Chapter Ten

Summary and Conclusions

10.1 Review of the New Results of these Studies

A summary of the new findings of these studies is given here. Most concern the classical dynamics of these kink excitations, as follows below.

The numerical simulations of easy-plane ferromagnetic kinks revealed a number of interesting properties of these modes. In general, the single kink energy dispersion is only described by sG theory in the limit of zero velocity, and only for fields $b = g\mu_B B/2AS$ less than the critical field $b_c = \frac{1}{3}$. For arbitrary fields below the critical field, the effective mass in this sG limit is greater than the sG mass. Also for $b < b_c$, the dispersion curve consists of three continuously connected branches. Branch I is the positive mass, positive velocity segment; branch II is the negative mass, positive velocity segment, and branch III is the negative mass, negative velocity segment. Above the critical field, only branch III exists. On all of these branches the kinks are dynamically stable. The instability predicted by Kumar (1982) and Magyari and Thomas (1982) does not cause a topological decay of the kink, but manifests itself in the unusual properties of the energy dispersion.

This instability also has its effect on the $K\bar{K}$ collisions. Generally, as a function of increasing magnetic field, the possible output states of a collision of an equal but opposite velocity $K\bar{K}$ pair range from sG-like transmission, to breather formation, to branch II to branch III reflection (and vice-versa below the critical field) to branch III reflection above the critical field. The sG transmission regime extends only to $b_1 \simeq 0.18\, b_c$. Most experiments have been done beyond this field,[1] and these results suggest that an interpretation in terms of a gas of perturbed sG kinks and antikinks is invalid. It is likely that breathers then become important for the thermodynamics.

The numerical simulations of xy kinks in the antiferromagnet have shown dynamic stability both above and below the critical field $\beta_c = 2\sqrt{\alpha}$. These kinks probably have an energetic instability similar to that of the branch I ferromagnetic kinks, in that the effective mass diverges and changes sign from positive to negative as the field is increased past the critical field.

By analytic linear stability analysis, it has been shown that static yz kinks in the antiferromagnetic are stable only if the field is greater than the critical field. Similarly, dynamic yz kinks are found to be stable only above a minimum velocity which decreases as the applied field increases. Or it can be said that they have a minimum field necessary for stabilty which decreases as the velocity increases. The more stable yz kinks are those whose sublattice planes are canted further toward the applied field direction compared to the ground state. These results were obtained by orienting the coordinate system such that the polar axis was parallel to the applied field, thereby explicitely taking the symmetry of yz kinks into account.

The xy and yz kinks are geometrically very similar, with only minor differences in the planes in which the sublattices move, such that a variational Ansatz has been made connecting the two. The Ansatz shows that the xy E(v) branch terminates into the yz branch, at the point corresponding to the stability limit for yz kinks. Only one of the two

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[1] For CHAB, b_c = 13.6 kG, b_1 = 2.5 kG, while for $CsNiF_3$, b_c = 18.6 kG, b_1 = 3.3 kG.

solutions given by the Ansatz always corresponds to a stable kink branch, as found by numerical simulation. The yz stability limits determined from the linear stability analysis were confirmed by the numerical simulations.

In Part II, quantum thermodynamics of spin-$\frac{1}{2}$ and spin-1 easy-plane ferromagnetic models in the presence of an applied magnetic field in the easy plane was studied using a quantum Monte Carlo method. In the checkerboard decomposition, vertex weights were found for a general 16 vertex spin-$\frac{1}{2}$ model, although its application to CHAB as a 16 vertex model was inefficient. A coordinate rotation resulted in a more efficient 8 vertex model, used to obtain the thermodynamics of CHAB. The effective Hamiltonian for the 2-D effective lattice was written out for the general 16 vertex model. Monte Carlo was applied to the 8 vertex model, and the results were compared with experimental data for CHAB. It was concluded that for this spin-$\frac{1}{2}$ system quantum effects are important, and that the sG phenomenological theory is of questionable applicability to CHAB.

Vertex weights have been found for a similar spin-1 easy-plane model that is equivalent to a 41 vertex model for the 2-D lattice. A flipping method was devised such that transitions to all possible output states for a given local move have equal a priori probability, a requirement for an unbiased algorithm. The model was used to study the thermodynamics of $CsNiF_3$, at low temperatures (less than 15 K) and fields less than 10 kG. The method was found to be inefficient for this problem -- an excessive amount of cpu time would have been necessary to reduce the statistical errors to a reasonable level. Therefore it is difficult to make any strong conclusions based on this study, although it is likely that quantum effects are important for a proper description of $CsNiF_3$. An encouraging result was that the positions of the peaks in ΔC vs. B_z at fixed T fit well to the available experimental data, although this result could be coincidental.

In conclusion, then, some unusual properties of the kink excitations in classical ferro and antiferromagnets with broken easy-plane symmetry have been demonstrated. These excitations are approximately described by sine-Gordon theory only for a small region of the parameter space, and more generally the energy dispersion can have both positive and negative effective mass regions, indicating very strong non-sG-like behavior. Curiously, the positive effective masses found are greater than the bare sG mass, in contrast to the standard (renormalized) reduced mass interpretation which has been given to much experimental data. The deviation from sG behavior is also apparent in the $K\bar{K}$ (computer) scattering experiments. These results provide cause for questioning the traditional soliton-spin wave gas interpretation of neutron scattering and specific heat experiments on materials such as $CsNiF_3$ -- a broader interpretation in terms of distorted kinks, breathers, and associated lifetimes may be necessary. Also, the quantum thermodynamics of spin-$\frac{1}{2}$ and spin-1 models for easy-plane broken symmetry ferromagnets has been studied using a quantum Monte Carlo technique. Results obtained for CHAB are consistent with experiment, although there are minor differences. Results obtained for $CsNiF_3$ are difficult to compare with experiment because of larger statistical fluctuations in the data. However, in both cases it is concluded that quantum effects play a strong role, and there should be further work done on these problems.

10.2 Possible Improvements and Extensions

There are a number of ways that these results can be extended and improved upon. Some ideas for obvious things to be done are given here.

It would be useful to have a complete solution of the dynamic stability equations for the static ferromagnetic kinks, equation (2-15). Then it might be easy to see how the instability found in the energetic stability analysis is capable of affecting the dynamics below the instability field. Also, for $b > b_c$, it is likely that a perturbation analysis starting from the exact known pulse modes of the isotropic limit with field might give the branch III kink properties approximately. Solutions of both of these problems will probably aid in understanding the dynamics of $K\bar{K}$ scattering. In any case, it would also be useful to determine the $K\bar{K}$ final state phase diagram in terms of the more appropriate parameter θ_m and b, in place of u_{sG} and b.

A slight improvement in the agreement between the results of the antiferromagnet Ansatz and the numerical simulation on a lattice might be obtained by including higher order terms in $\sqrt{\alpha}$, β and Δ which were previously dropped for simplicity. This is not expected to change the present results qualitatively, however.

More work is yet to be done concerning the analytic linear stability analysis of the static xy antiferromagnetic kinks, especially in solving the relevant stability equations. Also, there may be a possibility of obtaining an accurate dynamic xy kink solution, for which the dynamic kink stability analysis might be carried out.

Since the yz antiferromagnetic kinks are described accurately by an exact dynamic sG equation (in x-polar coordinates), probably a linear stability analysis of yz $K\bar{K}$ collisions can be performed analytically. Generally, however, we could also re-do the numerical study of antiferromagnetic $K\bar{K}$ collisions as was done for the ferromagnet, for both yz and xy kinks. The results presented here for the ferromagnet would suggest that sG transmission in general is not expected, especially for the xy kinks, since they appear to have an instability similar to that seen in the ferromagnet. Results of numerical $K\bar{K}$ collisions could then be compared with the yz $K\bar{K}$ stability analysis above and with the final state phase diagram for ferromagnetic kinks.

For the quantum Monte Carlo calculations, it seems likely that there may be more efficient flipping algorithms possible. One should know how to choose the proper proportions of column, row and square moves, or other types of moves, such that all microstates of the system are properly sampled.

In these calculations, the errors due to the finite in Trotter approximation were estimated only by looking at the trends with m in the data. Analytic calculations should be able to show specifically the functional dependence of the errors on m and the other parameters of the model.

It may be interesting to generalize the present Trotter formalism for two-site Hamiltonians to cases where there are next nearest neighbor interactions. In particular cases with competing nearest and next nearest interactions might be studied.

Finally, the transfer matrix approach could be used on the 2-D lattice in place of the Monte Carlo method, if an efficient, accurate method for determining the largest eigenvalue of the transfer matrix can be developed.

All of the above ideas are expected to lead to useful results, and are believed to be presently tractable. Work on these ideas is in progress.