Parallel execution of quantum gates in a long linear ion chain via Rydberg mode shaping

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(Received 15 August 2012; revised manuscript received 31 January 2013; published 6 May 2013)

We present a mechanism that permits the parallel execution of multiple quantum gate operations within a single long linear ion chain. Our approach is based on large coherent forces that occur when ions are electronically excited to long-lived Rydberg states. The presence of Rydberg ions drastically affects the vibrational mode structure of the ion crystal, giving rise to modes that are spatially localized on isolated subcrystals which can be individually and independently manipulated. We theoretically discuss this Rydberg mode shaping in an experimentally realistic setup and illustrate its power by analyzing the fidelity of two conditional phase flip gates executed in parallel. The ability to dynamically shape vibrational modes on the single-ion level might find applications in quantum simulators and quantum computation architectures.

DOI: 10.1103/PhysRevA.87.052304 PACS number(s): 03.67.Lx, 32.80.Qk, 33.80.Rv

I. INTRODUCTION

The ability to execute multiple quantum operations in parallel is believed to be a fundamental requirement for achieving large-scale quantum computation [1–3]. Among the many types of systems being considered for the physical implementation of a quantum processor [4], trapped ions have attracted much attention for the astonishingly high degree of experimental control that can be gained over their internal and external degrees of freedom [3]. One strategy for achieving parallelism is to build many local quantum processors. Current proposals envision setups where ions are confined in spatially separated wells provided by arrays of microtraps [5] or by traps with segmented electric field electrodes [6]. Few ions trapped within a given well form one of many local quantum processors that can be operated independently and in parallel [7]. Information can be exchanged among different local processors by rearranging the potential landscape such that previously disconnected ions have common vibrational modes. Such rearrangement is usually achieved by switching voltages applied to the ion trap electrodes [6]. In spite of the availability of microstructured arrays it remains a challenge to obtain fast switching times and a high spatial resolution of the local electric fields that would grant a manipulation of the potential landscape down to the level of a single ion.

In this work we introduce a scheme that permits the execution of multiple quantum gates in parallel on a long linear ion crystal. The method relies on the shaping of the vibrational crystal modes through the laser excitation of selected ions into electronically excited Rydberg states. Strong coherent forces acting on these excited ions [8,9] effectively break the long crystal into small subcrystals in the sense that vibrational modes emerge which are strongly localized on only a few ions. We illustrate the power of this Rydberg mode shaping by thoroughly analyzing the fidelity of two two-qubit conditional phase flip (CPF) gates that are executed in parallel on different subcrystals belonging to the same ion chain. A feature of our scheme is that decoupling between the localized modes and the remaining spectator modes permits us not only to achieve a high gate fidelity but also to drastically reduce the complexity of gate optimization protocols [10–12].

In view of the intrinsic stability of ion crystals [13], the ability to address single ions individually by lasers [14] and the long lifetime of Rydberg states, we believe that this dynamical mode shaping is particularly useful in digital quantum simulations [15] as these strongly benefit from the availability of robust parallelization approaches.

II. SETUP AND IDEA

Before providing details let us briefly outline the setup we have in mind. We consider a long linear crystal of 100 40Ca+ ions which is realized within a quartic electric potential (see details below). This choice is motivated by the proposal discussed in Ref. [13], which envisages the implementation of an ion quantum processor where a long ion chain is divided into two parts: Quantum computation is carried out in the central region where ions are nearly uniformly spaced. The remaining outer ions are continuously Doppler cooled to prevent heating. To describe the internal structure of the ions we consider the four states depicted in Fig. 1(a). The electronically low-lying (ELL) $S, P,$ and $D$ states are employed in numerous ion trap experiments for the storage, manipulation, and readout of quantum information [3]. Furthermore, we consider the Rydberg state $nP_J$ (with $J = 1/2$ and the principal quantum number $n$) which is excited from the $3D_{3/2}$ state via a single photon transition [14,16].

We envisage Rydberg excitations to be carried out in the central region of the ion chain and in Fig. 1(a) we illustrate a situation where four Rydberg ions enclose two pairs of ions in ELL states. Those ion pairs will form the subcrystals on which we are going to execute quantum gates in parallel. The underlying physical mechanism which we aim to exploit for this purpose becomes apparent in Figs. 1(b) and 1(c). Here we show the absolute values of the normal mode matrix of the vibrational crystal modes which provide a measure on how much each ion contributes to a vibrational mode. In Fig. 1(b), which shows the case in which all ions are in ELL states, we see that, in general, many ions contribute to each normal mode. Compared to this, the presence of Rydberg ions leads to a drastic change of the mode structure as can be seen in...
is the potential of a radio-frequency (rf) field with gradient $\alpha$ and frequency $\Omega$ and
\begin{equation}
\Phi_{\alpha}(\mathbf{r}) = \beta_2 \frac{2z^2 - r^2}{2} + \beta_4 \left[ z^4 - 3z^2 r^2 + \frac{3}{8} r^4 \right],
\end{equation}
with $r^2 = x^2 + y^2$, is a quartic static electric potential whose parameters $\beta_j (j = 2, 4)$ depend on the specifics of the field-generating electrodes, i.e., the gradient and higher derivatives of the field. Recently, similar potentials have been realized experimentally [17,18]. For a sufficiently fast rf frequency drive [19] an ion of mass $M$ experiences the ponderomotive potential
\begin{equation}
V_{\alpha}(\mathbf{r}) = e \frac{\alpha^2}{M \Omega^2} r^2 + \Phi_{\alpha}(\mathbf{r}).
\end{equation}
Within this trap an ion chain is formed along the $z$ axis provided that $\alpha \gg |[\beta_2/\beta_4]| > 0 (\beta_2 < 0)$. Here $l_z = (e(8\pi \epsilon_0 |\beta_2|))^{1/3}$ is the typical length scale associated with $V_{\alpha}(\mathbf{r})$ and $e$ and $\epsilon_0$ are the elementary charge and the vacuum permittivity, respectively. In addition, the tuning of the parameters $\beta_2$ and $\beta_4$ permits us to achieve a long ion crystal in which the equilibrium positions of ions in ELL states are approximately evenly spaced [13]. The equilibrium positions of the long ion crystal is determined by a parameter $k_4 = 2\beta_4 l_z^2/|\beta_2|$. In the following we set $k_4 = 1.343$ as this choice minimizes fluctuations of the nearest-neighbor separation within the central region of the ion chain [13].

In Ref. [9] we showed that ions excited to the $nP_{1/2}$-Rydberg state experience not only the ponderomotive potential but are also subject to an additional radial potential that is proportional to the Rydberg polarizability $V_{\alpha}(\mathbf{r}) \approx -e^2\alpha^2P_{a,p}r^2$, where $P_{a,p} \approx -0.25 \times n^2$ (in atomic units). There are also small corrections to the trapping potential along the $z$ axis but these are negligible in this linear ion trap. The ratio of the radial trap frequencies experienced by an ion in the Rydberg/ELL state is approximately given by
\begin{equation}
\frac{\omega_{Ryd}}{\omega_{ELL}} = \sqrt{1 - M \Omega^2 P_{a,p}}.
\end{equation}
In practice, ratios on the order of 2 and larger can be achieved. In the following we show that this is already sufficient for a Rydberg ion to effectively introduce a constriction of the linear ion chain which strongly affects the vibrational mode structure. Note that such state-dependent trap frequency change has also been theoretically reported for Rydberg atoms in inhomogeneous magnetic fields [20].

B. Collective modes and mode shaping

Let us now demonstrate the mode shaping considering the transverse phonon modes along the $x$ axis as an example. The treatment of the $y$ phonons is done accordingly. The phonon Hamiltonian is [7] $H_x = \sum_{n,j} \hbar \omega_{n,j} (b_{n,j}^\dagger b_{n,j} + 1/2)$. Here $b_{n,j}^\dagger (b_{n,j})$ is the creation (annihilation) operator of the $j$th phonon, whose frequency $\omega_j$ is calculated by diagonalizing the Hessian matrix $\sum_{m,n} \mathcal{H}_{mn} b_{n,j}^{(j,x)} = (\omega_j/\omega_{n,j})^2 B_{n,j}$ with
\begin{align}
\mathcal{H}_{mn} &= \left[ \frac{\omega_j}{\omega_{n,j}} \right]^2 + \frac{1}{2} - \frac{\Delta^2}{\omega_j^2} - \sum_{k \neq m} \frac{1}{|m - n|}, \quad n = m, \\
\mathcal{H}_{mn} &= \left[ \frac{\omega_j}{\omega_{n,j}} \right]^2 + \frac{1}{2} - \frac{\Delta^2}{\omega_j^2}, \quad n \neq m,
\end{align}

III. IMPLEMENTATION

A. A long linear ion crystal

Let us now provide a more detailed discussion of the practical implementation of the above idea. To achieve a long linear ion crystal we consider an ion trap formed by the time-dependent electric potential:
\begin{equation}
\Phi(r,t) = \Phi_{\text{el}}(r,t) + \Phi_{\alpha}(r).
\end{equation}
Here
\begin{equation}
\Phi_{\text{el}}(r,t) = \alpha \cos \Omega t (x^2 - y^2)
\end{equation}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{(Color online) (a) Level structure of Ca$^{+}$ and schematics of the envisioned setup. Red and blue symbols refer to ions in Rydberg states and ions in electronically low-lying (ELL) states, respectively. Subcrystals of ion pairs are isolated within a linear crystal formed by 100 ions by the excitation of selected ions to the Rydberg $nP_{1/2}$ state (here the 45th, 48th and 53rd, 56th). Using laser-induced spin-dependent forces, quantum gates can be executed on the two subcrystals in parallel. (b) Vibrational modes of a crystal formed by spin-dependent forces, quantum gates can be executed on the two states (here the 45th, 48th and 53rd, 56th). (c) Excitation laser subcrystals in parallel.}
\end{figure}
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and $B_{m}^{(j,x)}$ denoting the eigenvectors. The parameters $z_{m}$ are the $z$ component of the equilibrium position of the $m$th ion and $\omega_{m}^{(x)}$ is the state-dependent trapping frequency of the $m$th ion along the $x$ axis; i.e., $\omega_{m}^{(x)} = \omega_{\text{ Ryd}}(\omega_{\text{ ELL}})$ if the ion is in the Rydberg (ELL) state. For convenience, we have defined a reference frequency $\omega_{s} = \sqrt{2\epsilon|B_{j}|/M}$ and scaled length with $l_{j}$ such that the Hessian is dimensionless.

We start with a simple situation where in our chain of 100 ions the 45th and 56th are excited to the Rydberg state. The resulting change of the mode structure becomes directly apparent in the modulus of $B_{m}^{(j,x)}$ which is depicted in Fig. 2(a). Compared to the situation without mode shaping [Fig. 1(b)], the striking difference is that the 46th to 55th ions constitute a virtually isolated subcrystal hosting a series of spatially localized modes. The energies of these local modes are shown in Fig. 2(b) where we also undertake a comparison to the mode energies obtained from the full (circles) and truncated (diamonds) calculations. The largest discrepancy between these calculations is about 0.3%. The dots show the (quasicontinuous) energy spectrum of the ion chain without mode shaping. In all the calculations we use $\omega_{\text{ ELL}}/\omega_{s} = 150$ and $\omega_{\text{ Ryd}}/\omega_{s} = 198.5$.

C. Parallel conditional phase gates

Let us return to this initial example in which we had two subcrystals composed by the ion pairs \{46,47\} and \{54,55\}. Each of the subcrystals hosts two localized vibrational modes. The eigenvector corresponding to the localized mode with higher energy is displayed in the inset of Fig. 1(c). In the following we show that with these local modes, we can execute two two-qubit gates in parallel. Specifically, we discuss a $\sigma^{z}$-type [21] two-qubit CPF gate. Qubits are encoded in two ELL states of an ion, denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$. These can be hyperfine states as discussed in Refs. [22,23] or states coupled by optical quadrupole transitions as, e.g., in Ref. [24]. The CPF gate is implemented by a laser-induced coupling [see gate lasers in Fig. 1(a)] between the qubit states and the vibrational crystal modes/phonons. This results in a “spin-dependent” force [22–24] whose action is described by the spin-phonon Hamiltonian [11,25]

$$H_{1} = \sum_{m,j=1}^{N} \hbar \Omega_{m}(t) \sigma_{m}^{z} \eta^{(j)}(B_{m}^{(j,x)})(b_{j}^{\dagger} e^{i\omega j t} + \text{H.c.}).$$

Here $\Omega_{m}(t)$ is the time-dependent Rabi frequency of the gate laser that addresses the $m$th ion and $\eta^{(j)} = k_{j} l_{j}$ is the corresponding Lamb-Dicke parameter, with $k_{j}$ being the modulus of the laser wave vector and $l_{j} = \sqrt{2 \hbar M \omega_{s}}$ being the oscillator length associated with the $j$th phonon mode. The CPF gate is conducted by switching the gate lasers on for a given time $t$ during which the Rabi frequencies $\Omega_{m}(t)$ are varied. Using the Magnus formula [26], the evolution operator due to $H_{1}$ is then given by

$$U(t) = \exp \left[ i \sum_{m} Q_{m}(t) \sigma_{m}^{z} + i \sum_{mn} \phi_{mn}(t) \sigma_{m}^{x} \sigma_{n}^{x} \right].$$

The first term in the exponential characterizes the residual coupling of the $m$th qubit with the phonon modes and depends on $Q_{m}(t) = \sum_{j} [\alpha_{m}^{(j)}(t) b_{j}^{\dagger} + \text{H.c.}]$, where $\alpha_{m}^{(j)}(t)$ is a parameter that characterizes the coupling strength. The second term gives rise to a phonon-induced spin-spin coupling between the $m$th and $n$th qubit, thereby effectuating a CPF gate. A perfect CPF gate is realized when $\phi_{mn}(t) = \pi/8$ and $\alpha_{m}^{(j)}(t) = 0$. As shown in Refs. [10–12] this can be achieved via optimizing the time-dependent profile of the Rabi frequencies $\Omega_{m}(t)$. Such optimization is challenging since, in general, many phonon modes contribute even when only a single CPF gate operation is conducted within a long ion chain. Rydberg mode shaping has the potential to drastically reduce the complexity of such optimization procedure as even in long crystals only few vibrational modes actually couple to the qubit ions located on a subcrystal.

Let us now analyze the performance of two CPF gates that are executed in parallel on the two subcrystals depicted in Fig. 1(a). To assess the performance of the gate operation, we use the high-energy mode [inset of Fig. 1(c)] as “quantum bus.” The gate lasers are switched on for a time $\tau = 8 \tau_{0}$, where $\tau_{0} = 2\pi/\omega_{b}$ is the oscillation period of the bus mode and the Rabi frequency is assumed to follow $\Omega_{m}(t) = \Omega_{0} \sin(\nu t)$ (as also discussed in Ref. [23]). We optimize the fidelity with respect to the parameter $\nu$ of this simple ansatz. Imposing a two-qubit phase shift $\phi_{mn}(t) = \pi/8$ fixes the value of the amplitude $\Omega_{0}$ (for more detail see Ref. [25]). The qubits are prepared in a product state

$$|\Psi(0)\rangle = (|\psi_{m_{1}}\rangle \otimes |\psi_{n_{1}}\rangle \otimes |\psi_{m_{2}}\rangle \otimes |\psi_{n_{2}}\rangle),$$

with $|\psi_{m}\rangle = (|\uparrow\rangle_{m} + |\downarrow\rangle_{m})/\sqrt{2}$ and $\{m_{1},n_{1}\}$ being indices of ions forming the $j$th subcrystal. Ideally, the output state after
the parallel execution of the two CPF gates is

$$|\Psi(\tau)\rangle = \exp\left[i \frac{\pi}{4} (\sigma^z_{m1} \sigma^z_{n1} + \sigma^z_{m2} \sigma^z_{n2})\right] |\Psi(0)\rangle.$$  \hspace{4cm} (9)$$

However, due to the residual phonon-qubit coupling this state will be only reached with a certain probability, which we characterize through the fidelity

$$F = \langle \Psi(\tau)|\text{Tr}_v \rho(\tau)|\Psi(\tau)\rangle.$$  \hspace{4cm} (10)$$

Here, $\rho(\tau) = U(\tau) \rho(0) U^\dagger(\tau)$, with $\rho(0) = \rho_c \otimes |\Psi(0)\rangle \langle \Psi(0)|$ and $\text{Tr}_v$ denotes the trace over the vibrational modes whose density matrix is $\rho_c$. For calculating the fidelity we assume the following sequence: The ions are initially in ELL states and the phonon density matrix $\rho_c$ is a thermal distribution. Rydberg ions are subsequently excited via protocol that is highly nonadiabatic with respect to the phonons; i.e., the phonon density matrix $\rho_c$ is a thermal distribution. In Appendix A we provide more detail on such protocol. The gate fidelity is then calculated via a transformation that expresses $\rho_c$ in terms of the shaped vibrational modes [9]. The exact details of the calculation are provided in Appendix B.

Let us first consider a situation in which the two CPF gates start simultaneously. We find that the highest achievable fidelity within our simple ansatz is $F_{\text{max}} \approx 99.95\%$. As shown in Fig. 3(a), this maximum occurs at $\nu \tau = 2\pi \times K$ (with $K$ an integer). At these points the bus modes almost entirely return to their initial states [11,27]. The fact that such a high fidelity is achievable within this simple ansatz is a direct consequence of the fact that the Rydberg ions delimiting the subcrystal lead to a dramatic reduction of the number of vibrational modes that couple to the qubit ions. This reduction is clearly seen by the data presented in Fig. 3(a). Without this Rydberg mode shaping the highest fidelity that we can achieve is 93%.

The power of the mode shaping becomes even more apparent when introducing a start time delay $t_d$ of the second CPF gate with respect to the first one. $F_{\text{max}}$ slightly decreases with growing $t_d$ but always remains above 98%, as shown in Fig. 3(b). This demonstrates that the two CPF gates can be operated essentially independently. In the absence of mode shaping, however, $F_{\text{max}}$ quickly drops with increasing $t_d$ reaching a minimal value of $\approx 36.1\%$.

Finally, let us discuss additional sources that would influence the gate fidelity. First, the fidelity will be, in principle, reduced by the radiative decay of the Rydberg state. This is mitigated by the fact that CPF gates are inherently fast [25] and that Rydberg states are long lived. For example, choosing the $60P_{1/2}$ state, we obtain a Rydberg lifetime $\approx 270 \mu$s and with the trap parameters $\alpha = 7 \times 10^3$ V/m, $\Omega = 2\pi \times 25.2$ MHz, and $\beta_2 = -2.09 \times 10^3$ V/m we obtain a gate time $\tau \approx 3.7 \mu$s. Taking into account the Rydberg excitation time, the gate fidelity will be modified by an overall factor, about $0.982^{103 \mu s}$, with $N_{\text{Ryd}}$ the number of Rydberg ions that are excited during the gate operation. However, in principle, the gate operations can be accelerated by using a more sophisticated optimization protocol [13], and furthermore, optimized gate schemes can be imagined in which the Rydberg ions do not stay permanently excited. Second, infidelities are caused by other factors, such as the anharmonicity of the ionic motion and corrections beyond the Lamb-Dicke limit. These have been investigated in detail by Lin et al. in Ref. [13] and their contributions have been found to be marginal.

### IV. SUMMARY AND OUTLOOK

In conclusion, we showed that the transverse vibrational modes of a linear ion chain can be shaped by the selective excitation of Rydberg ions leading to the emergence of strongly localized modes. This Rydberg mode shaping can potentially be applied for implementing quantum simulation and processing schemes within a single large (possibly three-dimensional) ion crystal. One can envisage a scheme where dedicated ions are not used as qubits but only for segmenting the crystal. When excited they give rise to local modes that permit the parallel manipulation of sets of qubits. When deexcited the nonlocal character of the vibrational modes is restored permitting the entanglement of more distant qubits.

A drawback of the current scheme is that the gate execution follows the Rydberg excitation. This means that Rydberg ions are excited throughout the entire duration of the gate sequence which consequently leads to a reduced fidelity. A future goal is therefore to devise optimized control sequences which reduce the Rydberg excitation time but at the same time make use of the existence of localized modes. In addition, the Rydberg mode shaping is particularly applicable for parallel execution of multiple quantum gates with the Mølmer-Sørensen scheme [27]. If, instead, the gate is based on the Cirac-Zoller scheme [28], where phonons need to be cooled to the ground state initially, the consequent gate error will be severe as phonons can be significantly excited after the Rydberg excitation (see Appendix B).

### ACKNOWLEDGMENTS

We thank Peter Zoller for initial discussions which stimulated this work. We thank C. Ates and S. Genway for careful reading of the manuscript. Discussions with all members of the R-ION consortium are kindly acknowledged. This work...
is funded through EPSRC and the ERA-NET CHIST-ERA (R-ION consortium).

**APPENDIX A: EXCITATION OF RYDBERG IONS**

For the practical application of the mode shaping it is crucial to excite ions to the Rydberg state with high fidelity, which can be a challenge if the trapping potentials of ELL and Rydberg states are very different. In general, the (reduced) density matrix of the ion to be excited is given by \( |SD_{3/2}\rangle \otimes \rho_P \), where \( \rho_P \) is the density matrix of the external degrees of freedom. The Rydberg excitation needs to take the ion to the state \( |nP_{1/2}\rangle |nP_{1/2}\rangle \otimes \rho_P \) as the shaped modes are only present if the electronic population of the ion is entirely transferred to \( |nP_{1/2}\rangle \). Note that the density matrix of the Rydberg states can be obtained under the assumption that the excitation has been carried out the MW is switched on. After this process, the dressed states are very different: In general, the (reduced) density matrix of the ion to be excited is given by

\[
|SD_{3/2}\rangle \otimes \rho_P = \begin{pmatrix}
|N\rangle |+\rangle
|N\rangle |-\rangle
|P\rangle |+\rangle
|P\rangle |-\rangle
\end{pmatrix}
\]

where \( |N\rangle \) is the density matrix of the external degrees of freedom. In the extreme case the Franck-Condon factors become trivial and the laser becomes identical with that of the ions in ELL states. In this case the large energy splitting allows us to address the dressed states individually.

The scheme works as follows. Together with Rydberg laser, we apply a microwave field (MW), which creates dressed states. The Rydberg excitation is then independently of the phonon state. Both methods, however, can use a broadband laser excitation that does not resolve the individual phonon modes and thus performs the transfer with high fidelity: For example, one can cool all phonon modes to the ground state, such that the initial state \( \rho_P \) is precisely known. The excitation laser pulse (frequency, strength, and duration) can then be optimized to achieve perfect electronic state transfer. Alternatively, one can use a broadband laser excitation that does not resolve the individual phonon modes and thus performs the transfer independently of the phonon state. Both methods, however, are rather challenging with current technology. A currently feasible alternative is to remove the difference in the electronic population of Rydberg states through the application of a microwave field (MW), which creates dressed states of tuneable polarizability. The Rydberg excitation is then no longer different than the excitation of ELL states. After the excitation has been carried out the MW is switched off in a way that is adiabatic on electronic time scales but can be highly nonadiabatic on the time scale of the phonon dynamics.

The scheme works as follows. Together with Rydberg laser, we apply a MW field that couples the Rydberg \( |nP_{1/2}\rangle |nP_{1/2}\rangle \otimes \rho_P \) (denoted by \( |P\rangle \)) with a nearby state \( |n'S_{1/2}\rangle |n'S_{1/2}\rangle \otimes \rho_P \) (denoted by \( |S\rangle \)). The respective level scheme is depicted in Fig. 4. The corresponding ion-field interaction is given by

\[
V(t) = -eE_0 \cos \omega_0 t z - eE_1 \cos \omega_1 t z, \tag{A1}
\]

where \( E_0 \) (\( E_1 \)) is the laser (MW) electric field and \( \omega_0 \) (\( \omega_1 \)) is the Rydberg laser (MW) frequency. Both the Rydberg laser and the MW field are linearly polarized along the \( z \) axis. The field-free Rydberg energies are \( \epsilon_S \) and \( \epsilon_P \), respectively. To be concrete, we also assume \( \epsilon_S < \epsilon_P \).

\[
H = \Delta_S |S\rangle \langle S| + \Delta_P |P\rangle \langle P| + H_L, \tag{A2}
\]

where \( \Delta_S = \epsilon_S - (\omega_0 - \omega_1) \) and \( \Delta_P = \epsilon_P - \omega_0 \). \( \Omega_L = -eE_0 |P| z |D\rangle \) and \( \Omega_{MW} = -eE_1 |S| z |P\rangle \).

We consider a strong MW field, \( \Omega_{MW} \gg \Omega_L \), for which it is convenient to use the dressed state in order to describe dynamics of the Rydberg states. By diagonalizing the part of Hamiltonian (A2) that contains the MW coupling part, the dressed states are given by

\[
|\pm\rangle = N_{\pm} (C_{\pm} |P\rangle + |S\rangle), \tag{A3}
\]

where \( C_{\pm} = \frac{\Delta_{\pm} \sqrt{\Omega_{MW} + \Delta_{\pm}}}{\Delta_{\pm} \sqrt{\Omega_{MW} + \Delta_{\pm}}} \) with \( \Delta_{\pm} = \Delta_P \pm \Delta_S \) and \( N_{\pm} \) is the normalization constant. The dressed state energy is \( E_{\pm} = \frac{\Delta_{\pm} \sqrt{\Omega_{MW} + \Delta_{\pm}}}{\Delta_{\pm} \sqrt{\Omega_{MW} + \Delta_{\pm}}} \). With the dressed state at hand, the Hamiltonian Eq. (A2) becomes

\[
H \approx E_{\pm} |+\rangle \langle +| + E_{\pm} |\mp \rangle \langle \mp| + H_L', \tag{A4}
\]

\[
H_L' = -\frac{1}{2}(\Omega_{\pm} |+\rangle \langle D| + H.c.) + \frac{1}{2}(\Omega_{\pm} |-\rangle \langle D| + H.c.),
\]

with \( \Omega_{\pm} = \frac{\Omega_{MW}}{2 \sqrt{\Omega_{MW} + \Delta_{\pm} \Omega_L}} \). Thus, the low-lying \( D \) state is now coupled with the two dressed states. Here the large energy splitting allows us to address the dressed states individually with the Rydberg laser.

The polarizability of the dressed state is \( \mathcal{P}_{\pm} = N_{\pm}^2 (C_{\pm}^2 \mathcal{P}_P + \mathcal{P}_S) \). As \( \mathcal{P}_S > 0 \) for high-lying Rydberg states, the polarizability of the dressed state vanishes under certain conditions. For example, for \( n' = n \), \( \mathcal{P}_S = 0 \) when \( |C_{\pm}| < 0.68 \), which can be realized by controlling the MW frequency and/or Rabi frequency. On the other hand, when \( \mathcal{P}_S = 0 \), the trapping potential of the Rydberg ion in the dressed state becomes identical with that of the ions in ELL states. In this case the Franck-Condon factors become trivial and the laser excitation is not different than transitions driven among ELL states. In Fig. 5(a) we demonstrate the \( |\mp \rangle \) state excitation. After a \( \pi \) pulse, the ion is excited to the \( |\mp \rangle \) state.

Once the state \( |\mp \rangle \) is excited, the Rydberg laser is switched off and also the MW is switched off such that \( |\mp \rangle \) is adiabatically transferred to the state \( |P\rangle \). As an example, we show in Fig. 5(b) a case in which the MW detuning is changed according to \( \Delta_{SP}(t) = (\Delta_S - \Delta_P)(1 - c^2 t^2) \). The Rydberg ion is fully populating the \( P \) state after about 13 ns.

**APPENDIX B: CALCULATION OF THE GATE FIDELITY**

As shown in the previous section, the Rydberg excitation can be performed on a time scale that is highly nonadiabatic with respect to the vibrational dynamics. In the extreme case the spatial wave function of the ion does not change, i.e., is
frozen, in the course of the Rydberg excitation. In this section, we show how for this case the gate fidelity can be calculated by using a Duschinsky transformation that connects the phonon modes before the Rydberg excitation (bare phonon modes) to the shaped phonon modes.

Let us first describe the normal coordinate $Q_g$ and canonical momentum $P_g$ of the bare mode using the corresponding phonon creation and annihilation operators [7],

$$Q_g = L_g(A_i + A),$$

$$P_g = P_g(A_i - A),$$

where $A_i$ and $A$ are both column vectors, $A_i = (a_1^\dagger, a_2^\dagger, \ldots, a_N^\dagger)$ and $A = (a_1, a_2, \ldots, a_N)$, with $N$ the total number of ions and $i$ to be the transverse operation. $a_i$ ($a_i^\dagger$) is the annihilation (creation) operator of the $i$th bare phonon mode. $L_g$ and $P_g$ are diagonal matrices, whose matrix elements are $L_g(p, p') = \sqrt{h/2M_\alpha p^2}$ and $P_g(p, p') = i\sqrt{hM_\alpha p^2}$, where $\alpha p$ is the $p$th phonon frequency of the bare mode. Similarly, we obtain the result of normal coordinate $Q_e$ and momentum $P_e$ of the Rydberg shaped mode

$$Q_e = L_e(B_i + B),$$

$$P_e = P_e(B_i - B),$$

where $B_i = (b_1^\dagger, b_1^\dagger, \ldots, b_N^\dagger)$, $B = (b_1, b_2, \ldots, b_N)$, $L_e(p, q) = \sqrt{h/2M_\omega p^2}$, and $P_e(p, q) = i\sqrt{hM_\omega p^2}$ when $p = q$ and zero otherwise.

We now find the Duschinsky transformation between the bare and Rydberg modes. The displacement of the ions around their equilibrium positions is denoted by a column vector $\chi = (x_1, x_2, \ldots, x_N)^T$. We can obtain that $Q_g = A\chi$ and $Q_e = B\chi$, where $A$ ($B$) is the eigenvector of the bare (Rydberg) mode. Applying the Duschinsky transformation, one finds $Q_e = TQ_g$ with $T = BA^{-1}$. Examples of the $T$ matrix element are given in Fig. 6. Similarly, one obtains $P_e = TP_g$.

With Eqs. (B1)–(B4) and the Duschinsky transformation, we can find the transformation between the phonon operators of the Rydberg and bare mode,

$$B_i = \frac{1}{\sqrt{2}}[T_\alpha A_i + T_{-\alpha} A_i],$$

$$B_p = \frac{1}{\sqrt{2}}[T_\alpha A_i + T_{-\alpha} A_i],$$

where $T_\alpha = (I_\alpha - \text{TL}_e \pm \text{TP}_e)^{-1}$. This relation allows us to express the gate evolution operator Eq. (7) in the main text in terms of the phonon operators of the bare mode,

$$U(p) = \exp \left[ -i \left( C_e A_i + C_e^\dagger A + \sum_{m,n=1}^4 \phi_{mn} \sigma_m^\dagger \sigma_n^\dagger \right) \right]$$

$$= \exp \left[ -i \sum_{p=1}^N (c_p a_p^\dagger + c_p^\dagger a_p) + i \sum_{m,n=1}^4 \phi_{mn} \sigma_m^\dagger \sigma_n^\dagger \right],$$

where $C_e = \text{Re}(C_e)L_e^{-1}TL_e + i\text{Im}(C_e)P_e^{-1}TP_e$ and $c_p = \sum_{m=1}^4 C_e(m, p)$. $C_e$ is a diagonal matrix characterizing the residual phonon-qubit coupling, whose diagonal matrix elements are $C_e(p, p) = \sum_{m=1}^4 a_{m, p}^{(p)} \sigma_m$ with $a_{m, p}^{(p)}(\tau) = \int_0^\tau \Omega_m(t) B_m^{(p)} \eta^{(p)} e^{i\omega_p t} dt$, where $B_m^{(p)}$ is the $p$th mode vector of the $m$th ion and $\eta^{(p)} = k_l^p l_p$ is the corresponding Lamb-Dicke parameter. Here $\Omega_m(t) = \Omega_0 \sin(\nu t)$ is the time-dependent Rabi frequency of the gate laser that addresses the $m$th ion. The spin-spin phase is $\phi_{mn}(t) = \int_0^t dt' \int_0^{t'} dt' \int_0^{t''} dt'' \sum_p \Omega_m(t') \Omega_m(t) B_m^{(p)} B_n^{(p)} \eta^{(p)} \sin(\omega_p(t'' - t')).$
For convenience, we have denoted the index of the qubit ions (the 46th, 47th, 54th, and 55th ion in the 100-ion chain) with $m(n) = 1, 2, 3, 4$.

Equation (77) permits us to calculate the gate fidelity conveniently as the bare phonon modes are initially in a thermal state $\rho_0$. The qubits are in a product state $|\Psi(0)\rangle = (|\psi_m\rangle \otimes |\psi_n\rangle) \otimes (|\psi_m\rangle \otimes |\psi_n\rangle)$ with $|\psi_m\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ and $|m, n\rangle$ being indices of ions forming the $j$th subcrystal. Ideally, the output state after a gate time $t$ is $|\Psi(t)\rangle = \exp[i\pi/4(\sigma^z_m \sigma^z_n + \sigma^z_m \sigma^z_n)]|\Psi(0)\rangle$. The actual gate performance is characterized by the gate fidelity $F = \langle \Psi(t)|\text{Tr}(\rho(t))|\Psi(t)\rangle = 1/256 \sum_{j,k=1}^{16} \langle j|\rho|k\rangle$. Here $|j\rangle$ ($j = 1, \ldots, 16$) is the four-qubit basis (a full list of $|j\rangle$ is given in Table I), with $\sigma^z_n|j\rangle = \sigma^z_n|j\rangle$ and $\rho(t) = U(t)\rho(0)U^\dagger(t)$ with $\rho(0) = \rho_0 \otimes |\Psi(0)\rangle\langle\Psi(0)|$. $\text{Tr}$ denotes the trace over the vibrational modes. After some math, the gate fidelity is found explicitly as

$$F = \frac{1}{256} \sum_{j,k=1}^{16} \varphi_{jk} \times \exp \left[ \frac{1}{2} \sum_{p=1}^{N} \left( c^j_p c^k_p - c^{j+1}_p c^{k+1}_p - |c^j_p - c^k_p|^2 \coth \frac{\gamma_p}{2} \right) \right],$$

(B8)

where $c_{p,j} = c^j_p|j\rangle$ and $\gamma_p = h\omega_p/k_BT$ is the temperature factor ($k_B$ the Boltzman constant, $T$ phonon temperature)

The gate error here is mainly caused by the spin-phonon coupling, i.e., the $c^j_p$ term in Eq. (B8). We illustrate this with an example when $v\tau/2\pi = 1$ [see Fig. 3(a)]. We assume that initially all the bare modes share a same temperature $T$, in which the average phonon number of the highest energy mode is 3.25. The temperature factor is roughly $\gamma_p \sim 0.2$. The gate fidelity is calculated under two different situations, i.e., without and with Rydberg mode shaping. When the gate is performed with the bare mode, we find that $0 < |c^j_p| < 2.2 \times 10^{-3}$. Therefore, the maximal $|c^j_p|$ in the presence of the mode shaping is one order of magnitude smaller than that of the bare mode case. In both cases, $|\varphi_{jk}| \approx 1$ (the numerical value of the spin-spin phase $\varphi_{mn}$ is given in Table II), which results from the optimization of the laser Rabi frequency $\Omega_0$ [13].

With these data we find the gate fidelity $F = 0.85$ (in case of the bare mode) and $F = 0.9995$ (in case of the mode shaping), respectively.
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