Scientific Report

Coupled Cluster Method (CCM) Calculations of Frustrated Quantum Magnets: The Manchester/Magdeburg Approach

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Overview:

The Coupled Cluster Method (CCM – see, e.g., Refs. [1-8]) is a well-known and powerful technique of quantum many-body theory. A computer code [9] 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 classical "model states". A recent and possibly important breakthrough by DJJF has been that we may form dimer and plaquette solid ground states using this code from these classical states. Another recent breakthrough has been the application of the CCM in order to study the lattice magnetisation of quantum magnets as a function of external magnetic field – including those systems with frustration. In particular, systems showing a magnetisation plateau can be analyzed. The primary aim of the funded research was to exploit these new results via preparation and publication of articles.

Furthermore, there is wide experience of the application of the CCM to quantum spins systems in both research groups in Manchester and Magdeburg. We note that the CCM is one of the methods of quantum many-body theory which can deal with strongly frustrated spin systems in any dimension and it can be therefore the method of choice for systems where other many body techniques fail (e.g. QMC for frustrated systems, DMRG for higher dimensions etc.). The secondary aim of the proposed short visit was to further develop these recent and exciting new features of the CCM and bring together the experience of both groups in the field of the methodology and the exotic properties of frustrated quantum spin systems.

Description of work carried out during the visit:

- Writing scientific articles (see below) to be submitted to academic journals in the near future.
- DJJF explained new results and workings/formalism of the high-order CCM codes to JR and his students, especially as this relates to the behaviour of antiferromagnets in external magnetic fields and spin plateaux.
- New spin problems currently being worked on in Magdeburg were introduced to DJJF so that DJJF could apply high-order CCM to these problems: namely, an interpolating antiferromagnetic model between the frustrated maple leaf and bounce lattices by one of JR's students (Rachid Darradi), and a frustrated Kagome-lattice antiferromagnet with nearest-neighbour and other bonds with a three-dimensional CCM model state by JR.
- Validation of the current high-order CCM code + creation of an archive of common problems treated by both groups.
- Discussions regarding the development of high-order CCM code by DJJF, namely, to consider spin-spin correlations and excited states in future.
- Discussions regarding future visits of another of JR's students (Ronald Zinke) to the United Kingdom n 2009/2010 (and how to obtain financial support for any visit, e.g., from the UK's Engineering and Physical Sciences Research Council) and a possible return visit of DJJF to Magdeburg in 2009.

Main results obtained:

- Existing CCM codes were validated and error-checked.
- DJJF's new results for AFs in external magnetic fields were also validated.
- Articles in progress were pushed forward significantly (see below).
- Significant development of the underlying CCM code is now scheduled.
- New frustrated models to apply these codes to were discussed during the visit.
- This constitutes a good "exchange of information" during the visit – as planned originally.

Future Collaborations:

- A visit of Ronald Zinke to Manchester, UK and DJJF to Magdeburg, Germany is planned.

- Ongoing mutual development of the high-order CCM code via the Manchester/Magdeburg link will occur.
- New frustrated spin problems will be analysed using high-order CCM and academic articles written on the results of this research.

Projected publications from the visit:

1. One article entitled "High-Order Coupled Cluster Method (CCM) Calculations for Quantum Magnets with Valence-Bond Ground States," by D.J.J. Farnell (University of Manchester), J. Richter, R. Zinke (Otto-von-Guericke Universität Magdeburg) and R.F. Bishop (University of Manchester) completed during visit with submission deadline to the *Journal of Statistical Physics* of May 2008.
2. Another article entitled "Coupled Cluster Method (CCM) Simulation of Two-Dimensional Frustrated and Unfrustrated Quantum Magnets in External Magnetic Fields" by by D.J.J. Farnell (University of Manchester), J. Richter and R. Zinke (Otto-von-Guericke Universität Magdeburg) greatly enhanced during visit. Submission deadline July 2008 to the *International Journal Modern Physics C*.

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