CENTRAL PEAK SIGNATURES FROM VORTICES IN 2D EASY-PLANE ANTIFERROMAGNETS

F.G. Mertens, A. Völkel, G.M. Wysin*, A.R. Bishop[+]
University of Bayreuth, Germany, *Kansas State University, Manhattan, USA,
[+]Los Alamos National Laboratory, USA

We investigate the dynamics of a classical, anisotropic Heisenberg model. Assuming a dilute gas of ballistically moving vortices above the Kosterlitz-Thouless transition temperature, we calculate the dynamic form factors $S(\vec{q},\omega)$ and test them by combined Monte Carlo-molecular dynamics simulations. For both in-plane and out-of-plane correlations we predict and observe central peaks (CP) which are, however, produced by quite different mechanisms, depending on whether the correlations are globally or locally sensitive to the presence of vortices. The positions of the peaks in q-space depend on the type of interaction and on the velocity dependence of the vortex structure. For a ferromagnet both CP's are centered at q = 0; for an antiferromagnet the static vortex structure is responsible for a CP at the Bragg points, while deviations from it due to the vortex motion produce a CP at q = 0. By fitting the CP's to the simulation data we obtain the correlation length and the mean vortex velocity.

1. INTRODUCTION

A wide class of quasi-two-dimensional magnetic materials (e.g. layered magnets[1], graphite intercalation compounds[2], magnetic lipid layers[3]) can be described approximately by the classical anisotropic Heisenberg model

$$H = J \sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z) \qquad (1.1)$$

with $0 \leq \lambda < 1$. The spins $\vec{S}_i$ are coupled only to nearest neighbors on a square lattice and tend to be aligned in the xy-plane (easy-plane).

Below the Kosterlitz-Thouless transition temperature T_c bound vortex-antivortex pairs are thermally excited, but do not move. Above T_c the pairs begin to unbind and the single vortices move around due to the interaction with the other vortices.

For the static spin correlations many exact results from the Kosterlitz-Thouless theory are known. However, for the dynamic correlations

only a phenomenological treatment has been possible so far. Assuming a dilute gas of ballistically moving vortices above T_c, the dynamic form factors $S(\vec{q}, \omega)$ have been calculated for the case of a ferromagnetic coupling[4,5]. The typical signatures of moving vortices are central peaks (CP's), which have been observed both in combined Monte Carlo-molecular dynamics simulations[4] and in inelastic neutron scattering experiments[1,2].

In this paper we will shortly review these results and discuss the characteristic changes of the CP's for the case of an <u>antiferromagnetic</u> coupling.

2. ANTIFERROMAGNETIC VORTICES

We parametrize the classical spins by four angles[6]

$$S_n^x = (-1)^n S \cos[\Phi_n + (-1)^n \phi_n] \cos[\theta_n + (-1)^n \vartheta_n]$$

$$S_n^y = (-1)^n S \sin[\Phi_n + (-1)^n \phi_n] \cos[\theta_n + (-1)^n \vartheta_n] \qquad (2.1)$$

$$S_n^z = (-1)^n S \sin[\theta_n + (-1)^n \vartheta_n] ,$$

where the even n denote one sublattice, the odd n the other one. In the continuum approximation the capital angles $\Phi(\vec{r})$ and $\theta(\vec{r})$ describe a perfect local antiferromagnetic structure, while the small angles $\phi(\vec{r})$ and $\vartheta(\vec{r})$ describe deviations from this structure.

In a previous paper[7], we have derived the four equations of motion and we have found the following continuum limit vortex solutions (to first order in the vortex velocity u)

$$\Phi(\vec{r}) = \pm \arctan(y/x) , \qquad \phi(\vec{r}) = 0 , \qquad \theta(\vec{r}) = 0 \qquad (2.2)$$

$$\vartheta(\vec{r}) \sim \frac{u}{4(1+\lambda)JS} \frac{\sin(\varphi-\varepsilon)}{r} \quad \text{for large r} . \qquad (2.3)$$

Here r, φ are the polar coordinates of $\vec{r}$, and ε is the angle between $\vec{u}$ and the x-axis.

When placed on a lattice, this solution is stable only for $\lambda < \lambda_c \approx 0.72$ and is called "in-plane vortex" because the out-of-plane components of the spins are small, or even zero in the static limit. In this paper we do not

discuss the case $\lambda > \lambda_c$ for which "out-of-plane vortices" are stable, here θ is nonzero independent of the velocity.

3. IN-PLANE CORRELATION FUNCTION

Inserting the vortex solution (2.2/3) in the definition $S^{xx}(\vec{r},t) = \langle S^x(\vec{r},t)\, S^x(\vec{0},0)\rangle$ we obtain

$$S^{xx} = S^2 \langle e^{i\vec{K}\vec{r}} \cos \Phi(\vec{r},t) \cos[e^{i\vec{K}\vec{r}} \vartheta(\vec{r},t)] \cos \Phi(\vec{0},0) \cos \vartheta(\vec{0},0)\rangle. \tag{3.1}$$

Here $\exp(i\vec{K}\vec{r}) = \pm 1$, depending on the sublattice to which $\vec{r}$ belongs; $\vec{K} = (\pi,\pi)$ restricting ourselves to the first Brioullin zone.
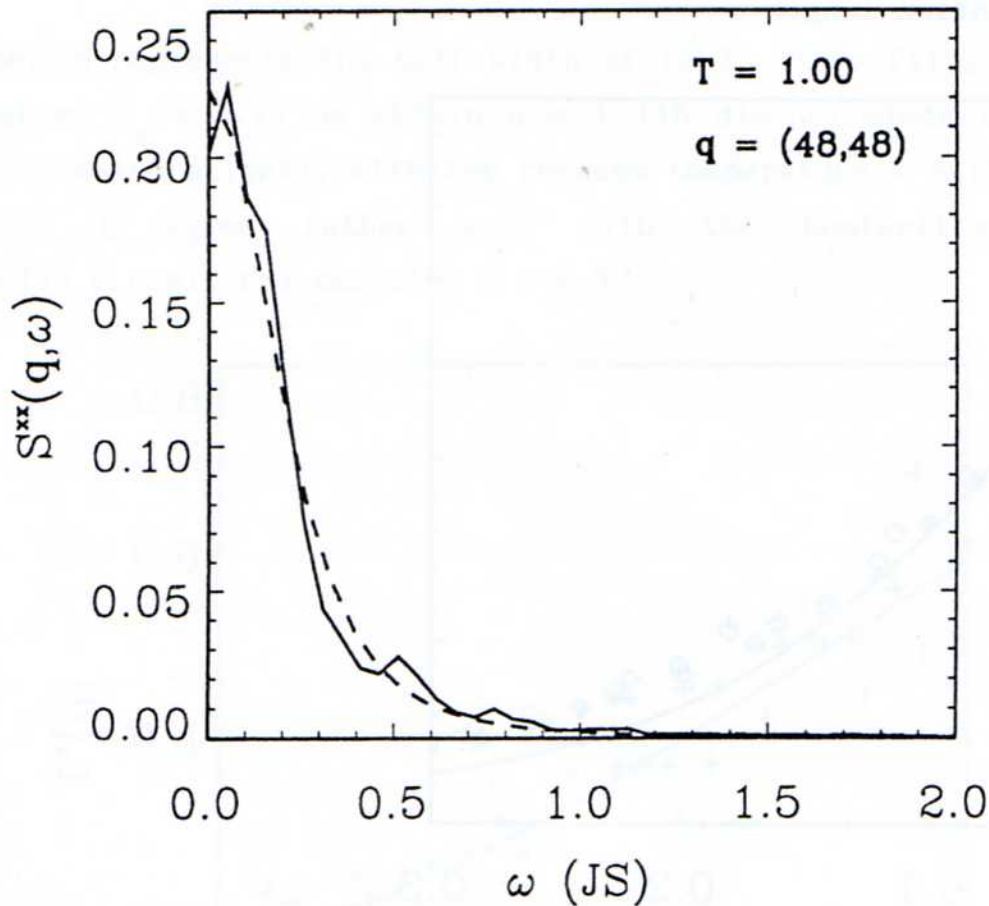

Fig. 1. In-plane dynamic form factor for $\lambda = 0$ (XY-model), $\vec{q}$ in units of $2\pi/L$ with lattice size $L = 100$ a. Solid line: simulation data; dashed line: fit of squared Lorentzian (3.3).

Similar to the ferromagnet[4], for large r the main effect of a vortex passing a lattice site is to flip the spin at this site, i.e. $\cos \Phi$ changes its sign. Compared to this big effect the small angle ϑ can be neglected and we obtain

$$S^{xx}(\vec{r},t) = S^2 e^{i\vec{K}\vec{r}} \langle\cos^2\Phi\rangle\langle(-1)^{N(\vec{r},t)}\rangle . \tag{3.2}$$

The first average is a static one and gives 1/2; the dynamics is contained in the second average: $N(\vec{r},t)$ is the number of vortices passing an arbitrary, nonintersecting contour between $(\vec{0},0)$ and $(\vec{r},t)$. The calculation proceeds in the same way as for the ferromagnet[4] and yields a squared Lorentzian CP for the dynamic form factor

$$S^{xx}(\vec{q},\omega) = \frac{S^2}{2\pi} \frac{\gamma^3 \xi^2}{\{\omega^2 + \gamma^2[1+(\xi q^*)^2]\}^2} \; , \tag{3.3}$$

the only difference is the appearance of $\vec{q}^* = \vec{K} - \vec{q}$ instead of $\vec{q}$. Here $\gamma = \sqrt{\pi}\ \bar{u}/(2\xi)$, with rms vortex velocity $\bar{u}$, and 2ξ is the average distance between two vortices (according to the Kosterlitz-Thouless theory, ξ is also the static correlation length).
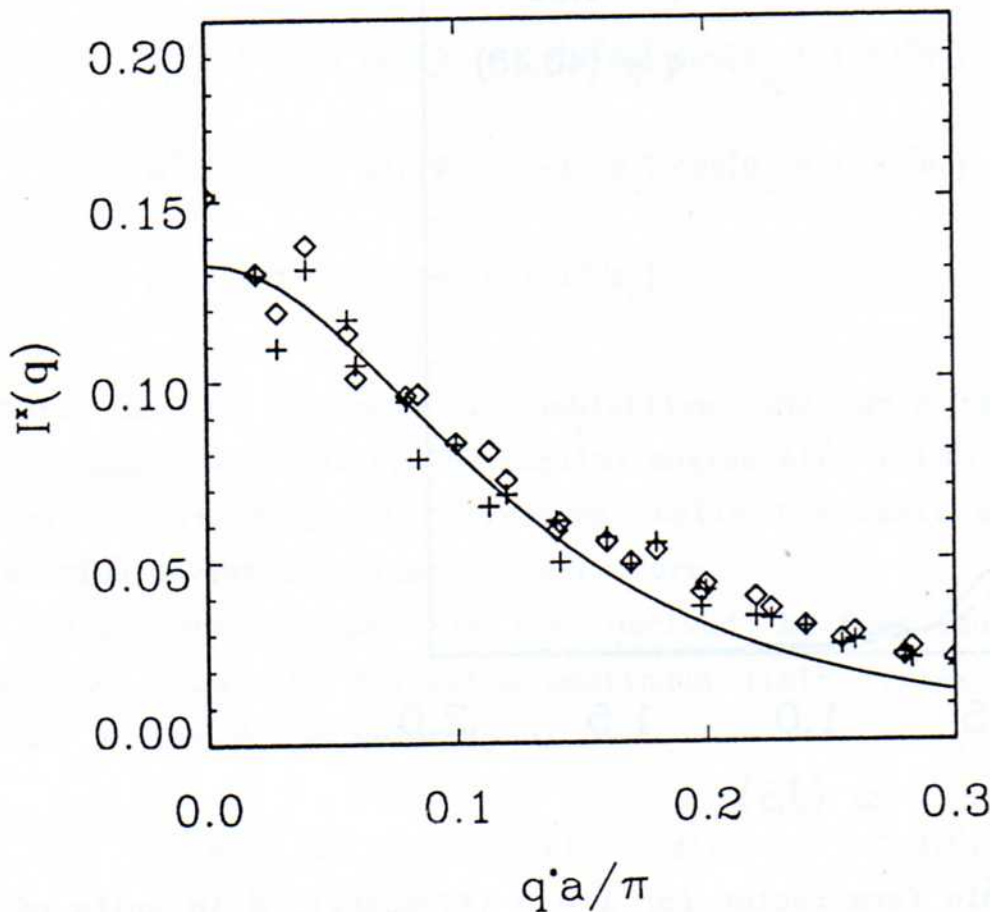

Fig 2. Integrated intensity of in-plane dynamic form factor for $T = 1.0$. +: intensity of fitted central peak (3.3); $\diamondsuit$: intensity from simulation data; solid line: fit to (3.4) for small q^*.

Since (3.3) contains no parameters characterizing the vortex structure, S^{xx} is only <u>globally</u> sensitive to the presence of vortices. In fact, the moving vortices disturb the local antiferromagnetic order and thus <u>diminish</u> the correlations. For this reason the integrated intensity

$$I^x(q^*) = \frac{S^2}{4\pi} \frac{\xi^2}{[1+(q^*\xi)^2]^{3/2}} \qquad (3.4)$$

is inversely proportional to the density $n_v \simeq (2\xi)^{-2}$ of free vortices.

The prediction (3.3) can be well fitted to the CP which we observe in simulations on a 100 x 100 lattice (Fig.1). The resulting data for the width Γ^x and intensity I^x are displayed in Figs. 2 and 3. Moreover, we have fitted these data for small q^* (because of our large-r approximation) to (3.4) and to

$$\Gamma^x(q^*) = \frac{1}{2} \sqrt{\pi(\sqrt{2}-1)} \frac{\bar{u}}{\xi} \sqrt{1+(\xi q^*)^2} \qquad (3.5)$$

which represents the half width of (3.3). This fit gives us $\bar{u}$ and ξ. Just above $T_c \simeq 0.79$ we obtain $\bar{u} \approx 1$ (in dimensionless units) and this value increases slightly with the reduced temperature $\tau = (T - T_c)/T_c$. The values for ξ agree rather well with the Kosterlitz-Thouless prediction $\xi(T) \simeq \exp(b/\sqrt{\tau})$ choosing $b \simeq 0.5$.
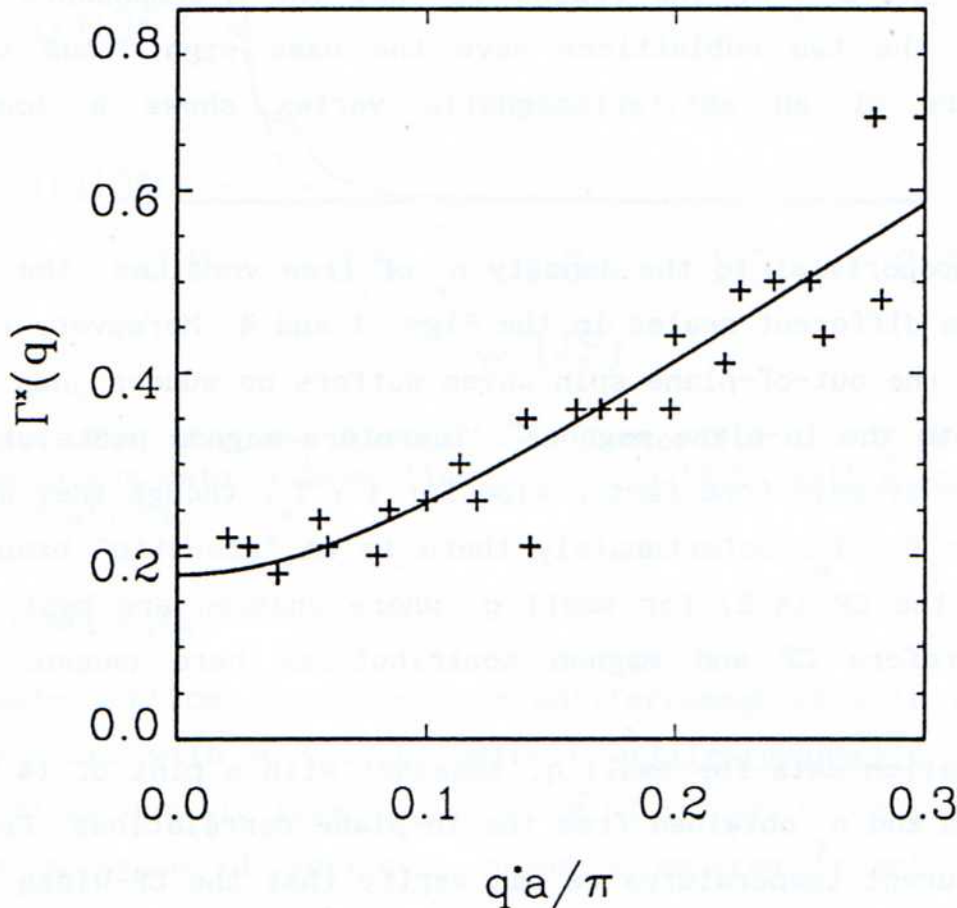

Fig 3. Width of in-plane dynamic form factor for T = 1.0. +: width of fitted central peak (3.3); solid line: fit to (3.5) for small q^*.

4. OUT-OF-PLANE CORRELATION FUNCTION

Contrary to the in-plane structure, the out-of-plane structure (2.3) of a vortex is <u>localized</u>. Therefore we expect that $S^{zz}(\vec{r},t)=\langle S^z(\vec{r},t)S^z(\vec{0},0)\rangle$ depends on the <u>shape</u> of this structure. We are mostly interested in small wave vectors and therefore we evaluate

$$S^{zz} = \langle e^{i\vec{K}\vec{r}} \sin [e^{i\vec{K}\vec{r}} \vartheta(\vec{r},t)] \cdot \sin \vartheta(\vec{0},0)\rangle \qquad (4.1)$$

for large r where ϑ is small, and obtain $\langle\vartheta(\vec{r},t)\vartheta(\vec{0},0)\rangle$. Using (2.3) we obtain in a vortex-gas approximation, similarly to the ferromagnetic case[5], a Gaussian CP

$$S^{zz}(q,\omega) = \frac{n_v\bar{u}}{32(1+\lambda)^2 J^2\sqrt{\pi}\ q^3} \exp \{-[\omega/(\bar{u}q)]^2\} . \qquad (4.2)$$

Here $1 + \lambda$ appears, instead of $1 - \lambda$ for the ferromagnet. However, otherwise the formula is the same, i.e. in both cases there is a CP with a maximum at $\vec{q} = (0,0)$ and $\omega = 0$. The reason is that the z-components of neighboring spins on the two sublattices have the same sign, thus the out-of-plane structure of an antiferromagnetic vortex shows a local <u>ferromagnetic</u> order.

Because (4.2) is proportinal to the density n_v of free vortices, the CP is very small, cf. the different scales in the Figs. 1 and 4. Moreover, the stiffness constant of the out-of-plane spin waves suffers no sudden jump to zero at T_c, contrary to the in-plane magnons[8]. Therefore magnon peaks show up in the out-of-plane dynamic form factor also for $T > T_c$, though they are much broader than for $T < T_c$. Unfortunately there is an "acoustic" branch that interferes with the CP (4.2) for small q, where chances are best to observe the CP. Therefore CP and magnon contributions here cannot be distinguished clearly.

Fig. 4 shows simulation data for small q, together with a plot of (4.2) using the values for $\bar{u}$ and n_v obtained from the in-plane correlations. From such figures for different temperatures we can verify that the CP-width is consistent with the prediction $\Gamma^z = \bar{u}q$ resulting from (4.2). However, the intensity

$$I^z(q) = \frac{n_v \bar{u}}{32(1+\lambda)^2 J^2 \sqrt{\pi} \, q^2} \tag{4.3}$$

cannot be tested because of the difficulty to separate the magnon contributions. (Remark: The singularity in (4.3) for $q \to 0$ can be avoided by introducing a cut-off in the order of ξ in order to account for the finite size of the vortices due to the presence of the other vortices[5].)
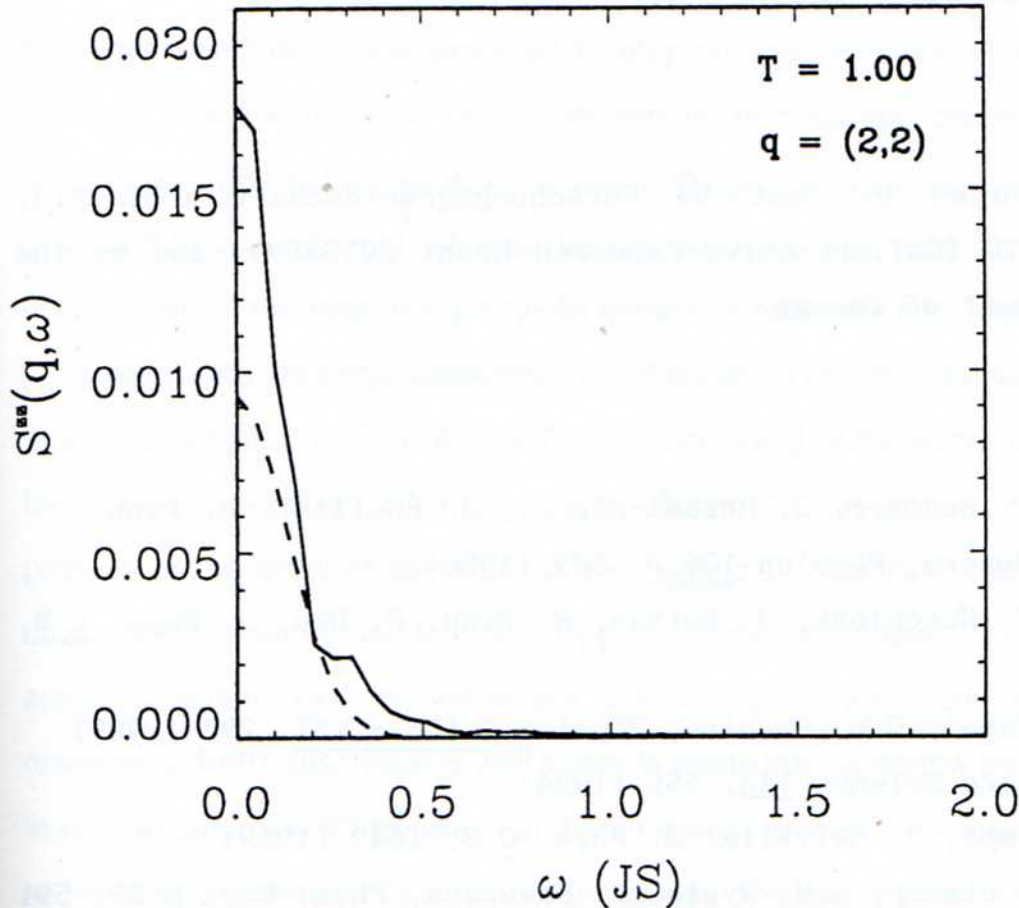

Fig 4. Out-of-plane dynamic form factor for $\lambda = 0$ (XY-model). Solid line: simulation data; dashed line: Gaussian (4.2) with $\bar{u}$ and ξ from the in-plane correlations.

5. CONCLUSION

Single vortices in easy-plane antiferromagnets with $\lambda < \lambda_c$ have a static structure with a locally perfect <u>antiferromagnetic</u> order. Therefore the in-plane dynamic form factor $S^{xx}(\vec{q}, \omega)$, which is only globally sensitive to the presence of vortices, shows a squared Lorentzian CP at the Bragg points.

The finite velocity of the vortices causes small deviations from the above structure, producing a localized out-of-plane structure with a _ferromagnetic_ character. Therefore the out-of-plane dynamic form factor $S^{zz}(\vec{q},\omega)$ shows a Gaussian CP at the _center_ of the Brioullin zone. The q-dependence of S^{zz} reflects the shape of the ferromagnetic out-of-plane structure and the ω-dependence reflects the velocity distribution of the vortices.

Both CP's are observed in computer simulations which allows to fit the phenomenological parameters ξ and $\bar{u}$.

ACKNOWLEDGEMENTS

REFERENCES

1. L.P. Regnault, J.P. Boucher, J. Rossat-Mignot, J. Bouillot, R. Pynn, J.Y. Henry, J.P. Renard, Physica 136 B, 329 (1986);
   S.T. Bramwell, M.T. Hutchings, J. Norman, R. Pynn, P. Day, J. Phys. C 8, 1435 (1988)
2. D.G. Wiesler, H. Zabel, S.M. Shapiro, Physica B 156 + 157, 292 (1989)
3. M. Pomerantz, Surface Science 142, 556 (1984);
   D.I. Head, B.H. Blott, D. Melville, J. Phys. C 8, 1649 (1988)
4. F.G. Mertens, A.R. Bishop, G.M. Wysin, C. Kawabata, Phys. Rev. B 39, 591 (1989)
5. M.E. Gouvêa, G.M. Wysin, A.R. Bishop, F.G. Mertens, Phys. Rev. B 39, 11840 (1989)
6. H.J. Mikeska, J. Phys. C 13, 2913 (1980)
7. A.R. Völkel, F.G. Mertens, A.R. Bishop, G.M. Wysin, Phys. Rev. B 43, 5992 (1991)
8. D.R. Nelson, J.M. Kosterlitz, Phys. Rev. Lett. 39, 1201 (1977)