Digital Quantum Simulation of the Holstein Model in Trapped Ions

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We propose the implementation of the Holstein model by means of digital methods in a linear chain of trapped ions. We show how the simulation fidelity scales with the generation of phononic excitations. We propose a decomposition and a stepwise trapped-ion implementation of the Holstein Hamiltonian. Via numerical simulations, we study how the protocol is affected by realistic gates. Finally, we show how measurements of the size of the simulated polaron can be performed.

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Quantum simulators[1, 2] are promising tools for the deep comprehension of complex quantum dynamics. In a quantum simulator, the higher control on the simulating system can allow to reproduce and recover non-trivial quantum behaviors. Recently, a significant boost to the field of quantum simulations has been provided by the use of digital approximations in trapped-ion setups[3, 4], based on stroboscopic decompositions of unitary operators[5, 6]. However, the digital simulation of coupled bosonic-fermionic systems, naturally described by unbounded Hamiltonians, has not been considered.

Strongly correlated quantum many body systems represent a challenge to both computational and analytic methods. Among them, correlated fermionic-bosonic models are of critical relevance. The importance of correlation between electrons and ion vibrations has been proven for a large number of condensed-matter systems[7]. Their role in high-temperature superconductors, as fullerides and cuprates, is still debated[8–10]. In solid state systems, the correlation between the presence of electrons in a lattice and deformations of the latter can result in the formation of polarons: electrons and phonons can no longer be considered as stand-alone particles. Depending on the strength of the electron-phonon couplings, the cloud of lattice displacements surrounding the electron can have different sizes. For strong couplings, the electrons can be trapped, with remarkable changes of global properties[11]. The Holstein model[12] has been proved to naturally describe the strong coupling case. This model has been recently addressed by heavy numerical simulations[13] and classical analog simulations for a reduced number of sites[14]. Perturbation methods based on the Lang-Firsov approximations[15] valid in the strong coupling limit, are known since long times. The dimensionality of the underlying lattice also raises critical features[16]. While involving a lot of efforts, the full and complete comprehension of the electron-phonon correlations is still an open problem. From a quantum mechanics point of view, when considering creation of phonons, even with few electron sites, the size of the simulated Hilbert space can dramatically grow. The quantum simulation of such a complex dynamics could represent an important step forward in the description of condensed matter systems.

Trapped-ion systems are among the most controllable quantum systems. They offer remarkable computational power to perform quantum simulations exponentially faster than their classical counterparts[17, 32].

In this Letter, we propose the implementation of the Holstein Hamiltonian in a chain of trapped ions, using digital-analog approximation methods, in which the fermionic part is digitized and the bosonic part is analog and provided naturally by the phonons. First, we address the problem of simulating unbounded Hamiltonians with digital-analog protocols. Then, we provide a convenient decomposition of the Holstein Hamiltonian, in that each step can be implemented in a trapped-ion setup. We discuss a possible experimental implementation, testing the whole protocol with numerical integration of the Schrödinger equation. We show how critical observables, as electron-phonon correlations, can be retrieved from the trapped ion setup, leading to an estimation of the polaron size.

Decomposition of the Model.- It is known that the dynamics of a quantum state under the action of a Hamiltonian \( H \) can be recovered by using combined fractal-stroboscopic symmetric decompositions[5, 6]. In most practical cases, one can assume a fractal depth of one. This will be the case through all the rest of our analysis. With these techniques, the target Hamiltonian \( H \) is decomposed in a set of \( m \) terms: \( H = \sum_{i=1}^{m} H_i \). Then, the symmetric decomposition for the unitary operator encoding the dynamics of Hamiltonian \( H \) reads

\[
U_r(t) = \left( \prod_{i=1}^{m} e^{-i\frac{H_i}{r}} \right)^r \left( \prod_{i=m}^{1} e^{-i\frac{H_i}{r}} \right)^r.
\]

Here \( r \) is the degree of approximation in terms of Trotter steps. It has been shown[6] that, using symmetric Suzuki fractal decompositions, the number of gates needed to approximate the exact time evolution of the quantum state grows with the norm of the simulated Hamiltonian. Therefore, it is a natural problem to think of a quantum simulation involving particle generation, in particular of
bosons, whose number can grow, in principle, indefinitely. However, in the standard approach to these problems, the dynamics of a bosonic Hilbert space can be recovered by truncating at a certain point of the number of possible bosonic excitations. Thus, the number of gates needed to achieve a certain fidelity for the simulated quantum state grows as more bosonic excitations are created.

The Holstein Hamiltonian \([12]\), of a chain of \(N\) sites (in the following \(\hbar = 1\)), reads

\[
H = -\hbar \sum_{i=1}^{N-1} \left( c_i^\dagger c_{i+1} + \text{h.c.} \right) + g \sum_{i=1}^{N} (b_i + b_i^\dagger) n_i + \omega_0 \sum_{i=1}^{N} b_i^\dagger b_i. \tag{2}
\]

Here, \(c_i(c_i^\dagger)\) is the annihilation (creation) operator in the electron site \(i\), and \(b_i(b_i^\dagger)\) is the phonon annihilation (creation) operator on the site \(i\); \(n_i = c_i^\dagger c_i\) is the electronic occupation number operator. The parameters \(\hbar\), \(g\) and \(\omega_0\) stand respectively for a nearest-neighbor (NN) site hopping for the electrons, electron-phonon coupling and free energy of the phonons.

To encode the model in a trapped-ion chain, we first map the fermionic operators through the Jordan-Wigner transformation, \(c_i \rightarrow \prod_{j=1}^{i-1} \sigma_j^x \sigma_i^z\) to tensor products of Pauli matrices. The mapped Hamiltonian describes now a coupled spin-boson system

\[
H = \hbar \sum_{i=1}^{N-1} \left( \sigma_i^x \sigma_{i+1}^x + \text{h.c.} \right) + g \sum_{i=1}^{N} (b_i + b_i^\dagger) \left( \frac{\sigma_i^z + 1}{2} + \omega_0 \right) + \sum_{i=1}^{N} b_i^\dagger b_i. \tag{3}
\]

The first term can be rewritten as \(\frac{\hbar}{2} \sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)\). We now decompose the Hamiltonian into three parts, \(H = H_1 + H_2 + H_3\). The single steps read

\[
H_1 = \hbar \sum_{i=1}^{N-1} \frac{1}{2} \sigma_i^x \sigma_{i+1}^x + \omega_0 \sum_{i=1}^{N} b_i^\dagger b_i, \\
H_2 = \hbar \sum_{i=1}^{N} \sigma_i^y \sigma_{i+1}^y + \omega_0 \sum_{i=1}^{N} b_i^\dagger b_i, \tag{4}
\]

\[
H_3 = g \sum_{i=1}^{N} (b_i + b_i^\dagger) \left( \frac{\sigma_i^z + 1}{2} + \omega_0 \right) + \sum_{i=1}^{N} b_i^\dagger b_i.
\]

According to Ref. [37], one can upper bound the number of gates \(N_g\) needed to achieve a simulation error smaller that \(\epsilon\), by giving an upper bound for the norm of \(H\)

\[
N_g \leq 3 \cdot 5^{2k} [3!(N-1) + 2g|N\sqrt{M-1} + \omega_0 N M) t^{1/2 + 2k}]. \tag{5}
\]

As mentioned before, the fractal depth \(k\) [5] can be set to one in most applications. Here, we show the dependence of the number of gates in the number of fermionic sites \(N\), and on the truncation in the number of bosons \(M\). As the number of created phonons increases, one needs a higher-level truncation, and a larger Hamiltonian norm. Nevertheless, this shows that we can efficiently simulate a \(2^N \times (M+1)^N\) Hilbert space, i.e., with a number of gates that grows at most polynomially in \(N\) and \(M\). To show the scaling of fidelities with the parameters considered, we plot in Fig. 1(a) the time dependence of the fidelity loss \(1-F(t) = 1-|\langle \Psi_E(t)|\Psi_S(t) \rangle|^2\) for a two site configuration, as a function of the electron-phonon coupling strength \(g\), for \(\omega_0 = \hbar/4\). As the coupling \(g\) increases, more phonons are created, the Hilbert space describing the dynamics enlarges and the fidelity decreases for a fixed number of approximant gates \((r = 10)\) here. (b) dependence of the fidelity loss in the number of sites. Here \(g = 0.3\ \hbar\), \(\omega_0 = 0.5\ \hbar\), and ten symmetric steps are considered \((r = 10)\). The initial state of both plots corresponds to a configuration in which an electron is injected in the site \(N/2\) (\(N\) even) or \((N + 1)/2\) (\(N\) odd), and there are no phonons.

\[
H_0 = \sum_{i=1}^{N+1} \frac{\omega_0}{2} \sigma_i^z + \sum_{i=1}^{N} \Delta_i b_i^\dagger b_i + \nu_{N+1} b_{N+1}^\dagger b_{N+1}. \tag{6}
\]

where \(\omega\) is the excitation energy of the individual ion taken as a two-level system, i.e., the carrier frequency. In this way, the free energies of \(N\) normal modes do not disappear in the interaction picture, and a flatterd part of them is still present in order to recover the dispersion-less phononic spectrum.

To simulate the dynamics associated to \(H_1\) and \(H_2\) of Eq. (4), one has to achieve a NN Ising coupling. The
Dynamics decoupled with respect to the phonons at time steps of \( \sim 333 \nu t \) and a negligible NNN interaction \( [37] \). At these times, the ion spins match the exact value, phonons are detached from spins and the fidelity oscillation (top black curve) \( F(t) = |\langle \Psi_E(t)|\Psi_I(t) \rangle|^2 \) reaches maxima, with peaks of \( \sim 0.995 \).

The initial state, as in all our numerical simulations, except where specified, is chosen to mimic a configuration in which one electron is injected at the center of a one-dimensional lattice provided with Holstein interactions. To this extent, all the spins are initialized in the opposite \( Z \) direction, except the one in site \( N/2 \), in case of even \( N \), or \((N+1)/2\) in case of odd \( N \). The spin of the last ion has to be initialized along the \( Z \) direction in order to be a passive ion with respect to the dynamics, according to the protocol for the implementation of \( H_3 \) given below. The vibrational modes are assumed to be initially cooled down to the ground state with resolved sideband cooling \( [33] \).

Notice that one can always implement a perfect NN coupling by using more stroboscopic steps. A possibility is to decompose the global NN into nearest-neighbor pairwise interactions. Another possibility is to design a counter, non-nearest-neighbor interaction step between pairs of non-nearest neighbor ions in order to eliminate the spurious NNN imperfections. Given that one has an unwanted \( \eta_{ij} \sigma^z_1 \sigma^z_2 \), one can add more Trotter steps to the protocol of the form \(-\eta_{ij} \sigma^+_i \sigma^-_j\) in order to have an Hamiltonian free of NNN couplings. The dynamics associated to the step with \( H_3 \) is implemented similarly to the one of \( H_1 \), with a different choice of the initial phases of the lasers, in order to achieve a YY interaction.

The Hamiltonian \( H_3 \) is realized as a combination of \( 2N \) red and blue detuned lasers with appropriate initial phases in order to recover a coupling of the \( i \)-th ion \((i=1,...N)\) with the \( m_i \)-th normal (shifted) mode \( \eta_{i,m} \Omega \sigma^z_i |b_{m_i}^+ + b_{m_i} \rangle \). The \( i \)-th ion is driven with red and blue detuned lasers to the \( m_i \)-th mode, establishing a one-to-one correspondence between the first \( N \) ions and the first \( N \) normal modes. Moreover, the last ion of the chain is driven by \( 2N \) lasers detuned in order to be coupled with the same modes of the ions in the chain. Two additional rotations of the spins of all ions around the \( Y \) axis are applied before and after coupling the spins to the phonons. They can be obtained by acting twice with a global beam upon all the \( N+1 \) ions at the same time. The Hamiltonian describing this process is,

\[
H_{c-p} = \sum_{i=1}^{N} (\Omega_i \eta_{i,m} \sigma^z_i + \Omega_{N+1,i} |\eta_{N+1,m_i} \sigma^z_{N+1} | (b_{m_i}^+ + b_{m_i}^\dagger))
\]

The Rabi frequencies of the lasers must be chosen according to \( \Omega_i = g/2 \eta_{i,m_i} \). \( \Omega_{N+1,i} = g/2 \eta_{N+1,m_i} \). If the last ion is initialized with the spin aligned along the \( Z \) axis and not addressed by spin flip gates during the simulation, the previous described gates result in the effective
Hamiltonian on the first $N$ ions subspace,

$$H_{e-p,N} = \sum_{i=1}^{N} g \frac{(\sigma_i^z + 1)}{2} (b_{m_i} + b_{m_i}^\dagger).$$  \hspace{1cm} (9)

Digital Simulation.- In general, digital protocols are much sensitive to the state fidelity that one can achieve at the end of the digital step. According to the mathematical theory, increasing the number of steps will result in an increased fidelity on the final simulated state. However, if one has an error on a single step, increasing the number of gates will result in the accumulation of these errors. Thus on one hand the use of more accurate single gates is required, on the other hand one has to get a compromise between the increased fidelity due to the increased number of steps and the fidelity loss due to the accumulated single gate error.

To have a quantitative estimation of the fidelity loss with the dynamics of the full ion Hamiltonian, we have realized numerical integrations for the Schrödinger equation for $N = 2+1$ \cite{37} and $N = 3+1$ ion setups. We point out that we consider this reduced number of ions because of numerical computation restrictions, and to prove the feasibility of our model. In general our formalism may be straightforwardly extended to several ions. In Fig.3 a simulation for $r = 2$ and $r = 3$ symmetric Trotter steps is realized. The fidelity loss $1 - |\langle \Psi_E(t)|\Psi_S(t)\rangle|^2$ for the Trotter protocol with perfect gates, i.e., associated to Hamiltonians $H_1$, $H_2$ and $H_3$, is plotted against points of fidelity loss $1 - |\langle \Psi_E(t)|\Psi_I(t)\rangle|^2$ obtained with realistic trapped-ion gates including the full laser interactions are plotted at various times. As can be appreciated, the fidelity loss for the ion gates is only slightly larger than for the exact Trotter gates, showing the feasibility of the protocol with realistic trapped-ion interactions. The total simulation time has been chosen in order to remain under the decoherence time for the ions \cite{34}. The frequency of the center of mass mode can be assumed to be $\nu_1 \simeq 2\pi \times 1$ MHz. The global rotation for the ion spins can be assumed to be done in 7 $\mu$s \cite{3]. The number of global rotations is $4r$. The step for the red and blue sideband Hamiltonian can be performed in the same time as the step for the NN XX gate (or even faster). Provided with these parameters, for a final simulated time of $2000/\nu_1 \sim 318 \mu$s, the time spent for the simulation can be taken of $\sim 1$ ms. Given that typical heating rates in trapped ion experiments \cite{3} are of about 1 phonon/s, we can assume that for the time of the proposed simulation heating will not be significant.

Tuning the coupling strength $g$ by setting the Rabi frequencies of the red and blue detuned lasers to various values, one can measure the different correlations between electron and phonon displacement at distant sites,

$$\chi(i, j) = \langle \Psi(t)|c_i^\dagger c_j (b_j + b_j^\dagger)|\Psi(t)\rangle.$$

This will amounts to a signature of the polaron size \cite{1]. Ranging from small to large $g$ will lead to a measure of the crossover between large/small polaron. Notice that these correlations are mapped in our ion setup onto

$$\chi(i, j) = \langle \Psi(t)|(b_{m_j} + b_{m_j}^\dagger)\frac{(\sigma_i^z + 1)}{2}|\Psi(t)\rangle,$$

which can be measured by mapping the motional onto the internal state of the auxiliary $N + 1$-th ion, and then detecting resonance fluorescence of ions $N + 1$ and $i$ \cite{22} \cite{24}. We notice that with our setup the possibility of simulating a 2D and 3D Holstein model is provided, by encoding two and three dimensional interactions into a linear chain by addressing distant ions with nonlocal gates \cite{4].

Currently, more than 100 gates have been implemented in a trapped-ion quantum simulation experiment with Trotter methods \cite{3}. In the near future, it should be possible to achieve hundreds or even thousands of gates per experiment \cite{38}, allowing our proposal to reach about ten qubits. It is noteworthy to mention that our proposed digital quantum simulation will already overcome the limits of classical computers with 10 ions and 5 phonons per ion. This will allow to study the formation of small polarons under these conditions. Future experiments involving 20 to 30 ions will permit to address the study of more complex dynamics, including electron-electron correlations mediated by phonons. In this manner, the trapped-ion quantum simulator will prove to be a remarkable tool for simulating fermions coupled to bosons and related condensed-matter or high-energy physics scenarios.

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SUPPLEMENTAL MATERIAL FOR "DIGITAL QUANTUM SIMULATION OF THE HOLSTEIN MODEL IN TRAPPED IONS"

UPPER BOUND FOR THE NORM

In this section, we give an upper bound for the norm of $H$ in Eq. (3) of the main text, in order to bound the error one makes with a Suzuki-Lie-Trotter expansion $[1]$. Consequently, we bound the number of gates one needs for achieving a given fidelity on the simulated quantum state. The norm is bounded by the sum of the norms of each term appearing in $H$. The computation of single norms amounts to finding the largest eigenvalue of the single terms

$$\|H\| \leq |h| \sum_{i=1}^{N-1} \|\sigma_i^+ \sigma_i^{-1} + h.c.\| + |g| \sum_{i=1}^{N} \|b_i b_i^\dagger\| + \omega_0 \sum_{i=1}^{N} \|b_i b_i^\dagger\|.$$  \hspace{1cm} (12)

Let us consider the various norms separately. The term expressed by $|h| \sum_{i=1}^{N-1} \|(-\sigma_i^+ \sigma_i^{-1} + h.c.)\| = |h|/2 \sum_{i=1}^{N-1} \|\sigma_i^+ \sigma_i^{-1} + \sigma_i^y \sigma_i^y\|$ represents a sum of $2(N-1)$ tensor products of Pauli matrices, with norm 1. Therefore, $|h| \sum_{i=1}^{N-1} \|(-\sigma_i^+ \sigma_i^{-1} + h.c.)\| \leq |h|(N-1)$.

The norm $\|b_i b_i^\dagger\|$ is bounded by the truncation in the number of bosons in the mode $i$, as is clear by the standard Fock representation

$$b_i^\dagger b_i \rightarrow \begin{pmatrix} 0 \\ 1 \\ \vdots \\ M \end{pmatrix}, \quad \|b_i b_i^\dagger\| = M.$$  \hspace{1cm} (13)

Therefore $\sum_{i=1}^{N} \|b_i b_i^\dagger\| = \sum_{i=1}^{N} M = NM$.

The norm $\sum_{i=1}^{N} \|b_i b_i^\dagger\| = \sum_{i=1}^{N} \|\sigma_i^+ \sigma_i^{-1} + \sigma_i^y \sigma_i^y\|$ is equivalent to $\sum_{i=1}^{N} \|b_i b_i^\dagger\|$, given that $\|\sigma_i^+ \sigma_i^{-1} + \sigma_i^y \sigma_i^y\| = 1$. The term $(b_i + b_i^\dagger)$ in the Fock basis reads

$$(b_i + b_i^\dagger) \rightarrow \begin{pmatrix} 0 & 1 & \sqrt{2} & \sqrt{2} & \cdots \\ 1 & 0 & \sqrt{2} & 0 & \cdots \\ \sqrt{2} & \sqrt{2} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix}.$$  \hspace{1cm} (14)

The characteristic polynomial of the matrix for the truncation to $M$ bosons is given in a recursively way,

$$D_0(\lambda) = 1, \quad D_1(\lambda) = -\lambda$$

$$D_n(\lambda) = -\lambda D_{n-1}(\lambda) - (n-1)D_{n-2}(\lambda).$$  \hspace{1cm} (15)

The $D_n(\lambda)$ are a $\sqrt{2}$ rescaled version of the Hermite polynomials. A simple bound for the largest zero of $D_M(\lambda)$ (i.e. the norm of the bosonic displacement operator) is given by the expression $2\sqrt{M-1}$ (see for example Ref. [2]). Summarizing, the norm for the Holstein Hamiltonian is upper bounded by

$$\|H\| \leq |h|(N-1) + 2|g|N\sqrt{M-1} + \omega_0NM.$$  \hspace{1cm} (16)

NUMERICAL SIMULATIONS

In this section, we provide additional numeric plots and further discussions for our simulation protocol for a 2+1 and 3+1 ion configuration. First of all, in all our numerical simulations, we have fixed the total simulated time to a maximum of $2000/\nu_1$, in units of the center of mass (COM) mode frequency $\nu_1$. Assuming $\nu_1 \sim 2\pi \times 1$ MHz, this gives a total simulated time of $\sim 318$ $\mu$s. We choose Trotter steps equally extended within a time $\tau = t/2$, where $t$ is the total simulated time. With these assumptions, to compute the total effective simulation time, one has to multiply the simulated time by the number of terms in the decomposition of the simulated dynamics, i.e. 3 in our case. Then we have to add the time contribution for the global $\pi/4$ rotations along the Y axis, necessary to achieve the Z-like coupling to the phonons, that can be estimated to be around $\sim 7$ $\mu$s each $[3]$. Considering four global rotations per symmetric Trotter step, this gives a total simulation time of the order $\sim 1$ ms for the $r = 1$ and $r = 2$ case. This is well below the typical decoherence times for a trapped-ion setup $[1]$. Notice that we have made assumptions on the time extension for the Trotter steps, but nothing prevents to set the duration for the Trotter step to shorter times, as long as one can adjust properly the Rabi frequencies of the lasers used $[3]$. This paves the way to the scalability of the protocol.

The dynamics described by Hamiltonians $H_1$ and $H_2$ can be achieved by using two pairs of counterpropagating lasers with opposite detunings $\pm \delta_i$ $[3]$, driving the $i$-th and the $i + 1$-th ions. One can switch between a nearest neighbor (NN) XX/YY Ising interactions by taking appropriate initial phases for the lasers. The effective spin-spin coupling generated by this kind of laser drivings has the form of Eq. (7) in the main text.

In order to have negligible phonon displacements at the Trotter step time $\tau$, one has to choose the detuning $\delta_i = \pm 2\pi/\tau + \Delta_m$ close to one of the modes of (shifted) frequencies $\Delta_m$ (thus $|\delta_i - \Delta_m| \ll |\Delta_m|, |\delta_i|$). We point out again here that in our protocol we deal with shifted frequencies, as explained in the main text, to take into account the desired dispersionless energies of the Holstein phonons. The $\pm$ sign in the choice of $\delta_i$ can be used to change the relative sign of the spin-spin interaction, depending on $\text{sgn} [\eta_{h,m} \eta_{h+1,m}]$. We assume in our simu-
lations a relative Lamb-Dicke parameter distribution for ions and modes as in [6], with an overall magnitude of 0.1. If one chooses $m = 1$ for the 2+1 ions setup, i.e. a detuning close to the COM mode, it must be set to $\delta = 2\pi/\tau + \Delta_1$, to obtain a positive $\hbar/2$ coupling in the Ising NN interaction, because $\text{sgn} [\eta_{11} \eta_{12}] = +$.

In Fig. 4 we show the numerical integration for the dynamics of the NN XX Ising interaction for a 2+1 ions configuration. The simulated strength for the Ising coupling is $\hbar/2 = 0.001 \nu_1$. For $\omega_0 = \hbar/4$, one has a shifted frequency for the COM mode of $\Delta_1 = \nu_1 - 0.0005 \nu_1/3$. By choosing $\tau = 500/\nu_1$, the detuning used in this case is $\delta = 2\pi \nu_1/500 + \Delta_1 = 1.0124 \nu_1$, i.e. for $\nu_1 \simeq 2\pi \times 1$ MHz, a frequency difference with the mode of $\delta - \nu_1 = 2\pi \times 12.4$ KHz. The Rabi frequencies of the lasers are chosen in order to recover the desired strength for the Ising coupling.

To have an idea of how real ion interactions affect the protocol for a 2+1 ion setup, we make a plot of the errors on the simulated state with perfect gates and with ion gates in Fig. 5. One clearly sees that the higher fidelities obtained by using the ion gates with respect to the 3+1 ion setup are due to the higher single gate fidelity for the 2+1 setup, which permits to explore better fidelity regimes. The simulated parameters here are $g = \hbar/10$, $\omega_0 = \hbar/4$, $\hbar = 0.002 \nu_1$. We remark that in the simulations we have used a small $g/\hbar$ ratio to reduce the complexity of the simulation (i.e., the necessary truncation for the Fock space is small). Nevertheless, in a trapped-ion experiment, big $g/\hbar$ ratios with large freedom for the choice of $\omega_0$ can be explored, thus recovering the typical self trapping line for the formation of small polarons [7]. The time points for the simulation range from $t = 1000/\nu_1$ to $t = 2000/\nu_1$. For $r = 1$ this gives Trotter steps ranging from $\tau = 500/\nu_1$ to $\tau = 1000/\nu_1$. The detuning for the NN interaction has to be set accordingly at each point, ranging from $1.0124 \nu_1$ to $1.0061 \nu_1$.

To obtain the plot of Fig. 3 in the main paper, with the same simulated parameter $g = \hbar/10$, $\omega_0 = \hbar/4$, $\hbar = 0.002 \nu_1$, we have used two simultaneous NN XX interactions as described above. One involves the first two ions with a detuning close to the COM mode, and another one driving the second and the third ion with a detuning close to the breathing mode, of frequency $\nu_2 = 1.731 \nu_1$ [6]. To obtain an Ising interaction with the proper sign for the second and the third ion, we have to set the detuning for the second laser below the shifted frequency $\Delta_2$. This is because for a 3+1 configuration (i.e., four ions in a linear trap), one has...
The detuning for the second set of lasers is therefore chosen to be \( \delta = -2\pi/\tau + \Delta_2 \). For example, for the simulation point at \( t = 1000/\nu_1 \), corresponding to \( \tau = 250/\nu_1 \) for \( r = 2 \), one has \( \delta_1 = 1.025 \nu_1 \) and \( \delta_2 = 1.7057 \nu_1 \). Using these parameters, it turns out that the non-nearest-neighbor coupling between the first and the third ion is negligible.

To get an insight of what happens to the phonons population of the COM mode inside a Trotter protocol, one can have a look to Fig. 6. Here, it is shown the mean number of phonons for a 2+1 ion setup using a symmetric decomposition at \( r = 1 \) of the Hamiltonian \( H = H_1 + H_3 \), where \( H_1 \) is a XX Ising interaction obtained with a detuning close to \( \Delta_1 \) and \( H_3 \) is a Z-like coupling to phonons. The decomposed evolution operator has the form

\[
U_2(t) = e^{-iH_1t/2}e^{-iH_3t/2}e^{-iH_3t/2}e^{-iH_1t/2}.
\]

We see that, in the first and the last step, the two Ising interactions create phonons, while relaxing them at the end of the step, because the laser detuning and Rabi frequencies are chosen to obtain detachment from the phonons at the end of the Trotter step. In the middle steps, the phonons are excited according to the \( H_3 \) Hamiltonian. The final mean value for the phonon number is recovered with respect to the dashed line value, which is the numerical value according to the exact evolution operator \( e^{-iHt} \), with an error of \( \sim 1\% \). Notice that since the decomposition involves symmetric Trotter steps, and each one is chosen to be of the same duration, the total simulation time is doubled.

### Estimation of Non-Nearest-Neighbor Couplings

In this paragraph we give an estimation of the NNN couplings that appear when one wants to generate the NN Ising interaction with the parameters that we use in the main text. We propose to address pairs of NN ions with independent counterpropagating couples of lasers detuned close to different modes, i.e. a different mode is assigned to a specific couple of NN ions. This gives rise to NNN coupling between distant ions, which we show being negligible for specific detunings and gate times. For a 3+1 ion configuration, for example, the total Hamiltonian is

\[
H = H_1 + H_2 = \sum_m \sin(\delta_1 t) \left( a_m e^{-i\nu_m t} + a_m^\dagger e^{i\nu_m t} \right) \sum_{i=1}^2 \Omega_1 \eta_{i,m} \sigma_i^x + \sum_m \sin(\delta_2 t) \left( a_m e^{-i\nu_m t} + a_m^\dagger e^{i\nu_m t} \right) \sum_{i=2}^3 \Omega_2 \eta_{i,m} \sigma_i^x,
\]

obtained by driving the first two ions with two pairs of counterpropagating lasers detuned to \( \pm \delta_1 \) [3], while the lasers driving the second and the third are detuned to \( \pm \delta_2 \). Therefore a second order Magnus expansion of the Hamiltonian in Eq. (17) leads to unwanted NNN terms in the evolution operator of the form

\[
\left( \int_0^t dt' \int_0^{t'} dt'' [H_1(t'), H_2(t'')] + \int_0^t dt' \int_0^{t'} dt'' [H_2(t'), H_1(t'')] \right) = \sum_m \sum_{i=1}^2 \sum_{j=1}^3 \left( Z_{1,m}(t) + Z_{2,m}(t) \right) \sigma_i \sigma_j S_{1,m} S_{2,m},
\]

where we have defined \( S_{1,m} = \sum_{i=1}^2 \Omega_1 \eta_{i,m} \sigma_i^x \), \( S_{2,m} = \sum_{i=2}^3 \Omega_2 \eta_{i,m} \sigma_i^x \). Some straightforward algebra leads to

\[
Z_{1,m}(t) = \frac{i}{2(\delta_1^2 - \nu_m^2)} \begin{pmatrix}
\sin(\delta_2 - \nu_m)t \\
-\nu_m \sin(\delta_2 - \delta_1)t
\end{pmatrix} + \begin{pmatrix}
\sin(\delta_2 + \nu_m)t \\
\nu_m \sin(\delta_2 + \delta_1)t
\end{pmatrix},
\]

\[
Z_{2,m}(t) = \frac{i}{2(\delta_2^2 - \nu_m^2)} \begin{pmatrix}
\sin(\delta_1 - \nu_m)t \\
-\nu_m \sin(\delta_1 + \delta_2)t
\end{pmatrix} + \begin{pmatrix}
\sin(\delta_1 + \nu_m)t \\
\nu_m \sin(\delta_1 - \delta_2)t
\end{pmatrix}.
\]

These contributions are negligible for the parameters that we use, i.e. first detuning close to the first mode and second detuning close to the second one, \( |\nu_1 - \delta_1| \ll \nu_1 \).
\[\nu_1, |\nu_2 - \delta_2| < \nu_2. \] For example, taking the strongest resonant term from the series in Eq. (18), \(m = 2\) for \(Z_{2,2}(t)\), the first term on the right side in Eq. (20) reads

\[
\frac{\delta_2 \sin(\delta_1 - \nu_2)t}{2(\delta_2^2 - \nu_2^2)(\delta_1 - \nu_2)} = \frac{\delta_2 \sin(\delta_1 - \nu_2)t}{2(\delta_2 + \nu_2)(\delta_2 - \nu_2)(\delta_1 - \nu_2)}.
\]

(21)

Since \(\Omega_i\eta_{i,m} \sim \Omega_j\eta_{j,n}\), the term is negligible in comparison to the desired NN terms, whose couplings go like \(-\frac{\nu_1t}{2(\delta_1^2 - \nu_1^2)}, -\frac{\nu_2t}{2(\delta_2^2 - \nu_2^2)}\), for sufficient large times,

\[
\begin{vmatrix}
\nu_2t \\
(\delta_2 + \nu_2)(\delta_2 - \nu_2)
\end{vmatrix} \gg \begin{vmatrix}
\delta_2 \\
(\delta_2 - \nu_2)(\delta_2 + \nu_2)(\delta_1 - \nu_2)
\end{vmatrix}.
\]

(22)

\[
t \gg \frac{\delta_2}{\nu_2 (\delta_1 - \nu_2)}.
\]

(23)

For realistic parameters the critical time is \(t \sim 1/\nu_1\). Since our gates are obtained at times \(\tau \sim 100/\nu_1\), these NNN terms can be neglected. We stress again that in the protocol some of the frequencies \(\nu_i\) have to be shifted, we have left the original frequencies to avoid a heavy notation. Same kind of considerations are valid for the other terms in the right side of Eq. (20) and Eq. (19). This also extends in a straightforward way to couplings between any two NNN ions in a configuration with an arbitrary number of ions, as long as conditions like Eq. (23) are satisfied.

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