Quantum simulating an experiment:
Light interference from single ions and their mirror images

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(Dated: May 15, 2019)

We widen the range of applications for quantum computing by introducing digital quantum simulation methods for coherent light-matter interactions: We simulate an experiment where the emitted light from a single ion was interfering with its mirror image [Eschner et. al., Nature 431, 495 (2001)]. Using the quantum simulation software qitsim we accurately reproduce the interference pattern which had been observed experimentally and also show the effect of the mirror position on the spontaneous emission rate of the ion. In order to minimize the number of required qubits we implement a qubit-reinitialization technique. We show that a digital quantum simulation of complex experiments in atomic and quantum physics is feasible with no more than seven qubits, a setting which is well within reach for advanced quantum computing platforms.

PACS numbers: 02.60.Cb, 03.65.Yz, 03.67.-a, 03.67.Lx, 12.20.-m, 42.50.-p, 42.50.Lc, 42.50.Pq

Typical applications of quantum simulation include open questions in solid state physics [1-3]. More recently, using trapped ion setups, high energy physics problems have been addressed in experimental quantum simulation [4-6] and in hybrid classical-quantum simulation methods for molecular chemistry calculations have been demonstrated [7,8]. Yet another set of applications investigates energy transport in the quantum regime, with implications for our understanding of biological systems [9-11]. Experimental realizations of open quantum systems require the ability to implement both coherent many-body dynamics and dissipative processes [12,13]. Quantum simulation has been proposed even for mimicking non-physical systems [14]. Using a superconducting circuit quantum computer problems in the financial sector have been addressed, e.g. for an analysis of market stability or for pricing financial derivatives [15,16]. Here, we widen the spectrum of applications for digital quantum simulation further and propose to digitally simulate an experimental outcome. Specifically, we are able to accurately reproduce by quantum simulation the outcome of a trapped single ion experiment, where an interference pattern has been observed experimentally [17]. We show in the digital quantum simulation – similar to the experiment – the strong influence of the mirror position on the spontaneous emission rate of the ion. Implementing an experimental setting which includes the coherent emission and absorption of a quantum light field, the optical excitation of two-level systems, the interference of light and backaction on the atomic electronic levels, we provide a wide and universal set of tools for digital simulation which may therefore be applied to predict results in many other atomic, ionic, molecular and optical experiments.

For simulating light-matter interactions in a digital quantum simulator, we divide the electromagnetic field into spatial slices, each containing either zero or one photon, or any coherent superposition of these states. In this way, the field is modelled by a tensor network of qubits. At the points where the electromagnetic field interacts with matter, e.g. a single atom, ion, or a collection of atomic emitters, we introduce a unitary interaction matrix that couples the field slice at that position with the matter system. This unitary interaction represents one time step of the simulation. As the electromagnetic field is propagating with the speed of light, qubits in the tensor network move to the next field slice in every new time step of the computation. The tensor network might contain loops, which means we can also model fully coherent feedback, e.g. when back-reflecting the emitted light by semi-cavities.

The paper is organized as follows: After sketching the experimental setup to be implemented by quantum simulation, we describe the model and its approximations.
We continue by a detailed discussion of the simulation calculation method and exemplify the accuracy of results from the fitting parameters to the simulated interference pattern, in comparison with the experimental findings.

As a case example of our open-system quantum simulation we model an experiment [17] in which a single ion is held in a Paul trap in front of a mirror. When laser-exciting the ion, resonance fluorescence is emitted, and two light paths towards a detector are established: light that returns to the ion via the mirror before arriving at the detector, and light directly being detected. If the optical path lengths of these two light paths differ by a non-integer multiple of the transition wavelength there will be destructive interference. By mounting the mirror on a piezo-electric stage and varying the distance to the mirror, an interference pattern as a function of the distance was observed.

In the experiment, a single Ba$^+$ ion is continuously laser-excited and laser-cooled on its $S_{1/2} \leftrightarrow P_{3/2}$ and $P_{1/2} \leftrightarrow D_{3/2}$ resonance lines of 493 nm and 650 nm, respectively, see Fig. 1(a).

**The model:** For the quantum simulation we ignore the $D_{3/2}$ state and model the Ba$^+$ ion as a two-level system at a fixed position in space. The excitation of the transition $S_{1/2}$ to $P_{1/2}$ induces Rabi oscillations as well as the emission of fluorescence photons near 493 nm, which are subsequently collected by two lenses. One lens collimates the light that is directed towards the mirror, such that light can re-interact after a time delay and the second lens focuses the outgoing light in the direction of the photo detector 1 [17], see Fig. 1(a). The coordinates are fixed such that the Ba$^+$ ion is located at the origin and we place the reflection at a position $-d$. This leads to a natural time scale: we define $T$ as the time it takes for a photon to make a round trip from the Ba$^+$ ion to the mirror and back, i.e. $T := 2d/c$, where $c$ stands for the speed of light. We divide the time interval $[0, T]$ in $N \in \mathbb{N}$ equal time slices and we define a discretization parameter $\lambda$ by

$$\lambda := \sqrt{\frac{T}{N}},$$

such that every time slice represents $\lambda^2$ seconds.

We divide the field, interacting with the single ion, into three channels: (C1) Photons traveling from the ion to the mirror, (C2) Photons returning from the mirror to the ion, and (C3) Laser light from the side exciting the ion. All three channels are represented by a doubly infinite string of qubits, see Fig. 2. The free time evolution $\Theta$ of the electromagnetic field C1 and C3 corresponds to left shift, i.e. in one time step all elements in the tensor network shift left by one position. For C2 a free time evolution time step is imaged as a shift to the right, see Fig. 2.

We now introduce an interaction $R : \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ between the Ba$^+$ ion and the field slices at the origin of the channels 1 and 2 (last two copies of $\mathbb{C}^2$ in the tensor product)

$$R := \sqrt{\kappa \lambda} (\sigma_+ \otimes \sigma_+ \otimes I - \sigma_- \otimes \sigma_- \otimes I + \sigma_- \otimes I \otimes \sigma_+ - \sigma_+ \otimes I \otimes \sigma_-).$$

Here $\kappa$ is the strength of the coupling between the Ba$^+$ ion and the two field channels. Without loss of generality we assume identical coupling strength for C1 and C2, corresponding to an identical focussing by lenses L1 and L2. Operators $\sigma_+$ and $\sigma_-$ denote standard raising and lowering operators on a two-level system.

We introduce the interaction $Q : \mathbb{C}^2 \otimes \mathbb{C}^2 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2$ between the Ba$^+$ ion and the laser field slice at the origin of the third channel

$$Q := \sqrt{\kappa_s} (\sigma_- \otimes \sigma_+ - \sigma_+ \otimes \sigma_-),$$

where $\kappa_s$ is the coupling strength between the Ba$^+$ ion and the side channel C3. Furthermore, the Ba$^+$ ion undergoes its own internal time evolution given by

$$L := e^{-i\omega \lambda^2}.$$

We initialize all field slices in C1 and C2 in the vacuum state before interaction with the ion. The side channel C3, however, is initialized in a coherent state representing the resonantly driving laser. A complex number $\alpha = |\alpha| e^{-i\omega \lambda^2}$ represents its amplitude and phase, where $l$ represents the time step. We now introduce the discrete
Figure 3: Closed loop interaction model: Initially, the laser qubit $q_{\text{laser}}$ interacts with the Ba$^+$ ion qubit $q_{\text{ion}}$ through interaction $Q$. Next, the ion interacts with the first and last field qubits $q_0$ and $q_N$ through interaction $R$. Afterwards, $q_{\text{laser}}$ is reset, the outgoing field qubit $q_N$ is measured and reset, and the field qubits are shifted.

Weyl (or displacement) operator acting on the qubit at the origin of $C^3$

$$M := e^{\lambda\alpha \sigma_z - \lambda\pi \sigma_\times}. \quad (5)$$

Acting with the operator $M$ on the vacuum vector of the slice of $C^3$ at the origin, we drive this slice in a coherent state that represents the resonant driving laser. In this way, Rabi oscillations are induced in the ion with frequency $\Omega = |\alpha|\sqrt{\kappa}.$

Combining contributions from Eqns. (2) - (5), we construct a time evolution which is given by an evolution $U_l := (\Theta LRQM)^l$. Repeated interactions as described by this evolution have been studied in literature [18–26] and it can be shown that such a repeated interaction converges to a Hudson-Parthasarathy quantum stochastic differential equation (QSDE) [27] in the limit where the discretization parameter $\lambda$ goes to 0. QSDE’s constitute the starting point for the quantum stochastic input-output formalism introduced by Gardiner and Collett [28]. Consequently, our quantum simulation may be interpreted as a discretization of input-output open quantum systems, optionally creating finite loops by connecting some of the inputs to some of the outputs. In this specific case, this is the backreflection of photons in $C_1$ by the mirror to interact again with the ion as $C_2$.

At the mirror, the field slices of $C_1$ are transferred to $C_2$. In this way a loop of $N + 1$ field qubits $q_0 \ldots q_N$ is created, see Fig. 3. In the experiment [17] the mirror is placed at a distance of about 0.25 m, however modelling such a long time delay would require a prohibitively large number of qubits in $C_1$ and $C_2$. Instead, we limit the distance $d$ to the wavelength of the atomic transition and capture two full cycles of the interference pattern. Note that by varying $d$ for given $N$, we also vary the time step $\lambda$ according to Eqn. (1).

As soon as the last qubit $q_N$ in $C_2$ has interacted with the ion we project it in the $\sigma_z$ basis. If the measurement result is $+1$ we rotate the qubit back to $|0\rangle$. Then, the qubit is shifted to $C_1$ at the origin. In this way we reinitialize the qubit and can re-use it in the quantum computation, keeping the total required number of qubits minimal. Employing a similar procedure for $C_3$, we can simulate the entire channel with a single qubit, see Fig. 3.

In the following we assume a 7 qubit quantum computer, such that one can model one wavelength with 5 qubits and resolve expected sinusoidal interference pattern sufficiently well. The 6th qubit represents the coherent laser driving and the 7th qubit the simplified two-level system of the ion.

Quantum circuit: To implement the interaction described by the evolution $U_l$ all contributions are mapped to elementary single- and two-qubit gate operations. Leaving the interaction $R$ between the ion and the two photon field slices unspecified for the moment, the circuit for time step $l$ is given by:

$$\begin{align*}
|0\rangle & \rightarrow R_z(-\omega l^2) \rightarrow R_y(-2\sqrt{\kappa}\lambda) \\
q_{\text{laser}} & \rightarrow R_y(2|\alpha|\lambda) \rightarrow R_z(-\omega l^2) \\
q_{\text{ion}} & \rightarrow R \\
q_0 & \rightarrow R \\
q_1 & \rightarrow R \\
\vdots & \\
q_{N-1} & \\
q_N & \\
\end{align*} \quad (6)$$

Here the first two rotation gates represent the initialization of the laser. Note that the $R_z(-\omega l^2)$ rotation set-
The interaction $R$ between the ion and the photon field, given by Eqn. (2), can be decomposed into elementary quantum gates as follows:

$$R = R_\phi(2\sqrt{2\kappa\lambda}).$$

**Results and discussion:** We have implemented the quantum circuit from Eqn. (6) on a quantum computer simulator developed by Q1t BV, called qitsim [29].

Two types of calculations have been performed. A direct simulation of the experiment was done by running over a long time period (25 ps), but using only a single run. The second type of calculation is more conducive to running on a real quantum computer, since it consists of shorter runs simulating only 100 fs, but averaging the results over multiple runs.

We set the transition frequency in the ion to the experimental value of $f = 2\pi c/493$ nm. To show that our approach may be experimentally feasible to implement on current-technology quantum computers, we restricted the calculations to using 5 qubits for representing the photon field. The results for the simulations are shown in Fig. 4(a) and 4(b). Both simulations clearly show the interference pattern that has been previously observed in the experiment [17]. Fitting the oscillation frequency of the interference pattern, we find 246.0 nm and 246.2 nm, respectively, both close to the expected value of 493/2 nm = 246.5 nm.

To prove that the observed pattern is indeed caused by interference, we have performed calculations with the value of the internal transition frequency raised to $\omega = 1.5f$. The results are shown in Fig. 4(c). As expected, the fit for the wave length of the interference pattern of 164.1 nm is shorter by the factor 1.5.

More interestingly, the interaction with the backreflected photon channel does not only result in an interference pattern, but its back-action affects the emission rate of the ion to be either enhanced or reduced, depending on the ion to mirror distance. This results in a modulation of the $P_{1/2}$ state occupation probability, which has been revealed from the observation of photons near 650 nm on the $P_{1/2}$ to $D_{3/2}$ transition [17]. The mirror coating in the experimental realization was chosen highly transmitting near 650 nm such that the detector 2 allows to detect such photons, see Fig. 1. To illustrate that our simulation captures this behavior, the calculated population of the upper state of the ion is evaluated, as a function of the ion to mirror distance. This results in a modulation near 650 nm such that the detector 2 allows to detect photons, see Fig. 4(d). It is easily seen that the $P_{1/2}$ lifetime of the ion perfectly anticorrelates with the emitted photon count rate at 493 nm.

Using the full circuit defined by Eqns (6) and (7), a single time step in the simulation requires $17 + N$ two-qubit operations, and two measurement operations, where SWAP gates and controlled rotations are each counted as one two-qubit operation. The number of time steps needed increases with the total simulated time. For the results in Fig. 4(b), between 120-600 steps have been taken for each data point to simulate up to 100 fs, except for the shortest distances below 100 nm. At $d = 10$ nm, the required number of time steps runs up to 6,000 due to the small value of $\lambda^2$. This may be mitigated though, by using a smaller number of field qubits at these short distances. Furthermore, the interaction circuit in Eqn. (7) can be approximated using two separate interactions between the ion and the field qubit,
reducing the number of single and double qubit gates to 3 and 6 + N respectively.

**Conclusion and outlook:** We have been able to reproduce the interference pattern which had been observed in experiment [17] using the q1tsim simulator of a quantum computer. Furthermore, we have shown that the presence of the mirror modifies the emission by and thus the lifetime of an excited state of the Ba+ ion. Our results demonstrate simulation of a quantum model including an optical feedback loop on a quantum computer. Using the methods we presented in this paper, it will be possible to model many more problems originating from quantum optics, and more specifically cavity QED, on a future quantum computer.

Furthermore, we demonstrated that qubit re-initialization within a computation run allows for reducing the number of required qubits, thus facilitating a simulation of the experiment [17] with ≤10 qubits. Circuits we have been simulating on the q1tsim simulator are ready to be implemented in the laboratory on state-of-the-art platforms.

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