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 us to reproduce and recover nontrivial 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 be different sizes. For strong couplings, the electrons can be trapped, with remarkable changes of the 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, have been widely used. The dimensionality of the underlying lattice also raises critical features [16]. Therefore, 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 integrations 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

$$U_r(t) = \left(\prod_{i=1}^{m} e^{-(iH_i t/2r)} \prod_{i=m}^{1} e^{-(iH_i t/2r)} \right)^r. \qquad (1)$$

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

$$H = -h\sum_{i=1}^{N-1}(c_i^\dagger c_{i+1} + \text{H.c.}) + g\sum_{i=1}^{N}(b_i + b_i^\dagger)n_i + \omega_0\sum_{i=1}^{N} b_i^\dagger b_i. \quad (2)$$

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 h, g, and ω_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, $c_i \to \prod_{j=1}^{i-1}\sigma_j^z\sigma_i^-$ to tensor products of Pauli matrices. The mapped Hamiltonian describes now a coupled spin-boson system

$$H = h\sum_{i=1}^{N-1}(\sigma_i^+\sigma_{i+1}^- + \text{H.c.}) + g\sum_{i=1}^{N}(b_i + b_i^\dagger)\frac{(\sigma_i^z + 1)}{2} + \omega_0\sum_{i=1}^{N} b_i^\dagger b_i. \quad (3)$$

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

$$H_1 = \sum_{i=1}^{N-1}\frac{h}{2}\sigma_i^x\sigma_{i+1}^x + \frac{\omega_0}{3}\sum_{i=1}^{N} b_i^\dagger b_i,$$
$$H_2 = \sum_{i=1}^{N-1}\frac{h}{2}\sigma_i^y\sigma_{i+1}^y + \frac{\omega_0}{3}\sum_{i=1}^{N} b_i^\dagger b_i, \quad (4)$$
$$H_3 = \sum_{i=1}^{N} g(b_i + b_i^\dagger)\frac{(\sigma_i^z + 1)}{2} + \frac{\omega_0}{3}\sum_{i=1}^{N} b_i^\dagger b_i.$$

According to Ref. [6], one can upper bound the number of gates N_g needed to achieve a simulation error smaller than ϵ, by giving an upper bound for the norm of H [33],

$$N_g \le 3\times 5^{2k}[3(|h|(N-1) + 2|g|N\sqrt{M-1} + \omega_0 NM)t]^{1+(1/2k)}/\epsilon^{1/2k}. \quad (5)$$

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 the time dependence of the fidelity loss $1 - F(t) = 1 - |\langle\Psi_E(t)|\Psi_S(t)\rangle|^2$ of the simulated wave function $|\Psi_S(t)\rangle$ versus the exact one $|\Psi_E(t)\rangle$ as a function of coupling g and of number of sites N. The particular decomposition has been chosen so that all terms in Eq. (4) can be implemented in a linear chain of trapped ions.

Trapped-ion setup.—We consider a set of $N+1$ trapped ions in a chain, in order to simulate N fermionic sites provided with Holstein interactions. The ions are bounded strongly in the radial direction, and confined longitudinally within a harmonic potential [34]. We define ν_i, $i = 1, 2, \ldots, N+1$, as the frequencies of the axial normal modes. We relate the ion normal mode energies with the dispersionless phonon energies in Eq. (2) via $\Delta_i = \nu_i - \frac{\omega_0}{3}$. The three Hamiltonian steps H_1, H_2, and H_3 are derived in the interaction picture with respect to

$$H_0 = \sum_{i=1}^{N+1}\frac{\omega}{2}\sigma_i^z + \sum_{i=1}^{N}\Delta_i b_i^\dagger b_i + \nu_{N+1}b_{N+1}^\dagger b_{N+1}, \quad (6)$$

where ω 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 part of them is still present in order to recover the dispersionless phononic spectrum.

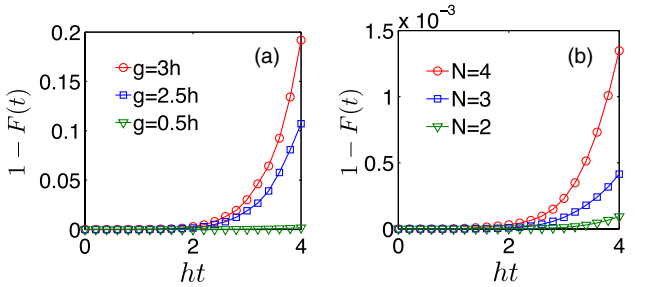

FIG. 1 (color online). (a) Behavior of the fidelity loss $1 - F(t) = 1 - |\langle\Psi_E(t)|\Psi_S(t)\rangle|^2$, for a two site configuration, as a function of the electron-phonon coupling strength g, for $\omega_0 = h/4$. As the coupling g increases, more phonons are created, the Hilbert space describing 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 $g = 0.3h$, $\omega_0 = 0.5h$, 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.

To simulate dynamics associated with H_1 and H_2 of Eq. (4), one has to achieve a NN Ising coupling. The possibility of obtaining an Ising field in linear chains of trapped ions has been proposed and realized [32,35]. However, in implementing NN interactions between more than two ions, one must be careful in designing an appropriate set of lasers and detunings in order to minimize the spurious non-nearest-neighbor (NNN) effects. To this extent, we have realized numerical simulations for a 3 + 1 ions setup [33], using one set of two pairs of counter-propagating lasers detuned close to the shifted center of mass mode of frequency $\Delta_1 = \nu_1 - \omega_0/3$ to drive the first two ions (detunings $\pm\delta_1$), and another set of lasers detuned close to a second mode of frequency Δ_2, that in the case of 3 + 1 ions can be chosen as the breathing mode, addressing the second and the third ion (detunings $\pm\delta_2$). For a generic number of ions, Rabi frequencies Ω_i of the lasers driving the ith and the $(i+1)$th ions are chosen to achieve the desired strength in the Ising coupling, according to [35],

$$H_{\mathrm{NN}} = \sum_{i=1}^{N-1} \Omega_i^2 \Bigg[\Bigg(\sum_{m=1}^{N} \frac{\eta_{i,m}\eta_{i+1,m}\Delta_m}{\delta_i^2 - \Delta_m^2} \Bigg) + \frac{\eta_{i,N+1}\eta_{i+1,N+1}\nu_{N+1}}{\delta_i^2 - \nu_{N+1}^2} \Bigg] \sigma_i^x \sigma_{i+1}^x. \quad (7)$$

In Fig. 2, the first and second ion are driven with two pairs of counterpropagating lasers with detuning close to the shifted center of mass mode ($\delta_1 = 1.0187\ \nu_1$ for $\omega_0 = h/4$). The Rabi frequencies are chosen properly in order to reach a NN interaction of $h/2 = 0.001\ \nu_1$. Lasers driving the second and the third ions are detuned close to the shifted breathing mode at $\nu_2 = 1.731\ \nu_1$ [34], with parameters $\delta_2 = 1.71196\ \nu_1$. Detunings are chosen to have

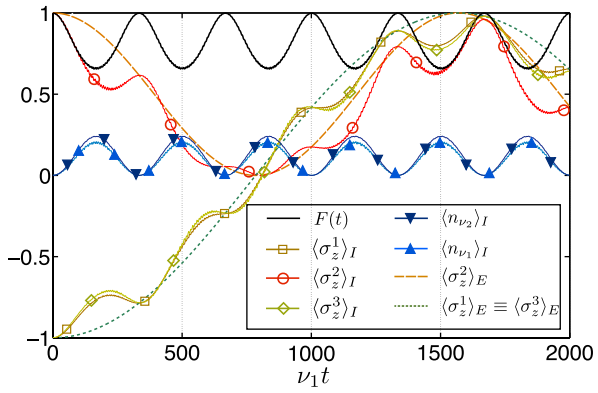

FIG. 2 (color online). Dynamics for the 3 + 1 ions configuration of the NN XX Hamiltonian. Dotted curves stand for $\langle\sigma_z^i\rangle_E$ for the exact dynamics, and solid curves stand for $\langle\sigma_z^i\rangle_I$ for realistic ion interactions ($i = 1, 2, 3$ for the first, second, and third ion). The parameters are chosen in order to have maxima in the fidelity $F(t) = |\langle\Psi_E(t)|\Psi_I(t)\rangle|^2$ of ∼0.995 (top black curve) at time steps of ∼333 $\nu_1 t$. These time steps can be chosen as Trotter steps.

a dynamics decoupled with respect to the phonons at time steps ∼333νt and a negligible NNN interaction [33]. 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 ∼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 [36].

Notice that one can always implement a perfect NN coupling by using more stroboscopic steps. A possibility is to decompose the global NN couplings 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 $h_{i,j}\sigma_x^i\sigma_x^j$, one can add more Trotter steps to the protocol of the form $-h_{i,j}\sigma_x^i\sigma_x^j$ in order to have a Hamiltonian free of NNN couplings. The dynamics associated with the step with H_2 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 ith ion ($i = 1, \ldots, N$) with the m_ith normal (shifted) mode $\eta_{i,m_i}\Omega_i\sigma_x^i(b_{m_i}^\dagger + b_{m_i})$. The ith ion is driven with red- and blue-detuned lasers to the m_ith 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 two times with a global beam upon all the $N+1$ ions at the same time. The Hamiltonian describing this process is,

$$H_{e\text{-}p} = \sum_{i=1}^{N} (\Omega_i\eta_{i,m_i}\sigma_z^i + \Omega_{N+1,i}\eta_{N+1,m_i}\sigma_z^{N+1})(b_{m_i} + b_{m_i}^\dagger). \quad (8)$$

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*,

$$H_{e\text{-}p,N} = \sum_{i=1}^{N} g \frac{(\sigma_z^i + 1)}{2} (b_{m_i} + b_{m_i}^\dagger). \tag{9}$$

Digital simulation.—In general, digital protocols are very 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 have 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 $N = 2 + 1$ [33] 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 which 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 [37]. The frequency

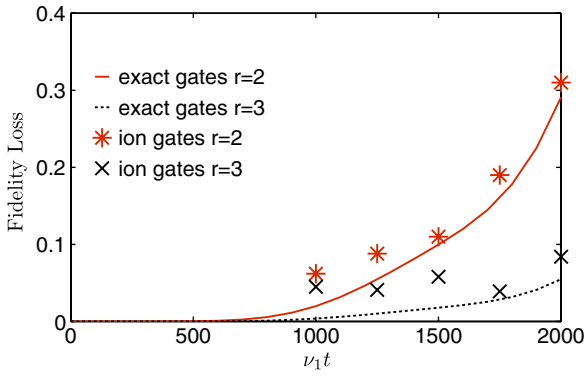

FIG. 3 (color online). Fidelity loss for 3 + 1 ion configuration, involving Trotter simulation with perfect gates and realistic ion interactions, for two and three symmetric Trotter steps.

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 μs [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 $2000/\nu_1 \sim 318$ μs, the time spent for the simulation can be taken to be of $\sim$1 ms. Given that typical heating rates in trapped ion experiments [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,

$$\chi(i, j) = \langle \Psi(t)|c_i^\dagger c_i (b_j^\dagger + b_j)|\Psi(t)\rangle. \tag{10}$$

This will amount to a signature of the polaron size [11]. Ranging from small to large g will lead to a measure of the crossover between large or small polaron. Notice that these correlations are mapped in our ion setup onto

$$\chi(i, j) = \langle \Psi(t)|(b_{m_j} + b_{m_j}^\dagger) \frac{(\sigma_i^z + 1)}{2} |\Psi(t)\rangle, \tag{11}$$

which can be measured by mapping the motional onto the internal state of the auxiliary $(N + 1)$th ion, and then detecting the resonance fluorescence of ions $N + 1$ and i [22,24]. 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 [4].

Currently, more than 100 gates have been implemented in a trapped-ion quantum simulation experiment with Trotter methods [3]. In the near future, it should be possible to achieve hundreds or even thousands of gates per experiment [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 us to study the formation of small polarons under these conditions. Future experiments involving 20 to 30 ions will permit us 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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