

## How vortices produce central peaks in the dynamic form factor of the 2-d anisotropic Heisenberg model

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The Kosterlitz-Thouless phase transition in the XY-model is caused by the unbinding of vortex-antivortex pairs. We consider a gas of freely moving vortices and show that the dynamic structure function exhibits a central peak for the in-plane as well as for the out-of-plane correlations. However, the mechanism producing these peaks is quite different in the two cases. The wavevector and temperature dependencies of the peaks agree with the results of a combined Monte Carlo-molecular Dynamics simulation as well as with recent neutron scattering experiments on two-dimensional easy-plane magnets.

### I. INTRODUCTION

In the last years magnetic materials like  $\text{Rb}_2\text{CrCl}_4$ ,  $\text{K}_2\text{CuF}_4$ ... or  $\text{BaCo}_2(\text{AsO}_4)_2$ ,  $\text{BaNi}_2(\text{PO}_4)_2$ ... have been produced, in which the magnetic ions are situated within planes. The measurement of spin-wave dispersion curves has shown that the intraplane coupling constants are by a factor of about  $10^3$  to  $10^6$  larger than the interplane coupling constants; this means that these materials are quasi two-dimensional concerning their magnetic properties.

The simplest classical model Hamiltonian for these systems has the form

$$H = -J \sum_{m,n} (S_x^m S_x^n + S_y^m S_y^n + \lambda S_z^m S_z^n) \quad (1.1)$$

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Here  $S_x^m$  is the x-component of the spin  $\vec{S}$  at the lattice site  $m$ ; all lattice sites lie in the xy-plane. For  $0 \leq \lambda < 1$  this is the 2-dimensional anisotropic Heisenberg model. The case  $\lambda = 0$  is called the XY-model; this should not be confused with the planar model, where the spins are confined to the xy-plane. For the above mentioned materials  $\lambda$  is in the range 0.4 to 0.99.

In two dimensions there is no spontaneous magnetization because every long-range order is destroyed by the spin waves (Mermin-Wagner theorem). Nevertheless there is a (topological) phase transition, predicted by Kosterlitz and Thouless (KT) (1). The idea is that below a transition temperature  $T_c$  there are vortices and anti-vortices which are bound in pairs, above  $T_c$  they become free.

For the static correlation function  $S_{xx}(r)$  the KT-theory predicts a power law below  $T_c$  and an exponential decay  $r^{-1/2} \exp(-r/\xi)$  above  $T_c$ , where the correlation length  $\xi$  has the form

$$\xi = \xi_0 \exp(b/\sqrt{\tau}) \quad \tau = (T - T_c)/T_c \quad (1.2)$$

$\xi_0$  is supposed to be in the order of the lattice constant  $a$ , and  $b \approx 1.3$ . However, more refined studies(2) have revealed that  $b$  is rather strongly temperature dependent.

The predicted form of the static correlations has been verified both by Monte Carlo simulations(3, 4) and by quasi-elastic neutron scattering experiments(5, 6). Thereby the existence of vortices has been proven indirectly.

However, direct evidence for the vortices can be expected from a study of the dynamic correlations. Recently some preliminary results from Molecular Dynamics simulations(7) and from inelastic neutron scattering(5, 8) have been published, which both show "central peak" structures in the dynamic structure function above  $T_c$ . The purpose of this paper is to study how these structures possibly are produced by free vortices.

So far, the dynamics is well known only for the spin waves(9), including renormalization effects by the vortex pairs(10). The only work on single vortices is that of Huber(11), who calculated several autocorrelation functions. However, this means that his dynamic struc-

ture functions have no wavevector dependence. Moreover, some of his results now seem to be questionable (see below).

## II. OUT-OF-PLANE CORRELATIONS

In a continuum approximation vortex spin configuration have the form(12)

$$\phi = \tan^{-1}(y/x)$$

$$v = \begin{cases} \pi [1 - \exp(-r/r_v)] & r \gg r_v \\ 0 & r \rightarrow 0 \end{cases} \quad (2.2)$$

where  $S_x = S \cos \phi \cdot \sin v$ ,  $S_z = S \cos v$ ,  $r^2 = x^2 + y^2$ , and

$$r_v = a [2(1 - \lambda)]^{1/2} \quad (2.3)$$

is a vortex core radius.

In contrast to  $S_x$  and  $S_y$  (see next section) the out-of-plane component  $S_z(\vec{r}, t)$  is localized which means that it has a spatial Fourier transform. Therefore we first consider the out-of-plane correlation function  $S_{zz}(\vec{r}, t) = \langle S_z(\vec{r}, t) \cdot S_z(\vec{0}, 0) \rangle$ .

We assume that an arbitrary field configuration can be represented by a sum of spin-wave and vortex contributions and that above  $T_c$  the latter is essentially produced by a gas of  $N_v$  free vortices with positions  $\vec{R}_v$  and velocities  $\vec{v}_v$ :

$$S_z(\vec{r}, t) \approx \sum_{v=1}^{N_v} \cos v (\vec{r} - \vec{R}_v - \vec{v}_v t) \quad (2.4)$$

Here, only incoherent scattering from independent vortices is considered.

Now the thermal average can be performed by integration over  $\vec{R}_V$  and  $\vec{v}_V$ , where we assume a Maxwellian velocity distribution. The calculation is straight-forward and gives for the Fourier transform

$$S_{ZZ}(\vec{q}, \omega) = \frac{S^2}{4\pi^{5/2}} \frac{n_V}{\bar{v}} \frac{|f(q)|^2}{q} \exp\left[-\frac{\omega^2}{(\bar{v}q)^2}\right], \quad (2.5)$$

which shows a Gaussian central peak. The vortex form factor  $f(q)$  is the Fourier transform of  $\cos v(r)$ ; we evaluate it approximately by extending the asymptotic solution in (2.2) to small  $r$  and by expanding about  $v = \pi/2$  up to the first order. This gives

$$f(q) = \frac{\pi^2 r_V^2}{[1 + (r_V q)^2]^{3/2}}, \quad qr_V \ll 1, \quad (2.6)$$

Apart from  $r_V$  there are only two other relevant parameters: the rms velocity  $\bar{v}$  and the correlation length  $\xi$  which appears in the density of free vortices  $n_V = \xi^{-2}$ .

Since we have made a phenomenological theory our predictions must be tested and the parameters must be determined. We have just learned(13) that a central peak has in fact been observed in  $S_{ZZ}(\vec{q}, \omega)$  for  $\text{Rb}_2\text{CrCl}_4$ , but we do not yet know any details. Therefore we compare with our Monte Carlo-Molecular Dynamics (MC-MD) simulations of a  $100 \times 100$  spin lattice. We have chosen the XY-limit  $\lambda = 0$  which should be representative for all  $\lambda$ -values up to about 0.7 because  $T_c$  and the static correlations depend only very weakly on  $\lambda$  in this regime (12, 14).<sup>1</sup> Below  $T_c$  ( $\approx 0.83$  in units of  $J/k_B$ ) there is only a spin-wave component. This is softened above  $T_c$ , but an additional central peak appears (Fig. 1).

From (2.5) we expect a width  $\Gamma'_Z = \bar{v} \cdot q$ . This linear prediction is in fact very well supported by the data (Fig. 2a). The rms velocity practically is a constant ( $\bar{v} \approx 1.6$  in units where  $J = \hbar = S = 1$ ) for  $0.9 \leq T \leq 1.1$ . (More closely to  $T_c$  the central peak is too weak to be

1. Extreme cases, like  $\lambda = 0.99$ , will be considered in a subsequent paper.

measured accurately). This behavior agrees qualitatively with a result of Huber(11) who calculated

$$\bar{v} = (\pi b)^{1/2} \frac{JS^2 a^2}{\hbar} (n_V)^{1/2} \tau^{-1/4} \quad (2.7)$$

from an equation of motion for free vortices, namely (2.7) shows a saturation as  $T \rightarrow 1.2$ . Even the numbers for  $\bar{v}$  are not too far off:  $\bar{v} = 0.74$  for  $T=1.0$ , with  $b \approx 0.3$  for this temperature(2), and  $\xi_0 = a$ . Since for  $\xi_0$  only the order of magnitude is known,  $\bar{v}$  could be fitted easily to the observed value of 1.6. On the other hand, this value is an upper limit because  $\Gamma_z$  might have been overestimated from plots like Fig. 1(b).

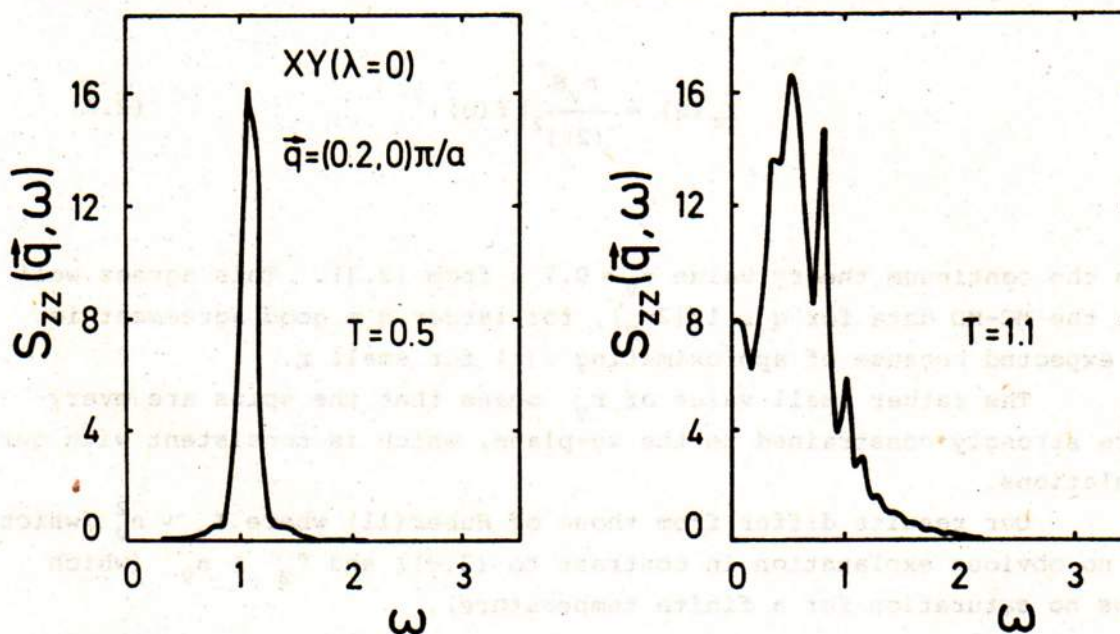


Figure 1. Dynamic form factor for out-of-plane correlations from a combined Monte Carlo-Molecular-Dynamics simulation of a  $100 \times 100$  lattice. (a) temperature  $T > T_c \approx 0.83$ , (b)  $T > T_c$ .

