A Novel 2-D Frustrated Antiferromagnet -- the Union Jack Lattice

C.J. Hamer, W.H. Zheng and J. Oitmaa

School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia.

We use series expansion methods to investigate a novel quantum spin-1/2 antiferromagnet, the Union-Jack lattice, at $T=0$. By expanding about the Ising ground state we investigate properties of the Néel phase and locate the quantum critical point where it becomes unstable.

1. Introduction

The physics of 2-dimensional quantum antiferromagnets on frustrated lattices is surprisingly rich, and not fully understood. There has been much study in recent year of the J_1-J_2 square lattice [1,2] (a model for Li_2VOSiO_4), the anisotropic triangular lattice [3] (a model for Cs_2CuCl_4), and the Shastry-Sutherland model [4] (a model for $SrCu_2(BO_3)_2$). These are shown in Figure 1.

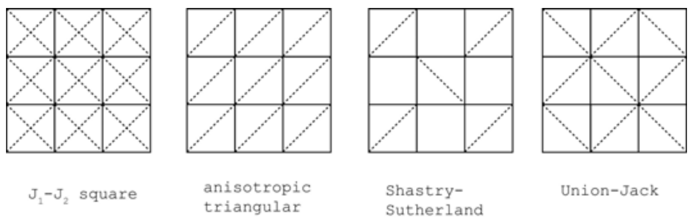


Fig. 1. Various frustrated antiferromagnets in 2-dimensions, with competing interactions J_1 (solid lines) and J_2 (dashed lines).

When the nearest neighbour interaction J_1 is dominant these systems have a Néel ordered ground state modified by quantum fluctuations. This will be destabilized by increasing the frustrating second neighbour interactions and Néel order will vanish at a **quantum phase transition** point. For large J_2 the ground state may show columnar order, spiral order or dimerization, depending on the model. All models show indications of an **intermediate phase**, sometimes referred to as a **spin liquid**, with no long range magnetic order.

To investigate this class of magnetic systems further we have introduced [5] another possible frustrated lattice, the **Union-Jack** lattice (Fig. 1). There is, as yet, no experimental realization of this model. This model will again exhibit Néel order for small J_2. Two questions suggest themselves:

- at what value $(J_2/J_1)_c$ does the Néel order vanish.
- what is the nature of the phase (or phases) for large J_2.

These questions have been addressed [5] using spin-wave theory with the following conclusions

- the Néel phase is stable up to $(J_2/J_1)_c \sim 0.84$, where a first-order transition occurs to a canted ferrimagnetic phase.
- two kinds of spin wave excitation exist (α and β bosons) with characteristic features.

However spin-wave theory is by no means always reliable for frustrated systems with strong quantum fluctuations.

In the present work we seek to confirm or correct the spin-wave predictions using the highly reliable systematic method of long series expansions [6], which our group at UNSW has developed and used for the last 15 years.

2. Method and Results

The Hamiltonian of the model is

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \bullet \mathbf{S}_j + J_2 \sum_{\langle kl \rangle} \mathbf{S}_k \bullet \mathbf{S}_l$$

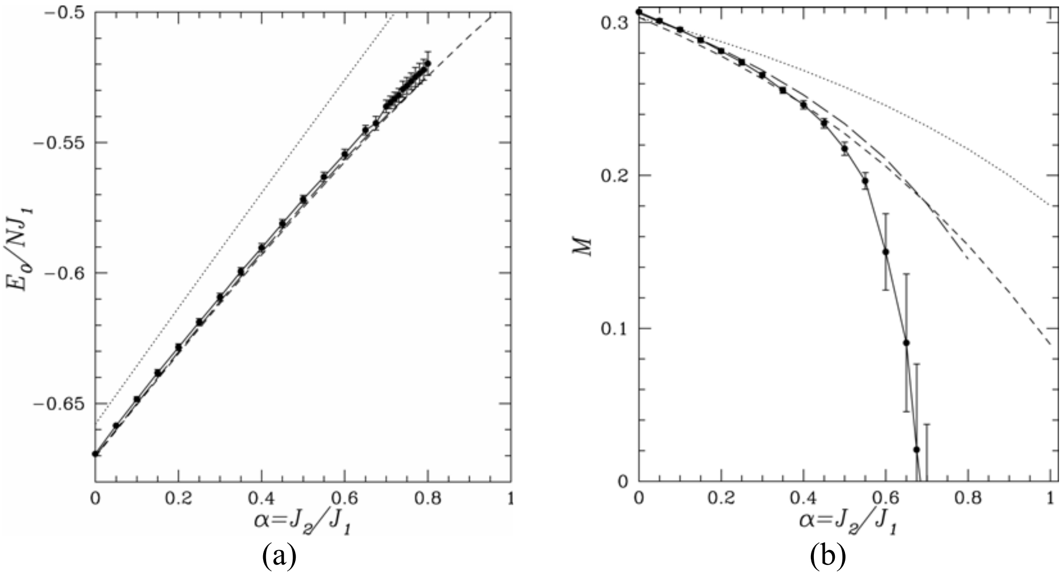
where the **S** are spin-1/2 operators and the summations are over the two types of bonds of strengths J_1 and J_2. To compute perturbation series we write this as $H=H_0+\lambda V$, with

$$H_0 = \sum_{\langle ij \rangle} S_i^z S_j^z + \alpha \sum_{\langle kl \rangle} S_k^z S_l^z$$

$$V = \frac{1}{2} \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + \frac{\alpha}{2} \sum_{\langle kl \rangle} (S_k^+ S_l^- + S_k^- S_l^+)$$

where $\alpha=J_2/J_1$ and, for convenience, we set $J_1=1$. This is an **Ising expansion**, in which the unperturbed Hamiltonian consists of the longitudinal (Ising) terms and the perturbation is the transverse quantum fluctuations. Series are derived, for fixed values of α, in powers of λ (up to order λ^{11}) for various quantities, and extrapolated via Padé and differential approximant methods to the isotropic limit $\lambda=1$.

We present various results and, where possible, compare them with the spin-wave predictions. Figure 2(a) shows the ground state energy. As is apparent, linear spin wave theory gives too high an energy, while 2nd order spin wave theory agrees rather well with the series results. Figure 2(b) shows the magnetization versus α. Here we see a clear discrepancy. The series results are suggestive of a second-order transition at $\alpha\sim 0.68$ whereas spin wave theory suggests a first-order transition at a larger value $\alpha\sim 0.84$.



(a) (b)

Fig. 2. Ground state energy (a) and magnetization (b) of the model, versus $\alpha=J_2/J_1$. The series results are shown as points (with error bars), while the dotted, short dashed and long dashed curves are the results of linear and two forms of 2nd order spin-wave theory.

To investigate the location and nature of the quantum phase transition further, we have derived and analysed series for the *correlator parameter*

$$\Delta C = | 3 \langle S_i^z S_j^z \rangle - \langle \mathbf{S}_i \bullet \mathbf{S}_j \rangle |$$

which is a measure of the breaking of spin rotational symmetry. This quantity is shown in Fig. 3, for both 1st and 2nd neighbours. In the Néel phase there is spontaneous breaking of spin rotational symmetry and $\Delta C \neq 0$. As is evident from the figure, ΔC appears to go to zero continously at $\alpha_c \sim 0.64(2)$, consistent with, but more precise than the estimate from the magnetization.

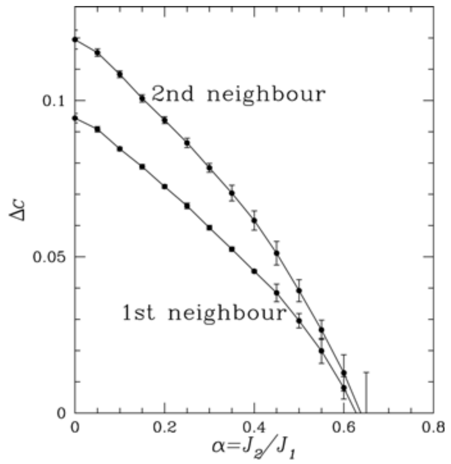


Fig. 3. Correlator parameter ΔC versus J_2/J_1.

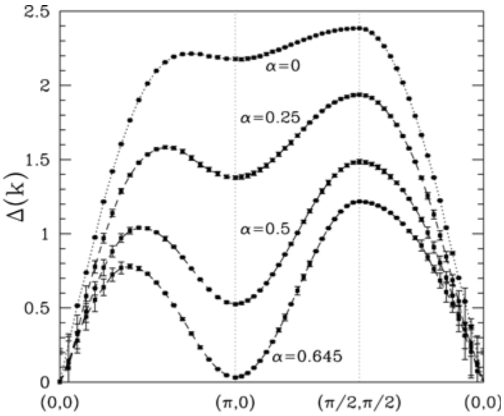


Fig. 4. Magnon dispersion curves.

The series method also permits calculation of the energies of elementary excitations. In Fig. 4 we show computed magnon (S=1) dispersion curves along symmetry lines in the Brillouin zone, for various α. The most striking feature is the softening of the energy at $(\pi,0)$ (and $(0,\pi)$) as α approaches the critical value $\alpha_c \sim 0.645$ where the gap vanishes.

3. Conclusions

The series expansion method gives a rather comprehensive picture of the Néel phase of the Union-Jack antiferromagnet, and indicates a second order transition at $\alpha_c \sim 0.645$, in contract to the first order transition at 0.84 predicted by spin wave theory. Further work will investigate the large J_2 canted phase and look for indications of a possible intermediate **spin liquid** phase.

Acknowledgments

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