DMRG studies of the ferromagnetic order in the ribbon and cylindrical geometry of CrI_3

Bartosz Rzepkowski[1], Michał Kupczyński[1], Paweł Potasz[1] and Arkadiusz Wójs[1]

[1] *Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Wrocław, Poland*

We investigate the magnetic properties of a monolayer chromium triiodide (CrI_3) [1]. CrI_3 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 CrI_3 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

[1] B. Huang et al *Layer-dependent ferromagnetism in a van der waals crystal down to the monolayer limit*, *Nature* **546** 270–3, (2017)

[2] J. L. Lado and J. Fernández-Rossier *On the origin of magnetic anisotropy in two dimensional CrI_3, 2D Mater.* **4** 035002, (2017)

[3] S. R. White *Density Matrix Formulation for Quantum Renormalization Groups*, *Phys. Rev. Lett.* **69**, (1992)

[4] A. E. Feiguin *The Density Matrix Renormalization Group*, A. Avella F. Mancini *Strongly Correlated Systems, Numerical Methods* pp 31-65, *Springer*, (2013)