

ESF-HFM short visit grant no. 3826 : Scientific report

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1 Purpose of the visit

The visit (from **17-01-2011 to 23-01-2011**) was undertaken with a view to start a scientific collaboration with Prof. Sylvain Capponi, Toulouse, on the spin-1/2 nearest-neighbour antiferromagnet on the *Kagomé* lattice. This report presents the research accomplished during this visit.

2 Details of research carried out during the visit

The main scientific objective of the visit was to explore the low energy phase diagram of the spin-1/2 *Kagomé* nearest-neighbour antiferromagnet using Contractor Renormalisation (CORE). The blocking unit we used for CORE is the 12 site "star" cluster shown in Fig 1. The *Kagomé* lattice is a triangular lattice of these clusters. This is a larger cluster than what was used in earlier studies [1, 2] and was first explored using perturbation theory in Ref. [3]. The symmetric and antisymmetric (and unimodular) linear combinations of two known exact ground states of the "star" cluster form the truncated basis for CORE.

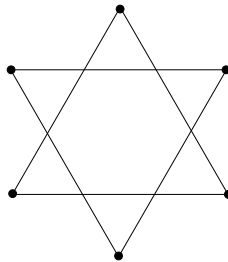


Figure 1: The blocking unit used for CORE

Prior to the visit preliminary results were obtained at the Technion (Auerbach, Chandra) concerning the effective Hamiltonian at range-2 of CORE. It

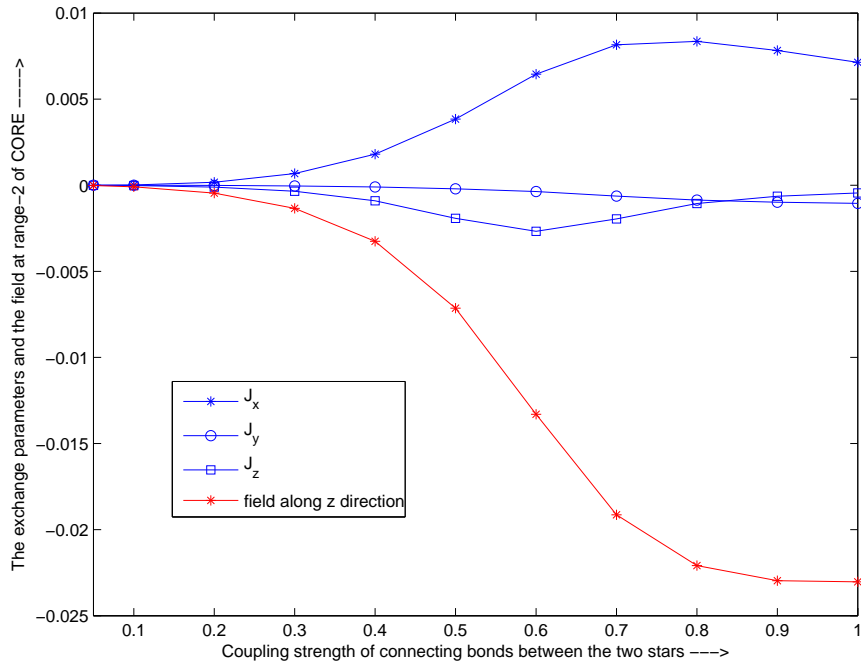


Figure 2: Variation of exchange and field terms of the range-2 effective Hamiltonian (Eq. 1) with coupling strength of bonds connecting the two stars. The energy scale is the set by the strength of the rest of the bonds which is 1.

was found that the effective Hamiltonian had anisotropic exchange and field terms.

$$H^{eff} = \sum_{\langle ij \rangle, \alpha} J_{\alpha} S_{i\alpha} S_{j\alpha} + h \sum_i S_{iz} \quad (1)$$

Where $\langle ij \rangle$ and α are the nearest-neighbour lattice site pairs and spin components respectively. The dominant terms correspond to a transverse field Ising model with the (large) field term dictating a ground state of the clusters all being in the symmetric state. In collaboration with Sylvain Capponi, we extended these calculations by weakening the bonds connecting the two stars and studying a range of coupling strengths of those bonds. The results of that calculation are shown in Fig. 2.

We found for most of the values of the coupling studied, including the isotropic point, that the nature of the effective Hamiltonian predicted using CORE at range-2 is different from the effective Hamiltonian obtained using degenerate perturbation theory in [3]. On general grounds one would expect the effective Hamiltonians to be similar at least for weak coupling between the two clusters. However, in contrast to our transverse field quantum model, the low energy effective model presented in [3] is a classical Ising ferromagnet on the

triangular lattice.

Following this, we computed for a three "site" connected cluster (36 sites of the original lattice) the energy eigenvalue approximations using range-2 CORE. The effective 8×8 Hamiltonian's spectrum was compared with existing exact diagonalisation spectra for 36 sites (Capponi) and we found that the range-3 contribution to the effective Hamiltonian is not negligible.

In light of these findings we decided to continue the collaboration along the following lines.

3 Future work

- We decided to revisit the perturbation theory presented in [3] and understand the origin of the different nature of the effective Hamiltonian at weak inter-block coupling when compared with a CORE calculation.
- Since we found the range-3 contribution in CORE to be important, we decided to evaluate the effective Hamiltonian at range-3. For computation of the spectrum and the necessary overlaps we plan to use either the Lanczos exact diagonalisation method using various symmetries or a new method for eigenvalue approximations presently under final stages of development [4].
- Ongoing studies on the *Kagomé* antiferromagnet using effective Quantum Dimer models indicate [5] that an additional weak next-nearest-neighbour coupling (ferromagnetic) might help to stabilise a 12-site valence bond crystal phase. In view of this we plan to extend the existing CORE calculations and include a weak next-nearest-neighbour-coupling and study both ferromagnetic and antiferromagnetic cases. This perturbation might thus help us in extracting a clearer picture of the phases of the nearest-neighbour model, which is currently under a lot of debate.

Our expectation is that the completion of these calculations will result in a significant body of results which can be published in the recent future.

References

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- [4] M. Weinstein, A. Auerbach, V. Ravi Chandra (in preparation)
- [5] D. Poilblanc, *Private communication*