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TITLE **DYNAMICS OF UNBOUND VORTICES IN THE 2-DIMENSIONAL XY AND ANISOTROPIC HEINSENBERG MODELS**

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Dynamics of Unbound Vortices in the 2-Dimensional XY and Anisotropic Heisenberg Models

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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.

two-dimensional magnets
nonlinear excitations
dynamical correlations

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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 $\vec{S}^m$ 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 ref [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

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

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

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

When a planar vortex starts moving it develops an out-of-plane structure (see next section). However, for $S_{xx}(\vec{r},t)$ this is not important because the dominant effect of moving vortices is to act like [illegible]d sign functions or [illegible]d kinks, i.e. every vortex that passes with its center between $\vec{O}$ and $\vec{r}$ 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 $S_{xx}(\vec{r},t)$ is published elsewhere [4] and gives a (squared) Lorentzian central peak for the dynamic form factor

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

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

$S_z(\vec{r},t)$ 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 $\vec{R}_i$ and velocities $\vec{u}_i$, and consider the incoherent superposition

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

The thermal average in $S_{zz}(\vec{r},t) = \langle S_z(\vec{r},t)\; S_z(\vec{0},0)\rangle$ is evaluated by integration over $\vec{R}$ and $\vec{u}$

$$S_{zz}(\vec{r},t) = n_v S^2 \iint d^2R\; d^2u\; P(\vec{u})\, \cos\theta(\vec{r}-\vec{R}-\vec{u}t)\, \cos\theta(R) \qquad (3.2)$$

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

$$S_{zz}(\vec{q},t) = \frac{S^2}{(2\pi)^2}\, n_v \int d^2u\; |f(\vec{q})|^2\, P(\vec{u})\, e^{-i\vec{q}\cdot\vec{u}t}. \qquad (3.3)$$

This can be evaluated easily if the <u>static</u> vortex solutions are inserted [3]. However, for $\lambda < 0.7$ 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 <u>velocity dependence</u> of $\theta(\vec{r})$ must be taken into account. For $\lambda < 0.7$ and small velocity u the equations of motion yield the asymptotic solution (in the moving frame, with time unit ħ/JS)

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

which has been checked by MD-simulations, $\delta = 1 - \lambda$, and $\vec{e}_\varphi$ 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 dependend form factor and eventually to

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

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

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

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 ξ (see Introduction), which can be taken into account e.g. by an ad-hoc cut-off function $\exp(-\epsilon r/\xi)$ with a free parameter ϵ. This gives an extra factor of κ^2 in (3.6), with $\kappa = 1 - 1/W$ and $W = [1 + (\xi q/\epsilon)^2]^{1/2}$. 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 ϵ 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.

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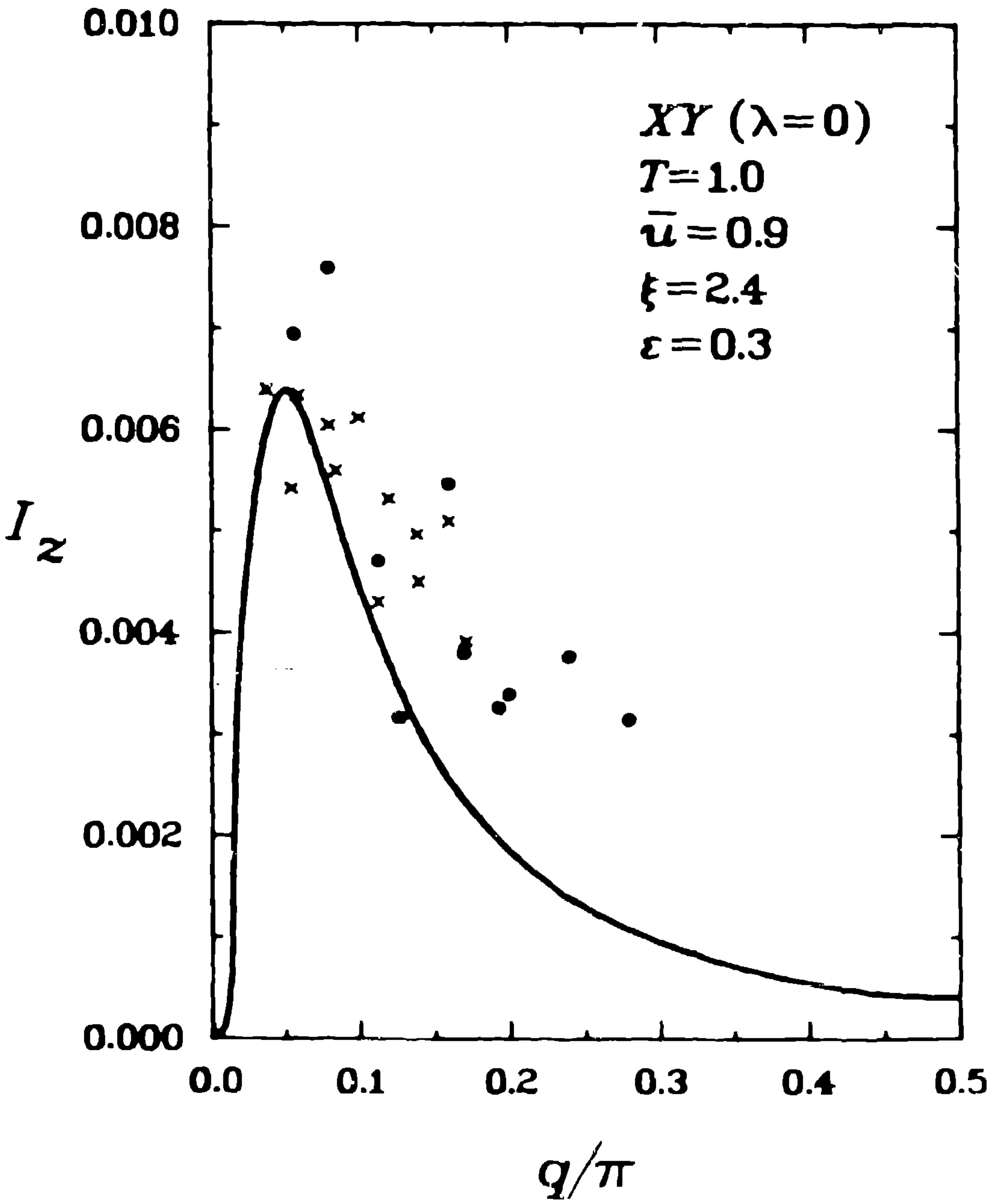
Captions

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



0.010
0.008
0.006
0.004
0.002
0.000
0.0
0.1
0.2
0.3
0.4
0.5
XY (λ=0)
T=1.0
ū=0.9
ξ=2.4
ε=0.3
I_z
q/π