Chapter 5: Digital quantum simulation

I. QUANTUM LOGIC GATES

While the possibilities for quantum simulation based on ultracold atoms outlined previously have great potential, they are also somewhat constrained by the limits imposed by the contact interaction. In principle, it is possible to also include different interaction mechanisms such as the long-ranged dipole-dipole interaction [1], but as the ultimate goal, we would like to have a quantum simulator capable of simulating "any" quantum system. For practical purposes, we restrict the definition of such a universal quantum simulator to the simulation of Hamiltonians with short-ranged interactions [2], as all physical interactions reduce to purely local interaction at some point. Similar to numerical simulations on classical computers, it is also helpful to introduce abstraction layers so that we can use suitable approximations for the inner workings of the quantum simulator. If we decide to ignore the actual physical implementation for now, the lowest level we can consider is given by quantum logic gates, which have originally been discussed in the context of quantum computing [3].

Quantum logic gates are represented by unitary matrices that transform the quantum state before the operation into another after the application of the quantum gate. As such, they can be seen as the time-evolution operator acting for discrete timesteps,

$$|\psi(\tau_{n+1})\rangle = U(\tau_n, \tau_{n+1})|\psi(\tau_n)\rangle. \tag{1}$$

The basis set for the quantum state $|\psi\rangle$ is given by a product basis of two-level systems (quantum bits or "qubits"),

$$|\psi\rangle = \sum_{i\in\{0,1\},j\in\{0,1\},\ldots} c_{ij\ldots}|ij\ldots\rangle. \tag{2}$$

We can also think of the operation U to be constructed out of several smaller building blocks,

$$U(\tau_n, \tau_{n+1}) = \prod_i^N U(\tau_{n+(i-1)/N}, \tau_{n+i/N}). \tag{3}$$

For simplicity, we want to restrict ourselves to a universal set of quantum gates that can be used to construct any other gate from it. This can be realized by a set of three quantum

gates, including the z rotation gate,

$$R_z(\phi) = \exp(i\phi\sigma_z) = \begin{pmatrix} e^{i\phi} & \\ & e^{-i\phi} \end{pmatrix}, \tag{4}$$

where ϕ is an arbitrary rotation angle. To construct any other single qubit quantum gate, we need a second gate that does not commute with R_z. The most convenient choice is the Hadamard gate given by

$$U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5}$$

The Hadamard gate can be used to transform σ_z into σ_x and vice versa, i.e.,

$$R_x(\phi) \;=\; \exp(i\phi\sigma_x) = \begin{pmatrix} \cos\phi & i\sin\phi \\ i\sin\phi & \cos\phi \end{pmatrix} = U_H R_z(\phi) U_H \tag{6}$$

$$R_z(\phi) \;=\; U_H R_x(\phi) U_H. \tag{7}$$

Note that while the Hadamard gate is Hermitian, $U_H^\dagger = U_H$, most quantum gates are not. Finally, rotations about the y axis can be constructed as

$$R_y(\phi) = \exp(i\phi\sigma_y) = R_z(-\pi/4) R_x(\phi) R_z(\pi/4). \tag{8}$$

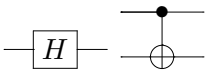
Single qubit rotation do not allow us to generate entanglement between the qubits. Therefore, it is necessary to include a two-qubit quantum gate, which is most coveniently chosen as the controlled-not (CNOT) gate, acting on two qubits A and B as

$$U_{CNOT} = |0\rangle\langle 0|_A \otimes 1_B + |1\rangle\langle 1|_A \otimes \sigma_B^x = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & & 1 \\ & & 1 & \end{pmatrix}. \tag{9}$$

Its function can be understood as follows: If the "control" qubit A is in the 0 state, nothing happens. However, if A is in 1, the "target" qubit B gets flipped by the σ_x operation. As an example, let us study the creation of entanglement between two qubits by a gate sequence consisting of a single Hadamard gate, followed by a CNOT operation. The qubits are initialized in the product state $|00\rangle$. Then, we have

$$|\psi\rangle = U_{CNOT} U_H^A |00\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \tag{10}$$

which is a maximally entangled state as its reduced density matrix is the maximally mixed state. The set of $R_z(\phi)$, U_H, and U_{CNOT} forms a universal set for all N-qubit quantum gates [4].



(a) (b)

FIG. 1: Circuit representation of the Hadamard gate (a) and the CNOT gate (b).

It is often convenient to use a pictorial representation for quantum gate networks, also known as quantum circuits. Each qubit is represented by a straight line, with the horizontal axis denoting time, and each single qubit gate is shown a rectangular box acting on the particular qubit. Two-qubit gates are represented in a similar way, with the control qubit being indicated by a small circle, see Fig. 1. In this notation, much more complex quantum circuits can be represented and analyzed, for instance the decomposition of the Toffoli gate,

$$U_T = \begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & & & & & 1 & \\ & & & & & 1 & & \end{pmatrix}, \tag{11}$$

which is a 3-qubit variant of the CNOT gate and is universal for all classical computations. It can be constructed from elementary gates, see Fig. 2, where $T = R_z(\pi/8)$ [3].

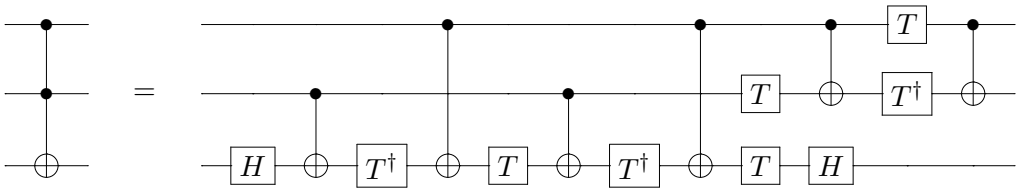


FIG. 2: Decomposition of the Toffoli gate into elementary quantum gates.

II. DIGITAL SIMULATION PROCEDURE

Suppose we want to simulate a four-body spin interaction of the form

$$H = E_0 \sigma_x^{(1)} \sigma_x^{(2)} \sigma_x^{(3)} \sigma_x^{(4)}. \tag{12}$$

This four-body spin operator has two eigenvalues, ± 1, which are eightfold degenerate. The key idea is to use an additional auxiliary particle and encode the eigenvalue into its spin state. If the auxiliary control spin is initially in $|0\rangle$, this can be done using the gate sequence

$$G = U_H^{(c)} \left(\prod_{i=1}^{4} U_{CNOT}^{(c,i)} \right) U_H^{(c)}. \tag{13}$$

To understand this in more detail, let us look at the behavior of the gate sequence on the spin state $|\pm 1, \lambda\rangle$, where λ labels the state within the degenerate manifold. The first Hadamard gate will yield

$$U_H^{(c)} |0\rangle_c | \pm 1, \lambda\rangle = \frac{1}{\sqrt{2}} (|0\rangle_c + |1\rangle_c) | \pm 1, \lambda\rangle. \tag{14}$$

Applying the sequence of CNOT gates will multiply the eigenvalue of the spin interaction, conditional on the control spin being in $|1\rangle$,

$$\prod_i U_{CNOT}^{c,i} \frac{1}{\sqrt{2}} (|0\rangle_c + |1\rangle_c) | \pm 1, \lambda\rangle = \frac{1}{\sqrt{2}} (|0\rangle_c \pm |1\rangle_c) | \pm 1, \lambda\rangle. \tag{15}$$

Finally, the second Hadamard gate will give us

$$\begin{aligned} U_H^{(c)} \frac{1}{\sqrt{2}} (|0\rangle_c + |1\rangle_c) | + 1, \lambda\rangle \;&=\; |0\rangle_c | + 1, \lambda\rangle \\ U_H^{(c)} \frac{1}{\sqrt{2}} (|0\rangle_c - |1\rangle_c) | - 1, \lambda\rangle &= |1\rangle_c | - 1, \lambda\rangle. \end{aligned} \tag{16}$$

Consequently, we have mapped the eigenvalue of the four-body interaction operator onto the state of a single auxiliary spin.

The full quantum simulation of the dynamics $U = \exp(-iHt)$ can then be realized by applying a z rotation to the control spin and reverse the mapping G,

$$U = \exp(-iE_0 \sigma_x^{(1)} \sigma_x^{(2)} \sigma_x^{(3)} \sigma_x^{(4)} t) = G R_z(-\phi) G. \tag{17}$$

The phase of the z rotation is related to the timescale of the simulation according to $\phi = E_0 t$.

For a many-body system, the full dynamics can be simulated if the gate sequences are applied in parallel (if they act on independent spins) or sequentially (if they act on the same

spins). However, in case of non-commuting operators, one has to ensure that this sequential operations does not introduce errors. This is true if the timestep τ of the simulation procedure is sufficiently small, as can be seen from the Suzuki-Trotter expansion

$$\exp[-i(H_A + H_B)\tau] = \exp(-iH_A\tau)\exp(-iH_B\tau) + O(\tau^2). \tag{18}$$

This completes the toolbox required for the realization of a universal quantum simulator.

III. IMPLEMENTATION BASED ON RYDBERG ATOMS

Let us now turn to a possible realization of such a universal quantum simulator based on ultracold Rydberg atoms [5]. The qubit states are formed by two hyperfine ground states. Single-qubit gates can be implemented using microwave driving described by the Hamiltonian

$$H = \begin{pmatrix} 0 & e^{i\phi}\Omega \\ e^{-i\phi}\Omega & \Delta \end{pmatrix}, \tag{19}$$

where Δ is the detuning of the microwave frequency from the resonance between the hyperfine levels, Ω characterizes the strength of the microwave field, and ϕ describes the phase of the microwave field at $t = 0$. This allows for the realization of arbitrary single-qubit gates.

For two-qubit gates, we need an interaction mechanism between the qubits. Ideally, we want the qubits to be separated by more than 500 nm, so they can be addressed independently using optical laser fields. Hence, we can think of the atoms being localized in individual sites of an optical lattice, forming the $n = 1$ Mott insulator. At such separations, however, the van der Waals interaction between ground state atoms is completely negligible. For dramatically increased interactions strengths, we will excite the atoms into a Rydberg state, which is an electronically excited state with a principal quantum number $n > 10$. In these highly excited states, the atoms behave almost hydrogen-like, and their eigenenergies are given by

$$E = -\frac{1}{2(n - \delta_l)^2}, \tag{20}$$

where δ_l is the quantum defect that accounts for deviations from the energy levels of hydrogen. For example, in rubidium in a $l = 0$ state, the quantum defect has been measured to be $\delta_0 = 3.1311$ [6].

In Rydberg states, the excited electron is only very loosely bound and therefore very sensitive to external perturbations. This is also true if the perturber is another Rydberg atom and leads to a dramatic increase in the van der Waals interaction coefficients, scaling as $C_6 \sim n^{11}$. At the same time, the lifetime limited by spontaneous emission also increases as $\tau \sim n^3$, leaving enough time to perform a quantum gate before the Rydberg atom decays. The strong interaction between Rydberg atoms leads to a blockade mechanism: if one atom has been excited to a Rydberg state, its neighbors can no longer be excited at the same time as the interaction energy changes the resonance condition [7]. To implement a CNOT gate, one first excites the $|0\rangle$ state of the control atom to the Rydberg state. Then, one tries to excite the target atom to the Rydberg state as well, which will only work if there are no interactions (i.e., the control atom is in $|1\rangle$), allowing for the conditional dynamics required for the implementation of the CNOT gate. The total gate requires a total of seven laser pulses and has been experimentally demonstrated in 2010 [8]. Scaling up to the case of many qubits required for a full-fledged quantum simulator is currently underway.

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