Rydberg Quantum Simulation
Ground State Preparation by Master Equation

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Quantum computation promises tremendous speedups compared to classical computation for certain tasks. Feynamn proposed that quantum computers can be used to simulate quantum system of the same class, i.e. with similar interactions. Albeit decoherence is normally tried to be avoided it can be used to imitate thermal effects in the system to be simulated. In this paper fundamental principles of quantum simulation are layed out and an implementation using Rydberg atoms is proposed. The Toric Code serves as a model Hamiltonian to show that dissipative dynamics can be simulated using the Rydberg quantum simulator.

Simulating dynamics of physical systems on a computer is a common way to study properties which measurement requires a high level of sophistication or to predict a behaviour to be reproduced by an experiment. This process is feasible for classical systems as the degrees of freedom increase linearly with the number of particles. Let $\mathfrak{S}$ be a system containing two particles p_1 and p_2, each having a number of degrees of freedom denoted by f_1, f_2. If these systems are coupled, even if the particles are to interact strongly, the total number of degrees of freedom is given by $f = f_1 + f_2$. In quantum mechanics we cannot apply this rule, because two systems are coupled by means of a *Kronecker product*, which results in an exponential growth of the Hilbert space with the number of particles, mathematically speaking $\mathscr{H}_1 \subset \mathbb{C}^{m\times n} \otimes \mathscr{H}_2 \subset \mathbb{C}^{p\times q} \to \mathscr{H}_{12} \subset \mathbb{C}^{mp\times nq}$. For a 40 spin one-half system the Hilbert space has a dimension of 2^{40} and to calculate the unitary time evolution one has to exponentiate a $2^{40} \times 2^{40} \approx 10^{24}$ matrix. The total number of particles in the universe is about 2^{300}, i.e. if we wanted to simulate more than 300 spin one-half particles we would need a computer that is larger than the universe.

It is strongly believed that the Fermi-Hubbard model describes high-T_c superconductors which are valuable for everyday life because the can transport electric current without any losses. Developments in recent years have pushed T_c more and more towards room temperature. It is still a game of trial and error to find the correct mixture of elements to obtain a high critical temperature. If one had a better understanding of the microscopic properties it would be much easier to engineer them for even higher temperatures. This knowledge could be obtained through quantum simulation. The Fermi-Hubbard model contains only nearest neighbour interactions it is hence a perfect candidate for quantum simulation. This paper will not directly deal with this model but provide simpler examples to lay the foundation for understanding the simulation of the Fermi-Hubbard model as proposed in [3–5].

In 1982 Feynman [1] conjectured that one could use quantum systems to simulate other quantum systems. He noted that analogies to phenomena of field theory can be found in solid state theory. He concluded that quantum systems form analogy classes where each can simulate any others dynamics, including a class that could simulate everything. Feynman furthermore devised that using a spin one-half system one could imitate any quantum system described by two base states. Lloyd [2] showed, that a quantum computer can simulate other quantum systems efficiently as long as the interactions are local and hence mutually commute.

In general decoherence and thermal effects are undesirable when doing computations with a quantum computer, because they shadow coherent effects, and a variety of quantum error correction algorithms have been developed to overcome this issue. In contrast, for the simulation of quantum systems one can exploit this property to imitate dissipation in the simulated system.

Every operation performed on a quantum system, such as a laser pulse, can be seen as a computational operation. The nature of the operation determines the effect on the system, it can either preserve coherence or introduce dissipation. The dissipative step is later introduced in terms of a master equation process. One can now choose these operations such that the system follows a particular interaction, which can then be used to realise a quantum logic gate.

Quantum simulation is viable if the Hamiltonian can be decomposed as follows

$$\mathcal{H} = \sum_{i=1}^{\ell} \mathcal{H}_i \,. \tag{1}$$

This is in general feasible for all Hamiltonian systems with local interactions. Because these local interactions mutually commute (approximately) the time evolution can be decomposed as well

$$\mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar} \approx \mathrm{e}^{\mathrm{i}\mathcal{H}_1 t/\hbar}\mathrm{e}^{\mathrm{i}\mathcal{H}_2 t/\hbar}\cdots\mathrm{e}^{\mathrm{i}\mathcal{H}_\ell t/\hbar}. \tag{2}$$

Rydberg atoms possess a large dipole moment which gives rise to strong Rydberg-Rydberg interactions. This stems from the fact that the van der Waals coefficient C_6

scales with the principal quantum number n[11]. When one atom is excited to a Rydberg state another atom in the vicinity cannot be excited to the Rydberg level at the same time because the aforementioned strong Rydberg-Rydberg interaction shifts the Rydberg level of the second atom out of resonance. This phenomenon is called the *Rydberg blockade* [6]. The blockade feature can be exploited to engineer quantum gates. In contrast to standard quantum gates, which can perform their respective operation only on one bit at a time, the long-range Rydberg-Rydberg interactions allow us to perform the gate operation on many atoms within the blockade radius, i.e. we can go massively parallel.

In the following text we're going to engineer a mesoscopic Rydberg CNOT gate. First of all we need to settle what the respective terms stand for. We start off with the CNOT gate: The CNOT gate is a two qubit gate where one qubit takes the role of a *control* qubit and the other of a *target* qubit. The target qubit is flipped depending on the state of the control qubit.

Let $|\alpha, \beta\rangle$ be a product of control and target qubit, where $\alpha \in \{0, 1\}$ denotes the control and $\beta \in \{A, B\}$ the target qubit, then the mapping of the CNOT operation is given by

$$\begin{aligned} \mathrm{CNOT}\,|0, A\rangle &= |0, A\rangle\,, \quad \mathrm{CNOT}\,|1, A\rangle = |1, B\rangle\,, \\ \mathrm{CNOT}\,|0, B\rangle &= |0, B\rangle\,, \quad \mathrm{CNOT}\,|1, B\rangle = |1, A\rangle\,. \end{aligned} \tag{3}$$

Above we already defined the term mesoscopic such that the gate will flip not only one but many target qubits.

$$\mathrm{CNOT} \to \mathrm{CNOT}^N\,. \tag{4}$$

The mapping rule needs to be modified then, as the single state of a sole target qubit is extended to a product state of all target qubits. Let $|A^N\rangle = \prod_i |A\rangle_i$, then

$$\begin{aligned} |0, A^N\rangle &\to |0, A^N\rangle\,, \quad |1, A^N\rangle \to |1, B^N\rangle\,, \\ |0, B^N\rangle &\to |0, B^N\rangle\,, \quad |1, B^N\rangle \to |1, A^N\rangle\,. \end{aligned} \tag{5}$$

The benefit in the realisation using Rydberg atoms is, that the gate is actually independent of the number and the position of the target qubits as long as they reside within the blockade radius of the control qubit.

The CNOT gate operator is defined as a product of control and target qubit operators [7].

$$U = |0\rangle\langle 0|_c \otimes \mathbb{1} + |1\rangle\langle 1|_c \otimes \prod_{i=1}^{N} \sigma_x^{(i)} \tag{6}$$

The first summand is the projection onto state $|0\rangle_c$ for the control qubit and unity for the target qubit, i.e. if the control qubit is in $|0\rangle_c$ nothing happens to the targets. The second summand is the projection onto $|1\rangle_c$ and a product of the σ_x-Pauli-matrices which perform a spin flip of the respective target qubit. The gate operation is unitary, so it can be reversed.

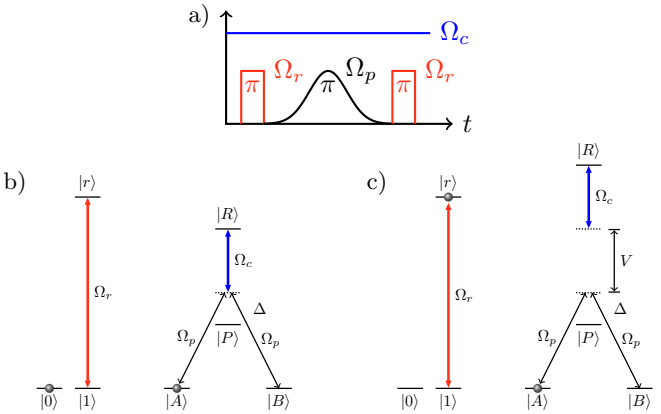

FIG. 1. Laser pulse sequence and level scheme for a Rydberg gate based on EIT. *a*) Ω_r is the excitation laser of the control atom, Ω_p is the Raman laser to perform the flip of the target atoms and Ω_c is the coupling laser to the Rydberg level of the target atoms. *b*) Level scheme for the scenario $|0\rangle_c$. *c*) Level scheme for the scenario $|1\rangle_c$.

The explicit level scheme and laser pulse sequence for such a setup is given in figure 1 as inspired by [3]. There are two possible scenarios

Control atom in $|0\rangle_c$: The π-pulse of the laser Ω_r is applied to excite the control atom from $|1\rangle$ to $|r\rangle$. This doesn't take place because the control atom is in $|0\rangle$. If we have a very strong laser field $\Omega_c \gg \Omega_p$ which couples to $|R\rangle$ then the atom is on two-photon resonance from the hyperfine ground states to the Rydberg state and the $|P\rangle$-level is dark. Thus the atom is transparent for the laser field Ω_p and nothing happens.

Control atom in $|1\rangle_c$: Now the control atom can be excited from $|1\rangle$ to $|r\rangle$. For the ensemble atoms we want to make a far off-resonant Raman transition from $|A\rangle$ to $|B\rangle$. Due to the Ryd-Ryd interaction the $|R\rangle$ level is shifted out of resonance and thus the EIT condition is violated. Two photon resonance is no longer feasible and the Raman transition takes place.

In the previous paragraph we exploited long-range Rydberg-Rydberg interactions to realise a many-body quantum gate. The question is then, can we use many-body gates to simulate many-body dynamics?

The prime example in condensed matter physics is the so called Toric Code. Actually the Toric Code was intended to serve as a fault tolerant quantum memory because information is encoded in topological properties, such as the winding number of a torus (hence the name "Toric Code"), but the system is also analytically solvable and exhibits interesting physical properties such as topological phases and anyonic exciations (depending on the boundary conditions) [4].

The Toric Code is a Hamiltonian which involves many body interactions [3–5]. It consists of spins located on the edges of a lattice. There are two types of local four-body interactions, so called stabilisers.

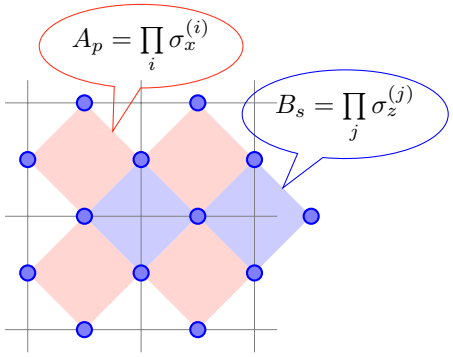

FIG. 2. Visualisation of a finite subset of the Toric Code Hamiltonian. In this and all other sketches involving the Toric Code the red squares correspond to plaquette interactions and the blue squares to star interactions.

- Plaquette interactions $A_p = \prod_i \sigma_x^{(i)}$
- Star interactions $B_s = \prod_j \sigma_z^{(j)}$

The Hamiltonian itself is a linear superposition of these local interactions

$$\mathcal{H} = -\sum_i A_p^{(i)} - \sum_j B_s^{(j)} \tag{7}$$

The model is exactly solvable and has a unique global ground state with the properties

$$A_p \left|\psi\right\rangle = \left|\psi\right\rangle \ , \quad B_s \left|\psi\right\rangle = \left|\psi\right\rangle . \tag{8}$$

The stabilisers of the Toric Code can be violated by flipping one of the spins taking part in the ineraction thus changing the sign of the eigenvalue. There are two types of exciations, viz. magnetic excitations $A_p \left|m\right\rangle = -\left|m\right\rangle$ and charge excitations $B_s \left|e\right\rangle = -\left|e\right\rangle$.

Before we move on to the dynamics of the excitations we introduce the dissipative state preparation [8, 9]. Dissipation is introduced by a coupling to a heat bath $V(t)$ with which energy can be exchanged. One can derive the Lindblad form by assuming that the system is Markovian (for more details see [8]), i.e. the system forgets its previous states really fast. Then the time evolution of the density matrix can be described as an exponential multiplied with the initial density matrix.

$$\varrho(t) = V(t)\varrho(0) = \mathrm{e}^{\mathcal{L}t}\varrho(0). \tag{9}$$

In the exponential one has the superoperator $\mathcal{L}$ which adds the dissipation to the system. Calculating the time derivative yields an equation similiar to the Liouville-van-Neumann equation [8, 9].

The Lindblad Master Equation is a generalised form of the Liouville-von-Neumann equation with an additional term which introduces the dissipation by jump operators

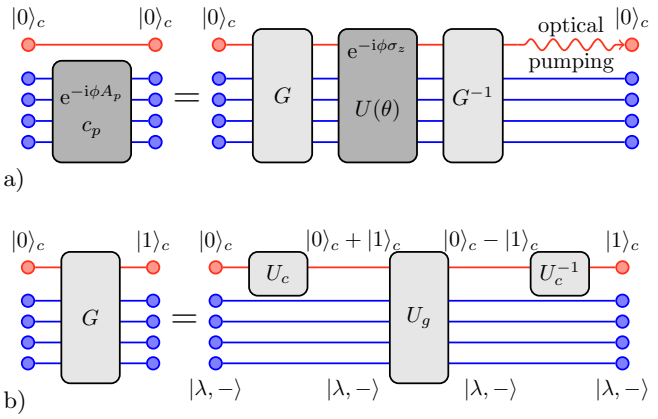

FIG. 3. Gate sequences. *a*) The decomposition of the whole time step into three gates and a dissipative step. *b*) Decomposition of the gate G into three processes, viz. entanglement U_c, mapping U_g and reversed entanglement U_c^{-1}.

c_i and decay rates γ_i [8, 9].

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho = -\frac{\mathrm{i}}{\hbar}[\mathcal{H}, \varrho] + \sum_i \gamma_i \left(c_i \varrho c_i^\dagger - \frac{1}{2}\{c_i^\dagger c_i, \varrho\} \right). \tag{10}$$

Here we define a dark state to be a state for which all coupling to the reservoir vanishes [4]

$$c_i \left|D\right\rangle = 0. \tag{11}$$

The dark state is now a stationary state of the system and the pure state $\left|D\right\rangle$ is a trivial solution to the master equation $\varrho = \left|D\right\rangle\left\langle D\right|$.

We want to find a jump operator which dark state is also the ground state of the whole system and which cools itself into the ground state, i.e. applying the jump operator on an arbitrary state a number of times should result in the ground state.

For the Toric Code plaquette interactions one chooses the jump operator

$$c_p = \frac{1}{2}\sigma_z^{(i)}(1 - A_p). \tag{12}$$

This operator is constructed in a manner $c_p = \mathrm{THEN} \cdot \mathrm{IF}$, i.e. it exhibits conditional behaviour. If the system is in the ground state the eigenvalue of A_p is $+1$, thus the second term vanishes (the ground state is the dark state in accordance with the definition above). If the system is in the excited state with eigenvalues -1 of A_p, then the second term will not vanish and the correction term $\sigma_z^{(i)}$ is applied to an arbitrary spin i on the plaquette. The correction term leads to the stabiliser condition ($A_p \left|\psi\right\rangle = \left|\psi\right\rangle$ for the plaquette) to be violated and a possibly present excitation will diffuse to the plaquette adjacent to the alternated spin i. If two excitations meet they annihilate each other.

Because all the interactions are local we can focus on a single plaquette to understand the quantum simulation. The Hamiltonian for a single plaquette reads [4]

$$\mathcal{H} = A_p = \sigma_x^{(1)}\sigma_x^{(2)}\sigma_x^{(3)}\sigma_x^{(4)}$$

The evolution of the system can be decomposed into a sequence of several quantum gates (see figure 3). One can show that the gate sequence is equivalent to the many-body interaction A_p, i.e.

$$\exp(-\mathrm{i}\phi A_p) = G^{-1}\exp(-\mathrm{i}\phi\sigma_z^{(c)})G. \tag{13}$$

Let us try to gain a better understanding of the depicted gate sequence. A coarse explanation of the sequence a) in figure 3 would be the following, cf. Weimer *et al.* [4]

- G entangles the control atom and the target atoms.
- The control atom is propagated coherently with $\mathrm{e}^{-\mathrm{i}\phi\sigma_z}$. A controlled spin flip $U_i(\theta)$ is performed onto the ensemble atom i.
- G^{-1} reverses the entanglement.
- Because dynamics of the system must not affect the state of the control atom it has to be optically pumped back into the $|0\rangle_c$ state which introduces the dissipative step.

Now for the detail. The gate G can be decomposed into three steps. First the control atom is rotated with U_c by $\pi/2$ into a superposition state. Then the gate U_g is performed which is given by (6), this will map the internal state of the ensemble atoms onto the control atom, viz. a state with eigenvalue $+1$ will not affect the control atom and a state with eigenvalue -1 will flip the sign of the $|1\rangle_c$ component. If then U_c^{-1} is applied to rotate back the control atom is reversed to either $|0\rangle_c$ or $|1\rangle_c$. If the ensemble atoms are in a state $|\lambda,+\rangle$, meaning in an arbitary state $|\lambda\rangle$ with eigenvalue $+1$ (which is the ground state), then the control atom will be in $|0\rangle_c$ at the end of G. Similarly the control atom will end up in $|1\rangle_c$ for the ensemble atoms being in $|\lambda,-\rangle$. This means that the gate is set up such that a flip of the control atom takes place if they are not in the ground state.

The aforementioned flip of one of the ensemble atoms is described by an operator $U_i(\theta)$ which functional form reads

$$U_i(\theta) = |0\rangle\langle 0|_c \otimes \mathbb{1} + |1\rangle\langle 1|_c \otimes \exp(\mathrm{i}\theta\sigma_z^{(i)}). \tag{14}$$

As already mentioned this operation, in combination with the mapping operation, leaves the ground state $|\lambda,+\rangle$ invariant. If the system is in the excited state a flip onto ensemble atom i is performed by $\exp(\mathrm{i}\theta\sigma_z^{(i)})$. One can see that the probability of the flip taking place depends on the angle θ. If the control qubit is mapped to $|1\rangle_c$ it resides there and the entanglement is not reversed by G^{-1}.

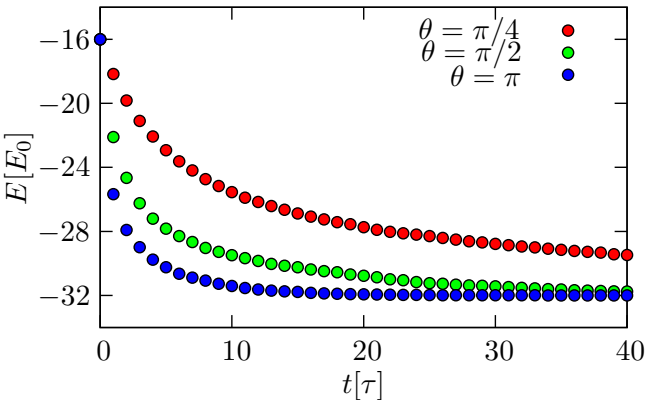

FIG. 4. Numerical simulation of the ground state preparation for a Toric Code with 32 spins, taken from [5]. This result makes clear that the fastest cooling is obtained for $\theta = \pi$.

If the control atom is now optically pumped back to state $|0\rangle_c$ the whole system evolves according to a Lindblad Master equation [4]

$$\partial_t\varrho = \gamma\left(c_i\varrho c_i^\dagger - \frac{1}{2}\{c_i^\dagger c_i, \varrho\}\right) + \mathcal{O}(\theta^3). \tag{15}$$

Each spin flip moves an excitation to the adjacent plaquette. For $\theta = \pi$ this move takes place with unity probability, i.e. one obtains the fastest cooling. This is obvious to see in figure 4, where the results for cooling a Toric Code containing 32 spins are depicted [5].

There are a couple of take-home messages in this paper. Feynman [1] and Lloyd [2] stressed that simulating quantum mechanics on a computer is exponentially hard and proposed the concept of quantum simulation. Weimer [3] contrived how to simulate many-body interactions using many-body gates based on the Rydberg blockade effect and EIT and conjectured that Rydberg atoms are very suitable tools for it, because the interactions are long-ranged and thus allow for large lattice spacings with superb single-site addressability. The implementation of a simple spin system—the Toric Code—was shown, more complex spin systems such as the Fermi-Hubbard model are presented in [3–5]. The dissipative preparation of the ground state, which is the key point of the quantum simulation here, was sketched for a single plaquette and results from [5] for larger systems were presented.

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