# Quantum Simulation

## I. INTRODUCTION

Feynman's discussion [1] of the computational difficulties associated with the simulation of quantum mechanical systems hinges on the exponential growth of the size of Hilbert space with the number of particles in the system. Keeping track of all degrees of freedom is thus a computationally expensive problem (e.g., the dimension of the Hilbert space of 20 qubits is $> 10^6$). As a result, classical computers cannot generally simulate such quantum systems. Without proof, Feynman suggested that a quantum mechanical system might not have this limitation. Other researchers, e.g. Benioff, Bennett, Deutsch, and Landauer contributed to the discussion, but only in 1996 Lloyd [2] could prove that universal quantum simulators can be built from quantum mechanical systems. The different scaling behavior of classical and quantum computers has deep implications for the theory of computability[3]. Part of the research in quantum simulation was devoted to proofs of existence of universal quantum computers [2, 4]. In addition, a number of specific proposals have been put forward for relevant physical processes and interactions that can be simulated more efficiently by quantum computers than by classical devices.

## II. METHOD

A general scheme for quantum simulation is summarized by the following diagram:

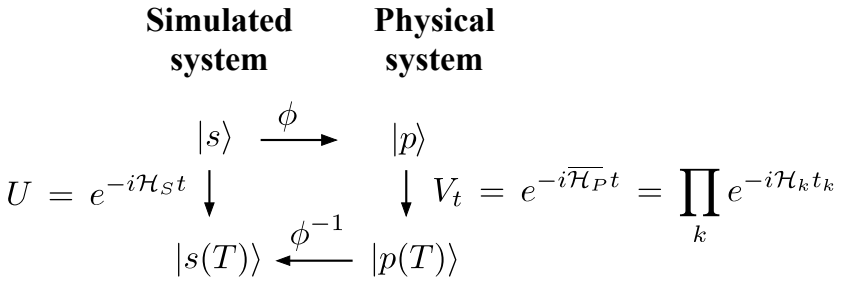


FIG. 1: Diagram of quantum simulation [5].

The task is to simulate the effect of the evolution $|s\rangle \xrightarrow{U} |s(T)\rangle$ using the physical system P. $\mathcal{H}_S$ is the desired Hamiltonian governing the simulated system, while $H_p$ is the Hamiltonian of the physical system we use. To do this, S is related to P by an invertible map $\phi$ that determines a correspondence between all the operators and states of S and P. Therefore, the challenge is to implement $V_T = \phi^{-1} U \phi$. In general, this evolution cannot be implemented in a single step. Instead, one decomposes the overall evolution into a series of steps, whose evolution $e^{-i\mathcal{H}_k t_k}$ can be generated in the system P using the available control operations. In our case (NMR), the control operations consist of radio frequency pulses, which rotate the spins, and free evolutions under the spin-Hamiltonian of the system.

One type of quantum simulation experiments has been established in NMR for a long time: Multiple pulse experiments, which were introduced by Carr and Purcell [6] and formalized and extended by Waugh and Haeberlen [7] and others. Experiments of this type are usually designed to simplify the Hamiltonian, keeping only a few of the spin-field and spin-spin interactions with specific properties. The resulting evolution $V_t = e^{-i\mathcal{H}_k t_k}$ can also be written as $V_t = e^{-i\bar{\mathcal{H}}_P t}$, where $\bar{\mathcal{H}}_P$ represents an effective or average Hamiltonian.

## III. RESULTS

### A. Quantum Phase Transitions

While classical phase transitions are usually driven by thermal fluctuations (energy vs. entropy) and occur at finite temperature, quantum phase transitions may occur at zero temperature and are driven by the change of a control parameter in the Hamiltonian of the system. An interesting aspect of these transitions is that the dynamic and static critical behaviors of quantum phase transitions are intimately linked. As a starting point for the simulation of quantum

phase transitions, we looked at the entangling transition of a Heisenberg spin chain: for large external magnetic fields, the ground state is ferromagnetic, but for small or vanishing external field, the spins pair antiferromagnetically and form an entangled state.

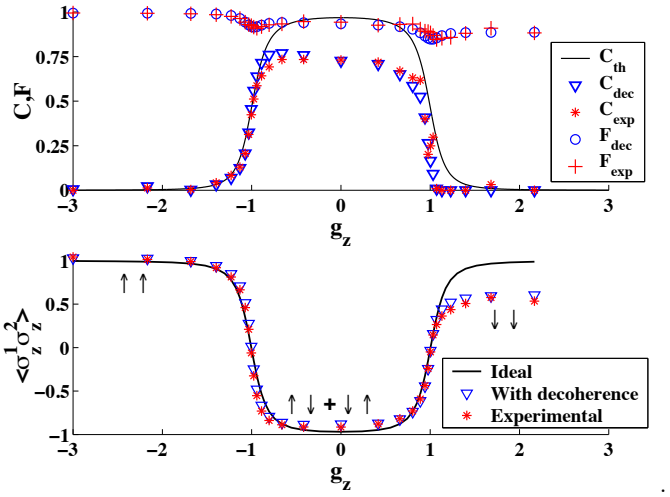


FIG. 2: Quantum phase transition of ground-state entanglement in Heisenberg spin chain [8].

This system can readily be simulated in an NMR quantum computer: a multiple pulse sequence generates the appropriate Hamiltonian, and by tuning the delays, it becomes possible to drive the system through the phase transitions. The results are shown in Fig. 2. For our simulation, we chose a system Hamiltonian that avoids degeneracies of the ground state. This allowed us to adiabatically change the Hamiltonian and observe how the phase change occurs in the system.

The first experiments were done on two- and three-qubit systems, and we now plan to proceed to longer chains and study changes in the systems' behavior as they get larger. Initial work is geared towards the examination of the ground state, but subsequent work will also look at excitations to study effects of finite (spin-)temperature. The finite-temperature behavior is predicted to scale with the size of the system [9]. It also leads naturally to the notion of a temperature-dependent dephasing length that governs the crossover between quantum and classical fluctuations.

### B. Localization

Localization transitions are among the most fascinating phase transitions. They relate to the fact that quantum mechanical ground states of ideal systems with no confining potential are often delocalized over the whole space, while random perturbations tend to result in localized ground states [10, 11]. The transition between the delocalized and the localized regime appears to show a critical behavior in many systems. However, analytical results are difficult to obtain, while numerical simulations are only meaningful if they use large systems, which results in difficult and costly computations.

NMR quantum simulators using magnetic dipole interactions between nuclear spins turned out to be a very attractive tool for studying localization [13, 14] and the associated phase transitions [12, 15]. In these simulations, an initially localized state is allowed to evolve under an effective Hamiltonian that generates correlations within a growing cluster of nuclear spins. Under these conditions, the size of the spin cluster appears to grow indefinitely. Perturbations can be added to this ideal evolution. This slows down the growth process and result in a finite equilibrium size of the spin cluster [12–15]. A detailed analysis of the dynamics of this quantum system reveals a distinctive critical behavior, which is a clear signature for the phase transition [12].

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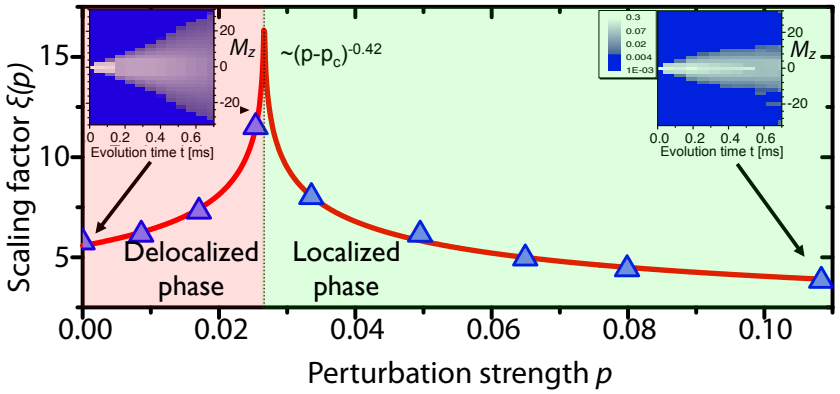


FIG. 3: Localization transition observed in a quantum simulator. The horizontal axis corresponds to the strength of a perturbation potential. For details see Ref.[12].


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