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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 Rb_2CrCl_4, K_2CuF_4... or $BaCo_2(AsO_4)_2$, $BaNi_2(PO_4)_2$... 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

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

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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 λ 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 ideas 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 ξ has the form

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

ξ_o is supposed to be in the order of the lattice constant a, and $b \simeq 1.3$, 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 teh 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 structure 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)

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

$$\upsilon = \begin{cases} \pi\left[1 - \exp(-r/r_v)\right] & r \gg r_v \\ 0 & r \to 0 \end{cases} \tag{2.2}$$

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

$$r_v = a\left[\,2(1-\lambda)\right]^{-1/2} \tag{2.3}$$

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 $\vec{R}_\nu$ and velocities $\vec{v}_\nu$:

$$S_z(\vec{r}, t) \simeq \sum_{\nu=1}^{N_v} \cos\upsilon\,(\vec{r} - \vec{R}_\nu - \vec{v}_\nu t)\,. \tag{2.4}$$

Here, only incoherent scattering from independent vortices is considered.

Now the thermal average can be performed by integration over $\vec{R}_\nu$ and $\vec{v}_\nu$, 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 $\cos \upsilon(r)$; we evaluate it approximately by extending the asymptotic solution in (2.2) to small r and by expanding about $\upsilon = \pi/2$ up to the first order. This gives

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

Apart from r_V there are only two other relevant parameters: the rms velocity $\bar{v}$ and the correlation length ξ 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 $Rb_2CrC\ell_4$, but we do not yet know any details. Therefore we compare with our Monte Carlo-Molecular Dynamics (MC-MD) simulations of a 100 × 100 spin lattice. We have chosen the XY-limit $\lambda = 0$ which should be representative for all λ-values up to about 0.7 because T_c and the static correlations depend only very weakly on λ in this regime (12, 14).[1] Bellow T_c ($\simeq$ 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 ($\bar{v} \simeq 1.6$ in units where $J = \hbar = S = 1$) for $0.9 \lesssim T \lesssim 1.1$. (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

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

from an equation of motion for free vortices, namely (2.7) shows a saturation as $T \to 1.2$. Even the numbers for $\bar{v}$ are not too far off: $\bar{v} = 0.74$ for $T = 1.0$, with $b \simeq 0.3$ for this temperature(2), and $\xi_o = a$. Since for ξ_o 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 Γ_z might have been overestimated from plots like Fig. 1(b).

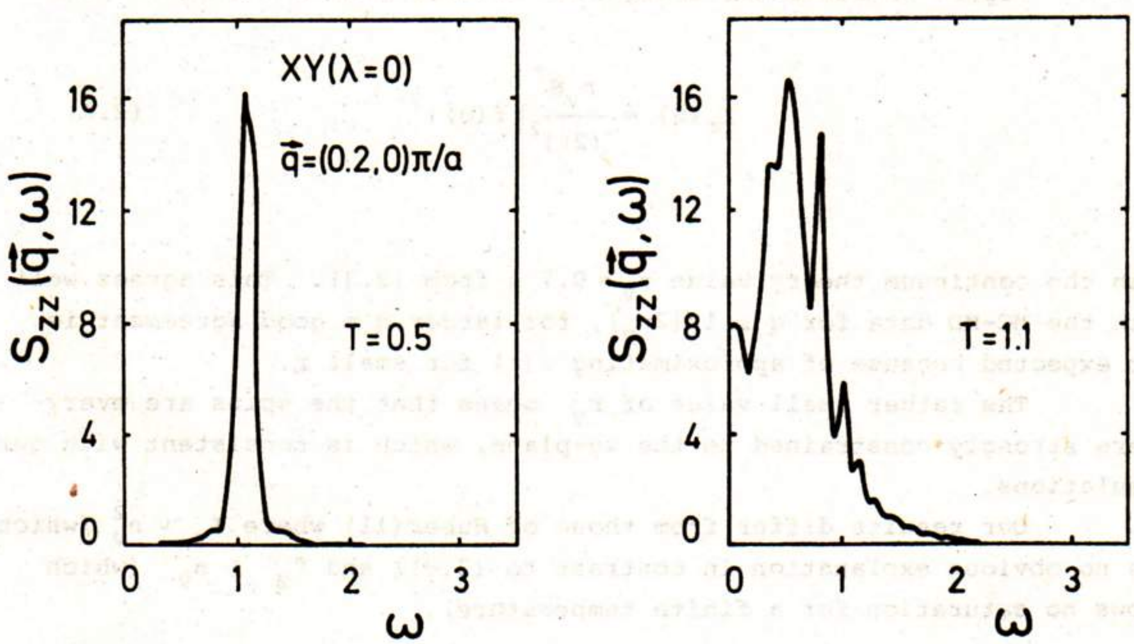

Figure 1. Dynamic form factor for out-of-plane correlations from a combined Monte Carlo-Molecular-Dynamics simulation of a 100 × 100 lattice. (a) temperature $T > T_c \simeq 0.83$, (b) $T > T_c$.

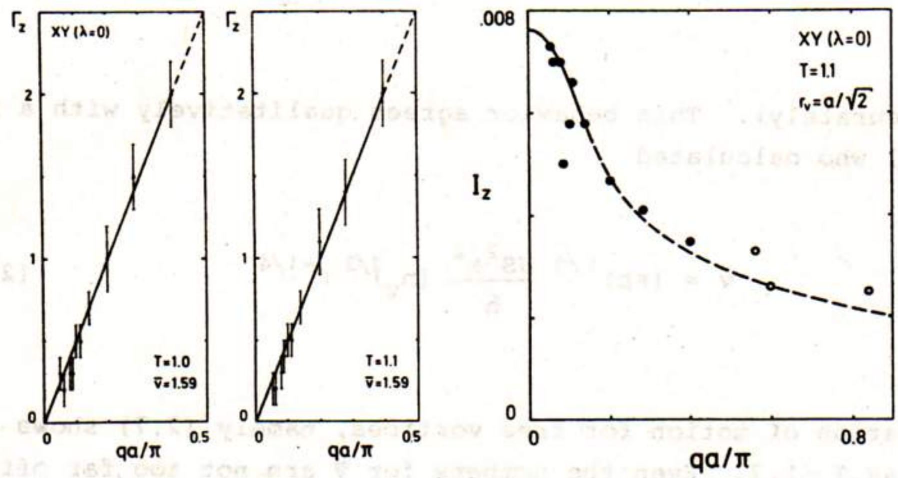

Figure 2. Width Γ_z and intensity I_z of the central peak in $S_{zz}(\vec{q}, \omega)$. The data points result from estimating these quantities from plots like Fig. 1. The solid lines are fits to $\Gamma_z = \bar{v}q$ from the Gaussian (2.5) and to I_z in (2.8). The dashed line is a guide to the eye and the open circles are upper bounds.

Figure 2b shows the integrated intensity of the central peak

$$I_z(q) = \frac{n_v S^2}{(2\pi)^2} |f(q)|^2 \qquad (2.8)$$

with the continuum theory value $r_v = 0.7$ a from (2.3). This agrees well with the MC-MD data for $q \leq 1/(2r_v)$, for larger q a good agreement is not expected because of approximating $\nu(r)$ for small r.

The rather small value of r_v means that the spins are everywhere strongly constrained to the xy-plane, which is consistent with our simulations.

Our results differ from those of Huber(11) where $I_z \sim n_v^2$ (which has no obvious explanation in contrast to (2.8)) and $\Gamma_z' \sim n_v$ (which shows no saturation for a finite temperature).

III. IN-PLANE CORRELATIONS

In contrast to S_z, the in-plane component $S_x = S\cos\phi$, sin υ with ϕ from (2.1) is not localized in space. This means that the correlation function $S_{xx}(\vec{r}, t) = \langle S_x(\vec{r}, t) \cdot S_x(\vec{0}, 0)\rangle$ is only globally sensitive to the presence of vortices. In fact all vortices which pass with its center through the point $\vec{r}$ in the time t diminish the correlation, namely by changing $\cos\phi$ by a factor of -1 (except for vortices moving along the x- or y- axis, which is a measure zero set only). If we work on a length scale $\gg r_V$ we can neglect effects due to the small out-of-plane components and due to the finite size of the vortices. In this sense the vortices act like 2-d-sign-functions. An ideal gas of vortices then has the effect that

$$S_{xx}(\vec{r}, t) = S^2 \langle \cos^2\phi \rangle \langle (-1)^{N(\vec{r}, t)} \rangle \quad . (3.1)$$

Here $N(\vec{r}, t)$ is the number of vortices which pass an arbitrary, non-intersecting contour connecting $(\vec{0}, 0)$ and $(\vec{r}, t)$.

Expressions like (3.1) were evaluated for the case of kinks in 1 - d models (e.g. ϕ^4 or sine-Gordon) by several authors; the most detailed investigation was made by Dorgovtsev(15), who also calculated such correlations numerically in two dimensions. We have now calculated(3.1) analytically: In contrast to (15) we use a velocity-independent contour, thereby we see various cancellation effects.

We wish to demonstrate this for the 1 - d case, the generalization to higher dimensions will then be obvious. For simplicity let all kinks have the same velocity v. Let us consider the case that the point (x, t) (with x, t $\geq$ 0) is situated outside the "light"-cone, which means x > vt. We choose the contour $(0, 0) \to (x, 0) \to (x, t)$. The contribution from the first part is

$$\langle (-1)^{N(x,t)} \rangle_1 = \sum_{n_\ell} (-1)^{n_\ell} p(n_\ell) \sum_{n_r} (-1)^{n_r} p(n_r) \quad . \quad (3.2)$$

for dilute gas of kinks we can use the Poisson-distribution

$$p(n_\ell) = \bar{n}_\ell \frac{e^{-\bar{n}_\ell}}{n_\ell!} \quad (3.3)$$

where $\bar{n}_\ell$ ($\bar{n}_r$) is the average density of kinks running to the left (right). Since the kinks pass this part of the contour at the same time ($t = 0$) but at different positions, these events are not correlated. Thus n_ℓ and n_r are independent and the two sums in (3.2) can be calculated separately, leading to the result

$$<(-1)^{N(x,t)}>_1 = e^{-2\bar{n}_\ell} = e^{-x/(2\xi)} \quad . \tag{3.4}$$

For the part $(x, 0) \to (x, t)$ of the contour we get formally again the expression (3.2). However, here the kinks pass the same point at different times, these events are correlated, as long as $t < x/v$ which was a prerequisite. Thus n_ℓ and n_r are not independent. As the number of left and right running kinks is the same, $n_\ell + n_r$ is even and the second part of the contour gives no contribution.

The other possible case, namely $x < vt$, is more complicated. Here we obtain the general result that vertical lines within the light cone give a contribution, whereas horizontal lines do not (just opposite to the previous case). The final result is $<(-1)^{N(x,t)}> = \exp(-vt/\xi)$.

In two dimensions, where the vortices play the role of the kinks, the same kind of argumentation can be applied, leading eventually to

$$<(-1)^{N(\vec{r},t)}> = \exp\left\{-\int_0^\infty \left[\frac{|r-vt|}{2\xi} + \frac{|r+vt|}{2\xi}\right] P(v)\, dv\right\} \tag{3.5}$$

Here the average over the velocities $v = |\vec{v}|$ is already included by means of $P(v)$. Assuming again a Maxwell velocity distribution we obtain

$$S_{xx}(\vec{r}, t) = \frac{1}{2} S^2 \exp\left\{-\frac{r}{\xi} - \frac{\sqrt{\pi}}{2}\frac{\bar{v}|t|}{\xi} \operatorname{erfc}\left(\frac{r}{\bar{v}t}\right)\right\} \tag{3.6}$$

with the complementary errorfunction erfc.

Similar to the 1-d case(16) one can find an excellent analytic approximation for the argument of the exponential

$$S_{xx}(\vec{r},\ t) = \frac{1}{2} S^2 \exp\{-\left[(r/\xi)^2 + (\gamma t)^2\right]^{1/2}\} \tag{3.7}$$

with

$$\gamma = \frac{\sqrt{\pi}}{2} \frac{\bar{V}}{\xi} \ . \tag{3.8}$$

This approximation preserves not only the correct integrated intensity (see below) but also the correct asymptotic behavior for r or $t \to \infty$.

For (3.7) the spatial and temporal Fourier transformations can be performed

$$S_{xx}(\vec{q},\ \omega) = \frac{S^2}{2\pi^2} \frac{\gamma^3 \xi^2}{\{\omega^2 + \gamma^2 \left[1 + (\xi q)^2\right]\}^2} \tag{3.9}$$

This is a squared Lorentzian central peak with a q-dependent (half)-width

$$\Gamma_x^{\cdot}(q) = \left(\sqrt{2} - 1\right)^{1/2} \gamma \left(1 + (\xi q)^2\right)^{1/2} \ . \tag{3.10}$$

Let us compare this with our MC-MD simulations for the XY-model (Fig. 3). Contrary to the out-of-plane case, the spin waves are strongly softened here for $T > T_c$ (this is consistent with the theoretical predictions(17), as well as with the experiments(5, 6, 8). Therefore we observe essentially a central peak, which could well be a Lorentzian. The q-dependence (3.10) is indeed observed (Fig. 4a) and we obtain numbers for the two parameters $\bar{v}$ and ξ in (3.9).

Using again Huber's result (2.7) for $\bar{v}$, $\Gamma_x^{\cdot}$ is predicted to increase with the temperature and to saturate at about $T \approx 1.2$ for $q \gg \xi^{-1}$, whereas an increase and no saturation at finite T occurs for $q \ll \xi^{-1}$; we indeed observe these behaviors in both cases, the former case has already been published(7).

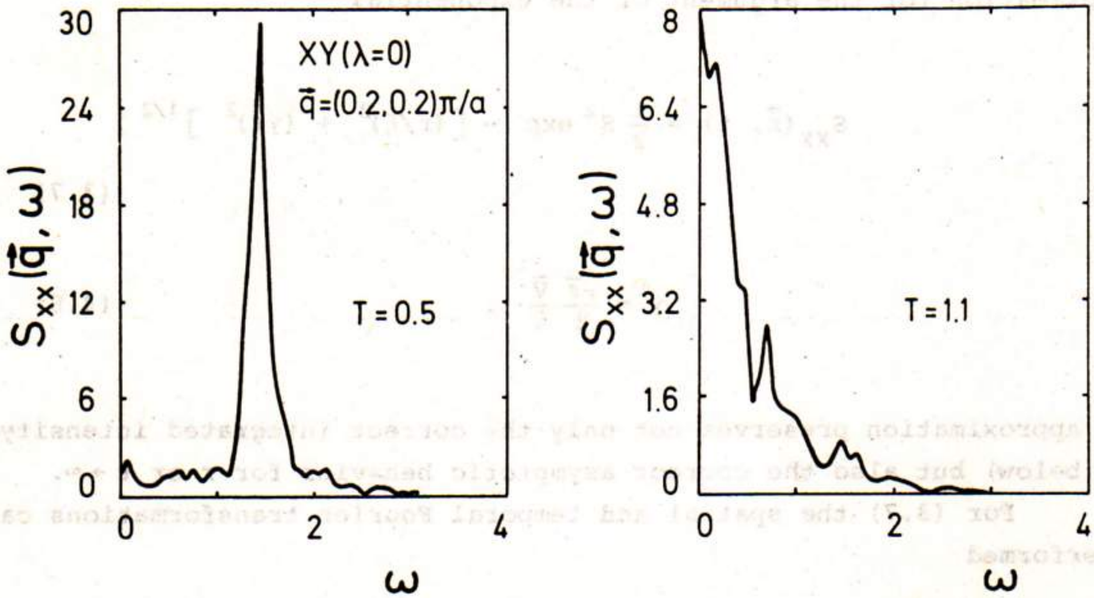

Figure 3. Dynamic form factor for in-plane correlations from MC-MD simulations; further explanations like in figure 1.

The integrated intensity of (3.9) is

$$I_x(\vec{q}) = \frac{S^2}{4\pi} \frac{\xi^2}{\left[1 + (\xi q)^2 \right]^{3/2}} \tag{3.11}$$

Since we are working on a length scale $\gg r_v$ we can fit (3.11) to our data for $q \ll \xi^{-1}$ (Fig. 4b) and obtain again values for ξ. They do not differ much from those previously obtained from Γ_x'. The values for ξ can be compared with theoretical values(2), where the unknown ξ_o is set equal to a, see table I.

Last, but not least, we can compare with inelastic neutron scattering experiments on XY-like quasi-2d magnets. Presently the published results are still rather incomplete, they contain each only one figure of $S_{xx}(q, \omega)$ and verbal statements on the q-dependence.

For $BaCo_2(AsO_4)_2$ a central peak has been measured(6) which can be fitted to a Lorentzian. The width Γ_x is a constant for small q, which agrees with (3.10). Using the experimental value for ξ and the

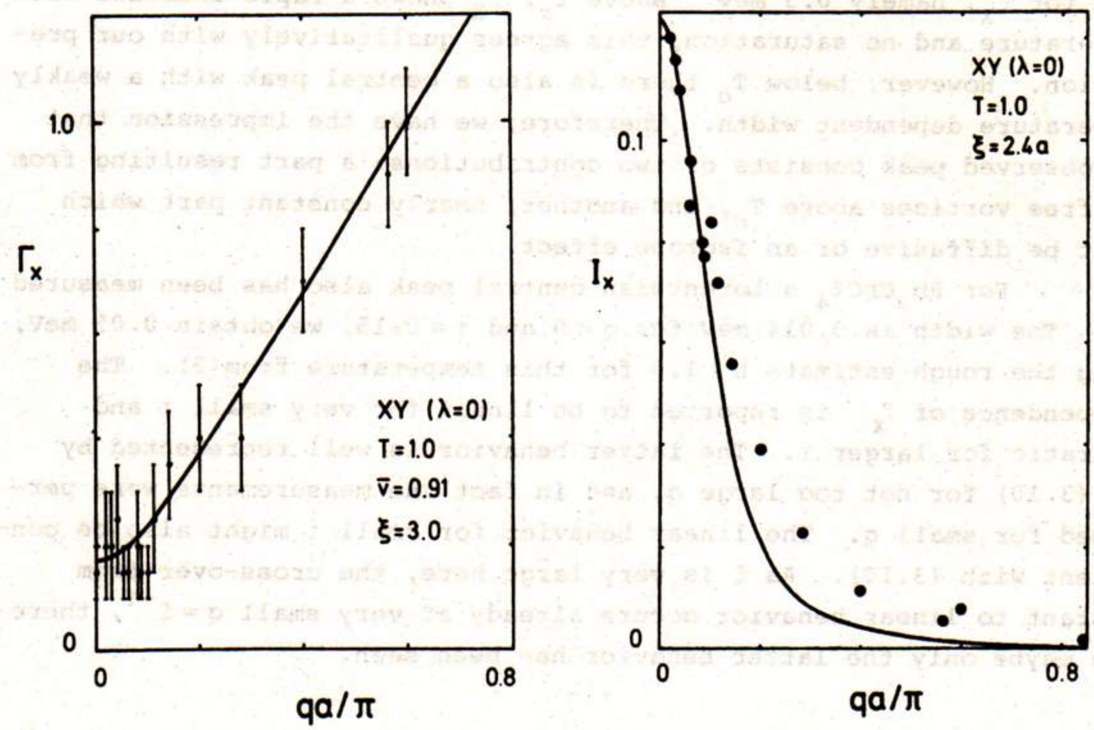

Figure 4. Width Γ_X and intensity I_X of the central peak in S_{XX}. The data points result from estimating these quantities from plots like figure 3. The solid lines are fits to (3.10) and to (3.11).

Table I

Parameter values obtained by fitting to our MC-MD data for the XY-model ($\lambda = 0$) for T = 1.0, compared to theoretical predictions.

from	$\bar{v}$	ξ/a	r_V/a
$\Gamma_Z(q)$	< 1.6	-	-
$I_Z(q)$	-	-	0.7
$\Gamma_X(q)$	0.91	3.0	-
$I_X(q)$	-	2.4	-
(1.2) with $b = 0.3$, $\xi_o = a$	-	1.9	-
(2.7) with $b = 0.3$, $\xi_o = a$	0.74	-	-
(2.3)	-	-	0.7

theoretical estimate (2.7) for $\bar{v}$ we obtain the correct order of magnitude for Γ_x', namely 0.3 meV. Above T_c, Γ_x' shows a rapid increase with temperature and no saturation, this agrees qualitatively with our prediction. However, below T_c there is also a central peak with a weakly temperature dependent width. Therefore, we have the impression that the observed peak consists of two contributions: a part resulting from the free vortices above T_c, and another, nearly constant part which might be diffusive or an isotope effect.

For $Rb_2CrC\ell_4$ a Lorentzian central peak also has been measured (8). The width is 0.014 meV for $q = 0$ and $\tau = 0.15$, we obtain 0.05 meV, using the rough estimate $b \approx 1.0$ for this temperature from(2). The q-dependence of Γ_x' is reported to be linear for very small τ and quadratic for larger τ. The latter behavior is well represented by Eq. (3.10) for not too large q, and in fact the measurements were performed for small q. The linear behavior for small τ might also be consistent with (3.10). As ξ is very large here, the cross-over from constant to linear behavior occurs already at very small $q = \xi^{-1}$, therefore maybe only the latter behavior has been seen.

IV. CONCLUSION

Our vortex-gas phenomenology predicts a Gaussian central peak for the out-of-plane correlations, and a Lorentzian peak for the in-plane ones. Both is in very good agreement with our MC-MD data.

Experimentally for the out-of-plane form factor only the existence of a central peak has been reported. For the in-plane case Lorentzian central peaks have been measured for two materials. From our theory we obtain the correct order of magnitude for the peak width, and qualitatively the same wavevector and temperature dependencies.

So far the experimental data have been fitted to an ad-hoc formula, namely a product of two Lorentzians, one for the ω-dependence and one for the q-dependence(8). We think that a fit to the squared Lorentzian (3.9) with its q-dependent width will allow a much more detailed comparison between theory and experiment.

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