Highly Frustrated Spin-Lattice Models of Magnetism and Their Quantum Phase Transitions: A Microscopic Treatment via the Coupled Cluster Method

Raymond F. Bishop

School of Physics and Astronomy, The University of Manchester, UK

The coupled cluster method[1] (CCM) is one of the most pervasive, most powerful, and most successful of all ab initio formulations of quantum many-body theory. It has probably been applied to more systems in quantum field theory, quantum chemistry, nuclear, subnuclear, condensed matter and other areas of physics than any other competing method. The CCM has yielded numerical results which are among the most accurate available for an incredibly wide range of both finite and extended physical systems defined on a spatial continuum. These range from atoms and molecules of interest in quantum chemistry, where the method has long been the recognized "gold standard", to atomic nuclei; from the electron gas to dense nuclear and baryonic matter; and from models in quantum optics, quantum electronics, and solid-state optoelectronics to field theories of strongly interacting nucleons and pions.

This widespread success for both finite and extended physical systems defined on a spatial continuum[2] has led to recent applications to corresponding quantum-mechanical systems defined on an extended regular spatial lattice. Such lattice systems are nowadays the subject of intense theoretical study. They include many examples of systems characterised by novel ground states which display quantum order in some region of the Hamiltonian parameter space, delimited by critical values which mark the corresponding quantum phase transitions. The quantum critical phenomena often differ profoundly from their classical counterparts, and the subtle correlations present usually cannot easily be treated by standard many-body techniques (e.g., perturbation theory or mean-field approximations). A key challenge for modern quantum many-body theory has been to develop microscopic techniques capable of handling both these novel and more traditional systems. Our recent work shows that the CCM is capable of bridging this divide. We have shown how the systematic inclusion of multispin correlations for a wide variety of quantum spin-lattice problems can be efficiently implemented with the CCM.[3] The method is not restricted to bipartite lattices or to non-frustrated systems, and can thus deal with problems where most alternative techniques, e.g., exact diagonalisation of small lattices or quantum Monte Carlo (QMC) simulations, are faced with specific difficulties.

In this talk I describe our recent work that has applied the CCM to strongly interacting and highly frustrated spin-lattice models of interest in quantum magnetism, especially in two spatial dimensions. I show how the CCM may readily be implemented to high orders in systematically improvable hierarchies of approximations, e.g., in a localised lattice-animal-based subsystem (LSUBm) scheme, by the use of computer-algebraic techniques. Values for ground-state (and excited-state) properties are obtained which are fully competitive with those from other state-of-the-art methods, including the much more computationally intensive QMC techniques in the relatively rare (unfrustrated) cases where the latter can be readily applied. I describe the method itself, and illustrate its ability to give accurate descriptions of the ground-state phase diagrams of a wide variety of frustrated magnetic systems via a number of topical examples of its high-order implementations, from among a very large corpus of results for spin lattices.

The raw LSUBm results are themselves generally excellent. I show explicitly both how they converge rapidly and can also be accurately extrapolated in the truncation index, m → infinity, to the exact limit.

[1] R.F. Bishop, in Microscopic Quantum Many-Body Theories and Their Applications, (eds. J. Navarro and A. Polls), Lecture Notes in Physics Vol. 510, Springer-Verlag, Berlin (1998), 1

[2] R.F. Bishop, Theor. Chim. Acta 80 (1991), 95; R.J. Bartlett, J. Phys. Chem. 93 (1989), 1697.

[3] D.J.J. Farnell and R.F. Bishop, in Quantum Magnetism, (eds. U. Schollwöck, J. Richter, D.J.J. Farnell and R.F. Bishop), Lecture Notes in Physics Vol. 645, Springer-Verlag, Berlin (2004), 307.