Bachelor Thesis - Project Description

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Supervisors

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Title

DMRG on ALPS: a computational approach to explore novel quantum states in low-dimensional materials

Description

Currently, the design of 1D carbon-based materials with novel electronic and magnetic properties is an important field of research [1]. Efficient research is connected to synergy between experiments and simulations. A typical quantity that is measured experimentally reflecting the excitation spectrum of the material is the conductance (dI/dV), as a function of the bias voltage (V). Simulation of this quantity requires solving the model Hamiltonian that describes the material. For 1D materials, density matrix renormalization group (DMRG) is the most efficient method. There are libraries, such as ITensor [2], that already implement the main routines of DMRG. Building on top of them a simulation tool that is efficient and easily accessible to computational scientists but also experimentalist active on this research field would be valuable. Successful completion of the work will deliver to the scientific community a computational tool easily accessible via Aiidalab [3].

Goal

The goal is to have a set of DMRG codes that can work efficiently on the CSCS supercomputer ALPS [4], helping computational scientists and experimentalists in their field of studies. Applications of DMRG to realistic systems may require huge amount of memory, thus careful parallelisation of the code will be needed. The project will be based on the existing ITensor library and will be coded in Julia.

References

[1] Mishra, S., et al. Nature 598, 287–292 (2021)

[2] Fishman, et al. SciPost Physics Codebases 2022, 004.

[3] Yakutovich, A. V.; et al. Computational Materials Science 2021, 188, 110165.

[4] `https://www.cscs.ch/computers/alps`