JOURNAL DE PHYSIQUE
Colloque C8, Supplément au n° 12, Tome 49, décembre 1988

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

F. G. Mertens [1], A. R. Bishop, M. E. Gouvea and G. M. Wysin

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.

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 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 $S_{xx}(\mathbf{r}, t)$ 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 $S_{zz}(\mathbf{r}, t) = \langle S_z(\mathbf{r}, t) S_z(\mathbf{0}, 0)\rangle$

[1] *Permanent address*: Physics Institute, University of Bayreuth, D-8580 Bayreuth, F. R. G.

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

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

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

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

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 ξ (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 ε. This gives an extra factor of κ^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 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.

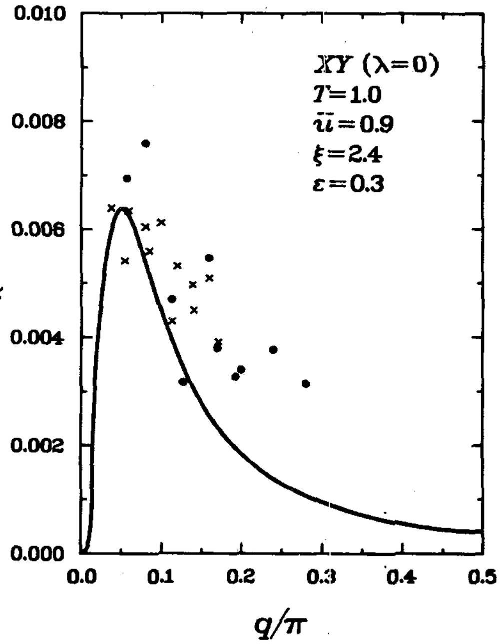

Fig. 1. – Intensity I_z of central peak for a temperature $T > T_c \simeq 0.8$. Data points result from MC-MD simulations on a 50×50 lattice (circles) and 100 × 100 lattice (crosses). Solid line from (3.6) including the cut-off, with $\bar{u}$ and ξ from reference [4].

Acknowledgments

The research of FGM and MEG was supported by DFG (Germany) and CNPQ (Brazil), respectively.

[1] Hutchings, M. T., Day, P., Janke, E. and Pynn, R., *J. Magn. Magn. Mater.* **54-57** (1986) 673.

[2] Regnault, L. P., Boucher, J. P., Rossat-Mignod, J., Bouillot, J., Pynn, R., Henry J. Y. and Renard, J. P., *Physica B* **136** (1986) 329.

[3] Mertens, F. G., Bishop, A. R., Wysin, G. M. and Kawabata, C., *Phys. Rev. Lett.* **59** (1987) 117.

[4] Mertens, F. G., Bishop, A. R., Wysin, G. M. and Kawabata, C., *Phys. Rev. B*, in press.

[5] Kawabata, C. and Bishop, A. R., *Solid State Commun.* **42** (1982) 595; *J. Phys. Soc. Jpn* **52** (1983) 27; *Solid State Commun.* **60** (1986) 169.

[6] Wysin, G. M., Gouvea, M. E., Bishop, A. R. and Mertens, F. G., Computer Simulation Studies in Condensed Matter Physics: Recent Developments (Springer, Berlin) 1988, in press.

[7] Huber, D. L., *Phys. Rev. Lett. A* **76** (1980) 406; *Phys. Rev. B* **26** (1982) 3758.

[8] Wiesler, D. G., Zabel, H. and Shapiro, S. M., Int. Conf. on Neutron Scattering, Grenoble, July 1988, preprint.