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Title: Hybrid quantum-classical method for simulating high-temperature dynamics of nuclear spins in solids

Abstract:

We propose a new hybrid quantum-classical method for computing the free induction decay (FID) for spin $1/2$ lattices measured by nuclear magnetic resonance (NMR). The method is based on the simulations of a finite cluster of spins $1/2$ coupled to an environment of interacting classical spins via a correlation-preserving scheme. Such simulations are shown to lead to accurate FID predictions for one-, two- and three-dimensional lattices with a broad variety of interactions. The accuracy of these predictions can be efficiently estimated by varying the size of quantum clusters used in the simulations.

References:

Starkov G.A., Fine B.V., PRB 98, 214421 (2018) Starkov G.A., Fine B.V., PRB 101, 024428 (2020) This work is supported by grant from Russian Science Foundation (Project No. 17-12-01587)