DMRG studies of the ferromagnetic order in the ribbon and cylindrical geometry of CrI₃

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We investigate the magnetic properties of a monolayer chromium triiodide (CrI₃) [1]. CrI₃ bulk crystal reveals a layer-dependent magnetic phase, highlighting thickness-dependent physical properties typical for van der Waals crystals. It was shown by magneto-optical Kerr effect microscopy, that the monolayer is an Ising ferromagnet with out-of-plane spin orientation [1]. Theoretically, magnetic order is prohibited in the two-dimensional isotropic Heisenberg model at finite temperatures by the Mermin–Wagner theorem, but magnetic anisotropy removes this restriction. The XXZ Hamiltonian with anisotropy was proposed as the adequate spin model of this system [2].

In this work, we analyze CrI₃ monolayer in a ribbon and cylindrical geometry, both in finite and infinite cases using density matrix renormalization group (DMRG) method [3, 4]. DMRG is a method intended to study 1D systems, so it is ideal for proposed geometries. We will determine the magnetic properties of the ground state and analyze them as a function of the XXZ Hamiltonian parameters. The role of the anisotropic interactions will be determined.

References

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