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Dynamics of vortices in quasi-two-dimensional classical Heisenberg magnets with weak easy-plane anisotropy

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Abstract. We present a discussion of the dynamical correlation functions for Heisenberg magnets with a weak easy-plane anisotropy for temperatures just above the Kosterlitz–Thouless phase transition. Compared to the XY-model we find here vortices which have in addition to the well known in-plane structure a localized out-of-plane profile around their centre. For the ferromagnetic case this structure produces an effective magnetic field which acts as a gyro force on the other vortices. Assuming a dilute gas of weakly interacting vortices, we find analytic expressions for the vortex contribution to the dynamical correlation functions. These results are compared (i) with numerical Monte Carlo–molecular dynamics simulations on a 100×100 square lattice allowing us to determine values for the vortex correlation length ξ and average vortex velocity $\bar{u}$ and (ii) with experiments performed on different quasi-two-dimensional magnetic materials. We find that our two calculations are in good agreement with the experiments and the Kosterlitz–Thouless theory on two-dimensional XY magnets as far as static properties are concerned. Data obtained by fitting the width of the central peak in appropriate dynamic structure functions, which reflect the dynamics, show a significant deviation from the results of our calculations, suggesting that here the parameters of the free vortex-gas *ansatz* are renormalized by additional interactions with vortex pairs (clusters) and/or in-plane spin waves at higher q-values.

1. Introduction

During the last few years an increasing number of quasi-two-dimensional (2D) magnetic materials have been found (a good overview over these materials is presented in the book by de Jongh (1990)) such as (i) layered magnets, like K_2CuF_4 (Hirakawa *et al* 1982), $(CH_3NH_3)_2CuCl_4$ (Aïn 1987) and $BaM_2(XO_4)_2$ with M = Co, Ni, ... and X = As, P, ... (Regnault *et al* 1989, Regnault and Rossat-Mignot 1990, Gaveau *et al* 1991); (ii) $CoCl_2$ graphite intercalation compounds (Wiesler *et al* 1989); (iii) magnetic lipid layers, like $Mn(C_{18}H_{35}O_2)_2$ (Pomerantz 1984, Head *et al* 1988); here even monolayers can be produced which are literally 2D magnetic systems. These various materials exhibit not only spatially extended modes (spin waves) as excitations, but also spatially local structures, such as vortices, domain walls, etc, characteristic of highly non-linear systems.

Most of the above mentioned materials can be well described in a first approximation by the anisotropic Heisenberg Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z \right) \tag{1.1}$$

where $\langle i, j \rangle$ label nearest-neighbour sites. $J > 0$ and $J < 0$ correspond to ferromagnetic (FM) and antiferromagnetic (AFM) exchange couplings, respectively. In this paper we will focus only on XY or 'easy-plane' symmetry with a corresponding $\lambda \in [0, 1[$. The non-linear excitations in this type of model are vortices which lead to a well known phase transition (Kosterlitz and Thouless 1973) at a temperature T_{KT}, where bound vortex pairs start to dissociate. Depending on the anisotropy parameter λ there exist two different types of vortices (Völkel *et al* 1991a): for $\lambda < \lambda_c \approx 0.72$ the static vortex structure is purely in-plane (hence, we call this type of vortex an 'in-plane vortex' (IPV)); however, for $\lambda > \lambda_c$ a well localized out-of-plane structure develops ('out-of-plane vortex' (OPV)).

As was shown by Völkel *et al* (1991a) the dynamics of single vortices of the two types are quite different: (i) due to their out-of-plane structure extending over a few lattice sites the OPVs 'feel' the discreteness of the underlying lattice much less than the IPVs and therefore move much more easily—this is true for both FM and AFM vortices; (ii) the out-of-plane structure of the FM OPVs acts like an effective magnetic field on the neighbouring vortices which leads to an additional gyro force between them—this is only true for FM vortices, because a (perfectly) AFM ordered structure does not yield an effective net magnetic field.

In previous papers (Mertens *et al* 1989, Gouvêa *et al* 1989, Völkel *et al* 1991b) we have investigated the contributions of the free vortices just above T_{KT} to the dynamical correlation functions for the small-λ regime for FM and AFM models. There we showed that an *ansatz* of a dilute gas of weakly interacting vortices yields central peaks (CP) which describe the results from numerical Monte Carlo–molecular dynamics (MC–MD) simulations quite well. However, most of the above mentioned materials contain only a small anisotropy, i.e. we expect them to have OPVs as non-linear excitations. In this paper we will extend our calculations to the large-λ regime and discuss the dynamical correlation functions just above T_{KT} from both analytical calculations and numerical simulations. A short comparison with experiments is also included.

The paper is organized as follows: in section 2 we will discuss the FM anisotropic Heisenberg model first by reviewing some analytic results, second by comparing these results with the numerical simulations and third by comparing with experiments. Section 3 contains the same for the AFM case. Section 4 briefly summarizes the results.

2. Ferromagnets

2.1. Some analytic results

To perform the analytic calculations we worked in the continuum limit using the angular fields $\Phi(\boldsymbol{r})$ and $\Theta(\boldsymbol{r})$, which are related to the spin field $\boldsymbol{S}(\boldsymbol{r})$ by

$$\boldsymbol{S}(\boldsymbol{r}) = (\cos\Phi(\boldsymbol{r})\cos\Theta(\boldsymbol{r}), \sin\Phi(\boldsymbol{r})\cos\Theta(\boldsymbol{r}), \sin\Theta(\boldsymbol{r})) . \tag{2.1}$$

For small temperatures the dynamics of (1.1) can be well described within a linear spin-wave theory (Holstein and Primakoff 1940). These linear excitations are characterized by the dispersion relation

$$\omega(q) = 4JS\sqrt{(1-\gamma(q))(1-\lambda\gamma(q))} \tag{2.2}$$

at $T = 0$ with $\gamma(q) = \frac{1}{2}(\cos q_x + \cos q_y)$ on a square lattice with lattice spacing $a = 1$. For the out-of-plane fluctuations this description is quite good even for larger temperatures, while in the plane the spin stiffness constant decreases to zero discontinuously at T_{KT} (Pokrovsky and Uimin 1974, Nelson and Kosterlitz 1977).

Due to the easy-plane symmetry of our model there exist also non-linear excitations, namely vortices. For $\lambda > \lambda_c$, i.e. a small anisotropy, the single static vortex shape is given by

$$\Phi = \hat{q} \arctan(y/x) \qquad \hat{q} = \pm 1, \pm 2, \dots$$
$$\Theta = \begin{cases} p(\pi/2 - c_2 r/r_v) & r \to 0 \\ pc_1\sqrt{r_v/r}\, e^{r/r_v} & r \to \infty \end{cases} \tag{2.3}$$

which has a well localized out-of-plane structure around its centre with width $r_v = \frac{1}{2}\sqrt{\lambda/(1-\lambda)}$; p denotes the sign of the z-components of the out-of-plane shape. This static structure is slightly distorted when the vortex is moving with finite velocity (Gouvêa *et al* 1989).

Assuming a dilute gas of weakly interacting vortices just above T_{KT} we can calculate their contributions to the dynamical correlation functions $S^{\alpha\alpha}(q,\omega)$, $\alpha = x, y, z$, which are mainly determined by the static structure (2.3). Considering length scales $r \gg r_v$, on which the in-plane structure acts like a sign function on the spins it is passing, we obtain for the in-plane correlations the same squared Lorentzian as in the case where $\lambda < \lambda_c$ (Mertens *et al* 1989):

$$S^{xx}(q,\omega) = (1/2\pi^2)\xi^2\gamma^3 / \left\{\omega^2 + \gamma^2[1 + (q\xi)^2]\right\}^2 \tag{2.4}$$

with width

$$\Gamma^x(q) = \left(\sqrt{2} - 1\right)^{1/2} \gamma\sqrt{1 + (q\xi)^2} \tag{2.5}$$

and integrated intensity

$$I^x(q) = (1/4\pi) / \left[1 + (q\xi)^2\right]^{3/2}. \tag{2.6}$$

Here $\gamma = \sqrt{\pi}\bar{u}/2\xi$ and the correlation length ξ and the average vortex velocity $\bar{u}$ are the two free parameters of the vortex-gas approach.

For the out-of-plane correlation function we obtain a Gaussian CP

$$S^{zz}(q,\omega) = \left(n_v/\sqrt{\pi}q\bar{u}\right) \exp[-(\omega/q\bar{u})^2]\{|f(q)|^2 + \tfrac{1}{2}(\bar{u}/[4(1-\lambda)Jq])^2\} \tag{2.7}$$

where

$$f(q) = S \int \frac{d^2 r}{(2\pi)^2} e^{iq\cdot r} \sin\Theta(r) \tag{2.8}$$

is the form factor of the static out-of-plane shape. This $|f(q)|^2$-term in $S^{zz}(q,\omega)$ is new for $\lambda > \lambda_c$ and dominates the vortex contributions to the out-of-plane correlations, while the velocity-dependent part of (2.7) is the same as in the case with $\lambda < \lambda_c$. $n_v \cong (2\xi)^{-2}$ is the density of free vortices (Bishop and Reppy 1978).

2.2. Comparison with MC–MD simulations

The results discussed above will now be compared to a combined MC–MD simulation on a 100×100 square lattice with anisotropy parameter $\lambda = 0.8$ ($> \lambda_c$). The MC algorithm is used to bring the system for a given temperature into thermal equilibrium. From these configurations we start a fourth-order Runge–Kutta method to integrate the equations of motion from which we can derive the dynamical correlation functions by Fourier transformation of the spin–spin corelations

$$S^{\alpha\alpha}(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \sum_{(i,j)} e^{i[q\cdot(r_i - r_j) - \omega t]} \langle S_i^\alpha(t)\, S_j^\alpha(0)\rangle . \tag{2.9}$$

A more detailed description of the simulation procedure is given by Wysin and Bishop (1990).

For $T < T_{KT}$ we observe only a single peak in the correlation functions which can be well identified with spin waves. Figure 5 in the paper of Mertens *et al* (1989) shows data obtained from the simulation for various temperatures. A crossover from XY-type to isotropic Heisenberg-type behaviour can be clearly seen at $q_c \cong 0.2\pi \cong \sqrt{2(1-\lambda)}$ (cf Hirakawa *et al* 1982). The bound vortex pairs cause only a renormalization of the spin-wave peaks (Kosterlitz and Thouless 1973, Côte and Griffin 1986).

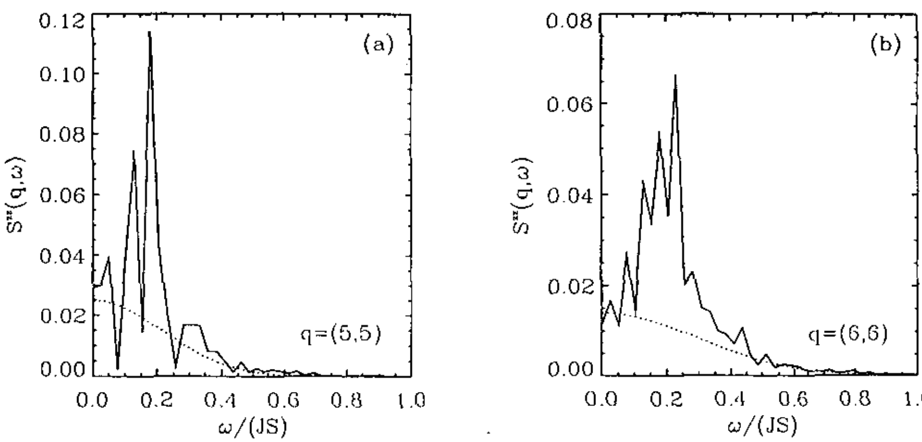

Figure 1. Out-of-plane correlation function S^{zz} for the FM model at $T = 0.85$. The dashed line is an estimate of the vortex CP.

Above T_{KT} there is still a spin-wave peak present in $S^{zz}(q,\omega)$. But now there is additional weight around $\omega \cong 0$ for small q-values (figure 1). These new contributions coincide with our expectations from the vortex-gas approach. However, from the simulation we observe no clear picture of this CP because of the strong overlap with the spin waves.

On the other hand the stiffness constant of the in-plane spin waves suffers a sudden decrease to zero above the Kosterlitz–Thouless transition temperature. Therefore we find only a single CP above T_{KT} in the planar correlations which can be well described by our free vortex-gas approach, i.e. this peak can be fitted very well to a squared Lorentzian over quite a large temperature range. An analysis

Table 1. Fitted data for the FM case. ξ_w: correlation length obtained by fitting the width. $\bar{u}$: vortex average velocity obtained by fitting the width. ξ_{int}: correlation length obtained by fitting the integrated intensity. $\bar{u}_H$: vortex average velocity obtained from (2.11) using ξ_{int}. A_{int}: amplitude obtained by fitting the integrated intensity. $A_t = \xi_{int}^2/4\pi$: theoretical amplitude of the integrated intensity.

T	ξ_w	$\bar{u}$	ξ_{int}	$\bar{u}_H$	A_{int}/A_t	A_p
0.82	12.54	0.49	4.69	0.28	0.31	0.70
0.83	10.19	0.44	3.63	0.33	0.35	0.70
0.85	6.60	0.39	2.80	0.40	0.40	0.60
0.87	5.62	0.38	2.79	0.40	0.37	0.63
0.90	9.53	0.47	2.03	0.49	0.46	0.51
0.95	4.32	0.43	1.72	0.54	0.45	0.40

of the width obtained in this way and the integrated intensity using equation (2.5) and equation (2.6) gives us values for the parameters ξ and $\bar{u}$ which are listed in table 1. We find, as in the previous cases (Mertens *et al* 1989, Völkel *et al* 1991b), a difference in the absolute values of the correlation length, depending on whether it was fitted from the width (ξ_w) or from the intensity (ξ_{int}). In addition, there is a quantitative difference for large temperatures: ξ_{int} agrees with the Kosterlitz–Thouless (KT) formula (Kosterlitz and Thouless 1973),

$$\xi(T) = \xi_0 \exp\left(b/\sqrt{T/T_{KT} - 1}\right) \tag{2.10}$$

quite well over the whole temperature range under consideration with $T_{KT} = 0.79$ and $b \cong 0.28$ (this b-value is very small compared to the prediction of KT. However, their result is only valid at $T = T_{KT}$, while for larger temperatures this parameter is slightly T-dependent (Heinecamp and Pelcovitz 1985) and only about 0.5 even for $\lambda = 0$), but we find an agreement of ξ_w with (2.10) only for $0.82 \lesssim T \lesssim 0.87$ (with $b = 0.59$); above $T \approx 0.87$ ξ_w jumps to a larger value. This change in ξ_w for a temperature above T_{KT} is expected (Hirakawa *et al* 1982) and indicates a crossover from the XY-like to a more isotropic Heisenberg behaviour of the system. This crossover can also be seen in the average vortex velocity $\bar{u}$ which suddenly jumps to larger values above $T \cong 0.87$. In the range $0.82 \lesssim T \lesssim 0.87$ the fitted $\bar{u}$ is decreasing with increasing temperature (table 1). The only available theory we can compare these values with is from Huber (1982) who obtained for the vortex velocity

$$\bar{u}_H = (1/2\xi)\sqrt{(\pi/2)\ln(4\xi^2 T_{KT})} \tag{2.11}$$

by assuming a dilute gas of freely moving vortices which interact via an attractive or repulsive force

$$\boldsymbol{F} \propto \hat{q}_1 \hat{q}_2 (\boldsymbol{r}_1 - \boldsymbol{r}_2)/|\boldsymbol{r}_1 - \boldsymbol{r}_2|^2 \tag{2.12}$$

and the gyro force (caused by the static out-of-plane shape)

$$\boldsymbol{G} \propto \hat{q} p \boldsymbol{e}_z . \tag{2.13}$$

If we insert ξ_{int} into equation (2.11) we obtain values for $\bar{u}$ which reproduce the fitted data quite well for $0.85 \lesssim T \lesssim 0.87$, but near the phase transition $\bar{u}$ is decreasing which is just the opposite behaviour to that observed in the simulation data.

From table 1 we also see that the ratio of the simulated amplitude of $I^x(q)$ is only about 0.4 times the expected value of $\xi^2/4\pi$. So far we have considered only the freely moving vortices in our calculations of the in-plane correlation function. A straightforward extension is to include the out-of-plane fluctuations in a perturbative way (appendix A). The first-order corrections only renormalize the amplitude of the CP

$$S^{xx}_{\mathrm{new}}(q,\omega) = S^{xx}(q,\omega)\{1 - \pi/(2\xi)^2[1 + (\bar{u}/4(1+\lambda))\ln\xi] - (T/2\pi)K(\lambda)\} = S^{xx}(q,\omega)A_p \tag{2.14}$$

and correspondingly the integrated intensity $I^x(q) = \int_{-\infty}^{+\infty} \mathrm{d}\omega\, S^{xx}(q,\omega)$. The first deviation from the old result on the right-hand side of (2.14) is due to the out-of-plane vortex shape and the second one is due to harmonic out-of-plane spin waves; $K(\lambda)$ is the complete elliptic integral of the first kind. These corrections can only partly account for the decrease of the amplitude (cf table 1), however, harmonic spin waves are a crude approximation for temperatures above T_{KT} (Menezes *et al* 1991). The second-order perturbations also change the width of the CP, but their influence is much too weak to change any of the parameters, which we obtained by using the unperturbed analytical results, in such a way that the data fitted from the width and intensity become more consistent (and even a more advanced spin-wave technique does not seem to improve this result).

We therefore conclude that because of the presence of vortex pairs (and clusters) and in-plane spin waves at higher q-values we obtain not the parameters due to our vortex-gas *ansatz*, but rather properly renormalized values of ξ and $\bar{u}$.

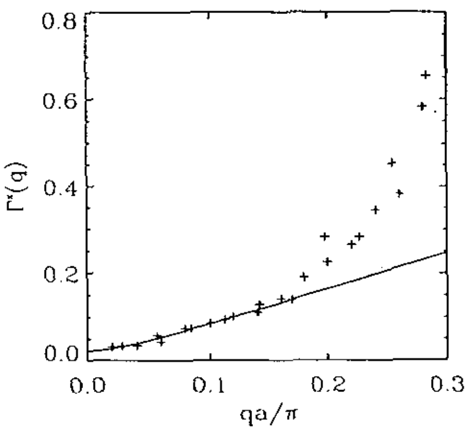

Figure 2. Width $\Gamma^x(q)$ of the in-plane correlation function of the FM model at $T = 0.83$; +: data from fitting S^{xx}; solid line: fit for small q to (2.5).

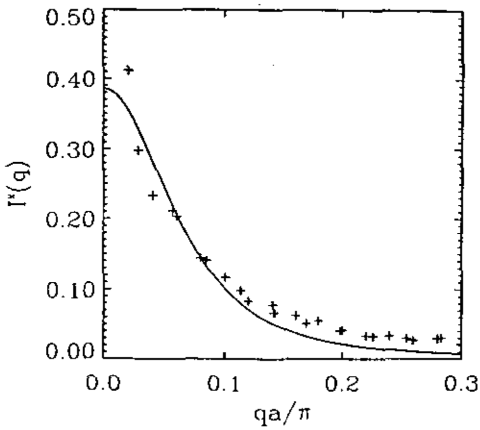

Figure 3. Integrated intensity $I^x(q)$ of the in-plane correlation function of the FM model at $T = 0.83$; +: data from fitting S^{xx}; solid line: fit for small q to (2.6).

If we examine the width $\Gamma^x(q)$ we also find a well-defined crossover in q-space from the XY-like to the isotropic Heisenberg behaviour (figure 2). Below a certain q-value we can fit the width very well with the function (2.5), while above this wave vector it has a much steeper slope. This 'critical' q is a little smaller than that for the spin waves. The crossover also occurs in the data of the integrated intensity. However, here the change in the functional behaviour of $I^x(q)$ is much smoother and hard to see by eye (figure 3) – but a fit of these data with equation (2.6) shows a change in the fit parameter, if we include data at higher q-values.

2.3. Comparison with experiments

A good representative of 2D FMs with easy-plane symmetry is K_2CuF_4 (Hirakawa *et al* 1982). Here the magnetic planes interact via a small exchange coupling $J' \approx 6.7 \times 10^{-4}$ J which becomes dominant at low temperatures leading to 3D ordering below a critical $T_c = 6.25$ K. The KT phase transition occurs just below T_c. However, there is still a temperature range above T_c where the system displays mainly XY-like behaviour, although the easy-plane anisotropy is very small for this material ($1 - \lambda = 0.01$ and $\lambda = 1$ denotes the isotropic limit). Regnault *et al* (1989) performed a neutron-scattering study of the *static* properties of K_2CuF_4 in the vicinity of the phase transition and found a good agreement with the KT theory just above T_c. The crossover to isotropic behaviour occurs at a temperature T_{c1} where $\xi(T_{c1}) \cong (1-\lambda)^{-1/2}$. In our model this gives a $\xi(T_{c1}) \approx 2.24$ corresponding to a temperature $T_{c1} \gtrsim 0.87$, if we compare with ξ_{int} (which makes sense, because this was fitted from the integrated intensity which is also a *static* quantity).

Wiesler *et al* (1989) performed measurements of the dynamical correlation function on $CoCl_2$ intercalated graphite which is another example of a 2D FM with easy-plane symmetry. The anisotropy here is of intermediate size ($1 - \lambda = 0.44$) and we expect that only fast moving vortices develop the well localized out-of-plane structure (2.3). On the other hand this is the only material on which the dynamical correlation function was explicitly measured. Wiesler *et al* (1989) could fit the measured CPs well to a squared Lorentzian above T_{KT} (≈ 9.6 K). However, for temperatures just above the phase transition they found an additional contribution to the CP which is sharp in ω-space, but broad in q-space, and which they suggest is a result of the pinning of vortices by defects or different spin diffusion time scales. If we translate their system parameters into our units we find that the temperature regime from 0.82 to 0.99, for which they observe the additional CP-contribution, is just the range where we expect the XY-like behaviour, while at $T_{c1} \approx 0.99$ we obtain $\xi_{int} \approx 1.50 \cong (1-\lambda)^{-1/2}$ for $\lambda = 0.56$ by extrapolating our data. This agrees very well with the crossover condition to isotropic behaviour suggested by Hirakawa *et al* (1982). Because we also observe these deviations from our vortex-gas results in the numerical simulations, where we have no defects, we conclude that the pinning effects do not alone explain this modified CP.

3. Antiferromagnets

The analytic approach for calculating the vortex contributions to the dynamical correlation functions in the AFM model is similar to the FM case (Gouvêa *et al* 1989, Völkel *et al* 1991b). In contrast, here the static structure is (on a local scale) perfectly AFM ordered, thus leading to peaks centred around $q = (\pi, \pi)$, while the deviations of this structure due to a finite velocity are (on a local scale) FM ordered and therefore give contributions near $q = (0, 0)$. Using an equivalent vortex-gas *ansatz* as explained in the last section we end up with the same squared Lorentzian CP for the in-plane correlation function (cf equation (2.4)), but here centred at the AFM Bragg point. The out-of-plane correlations also show a similar form as in (2.7). From the velocity induced z-components we obtain a contribution $\propto (\bar{u}/[4(1+\lambda)Jq])^2$. The main contribution, however, comes from the static out-of-plane structure with the same form factor $f(q)$ as in (2.8), but now centred at $q = (\pi, \pi)$. Because both parts are

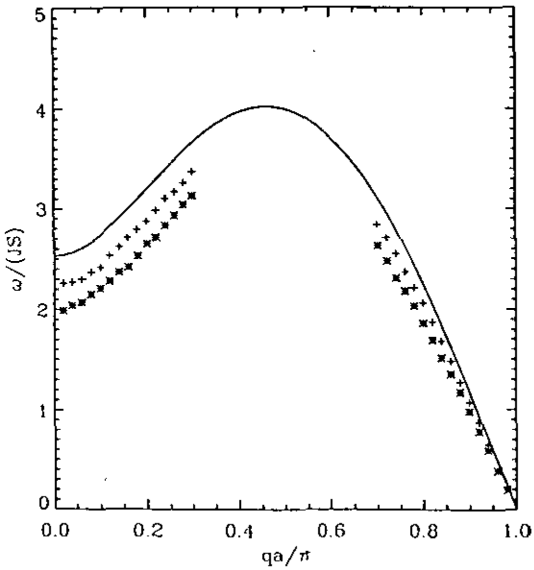

Figure 4. Spin-wave dispersion $\omega_2(q)$ along the (q,q) direction for $\lambda = 0.8$; $+$, $*$: simulation data obtained from the in-plane correlation function for $T = 0.3$ and $T = 0.5$, respectively; solid line: linear spin-wave theory for $T = 0$. The data are plotted in an extended zone scheme to emphasize the fact that one observes only a single spin-wave peak in the in-plane correlation function (2.4) for a given q-value. The data from the out-of-plane correlations show the same result within numerical accuracy, but following the ω_1-dispersion.

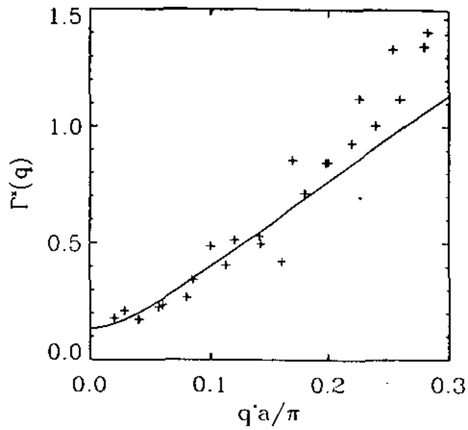

Figure 5. Width $\Gamma^x(q)$ of the in-plane correlation function of the AFM model with $\lambda = 0.8$ at $T = 0.85$; $+$: data from fitting S^{xx}; solid line: fit for small q to (2.5).

multiplied by the same Gaussian function, the width of which is increasing with q, the combined peak has its maximum intensity, but also its maximum width, at $q = (\pi, \pi)$.

Below T_{KT} (≈ 0.79) we observe only spin waves, and, because of the symmetry of the two dispersion branches (Völkel *et al* 1991b)

$$\omega_{1,2}(q) = 4JS\sqrt{(1 \mp \gamma(q))(1 \pm \lambda\gamma(q))}, \tag{3.1}$$

we find only one spin-wave peak in each of the two different correlation functions (figure 4). Above T_{KT} there is again a strong overlap of spin-wave and vortex contributions in $S^{zz}(q,\omega)$. In $S^{xx}(q,\omega)$, due to the sudden softening of the spin stiffness constant, only a CP at $q = (\pi, \pi)$ can be found†. Fitting this peak to our theoretical prediction provides us with values for the correlation length and the vortex average velocity (table 2). Again the values of ξ_{int} for various temperatures show no significant deviations from the KT prediction (2.10), while there seems to be a 'soft' change in the functional form of $\xi_w(T)$ at $T_{cl} \lesssim 0.9$, where $\xi_{int}(T_{cl}) \gtrsim 2.24 \cong (1-\lambda)^{-1/2}$. We also observe no sudden deviation of the fitted width from our theory for a certain q, as happened in the FM case (figure 5). This softening of the two crossovers

† There is also a CP around $q = (0, 0)$ basically caused by the small motion-induced deviations from the static in-plane structure, but this peak has a very small intensity compared to the peak at $q = (\pi, \pi)$ and is hard to investigate.

Table 2. Fitted data for the AFM case. ξ_w: correlation length obtained by fitting the width. $\bar{u}$: vortex average velocity obtained by fitting the width. ξ_{int}: correlation length obtained by fitting the integrated intensity. A_{int}: amplitude obtained by fitting the integrated intensity. $A_t = \xi_{int}^2/4\pi$: theoretical amplitude of the integrated intensity.

T	ξ_w	$\bar{u}$	ξ_{int}	A_{int}/A_t
0.83	7.53	1.00	3.46	0.39
0.85	6.87	1.23	3.29	0.38
0.87	3.75	0.93	2.91	0.37
0.90	3.74	1.05	2.25	0.42
1.00	2.26	0.93	1.56	0.52

from XY-like to isotropic Heisenberg behaviour is probably caused by the presence of the additional spin-wave branch and consequent bigger fluctuations in space.

As for the small-λ case (Völkel *et al* 1991b), we find quite a large vortex velocity (about twice as large as in the FM case) and this appears to be constant in the temperature range under consideration‡. This possibly reflects the different dynamic behaviour of the AFM vortices compared to the FM ones. A microscopic theory for $\bar{u}$ for the AFM is not available as far as we are aware.

A good candidate for a 2D easy-plane AFM is $BaNi_2(PO_4)_2$, which can be well described by the Hamiltonian (Regnault *et al* 1990)

$$H = J\sum_{(i,j)} S_i \cdot S_j + D\sum_i (S_i^z)^2 \tag{3.2}$$

with $J = 11K$, $D = 7.3K$, and $S = 1$. Though here the XY-anisotropy is caused by an on-site interaction of the z-components of the spins we find the same dynamical behaviour as in the model described by (1.1), but with slightly modified parameters (appendix B); and for $D > D_c \approx 0.5J$ we again expect OVPs as non-linear excitations.

Both neutron-scattering studies (Regnault *et al* 1989) and NMR experiments (Gaveau *et al* 1991) on $BaNi_2(PO_4)_2$ are presented. For the resonance experiment an external magnetic field was applied, but we do not expect it to change the vortex dynamics significantly as long as it is weak and is directed perpendicular to the easy-plane. The nuclear spin relaxation time T_1 is, after some aproximations, inversely proportional to $\int d^2q\, S^{xx}(q,\omega_N)$, where ω_N is the nuclear Larmor frequency. This is small compared to the typical (electronic) spin fluctuations in this material and thus

$$1/T_1 \propto 1/\gamma = 2\xi/(\sqrt{\pi}\bar{u}). \tag{3.3}$$

After expressing ξ and $\bar{u}$ by equations (2.10) and (2.11), respectively, the experimental data are fitted very well by (3.3) with $b = 0.95$. It is interesting to note that here the Huber formula for the vortex average velocity seems to fit the data quite well, although it was obtained for the FM case where the additional gyro force between the vortices was present. On the other hand, in this case we have the external field which is applied perpendicular to the easy planes, thus causing the system to develop a net magnetization in the z-direction, with the magnitudes of the z-components of the spins depending on where the spins are located relative to the vortex centres.

Neutron scattering was used to explicitly probe the dynamical correlation function $S^{xx}(q,\omega)$. Above T_{KT} a CP was clearly detected. However, this was better fitted by

‡ These data were obtained by fitting the width for $0 \leqslant q^* \leqslant 0.1\pi$. If we expand the fit to higher values of q^*, then we obtain larger values for $\bar{u}$, and for a fit in the range $0 \leqslant q^* \lesssim 0.17\pi$ we find $\bar{u} \cong 2.0$ (Völkel *et al* 1991b).

a Lorentzian rather than the squared Lorentzian (2.4). With a second experiment, using the neutron-spin echo technique (Regnault *et al* 1989), the local, time-dependent correlation function

$$S^{xx}(r = 0, t) \propto \exp(-\gamma t) \tag{3.4}$$

was measured. The investigation of these data yielded two time scales corresponding to 2D and 3D fluctuations (as expected for temperatures just above the 3D ordering). After separating the contributions of the 3D fluctuations, Regnault *et al* (1989) obtained quite large values for γ which account for a vortex average velocity of $1.5 \ldots 2.0\bar{u}$, where $\bar{u}$ corresponds to the simulation data of table 2. However, this method yields data integrated over the whole q space, including large values of q^*, where our approach is no longer valid. If we use a larger q^*-range for our fitting procedure we obtain values of $\bar{u}$ which are comparable to the results of Regnault *et al* (1989, see footnote ‡).

Another approach to explain the spin dynamics of $BaNi_2(PO_4)_2$ was made by Boucher *et al* (1992) in a recent paper. Those authors extended methods to the two-dimensional easy-plane Heisenberg AFM which were previously used for the one-dimensional AFM chain (Mikeska 1980, Maki 1981) and which can describe both a ballistic and a diffusive vortex motion. Boucher *et al* conclude that at small values of q^* the vortex dynamics become more ballistic. This result is based (i) on the fact that they could fit the CP in $S^{xx}(q, \omega)$ at small q^* better with a Lorentzian (rather than a squared Lorentzian) as expected from a diffusive vortex dynamics, and (ii) on the good agreement of the 'diffusive vortex average velocity' for small q^* and the 'ballistic vortex average velocity' for larger q^*.

4. Conclusions

In the present paper we have investigated the dynamical correlations in 2D Heisenberg magnets with weak easy-plane symmetry. In these systems there are, in addition to extended small-amplitude excitations (i.e. spin waves), also localized excitations (vortices) present which undergo a KT-like phase transition. We have focused our attention on the temperature range just above the transition temperature T_{KT}. Here we have found CPs as contributions from the vortices to the dynamical correlation functions by using an *ansatz* of a dilute gas of weakly interacting vortices.

A comparison of the FM model with MC–MD simulations shows that our phenomenological approach describes the static properties, e.g., the integrated intensity, quite well. However, the parameters ξ and $\bar{u}$ fitted from the width of the in-plane CP (which reflects the dynamics of the system) show significant deviations from our expectations, i.e. $\xi_w > \xi_{int}$, though ξ_w also fits to the KT formula (2.10), and $\bar{u}$ is increasing with decreasing temperature (above T_{KT})—this is just the opposite behaviour to that predicted by equation (2.11). A perturbative calculation shows that the interactions of the out-of-plane fluctuations with the in-plane vortex structure cannot explain these deviations. Our numerical results also agree with experimental results on K_2CuF_4 and $CoCl_2$ intercalated graphite compounds. Thus a more advanced *ansatz* for the vortex dynamics, including, e.g., interactions of freely moving vortices with vortex pairs (clusters) and in-plane spin waves at higher q-values, is necessary to properly describe the CPs in the *dynamical* correlation functions. However, from our fits of the numerical data to the present analytic results we suspect that this improved *ansatz* will lead only to a renormalization of the parameters ξ and $\bar{u}$, rather than a change in the functional form of the CP in $S^{xx}(q,\omega)$.

We find a similar behaviour in the AFM model. But here the vortex average velocity is much higher than in the FM case and roughly constant in the whole temperature range under consideration. This probably reflects the different dynamics in this system: (i) here the vortices interact only via the central force (2.12), while there is no additional gyro force as in the FM case; and (ii) there is a second spin-wave branch which results in extra interactions with the vortices.

In both systems we observe a crossover from XY-like to isotropic Heisenberg behaviour at a temperature $T_{c1} \approx (1-\lambda)^{-1/2}$ and at $q_{c1} \approx 0.167\pi < \sqrt{2(1-\lambda)}$. These crossovers are much smoother in the AFM case due to the additional spin-wave branch. In real systems there is usually also a small coupling between the magnetic planes present which leads to a 3D ordering just above the KT phase transition. XY-like behaviour can therefore only be observed in a certain temperature range above the phase transition and this range becomes smaller for weaker anisotropies.

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Appendix A.

To include out-of-plane fluctuations in the calculations of the in-plane correlation function for the FM case we make the *ansatz* (cf Menezes *et al* 1991)

$$\begin{aligned} \Phi(\boldsymbol{r}) &= \Phi_{\mathrm{v}}(\boldsymbol{r}) \\ \Theta(\boldsymbol{r}) &= \Theta_{\mathrm{v}}(\boldsymbol{r}) + \Theta_{\mathrm{s}}(\boldsymbol{r}) \end{aligned} \tag{A1}$$

where the index v (s) denotes the vortex (spin-wave) part of the angle fields. From the in-plane vortex structure we still consider only the effect of spin flips, thus we can separate the Φ from the Θ correlations. We therefore find for the dynamical in-plane correlation function

$$\begin{aligned} \tilde{S}^{xx}(\boldsymbol{r},t) &= \langle \cos\Phi(\boldsymbol{r},t)\cos\Theta(\boldsymbol{r},t)\cos\Phi(0)\cos\Theta(0)\rangle \\ &\cong \langle \cos\Phi(\boldsymbol{r},t)\cos\Phi(0)\rangle\langle \cos\Theta_{\mathrm{v}}(\boldsymbol{r},t)\cos\Theta_{\mathrm{v}}(0)\cos\Theta_{\mathrm{s}}(\boldsymbol{r},t)\cos\Theta_{\mathrm{s}}(0) \\ &+ \sin\Theta_{\mathrm{v}}(\boldsymbol{r},t)\sin\Theta_{\mathrm{v}}(0)\sin\Theta_{\mathrm{s}}(\boldsymbol{r},t)\sin\Theta_{\mathrm{s}}(0)\rangle . \end{aligned} \tag{A2}$$

In a further approximation we also decouple the correlations of Θ_{v} and Θ_{s}. Moreover, we assume that $\Theta(\boldsymbol{r}) \ll 1$ which is always true for Θ_{s}, but also for Θ_{v} for $r \gg r_{\mathrm{v}}$, and finally arrive at

$$\begin{aligned} \tilde{S}^{xx}(\boldsymbol{r},t) \cong \langle \cos\Phi(\boldsymbol{r},t)\cos\Phi(0)\rangle \{ 1 &- \langle\Theta_{\mathrm{v}}^2\rangle - \langle\Theta_{\mathrm{s}}^2\rangle \\ &+ \tfrac{1}{12}\left(\langle\Theta_{\mathrm{v}}^4\rangle + \langle\Theta_{\mathrm{s}}^4\rangle\right) + \langle\Theta_{\mathrm{v}}^2\rangle\langle\Theta_{\mathrm{s}}^2\rangle + \tfrac{1}{4}\langle\left(\Theta_{\mathrm{v}}^2(\boldsymbol{r},t)\Theta_{\mathrm{v}}^2(0)\right)^2\rangle \\ &+ \tfrac{1}{4}\langle\left(\Theta_{\mathrm{s}}^2(\boldsymbol{r},t)\Theta_{\mathrm{s}}^2(0)\right)^2\rangle + \langle\Theta_{\mathrm{v}}^2(\boldsymbol{r},t)\Theta_{\mathrm{v}}^2(0)\rangle\langle\Theta_{\mathrm{s}}^2(\boldsymbol{r},t)\Theta_{\mathrm{s}}^2(0)\rangle + \ldots \} . \end{aligned} \tag{A3}$$

Appendix B.

Using the same *ansatz* for the angle fields as proposed in an earlier paper (Völkel *et al* 1991b) we derive similar equations of motion from equation (3.2) as for the model described by (1.1). With a proper renormalization of the length scale we obtain the same unitless differential equations leading us to the following vortex structure up to first order in the velocity u

$$\begin{aligned}
\Phi(\boldsymbol{r}) &= \hat{q}\arctan(y/x) + \Phi_c \\
\Theta(\boldsymbol{r}) &= p\begin{cases} \pi/2 - c_3 r/r_v & r \to 0 \\ c_4\sqrt{r_v/r}\,\mathrm{e}^{-r/r_v} & r \to \infty \end{cases} \\
\phi(\boldsymbol{r}) &= (u/JS)\cos(\varphi-\epsilon)\begin{cases} r/2 & r \to 0 \\ [pc_4 r_v/(8r_v^2+1)]\sqrt{r_v/r}\,\mathrm{e}^{-r/r_v} & r \to \infty \end{cases} \\
\theta(\boldsymbol{r}) &= (u\hat{q}/JS)\sin(\varphi-\epsilon)\begin{cases} (c_3/r_v)r^2 & r \to 0 \\ -[r_v/(8r_v^2+1)]r_v/r & r \to \infty. \end{cases}
\end{aligned} \tag{B1}$$

with the vortex core radius $r_v = 1/\sqrt{2D/J}$.

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