

# INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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SOLITONS AND VORTICES

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SOLITONS AND VORTICES \*

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The primary purpose of this report is to outline our recent results [1,2] on the dynamics of easy-plane classical ferromagnetic spins in two spatial dimensions - particularly signatures of unbound vortices above a Kosterlitz-Thouless topological phase transition [3]. However, for completeness we briefly place this in the context of our wider studies of low-dimensional magnetism since the last meeting in this series. These may be summarized as:

(i) 0-dimensional systems. Here we include single spins [4] and small spin clusters [5], which have been studied with both free and externally-driven dynamics, and for both classical and spin-S quantum cases. The aim has been to probe the quantum analogs of classically "chaotic" dynamics by taking advantage of some special features of certain spin systems -- the Hilbert space is compact so numerical accuracy is assured; and both the degrees of "quantumness" ( $\pi \sim S^{-1}$ ) and "integrability" can be controlled (including totally integrable limits). In this way new scaling behaviours (motivated by dynamical systems theory in classical problems) has been suggested for both energy level structures [5] and wave-functions [4] in the semiclassical regime  $S \gg 1$ .

(ii) 1-dimensional systems. We have examined both ferromagnetic and antiferromagnetic easy-plane spin chains with an in-plane magnetic field (modeling, e.g., CsNiF<sub>3</sub> and TMMC, respectively), and both classical dynamics and quantum thermodynamics. Concerning dynamics, we have focused most recently on the kink-solitons in the antiferromagnetic case and on their interactions [6]. For the Hamiltonian

$$H = \sum_n J \mathbf{S}_n \cdot \mathbf{S}_{n+1} + A(S_n^z)^2 - BS_n^x, \quad (1)$$

( $J, A > 0$ , site index  $n$ ) there are both "XY" and "YZ" solitons, corresponding to sublattice rotations by  $\pi$ , principally in the XY and YZ plane, respectively -- at  $B = B_c = (2/JS)(2A/J)^{1/2}$  (where the rest kink energies are equal [6]) there is a natural crossover. Using an analytic ansatz [6], we have found that both dynamic branches can be incorporated in a unified manner and that: (a) the XY and YZ branches always merge at a field-dependent kink velocity; and (b) the XY solutions have a "negative effective mass" branch for  $B > B_c$ , similar to the ferromagnetic case [7]. Kink-antikink collisions may be summarized as generally transmitting for YZ kinks (which are more sine-Gordon-like in character), whereas for XY they transmit for small  $B$ , bind (into "breathing" states) or annihilate for larger  $B$  ( $< B_c$ ), and reflect for  $B > B_c$  (i.e. for the negative mass branch): thus the XY kinks behave in these respects much as for the XY kink solitons in the corresponding ferromagnetic case [7].

Using quantum MC or quantum transfer matrix methods [8] has been instructive for the thermodynamic of materials such as CHAB or CsNiF<sub>3</sub> in magnetic fields, since precise experimental measurements of specific heat differences (i.e. with and without a magnetic field) are now available. Thus an important test of proposed magnetic Hamiltonians is possible. Although agreements between the experiments and quantum simulations are very good, the systematic differences are important. They are outside the respective errors and of a percentage magnitude consistent with differences between various theoretical treatments (of semiclassical quantization, out-of-plane spin fluctuations, etc.). Thus, for these theoretical "disputes" to be meaningful requires that the original Hamiltonian be agreed to even greater accuracy -- including additional small terms (e.g. dipolar, in-plane symmetry-breaking).

(iii) 2-dimensional systems. Here again we have focused on easy-plane Heisenberg models and their classical thermodynamics [9], including crystalline symmetry-breaking terms in the easy-plane as appropriate (e.g. for magnetically-intercalated graphite or the layered magnet  $\text{Rb}_2\text{CrCl}_4$  [10]). We have also made preliminary studies [11] of transverse instabilities and their nonlinearly saturated forms on moving domain walls. This is a topic of considerable general importance in the field of pattern formation and extended dynamical systems, and the magnetic examples deserve more careful reassessment and measurement in the light of current advances in this field. However, the remainder of this report will deal with recent attempts [1,2] to study classical spin dynamics above the Kosterlitz-Thouless transition in easy-plane Heisenberg models, emphasising possible signatures of unbound vortices. This is also a topic which has reached a stage of great opportunity because of improved and more varied quasi-2-d materials, and because of increased interest in making inelastic neutron scattering measurements at small frequency and wave-vector [12].

As in 1-d soliton systems, we adopt an "ideal gas phenomenology" as a first step, so as to explicitly recognize the vortex collective structures -- i.e. the spin field is decomposed into additive spin wave and vortex contributions [13]. Here we treat only the vortex contribution, which is itself considered as a noninteracting dilute gas of unbound vortex-antivortex pairs ( $T > T_c$ ) moving in a screening background of the remaining bound pairs.

We consider the anisotropic ferromagnetic Heisenberg Hamiltonian

$$H = -J \sum_{(m,n)} [S_x^m S_x^n + S_y^m S_y^n + \lambda S_z^m S_z^n] \quad (2)$$

with (m,n) near-neighbor pairs on a square lattice. In a continuum approximation, unit strength vortex configurations behave as  $\phi = \tan^{-1}(y/x)$  and  $\theta = \frac{1}{2}\pi(1 - \exp(-r/r_v))$  for  $r \gg r_v$ ,  $\theta \rightarrow 0$ , as  $r \rightarrow 0$ , where  $S_x = S \cos\phi \sin\theta$ ,  $S_z = S \cos\theta$ ,  $r^2 = x^2 + y^2$ , and  $r_v$  is a vortex "core radius"  $a [2(1-\lambda)]^{-\frac{1}{2}}$  (lattice constant  $a$ ). It follows that  $S_z$  is only locally sensitive to the presence of vortices, whereas  $S_x$  and  $S_y$  are globally sensitive -- i.e. out-of-plane and in-plane spin correlations will reflect the vortex structure and mean separation (correlation length), **respectively** (c.f. solitons in 1-d easy-plane ferromagnets and antiferromagnets, respectively) and therefore the corresponding dynamic structure factors,  $S(\vec{q}, \omega)$ , are quite distinct.

Calculations of  $S_{xx}(\vec{q}, \omega)$  and  $S_{zz}(\vec{q}, \omega)$ , within the ideal vortex gas phenomenology, are given in Refs. [2]. The results are

$$S_{xx}^{\text{vortex}}(\vec{q}, \omega) \simeq \frac{S^2}{2\pi^2} \frac{\gamma^3 \ell^2}{\{\omega^2 + \gamma^2 [1 + (q\ell)^2]\}^2} \quad (3)$$

$$S_{zz}^{\text{vortex}}(\vec{q}, \omega) \simeq \frac{S^2 \pi^{3/2}}{4} \cdot r_v^2 \cdot \frac{n_v r_v^2}{\bar{u}/r_v} \cdot \frac{e^{-\omega^2/q^2 \bar{u}^2}}{qr_v [1 + (qr_v)^2]^3} \quad (4)$$

where  $\gamma = \frac{1}{2}\pi^2 \bar{u}/\ell$ , (correlation length)  $= \ell_0 \exp(b\tau^{-1/2}) = n_v^{-1/2}$ ,  $\ell_0 = O(a)$ , and  $\bar{u}$  is the rms vortex speed.  $\bar{u}$  and the forms (3,4) are calculated within an assumed Maxwellian vortex velocity distribution and fitted to the calculation of HUBER [13]:

$u(\tau) = (\pi b)^{1/2} (Ja/\hbar) \tau^{-1/2} (\exp(-b\tau^{-1/2}))$ . Here we have assumed the equilibrium temperature ( $\tau = T - T_c/T_c$ ) dependencies from Kosterlitz-Thouless thermodynamics. For the temperatures below,  $b$  is weakly  $\tau$ -dependent in the range (0.3, 0.5) [14].

Note the (squared) Lorentzian and Gaussian forms of the predicted central peaks (3,4), which we may characterize with widths ( $\Gamma$ ) and integrated intensities ( $I$ ):

$$\Gamma_z \approx uq \quad (5a)$$

$$\Gamma_x \approx \begin{cases} \bar{u}/\xi, & q\xi \ll 1 \\ \bar{u}q, & q\xi \gg 1 \end{cases} \quad (5b)$$

$$I_z \approx \frac{1}{2} S^2 \pi^2 n_v r_v^4 [1 + (qr_v)^2]^{-3} \quad (6a)$$

$$I_x \approx (S^2/4\pi) n_v \xi^4 [1 + (\xi q)^2]^{-3/2} \quad (6b)$$

We clearly observe the anticipated length scales  $r_v$  and  $\xi$  for out-of-plane and in-plane cases, respectively, yielding much larger intensities for in-plane scattering ( $\sim (\xi/r_v)^4$  relative to out-of-plane). Recent MC-MD simulation [1,2,15] have indeed observed central peaks for  $T > T_c$  and provided some striking agreements with the predicted forms (5) and (6). Examples are shown in Figs. 1(a) and 1(b) for the XY limit ( $\lambda = 0$ ), where we have also indicated predictions assuming  $b = 0.5$  and  $\xi_0 = a$ . Even better agreement may be obtained by fitting these parameters (since they are not exactly available from Kosterlitz-Thouless theory at these temperatures [14]). Remarkably, independent fitting for  $S_{xx}$  and  $S_{zz}$  gives agreement to within 20% for the parameters at several temperatures.

Theoretically, there are several important issues under continuing study, including: (i) a self-consistent calculation of the vortex velocity distribution function; (ii) vortex-vortex, vortex-spinwave, and multimagnon effects which appear to have significant effects on scattering intensity and  $q$ -dependence (especially for  $S_{zz}$ , c.f. 1-d easy-plane ferromagnets); (iii) extrinsic dissipation and impurity pinning effects; (iv) 3-d and Heisenberg crossovers; and (v) symmetry breaking (e.g. crystalline) fields which produce important additional collective **structures with slow** dynamics, e.g. domains, interacting with the vortices. (These are important, e.g., in  $Rb_2CrCl_4$  [12] and  $CoCl_2$ -intercalated graphite [10,16].) In addition, several quasi-2-d magnets are low-spin (e.g.  $K_2CuF_4$  [17] and  $BaCo_2(AsO_4)_2$  [12] are  $S = \frac{1}{2}$ ) so that quantum effects should be significant. Thermodynamic studies [18] suggest that, as in 1-d [8], the main quantum effects are reductions of **fluctuations intensities** (e.g. of specific heat). However, adequate description of quantum dynamics remains a major challenge in all dimensions.

Regarding inelastic neutron scattering data on real materials, conclusions must be tentative at this stage because systematic information on central peaks as functions of  $q$  and  $T$  is only now being gathered. However, as discussed elsewhere [2], preliminary evidence for  $K_2CuF_4$ ,  $Rb_2CrCl_4$  and  $BaCo_2(AsO_4)_2$  is quite consistent with our predictions at small  $q$  as far as central peak widths and some other trends (e.g. crossover from XY to Heisenberg behavior as  $q$  is increased at fixed  $\lambda < 1$ ) are concerned. Much more data and less ad hoc form fitting is anticipated in the near future. It will be especially helpful if the (weak)  $S_{zz}$  correlations can be measured. A very attractive possibility is that quasi-2-d magnets may provide good candidates [12]

for studying frustration dynamics - another context where collective structures are expected to control global response time scales but where current theoretical understanding is extremely poor.

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## REFERENCES

- [1] C. Kawabata, M. Takeuchi and A.R. Bishop, *J. Mag. Mag. Mat.* 54-57, 871 (1986).
- [2] F.G. Mertens, A.R. Bishop, G.M. Wysin and C. Kawabata, preprints (1987).
- [3] J.M. Kosterlitz and D.J. Thouless, *J. Phys.* C6, 1181 (1973).
- [4] K. Nakamura, Y. Okazaki and A.R. Bishop, *Phys. Rev. Lett.* 57, 5 (1986).
- [5] K. Nakamura, Y. Okazaki and A.R. Bishop, *Phys. Rev.* B33, 1963 (1986); *Phys. Lett.* A117, 459 (1986).
- [6] G.M. Wysin and A.R. Bishop, *J. Phys.* C19, 221 (1986); and in press.
- [7] G.M. Wysin and A.R. Bishop, *J. Phys.* C17, 5975 (1984).
- [8] G.M. Wysin and A.R. Bishop, *Phys. Rev.* B34, 3377 (1986),
- [9] C. Kawabata and A.R. Bishop, *Solid State Comm.* 60, 169 (1986).
- [10] C. Kawabata and A.R. Bishop, *Z. Physik* B65, 225 (1986).
- [11] J.C. Ariyasn and A.R. Bishop, *Phys. Rev. B* (in press);  
J. Pouget, S. Aubry, A.R. Bishop and P.S. Lomdahl, preprint.
- [12] E.g. L.P. Regnault and J. Rosat-Mignod, in Magnetic Properties of Layered Transition Metal Compounds, Eds. L.J. de Jongh and R.D. Willet;  
M.T. Hutchings et al., *J. Mag. Mag. Mat.* 54-57, 673 (1986).
- [13] See also earlier steps in this direction by D.L. Huber, e.g. *Phys. Rev.* B26, 3758 (1982).
- [14] S.W. Heinekamp and R.A. Pelcovits, *Phys. Rev.* B32, 4258 (1985).
- [15] A standard MC algorithm is used to initialize an equilibrium state for MD. Typically 5 averages on square lattices up to 100 x 100 have been used.
- [16] E.g. M. Elahy and G. Dresselhaus, *Phys. Rev.* B30, 7225 (1984).
- [17] E.g. K. Hirakawa et al., *J. Phys. Soc. Jpn.* 51, 2151 (1982).
- [18] E. Loh, Jr., D.J. Scalapino and P.M. Grant, *Phys. Rev.* B31, 4712 (1985).

FIGURE CAPTION

Fig.1 Widths ( $\Gamma_z$  and  $\Gamma_x$ ) and intensities ( $I_z$  and  $I_x$ ) of central peaks obtained in a numerical MC-MD simulation of the XY model ( $\lambda = 0$ ) on a 100 x 100 lattice for (a)  $S_{zz}(\vec{q}, \omega)$ , and (b)  $S_{xx}(\vec{q}, \omega)$  at a temperature  $T/J = 1.1$  ( $T_c/J \simeq 0.8$ ). Numerical data is shown as solid points. Solid lines result from Eqs.(5) and (6) without fitting parameters. The dashed line in (a) is a guide to the eye only - Eq.(6a) yields a significantly lower value at large  $q$  [2].



