Experimental Realization of a Compressed Quantum Simulation of a 32-Spin Ising Chain

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Certain n-qubit quantum systems can be faithfully simulated by quantum circuits with only $O(\log(n))$ qubits [B. Kraus, Phys. Rev. Lett. 107, 250503 (2011)]. Here we report an experimental realization of this compressed quantum simulation on a one-dimensional Ising chain. By utilizing an nuclear magnetic resonance quantum simulator with only five qubits, the property of ground-state magnetization of an open-boundary 32-spin Ising model is experimentally simulated, prefacing the expected quantum phase transition in the thermodynamic limit. This experimental protocol can be straightforwardly extended to systems with hundreds of spins by compressing them into up to merely 10-qubit systems. Our experiment paves the way for exploring physical phenomena in large-scale quantum systems with quantum simulators under current technology.

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Simulating quantum systems is one of the most essential issues in quantum science. However, simulating large-scale quantum systems with classical computers is unsustainable, due to the tremendous computational cost which grows exponentially with the size of the quantum system. By using quantum computation architecture, a universal quantum simulator only requires resources that grow polynomially with the size of the quantum systems [1,2]. In the past, quantum simulations of various interesting physical phenomena in small quantum systems have been well investigated experimentally, using several different physical systems [3–9]. Recently, there have been efforts to engineer the quantum simulator with hundreds of spins [10]. However, experimental quantum simulations of large-scale quantum systems are still a great challenge due to the limitation of controllability and scalability [11,12].

Recently the idea of compressed simulation was proposed [13], showing that a quantum simulator could be employed to simulate an exponentially larger system in certain cases. Explicitly, a matchgate circuit (MGC) running on n qubits could be simulated using $O(\log(n))$ qubits. By applying the compressed gates subsequently, the evolution of the original system is reproduced, which gives the observation of many quantities, such as magnetization and correlation functions. Moreover, the compressed simulation is an exact simulation of the original one without producing additional errors. Reference [14] proved that a one-dimensional (1D) Ising model and an XY model with size up to $n = 2^m$ particles can be simulated using only m qubits. Further theoretical investigations show that the simulation of several dynamical processes, like quantum quenching and finite time evolution, could also be compressed [15]. However, to our best knowledge, the experimental realization of compressed quantum simulation remains elusive.

In this Letter we report an experimental realization of the quantum simulation of a 2^5-spin Ising chain by using a 5-qubit NMR simulator. We develop a general quantum circuit running on $\log(n)$ qubits to mimic the behavior of an n-spin Ising model. A 5-spin NMR molecule is employed to simulate the adiabatic evolution of a 32-spin Ising chain. The magnetization of the Ising model is obtained by measuring the expectation value of the fifth qubit of the simulator. The experimental results are compared to the exact solution, which has demonstrated their reliability. This successful experimental implementation implies that the investigation of a variety of quantum systems with tens to hundreds of particles is accessible with current technology.

A quantum circuit running on n qubits could be compressed if it fulfills the following conditions [13]: (i) the quantum circuit only consists of nearest-neighbor matchgates (see note [16] for details); (ii) the input state of the circuit is the computational basis state, and (iii) the output is the result of a measurement on a single qubit of the computational basis. Then, the simulation could be implemented by using only $O(\log(n))$ quantum qubits. Generally, a MGC running on n qubits could be compressed to

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$R \in \mathrm{SO}(2n)$ acting on a Clifford algebra C_{2n} with $2n$ generators $c_{2k-1} = (\prod_{i=1}^{k-1} \sigma_z^i)\sigma_x^k$ and $c_{2k} = (\prod_{i=1}^{k-1} \sigma_z^i)\sigma_y^k$, where $k = 1, 2, \ldots, n$ and $\sigma_{x,y,z}^i$ denotes the Pauli operators for the ith spin.

Consider a matchgate U acting on the qubits $(k, k+1)$. Then we have

$$U^\dagger c_j U = \sum_{l=1}^{2n} R_{jl} c_l, \tag{1}$$

which holds for $j = 2k-1$, $2k$, $2k+1$, and $2k+2$. R is a real orthogonal matrix of $2n \times 2n$ associated with U. For a matchgate circuit $U = U_N \ldots U_1$, the compressed quantum circuit, denoted as W, is then $R_N \ldots R_1$, where R_i denotes the orthogonal matrix associated with U_i. When the final measurement can be represented by this Clifford algebra, e.g., the magnetization $\sigma_z^k = -ic_{2k-1}c_{2k}$, we have

$$\langle \sigma_z^k \rangle = \langle \Psi_{\mathrm{ini}} | U^\dagger \sigma_z^k U | \Psi_{\mathrm{ini}} \rangle = \langle 2k-1 | WSW^T | 2k \rangle, \tag{2}$$

where S is a $2n \times 2n$ matrix corresponding to the initial state $|\Psi_{\mathrm{ini}}\rangle$ of the original circuit. Hence, the MGC could be simulated using $O(\log(n))$ qubits by mapping the right hand of Eq. (2) into a quantum circuit.

Here we take the simulation of the 1D Ising chain as an example. Since the Ising model is solvable, it is a good example for the experimental validation of the compressed quantum simulation. The 1D quantum Ising model exhibits a phase transition when the control parameter is the ratio of the spin-spin coupling strength and the external magnetic field strength [17]. At the critical point, the second derivative of the magnetization is no longer continuous when the size of the model goes towards infinity. For finite system with size n, the crossover from paramagnetism to ferromagnetic order sharpens when n grows, as shown in Fig. 1. The ground-state magnetizations of the Ising model for size up to $n = 9$ have been simulated experimentally [18–20].

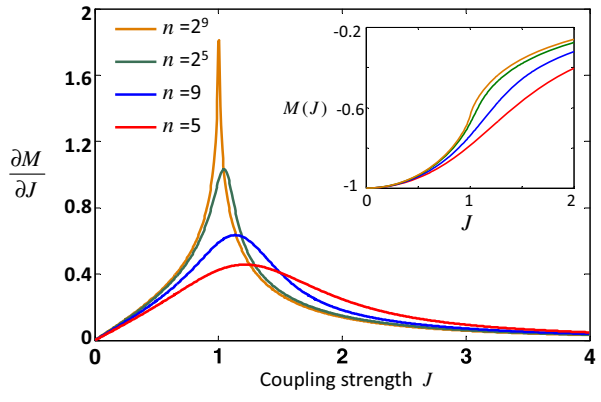

FIG. 1 (Color online) (color online). The ground-state magnetization $M(J)$ (inset) and its derivative with respect to coupling strength J in n-spin Ising chain.

The ground-state magnetization could be measured using the widely used adiabatic simulation method [21–23]. The Hamiltonian of the 1D quantum Ising model with open boundary conditions can be denoted by $H(J) = H_0 + JH_1$, where $H_0 = \sum_i \sigma_z^i$, $H_1 = \sum_i \sigma_x^i \sigma_x^{i+1}$ and J is the spin-spin coupling strength. The adiabatic evolution was approximated by L discrete steps. In the range $0 < J \leq 2$, we utilized the linear interpolation $J(l) = 2l/L$, $(l = 1, 2, \ldots, L)$. Thus the propagator for each step is $U_l = e^{-iH_l\tau}$, where τ is the duration of each step, and $H_l = H_0 + (2l/L)H_1$ is the intermediate Hamiltonian of the lth step. In each step, the Suzuki-Trotter expansion is used to decompose the unitary operation as

$$U_l = \sqrt{V_0} V_l \sqrt{V_0} + O(\tau^3), \tag{3}$$

with $V_0 = e^{-iH_0\tau}$ and $V_l = e^{-iJ(l)H_1\tau}$. The adiabatic condition and the Suzuki-Trotter approximation are satisfied when $L\tau \to \infty$ and $\tau \to 0$.

Starting from the ground state of H_0 (i.e., $|\uparrow\rangle^{\otimes n}$), the ground state $|\Psi_J\rangle$ of $H(J)$ could be obtained by applying U_l successively, from $l = 1$ to $l = JL/2$:

$$|\Psi_J\rangle = \left(\prod_l U_l\right) |\uparrow\rangle^{\otimes n}. \tag{4}$$

Then the magnetization of the ground state could be obtained by $M(J) = \sum_i \langle \Psi_J | \sigma_z^i | \Psi_J \rangle / n$.

Specifically, the adiabatic evolution of the n-spin Ising chain could be compressed to $m = \log(n)$ qubits [14,24]. The corresponding matrix of the initial state $|\uparrow\rangle^{\otimes n}$ is $S = -i\sigma_y^m + \mathbb{1}^{\otimes m}$, which equals $\rho_{\mathrm{ini}} = 2^{1-m}\mathbb{1}^{\otimes m-1} \otimes |+\rangle\langle+|$ in the m-qubit space, up to an ignorable factor. Here $|+\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$, being the eigenstate of σ_y with eigenvalue 1. Then we have the magnetization

$$M(J) = -\mathrm{Tr}[W(J)\rho_{\mathrm{ini}} W(J)^\dagger \sigma_y^m)], \tag{5}$$

with

$$W(J) = \prod_{l=1}^{JL/2} (U_d R_l R_0), \tag{6}$$

where R_0 and R_l are the compressed counterparts of V_0 and V_l in Eq. (3), respectively. Here $U_d = \mathbb{1}^{\otimes m} + (e^{i\phi_l} - 1)|1\rangle\langle 1|^{\otimes m}$ denotes a controlled phase gate. The magnetization $M(J)$ could be obtained by measuring the expectation value of $-\sigma_y^m$.

The compressed gates corresponding to V_0 and V_l are given by $R_0 = \exp(-2i\tau\sigma_y^m)$ and $R_l = [1 - \cos(\phi_l)](|1\rangle\langle 1| + |n\rangle\langle n|) + \cos(\phi_l) \times \mathbb{1}^{\otimes m} + \sin(\phi_l) \times \sum_{k=1}^{(n/2)-1} (|2k\rangle\langle 2k+1| - h.c.)$, with $\phi_l = 2J(l)\tau$ [24,25]. R_0 could be easily realized with a rotation along the y axis of the mth qubit. For R_l, by using the operators $T_+ = |1\rangle\langle n| + \sum_{k=1}^{n-1} |k+1\rangle\langle k|$ and $T_- = {T_+}^\dagger$, we have

$$T_+ R_l T_- = \mathbb{1}^{\otimes m-1} \otimes B_l - (|0\rangle\langle 0|^{\otimes m-1}) \otimes (B_l - \mathbb{1}), \quad (7)$$

where $B_l = e^{i\phi_l \sigma_y}$ is a single qubit gate. The right hand of Eq. (7) can be realized with a rotation on the last qubit $e^{i\phi_l \sigma_y^m}$ followed by an opposite rotation acting only on the subspace $|0\rangle\langle 0|^{\otimes m-1}$. The effective decomposition of compressed quantum circuit is depicted in Fig. 2.

The protocol of compressed quantum simulation is summarized as follows: (1) prepare the initial state $\rho_{\text{ini}} = 2^{1-m}\mathbb{1}^{\otimes m-1} \otimes |+\rangle\langle +|$; (2) evolve the system up to a certain value of J by applying $W(J)$; (3) measure the expectation value of $-\sigma_y^m$, i.e., the magnetization $M(J)$.

Now we turn to the experimental realization of the aforementioned scheme. With the well-developed control technology [27], nuclear magnetic resonance (NMR) has been widely utilized for many of the first demonstrations in quantum simulation. Here we use a 5-qubit NMR quantum system that consists of two ^{1}H nuclear spins and three ^{19}F nuclear spins. The experiments were carried out at 307 K on a Bruker AV-400 spectrometer. The sample we used is the 1-bromo-2,4,5-trifluorobenzene dissolved in the liquid crystal N-(4-methoxybenzylidene)-4-butylaniline (MBBA). The structure of the molecule is shown in Fig. 3. Due to the partial average effect in the liquid crystal solution, the direct dipole-dipole interaction will be scaled down by the order parameter [28]. As a result, the homonuclear dipolar coupling is much smaller than the difference between the chemical shifts of related nuclear spins. Therefore, in the rotating frame, the Hamiltonian for the homonuclear dipolar interaction reduces to the form of $\sigma_z^j \sigma_z^k$, as well as the heteronuclear situation. The effective Hamiltonian of this 5-qubit system in the rotating frame is

$$H_{\text{NMR}} = \sum_{j=1}^{5} \pi \nu_j \sigma_z^j + \sum_{1 \le j < k \le 5} \frac{\pi}{2} (J_{jk} + 2D_{jk}) \sigma_z^j \sigma_z^k, \quad (8)$$

with the parameters shown in Fig. 3. The deviation density matrix of thermal equilibrium state is $\rho_{\text{eq}} = \sum_{i=1}^{5} \gamma_i \sigma_z^i$, where γ_i represents the gyromagnetic ratio of each nuclear spin.

The experimental procedure consists of three parts: (i) state initialization (preparing the system to σ_y^5, which is equivalent to ρ_{ini} in NMR system), (ii) compressed simulation of the adiabatic evolution, and (iii) readout of the expectation value of $-\sigma_y^m$, i.e., the magnetization $M(J)$.

Starting from the thermal equilibrium ρ_{eq}, spin-selective pulses were applied to excite all the spins except for the fifth. Then a z-direction gradient pulse with length 1 ms was utilized to average out undesired excitations, leaving

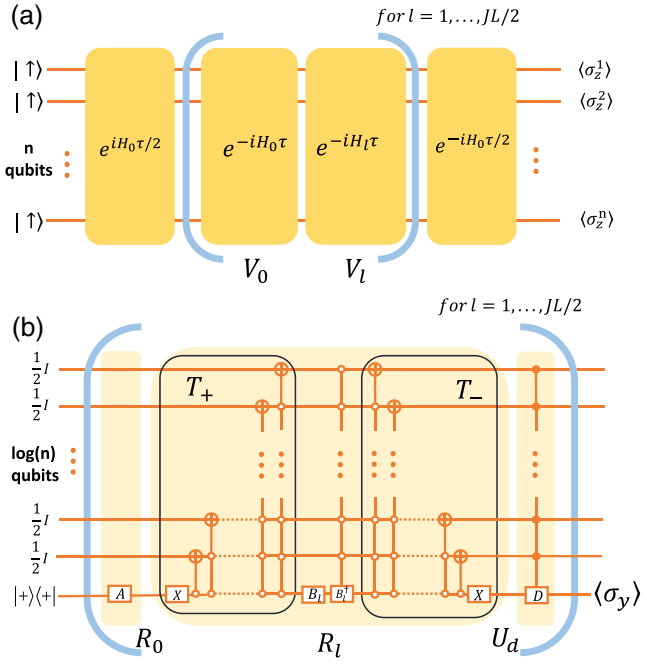

FIG. 2 (Color online) (color online). (a) Outline of the adiabatic simulation process of an n-spin Ising chain using n qubits. The initial state is prepared to the ground state of H_0, and the magnetization $M(J)$ is obtained by measuring the expectation value of σ_z for each qubit. (b) The quantum circuit of the compressed quantum simulation. Here, R_0 and R_l are the compressed counterparts of V_0 and V_l in (a), respectively. U_d is a controlled phase gate as defined in main text. X is a NOT gate, and $A = e^{-2i\tau\sigma_y}$, $B_l = e^{i\phi_l\sigma_y}$, $D = |0\rangle\langle 0| + e^{i\phi_l}|1\rangle\langle 1|$. All elementary gates in this circuit could be realized efficiently [26]. The magnetization is obtained by measuring the expectation value of $-\sigma_y^{\log(n)}$.

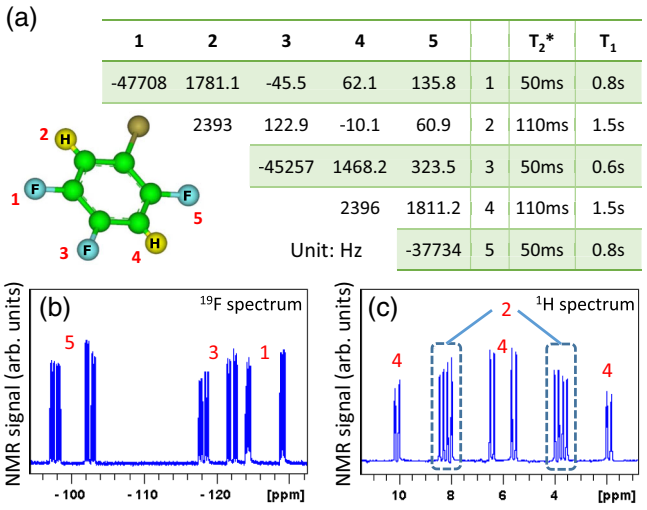

FIG. 3 (Color online) (color online). (a) Properties of the 1-bromo-2,4,5-trifluorobenzene molecule. The chemical shifts ν_i and effective coupling constants $(J_{jk} + 2D_{jk})$ are on and above the diagonal in the table, respectively. The chemical shifts are given with respect to reference frequencies of 376.48 MHz (fluorine atoms) and 400.16 MHz (hydrogen atoms). (b)(c) Equilibrium spectra of ^{19}F and ^{1}H nuclear spins. The numbers above the peaks are the indices of qubits.

only σ_z^5. Finally, a $\pi/2$ hard pulse along the x axis was applied to prepare the initial state σ_y^5.

In the second step, the adiabatic evolution of the Ising model was approximated by $L = 2400$ discrete steps. The propagator U_l for each step is displayed in Eq. (3) with $\tau = 0.1$. The numerical simulated results are shown in Fig. 4, showing a reliable approximation accuracy. The quantum circuit for adiabatic evolution is then compressed to the unitary operator $W(J)$ [Eq. (6)], whose effective decomposition is shown in Fig. 2. In experiment, we packed the circuit for each $W(J)$ into one shaped pulse calculated by the gradient ascent pulse engineering (GRAPE) method [29], with the length of each pulse being 50 ms and the number of segments being 1000. All the pulses have theoretical fidelities over 98% and are designed to be robust against the inhomogeneity of radio-frequency pulses.

Finally, we measured the expectation values of σ_y^5 for different values of J. The experimental NMR spectra for $J = 0$, 1, and 2 are shown in Fig. 4, along with theoretically simulated spectra. The sum of the intensities of all the peaks will produce the expectation value of σ_y^5. In our experiment, all the peaks suffer an obvious signal attenuation due to the decoherence effect in the process of the shaped pulses. Here we adopted the approach of Ref. [30] to characterize the decoherence effect. In the approach, the NMR experiment is divided into several slices where the power of the rf pulse is constant in every slice. Then every segment of slices is modeled by an ideal Hamiltonian evolution with an external rf field, followed by a phase damping channel acting on the spins with the same duration. By simulating the dynamical processes in each slice sequentially, the overall effect originate from decoherence could be estimated numerically. Firstly we measured the relaxation times in independent test experiments, and then utilized this approach to derive the reduction factor η for each shaped pulse in this experiment. The derived η was applied to rescale the experimental results. Figure 4(a) shows the experimentally acquired ground-state magnetization of the Ising model for various J values between $J_{\min} = 0$ and $J_{\max} = 2$.

The theoretical errors of this algorithm originate from the imperfection of the adiabatic simulation and the approximation of Trotterization. In our configuration, the adiabatic condition is well satisfied, and the produced errors are ignorable. The Trotterization will generate a fluctuation of magnetization around 0.01. In Fig. 4(a) the red curve shows the numerically simulated results taking these errors into account, compared to the exact solution (blue). We note that the compressed simulation is exactly equivalent to the original simulation without producing errors in the algorithm. This is also confirmed by a comparison experiment [24]. The signal attenuation in the experiment is mainly attributed to the spin-spin relaxation effect of the ^{1}H bath in the solution. The error originated from the statistic

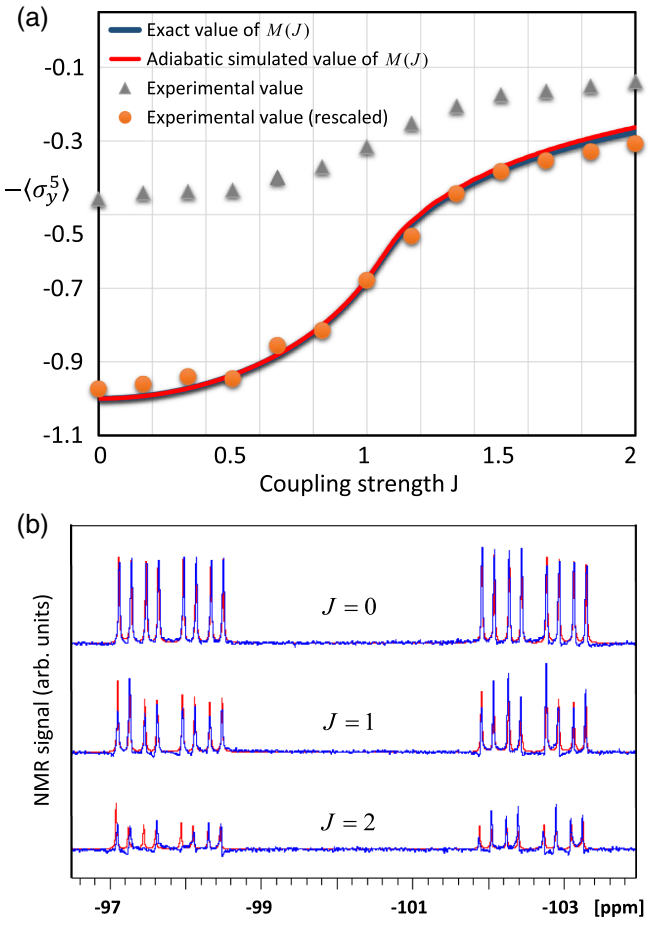

FIG. 4 (Color online) (color online). (a) The experimentally detected magnetization of 32-spin Ising chain for different J. The exact and adiabatic simulated solution are shown in blue (light) and red (dark) curves. Filled circles show the experimental results simulated by the 5-qubit NMR simulator, where rescaling was performed to extract the effect of decoherence. (b) The experimental spectra (blue) of the fifth qubit of final states for $J = 0$, 1, 2, compared with the simulated spectra (red). The vertical axes have arbitrary units but the same scale. Phase correction is performed to ensure that the sum of intensities of all peaks produces the expectation value of σ_y^5 .

fluctuation of signal strength is around 0.02. The inhomogeneity of magnetic fields is mostly diminished owing to the robustness of the GRAPE pulses. The theoretical infidelity of GRAPE pulses of no more than 0.02 will also contribute to the errors.

In conclusion, we have presented an experimental realization of a compressed quantum simulation which could mimic the behavior of an n-spin quantum system using $O(\log(n))$ qubits. In this experiment, a 32-spin Ising chain is successfully simulated by utilizing an NMR simulator with only 5 qubits. The experimental results are compared to exact solution and this has demonstrated the reliability. It is noted that (i) this experimental protocol could be straightforwardly extended to some other important quantum systems, such as the XY model [15] and Ising

model with inhomogeneous interactions and magnetic field strengths, (ii) the simulation is not limited to observation of magnetization or ground-state properties, and (iii) the compressed quantum simulation can be applied to several other important dynamical processes, like quantum quenching and finite time evolution. Our experiment implies that by using an exponentially smaller system, the investigation of a variety of quantum systems with hundreds of particles or more is accessible by using current technology. This marks an important step towards the quantum simulation of quantum systems in large scale.

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