## Spin-S Kitaev-Heisenberg model on the honeycomb lattice: A high-order treatment of its phase diagram via the coupled cluster method

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The coupled cluster method (CCM) [1] has become 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 chemistry, quantum field theory, atomic, nuclear, subnuclear, condensed matter and other areas of physics than any other competing method. It has yielded numerical results that 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 atomic physics and quantum chemistry, where the CCM 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 physical systems defined over a spatial continuum [2] has spurred recent applications to similar quantum-mechanical systems defined on an extended regular spatial lattice. Such lattice systems are the subject of intense theoretical study. They include many examples of systems characterized by novel ground states which display different forms of quantum order in different regions of the Hamiltonian parameter space, delimited by critical values that mark the respective quantum phase transitions.

We first discuss how the CCM may be applied in general to strongly interacting and highly frustrated spin-lattice models of interest in quantum magnetism, especially in two spatial dimensions [3]. We then describe very recent work [4] that has applied it to the spin-*S* Kitaev-Heisenberg model on the honeycomb lattice for values of the spin quantum number, S = 1/2, 1 and 3/2. This system is one of the earliest extensions of the Kitaev model and it contains two extended spin liquid phases. We show that the CCM fully captures the effects of the strong quantum-mechanical fluctuations that are present in generalized Kitaev models with competing bond-dependent anisotropies. We demonstrate that it predicts the phase boundaries of the two spin liquid phases accurately, as well as other transition points in the (zero-temperature) quantum phase diagram. Moreover, we find evidence of two narrow intermediate phases for S = 1/2: one is sandwiched between the zigzag and ferromagnetic phases, and the other lies between the Néel and the stripy phases.

[4] M. Georgiou, I. Rousochatzakis, D.J.J. Farnell, J. Richter and R.F. Bishop, "Spin-S Kitaev-Heisenberg model on the honeycomb lattice: A high-order treatment via the many-body coupled cluster method," <u>eprint arXiv: 2405.14378 (2024).</u>

<sup>[1]</sup> R.F. Bishop, "The Coupled Cluster Method," in <u>Microscopic Quantum Many-Body Theories and</u> <u>Their Applications, (eds. J. Navarro and A. Polls), Lecture Notes in Physics Vol. 510, Springer-Verlag, Berlin (1998), 1–70.</u>

<sup>[2]</sup> R.F. Bishop, "An Overview of Coupled Cluster Theory and its Applications in Physics," <u>Theor.</u> <u>Chim. Acta</u> 80 (1991), 95–148; R.J. Bartlett, "Coupled-Cluster Approach to Molecular Structure and Spectra: A Step Toward Predictive Quantum Chemistry," <u>J. Phys. Chem.</u> 93 (1989), 1697–1708.

<sup>[3]</sup> D.J.J. Farnell and R.F. Bishop, "The Coupled Cluster Method Applied to Quantum Magnetism," in <u>Quantum Magnetism</u>, (eds. U. Schollwöck, J. Richter, D.J.J. Farnell and R.F. Bishop), Lecture Notes in Physics Vol. 645, Springer-Verlag, Berlin (2004), 307–348.