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# DYNAMICS OF UNBOUND VORTICES IN THE 2-DIMENSIONAL $XY$ AND ANISOTROPIC HEISENBERG MODELS

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**Abstract.** – Assuming an ideal gas of vortices above the Kosterlitz-Thouless transition temperature, the dynamic form factors are calculated. For the in-plane correlations a Lorentzian central peak is predicted which is independent of the vortex size and shape. However, for the out-of-plane correlations the velocity dependence of the vortex structure is decisive for the occurrence of a Gaussian central peak. Both results are in good agreement with combined Monte Carlo-molecular dynamics simulations.

## 1. Introduction

Quasi-two-dimensional magnetic materials with easy-plane symmetry, e.g. $Rb_2CrCl_4$ or $BaCo_2(AsO_4)_2$, have been studied recently both by inelastic neutron scattering experiments [1, 2, 8] and by a phenomenological theory for the *dynamic* correlations [3]. In this theory the anisotropic Heisenberg model with nearest-neighbor interactions

$$H = -J \sum_{m,n} \left[ S_x^m S_x^n + S_y^m S_y^n + \lambda S_z^m S_z^n \right] \qquad (1.1)$$

is considered, where $\mathbf{S}^m$ is a classical spin vector and $0 \leq \lambda < 1$; $\lambda = 0$ corresponds to the $XY$-model.

At a critical temperature $T_c(\lambda)$ Monte Carlo (MC) data [5] show a Kosterlitz-Thouless phase transition. Above $T_c$ a part of the vortex-antivortex pairs unbind and the unbound vortices are in motion due to their interactions. Assuming that the positions are random locally, the velocity distribution is Gaussian [4], therefore the unbound vortices can be treated phenomenologically as an ideal gas, in the same spirit as the soliton-gas approach for 1-d magnets.

The correlations for the in-plane components $S_x$ or $S_y$ are quite distinct from those for the out-of-plane component $S_z$. We show here that the *velocity dependence* of the vortex structure is decisive for the out-of-plane correlations, in contrast to reference [3] where only the static structure has been considered.

## 2. In-plane correlations

We use a continuum description and spherical coordinates for the spin configuration

$$\mathbf{S}(\mathbf{r},t) = S\,(\cos\phi \sin\theta,\ \sin\phi\sin\theta,\ \cos\theta) \qquad (2.1)$$

where $\mathbf{r} = (x,y)$. The equations of motion have *two static* vortex or antivortex solutions [6] $\phi(\mathbf{r}) = \pm\tan^{-1}(y/x)$. Molecular dynamics (MD) simulations have shown [6] that for $0 \leq \lambda \lesssim 0.7$ only a planar solution $\theta(\mathbf{r}) \equiv \pi/2$ is stable, whereas for $\lambda \gtrsim 0.8$ only a solution which has an out-of-plane structure $\theta(\mathbf{r}) \neq \pi/2$ is stable; only the former case is considered here.

$S_x$ and $S_y$ are *not localized*, i.e. they have no spatial Fourier transform. Therefore the in-plane correlation function $S_{xx}(\mathbf{r},t) = \langle S_x(\mathbf{r},t)\, S_x(\mathbf{0},0)\rangle$ is only *globally* sensitive to the presence of vortices. Thus the characteristic length is the average vortex-vortex separation $2\,\xi$, where $\xi$ is the Kosterlitz-Thouless correlation length.

When a planar vortex starts moving it develops an out-of-plane structure (see next section). However, for $S_{xx}(\mathbf{r},t)$ this is not important because the dominant effect of moving vortices is to act like "2-d sign functions" or "2-d kinks", i.e; every vortex that passes with its center between $\mathbf{0}$ and $\mathbf{r}$ in time $t$ diminishes the correlations, changing $\cos\phi$ by a factor of $(-1)$, independent of the direction of movement and independent of the internal structure of the vortex [3].

The detailed calculation of $S_{xx}(\mathbf{r},t)$ is published elsewhere [4] and gives a (squared) Lorentzian central peak for the dynamic form factor

$$S_{xx}(\mathbf{q},\omega) = \frac{S^2}{2\pi^2} \frac{\gamma^3\xi^2}{\left\{\omega^2 + \gamma^2\left[1 + (\xi q)^2\right]\right\}^2} \qquad (2.2)$$

with $\gamma = \sqrt{\pi}\bar{u}/(2\xi)$. Here $\bar{u}$ is the rms velocity of the vortices which can be taken from Huber [7] who calculated the velocity auto-correlation function. The central peak (2.2) is in excellent agreement with data obtained from combined MC-MD simulations [4]. Moreover there is a qualitative agreement with the above mentioned neutron scattering experiments 1, 2].

## 3. Out-of-plane correlations

$S_z(\mathbf{r},t)$ is *localized* for a single vortex, therefore correlations are sensitive to the vortex size and structure. We assume a dilute gas of $N_v$ unbound vortices with positions $\mathbf{R}_i$ and velocities $\mathbf{u}_i$ and consider the incoherent superposition

$$S_z(\mathbf{r},t) = S\sum_{i=1}^{N_v} \cos\theta\,(\mathbf{r} - \mathbf{R}_i - \mathbf{u}_i t)\,. \qquad (3.1)$$

The thermal average in $S_{zz}(\mathbf{r},t) = \langle S_z(\mathbf{r},t)\, S_z(\mathbf{0},0)\rangle$

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is evaluated by integration over $\mathbf{R}$ and $\mathbf{u}$

$$S_{zz}(\mathbf{r},t) = n_v S^2 \int\int \mathrm{d}^2R\mathrm{d}^2u P(\mathbf{u}) \cos\theta(\mathbf{r}-\mathbf{R}-\mathbf{u}t) \times \times\cos\theta(\mathbf{R}) \quad (3.2)$$

where $n_v$ is the vortex density and $P(\mathbf{u})$ is the velocity distribution. Introducing the vortex form factor $f(\mathbf{q})$ = Fourier transform of $\cos\theta(\mathbf{r})$, we get

$$S_{zz}(\mathbf{q},t) = \frac{S^2}{(2\pi)^2} n_v \int \mathrm{d}^2u \left|f(\mathbf{q})\right|^2 \times \times P(\mathbf{u})\,\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{u}t}. \quad (3.3)$$

This can be evaluated easily if the *static* vortex solutions are inserted [3]. However, for $\lambda \lesssim 0.7$ only the planar solution turns out to be stable [6] and $S_{zz}$ would then vanish, in contradiction to the MC-MD simulation [3].

Therefore the *velocity dependence* of $\theta(\mathbf{r})$ must be taken into account. For $\lambda \lesssim 0.7$ and small velocity $u$ the equations of motion yield the asymptotic solution (in the moving frame, with time unit $\hbar/JS$)

$$\cos\theta = \frac{-1}{4\delta}\frac{\mathbf{u}.\mathbf{e}_\varphi}{r}, r \to \infty \quad (3.4)$$

which has been checked by MD-simulations; $\delta = 1-\lambda$, and $\mathbf{e}_\varphi$ is the azimuthal unit vector in the $xy$-plane. The solution for $r \to 0$ can be obtained also, but we are interested here only in the correlations for small $q$ where the asymptotic solution should be a good approximation. This leads to a velocity dependent form factor and eventually to

$$S_{zz}(\mathbf{q},\omega)\frac{n_v}{32\sqrt{\pi}\delta^2}\frac{\bar{u}}{q^3}\exp\left\{-\left(\frac{\omega}{\bar{u}q}\right)^2\right\}. \quad (3.5)$$

This is a Gaussian central peak which reflects the velocity distribution. The width $\Gamma_z = \bar{u}q$ has a linear $q$-dependence, which is very well supported by the MC-MD data [3]. The integrated intensity is

$$I_z(q) = \frac{n_v}{32\delta^2}\frac{\bar{u}^2}{q^2}. \quad (3.6)$$

Here the divergence for $q \to 0$ results from the infinite range of the structure (3.4). However, the actual radius of a vortex must be on the order of $\xi$ (see introduction), which can be taken into account e.g. by an ad-hoc cut-off function $\exp(-\varepsilon r/\xi)$ with a free parameter $\varepsilon$. This gives an extra factor of $\kappa^2$ in (3.6), with $\kappa = 1 - 1/W$ and $W = \left[1+(\xi q/\varepsilon)^2\right]^{1/2}$. The final result for $I_z(q)$ is consistent with our MC-MD data for small $q$ (Fig. 1). Note that *absolute* intensities are compared here; we have chosen $\varepsilon$ such that $I_z$ is smaller than the data because other effects can also contribute to the central peak, e.g. 2-magnon difference processes and vortex-magnon interactions which will be treated in future publications.

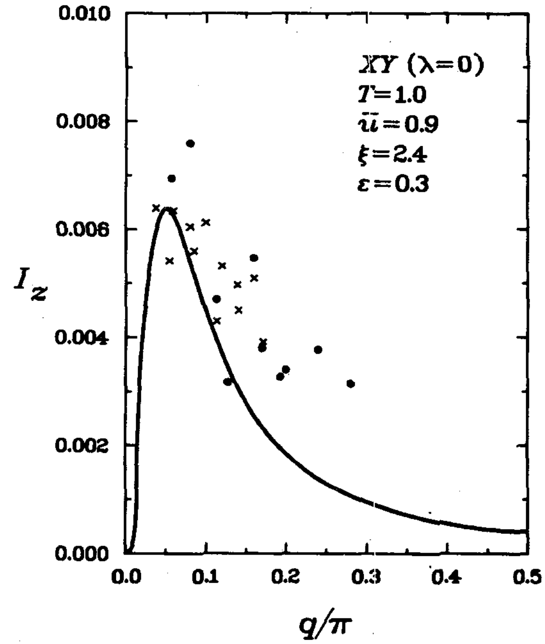


Fig. 1. – Intensity $I_z$ of central peak for a temperature $T > T_c \simeq 0.8$. Data points result from MC-MD simulations on a 50×50 lattice (circles) and 100 × 100 lattice (crosses). Solid line from (3.6) including the cut-off, with $\bar{u}$ and $\xi$ from reference [4].

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