Scientific Report:

Approximate Theoretical Methods Applied to Problems in Frustrated Quantum Magnetism

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Overview:

The Coupled Cluster Method (CCM; see, e.g., Refs. [1] chapter 7 and Ref. [2] chapter 10) is a well-known and powerful technique of quantum many-body theory. A computer code [3] has been developed by us that allows us to consider quantum spin systems, in principal, on any crystallographic lattice (including strongly frustrated spin systems) by using a range of "model states". Exact diagonalisations (ED; see, e.g., Ref. [1] chapter 2) provide another extremely useful method for treating a wide range of quantum spin systems. Another efficient ED computer code has been written by Joerg Schulenburg in Magdeburg [4]. Both CCM and ED methods may be applied to highly frustrated systems. The use of exact diagonalisations in tandem with the coupled cluster method (CCM) has been seen previously to provide an enormous insight into highly frustrated quantum magnets at T=0, e.g., as described in the final chapter of Ref. [2] chapter 11 where various methods are compared and contrasted for a wide range of (especially frustrated) quantum magnetic systems. A key part of this work has been the ongoing collaborations between theory groups in Manchester, UK (now also Glamorgan, Wales) and Magdeburg, Germany. The visit of DJJF to Magdeburg furthered our research into a wide range of problems in frustrated quantum magnetism.

Description of work carried out during the visit and anticipated resulting papers:

- An article [5] on an interpolating spin model between the maple-leaf and "bounce" lattices completed during visit. Awaiting full publication of a related experimental material before submission to *Phys. Rev. B* (thus, likely to be February/March 2011).
- Completed calculations and discussions regarding the spin-half frustrated J_1-J_2-J_3 model on the honeycomb lattice. First article now almost completed [6]. To be submitted to *Phys. Rev. Letts.* (probably March/April 2011). Second follow-up article [7] to be submitted to *Phys. Rev. B* (mid-2011).
- New CCM results obtained for the spin-half 1D J_1-J_2 model showing that collinear ordering wins over no-collinear ordering for $J_2/J_1>0.5$ – a probable case of "order-from-disorder." Article [8] written for submission to *Phys. Rev. Letts.* (March 2011).
- Article [9] written on CCM "benchmark" results for the spin-half square-lattice XXZ model. Submission early- to mid-2011.
- Discussion of ongoing CCM calculations for the spin-half Kagomé lattice antiferromagnet in an external field was completed. New calculations now underway. Paper [10] to be written in mid- to late-2011.
- Talk given during visit on the spin-half frustrated J_1-J_2 model on the square lattice comparing and contrasting results of CCM, ED, and cumulant series expansions. (New results for the excitation energy gap and "sign rules" are presented.) Article [11] describing these new results planned for late-2011/early-2012.

Future Collaborations and Mutual Projects:

- Ongoing visits of JR and/or his students to the University of Glamorgan, Cardiff, Wales, UK and DJJF to Magdeburg, Germany and DJJF to Magdeburg, Germany.
- Ongoing mutual development of the high-order CCM code via the Manchester/Glamorgan/Magdeburg "link" will occur.
- New frustrated spin problems will be analysed using high-order CCM and ED codes and academic articles written on the results of this research.
- Submission of an application for WE-Hereaus Workshop on "Quantum Magnetism in Low Spatial Dimensions." Physikszentrum, Bad Honnef, early-2012, Organisers: Prof. Raymond F. Bishop (raymond.bishop@manchester.ac.uk); Dr. Damian Farnell (d_j_j_farnell@yahoo.co.uk); Prof. Johannes Richter (johannes.richter@physik.uni-magdeburg.de); and, Dr. Juergen Schnack (jschnack@uni-bielefeld.de).

- Possible future, mutual grant applications to UK, German, and European research funding councils and other sources.

References

Books:

1. *Quantum Magnetism*, Series: Lecture Notes in Physics, Vol. 645, Schollwoeck, U.; Richter, J.; Farnell, D.J.J.; Bishop, R.F. (Eds.), (Springer Verlag, Heidelberg, 2004). Hardcover ISBN: 3-540-21422-4.
2. *An Introduction to Quantum Spin Systems*, Series: "Lecture Notes in Physics" Vol. 816. Written by J.B. Parkinson and D.J.J. Farnell. (Springer Verlag, Heidelberg, 2010). (Softcover ISBN: 978-3-642-13289-6).

Computer Codes:

3. The CCCM code: http://www-e.uni-magdeburg.de/jschulen/ccm/index.html
4. The Spinpack code: http://www-e.uni-magdeburg.de/jschulen/spin/

Some Recent Published Articles:

5. Coupled Cluster Treatment Of An Interpolating Maple Leaf/Bounce Heisenberg Antiferromagnet, R. Darradi, D. J. J. Farnell, R. Schmidt, and J. Richter, to be submitted to *PRB* (February/March 2011).
6. Deconfined Phase Transition of The J_1-J_2-J_3 Model on the Honeycomb Lattice, D.J.J. Farnell, J. Richter, R.F. Bishop, and P.Y. Li, , to be submitted to *PRL* (March/April 2011).
7. Phase Diagram of The J_1-J_2-J_3 Model on the Honeycomb Lattice, D.J.J. Farnell, J. Richter, R.F. Bishop, and P.Y. Li, to be submitted to *PRL* (mid-2011).
8. Collinear Versus Spiral Ordering In The One-Dimensional Spin-Half J_1-J_2 Model, D. J. J. Farnell, to be submitted to *PRL* (March/April 2011).
9. CCM Results for The Spin-Half XXZ Model on the Square Lattice, J. Richter, R. Zinke, J. Schulenburg, R. Darradi, and D. J. J. Farnell, article underway. Submission likely early- to mid-2011.
10. Spin-Plateau in the Spin-Half Kagomé-Lattice Antiferromagnet, O. Goetze, J. Richter, and D.J.J. Farnell. Article planned for mid- to late-2011.
11. Phase Diagram of the Spin-Half Frustrated J_1-J_2 Model on the Square Lattice, D.J.J. Farnell. Article planned for late-2011 to early-2012.