Digital Quantum Simulation of the Statistical Mechanics of a Frustrated Magnet

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Many interesting problems in physics, chemistry, and computer science are equivalent to problems of interacting spins. However, most of these problems require computational resources that are out of reach with classical computers. A promising solution to overcome this challenge is quantum simulation. Several “analog” quantum simulations of interacting spin systems have been realized experimentally. However, relying on adiabatic techniques, these simulations are limited to preparing ground states. Here we report the first “digital” quantum simulation of thermal states; we used an NMR quantum information processor to simulate a three-spin frustrated magnet with Hamiltonian

\[ H = J(Z_1Z_2 + Z_2Z_3 + Z_1Z_3) + h(Z_1 + Z_2 + Z_3) \]

where $Z_k$ is the $z$-Pauli matrix of spin $k$, and for antiferromagnetic coupling ($J>0$), the ground state at zero field ($h=0$) and zero temperature is frustrated. Our implementation is able to explore the phase diagram of the system at any simulated temperature and external field. The results serve as a guide to identify the challenges for performing quantum simulation on physical systems at finite temperatures, and may lead to new methods for simulating open quantum systems in condensed matter physics and chemistry.

Experimental results for simulated entropy. (a) Entropy $S$ as a function of magnetic field $h$ at low temperature, $\beta=11=1/T$ (where $k_B=1$, and $h$ is given in units of the coupling $J$). The experimental data is plotted together with numerical simulation results that include effects of relaxation and decoherence of the nuclear spin qubits. The theoretical result is shown as the solid curve. The sharp changes of $S$ around $h=\pm2$ and $h=0$ indicate phase transitions. The points labeled “\textsuperscript{II}Experiment (R)\textquotedblright are obtained from the experimental data using a simple decoherence model (with no free parameters) that partially removes the effects of decoherence. (b-e) Surface plots of entropy as a function of $h$ and $\beta$ from theory (b), experiment (c) and simulation (d). Modified experimental results that partially remove decoherence effects are shown in (e).