n^{(1)}(q)=-\frac{\pi}{2}\int_0^\infty r\,dr\langle J_{|n|}(qr)e^{-in\varphi}V(r)e^{in\varphi}J_{|n|}(qr)\rangle_\varphi, \tag{13}$$

where the symbol $\langle\cdots\rangle_\varphi$ denotes an angular average. Since the ''out-of-plane'' spin waves ''feel'' a potential $V(r)=-1/r^2$, we get for $n\neq 0$

TABLE I. Comparison between the Born approximation and exact result for five momentum angular channels.

Phase shift	Exact results	Born approximation
Δ_1	$\pi/2$	$1/2(\pi/2)$
Δ_2	$0.268(\pi/2)$	$0.25(\pi/2)$
Δ_3	$0.171(\pi/2)$	$0.166(\pi/2)$
Δ_4	$0.127(\pi/2)$	$0.125(\pi/2)$
Δ_5	$0.101(\pi/2)$	$0.100(\pi/2)$

$$\Delta_n^{(1)}=\frac{\pi}{4|n|} \quad (n\neq 0). \tag{14}$$

For $n=0$, the integral (13) diverges because the vortex core is a singularity in a continuum limit. Usually this means that a short-distance cutoff[1,15] must be applied *ad hoc* to integrals over the spin field, but the cutoff radius itself is not well known.

The agreement between the approximation [Eq. (14)] and the exact result [Eqs. (11)] for large angular momentum channels ($|n|\geq 2$) is presented in Table I. For $|n|=1$ the error is 50%.

As we could expect the Born approximation (first order) is not good for $n=0,\pm 1$ angular momentum (s and p waves). In fact, in these cases the centrifugal barrier given by n^2/r^2 [see Eq. (7)] is small and hence the s and p waves can approach the zone of strong influence of the potential, where the Born approximation may fail. For $|n|\geq 2$, the centrifugal barrier is large and expels the spin waves from the center of the vortex, where $V(r)\gg 1$. It is easy to see that, when $|n|\gg 1$, Eqs. (11) reduce to Eq. (14). This result is physically important for it implies that an ''out-of-plane'' spin wave in the state $\xi_{n,q}(\mathbf{r},t)$ is practically unaffected by what happens inside a circle centered at the origin (vortex-center) of the radius $R_n(q)=n/q$.

In order to improve the calculations for $\Delta_0^{(1)}(q)$ and $\Delta_1^{(1)}(q)$ we have to consider the second-order Born terms $\Delta_0^{(2)}(q)$ and $\Delta_1^{(2)}(q)$. However, these calculations present the same difficulty we have met in calculating $\Delta_0^{(1)}(q)$, since the cutoff radius is not well known. In using a value proportional to a (lattice constant), we get results that depend on this value and then it seems to be artificial.

In summary, we have obtained the exact phase shifts (and hence the exact wave forms) of linear spin waves in the presence of a planar vortex in 2D easy-plane antiferromagnets. This has been theoretically described in the continuum limit, and hence, for the discrete case, the wave forms are correct only for sufficiently large values of r, far from the vortex center.[14] The results were compared with the Born approximation, leading to the conclusion that this approximation works very well for large momentum angular channels ($|n|\geq 2$) but it may fail for s and p waves. In addition to the scattering states, two modes with a well-defined frequency $\omega_b=\sqrt{2\lambda}c$ were found. Resonances at characteristic frequencies of an internal motion can be observed in EPR or INS experiments. Then, if vortices are present in the system, EPR linewidth measurements provide an indirect method to experimentally detect vortices. In fact, this method could check if vortices dominate the thermodynamics in the fluctuation region immediately above the Kosterlitz-Thouless temperature[1] T_{KT}. Finally, we would like to mention that the bound state(s) and scattering or continuum states may be of fundamental importance not only for the spin dynamics but also for use in statistical mechanics,[28] as well as quantizations procedures for soliton states[11,29] and perturbation theories[30] involving soliton responses to external perturbations.

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