Computational Studies on the Static and Dynamical Properties of One Dimensional Integer Spin Quantum Magnets

One dimensional quantum magnets have always been an active area of research due to their experimental realizability and the rich physics that they offer. By including geometrical frustration and additional interactions, it leads to even more novel and exotic quantum phases. In this thesis, we present the results of our investigations conducted by extending the quantum systems to spin-1. We conducted static, topological and dynamical calculations numerically on the spin-1 Heisenberg chain with Dzyaloshinskii–Moriya interaction in a uniform magnetic field in the form of a spin-1 Heisenberg chain in a helical magnetic field as well as the spin-1 Heisenberg model on the spin diamond and orthogonal dimer lattices. For the spin-1 Heisenberg chain in a helical field, we obtained the phase diagram using the density matrix renormalization group method and showed conclusively that the helical field destroys any topological order. We also obtained the dynamical spin structure factor spectra to study the magnon band structures and the softening of the modes near phase transitions. We then investigated the spin-1 Heisenberg model on the spin diamond and orthogonal dimer lattices using both exact diagonalization and the density matrix renormalization group method. We obtained the phase diagrams for both systems and explicitly calculated the magnetization, static spin structure and topological order of the different phases. Similar to the spin-1 Heisenberg chain in a helical magnetic field, we also obtained the dynamical spin structure factor spectra to study the characteristics of the lowest excitation occurring in both quantum systems.

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