The physics of Ion Coulomb Crystals: Thermodynamics, Quantum control, and Quantum Simulators

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Protocols for quantum state preparation of ICC and experimental route to their realization

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Title: Protocols for quantum state preparation of ICC and experimental route to their realization

Short Description: Report on robust laser-cooling protocols for preparing an ion string in the quantum regime.

Work achieving the deliverable: Ref. [1] constitutes the main contribution to the deliverable and fulfills its central goal. Here, the dynamics of an ion chain confined in a high-finesse resonator are analysed, and parameter regimes are identified in which the chain can be cooled to a state, where photonic and vibrational excitations are entangled. The model includes noise on the atomic motion and cavity decay, and the predictions show that entanglement can be found for parameter regimes which are experimentally feasible. In Ref. [2], it is proposed to use an interplay between cavity-enhanced scattering and electromagnetically induced transparency in order to obtain a high-fidelity cooling mechanism for trapped atoms and ions. Refs. [3-4] characterise the use of quantum quenches for quantum state-preparation engineering of ICC. The quenches are realized by driving the transition of one ion in the crystal in presence of spin dependent forces, such that a coherent superposition of the electronic states evolves into an entangled state between the chain's internal and external degrees of freedom. It is shown that the creation of such an entangled state can be revealed by performing Ramsey interferometry with one ion of the chain. Refs. [5-6] introduce robust numerical tools for state preparation which embed concepts of signal response theory and quantum information theory. They have been tailored for quantum many body system, and show promising features for application to ICC.

References:
Structural transitions of ion strings in quantum potentials

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We analyse the stability and dynamics of an ion chain confined inside a high-finesse optical resonator. When the dipolar transition of the ions strongly couples to one cavity mode, the mechanical effects of light modify the chain properties close to a structural transition. We focus on the linear chain close to the zigzag instability and show that linear and zigzag arrays are bistable for certain strengths of the laser pumping the cavity. For these regimes the chain is cooled into one of the configurations by cavity-enhanced photon scattering. The excitations of these structures mix photonic and vibrational fluctuations, which can be entangled at steady state. These features are signalled by Fano-like resonances in the spectrum of light at the cavity output.

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Crystals of singly-charged ions in traps are remarkable realisations of the phenomenon first predicted by Wigner [1]. The level of control experimentally achieved on these systems is impressive even at the quantum level and makes them promising candidates for several applications ranging from metrology to quantum information processing [24]. Their versatility also offers the possibility to study paradigmatic models of strongly-correlated many-body systems [3, 4].

Structural transitions in ion crystals have recently attracted renewed interest [10,11]. They are due to the interplay between the repulsive Coulomb interaction and the confining potential of Paul or Penning traps and can be controlled by varying, for instance, the aspect ratio of the trap potential. A prominent example is the linear-zigzag transition, that is classically described by Landau model [10], while its quantum analogue belongs to the universality class of a one-dimensional ferromagnet [19]. Studies of quenches across the instability in the classical regime showed that formation of defects follows the predictions of the Kibble-Zurek mechanism [15, 16].

The combination of ion and dipolar traps [17, 18] opens further perspectives, such as the possibility of realising the Frenkel-Kontorova model [19, 20] and of coupling ultracold atomic systems with ions [21, 22]. In Refs. [17, 18] the dipolar potential is classical, the quantum fluctuations of the electromagnetic field being very small. A very different scenario can be reached in presence of a cavity. Experiments with trapped ions in front of a mirror showed a mirror-mediated dipole-dipole interaction [29] and demonstrated the mechanical effect of the vacuum state of the electromagnetic field on a single ion [24]. The recent achievement of strong coupling between the optical transitions of ions forming a Wigner crystal and one mode of a high-finesse resonator [25, 26] sets the stage for the observation of novel self-organised structures. In this regime, mechanical forces due to multiple scattering of a cavity photon can be infinitely long-ranged and may modify the structural stability even at the single photon level. The understanding of such dynamics can allow one to identify new control tools as well as to access new strongly-correlated states. The competition of long-range potentials of different nature, however, gives rise to a theoretical problem of considerable complexity.

![FIG. 1. The dipolar transitions of ions forming a chain couple with one mode of a high-finesse optical cavity. The depth of the optical potential inside the resonator depends on the ions’ transverse positions and on the strength of the laser pumping the cavity. This property gives rise to hysteresis in the structural configuration and to quantum correlations between photonic and mechanical fluctuations. The scheme can be implemented in setups like the ones realised in [24, 25].](image)

In this Letter we theoretically characterise structural properties of crystalline structures inside a standing-wave resonator, analysing in particular how the crystal structure close to the linear-zigzag instability is modified in this environment. Figure 1 displays the main features of the system. A string of $N$ ions of mass $m$ and charge $q$ is confined within an optical resonator by a radiofrequency trap, here described by a harmonic potential with axial and transverse frequencies $\omega_a$ and $\omega_t$, respectively. The dipolar transition of the ions interacts with a mode of the cavity field which is pumped by a laser with strength $\eta$. When cavity and pump are sufficiently out of resonance from the atomic dipole transition, the dynamical variables of ions and cavity field are described by the operators $\hat{r}_j$ and $\hat{p}_j$, denoting the position and momentum of the center of mass of the $j$-th ion in the array, and by the annihilation and creation operators $a$ and $a^\dagger$ of a cavity photon at frequency $\omega_c$. Their coherent dynamics are governed by Hamiltonian $H = H_{cav} + H_{\text{ions}} + H_{\text{int}}$. Here, $H_{\text{cav}} = -\hbar\Delta_c a^\dagger a - \hbar\eta(a - a^\dagger)$ is the Hamiltonian for the cavity mode in absence of atoms and in the reference frame rotating at the pump frequency $\omega_p$ with
\[ \Delta_c = \omega_p - \omega_c, \] the Hamiltonian for the ions is given by
\[ H_{\text{ions}} = \sum_{j=1}^{N} \left[ \frac{\vec{p}_j^2}{2m} + V_{\text{trap}}(\vec{r}_j) + \sum_{k=j+1}^{N} V_{\text{Coul}}(|\vec{r}_j - \vec{r}_k|) \right], \tag{1} \]
and includes the kinetic energy, the trap potential \( V_{\text{trap}} \), and the Coulomb repulsion \( V_{\text{Coul}} \). Finally, \( H_{\text{int}} = \hbar^2 a U_0 (\vec{r}_1, \ldots, \vec{r}_N) \) describes the interaction between ions and cavity field, with
\[ U_0(\vec{r}_1, \ldots, \vec{r}_N) = \frac{g_0^2}{\Delta_0} \sum_{j} \cos^2(kx_j) e^{-\eta^2/\sigma^2}. \tag{2} \]

Here, \( g_0 \) is the strength of the coupling between the cavity and the ions’ transition at frequency \( \omega_i \), \( k \) the cavity wave vector, \( \Delta_0 = \omega_p - \omega_c \) the detuning of the pump from the dipolar transition, and \( \sigma \) denotes the width of the cavity mode, that is generally smaller than the chain length. The number of ions coupling to the cavity mode, and hence contributing to \( U_0 \), is \( N_{\text{eff}} \), with \( N_{\text{eff}} < N \). Frequency \( U_0 \) weights the nonlinear coupling between motion and cavity mode: It is the shift of the cavity frequency due to the ions inside the resonator, and conversely it is the mechanical potential exerted on these ions by a single cavity photon \[ 29 \]. This term gives rise to mechanical effects that, for strong coupling, can be significant at the single-photon level. Incoherent effects arise from spontaneous decay of the dipolar transition at rate \( \gamma \), cavity decay at rate \( 2\kappa \), and thermalization of the ions’ motion with an external reservoir which may be due to patch potentials at the trap electrodes \[ 2 \ 30 \]. We choose the detuning \( |\Delta_0| \) to be the largest parameter, corresponding to the inequality \( |\Delta_0| \gg \gamma, \kappa, |\Delta_c|, g_0 \sqrt{n} \), with \( n \) the mean intracavity photon number. In this regime the cavity-ion interaction is mainly dispersive and spontaneous emission can be neglected \[ 31 \].

The Hamiltonian \( H \) formally agrees with the one derived for neutral atoms \[ 29 \ 32 \]. However, while in \[ 29 \ 32 \] the atomic interaction is a contact potential, here the ions repel via the long-range Coulomb repulsion. Therefore, in the first case the strength of the pump determines the quantum phase of the atoms in a non-trivial way \[ 33 \]. For ions, on the other hand, quantum degeneracy is irrelevant but the strength of the cavity potential can substantially modify the crystalline structure. An effective dispersive potential for the particles can be derived when retardation effects can be discarded. In this limit the cavity field is determined by the instantaneous set of positions of all ions coupled with the cavity mode and reads \( \tilde{a} = \eta/(\kappa - i \Delta_{\text{eff}}) \), with \( \Delta_{\text{eff}} = \Delta_c - U_0 \), while the corresponding effective potential takes the form
\[ V_{\text{eff}} = (\hbar \omega / \kappa) \arctan(-\Delta_{\text{eff}}/\kappa). \tag{3} \]

This potential gives rise to an effective long-range force between these ions whose strength scales with the cooperativity \( C = g_0^2 N_{\text{eff}}/(\kappa |\Delta_0|) \). The ions’ structure is then determined by the positions at which the total potential \( V_{\text{tot}} = V_{\text{trap}} + V_{\text{Coul}} + V_{\text{eff}} \) exhibits minima.

Two situations can be identified depending on the value of the cooperativity \( C \). For \( C \ll 1 \), the potential in Eq. \[ 3 \] approaches a classical potential whose depth is independent of the ions’ positions. In this limit, when the ion string is parallel to the cavity axis (which corresponds to setting all values \( y_j = 0 \)), the system provides a realisation of the Frenkel-Kontorova model with trapped ions \[ 19 \]. When the string is instead orthogonal to the cavity mode wave vector, as in Fig. \[ 1 \] the optical potential generates a transverse force. This force is symmetric about the chain axis when the chain is at a node or antinode of the cavity standing wave. Then, close to the linear-zigzag mechanical instability the optical potential shifts the critical value of the transverse trap frequency with respect to the free-space value \( \omega_{tc} \) \[ 24 \]. In the following we shall assume that the equilibrium positions of the ions in the linear array are located at an antinode of the cavity standing wave. This can be realised, for instance, with the setups of Refs. \[ 27 \ 28 \]. For blue-detuned pumps, with \( \Delta_0 > 0 \), the antinode is a maximum of the cavity potential and a mechanical instability thus appears at frequencies larger than \( \omega_{tc} \), while a red-detuned pump field will have the opposite effect \[ 35 \]. This behaviour is significantly modified at large cooperativities, \( C \gtrsim 1 \), where the cavity-mediated interaction between the ions becomes relevant. We consider \( \Delta_c = 0 \), \( \Delta_0 > 0 \): In this case the intracavity field is minimum when the ions form a linear array, while it increases when their equilibrium positions arrange in a zigzag. This property can give rise to bistability of the linear and zigzag structures which can be observed in the mean value of the intensity \( I_{\text{out}} \) of the field at the cavity output. An example of this behaviour is shown in Fig. \[ 2 \]a) where \( I_{\text{out}} \) is plotted as a function of the pump intensity \( \eta^2 \) for a chain of 60 ions in a harmonic trap, assuming that the central region of the chain couples to the cavity mode and \( N_{\text{eff}} \sim 5.7 \).

Further insight is gained by analysing the effective potential \( V_s \) of the zigzag mode which is the soft mode of the linear-zigzag transition in free space \[ 10 \]. We first consider the simplest limit when the ions can be assumed to be equidistant (which describes the chain central region or a chain in an anharmonic axial trap \[ 30 \] ) and the mode amplitude reads \( x_s = \sum_j (-1)^j x_j/\sqrt{N} \). Denoting by \( \omega_s = \sqrt{\omega_i^2 - \omega_{tc}^2} \) the frequency of the soft mode above the critical point in free space, the potential \( V_s \) when the ions are uniformly illuminated by the cavity field and for \( \omega_i > \omega_{tc} \) reads
\[ V_s = \frac{m}{2} \omega_s^2 x_s^2 + \frac{\hbar \eta^2}{\kappa} \arctan \left[ \cos^2 \left( \frac{kx_s}{\sqrt{N}} \right) \right]. \tag{4} \]

The second term on the right-hand side of Eq. \[ 4 \] describes the effect of the optical field. For \( \eta = 0 \) the cavity mode is in the vacuum state and the linear array is stable. The soft mode becomes unstable when the optical power is increased above the threshold value \( \eta_{th}^2 = N(1 + C^2)/(4C \omega^2_{tc} \kappa) \), with \( \omega_R = \hbar k^2/(2m) \) the recoil frequency. For \( C > 1 \) parameters can be found where both linear and zigzag configurations are stable. In
a finite chain the amplitude of the soft mode and the coupling of the ions to the cavity are not uniform along the chain. However, the potential energy as a function of the soft-mode amplitude gives similar qualitative results, as shown in Fig. 2(b). Here, for certain values of $\eta$ the potential can exhibit three minima, corresponding to stable linear and zigzag arrays. We remark that the observed bistability is a consequence of the nonlinear dependence of the optical forces on the positions of the atoms within the standing-wave field. In the thermodynamic limit, if the region of the chain interacting with the cavity mode is finite, the effect of this coupling is a localized defect in the chain. For a finite system, nevertheless, forces acting on few ions can generate arrays close to zigzag configurations due to the long-range Coulomb repulsion.

The three metastable configurations can be observed when $\Delta \epsilon = 0$, $\Delta_0 \gg \gamma$ as the result of a cooling process due to the strong coupling with the cavity \cite{39}. In this regime the excitations of the emergent crystalline structure reach a stationary state mixing photonic and vibrational modes. We analyse their behaviour by considering the coupled dynamics of the quantum fluctuations of field and motion. Be $\delta a = a - \bar{a}$ the quantum fluctuations of the field about the mean value $\bar{a}$, and $\{ \delta x_j, \delta y_j \}$ the displacement of the ion localized at the equilibrium position $\delta_{ij}^{(0)}$ determined by the balance of harmonic, Coulomb and mean optical forces. For convenience we introduce the normal modes of the crystal, that characterise the dynamics of the ions when the coupling with the quantum fluctuations of the cavity field can be neglected. Let $\delta_{ij} = \sum_n M_{jn}^{(c)} B_{n0} (b_n + b_n^\dagger)$ with $\zeta = x, y$ and $b_n (b_n^\dagger)$ the bosonic operator annihilating (creating) a phonon of the normal mode at frequency $\omega_n$, $B_{n0} = \sqrt{\hbar/(2m\omega_n)}$, and $M_{jn}^{(c)}$ the element of the orthogonal matrix relating the local coordinates with the normal modes. The dynamics of normal modes and field fluctuations are governed by the Heisenberg-Langevin equations \cite{40,41}:

$$\dot{\delta a} = (i\Delta_{\text{eff}} - \kappa)\delta a - i \sum_n c_n \delta_{ij} (b_n + b_n^\dagger) + \sqrt{2\kappa} a_{\text{in}}, \quad (5)$$

$$\dot{b}_n = -\left( i\omega_n + \Gamma_n \right) b_n - ic_n (\bar{a}^\dagger \delta a + \bar{a} \delta a^\dagger) + \sqrt{2\Gamma_n} b_{\text{in},n}, \quad (6)$$

that include quantum noise on the cavity at rate $\kappa$ with corresponding input noise $a_{\text{in}}$, and on the motion at rate $\Gamma_n$ with input noise $b_{\text{in},n}$, simulating the presence of a reservoir with which the ions' vibrations couple, such that $(b_{\text{in},n}(t) b_{\text{in},n}(t')) = N_n \delta_n \delta(t-t')$ \cite{42}, with $N_n$ the mean phonon number at the temperature of the reservoir. Vibrations and field fluctuations couple with strength $c_n$, where

$$c_n = \frac{B_{n0}}{\Delta_0} \sum_j \left[ M_{jn}^{(x)} \partial_x g_j^2 + M_{jn}^{(y)} \partial_y g_j^2 \right] \quad (7)$$

and $g_j = g_0 e^{-(kx)^2/(2\sigma^2)}$. The coefficients $c_n$ vanish when all equilibrium positions are at field nodes, where $g_j = 0$. If the particles are located at antinodes, the coupling is determined by the derivatives in y direction which are assumed to be much smaller than those along x ($k\sigma \gg 1$). Thus, for the chosen setup the coupling between vibrations and field fluctuations is stronger in the zigzag configuration, while it is a very small perturbation when the ions form a linear chain. We remind that for the parameters considered the cavity field cools the normal modes coupled to it, so that cavity and crystal reach a stationary state \cite{39}.

We study the effect of this coupling in the spectrum at the cavity output, $S(\nu) = \langle a_{\text{out}}(\nu) a_{\text{out}}(\nu') \rangle/I_0$, with $I_0 = 2\kappa|\bar{a}|^2$ the zero-order intensity of the output field and $a_{\text{out}} = a_{\text{in}} + \sqrt{2\kappa} \rho \delta_{ij}^{(0)}$. The steady-state spectrum exhibits negligible fluctuations in the linear phase, while in the zigzag configuration it reads

$$S(\nu) = S_0(\nu) \left\{ \frac{4\kappa|\theta(\nu)|^2|\bar{a}|^2}{\kappa^2 + (\nu - \Delta_{\text{eff}})^2} \right. + \sum_n c_n^2 \Gamma_n \left[ \frac{N_n}{\Gamma_n^2 + (\omega_n - \nu)^2} + \frac{N_n + 1}{\Gamma_n^2 + (\omega_n + \nu)^2} \right] \right\} \quad (8)$$

where the first term is the contribution due to the coupling of the quantum vacuum with the crystal vibrations, with $\theta(\nu) = \sum_n c_n^2 \omega_n / |\bar{a}|^2 - (\gamma_n - i\nu)^2$, and the second is due to thermal noise coupling to the modes. The common prefactor takes the form

$$S_0(\nu) = \frac{2}{\kappa^2 + (\nu - \Delta_{\text{eff}})^2} \left[ 1 + \frac{4\Delta_{\text{eff}} \theta(\nu)|\bar{a}|^2}{(\kappa - i\nu)^2 + \Delta_{\text{eff}}^2} \right]^{-2} \quad (9)$$
FIG. 3. Spectrum $S(\nu)$ of the field at the cavity output (in units of $S_0 = 1/\omega_a$) for a zigzag chain of 3 ions when only one ion at the chain edge, the right one in (c), couples significantly to the cavity mode (with Lamb-Dicke parameter $\sim 0.1$) and the ions’ motion is cooled by the cavity field. The parameters are the same as in Fig. 2 except for $\omega_a = \kappa = 2\pi \times 1$ MHz, $\omega_i = 2\pi \times 1.57$ MHz, and (a) $C = 0.5$, $P = 1$; (b) $C = 3$, $P = 0.22$; the mode width $\sigma$ is 0.65 times the interparticle distance in the linear array, so $N_{\text{eff}} \approx 1.1$. The equilibrium positions are the same in (a) and (b). The motional modes contributing to the spectral peaks are sketched in panel (c) (not to scale; the resonance corresponding to mode 2 is not visible, because this mode is too weakly coupled to the cavity). The Rayleigh peak is not shown.

and gives a Lorentz curve when $C \ll 1$. Its functional behaviour is strongly modified when the cooperativity is increased: Then, motional and quantum noise do not simply add up, but nonlinearly mix to determine the spectral properties of the output field.

Figure 3 displays the spectra for a chain of three ions for different parameter choices: as $C$ is increased the spectral lines change the relative heights, width, and shape. We first note the asymmetry in the spectra with respect to $\nu = 0$: This is due to the (weak) coupling of the ions’ motion to the thermal bath [43]. The broadening at large cooperativity is a consequence of the vacuum input noise on the cavity field and indicates the rate at which the cavity cools the corresponding vibrational mode [44]. It is accompanied by the appearance of Fano-like resonances which result from the dispersive effect of the cavity back-action and are a signature of quantum interference in the fluctuations of motion and field [45]. This interference is due to quantum correlations established by the dynamics described in Eqs. (5)-(6), which can generate entanglement between vibrational and photonic modes [46]. In fact, for the parameters of Fig. 3 (b) we find in the steady-state a logarithmic negativity of 0.15 [47] between cavity and phononic excitations. We remark that the field at the cavity output allows one to monitor the stationary state in a non-destructive way, it can be measured in existing experimental setups [48] and could be used to realise feedback on the ion crystal, for instance by means of an appropriate generalization of the procedure in Ref. [49].

In summary, the structural properties and quantum fluctuations of an ion Coulomb crystal inside a resonator are strongly affected by the nonlinearity of the cavity coupling. This effect is particularly visible close to structural instabilities. We have focused on the linear chain close to the zigzag instability and shown that for large cooperativity also the zigzag array can be made stable by the photon-mediated interaction between the ions (when a small region of the chain is coupled to the cavity, this coupling induces a localized defect in the chain with a zigzag form). This behaviour can be detected by hysteretical behaviour of the intensity of the field at the cavity output as a function of the pump strength. The excitations of these structures reach a stationary state where phonons and photons are strongly correlated and can exhibit entanglement. At even larger cooperativity the dynamics studied in this work could be induced by one photon inside the resonator, thereby providing an unprecedented control of many-body systems at the single-photon level.

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Cavity cooling of a trapped atom using electromagnetically induced transparency

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\textbf{Abstract.} A cooling scheme for trapped atoms is proposed, which combines cavity-enhanced scattering and electromagnetically induced transparency. The cooling dynamics exploits a three-photon resonance, which combines laser and cavity excitations. It is shown that relatively fast ground-state cooling can be achieved in the Lamb–Dicke regime and for large cooperativity. Efficient ground-state cooling is found for parameters of ongoing experiments.

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1. Introduction

Control of the quantum dynamics of physical objects is a prerequisite for quantum technological applications. One important requirement is high-fidelity quantum state preparation. This often relies on cooling the physical system of interest to sufficiently low temperatures, such that a single quantum state, the ground state, is occupied with probability approaching unity. Laser cooling constitutes in this respect a successful technique, which is routinely used in the preparation stage of experiments with atoms and ions [1, 2]. Furthermore, the various laser-cooling concepts and schemes that have been proposed and partly tested over the years are being considered for cooling molecules [3] and more complex objects, such as, for instance, phononic modes of micromechanical resonators to ultralow temperatures [4] and condensed-phase systems [5, 6].

The idea at the basis of laser cooling of trapped particles is to enhance scattering processes leading to a net transfer of the oscillator mechanical energy to the electromagnetic-field modes. Ground-state cooling of a harmonically trapped particle, in particular, relies on a strong enhancement of the scattering processes that cool the oscillator, over the ones that heat the motion. Several ground-state cooling techniques have been discussed that apply this basic concept in various ways [2, 7–9]. One scheme that is relevant to the study carried out in this work is known in the literature as electromagnetically induced transparency (EIT) cooling [10], and it uses coherent population trapping [10, 11] due to quantum interference between laser-driven electronic transitions, in order to tailor the scattering cross section of the atoms to pursue...
ground-state cooling \([12, 13]\). The EIT cooling scheme extends the basic concepts of velocity-selective coherent population trapping for free atoms \([14, 15]\) to trapped atoms and has been experimentally demonstrated in \([16–18]\). Further studies can also be found in \([19–21]\).

A further tool that is being increasingly considered in order to enhance the scattering processes leading to the trapping and cooling of atoms is the strong coupling of one or more atomic transitions to a high-finesse optical resonator \([22–30]\). For such a system it has been predicted that quantum interference effects can emerge from the quantized nature of the cavity mode \([31, 32]\). When, in addition, the field is interfaced with the atomic vibration in a trap via the mechanical action of light, further interference effects can emerge that can increase the cooling efficiency \([33, 34]\). The most recent observation of cavity-induced EIT \([35, 36]\), and of mechanical effects associated with it \([37, 38]\), leads to the natural question of whether and how EIT and cavity quantum electrodynamics can concur together to provide novel tools for control of the mechanical effects of atom–photon interactions.

In this paper, we present a theoretical study of the mechanical effects of light on a trapped atom in a setup that supports cavity-induced EIT. We show that the combination of EIT and cavity quantum electrodynamics can give rise to a cooling mechanism, which for an accurate choice of parameters allows one to prepare the atoms in the ground state of the potential with a probability approaching unity. Remarkably, high efficiencies are found for the parameters of the experimental setup reported in \([37]\). We show that the cooling dynamics can often be explained by means of a three-photon resonance \([39–42]\), which involves cavity and laser photons. For certain parameter choices cooling results from interference in the mechanical effects of the atomic interaction with the cavity and laser fields.

This paper is organized as follows. In section 2 the physical system and the theoretical model are introduced. The assumptions are discussed, which are at the basis of the theoretical treatment in this paper. In section 3 the dark resonances and dressed states of the Hamiltonian for the electronic and cavity levels are reported, and the cavity and atom excitation spectra are discussed. In section 4 the basic equations of cooling are derived, and in section 5 the corresponding predictions are reported for experimental parameters based on \([37]\). The conclusions are drawn in section 6, and in the appendices the details of the calculations in sections 2–4 are presented.

2. The theoretical model

A single atom of mass \(M\) is confined inside an optical resonator by an external harmonic trapping potential and is irradiated by a laser field, while the cavity is pumped by a second laser field at strength \(\Omega_p\). Two atomic dipolar transitions couple to the laser and the cavity mode, respectively, and share the same excited state, forming a \(\Lambda\)-shaped configuration of levels. The atomic center-of-mass motion is treated in one dimension along the \(x\)-axis. Although the one-dimensional treatment seems to be a strong restriction, in the Lamb–Dicke regime that we will assume here, the rate equations for the cooling dynamics can be split into three independent sets of rate equation, one for each direction of motion. Thus, in this limit each spatial dimension can be treated separately \([43]\). Figure 1 illustrates the setup and the level configuration, highlighting the geometry of the laser beam and the cavity axis with respect to the axis of the motion.

In the following, we report some of the relevant parameters and introduce the basic notation. The atomic level configuration is reported in figure 1(b). The atomic levels are denoted by the stable states \(\mid g_1\rangle\) and \(\mid g_2\rangle\) which are coupled by a dipolar transition with moments \(\vec{p}_1\) and \(\vec{p}_2\), respectively, to the common excited state \(\mid e\rangle\). We denote the level frequencies by \(\omega_1\), \(\omega_2\)
Figure 1. (a) The setup of the system. An atom is confined inside an optical resonator by a harmonic trap with frequency $\nu$. The atom is transversally driven by a laser at the Rabi frequency $\Omega_L$ and couples to the cavity mode with the vacuum Rabi frequency $g$. The cavity mode is pumped by a laser (coupling strength $\Omega_P$) and decays with rate $\kappa$. $\phi_L$ ($\phi_C$) denotes the angle between the axis of the motion and the laser (cavity) wave vectors. (b) Relevant electronic transitions. The transverse laser (cavity mode) drives the transition $|g_1\rangle \rightarrow |e\rangle$ ($|g_2\rangle \rightarrow |e\rangle$). The excited state $|e\rangle$ decays spontaneously into the stable states $|g_1\rangle$ and $|g_2\rangle$ with rates $\gamma_1$ and $\gamma_2$, respectively.

and $\omega_c$. The atomic dipole transition $|g_1\rangle \leftrightarrow |e\rangle$ is driven by a laser with frequency $\omega_L$ and Rabi frequency $\Omega_L$. The transition $|g_2\rangle \leftrightarrow |e\rangle$ is coupled to a mode of the optical resonator with frequency $\omega_C$, linewidth $2\kappa$ and vacuum Rabi frequency $g$. The excited state has radiative linewidth $\gamma$ and decays into the state $|g_j\rangle$ with rate $\gamma_j$ ($j = 1, 2$) such that $\gamma = \gamma_1 + \gamma_2$.4

The atomic center-of-mass motion is confined by a harmonic potential of frequency $\nu$ which is independent of the electronic state of the atoms. This situation can be realized when the single particle is an ion in a Paul or Penning trap [44], or a neutral atom when the confining potential is a dipole trap under specific conditions (such as the magic wavelength) [45, 46]. The geometry of the setup is fixed by the angles $\phi_L$ and $\phi_C$ which give the orientations of the laser and cavity wave vectors with respect to the axis of motion; see figure 1.

The dynamics of the system include the mechanical coupling of the atom with the electronic transition via absorption and/or emission of photons. Moreover, it describes the

4 The assumption of a closed configuration is not necessary if an appropriate pumping scheme can be used.
coupling of the cavity mode with the longitudinal modes of the electromagnetic field by the finite transmittance of the mirrors. Correspondingly, the Hamiltonian $\mathcal{H}$ governs the dynamics in the Hilbert space of the degrees of freedom of the atom, the cavity mode and external modes of the electromagnetic field. It can be decomposed into the sum

$$\mathcal{H} = H + W_\gamma + W_\kappa + H_{\text{emf}}.$$  

Here, $H$ is the Hamiltonian for the dynamics of the system, composed of the cavity mode, electronic bound states and center-of-mass motion of the atom, and contains the coupling with the lasers, which are treated as classical fields. The term $H_{\text{emf}}$ describes the Hamiltonian of the modes of the electromagnetic field external to the resonator. The coupling between the atomic dipole transitions and these modes is given by $W_\gamma$, which is responsible for the radiative instability of excited state $|e\rangle$ at rate $\gamma$. The longitudinal modes of the external electromagnetic field couple to the cavity mode via the finite mirror transmittance. This coupling is incorporated by the term $W_\kappa$ and gives rise to cavity losses at rate $\kappa$. In what follows, we discuss in detail the form of the individual terms.

### 2.1. The Hamiltonian of the atom–cavity system

The Hamiltonian

$$H = H_{\text{ext}} + H_{\text{int}} + H_{\text{cav}} + W$$  

(2)

governs the dynamics of the composite system of the atom and the cavity. In a frame rotating with the lasers’ frequencies, the individual terms on the right-hand side of equation (2) read

$$H_{\text{ext}} = \hbar \nu (b^\dagger b + \frac{1}{2}),$$  

(3)

$$H_{\text{int}} = -\hbar \delta c_2 |e\rangle\langle e| + \hbar \delta_1 |g_1\rangle\langle g_1| + \hbar \Delta |g_2\rangle\langle g_2|,$$  

(4)

$$H_{\text{cav}} = -\hbar \Delta a^\dagger a$$  

(5)

and describe the center-of-mass motion of the atom in the harmonic potential of frequency $\nu$, the unperturbed dynamics of the internal electronic states and the dynamics of the cavity mode, respectively. The operators $b$ and $b^\dagger$ in equation (3) annihilate or create single vibrational excitations and are connected with the atom’s position operator by the relation

$$x = \xi (b + b^\dagger),$$  

(6)

where $\xi = \sqrt{\hbar/2M\nu}$ denotes the size of the ground-state wave packet. The operators $a$ and $a^\dagger$ in equation (5) annihilate and create, respectively, a photon in the considered mode, and

$$\Delta = \omega_P - \omega_C$$  

(7)

is the detuning between the cavity and the probe. The other detunings occurring in equation (4) are

$$\delta_1 = \omega_L - (\omega_e - \omega_1),$$  

(8)

$$\delta_c = \omega_C - (\omega_e - \omega_2).$$  

(9)

The interaction part

$$W = W_\gamma + W_L + W_C$$  

(10)
is composed of
\[
W_p = \frac{\hbar \Omega_p}{2} [a + a^\dagger],
\]
\[
W_L(x) = \frac{\hbar \Omega_L}{2} [|e\rangle \langle g_1| e^{\mathrm{i} k x \cos \phi_c} + \text{H.c.}],
\]
\[
W_C(x) = \hbar g(x) [|e\rangle \langle g_2| a + \text{H.c.}],
\]
where \(W_p\) is the drive of the cavity field by the probe of power \(P\) with strength \(\Omega_p = 2 \sqrt{\frac{P}{\hbar \omega_p}}\). \(W_L(x)\) is the coupling of the atomic dipole \(|g_1\rangle \leftrightarrow |e\rangle\) to the control laser with Rabi frequency \(\Omega_L\), and \(W_C(x)\), is the Jaynes–Cummings interaction between the cavity mode and the transition \(|g_2\rangle \leftrightarrow |e\rangle\) with the coupling constant
\[
g(x) = g \cos(k x \cos \phi_C + \varphi).
\]

The quantity \(k\) is the wavenumber of the control laser field and of the cavity mode\(^5\). Moreover, \(\varphi\) determines the equilibrium position of the atom in the trapping potential with respect to the cavity mode function.

2.2. Coupling to the electromagnetic field external to the resonator

We include the electromagnetic field outside the cavity into the theoretical model using a Hamiltonian description instead of a master equation. This provides more insight into the basic processes underlying the cooling dynamics. The Hamiltonian
\[
H_{\text{emf}} = \sum_{\kappa, \epsilon}^{(y_1)} \hbar [\omega_\kappa - \omega_\epsilon] c_\kappa,\epsilon^\dagger c_\kappa,\epsilon + \sum_{\kappa, \epsilon}^{(y_2)} \hbar [\omega_\kappa - \omega_p] c_\kappa,\epsilon^\dagger c_\kappa,\epsilon + \sum_{\kappa, \epsilon}^{(\kappa)} \hbar [\omega_\kappa - \omega_p] c_\kappa,\epsilon^\dagger c_\kappa,\epsilon
\]
accounts for the energy of the transversal and longitudinal field modes that couple independently to the atomic dipoles and the cavity, respectively. The superscript \(y_j(\kappa)\) indicates that the sum is restricted to the modes that couple quasi-resonantly with transition \(|g_j\rangle \leftrightarrow |e\rangle\) (with the cavity mode) and the Hamiltonian is reported in the reference frame at which the corresponding transition rotates at the frequency of the driving laser. The quantity \(\omega_\kappa = c|\kappa|\), with the speed of light in vacuum \(c\), denotes the frequency of the electromagnetic-field mode, and \(c_\kappa,\epsilon\) is the annihilation operator of the mode labeled by the wavevector \(\kappa\) and polarization \(\epsilon_\kappa,\epsilon\) with \(\epsilon = 1, 2\).

The interaction between the atomic dipole \(|g_j\rangle \leftrightarrow |e\rangle\) and the external electromagnetic field reads
\[
W_{\gamma_j}(x) = W_{\gamma_1}(x) + W_{\gamma_2}(x)
\]
\[
= \sum_{j=1,2} \sum_{\kappa, \epsilon}^{(y_j)} \hbar [g_{\kappa, \epsilon}^{(y_j)} |e\rangle \langle g_j| e^{\mathrm{i} \kappa \cdot \mathbf{e}_\kappa} c_\kappa,\epsilon + \text{H.c.}],
\]
where the coupling constant \(g_{\kappa, \epsilon}^{(y_j)} = \tilde{\gamma}_j \cdot \mathbf{e}_\kappa \mathbf{E}_\kappa / \hbar\) is proportional to the scalar product of the atomic dipole moment \(\tilde{\gamma}_j\) with the vacuum electric field \(\mathbf{E}_\kappa \mathbf{e}_\kappa\). The coupling of the cavity mode to the longitudinal modes of the external electromagnetic field is given by
\[
W_{\kappa} = \hbar \sum_{\kappa, \epsilon}^{(\kappa)} [s_{\kappa, \epsilon}^{(\kappa)} a^\dagger c_\kappa,\epsilon + \text{H.c.}],
\]
\(^5\) We assume that the two lower states \(|g_j\rangle\) are atomic hyperfine states. Then, the wavenumbers of cavity \(k_c\) and the lasers \(k_L, k_P\) can be assumed to be approximately equal: \(k \approx k_c \approx k_L \approx k_P\).
with coupling constant $g_{\vec{k}, \epsilon}$ (a detailed form in terms of the physical parameters can be found, for instance, in [47]). We remark that the operator $W_\kappa$ does not depend on the atomic motion, but describes dissipation processes that will be instrumental for cooling the atomic motion [24]. We furthermore emphasize that quantum noise due to fluctuations of the atomic dipoles and the cavity field is systematically incorporated in the theoretical description by the coupling equations (15) and (16).

2.3. Basic assumptions and perturbative expansion

Throughout the paper we focus on the regime where: (i) the atom is tightly confined: the size of the atomic wavepacket $\Delta x$ is much smaller than the lasers’ wavelengths. This is the so-called Lamb–Dicke regime [2, 48]. It is found when the inequality $k\Delta x \ll 1$ is satisfied. Using that $\Delta x = \xi \sqrt{2\langle m \rangle + 1}$ by averaging over a thermal state with mean occupation number $\langle m \rangle$, the inequality can be rewritten as

$$\eta \sqrt{2\langle m \rangle + 1} \ll 1,$$

where $\eta = k\xi$ is the Lamb–Dicke parameter, which scales the mechanical effects of light on the atomic motion [48]. For later convenience we define

$$\eta_L = \eta \cos \phi_L,$$

$$\eta_C = \eta \cos \phi_C,$$

which account for the geometry of the mechanical coupling of laser and cavity to the axis of motion, respectively.

We further assume that (ii) the laser driving the cavity is sufficiently weak such that the average photon number of the cavity mode is much smaller than unity. This corresponds to taking the small parameter

$$|\epsilon|^2 \equiv \left| \frac{\Omega P/2}{\Delta + i\kappa} \right|^2 \ll 1,$$

which gives the mean number of intracavity photons when no atom is present. The requirement (18) can be achieved for high-finesse cavities by adjusting the parameters $\Omega P$ and $\Delta$ accordingly.

This regime allows for a perturbative treatment of the dynamics. We expand the total Hamiltonian into different orders of the Lamb–Dicke parameter by performing a Taylor expansion in $\eta$ of the exponentials $\exp[\ldots x]$ in equations (12) and (15) and the function $g(x)$ in equation (13) [49]. Moreover, we separate the weak driving term $W_P$, i.e. the first-order term in $|\epsilon|$, from $\mathcal{H}_0$, so that the Hamiltonian takes on the form

$$\mathcal{H} = \mathcal{H}_0 + W_P + \mathcal{H}_1 + O(\eta^2).$$

The term $\mathcal{H}_0$ is in lowest order in $\eta$ and $|\epsilon|$ and reads

$$\mathcal{H}_0 = H_0 + W_\gamma(0) + W_\kappa.$$

Here,

$$H_0 = H_{\text{ext}} + H_{\text{opt}} + H_{\text{emf}}$$

(21)

$$H_{\text{opt}} = H_{\text{int}} + H_{\text{cav}} + W_L(0) + W_C(0),$$

(22)
which is given in zero order in the perturbative expansion. In this order of perturbation theory, the stable state of the atom–cavity system is

$$|\Psi_{st}\rangle = |g_2, 0\rangle,$$

which is the product state of the atom in \( |g_2\rangle \) and no cavity photon, \(|n = 0\rangle\). Under the influence of \( H_0 \) (assuming the regime in which the Wigner–Weisskopf approximation can be applied [47]), the atom–cavity system relaxes into the state \( |\Psi_{st}\rangle \), while the atomic center-of-mass motion evolves coherently and is decoupled from the electronic dynamics.

Coupling between the center-of-mass motion and the light is introduced in first order in the Lamb–Dicke parameter \( \eta \). The corresponding term of the total Hamiltonian reads

$$\mathcal{H}_1 = Fx + \sum_{j=1,2} F_{\gamma j} x.$$

It accounts for the mechanical effects due to absorption and emission of photons from/to the control laser and the cavity mode, where the operator \( F \)

$$F = F_L + F_C$$

$$= \frac{d}{dx} (W_L(x) + W_C(x))|_{x=0}$$

(25)

can be interpreted as a force operator [50], while

$$F_{\gamma j} = \vec{e}_x \cdot \left[ \vec{\nabla} W_{\gamma j}(x) \right]|_{x=0}$$

(26)

gives rise to the stochastic force, which is associated with the recoil due to spontaneous emission [50]. Here, \( \vec{e}_x \) is the unit vector along the axis of the motion.

The Lamb–Dicke regime is found when the condition set by equation (17) is fulfilled, and it allows one to assume the separation of time scales which determine the center-of-mass motion of the atom, and the common, internal-state dynamics of the atom–cavity system. At lowest order in the Lamb–Dicke expansion, the internal and external atomic degrees of freedom evolve independently. The relevant time scale is given by the smallest relaxation time of the atom–cavity system. At higher order, the atomic center-of-mass motion experiences the force due to the gradient of the electromagnetic field over the extension of its wave packet. These processes take place on a time scale that is slower by a factor of \( \eta^2 \) with respect to the time scale of the internal motion. In this regime the internal motion follows the external motion adiabatically [13, 48, 51]. It is therefore instructive to first study the internal dynamics, neglecting the coupling with the external motion: this permits one to identify scattering processes which leads to cooling.

3. Level structure and properties of the atom–cavity system

We now discuss the dressed states of the Hamiltonian \( H_{opt} \), equation (22). Condition (18) allows one to restrict the cavity–atom Hilbert space to states that contain at most one excitation of the cavity mode. The dynamics then takes place within the subspace spanned by the states

\[ \{|g_2, 1\}, \{|e, 0\}, \{|g_1, 0\}, \{|g_2, 0\} \}. \]

These coupled levels constitute an effective four-level system, which is depicted in figure 2. Such a configuration of levels has been studied in the literature for the case when the states are
Figure 2. Level scheme of the atom–cavity system in (a) the laboratory and (b) the rotating frame. The vertical axis gives the frequency $\omega$. Downward arrows denote negative detuning. In (b) the dressed states $|g_1, \pm\rangle$ and the states $|g_2, \epsilon'\rangle$ with their corresponding frequency shifts are reported (see text). The detunings are defined in equations (7)–(9) and (29).

The eigenspectrum of $H_{opt}$, equation (22), within the considered subspace is displayed in figure 3 as a function of the frequency of the transverse laser, under the assumption that the state $|g_2, 0\rangle$ is weakly coupled to the other states. The frequencies of the states $|e, 0\rangle$, $|g_1, 0\rangle$, $|g_2, 1\rangle$, which diagonalize $H_{opt}$ when the coupling to laser and cavity is set to zero, are indicated by the dashed curves. In the presence of the coupling with the fields, the frequencies are shifted and degeneracies become avoided crossings. The resulting eigenfrequencies are $\omega_{\pm}$, $\omega_c$, which correspond to the eigenvectors $|\pm\rangle$ and $|c\rangle$, being a superposition of the three states $|e, 0\rangle$, $|g_1, 0\rangle$, $|g_2, 1\rangle$. The horizontal part of the curves, in particular, denotes the frequency of the dressed states of the Jaynes–Cummings Hamiltonian, namely a superposition of the states $|g_2, 1\rangle$ and $|e, 0\rangle$. These states appreciably mix with state $|g_1, 0\rangle$ at the level crossing with the curve $\delta_1 - \delta_{c2}$. This is also visible by inspecting the linewidth, indicated in the figure by the breadth of the curves.

We now analyze the excitation spectra of the cavity and the atom, namely the rate of photon emission by the cavity and the atom, as a function of the probe frequency $\Delta$. For this case it has been found that this level scheme can exhibit dark resonances due to quantum interference between excitation paths involving three photons. The purpose of this section is to analyze the spectroscopic properties of the four-level system arising from the atom–cavity coupling, in the regime in which we can neglect the coupling with the center-of-mass motion. We will focus, in particular, on the conditions under which dark states exist as they will turn out to be relevant for the cooling dynamics; for an extensive analysis, see [42].
Figure 3. Frequencies and linewidths of the dressed states of the atom–cavity system as a function of $\delta_1$. The frequencies are found diagonalizing $H_{\text{opt}}$, equation (22), over the basis of the unperturbed states $\{|e, 0\rangle, |g_1, 0\rangle, |g_2, 1\rangle\}$, and correspond to the centers of the black curves. The corresponding linewidths determine the curves’ width. The horizontal dashed-dotted lines and the dashed diagonal line give the frequencies of the unperturbed states as a function of $\delta_1$. The arrows mark the frequencies of the resonances shown in figure 4. The parameters are $\kappa = 2\nu$, $\gamma = 10\nu$, $g = 20\nu$, $\Omega_L = 12\nu$, $\varphi = 0$ and $\delta_{c2} = 20\nu$.

They are evaluated for the stationary state of the (internal) atom–cavity system, and are proportional to the probability that the cavity contains one photon and that the atom is in the excited state, respectively. In appendix A a detailed calculation is reported, which shows that they take on the form

$$S_{\text{exc}}^\kappa(\Delta) \propto |F_\kappa(\Delta)|^2,$$

$$S_{\text{exc}}^\gamma(\Delta) \propto |F_\gamma(\Delta)|^2$$

with

$$F_\kappa(\Delta) = \frac{(\delta_{c2} + \Delta - \delta_1) \left[ \delta_{c2} + \Delta + i\frac{\gamma^2}{4} \right] - \frac{\Omega_L^2}{4}}{f(\Delta)},$$

$$F_\gamma(\Delta) = g \frac{\delta_{c2} + \Delta - \delta_1}{f(\Delta)},$$

where the superscript $\kappa(\gamma)$ indicates that it refers to cavity (atom) emission; see appendix A for details. The relevant resonances can be identified with the poles of the function $f(\Delta)$ that correspond to the frequencies of the dressed states of $H_{\text{opt}}$.

The excitation spectra for the cavity and the atom are displayed in figures 4(a) and (b), respectively, as a function of $\Delta$. We recall that in the absence of the atom, the cavity excitation spectrum is a Lorentz curve centered at the mode frequency with full-width $2\kappa$, and corresponds to the gray curve reported in the figure. The solid curve corresponds to the cavity excitation spectrum in the presence of the atom. The three peaks are identified with the dressed states of
Figure 4. Excitation spectra of (a) the cavity and (b) the atom, in arbitrary units, as a function of the probe frequency $\Delta$, in units of $\nu$, for $\delta_{c_2} = 20\nu$ and $\delta_1 = 10\nu$ (black solid line) and $\delta_1 = \delta_{c_2} = 20\nu$ (dashed line). The gray curve in (a) gives the Lorentzian excitation spectrum of the unperturbed cavity and is plotted for comparison. The spectra consist of three peaks at the frequencies of the dressed states of the manifold $\{|e, 0\rangle, |g_1, 0\rangle, |g_2, 1\rangle\}$, which are marked with arrows. The circles mark the frequencies for which the excitation spectra exhibit local minima, corresponding to approximate dark resonances. In (b) the atomic excitation spectrum vanishes at $\Delta = \delta_1 - \delta_{c_2}$ (small circle), due to three-photon resonance between $|g_1, 0\rangle$ and $|g_2, 0\rangle$. The other parameters are $\kappa = 2\nu$, $\gamma = 10\nu$, $g = 20\nu$, $\Omega_\perp = 12\nu$ and $\varphi = 0$.

Moreover, the cavity excitation spectrum exhibits two points, where the cavity response is minimal. These minima are marked with two circles in figure 4(a).

The Fano-like profile and the minima in the cavity excitation spectrum can be understood in terms of quantum interference between the dressed states and state $|g_2, 0\rangle$, which can give
rise to significant effects even though state $|g_2, 0\rangle$ is very weakly coupled to the other levels. In order to gain more insight, we first analyze the atom–cavity levels in a unitarily equivalent scheme, where $H_{\text{cav}} + W_P$ is diagonal. We consider the states

$$|g_j, \epsilon\rangle = D_c(\epsilon^\prime)|g_j, 0\rangle$$

(30)

with the displacement operator $D_c(\epsilon) = \exp(\epsilon a^\dagger - \epsilon^\ast a - i\epsilon^\prime t)$ for the cavity mode and $\epsilon^\prime = \Omega_p/2\Delta$. For $\delta_{c2} + \Delta - \delta_1 = 0$, the states equation (30) are resonantly coupled, such that

$$|D\rangle \propto \epsilon^\prime g \cos \varphi |g_1, \epsilon\rangle - \frac{\Omega_L}{2} |g_2, \epsilon\rangle$$

(31)

is an eigenstate of the Hamiltonian $H_{\text{opt}}$ that has zero projection onto the electronic excited state. In the limit in which the pump is weak and out of resonance, the state $|D\rangle$ is to a good approximation the stationary state of the system and is in a dark state. Equation (29) then gives the correct resonance condition and explains the position of the minimum in the atomic excitation spectrum. Similarly, the cavity excitation spectrum exhibits minima when the state $|g_2, 0\rangle$ is resonantly coupled to one of the dressed states $|g_1, \pm\rangle$, which diagonalize the laser interaction $H_{\text{int}} + W_L(0)$.

Another dark resonance is found when the states $|g_2, 1\rangle$ and $|g_1, 0\rangle$ are resonantly coupled, namely when $\delta_1 = \delta_{c2}$. We denote this situation by ‘two-photon resonance’. In this case the state

$$|D_M\rangle \propto g \cos \varphi |g_1, 0\rangle - \frac{\Omega_L}{2} |g_2, 1\rangle$$

(32)

is an eigenstate of the Hamiltonian $H_{\text{opt}}$ and is stable over a time scale, in which cavity decay can be neglected. This situation is reported by the dashed curves in figures 4(a) and (b). In this case, the atomic excitation spectrum exhibits only two peaks, and the dark resonance is at the frequency where the cavity output is maximal.

In the next section we take into account the motion of the atom, and trace back the properties of the rates of heating and cooling transitions to the characteristics identified in the excitation spectra.

4. Theory of cooling in the Lamb–Dicke limit

In the Lamb–Dicke regime, the atom’s external and internal degrees of freedom are weakly coupled. In this limit, one can assume that the system, composed of cavity and electronic excitations of the atom, reaches a steady state over a time scale that is much faster than the one at which the motion evolves. The corresponding theoretical treatment has been discussed in detail in [13, 51, 53] for instance. This justifies the formulation of the dynamics of the external degrees of freedom in the form of a rate equation for the occupations $p_m(t)$ of the vibrational state $|m\rangle$, which reads

$$\frac{dp_m}{dt} = (m + 1)A_- p_{m+1} - [(m + 1)A_+ + mA_-]p_m + mA_+ p_{m-1}.$$ 

(33)

The average phonon number obeys the equation $\langle m \rangle(t) = -\Gamma \langle m \rangle(t) + A_+$ with the cooling rate

$$\Gamma = A_- - A_+.$$ 

(34)
When $\Gamma > 0$, i.e. $A_- > A_+$, a stationary state exists. At steady state, the flow of population fulfills the detailed balance condition, and the mean occupation at the steady state reads [48, 54]

$$p^s_m = \left(1 - \frac{A_+}{A_-}\right) \left(\frac{A_+}{A_-}\right)^m$$

with mean phonon occupation

$$\langle m \rangle^s = \frac{A_+}{A_- - A_+}.$$

These formulae show that high cooling rates are reached by maximizing the value of $A_-$ as well as the ratio $A_-/A_+$, while the ratio $A_-/A_+$ alone controls the final temperature. Various cooling schemes resort to different control tools in order to achieve either fast cooling and/or low temperatures. In the following, we will characterize the dynamics which can lead to efficient ground-state cooling in this setup.

4.1. Cooling and heating rates

The transition rates $A_{\pm}$ in equation (33) can be calculated in perturbation theory using the resolvent of the Hamiltonian; for the detailed evaluation see appendix A. They describe absorption of a photon of the probe laser pumping the cavity, followed by emission into the modes of the external field either by atomic or by cavity decay, and can be written as the sum of various contributions of different physical origin:

$$A_{\pm} = D + \sum_{r=1,2} \gamma_r |\tilde{T}_L^{\ell,\pm} + \tilde{T}_C^{\ell,\pm}|^2 + 2\kappa |\tilde{T}_L^{\ell,\pm} + \tilde{T}_C^{\ell,\pm}|^2.$$

The quantity $D$ is a diffusion coefficient, originating from the mechanical effects of the spontaneously emitted photon, while $\tilde{T}_F^{\ell,\pm}$ denote the transition amplitude associated with the absorption (−) or emission (+) of a vibrational phonon either by scattering the probe photon into the external modes by cavity decay ($\ell = \kappa$) or by spontaneous emission along one of the two transitions ($\ell = \gamma_{1,2}$). The subscript $F$ indicates whether the mechanical effect is due to the laser photon ($F = L$) or to the cavity photon ($F = C$). For a given scattering process, these mechanical effects can interfere constructively, as one observes from the fact that the corresponding contribution, $|\tilde{T}_L^{\ell,\pm} + \tilde{T}_C^{\ell,\pm}|^2$, is the coherent sum of the individual amplitudes. A schematic representation of the corresponding scattering processes is depicted in figure 5.

A similar decomposition as the one in equation (37) was identified for the heating and cooling rates of a trapped atom whose two-level, dipole transition couples simultaneously to the cavity mode and to a transversal laser [53]. In such a setup several interference processes have been identified which can be tuned in order to enhance the cooling efficiency. In the present system, where an additional electronic transition is involved, a further interference process can take place, which is analogous to EIT.

Below we discuss in detail the individual terms for the system considered in this work. In the following, we neglect the decay along the transition $|e\rangle \rightarrow |g_1\rangle$, and take $\gamma_2 = \gamma$, unless otherwise specified. This assumption leads to a considerable simplification of the analytical expressions we are going to report and does not affect qualitatively the cooling dynamics for the parameter regime explored here, as numerical checks show.
Figure 5. Schematic representation of the scattering processes leading to a change of the motional state, corresponding to equations (39), (40) and (42). The arrows show the sequence of processes leading to a transition $|\Psi_{st}, m\rangle \rightarrow |\Psi_{st}, m \pm 1\rangle$. The intermediate internal states are denoted by the rounded box. The process in (a) terminates by a spontaneous decay, in which the mechanical effect is due to the spontaneously scattered photon. In (b) and (c), the transition is terminated by the emission of a photon by spontaneous emission and cavity decay, respectively, and the mechanical effects are due either to absorption or emission of a photon of the control laser ($F = L$) or of the cavity mode ($F = C$).

We first consider the diffusion term $D$ in equation (37). This term describes scattering processes where a probe photon is spontaneously emitted by the atom and where the mechanical effect is due to photon recoil by spontaneous decay. It can be written in the form

$$D = \gamma W_2 |\tilde{T}_D|^2,$$

where $W_2$ is a geometrical factor that depends on the atomic dipole pattern of radiation and

$$\tilde{T}_D = -i\eta \frac{\Omega_p}{2} \cos \varphi F_\gamma(\Delta)$$

is the transition matrix element (apart from some constant factors), where the function $F_\gamma(\Delta)$ is given in equation (28b). Hence, $D$ is proportional to the atomic excitation spectrum in equation (27a), and thus to the probability that the excited state is occupied. In particular, it vanishes at a node of the cavity mode function where $\cos \varphi = 0$, since there, the state $|g_2\rangle$ does not couple to the excited state in zero order in the Lamb–Dicke expansion. Moreover, for general values of $\varphi$, $D$ becomes zero when the atomic excitation spectrum vanishes, which is verified when $\Delta = \Delta_0$, with

$$\Delta_0 \equiv \delta_1 - \delta_{c2},$$

namely when states $|g_2, 0\rangle$ and $|g_1, 0\rangle$ are resonantly coupled. For these parameters the population of the atomic excited state is zero because of destructive interference between the excitation paths. Consequently, diffusion can be suppressed. This property is also at the basis of the so-called EIT-cooling mechanism [13]. Differing from EIT cooling, suppression of diffusion is here due to a three-photon interference process.
We now turn our attention to the transition amplitudes

\[ \tilde{T}_L^{\gamma, \pm} = \mp i n_L \frac{\Omega p}{2} \frac{\Omega_1^2}{4} \frac{\nu (\nu + \Delta \mp \nu) g \cos \varphi}{f(\Delta \mp \nu) f(\Delta)} , \]  

(40a)

\[ \tilde{T}_L^{\kappa, \pm} = \mp i n_L \frac{\Omega p}{2} \frac{\Omega_1^2}{4} \frac{\nu g^2 \cos^2 \varphi}{f(\Delta \mp \nu) f(\Delta)} , \]  

(40b)

They describe the scattering processes where absorption or emission of a photon of the transverse laser leads to a change in the vibrational motion and are depicted in figures 5(b) and (c). These scattering amplitudes vanish at the node of the mode function where \( \cos \varphi = 0 \), and when the control laser is perpendicular to the axis of motion \((\eta_L = 0)\), namely when there is no mechanical effect of the control laser along the direction of the motion. When this is not verified, these amplitudes may become maximal when the parameters are chosen so that the energy defect of the intermediate scattering states becomes minimal. Cooling transitions are enhanced over heating transitions, in particular for the parameters for which the equation

\[ \text{Re} \{ f(\Delta + \nu) \} = 0 \]  

(41)

is fulfilled.

Finally, the transition amplitudes

\[ \tilde{T}_C^{\gamma, \pm} = -\eta_C \frac{\Omega p}{2} \sin \varphi \mathcal{F}_\gamma(\Delta \mp \nu) \left[ g \cos^2 \varphi \mathcal{F}_\gamma(\Delta) + (\nu + \Delta \mp \nu) \mathcal{F}_\kappa(\Delta) \right] , \]  

(42a)

\[ \tilde{T}_C^{\kappa, \pm} = -\eta_C \frac{\Omega p}{2} \sin 2 \varphi \frac{2}{2} g \left[ \mathcal{F}_\gamma(\Delta \mp \nu) \mathcal{F}_\gamma(\Delta) + \mathcal{F}_\gamma(\Delta) \mathcal{F}_\kappa(\Delta \mp \nu) \right] \]  

(42b)

describe the scattering processes where absorption or emission of a photon of the cavity field leads to a change in the vibrational motion. They are depicted in figures 5(b) and (c). These transition amplitudes vanish when the cavity axis is perpendicular to the axis of motion \((\eta_C = 0)\), namely when there is no mechanical effect of the cavity photon along the direction of the motion or alternatively when the atom is situated at an antinode of the mode function, so that the derivative of the cavity–ion potential vanishes and the corresponding force operator is zero. The term \( \tilde{T}_C^{\kappa, \pm} \), equation (42b), also disappears at a node of the cavity standing wave. Interestingly, both terms are products of the Fano-like factors \( \mathcal{F}_\gamma \), equation (28b), connected with the atomic excitation spectrum, and \( \mathcal{F}_\kappa \), equation (28a), which reflects the characteristics of the excitation spectrum \( S_{\text{exc}}^\kappa \), equation (27b).

We now identify some conditions under which ground-state cooling can be implemented.

4.2. Three-photon resonance: electromagnetically induced transparency cooling and beyond

In this section we study the cooling dynamics under the assumption of three-photon resonance,

\[ \delta_{TP} = \Delta + \delta_{\omega 2} - \delta_1 = 0 , \]

corresponding to setting \( \Delta = \Delta_0 \). In this case the transition rates simplify considerably: due to destructive interference of the excitation paths, the excited state \( |e\rangle \) is not occupied and the diffusion term \( D \) in equation (37) vanishes. This property also leads to a considerable
simplification of the transition amplitudes $\tilde{T}_C^{\pm}$, since $\mathcal{F}(\Delta_0) = 0$. In this case the rates take on the form\(^6\)

$$A_{\pm} = |\epsilon|^2 \tilde{\eta}^2 g^2 \gamma \frac{1 + C_{\pm}}{\nu^2 \left( 1 + C_{\pm} \right)^2 + \left( \frac{\Omega_i^2}{4\nu} - \nu \pm \delta_1 + \frac{\nu}{2\kappa} C_{\pm} (\nu \mp \Delta) \right)^2}, \quad (43)$$

where

$$\tilde{\eta}^2 = \eta_L^2 \cos^2 \varphi + \eta_C^2 \sin^2 \varphi \quad (44)$$

contains the dependency on the geometry of the setup, and the parameters

$$C_{\pm} = C \frac{\kappa^2}{\kappa^2 + (\Delta \mp \nu)^2} \quad (45)$$

are proportional to the single-atom cooperativity

$$C = \frac{g^2 \cos^2 \varphi}{\kappa \gamma / 2}. \quad (46)$$

The rate of cooling (heating) is maximum when state $|g_2, 0\rangle$ is set on resonance with the red (blue) sideband of one of the dressed states of $H_{\text{opt}}$. Cooling is enhanced, for instance, when the denominator of rate $A_-$ in equation (43) becomes minimal, which is satisfied when the relation

$$\delta_1 = \frac{\Omega_i^2}{4\nu} - \nu + (\nu + \Delta) \frac{g^2 \cos^2 \varphi}{\kappa^2 + (\Delta + \nu)^2} \quad (47)$$

is fulfilled.

4.2.1. Cavity EIT cooling. In order to acquire a better understanding of the role of the resonator and identify the regimes in which cooling occurs, we first analyze the case $C_{\pm} \ll 1$.

The parameters $C_{\pm}$ become small (i) for small cooperativities $C$, (ii) when the pump on the cavity is far-off resonant or (iii) for $\kappa \ll |\Delta \pm \nu|$. Then, the rates are given by

$$A_{\pm}^{\kappa} = |\epsilon|^2 \tilde{\eta}^2 \frac{\gamma g^2 \nu^2}{\nu^2 \nu^2 + \left[ \frac{\Omega_i^2}{4\nu} - \nu (\nu \mp \delta_1) + \frac{\nu}{2\kappa} C \frac{\nu (\nu \mp \Delta)}{\kappa^2 + (\Delta + \nu)^2} \right]^2}. \quad (48)$$

For asymptotically small values of $C$, case (i), or large detunings $|\Delta| \gg \nu, \kappa$, case (ii), the rates assume the form

$$A_{\pm}^{\kappa} = |\epsilon|^2 \tilde{\eta}^2 \frac{\gamma g^2 \nu^2}{\nu^2 \nu^2 + \left[ \frac{\Omega_i^2}{4\nu} - \nu (\nu \mp \delta_1) \right]^2}. \quad (49)$$

whose functional dependence on the parameters is the same as that in EIT cooling [13]. For analyzing case (iii), we use the definition of $C$, equation (46), yielding

$$A_{\pm}^{\nu} = |\epsilon|^2 \tilde{\eta}^2 \frac{\gamma g^2 \nu^2}{\nu^2 \nu^2 + \left[ \frac{\Omega_i^2}{4\nu} + \frac{\nu g^2 \cos^2 \varphi}{\nu \mp \Delta} - \nu (\nu \mp \delta_1) \right]^2}. \quad (50)$$

\(^6\) We note that equation (43) and the following formulae derived from it acquire the same form also for $\gamma_1 \neq 0$: the parameter $\gamma$ appearing there is the total radiative linewidth of the excited state.
For $\Delta = 0$ it corresponds to EIT cooling with a modified Rabi frequency $\Omega_1^2/4 \rightarrow \Omega_1^2/4 + g^2 \cos^2 \varphi$.

All cases discussed here correspond to a mean phonon number at steady state
\[ \langle m \rangle_{st} = \frac{[\Omega^2/4 - \nu(v(\nu + \delta_1))]^2 + \gamma^2 \nu^2/4}{4\nu \delta_1 (\Omega^2/4 - \nu^2)}, \tag{51} \]
where $\Omega$ denotes the corresponding (modified) Rabi frequency. It achieves the minimum value, $\langle m \rangle_{st,\text{min}} = (\gamma/4\delta_1)^2$, when $\Omega^2/4 = v(\nu + \delta_1)$. The corresponding cooling rate at this value reads $W = A_+ - A_+ \sim |e|^{2\tilde{\eta}^2/4} g^2/\gamma$.

Resonant driving, $\Delta = 0$, also leads to EIT-like cooling even for arbitrary values of the cooperativity $C$, which is especially interesting for $C_0 = C \pm |\Delta = 0 \gg 1$. Then, the transition rates between the vibrational levels are given by
\[ A_\pm = |e|^{2\tilde{\eta}^2} \frac{\gamma' g^2 \nu^2}{\nu^2/4 + \left[\frac{\Omega_1^2}{4} - \nu(v \pm \delta_1) + \frac{\nu^2 \gamma^2}{2} \right]^2}, \tag{52} \]
with the modified Rabi frequency $\Omega_1^2/4 \rightarrow \Omega_1^2/4 + \gamma' \nu^2/2\kappa$ and the modified atomic linewidth $\gamma' = \gamma C_0$. For asymptotically large $C_0$, this case leads to the minimal mean vibrational occupation number at steady state of $\langle m \rangle_{st,\text{min}} = (\kappa/2\nu)^2$, which can be very small provided that the cavity linewidth is much smaller than the trap frequency.

4.2.2. Cavity EIT cooling in the strong coupling regime. We now consider the case of large cooperativities, $C \gg 1$, and small cavity linewidths, such that $\kappa \ll \nu$. Moreover, we assume that the system is driven at three-photon resonance, $\delta_{TP} = 0$.

When the pump is tuned on the blue sideband transition of the cavity, $\Delta = \nu$, one encounters the situation $C_+ = C$ and $C_- \approx C \frac{\nu^2}{4\nu^2}$, fulfilling $C_+ \gg C_-$. The resulting transition rates between the vibrational levels take on the form
\[ A_+ \sim |e|^{2\tilde{\eta}^2} \frac{4 g^2}{C \gamma}, \tag{53} \]
\[ A_- = |e|^{2\tilde{\eta}^2} \frac{g^2 \gamma (1 + C_-)}{\nu^2 (1 + C_-)^2 + (\delta_1 - \delta_{\text{opt}})^2}, \tag{54} \]
where
\[ \delta_{\text{opt}} = \Omega_1^2/(4\nu) + g^2 \cos^2 \varphi/(2\nu) - \nu. \]

This corresponds to the case when the weak pump is in resonance with the red sideband of the dressed state $|+\rangle$ of $H_{\text{opt}}$. It becomes clear from equation (53) that the cooling is larger than the heating rate by the factor
\[ \frac{A_-}{A_+} \sim \left(C^{-1} + \frac{\nu^2}{4\nu^2}\right)^{-1}. \]

Additionally, diffusive processes are suppressed due to three-photon resonance. In this regime, the mean occupation number reads
\[ \langle m \rangle_{st} = \left[C \frac{1 + C_-}{(1 + C_-)^2 + 4(\delta_1 - \delta_{\text{opt}})^2/\gamma^2} - 1\right]^{-1}, \tag{55} \]
Figure 6. Transition rates of cooling $A_-$ (solid line) and heating $A_+$ (dashed line), for large cooperativity $C \gg 1$ and small cavity decay rate, $\kappa \ll \nu$. The arrows and circles mark the dressed states’ frequencies and the dark resonances, in correspondence to figure 3. The parameters are $\gamma = 10 \nu$, $\kappa = \nu/10$, $g = 10 \nu$, $\Omega_L = 12 \nu$, $\delta_1 = \delta_{\text{opt}} = 47.5 \nu$, $\delta_{c2} = \delta_1 - \nu$, $\varphi = \pi/3$ and $\phi_L = \phi_C = 0$. The transition rates are given in units of $\alpha$, equation (57), and $\Delta$ in units of $\nu$.

and it takes on the minimal value $\langle m \rangle_{\text{st,min}} \approx 1/C$ for $\delta_1 = \delta_{\text{opt}}$ and $C_- \ll 1$. In this limit the cooling rate reads $W \sim A_- = |\epsilon|^2 \tilde{T}_\gamma^2 / \gamma$. Figure 6 displays the transition rates $A_\pm$ for $\delta_1 = \delta_{\text{opt}}$. For this choice of $\delta_1$ the rate $A_-$ has a pronounced maximum at $\Delta = \nu$. This maximum is displaced from the resonance around $\Delta \approx 2 \nu$ by the trap frequency $\nu$, and corresponds to the case when the pump laser is resonant with the red sideband of a dressed state. The transition rate of heating is strongly suppressed at $\Delta = \nu$ due to three-photon resonance.

4.3. Double dark resonances

A peculiar characteristic of this specific setup is found when the mechanical effects are predominantly governed by the interaction with the cavity field. In this case the transition rates read

$$A_\pm \approx A_{C,\pm} = \gamma_2 |\tilde{T}_C^{\gamma,\pm}|^2 + 2\kappa |\tilde{T}_C^{\kappa,\pm}|^2$$  \hspace{1cm} (56)

with the amplitudes $\tilde{T}_C^{\gamma,\pm}$, $\tilde{T}_C^{\kappa,\pm}$, given in equations (42). These scattering amplitudes are connected to products of the functions $F_\gamma$ and $F_\kappa$, equations (28), which determine the excitation spectra of the atom and the cavity.

Figure 7 displays the rates $A_{C,\pm}$ for different values of the detuning $\delta_1$ and as a function of $\Delta$. Cooling is found whenever $A_{C,-} > A_{C,+}$, i.e. when the black curve overtops the dashed curve. This is the case on the left edge of the broad resonance around $\Delta \approx 4 \nu$. More interesting is the behavior around three-photon resonance $\Delta = \delta_1 - \delta_{c2}$, marked by the black arrow. In particular in the graphs (b) and (c), the rates $A_{C,\pm}$ oscillate with poles at a distance of the order of the trap frequency $\nu$. These oscillations are a consequence of Fano-like profiles in the scattering cross-section of the system and are visible in the excitation spectra of the atom and the cavity.
Figure 7. Transition rates of cooling $A_{C-}$ (solid line) and heating $A_{C+}$ (dashed line) in units of $\alpha$, equation (57), as a function of $\Delta$ in units of $\nu$. The rates are evaluated from equation (56) for (a) $\delta_1 = \delta_{c2}/2$, (b) $\delta_1 = \delta_{c2}$ and (c) $\delta_1 = 3\delta_{c2}/2$. The other parameters are $\gamma = 10\nu$, $\kappa = 2\nu$, $g = 20\nu$, $\Omega_L = 12\nu$, $\delta_{c2} = 20\nu$, $W_2 = 1$, $\phi = \pi/3$, $\phi_C = 0$. The small arrows in the plots mark the positions of three-photon resonance (black) and of the corresponding sidebands, shifted by $\pm \nu$ (gray).

Here, these approximate double dark resonances lead to alternating cooling and heating regions around three-photon resonance.

It is interesting to consider whether the parameter can be adjusted, to suppress both carrier and blue sideband transitions, thereby increasing the cooling efficiency. An example of such a situation is the cooling scheme discussed in section 4.2.2. This could constitute a more accessible realization of a cooling process, which has been proposed so far in a tripod level configuration [20] and for a two-level atomic transition confined in a resonator and at the node of the laser standing wave [34].
4.4. Large three-photon detuning

The case when the control laser is far detuned from the atomic transition $|g_1\rangle \leftrightarrow |e\rangle$ corresponds to a closed two-level system consisting of the atomic levels $|g_2\rangle$ and $|e\rangle$ (in the presence of a finite decay probability into state $|g_1\rangle$, the control laser acts as a repump). In our model, this case corresponds to taking large three-photon detunings $\delta_{TP}$ and large values of the detuning $|\delta_1|$. In this limit the mechanical effects are due to coherent atom–cavity interaction and to spontaneous decay, while the effect of the transverse laser coupling to the atom can be neglected. The atomic system thus reduces to an effective two-level transition coupled to a cavity which is pumped. This situation differs from the one considered in [34, 53] where the two-level atom is driven by a transverse laser. The case of a trapped two-level system whose center-of-mass motion is cooled in a driven cavity shows interesting features on its own, and its dynamics will be the object of future investigations.

5. Discussion of the results

In this section we report the graphs of the cooling rate and the average vibrational number at steady state, $\langle m \rangle_{st}$. These quantities, defined in equations (34) and (36), determine the velocity of the cooling process and the final temperature, and are found by evaluating the rates in equations (37) as a function of the physical parameters. For convenience, we report the cooling rate $\Gamma$ scaled with the frequency

$$\alpha = \eta^2 \Omega_P^2 / \nu.$$  \hfill (57)

The parameters we consider are based in most cases on the experiment in [37]. Typical values for $\alpha$, which are in accordance with equation (18), are of the order of $10^{-6} \nu$ to $10^{-4} \nu$.

We first consider the three-photon resonance condition. This is achieved by appropriately setting the frequencies of the transverse laser and of the laser pumping the cavity. In this regime we expect that cooling is dominated by the mechanical effect stemming from the laser and cavity interaction, which mutually interfere, while the diffusion processes due to spontaneous emission are suppressed.

Figure 8 displays the contour plots of the cooling rate $\Gamma$ and of the corresponding stationary mean phonon number $\langle m \rangle_{st}$ as a function of the detuning $\Delta$ between the probe and the cavity, and of the detuning $\delta_1$ between control laser and the atomic transition $|g_1\rangle \leftrightarrow |e\rangle$. The solid line corresponds to the condition given in equation (47), which relates $\Delta$ and $\delta_1$ and which maximizes the value of $A_-$. Indeed, the lowest values of $\langle m \rangle_{st}$, and correspondingly the maxima of the cooling rate, are found along the solid line. The largest value of the cooling rate $\Gamma$, figure 8(a), is found at the intersection between this curve and $\Delta = 0$, namely when the pump laser drives resonantly the cavity mode and the states $|g_2, 1\rangle$ and $|g_1, 0\rangle$ are hence also resonantly coupled. This behavior can be understood considering that the atom appears transparent to the cavity at three-photon resonance and in zero order in the Lamb–Dicke expansion. In this regime, hence, the cavity resonance line, which scales the cooling rate, is given by a Lorentzian shape and has its maximum when $\Delta = 0$. Figure 8(c) displays the mean phonon number as a function of $\delta_1$ when $\Delta = 0$ (solid curve). This value is compared with that one found for $\Delta(\delta_1)$, which satisfies equation (47) and is indicated by the dashed curve. In both cases the system is driven at three-photon resonance. One observes that the temperature is minimal for the values predicted by equation (47).

Figure 8. (a) The cooling rate $\Gamma$ and (b) mean phonon number $\langle m \rangle_{\text{st}}$ as a function of the detunings $\delta_1$ and $\Delta$ when the three-photon resonance condition is satisfied, $\delta_{\text{TP}} = 0$. The solid curves in (a) and (b) correspond to the resonance condition from equation (47) which maximizes $A_-$ (the dashed line reports the curve where $A_+$ is maximum). In the hatched area the cooling rate is negative and corresponds to the region where the atomic motion is heated. (c) $\langle m \rangle_{\text{st}}$ as a function of the detunings $\delta_1$ for $\Delta$ fulfilling equation (47) (solid line) and $\Delta = 0$ (broken line). The other parameters are $\gamma = 2\nu$, $\kappa = \nu/4$, $g = 12\nu$, $\Omega_L = 11.2\nu$, $\varphi = \pi/3$.

Figure 9 displays the cooling rate and mean vibrational number at steady state for the same parameters as in figure 8, but a larger spontaneous emission rate $\gamma = 20\nu$ and a smaller cavity decay rate $\kappa = 0.01\nu$. With respect to the results found in figure 9, we observe that the cooling region about $\Delta = -\nu$ and $\delta_1 < 0$ becomes smaller. More striking is the appearance of a cooling region which stretches around $\Delta = \nu$ across all considered values of the detuning $\delta_1$. This is understood in terms of the cooling dynamics discussed in section 4.2.2: in fact, for the considered parameters the rate $A_-$ is more than two orders of magnitude larger than the rate $A_+$. In this case, the cooling transition is enhanced because the pump is tuned to the red sideband of a resonance, while the heating is suppressed because the corresponding transition coincides with a dark resonance.
Figure 9. The same as figure 8 but for $\kappa \ll \nu$. The plot (c) shows cuts along the line $\Delta = 0$ (broken), $\Delta = \nu$ (dash-dotted) and for $\Delta$ fulfilling equation (47) (solid line). The other parameters are $\gamma = 20\nu$, $\kappa = \nu/100$, $g = 12\nu$, $\Omega_L = 11.2\nu$, $\varphi = \pi/3$.

Figure 9(c) displays the mean phonon number as a function of the detuning $\delta_1$ for various values of $\Delta$. The broken line corresponds to the case $\Delta = 0$ and shows a similar behavior as in figure 8. The thick dashed-dotted line is found for $\Delta = \nu$: here, not only diffusion is suppressed due to the three-photon resonance condition, but also the heating rate is strongly reduced. Indeed, the temperature is minimal for the value of $\delta_1$ fulfilling equation (47) at $\Delta = \nu$. Further insight can be gained by inspecting the dressed states shown in figure 3: one finds that the cooling regions mostly correspond to the probe laser being set in resonance with the red sideband of a narrow-line dressed state. We note, in particular, that the condition of optimal cooling can be identified in figure 3 at the intersection of the curve $\Delta = \delta_1 - \delta_{c2}$ with the curve showing the frequency of the dressed state, shifted downwards by the trap frequency. This intersection determines the curves of optimal cooling in figure 8(b).
We finally analyze the cooling dynamics when the three-photon resonance condition is not satisfied, restricting to some specific parameter regimes. Figure 10 displays the mean phonon number at steady state as a function of $\Delta$ and $\delta_1$ at a fixed value $\delta_{c2} = 20\nu$. The solid line corresponds here to the values of $\Delta$ and $\delta_1$ fulfilling equation (41). For comparison, the curve corresponding to three-photon resonance is reported and corresponds to the diagonal line. Minimal temperatures are mostly found along this curve, demonstrating that EIT cooling is in most parameter regimes an efficient cooling scheme. Further parameter intervals where low temperatures are encountered are close to the curves $\Delta = -30\nu$ and $\Delta = 0$. These regimes correspond to dynamics which can be understood in terms of Doppler cooling: the probe laser is here tuned on the red of the corresponding dressed state, whose linewidth is larger than the trap frequency. A strikingly different behavior is found close to the intersection between the three-photon resonance curve and $\Delta = 0$: this parameter region is reported in the inset. Here, we observe that heating and cooling regions alternate. The cooling dynamics is here determined by interference processes: the corresponding rates $A_{\pm}$ are displayed in figure 7(b), showing that the cooling rate is characterized by a double Fano-like profile.

6. Conclusions

A cooling scheme has been presented and characterized, which combines cavity quantum electrodynamics and electromagnetic induced transparency. Novel dynamics have been identified, which may allow one to efficiently cool the atomic motion. These originate from the composite action of cavity, laser and quantized atomic motion, giving rise to interference processes that allow one to efficiently cool the motion. The cooling dynamics is robust against fluctuations of the parameters for most situations identified. Moreover, efficient ground-state cooling has been predicted for parameters that are consistent with these reported in [37].

The theory we presented here should also be applicable to current experimental setups, where the atom is confined in traps with different potentials for the relevant atomic states,
as is often the case for a dipolar trap setup. The fluctuations of the state-dependent trapping potential may be accounted for by a modified diffusion coefficient in the rate equations, as initial considerations suggest [13]. Moreover, the theory can be extended to the case when the motion is only strongly confined along the cavity axis. The perpendicular motion of the atom can be taken into account by averaging $g$ over the corresponding slice of the cavity’s mode function.

Future work shall address the properties of the scattered light. For several cavity-based systems it has already been demonstrated that photons can be emitted from a single atom in a controlled way [55–57]. Furthermore, quantum interference sustains the creation of non-classical features in the emitted light [58, 59]. Therefore, the system presented here exhibits several requirements to be potentially operating as a quantum emitter. In general, given the large number of control parameters at hand, and the possibility of interfacing it with several fields, this system can result to be a very useful element for a quantum network [60] for which further building blocks based on elementary light–atom interaction have recently been realized [61–63].

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Appendix A. Evaluation of the scattering rates

A.1. Calculation of the transition amplitudes for cooling

The transition amplitudes

$$T_{\tilde{n}} = \langle \phi_{\tilde{f}} | \left( V + \frac{1}{E_i - H} V \right) | \phi_{\tilde{i}} \rangle$$

(A.1)

of a scattering process are evaluated using the resolvent of the Hamiltonian [64]. The corresponding transition rates are

$$R_{\tilde{n}} = \frac{2\pi}{\hbar} \sum_{\tilde{f}} |T_{\tilde{n}}|^2 \delta(E_i - E_{\tilde{f}}),$$

(A.2)

where the $\delta$-function ensures energy conservation, and the sum goes over all relevant, different final states. The initial and final states $|\phi_{\tilde{i}}\rangle$ and $|\phi_{\tilde{f}}\rangle$ have defined energies $E_i$ and $E_{\tilde{f}}$ with respect to the unperturbed Hamiltonian $H_0$, equation (21). The total Hamiltonian $\mathcal{H} = H_0 + V + O(\eta^2)$ contains the interaction part

$$V = [H_0 - H_0] + \mathcal{H}_1 + W_P$$

$$= W_\nu(0) + W_\kappa + F_\chi + \sum_{j=1,2} F_{\gamma_j} x + W_P,$$

(A.3)

which includes the mechanical effects of laser and cavity, $F$, equation (25), and the mechanical effects denoted by $F_{\gamma_j}$, equation (26), of the interaction with the free radiation field in first order in $\eta$. 

We regard scattering processes with initial state

$$|\varphi_i\rangle = |\Psi_{st}, m; 0_{k,e}\rangle,$$  \hspace{1cm} (A.4)

where the atom and cavity modes are in the state $|\Psi_{st}\rangle$, equation (23), $m$ phononic excitations are present in the center-of-mass motion of the atom, and the free radiation field is in the vacuum state. The initial energy is $E_i = (m + \frac{1}{2})\hbar \nu + \hbar \Delta$. We are interested in the processes that change the motional state of the atom by one phonon, corresponding to the final states,

$$|\varphi_i^{\gamma,\pm}\rangle = |\Psi_{st}, m \pm 1; 1^{(\gamma)}_{k,e}\rangle,$$  \hspace{1cm} (A.5a)

$$|\varphi_i^{\epsilon,\pm}\rangle = |\Psi_{st}, m \pm 1; 1^{(\epsilon)}_{k,e}\rangle.$$  \hspace{1cm} (A.5b)

These are states where a photon is scattered into the modes of the electromagnetic field external to the resonator, either by spontaneous decay along $|e\rangle \leftrightarrow |g_2\rangle$ or cavity losses.

If one neglects the decay along the transition $|g_1\rangle \leftrightarrow |e\rangle$, the states (A.5) are the only final states for processes in first order of $\epsilon$ and $\eta_j$ where the motional state is changed by one quantum. We make the assumption $\gamma_1 = 0$ to avoid multi-photon scattering at the transition driven by the strong control laser. This simplification allows for a less involved analytical treatment. Comparisons with numerical results show that the results are not significantly altered in the parameter range we are interested in.

The evaluation of the scattering amplitude $T_\hbar$, equation (A.1), using the initial and final states from equations (A.4) and (A.5), is performed perturbatively in a Born series expansion

$$T_\hbar \approx \langle \varphi_i | [V G_0(E_i) V + V G_0(E_i) V G_0(E_i) V] |\varphi_i\rangle$$  \hspace{1cm} (A.6)

using the unperturbed resolvent

$$G_0(z) = \frac{1}{z - H_0^{\text{eff}}},$$  \hspace{1cm} (A.7)

containing the effective Hamiltonian

$$H_0^{\text{eff}} = H_0 - i\hbar \frac{\gamma}{2}|e\rangle \langle e| - i\hbar \kappa a^\dagger a,$$  \hspace{1cm} (A.8)

which accounts for radiative losses. The evaluation of equation (A.6), using the initial and final states (A.4) and (A.5), reveals that only three processes described by the amplitudes

$$T_D^{\pm} = \langle \varphi_i^{\gamma,\pm}|F_{g_2} G_0 W_p |\varphi_i\rangle,$$  \hspace{1cm} (A.9a)

$$T_F^{\gamma,\pm} = \langle \varphi_i^{\gamma,\pm}|W_{g_2}(0) G_0 F G_0 W_p |\varphi_i\rangle,$$  \hspace{1cm} (A.9b)

$$T_F^{\epsilon,\pm} = \langle \varphi_i^{\epsilon,\pm}|W_{g_2} G_0 F G_0 W_p |\varphi_i\rangle$$  \hspace{1cm} (A.9c)

contribute. Here, $G_0 \equiv G_0(E_i)$. Equation (A.9a) represents the diffusive process due to the mechanical effect of spontaneous emission, whereas equations (A.9b) and (A.9c) stand for the lowest order mechanical effects of the control laser and the cavity.

With the specific definitions given in this appendix, it is easy to check that the scattering amplitudes, equations (A.9), are the only contributions to light scattering including mechanical interaction up to first order in $\eta$ and $\epsilon$. They are straightforwardly evaluated by substituting the various operators by the explicit expressions from equations (11), (15), (25) and (26). The matrix elements of $G_0(E_i)$ are evaluated in appendix B, in particular equations (B.1) and (B.4).
with \( E_i = \hbar \Delta + \hbar (m + \frac{1}{2}) \nu \). One finds

\[
\mathcal{T}_D^\pm = \hbar \sqrt{m + \delta_\pm [\vec{e}_x \cdot \vec{e}_k, e]} g^{(\gamma)}_{k,\epsilon} \mathcal{T}_D(|\vec{k}|),
\]

\[
\mathcal{T}_F^{\gamma,\pm} = \hbar \sqrt{m + \delta_\pm g_{k,\epsilon}^{(\gamma)} \mathcal{T}_F^{\gamma,\pm}(|\vec{k}|),}
\]

\[
\mathcal{T}_F^{\epsilon,\pm} = \hbar \sqrt{m + \delta_\pm g_{k,\epsilon}^{(\epsilon)} \mathcal{T}_F^{\epsilon,\pm}(|\vec{k}|),}
\]

after collecting all the remaining factors—which are independent of the polarization \( \vec{e}_{k,\epsilon} \) and direction \( \vec{k}/|\vec{k}| \) of the scattered photon and the vibrational quantum number \( m \)—in the tilded quantities. The abbreviation \( \delta_\pm \) yields 1 for the ‘+’ case and otherwise vanishes.

The corresponding rates are found using equation (A.2), where one has to sum over all relevant polarizations and wave vectors,

\[
R_D^\pm = 2\pi (m + \delta_\pm) \sum_{k,\epsilon} (g^{(\gamma)}_{k,\epsilon})^2 \delta(c|\vec{k}| - \omega_{c,2}) |\mathcal{T}_D|^2,
\]

\[
R_F^{\gamma,\pm} = 2\pi (m + \delta_\pm) \sum_{k,\epsilon} (g^{(\gamma)}_{k,\epsilon})^2 \delta(c|\vec{k}| - \omega_{c,2}) |\mathcal{T}_F^{\gamma,\pm}|^2,
\]

\[
R_F^{\epsilon,\pm} = 2\pi (m + \delta_\pm) \sum_{k,\epsilon} (g^{(\epsilon)}_{k,\epsilon})^2 \delta(c|\vec{k}| - \omega_C) |\mathcal{T}_F^{\epsilon,\pm}|^2.
\]

Moreover, we used \( \omega_P \approx \omega_C \approx \omega_{c,2} \gg \nu \) to approximate the argument of the delta function, and \( \omega_{c,2} = \omega_C - \omega_2 \). The quantities \( \mathcal{T}_D, \mathcal{T}_F^{\gamma,\pm} \) and \( \mathcal{T}_F^{\epsilon,\pm} \) in the latter equations are evaluated at the \( |\vec{k}| \)-value determined by the delta function. Taking into account the definitions [64]

\[
\gamma_2 = \frac{2\pi}{\hbar} \sum_{k,\epsilon} |\hbar g^{(\gamma)}_{k,\epsilon}|^2 \delta(h c|\vec{k}| - \hbar \omega_{c,2}),
\]

\[
\kappa = \frac{\pi}{\hbar} \sum_{k,\epsilon} |\hbar g^{(\epsilon)}_{k,\epsilon}|^2 \delta(h c|\vec{k}| - \hbar \omega_C)
\]

and \( A_\pm (m + \delta_\pm) = R_D^\pm + R_F^{\gamma,\pm} + R_F^{\epsilon,\pm} [48] \) leads to expression (37), where \( \mathcal{W}_2 \) was introduced as a geometrical factor characterizing the atomic dipole radiation pattern [65].

A.2. Calculation of the excitation spectra

The excitation spectra of the atom at rest give the rate of photon scattering as a function of the probe frequency \( \omega_P \) either at the cavity output, giving \( S^x_{\text{exc}}(\omega_P) \), or from the resonance fluorescence of the atom integrated over the solid angle involving the modes external to the resonator, which we label by \( S^y_{\text{exc}}(\omega_P) \). It has the form \( S^j_{\text{exc}} \propto R^j(\omega_P) \), for \( j = \kappa, \gamma \), whereby \( R^j(\omega_P) \) is the rate of scattering a probe photon, assuming that the atom–cavity system is in the initial state \( |g_2, 0\rangle \) at energy \( E_i = \hbar \Delta \) and that the atomic motion is neglected. They are connected to the scatter amplitudes

\[
\mathcal{T}^j = \langle \varphi_i | W_j(0) G_0(E_i) W_P | \varphi_i \rangle
\]

by equation (A.2), evaluated up to first order in the small parameter \( \epsilon \). These amplitudes correspond to processes where, starting from the state \( |\varphi_i\rangle \), equation (A.4), the cavity is excited...
by the probe laser as described by $W_p$. The subsequent evolution determined by $G_0(E_i)$ couples the states of the manifold $\{ |e, 0 \rangle, |g_1, 0 \rangle, |g_2, 1 \rangle \}$ due to the strong cavity–atom and control laser interaction. Generally, all states of the manifold can be populated at this intermediate state, and a photon can leave the atom–cavity system either by spontaneous emission ($W_f = W_{\gamma_2}(0)$) or by leaking through the cavity mirrors ($W_f = W_k$), leading to the final state $|\phi_f\rangle = |g_2, 0, m; \bar{k}_\epsilon\rangle$.

We note that for spontaneous decay it is sufficient to take into account only $W_{\gamma_2}(0)$, even for $\gamma_1 \neq 0$: both scattering amplitudes differ only by a constant prefactor.

Evaluating equation (A.15) yields

$$
T^\gamma = \hbar \frac{\Omega_p}{2} g_{\bar{k}_\epsilon}^{(\gamma_2)} \hbar \langle e, 0 | G_{\text{opt}}^{(1)}(\hbar \Delta) | g_2, 1 \rangle,
$$

(A.16)

$$
T^\epsilon = \hbar \frac{\Omega_p}{2} g_{\bar{k}_\epsilon}^{(\epsilon)} \hbar \langle g_2, 1 | G_{\text{opt}}^{(1)}(\hbar \Delta) | g_2, 1 \rangle,
$$

(A.17)

where the required matrix elements of $G_{\text{opt}}^{(1)}(\hbar \Delta)$, calculated in appendix B, give the functions $\cos \varphi \mathcal{F}_Y(\Delta)$, equation (28b), and $\mathcal{F}_h(\Delta)$, equation (28a), respectively. Using equation (A.2) and after summing over all relevant modes $\bar{k}_\epsilon$ of the emitted photon, one finds the excitation spectra in the form of equations (27).

### Appendix B. Matrix elements of the resolvent

In this appendix the relevant matrix elements of the resolvent $G_0(z)$, equation (A.7), are calculated. We first rewrite

$$
G_0(z) = G_{\text{opt}}(z - H_{\text{ext}} - H_{\text{free}})
$$

using $G_{\text{opt}}(z) = [z - H_{\text{opt}}]^{-1}$ and

$$
H_{\text{opt}}^\epsilon = H_{\text{opt}} - i\hbar \gamma \frac{\hbar}{2} |e\rangle \langle e| - i\hbar \kappa a^\dagger a.
$$

(B.2)

The operator $G_{\text{opt}}(z)$ has block diagonal form ($P_m H_{\text{opt}} P_n = 0$ for $n \neq m$) when considering the subspaces of the state $|g_2, 0\rangle$ and the manifolds

$$
\mathcal{M}_n = \{ |g_2, n\rangle; |e, n-1\rangle, |g_1, n-1\rangle \} \quad (n > 0),
$$

(B.3)

where we have denoted the corresponding projectors by $P_0 = |g_2, 0\rangle \langle g_2, 0|$ and $P_n$, respectively.

For the dynamics analyzed in this work it is sufficient to calculate the matrix elements belonging to the case $n = 1$. The relevant matrix elements are found by inverting $z - P_1 H_{\text{opt}} P_1$, yielding

$$
G_{\text{opt}}^{(1)}(\hbar \xi) = \frac{1}{\hbar f(\xi)} \begin{bmatrix}
|e, 0\rangle \langle e, 0| & \{ (\delta_{c2} - \delta_1 + \xi)(\imath \kappa + \xi) \\
+ |g_2, 1\rangle \langle g_2, 1| & \left\{ \left( \delta_{c2} + \imath \frac{\gamma}{2} + \xi \right) \left( \delta_{c2} - \delta_1 + \xi \right) - \frac{\Omega_1^2}{4} \right\} \\
+ |g_1, 0\rangle \langle g_1, 0| & \left\{ \left( \delta_{c2} + \imath \frac{\gamma}{2} + \xi \right) (\imath \kappa + \xi) - g^2 \cos^2 \varphi \right\} \\
+ g \cos \varphi \frac{\Omega_1}{2} |[|g_1, 0\rangle \langle g_2, 1| + \text{H.c.} \rangle \langle e, 0| + \hbar \text{c.} \right\} \\
+ g \cos \varphi (\delta_{c2} - \delta_1 + \xi) |[|g_2, 1\rangle \langle e, 0| + \hbar \text{c.} \right]\right] .
$$

(B.4)
All the matrix elements of equation (B.4) are inversely proportional to the function

\[ f(\zeta) = \det[\zeta - P_1 H_{\text{opt}} P_1 / \hbar] = \prod_{\ell = \pm, 0} (\zeta - \omega_\ell^{\text{eff}}) = (i\kappa + \zeta) \left\{ \left[ \delta_{c2} + \zeta + i \frac{\gamma}{2} \right] (\delta_{c2} + \zeta - \delta_1) - \frac{\Omega_1^2}{4} \right\} - g^2 \cos^2 \varphi (\delta_{c2} + \zeta - \delta_1). \]  

(B.5)

Its poles are the complex eigenfrequencies \( \omega_\ell^{\text{eff}}, \omega_\circ^{\text{eff}} \) of the non-Hermitian operator \( H_{\text{opt}} \), equation (B.2), reduced to the states within the manifold \( \mathcal{M}_1 \). The real and imaginary parts of these eigenfrequencies are plotted in figure 3 and determine the relevant resonances of the scattering processes.

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Quantum superpositions of crystalline structures

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A procedure is discussed for creating coherent superpositions of motional states of ion strings. The motional states are across the structural transition linear-zigzag, and their coherent superposition is achieved by means of spin-dependent forces, such that a coherent superposition of the electronic states of one ion evolves into an entangled state between the chain’s internal and external degrees of freedom. It is shown that the creation of such an entangled state can be revealed by performing Ramsey interferometry with one ion of the chain.

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I. INTRODUCTION

The superposition principle is one of the fundamental elements of quantum mechanics, most fascinating as it defies the everyday experience of physical reality. A paradigmatic example is Schrödinger’s Gedankenexperiment, which pushes the quantum-mechanical predictions to their ultimate consequences, by envisioning an experiment that would lead to a quantum superposition involving a photon and a cat [1–3]. The “cat paradox” has been extensively discussed in the literature. The realization of quantum superpositions of physical objects having size bigger than a single atom or photon has been experimentally pursued in several milestone experiments, some of which are reported in Refs. [4–10]. These efforts ultimately aim at controlling the quantum dynamics of increasingly large systems, applying mostly a bottom-up approach. The goal is to warrant scalability of quantum mechanical operations, a basic requisite for quantum technological applications.

Strings of trapped ions are one of the most promising platforms for quantum technologies. Among several remarkable achievements, we mention here that the collective vibrations of small arrays of ions have been cooled to the zero-point energy [11], quantum teleportation of an ion’s internal state has been realized [12–14], and entangled states of the internal excitations have been demonstrated [15,16]. First realizations of quantum simulators with these systems have been reported most recently [17–21]. This progress is mostly based on scaling-up techniques, whose efficiency has been demonstrated for few particles, and points toward the need for identifying novel tools, which can allow one to control the quantum dynamics of mesoscopic systems.

In this article we propose a scheme for creating quantum superpositions of two different structures of a trapped ion crystal: the linear and the zigzag order [22]. The superposition is accessed by driving the electronic transition of one ion in the chain, in a setup where an external field makes the trap frequency spin dependent. The setup is sketched in Fig. 1. The corresponding stability diagram is derived for three ions; a measurement scheme, to reveal the presence of entanglement, is discussed, which is based on Ramsey interferometry.

Before we start, we note that the structural transition from a linear to a zigzag chain has been extensively studied in the literature [23–26]. In Ref. [24] it was shown that in the thermodynamic limit this is a second-order phase transition, which is classically described by the Landau model and whose control fields are the transverse trap frequency and the interparticle distance. If the system is quenched, the density of defects is well reproduced by the Kibble-Zurek model [27–30]. Our study is a first step toward creating a quantum superposition of two phases across the quantum phase transition, while the quenching here is realized by coupling to a quantum degree of freedom: a two-level transition of one ion in the chain. In this respect, our proposal extends to the ion-trap setup in previous studies which considered this idea for spin chains coupled to a qubit [31–33].

This article is organized as follows. In Sec. II we introduce the setup and the corresponding model. In Sec. III schemes for preparing quantum superpositions of crystalline structures are proposed, while the details on how state-dependent crystalline structures can be created are reported in Sec. IV. Measurement protocols for detecting the quantum superposition are discussed in Sec. V. The conclusions are drawn in Sec. VI, while the appendix provides further details on the stability diagrams.

II. THEORETICAL MODEL

We consider $N$ atomic ions of mass $m$ and charge $q$, which are confined by an anisotropic harmonic potential (generated by a linear Paul trap [34] or a linearized Penning trap [35]). We denote by $r_j$ and $p_j$ the position and canonically conjugate momentum of the $j$th ion, with $j = 1, \ldots, N$. The internal degrees of freedom of the ions, which are relevant to the dynamics, are the electronic states $|e\rangle$ and $|g\rangle$, which we assume to be stable. They are driven by external laser pulses, which manipulate the quantum state of each ion’s two-level transition in a controlled way.

The total Hamiltonian $H$ describing the dynamics of the ions’ internal and external degrees of freedom (excluding the
laser pulses) can be decomposed into the sum,
\[ H = H_{\text{int}} + H_{\text{kin}} + V, \]  
(1)
where \( H_{\text{int}} = \sum_{j=1}^{N} \hbar \omega_j |g\rangle_j \langle g| \) and \( H_{\text{kin}} = \sum_{j=1}^{N} p_j^2/(2m) \) are the internal and the kinetic energy of the ions, respectively, while \( V \) is the mechanical potential. The latter takes the form,
\[ V = V_{\text{Coul}} + V_{\text{pot}}, \]
(2)
with
\[ V_{\text{Coul}} = \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} \frac{q_j^2}{4\pi\varepsilon_0} \frac{1}{|r_j - r_k|} \]
(3)
the unscreened Coulomb repulsion, and with \( \varepsilon_0 \) the vacuum permittivity. The term \( V_{\text{pot}} \) denotes an external, harmonic potential that is assumed to be anisotropic. In the rest of this work we assume that the confinement along the \( z \) direction is so tight, that the motion along this direction can be considered to be frozen out. In the \( x-y \) plane, the potential depends on the internal state of the ions and takes the form,
\[ V_{\text{pot}} = \sum_{j=1}^{N} |g\rangle_j \langle g| V_{g}(r_j) + |e\rangle_j \langle e| V_{e}(r_j), \]
(4)
where
\[ V_{g}(r_j) = \frac{1}{2} m v_x^2 \left( x_j^2 + \alpha^2 y_j^2 \right), \]
(5)
\[ V_{e}(r_j) = \frac{1}{2} m v_y^2 \left[ x_j^2 + (\alpha + \delta\alpha)^2 y_j^2 \right], \]
(6)
Here \( v_x \) is the trap frequency along the \( x \) axis, \( \alpha = v_y/v_x \) is the aspect ratio between transverse and axial trap frequency when the ion is in the internal state \( |g\rangle \), and \( \alpha + \delta\alpha \) is the aspect ratio when the ion internal state is \( |e\rangle \).

The potential (4) can be obtained by superimposing an optical potential to the ion trap. Such potential can be generated by a laser which is far detuned from a dipole transition between the state \( |e\rangle \) and an additional auxiliary electronic level, while it does not affect the dynamics when the ion is in state \( |g\rangle \) [36,37]. Alternatively, the state-dependent potential can be realized by means of magnetic fields, by appropriately coupling a magnetic dipole transition [19].

In this article we assume that the ions are sufficiently cold, such that they are localized around the equilibrium positions of the total potential, composed of \( V_{\text{Coul}} + V_{\text{pot}} \). The ordered structures they form depend on the potential, and thus also on the ions’ internal state. The potentials we will discuss support the linear and zigzag structures, which are illustrated on the top of Fig. 2.

For later convenience, we introduce dimensionless variables: The lengths are scaled by a characteristic scale,
\[ l = q^{2/3}/(4\pi\varepsilon_0 m v_x^2) \]
which is the typical interparticle distance along the chain axis, while the energies by the scale \( \mathcal{E} = m v_x^2 l^2 \). The dimensionless potentials read
\[ V_{\text{Coul}} = \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} \frac{1}{|r_j - r_k|}, \]
(7)
III. CAT STATES OF ION CHAINS

In this section we describe a possible scheme for preparing and measuring a coherent superposition of different motional states by manipulating the ions with lasers. We are interested in the case in which the chain is composed by few ions, for instance, three. We assume that the superimposed optical potential is sufficiently tight such that, when an ion in the zigzag chain is excited, the structure becomes linear. In this regime the cat state is achieved by preparing a single ion in a superposition state. The parameters required in order to access this regime will be analyzed in the next section.

A. Creation of cat states

The initial state of the crystal is assumed to be, unless otherwise stated, given by all ions in their electronic ground state and the chain in the ground state of the zigzag structure, which we denote by $|\phi(0)\rangle = |0\rangle_{zz}$. A laser pulse addresses one of the ions in the chain and drives the two-level transition $|g\rangle \rightarrow |e\rangle$, performing the rotation $|g\rangle \rightarrow |g\rangle \cos \theta/2 + |e\rangle \sin \theta/2$. Assuming that the duration of the pulse is much shorter than the typical scales of the vibrational motion, the state of crystal after the pulse is $|\Psi\rangle = |\psi(t)0\rangle_{zz}$, with (for $\theta = \pi/2$)

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}(|ggg\rangle + |geg\rangle).$$

After the pulse, the motional and internal degrees of freedom get entangled by the unitary evolution governed by Hamiltonian $H$, Eq. (1), creating states of the form,

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}(|ggg\rangle|0\rangle_{zz} + |geg\rangle|\phi(t)\rangle),$$

with

$$|\phi(t)\rangle = e^{-iH_{t}/\hbar}|0\rangle_{zz},$$

and $H_{c} = \langle ge|H|ge\rangle$ the Hamiltonian projected over the excited state. Here, the energy of state $|ggg\rangle|0\rangle_{zz}$ is set equal to zero, and the state is in the reference frame of Hamiltonian $H_{at}$.

Entanglement between internal and external degrees of freedom is achieved for times over which the overlap,

$$I(t) = \langle \phi(0)|\phi(t)\rangle,$$

has modulus smaller than unity. This entanglement can also be interpreted in terms of which-way information. Entanglement between internal and external degrees of freedom, in fact, diminishes the visibility of the Ramsey signal introducing a “distinguishability” (which-way information) in the interferometric path. Maximal distinguishability, and correspondingly zero visibility, is found for $I = 0$. We refer the reader to Refs. [38, 39] for a more detailed discussion.

B. Ramsey interferometry

The overlap $I(t)$ can be measured by means of Ramsey interferometry, according to the scheme proposed in Ref. [38] and in [40] to study spin-dependent dynamics in ion chains. Let us assume that, after obtaining state (11) for a given evolution time $t$, we apply a $-\pi/2$ pulse (i.e., the inverse operation of a $\pi/2$ pulse). The resulting state reads

$$|\psi_{f}(t)\rangle = \frac{1}{2}(|ggg\rangle|\phi(0)\rangle + |\phi(t)\rangle - |geg\rangle|\phi(0)\rangle - |\phi(t)\rangle),$$

and the corresponding probability to find the addressed ion in state $|g\rangle$ is given by

$$P_{1}(g) = \frac{1 + \text{Re}[I(t)]}{2}.$$  

Alternatively, after obtaining the state (11), we can first apply a phase gate on the addressed ion, namely an operation that maps the internal states according to the rule: $|g\rangle \rightarrow |g\rangle, |e\rangle \rightarrow -i|e\rangle$. After an elapsed time $t$, the $-\pi/2$ pulse is applied and the probability to find the ion in $|g\rangle$ reads

$$P_{2}(g) = \frac{1 + \text{Im}[I(t)]}{2}.$$  

From these two measurements the overlap $I(t)$ is obtained. We note that this quantity is sometimes called “Loschmidt echo” or also “quantum fidelity,” and has been studied extensively in other systems, for instance, in Refs. [31,41–43].

C. Discussion

Some remarks are now in order. First of all, in the example provided here it is the ion in the middle of the chain which is addressed by the laser pulses. The reason for this choice is rather natural, as the type of excitation does preserve the symmetry by reflection about the center of the trap, which characterizes both linear and zigzag chain. Control of the internal excitation is a necessary condition for the implementation of the protocol. The selective driving of the central ion could be implemented by a focused laser beam, as realized, for instance, in Ref. [13], or by means of a magnetic field gradient, which tunes only the central ion’s transition in resonance with an external microwave field [44]. In this regime mechanical effects of the coupling to radiation can be taken to be very small and can be neglected. The Hamiltonian for the pulse reads

$$H_{L} = \frac{i\hbar}{2}(|g\rangle|e\rangle - |e\rangle|g\rangle)\theta(t)(t - t_{\text{pulse}})$$

in the reference frame rotating at the laser frequency; $\theta(t)$ is the Heaviside function, describing the steplike form of the pulse with duration $t_{\text{pulse}}$. Here, $\Omega$ is the Rabi frequency, and the rotation angle of the dipole is $\theta = 2\Omega t_{\text{pulse}}$.

Neglecting the evolution of the vibrational motion during the pulse is justified provided that the largest vibrational frequency scale $\nu_{\text{max}}$ is much smaller than the pulse duration of the pulse, $\nu_{\text{max}}t_{\text{pulse}} \ll 1$. Considering that $\Omega t_{\text{pulse}} = \pi/4$ for the example here considered, the

\[1\] Neglecting the mechanical effects of the laser pulse simplifies the theoretical treatment but does not limit the feasibility of the protocol.
requirement can be rewritten in terms of the inequality $v_{\text{max}} \ll \Omega$.

We note that the scheme here proposed is based on creating a local defect when the central ion is in the excited state. This defect will induce another ordering (e.g., when starting from a zigzag array, the ion excitation induces a transition to a linear chain) provided that the length of the string is shorter than the correlation length [24]. However, as the number of ions is scaled up, a linear superposition like the state in Eq. (10) will present a central deformation of finite size. This problem could be solved by creating a Greenberger-Horne-Zeilinger (GHZ) state, namely,

$$\frac{1}{\sqrt{2}}(|\text{ggg}\rangle + |\text{eee}\rangle),$$

which warrants that all ions feel the same potential. This kind of state has been realized in [45,46]. The preparation of this class of states becomes increasingly difficult for larger ion chains [45,46], and the entanglement of GHZ states is in general not robust [47].

To conclude this section, we mention that an alternative procedure for generating a cat state could be implemented by (i) first preparing the superposition state (10) for the internal degrees of freedom, and then (ii) slowly switching on the additional state-dependent potential, such that the vibrational state follows adiabatically the change in the (state-dependent) vibrational Hamiltonian. In this form, it would be possible to prepare a superposition of two different structures in their respective ground state. This proposal poses several challenges and it will be elaborated in more detail in a subsequent publication.

IV. STATE-DEPENDENT CRYSTALLINE STRUCTURES

In this section we shall analyze the equilibrium configuration and normal modes of the ion chain in the harmonic trapping potential. The stationary equilibrium positions $r_i^{(0)}$ satisfy the equations \( \frac{\partial V}{\partial r_i}(r_i^{(0)}) = 0 \), and they are stable when the eigenvalues of the Hessian matrix of $V$ evaluated at $r_i^{(0)}$ are larger than zero. In this case the eigenvalues give the frequencies of the normal modes, and the corresponding eigenvectors are the eigenmodes [48]. Clearly, in our case there will be different sets of solutions depending on the ions’ internal state.

In the following we will consider that the ion excitation couples the ground states of the classical phase transition [24]. We will hence discard the regime, in which one would observe the disordered phase, predicted for the quantum phase transition, and which is observed when the trap frequency is close but below the critical value, yet quantum fluctuations destroy the zigzag order [26,49]. This would correspond to a narrow interval of values, that has been characterized in detail in Ref. [49]. In Ref. [25] a characterization of the parameters required for small chains of ions can be found.

A. Spatial organization of the ions in harmonic potentials

We first examine the equilibrium structures for three trapped ions in the case in which the internal state of all particles is $|g\rangle$ and the confinement in the $y$ direction is tighter than that along $x$ (i.e., $\alpha > 1$). The following discussion reviews results which have been reported, for instance, in [24,50,51]. For this case there are two different possible types of solutions for the equilibrium positions: the linear chain, with all ions aligned along the $x$ axis, and a planar structure, where the ions form the extremes of an isosceles triangle whose symmetry axis is aligned along the $y$ axis. We refer to this planar structure as zigzag configuration. More specifically, the equilibrium positions of the linear chain are

$$x_i^{(0)} = -x_0^{(0)} = \sqrt{\frac{5}{74}}, \quad y_i^{(0)} = 0.$$  

This configuration is stable when $\alpha > \alpha_c$, with $\alpha_c = \sqrt{12/5} \approx 1.5492$. In this case, the axial normal mode frequencies are \{1, $\sqrt{3}$, $\sqrt{29/5}$\} and the transverse ones are \{\sqrt{\alpha^2 - \alpha_c^2}, \sqrt{\alpha^2 - 1}\alpha\}.

For $\alpha < \alpha_c$ (and $\alpha > 1$) the chain is in a zigzag configuration, with equilibrium positions,

$$x_i^{(0)} = -x_0^{(0)} = \bar{x}, \quad y_i^{(0)} = 0.$$  

where

$$\bar{x} = \left[4 \left(1 - \frac{\alpha^2}{3}\right)\right]^{-1/3},$$

$$\bar{y} = \pm \sqrt{\frac{3}{\alpha^2} - \bar{x}^2}.$$  

The analytic expressions for the normal mode frequencies are rather cumbersome and are reported, for instance, in Ref. [24] for the case of $N$ ions in a ring. Figure 2 displays the frequencies of the normal modes as a function of the aspect ratio $\alpha$.

B. Spatial organization in state-dependent harmonic potentials

We now extend the previous considerations to the case in which the internal state of the three ions is not the same, so that the ions experience different trapping potentials. We shall consider only the case in which one of the three ions is excited. In particular, we will discuss the case in which the excited ion is in the middle of a linear chain. The configurations found for the case, in which the excited ion is at one edge of the chain, are reported for completeness in the appendix.

When the ions form a linear array, the equilibrium configurations corresponding to state $|\text{geg}\rangle$ are the same as in the homogeneous case, and are thus given by Eqs. (19) and (20). In this case, in fact, the central ion is located in the center of
the trap where the external potential is zero. For this case the

eigenfrequencies read

\[
\{1, \sqrt{3}, \sqrt{29/5}, \sqrt{\alpha^2 - 4}, \sqrt{\alpha^2 - 1},
\sqrt{\alpha^2 + \alpha \delta \alpha - (12 - 5 \delta \alpha^2 - \rho)/10},
\sqrt{\alpha^2 + \alpha \delta \alpha - (12 - 5 \delta \alpha^2 + \rho)/10},
\]

(25)

with \(\rho = \sqrt{128 + [5\delta \alpha(2 \alpha + \delta \alpha) - 4]^2}\). By imposing that the
eigenfrequencies are real and positive, one finds that the linear
chain is stable for \(\delta \alpha > \delta \alpha_c\), with

\[
\delta \alpha_c = \left(2 \frac{2}{5 \alpha^2 - 4} - 1\right) \alpha,
\]

(26)

where \(\alpha \geq 1\). The corresponding curve is reported in the
stability diagram of Fig. 3. Here, one observes that for most
values of \(\delta \alpha < \delta \alpha_c\), the chain is in a zigzag structure along the
x axis (i.e., symmetric about the y axis), whose equilibrium
positions read

\[
x_1^{(0)} = \bar{x}, \quad x_2^{(0)} = 0, \quad x_3^{(0)} = -\bar{x},
\]

\[
y_1^{(0)} = \bar{y}, \quad y_2^{(0)} = -2 R \bar{y}, \quad y_3^{(0)} = \bar{y},
\]

(27)

(28)

with

\[
\bar{x} = \left[4 \left(1 - \frac{\alpha^2}{1 + 2 R} \right) \right]^{-1/3},
\]

(29)

\[
\bar{y} = \pm \frac{1}{1 + 2 R} \left[\frac{1 + 2 R}{\alpha^2} \right]^{2/3} \bar{x}^{2/3},
\]

(30)

and

\[
R = \frac{\alpha^2}{(\alpha + \delta \alpha)^2}.
\]

(31)

The homogeneous case is recovered in the formula by setting
\(\delta \alpha = 0\): In this limit, \(R = 1\), and Eqs. (29) and (30) coincide
with Eqs. (23) and (24), respectively.

The region in the upper left corner of Fig. 3 corresponds to the
appearance of zigzag configurations along the y direction.
The corresponding stability boundary is evaluated by imposing
that the Hessian matrix, giving the normal modes, has
vanishing determinant, which leads to the equation:

\[
\frac{\alpha^2}{2 R + 1} = -\left(\frac{y}{D}\right)^2 + \frac{1}{3} + \frac{(3\bar{x} \bar{y})^2}{D^2 [2 - \alpha^2 - (\frac{\bar{y}}{R})^2]},
\]

(32)

where \(\bar{x}, \bar{y}, \) and \(D\) correspond to the equilibrium positions in
this configuration and are given by

\[
\bar{x} = \frac{1}{3} (32^{1/3} - \bar{y}^2)^{1/2},
\]

(33)

\[
\bar{y} = \left[4 \left(\alpha^2 - \frac{1}{3} \right) \right]^{-1/3},
\]

(34)

\[
D = (9 \bar{x}^2 + \bar{y}^2)^{1/2} = 3^{1/3}.
\]

(35)

We note that, as opposed to the case when all ions experience
the same potential, more than one configuration can be stable
in the same region.

V. LOSCHMIDT ECHO

A clear demonstration of the creation of cat states would
require quantum tomography of the crystal state [8,52–54].
Nevertheless, signatures of the quantum superposition can be
obtained by means of Ramsey interferometry. This scheme
allows one, as we have shown, to determine the overlap
\(I(t)\) as a function of the elapsed time \(t\) between the two
laser pulses. In this section we analyze the behavior of the
absolute value of the overlap \(|I(t)|\) for different values of the
axial and spin-dependent potential. This is performed by
scanning through various regions of the phase diagram of the
linear-zigzag structural instability for the case of three ions.
For this calculation, the potentials were approximated by their
quadratic expansions about the corresponding equilibrium
positions, and the vibrations have been quantized according
to the procedure reported, for instance, in Ref. [50].

In the following discussion we will assume that the chain
is initially either in the zigzag or in the linear configuration,
depending on the value of the aspect ratio \(\alpha\), and that the ions
are prepared in state (11) at \(t = 0\), as described in Sec. III.
The strength of the harmonic potential trapping the central ion
is given by the frequency \(\nu' = \nu_y + \delta \nu_y\), with \(\delta \nu_y = \delta \alpha \nu_y\).
We first focus on the signal for different values of \(\alpha\), fixing the
quant \(\delta \alpha\). This corresponds to analyzing the Ramsey
signal by keeping constant the frequency shift \(\delta \nu_y\) (due to
the spin-dependent potential) but varying the potential at the
electrodes.

Figure 4 displays \(|I(t)|\) for different values of \(\alpha\) when
the excitation of the central ion gives rise to a transition
(a) between two zigzag structures (where the second one is more tightly confined), (b) from a zigzag to a linear string, and (c) between two linear strings (where the second one is more tightly confined). We note that the observed time-dependent behavior is determined by the modes of the crystalline structure that is generated by exciting the central ion. In fact, the initial structure, which corresponds to the structure when all ions are in state $|\text{g}\rangle$, is the ground state of the corresponding array. In (a) revivals of the overlap signal are observed. These revivals become more distant in time the closer the zigzag array is to the mechanical instability, where the time intervals scale with the period of the lowest eigenfrequency of the tighter zigzag chain. In (b), where the excitation corresponds to a quench across the transition connecting zigzag and linear chain, one still observes revivals of the overlap, whereby the signal exhibits a more complex, quasiperiodic structure. When the transition is instead between two linear arrays with different transverse confinement (c), the overlap exhibits a periodic modulation whose maximal amplitude is unity and at twice the frequency of the lowest frequency eigenmode: the zigzag mode of the linear chain. This modulation is a manifestation of squeezing induced by the sudden change of the trap potential.

This behavior can be further characterized using the Fourier spectra of the overlap signal. These are shown in Fig. 5 for each of the three cases displayed in Fig. 4. A first look shows that the spectral components of the transition between the zigzag structures are dominated by a comb of frequencies [Fig. 4(a)] with a background signal. The comb is at frequencies that are multiples of the lowest frequency of the tight zigzag array. This structure splits up into more components when the transition couples two different structures [Fig. 4(b)]. Finally, when the transition couples two linear structures [Fig. 4(c)], the spectrum is much more regular and composed of only a few frequency components, dominated by the lowest one. Further analysis shows that the dominant contribution in Figs. 4(a) and 4(c) is from the zigzag mode, which is also the soft mode of the structural phase transition. This mode seems to play a relevant role also when the transition couples two structures across the structural instability [Fig. 4(b)]. The revivals are associated with the oscillations of this mode, which is mostly excited by the quench.

We note that the appearance of the revival signal is a signature of the quantum superposition: This signal would be absent if there is no quantum coherence between the two crystalline states. We then focus on its features, and characterize them in detail considering electronic excitations that couple a crystal with an equilibrium zigzag structure to a crystal with a linear array.

The figures discussed in the following refer to the situations in which ground and excited states correspond to equilibrium structures across the mechanical instability, namely, when the initial state is a zigzag array and the excited state is a linear chain. Figure 6 shows the overlap signal for different frequencies of the spin-dependent potential, corresponding to different values of the parameter $\delta \alpha$ (larger absolute values correspond to larger variations). The distance between the revival signals decreases as $\delta \alpha$ increases, namely, the excited state is deeper in the linear phase. Moreover, for $\delta \alpha = 0.1$ one observes the onset of a periodic signal. The form of the signal at $\delta \alpha = 0.02$ is further characterized in Fig. 7 as a function
of the axial trap frequency, showing a slight increase of the revival signals as $v_x$ is increased, and correspondingly as the ions are more tightly confined in the $x$ direction.

Finally, the form of the revivals is reported in Fig. 8 as a function of the ion species, that is, of the mass determining the spread of the motional wave packet. In this case, for lighter ions (i.e., for larger quantum fluctuations), one observes a slight increase in the revival signal.

The dynamics we considered so far is unitary: decay of the overlap signal is solely due to dephasing in the dynamics of internal and external degrees of freedom. Decoherence and noise sources have been neglected. These would affect both internal and external degrees of freedom. They are expected to introduce a damping factor in the overlap signal, setting an upper bound for partial revivals decreasing with time, such as those reported in Fig. 8.

FIG. 5. (Color online) Fourier transform of the overlap signal $|I(t)|$ in Fig. 4. Here, (a) corresponds to the curve at $\alpha = 1.49$, (b) to $\alpha = 1.547$, and (c) to $\alpha = 1.55$.

FIG. 6. (Color online) Same as Fig. 4 but for $\alpha = 1.547$ ($v_x = 2\pi \times 773.5$ kHz) and $\delta \alpha = \{0.01, 0.04, 0.10\}$ (corresponding to $\delta v_x = 2\pi \times (5, 20, 50)$ kHz). In this case the equilibrium structures for ground and excited states are a zigzag and a linear array, respectively.

FIG. 7. (Color online) Same as Fig. 6 but for $\delta \alpha = 0.02$ and different axial trap frequencies $v_x$ (the values are reported in the box). The value for $\alpha$ corresponds to $v_x = 2\pi \times \{154.7, 309.4, 773.5, 1547\}$ kHz, the frequency shift due to the optical potential is $\delta v_x = 2\pi \times (2, 4, 10, 20)$ kHz (ordering corresponds to the values of $v_x$, reported in the legends in the box, from bottom to top). The different abscissae indicate the time (in $\mu$s) for the corresponding curves.

FIG. 8. (Color online) Same as Fig. 4 but for $\alpha = 1.547$ and different axial trap frequencies $v_x$ (the values are reported in the box). The value for $\alpha$ corresponds to $v_x = 2\pi \times \{154.7, 309.4, 773.5, 1547\}$ kHz, the frequency shift due to the optical potential is $\delta v_x = 2\pi \times (2, 4, 10, 20)$ kHz (ordering corresponds to the values of $v_x$, reported in the legends in the box, from bottom to top). The different abscissae indicate the time (in $\mu$s) for the corresponding curves.
that a measured revival in an experiment in turn would give an estimated bound on decoherence effects. In order to observe the curves reported in Fig. 4, one needs coherence times longer than $100\nu_{x}^{-1}$ for both internal and external degrees of freedom. Taking $\nu_{x} \simeq 2\pi \times 500$ kHz, the state would need to remain coherent for times longer than $30$ $\mu$s. This assumption seems reasonable given the coherence times reported for instance in [9,55,56]. The requirements of our proposal in terms of optical power are very moderate: For the values corresponding to Fig. 4, the optical potential should have an associated motional frequency of the order of $2\pi \times 100$ kHz, well within present reach. Finally, we note that the ability to combine optical potentials and ion traps has already been demonstrated [37,57].

**VI. CONCLUSIONS**

In this paper we have studied the dynamics of the structural phase transition from the linear to the zigzag configuration in a chain of trapped ions, with the aim of creating a coherent superposition of different mesoscopic crystalline structures. Among several possibilities to achieve that goal, we have chosen to exploit spin-dependent trapping potentials, which influence each ion’s motional state as a function of its internal electronic state. This allows one in particular to create an entangled state from coherent superpositions of one degree of freedom.

Specifically, our protocol starts with an ion chain at rest under external confinement in a regime near the chain’s structural phase transition. Excitation of one particular ion from the chain into a superposition of metastable electronic states affects, via the state dependence of the external potential, this ion’s motion, entangling its vibrational and internal state. As a result of Coulomb repulsion, the other ions in turn rearrange their motion according to this ion’s new state, thereby becoming entangled with it as well.

This realizes, under appropriate conditions described in the text, a mesoscopic superposition (a cat state) of different crystalline structures, something that to our knowledge has not been observed or proposed before. Signaturers of the generated cat state can be obtained by means of Ramsey interferometry, according to the scheme discussed in [38]. Our analysis shows that these dynamics could in principle be observed in current experiments, using crystals of three ions.

Future work will focus on the properties of the Ramsey signal measured for longer chains when the ions are in the disordered phase of the quantum phase transition [26,49]. Moreover, the efficiency of the protocol will be characterized as a function of the temperature of the chain, including also heating and decoherence effects systematically in the theoretical model. The control tools proposed here open the way to the application of optimal control techniques in the spirit of the proposals in Refs. [58,59], for the purpose of creating robust mesoscopic quantum states on demand.

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3Recently, we became aware of work along related lines carried out in W. Li and I. Lesanovsky [arXiv.1108.3591 (to be published)], where the creation of a three-ion state-dependent structure was proposed by means of Rydberg excitation of the central ion.
**APPENDIX: EQUILIBRIUM CONFIGURATIONS WHEN ONE OUTER ION IS EXCITED**

We now determine the stability diagram when one of the outer ions is excited and experiences a state-dependent potential. We distinguish between three different cases: (1) a linear chain configuration along the $x$ direction, which we denote by $\text{LIN X}^*$; (2) a linear chain configuration along the $y$ axis, which we denote by $\text{LIN Y}^*$; and (3) a triangular configuration which we label by $\text{TRIA}^*$ (here we choose not to distinguish between orientation along $x$ or $y$). The asterisk always denotes the structures where one of the outer ions is excited. As in the previous cases, we focus on the parameter region $\alpha \gg 1$, for which a linear chain along the $y$ axis is never stable.

For the LIN X* we obtain again the same equilibrium positions as in Eqs. (19) and (20). It is possible to determine the stability boundary analytically by solving equation,

$$\frac{\alpha^2}{R^2} = \frac{9}{20} \left( \frac{65/8}{5\alpha^2 - 25\alpha^2/2 + 4} \right),$$

where $R$ is defined as in Eq. (31).

The triangular structure $\text{TRIA}^*$ does not exhibit the symmetry properties of the zigzag structure. The corresponding equilibrium positions, as well as the stability boundary shown in Fig. 9, were calculated numerically using a Metropolis algorithm with random initial positions followed by a constraint minimization setting the asymmetry as a constraint. However, as the structures transform smoothly, one has to allow a certain tolerance on the constraint. On the other hand, the algorithm might run into a minimum corresponding to another structure satisfying accidentally this constraint. We believe this is the reason why scattered singular solutions are observed in the stability diagram for the triangular configuration.

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Quantum quenches of ion Coulomb Crystals across structural instabilities

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Quenches in an ion chain can create coherent superpositions of motional states across the linear-zigzag structural transition. The procedure has been described in [Phys. Rev. A 84, 063821 (2011)] and makes use of spin-dependent forces, so that a coherent superposition of the electronic states of one ion evolves into an entangled state between the chain’s internal and external degrees of freedom. The properties of the crystalline state so generated are theoretically studied by means of Ramsey interferometry on one ion of the chain. An analytical expression for the visibility of the interferometric measurement is obtained for a chain of arbitrary number of ions and as a function of the time elapsed after the quench. Sufficiently close to the linear-zigzag instability the visibility decays very fast, but exhibits revivals at the period of oscillation of the mode that drives the structural instability. These revivals have a periodicity that is independent of the crystal size, and they signal the creation of entanglement by the quantum quench.

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I. INTRODUCTION

Quenches of quantum many-body systems provide important information on the thermodynamic properties of physical objects close to phase transitions. They give insight into the statistical mechanics of closed systems, and can find applications for quantum information [1–3]. Among several proposals discussed in the literature, some setups make use of the coupling with a quantum system, a spin, to drive a quantum phase transition in a larger physical object acting as environment. These dynamics are associated with decay of spin coherence that has been shown to exhibit universal features [4–7].

A recent article studied these dynamics for the case where the spin was the internal transition of a trapped ion embedded in a chain, while the vibrational excitations of the chain itself acted as environment [8]. That work proposed to use the visibility of a Ramsey-type of interferometry in order to measure thermodynamic properties of the crystal. It was shown that close to the critical point where the chain undergoes a classical second-order phase transition to a zigzag structure [9], the visibility allows one to study the behaviour at criticality. In Ref. [10] it was proposed to use the spin excitation to create a superposition of two different crystalline structures across the linear-zigzag structural transition. The superposition can be accessed by driving the electronic transition of one ion of the chain in a set-up where an external field makes the trap frequency spin-dependent [10] [11]. In this case the visibility of the interferometric signal exhibits a fast decay, in agreement with studies performed in other settings [5–7], while for longer times quasi-periodic revivals of the visibility appear.

In this paper we analyse the dependence of the signal visibility on the system parameters, for the setup proposed in Ref. [10] and sketched in Fig. 1. We determine analytically the expression of the visibility and study its behaviour close to and across the classical linear-zigzag instability, for different numbers of ions. We find that

FIG. 1. (Color online) A quench across the linear-zigzag instability is performed by exciting the central ion with a laser pulse in presence of spin-dependent forces. In (a) the collective motion is initially in the ground state of a zigzag structure, and the central ion in the internal state $|g\rangle$. A $\pi/2$ laser pulse prepares it in the superposition $(|g\rangle + |e\rangle)/\sqrt{2}$. (b) A tighter state-dependent potential, acting only when the ion is in state $|e\rangle$, induces conditional dynamics such that the ions’ internal and external degrees of freedom get entangled. When the state-dependent potential is sufficiently tight, the excited component will start oscillating around the equilibrium positions of the linear chain. (c) A laser pulse performs a $-\pi/2$ rotation on the central ion. The final occupation of the ground state $|g\rangle$ as a function of the time between the two pulses contains information on the properties of the chain across the linear-zigzag instability.
the revivals observed in the visibility as a function of the time $t$ elapsed after the quench are characterized by the frequency of the zigzag mode, and persist when the number of ions is increased. The analysis of the spectrum of the visibility signal as a function of $t$ shows the presence of squeezing and entanglement that are generated by the quantum quench.

The article is organized as follows: In Sec. II the proposal of Ref. [10] is summarized. The theoretical model is presented in Sec. III which also includes the detailed evaluation of the visibility signal. The behaviour of the visibility is analysed in Sec. IV, and the conclusions are drawn in Sec. V. Theoretical details for the derivation of the results in Sec. III are given in the appendices.

II. RAMSEY INTERFEROMETRY WITH AN ION COULOMB CRYSTAL

In this section we briefly review the physical model at the basis of this work. A string of $N$ ions of mass $m$ and charge $q$ is confined in a trap, forming a zigzag structure close to the linear-zigzag mechanical instability. A two-level transition of the central ion is driven by two laser pulses separated by a time interval $t$ and for which perform a $\pi/2$ and $-\pi/2$ rotation of the dipole, respectively. The pulses are short so that the crystal dynamics can be neglected during their duration [8, 10]. Under the assumption that both internal states of the dipolar transition are stable, a spin-dependent force is applied, such that the stable configuration of a finite chain is a linear structure when the ion is in the excited state [10]. Therefore, during the time elapsed between the two pulses, the crystalline state undergoes conditional dynamics depending on the internal state, that lead to entanglement between internal and external degrees of freedom.

In the following we denote by $|g\rangle$ and $|e\rangle$ the two internal states of the central ion, and omit to write the internal state of the other $N - 1$ ions since this remains unchanged. Before the first pulse, the state of the central ion and crystal motion reads $|\psi(0)\rangle = |g\rangle \phi(0)\rangle$ where $|\phi(0)\rangle$ can be either the ground state of the linear or of the zigzag configuration, as shown in Fig. 3(a). The pulse performs a quantum quench by bringing the central ion into a superposition of ground and excited states. In fact, at a time $t$ after the first pulse the state takes the form:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( |g\rangle \phi_g(t)\rangle + e^{i\varphi} |e\rangle \phi_e(t)\rangle \right),$$

(2.1)

where $\varphi$ is a controllable phase and

$$|\phi_x(t)\rangle = \exp \left( -i H_{x} t / \hbar \right) |\phi(0)\rangle,$$

(2.2)

with $s = g, e$ and $H_{g}, H_{e}$ the Hamiltonians for the external degrees of freedom, accounting for the state-dependent potential. The free evolution is pictorially shown in Fig. 1(b) and leads to entanglement between internal and external degrees of freedom. After the second pulse, which performs a $-\pi/2$ rotation of the dipole as sketched in Fig. 1(c), the probability of measuring the central ion in state $|g\rangle$ reads

$$P_g(\phi) = \frac{1}{2} \left\{ 1 + \text{Re} \left[ e^{i\varphi} O(t) \right] \right\},$$

(2.3)

where

$$O(t) = \langle \phi_g(t)|\phi_e(t)\rangle$$

(2.4)

is the overlap between the two motional states. The contrast of the Ramsey fringes is given by

$$V(t) = |O(t)|,$$

(2.5)

and depends on the time $t$ elapsed between the two Ramsey pulses. We note that the visibility of the interference signal is directly related to the Loschmidt echo, frequently used to describe the loss of coherence as a consequence of the interaction between a system and its environment [13].

Figure 2 displays the visibility of the interferometric signal, given by Eq. (2.5), as a function of the time elapsed between the two pulses. The visibility is evaluated using the formula derived in Sec. III. The three plots correspond to three regimes we consider in this paper. In (a) the equilibrium configuration of the crystal is always a linear chain, which experiences a tighter potential when the central ion is excited. Therefore the first quench does not change the equilibrium positions but rather the frequencies of the normal modes. The corresponding visibility exhibits sinusoidal oscillations and is close to unity. Figure 2(b) shows the case when the equilibrium configuration is a zigzag if the central ion is in the ground state, while it is a linear chain when the central ion is excited. The visibility decays quickly to zero, in agreement with the theoretical predictions for the decoherence of a spin coupled to an environment close to criticality [4, 5], but exhibits revivals with different peak heights. Figure 2(c), finally, corresponds to the situation when the equilibrium configuration of the crystal is always a zigzag, which experiences a shallower potential when the central ion is excited. Here, the quench is also associated with a displacement of the equilibrium positions. Similar to case (b), the signal decays and exhibits revivals. The decay of the visibility in (b) and (c) arises from the entanglement of the spin excitation with the crystal degrees of freedom, and the revivals are a signature of quantum coherence that is stored in the whole system. Similar revivals have been experimentally observed for a single trapped ion [14]. They are here an intrinsic property of the many-body system and, as we will argue in the following, are a scalable feature that appears close to criticality.

The details of the model that determine the properties of the overlap integral, and thus of the visibility, are reported in the next Section. We note that in Eq. (2.4) we assumed that there is no mechanical effect associated with photon absorption and emission. This is the case
the internal transition is excited by means of a radiofrequency field\textsuperscript{15}, or by a Raman transition with copropagating beams\textsuperscript{16}. The mechanical effects can also included in our formalism, see for instance Ref.\textsuperscript{8}, but will not change substantially the results for the cases illustrated in Figs. 2(b) and (c). If the equilibrium structure is a linear chain independently of the internal state of the ion, as in Fig. 2(a), a momentum kick would induce an oscillation about the equilibrium positions that would modify the signal. We refer the reader to Ref.\textsuperscript{8}, where a similar situation was studied.

III. THEORETICAL MODEL

We now give the detailed form of the Hamiltonian $H$ that determines the evolution of the system. In the following we will restrict the motion of the crystal to the $x$-$y$ plane assuming a tight confinement in the $z$ direction, so that the motion along this axis can be considered frozen out. The coordinates $r = (x, y)$ give the position in the plane $z = 0$. This assumption is made for convenience: The calculations of this paper can be straightforwardly extended to three dimensions.

A. Hamiltonian

We first consider the internal degrees of freedom. We shall assume that only the central ion can be excited, while all other ions remain always in the ground state. The internal dynamics between the pulses can be restricted to the central ion, with Hamiltonian:

$$H_{el} = \hbar \omega_{eg}|e\rangle\langle e|,$$

where $\omega_{eg} = \omega_e - \omega_g$ is the transition frequency. The pulses are applied at time $t = 0$ and $t$ and correspond to a unitary operation given by the Pauli matrix $\sigma_x$.

The Hamiltonian for the external degrees of freedom of the ions, $H_{mot}$, depends on the internal state of the central ion. We denote by $r_i$ the position and by $p_i$ the canonically conjugate momentum of the ion labelled by $i$. The corresponding energy reads

$$H_{mot} = H_{kin} + V_{pot} + V_{Coul},$$

where $H_{kin} = \sum_{i=1}^{N} p_i^2/(2m)$ is the total kinetic energy,

$$V_{Coul} = \frac{1}{2} \sum_{i=1}^{N} \sum_{l \neq i}^{N} \frac{q^2}{4\pi\epsilon_0 |r_i - r_l|}$$

is the Coulomb repulsion, while the energy associated to the external potential takes the form

$$V_{pot} = \sum_{i=1}^{N} V_{\text{trap}}(r_i) + V_{\text{dip}}(r_i) |e\rangle\langle e|.$$

Here, the trap potential is

$$V_{\text{trap}}(r_i) = \frac{m}{2} \left( \nu_x^2 x_i^2 + \nu_y^2 y_i^2 \right)$$

with $\nu_x$, $\nu_y$ the trap frequencies along the axes $x$, $y$ respectively, and the spatial part of the spin-dependent potential reads

$$V_{\text{dip}}(r_{ic}) = \frac{m}{2} \nu_{\text{dip}}^2 y_{ic}^2,$$

where the subscript $i_c$ labels the central ion. We assume $\nu_{\text{dip}}$ is small compared to $\nu_y$. The total Hamiltonian which governs the dynamics between the laser pulses takes then the form

$$H = H_{el} + H_{kin} + V_{pot} + V_{Coul}.$$

In particular, the Hamiltonian $H_s = \langle s|H_{mot}|s\rangle$ determines the dynamics of the external degrees of freedom when the central ion is in the internal state $|s = g, e\rangle$. 

![Diagram](image-url)
B. Spin-dependent crystalline structures

We shall consider that the ions vibrate about their classical equilibrium positions, with displacements from equilibrium that are much smaller than the interparticle distance [17]. This situation can be achieved by laser cooling a hot cloud of ions confined in an electromagnetic trap, e.g. a Paul or Penning trap [18] [19]. The spin-dependent potential can be an optical potential, like a tightly focused laser beam propagating along and aligned with the chain axis, as discussed in [10]. Since this potential depends on the internal state, so does the crystal equilibrium structure. For a fixed number of ions the relevant parameters controlling the structure of the crystal are the aspect ratio \( \alpha = \nu_y^2/\nu_x^2 \) and the state-dependent shift to the aspect ratio \( \alpha_{\text{dip}} = \nu_{\text{dip}}^2/\nu_x^2 \), where we consider that the spin-dependent force steepens the potential for the central ion. When all ions are in the ground state and \( \alpha \) is larger than a critical value \( \alpha_c(N) \), the linear chain is stable, while at \( \alpha_c(N) \) it undergoes a continuous transition to a zigzag [20] [22]. We shall assume that \( \alpha \) is close to this critical value, so that the equilibrium structure depends on the internal state. To study quenches across the phase transition by exciting the central ion, an accurate knowledge of the dynamical properties of the crystalline structures in both configurations is necessary.

C. Spin-dependent normal modes

In the following we introduce the notation for the normal modes of the state-dependent ion crystal, using \( s = g, e \) to indicate the internal state of the central ion. We denote by \( r^s_i \) the equilibrium position of the \( i \)-th ion in the crystal for each internal state. A Taylor expansion of the potential \( V_{\text{pot}} + V_{\text{Coul}} \) is performed to second order for small displacements \( q^s \) around the equilibrium positions, \( q^s_i = r^s_i - r^s_1 \). For convenience we will use the notation \( q_{i,x} \leftrightarrow q_j \) with \( j = 1, \ldots, N \) and \( q_{j,y} \leftrightarrow q_j \) with \( j = N + 1, \ldots, 2N \). The following relation links the displacements between the crystal with the central ion in state \( g \) and \( e \):

\[
r_j = r^g_j + q^g_j = r^e_j + q^e_j.
\] (3.8)

The Hamiltonian of the crystal conditioned to whether the central ion is in state \( s = g, e \) takes the form

\[
H_{\text{eff}}^{(s)} \approx \sum_{j=1}^{2N} \frac{P_j^2}{2m} + \sum_{j,k} \frac{m}{2}\tilde{V}^s_{jk}q^g_j q^e_k,
\] (3.9)

where \( \tilde{V}^s_{jk} \) is defined as

\[
\tilde{V}^s_{jk} = \frac{\partial^2}{\partial r_j \partial r_k} (V^s_{\text{pot}} + V_{\text{Coul}}) \big|_{r^s_i}.
\] (3.10)

and \( V^s_{\text{pot}} = \langle s | V_{\text{pot}} | s \rangle \).

Hamiltonian [3.9] is transformed into a set of uncoupled oscillators by an orthogonal matrix \( M^s \) such that:

\[
\sum_{jk} M^s_{j,k} \tilde{V}^s_{jk} M^s_{k,n} = m (\omega_i^s)^2 \delta_{in},
\]

where \( \omega_i^s \) are the normal modes frequencies and the corresponding coordinates are related to the original displacements by the transformation \( Q^s_j = \sum_k M^s_{jk} q^s_k \), with \( l = 1, \ldots, 2N \). The second-quantized form of the Hamiltonian is found introducing annihilation (creation) operators \( b^s_j (b^{s \dagger}_j) \), with \( b^s_j = \sqrt{m \omega_j^s/(2h)} [Q^s_j + i P^s_j/(m \omega_j^s)] \) and \( [b^s_j, b^{s \dagger}_l] = \delta_{ji} \):

\[
H^{(s)}_{\text{eff}} = \sum_{s=g,e,j=1}^{2N} \sum_{s=g.e} |s\rangle \langle s| \hbar \omega_j^s \left( b^{s \dagger}_j b^s_j + \frac{1}{2} \right).
\] (3.11)

The eigenstates are the number states \( \{|n_1, \ldots, n_{2N} \rangle_s \} \) with \( b^{s \dagger}_j b^s_j |n_1, \ldots, n_{2N} \rangle_s = n_j |n_1, \ldots, n_{2N} \rangle_s \) and \( n_j = 0, 1, 2, \ldots \), which form a complete and orthonormal basis for fixed \( s \). The eigenstates of \( H_{\text{eff}}^{(g)} \) and \( H_{\text{eff}}^{(e)} \) are related by a transformation which is specified below and will be needed in order to study the dynamics of the system after the quench.

D. Mapping between the normal modes of the two crystalline structures

The transformation relating the normal modes \( Q_j^g \) and \( Q_j^e \) is found starting from Eq. (3.8) and rewriting it as

\[
q^g_j = q^e_j + d^g_j,
\] (3.12)

where \( d^g_j = r^e_j - r^g_j \) is the difference between the equilibrium values for the coordinate \( r_j \). Inserting the definition of the normal modes one finds

\[
Q_j^g = \sum_k T_{jk} Q_k^e + D_j^g,
\] (3.13a)

\[
P_j^g = \sum_k T_{jk} P_k^e,
\] (3.13b)

with \( T_{jk} = \sum_k M^g_{jk} M^e_{kl} \) an orthogonal matrix and \( D_j^g = \sum_k M^g_{jk} d^g_l \) the mode displacements. The transformation of the corresponding normal-mode annihilation and creation operators is given by a Bogoliubov transformation, obtained by inserting the definitions of the operators into relations (3.13), and which takes the form:

\[
b_j^g = \sum_k u_{jk} b_k^e - \sum_k v_{jk} b_k^{e \dagger} + \beta_j^g,
\] (3.14a)

\[
b_j^{g \dagger} = \sum_k u_{jk} b_k^e - \sum_k v_{jk} b_k^{e \dagger} + \beta_j^g.
\] (3.14b)
Here, the real dimensionless coefficients \( u_{jk}, v_{jk} \) read:

\[
\begin{align*}
\quad u_{jk} &= \frac{\mathbf{T}_{jk}}{2} \left[ \sqrt{\frac{\omega_k^2}{\omega_j^2}} + \sqrt{\frac{\omega_k^2}{\omega_j^2}} \right], \quad (3.15a) \\
\quad v_{jk} &= \frac{\mathbf{T}_{jk}}{2} \left[ \sqrt{\frac{\omega_k^2}{\omega_j^2}} - \sqrt{\frac{\omega_k^2}{\omega_j^2}} \right], \quad (3.15b)
\end{align*}
\]

and fulfill the equations [23]

\[
\begin{align*}
\sum_k (u_{jk} u_{lk} - v_{jk} v_{lk}) &= \delta_{jl}, \quad (3.16a) \\
\sum_k (u_{jk} v_{lk} - v_{jk} u_{lk}) &= 0 \quad \forall j, l. \quad (3.16b)
\end{align*}
\]

Coefficient \( \beta_j^g \) describes a displacement of the corresponding normal mode:

\[
\beta_j^g = \sqrt{\frac{m \omega_j^g}{2h}} D_j^g. \quad (3.17)
\]

After having obtained these relations we can now identify the transformation connecting the basis states \( \{|n_1, n_2, \ldots \rangle \} \) and \( \{|n_1, n_2, \ldots \rangle \} \). Since every state of the bases can be generated from the corresponding ground state by applying repeatedly the corresponding creation operators, it is sufficient to find a mapping between the ground states \( |0, 0, \ldots, 0 \rangle_e \equiv |0 \rangle_e \) and \( |0, 0, \ldots, 0 \rangle_g \equiv |0 \rangle_g \). Such mapping is given by a unitary transformation \( \mathbf{U} \) such that

\[
|0 \rangle_g = \mathbf{U} |0 \rangle_e. \quad (3.18)
\]

Operator \( \mathbf{U} \) connects two Gaussian states and can thus be written as:

\[
\mathbf{U} = \mathbf{D}(\gamma_1, \ldots, \gamma_{2N}) \mathbf{S}(\xi_{11}, \xi_{12}, \ldots, \xi_{2N, 2N}), \quad (3.19)
\]

where \( \mathbf{D} \) is a displacement operator and \( \gamma_j \) are real scalars, while \( \mathbf{S} \) is a squeezing operator that takes the form

\[
\mathbf{S} = \exp \left( \frac{1}{2} \sum_{jk} \xi_{jk} b_j^\dagger b_k^\dagger - \xi_{jk}^* b_j^\dagger b_k^\dagger \right), \quad (3.20)
\]

with squeezing parameters \( \xi_{jk} \) to be determined. With the help of the disentangling theorem, Eq. (3.20) can be recast into the convenient form

\[
\mathbf{S} = Z e^{\mathbf{A} b^\dagger} e^{-\mathbf{A}^\dagger}, \quad (3.21)
\]

where \( Z \) is a scalar while

\[
\begin{align*}
\quad \mathbf{A} &= \frac{1}{2} \sum_{jk} A_{jk} b_j^\dagger b_k^\dagger, \quad (3.22a) \\
\quad \mathbf{B} &= -\sum_{jk} B_{jk} b_j^\dagger b_k^\dagger, \quad (3.22b)
\end{align*}
\]

are operators, with \( A_{jk} \) a symmetric matrix. Details of the derivation are provided in Appendix A. Application of operator (3.21) to the state \( |0 \rangle_e \) gives

\[
|0 \rangle_g = \mathbf{W} |0 \rangle_e, \quad (3.23)
\]

with the non-unitary operator \( \mathbf{W} \) defined as:

\[
\mathbf{W} = \mathbf{Z} \mathbf{D}(\gamma_1, \ldots, \gamma_{2N}) e^\mathbf{A}. \quad (3.24)
\]

We note that this operator was first introduced in [24] for evaluating the thermodynamics of interacting condensates.

We now determine the coefficients \( A_{jk} \), the displacements \( \gamma_j \) and the normalization constant \( Z \). For this purpose we make use of relation \( b_j^g |0 \rangle_g = 0 \) which must hold for any mode \( j \) of \( H_{ef}^{(g)} \). Using Eqs. (3.14a) and (3.23), one obtains:

\[
0 = b_j^g |0 \rangle_g = \left[ \sum_k (u_{jk} b_k^g - v_{jk} b_k^g), + \beta_j^g \right] \mathbf{W} |0 \rangle_e, \quad (3.25)
\]

which can be recast in the form

\[
\mathbf{W} \left[ \sum_k u_{jk} \left( \sum_l A_{kl} b_l^g, - \sum_k v_{jk} b_k^g \right) \right] + \left[ \sum_k (u_{jk} - v_{jk}) \gamma_k + \beta_j^g \right] |0 \rangle_e = 0 \quad (3.26)
\]

The latter equation has been derived from (3.25) multiplying by \( \mathbf{I} = \mathbf{W} \mathbf{W}^{-1} \) on the left side and making use of the relations

\[
\mathbf{W}^{-1} b_k^g \mathbf{W} = b_k^g + \sum_l A_{kl} b_l^g + \gamma_k, \quad (3.27a) \\
\mathbf{W}^{-1} b_k^g \mathbf{W} = b_k^g + \gamma_k. \quad (3.27b)
\]

Equation (3.26) is equivalent to:

\[
\begin{align*}
\sum_k u_{jk} A_{kl} - v_{jl} &= 0 \quad (3.28) \\
\sum_k (u_{jk} - v_{jk}) \gamma_k + \beta_j^g &= 0. \quad (3.29)
\end{align*}
\]

which must hold for all \( j, l = 1, \ldots, 2N \). From Eq. (3.28) one finds the coefficients

\[
A_{jk} = \sum_l (u^{-1})_{jl} v_{lk}, \quad (3.30)
\]

where one sees that \( A \) is real, with symmetry following from (3.16b), while from Eq. (3.29) one obtains

\[
\gamma_j = -\sum_k (u_{kj} + v_{kj}) \beta_j^g = : \beta_j^g, \quad (3.31)
\]

where \( \beta_j^g \) has been defined. Finally, the constant \( Z \) is found from the condition that the norm of the ground
Using Eq. (3.34), expression (3.37) can be cast in the form 
\[ \langle \beta^e \rangle = \frac{1}{2} \sum_j A_{jk} (b_j^e - b_j^e)^* (b_j^e - b_j^e)^* \]  
which leads to: 
\[ Z = \det \left[ (1 - A^2)^{1/4} \right] \]  
(details are given in Appendix B). 
Using this result, we find: 
\[ |0\rangle_g = Z D_e(\beta^e) e^A |0\rangle_e \]  
(3.34) 
with \( A_{jk}, \beta_j^e \), and \( Z \) given in Eqs. (3.30), (3.31) and (3.33), respectively. Using this formalism we can now evaluate the visibility (which we defer for Sec. III E) as well as the overlap between the two ground states: 
\[ \langle \phi_e | 0 \rangle | \beta \rangle = Z \langle \beta | D(\beta^e) e^A |0\rangle_e \]  
(3.35) 
Before we conclude this section, we also give the form of the squeezing parameters \( \xi_{jk} \) in operator \( \mathcal{S} \) (3.21): 
\[ \xi_{jk} = \sum_l A_{jl} \arctanh(\alpha_l) \Lambda_{lk} \]  
where \( \Lambda_{lk} \) is the orthogonal transformation diagonalizing \( A \) and \( \alpha_l \) are the corresponding eigenvalues. The parameters \( \xi_{jk} \) are real, since \( A_{jk} \) is real and symmetric. The derivation of Eq. (3.36) can be found in Appendix A. 

E. Evaluation of the visibility

We now derive an analytical expression for the visibility. Our starting point is the overlap as a function of the time \( t \) between the pulses, as given in Eq. (2.4). Using \( |\phi\rangle_s = \exp \{ H_{\text{eff}}(s) / \hbar \} |0\rangle_g = U_s(t) |0\rangle_g \), we rewrite it as 
\[ \mathcal{O}(t) = g |0\rangle_g U_g(t) U_e(t) |0\rangle_g = g |0\rangle_e U_e(t) |0\rangle_g \]  
(3.37) 
We note that this expression is given up to a time-dependent phase, which depends on the difference between the (classical) ground-state energies of the two equilibrium configurations [9]. Since this factor is irrelevant for the visibility, it will be omitted from now on. Using Eq. (3.34), expression (3.37) can be cast in the form: 
\[ \mathcal{O}(t) = Z^2 e(0) e^{A^t} D_e(\beta^e) U_e(t) D_e(\beta^e) e^A |0\rangle_e \]  
(3.38) 
where \( D_e(\beta^e) = D_e(\beta^e) |0\rangle_e \) and from the first to the second line we employed the relation 
\[ D_e(\beta^e) e^A = e^{\tilde{A}(\beta^e)} D_e(\beta^e) \]  
(3.39) 
with 
\[ \tilde{A}(\beta) = \frac{1}{2} \sum_{jk} A_{jk} (b_j^e - b_j^e) (b_j^e - b_j^e)^* \]  
(3.40) 
Using the overcompleteness of the multimode coherent states, Eq. (3.38) takes the form 
\[ \mathcal{O}(t) = \frac{Z^2}{\pi^{2N}} \int d^2 \alpha_1 \ldots d^2 \alpha_N \]  
\[ e^{\langle \beta^e \rangle e^{\tilde{A}(\beta^e)} U_e(t) |\alpha\rangle_e \langle \alpha| e^{\tilde{A}(\beta^e)} |\beta^e\rangle} \]  
\[ = \frac{Z^2}{\pi^{2N}} \int d^2 \alpha_1 \ldots d^2 \alpha_N \]  
\[ e^{\langle f(\alpha(t) - \beta^e) | f(\alpha(t) - \beta^e) \rangle} C_{\beta^e, \alpha(t)} C_{\alpha, \beta} \]  
(3.41) 
Here, we have defined 
\[ C_{\alpha, \beta} = e^{\langle \alpha | \beta \rangle} = e^{-\sum_j (|\alpha_j|^2 + |\beta_j|^2 - \alpha_j^* \beta_j)} \]  
(3.42) 
and used 
\[ e^{\langle \beta^e | e^{\tilde{A}(\beta^e)} | \alpha(t) \rangle} = e^{\langle f(\beta(t) - \beta^e) \rangle} e^{\langle \beta^e | \alpha(t) \rangle} \]  
(3.43) 
where \( |\alpha_j(t)\rangle = |\alpha_j \exp \{-i \omega_j t\} \rangle \) is the time-evolved coherent state and \( f(\alpha) = \frac{1}{2} \sum_{jk} A_{jk} \alpha_j^* \alpha_k \) a \( 2N \)-dimensional complex-valued function. The evaluation of Eq. (3.41) is just a matter of algebra and is shown in Appendix C. The result reads 
\[ \mathcal{O}(t) = e^{\frac{i}{2} w^T \Omega^{-1} w} \frac{\mathcal{G}_0}{\sqrt{|\det \Omega|}} \]  
(3.44) 
where the complex symmetric \( 4N \times 4N \) matrix \( \Omega \) and the \( 4N \)-dimensional vector \( w \) are defined as 
\[ \Omega = \begin{pmatrix} 1 - \Lambda^+ & -i \Lambda^- \\ -i \Lambda^+ & 1 + \Lambda^+ \end{pmatrix}, \quad w = \left( S^+ \right. \left. S^- \right) \]  
(3.45) 
Here, 
\[ \Lambda_{jk}^\pm = \frac{1}{2} A_{jk} \left[ e^{-i (\omega_j^e + \omega_k^e) t} \pm 1 \right] \]  
(3.46a) 
\[ S_j^\pm = S_j(\beta^e) \pm S_j(\beta^e) e^{-i \omega_j^e t} \]  
(3.46b) 
and 
\[ S_j(\beta) = \sum_k A_{jk} \beta_k - \beta_j^e \]  
(3.47) 
Equation (3.44) determines the visibility, that is plotted in Sec. IV for several parameter regimes in which this formula is valid. 

The short-time behaviour of the visibility is found by performing a Taylor expansion of (3.37), and reads: 
\[ V(t) \approx 1 + \eta t^2 / 2. \]  
(3.48)
Quantity $\eta < 0$, denoted in Sec. IV as the curvature, is determined by the variance of $H^{(e)}_{\text{eff}}$ in the initial state:

$$\eta = -\frac{1}{\hbar^2} \left[ g \langle 0 | H^{(e)}_{\text{eff}} | 0 \rangle_g - \langle g | H^{(e)}_{\text{eff}} | 0 \rangle_g \right]^2 .$$

(3.49)

The functional dependence of $\eta$ on the parameters in Eq. (3.44) is derived and given in Appendix C.

IV. QUANTUM QUENCHES AT THE LINEAR-ZIGZAG TRANSITION

We shall now examine the visibility of the interferometric signal when the chain is close to the linear-zigzag instability. We assume that a quench is performed by exciting the central ion in presence of a spin-dependent force. Due to the long-range interaction, the force on the central ion can induce a change of the equilibrium configuration of the entire crystal. In particular, if $\nu_c^2 < \nu_c^2 < \nu_c^2 + \nu_{\text{dip}}^2$, the two equilibrium configurations corresponding to the different internal states can be a zigzag and a linear chain, respectively, provided that the correlation length is larger than the size of the system $[9, 25]$. The equilibrium configurations corresponding to the central ion excitation are represented in the diagram of Fig. 3. Here, the horizontal axis gives the dimensionless parameter $g$, which is defined as

$$g = \frac{\nu_c^2 - \nu_c^2}{\nu_c^2} .$$

This parameter determines whether the equilibrium configuration corresponding to the central ion in state $|g\rangle$ is a linear ($g > 0$) or a zigzag chain ($g < 0$). The vertical axis gives the dimensionless parameter $\Delta$, defined as

$$\Delta = \frac{\nu_{\text{dip}}^2}{\nu_c^2} ,$$

and related with the change in the potential on the central ion when it is in state $|e\rangle$. The equilibrium configuration when the ion is in state $|e\rangle$ is shown in the diagram as a function of $g$ and $\Delta$. We restrict to the case $\Delta > 0$, consistently with the choice that the spin-dependent force is restoring. The ion in the excited state feels thus a change of the transverse potential corresponding to a vertical shift in the diagram as sketched by the green arrow.

Three situations will be discussed in the regime close to the linear-zigzag instability, indicated by the solid line of Fig. 3. The first one corresponds to the case in which the crystal is initially forming a linear chain ($g > 0$). The spin excitation then does not change the equilibrium configuration, nevertheless it modifies the frequencies of the normal modes. An example of the visibility one measures in this case is displayed in Fig. 2(a). When $g < 0$, the equilibrium configuration of the initial state is a zigzag. Whether the equilibrium configuration of the excited state is a zigzag or a linear, depends here on whether the shift $\Delta$ is below or above the instability line. For a fixed $\Delta$, this defines a critical value $g_c(\Delta)$, hence, the crystal equilibrium configuration for the excited state is exactly on the instability line (note that $g_c$ depends on the number of ions $N$). If $g > g_c(\Delta)$, the crystal equilibrium configuration in the excited state is also a zigzag (with however different transverse displacement as the initial one). An example for the visibility found in this case is shown in 2(c).

If $0 > g > g_c(\Delta)$, instead, the crystalline structures of ground and excited states are a zigzag and a linear chain, respectively. The quench hence drives the chain across the critical point, and a typical visibility signal is shown in Fig. 2(b).

The behaviour of the visibility for short times is characterized by a decay with quadratic dependence on the elapsed time, according to Eq. (3.48). Figure 4(a) displays the parameter $\eta$ as a function of $g$ and $\Delta$. Decay is faster in the region where the quench is performed across the phase transition, where the overlap between initial and final states is small. The plot is reminiscent of the features of the stability diagram in Fig. 3 as is visible by inspecting the contour plot in Fig. 4(b).

We now analyse the behaviour for long times. Figure 5 displays the density plot of the visibility as a function of the rescaled aspect ratio $g$ and of the time $t$ between the pulses. Three distinct behaviours are observed corresponding to the three regimes we identified. For $g < g_c$ the appearance of the revivals is periodic. The corresponding period diverges as $g$ approaches $g_c$. Each curve indicating a maximum of the visibility, moreover, ex-
hbits an additional modulation, showing that the height of the revival peaks varies with \( g \). The inset shows the behaviour at \( g = g_c \): Here, several peaks of the visibility appear at short elapsed times, with rapidly vanishing height. In the interval \( g_c < g < 0 \) the periodic structure of the revivals is also observed, with decreasing period as \( g \) approaches 0. Finally, for \( g > 0 \) the visibility is close to unity and exhibits some modulation for small positive \( g \), with an amplitude that vanishes as \( g \) increases.

Let us now make some considerations. In the first place, the value of \( g_c \) depends on \( \Delta \). Nevertheless, the behaviour found in Fig. 5 is encountered for different values of \( \Delta \), as is visible in Fig. 6, where we show the revival times at which the visibility is different from zero. This behaviour is also to large extent independent of the number of ions composing the crystal, as is indicated by Fig. 6. Here, one observes that all curves giving the first revival time for different numbers of ions exhibit a similar functional dependence as \( g \) approaches \( g_c \) (which depends also on the number of ions \( N \)). This behaviour becomes evident by appropriately rescaling the curves as shown in the inset. The width of the peak at \( g_c \) in turn decreases as the number of ions is increased.

Further information is gained by inspecting the Fourier transform of the visibility and of its logarithm, respectively defined as

\[
\mathcal{F}(\omega_n) = \frac{1}{T} \int_{0}^{T} dt \ V(t) \ e^{-i\omega_n t},
\]

\[
\mathcal{F}_L(\omega_n) = \frac{1}{T} \int_{0}^{T} dt \ \ln |V(t)| \ e^{-i\omega_n t},
\]

where \( \omega_n = 2\pi n/T \) with \( n \in \mathbb{N}_0 \) and \( T \) is a time interval such that \( T\nu_{\text{min}} > 1 \), with \( \nu_{\text{min}} \) the smallest gap in Hamiltonian \( H^{(c)} \). Figure 7 displays the spectra corresponding to the visibility as a function of time in Fig. 2 and its logarithm. For \( g > 0 \), shown in (a), the main peak is located at twice the eigenfrequency of the zigzag mode, while for \( g < 0 \) it is at the eigenfrequency of the corresponding lowest frequency mode, see (b) and (c), which becomes unstable when the critical value is approached. The behaviour for \( g > 0 \) hints to the presence of squeezing, originated by quenching the trap frequency.
that some entanglement between the modes is generated due to the quenching, suggesting multimode squeezing. They hint at the presence of single-mode and the zigzag mode frequency with the axial breathing mode. In (b) and (c) minor peaks are present at the eigenfrequencies which couple to the zigzag mode and in (b) also at sums of eigenfrequencies.

![Density plot of the logarithmic spectrum](image)

**FIG. 8.** Color online) Density plot of the logarithmic spectrum \( \mathcal{F}_L(\omega) \) of the visibility, \( \mathcal{F}_L(\omega) \) in Eq. (4.2), corresponding to the plots in Fig. 2. The vertical dashed red lines indicates the normal-mode frequencies of the crystal when the central ion is excited, the dashed green lines give the doubled frequencies. The magenta dash-dotted lines show sums of frequencies. The insets show the corresponding spectrum of the visibility, \( \mathcal{F}(\omega, \Delta) \) in Eq. (4.1). The parameter \( g \) is, from left to right, 0.02, −0.005, and −0.1, while the critical value is \( g_c = −0.0165 \), and \( \Delta = 0.025 \).

The spectrum of the logarithmic signal as a function of \( g \) is displayed in Fig. 8 for \( g < 0 \) and \( \Delta \) constant. One observes a main peak corresponding to the mode whose frequency goes to zero when \( g \) approaches \( g_c \), and the crystal in the excited state becomes unstable. Close to \( g_c \) one observes two signals which become more visible, that are at twice the zigzag eigenfrequency and at the sum of the zigzag mode frequency with the axial breathing mode frequency. They hint at the presence of single-mode and multimode squeezing due to the quenching, suggesting that some entanglement between the modes is generated by the quench.

We now summarize our findings. In the first place, the visibility decays fast to zero when the quench is performed between motional states whose classical equilibrium configurations differ. The decay is faster when the two structures have different symmetries, and thus different spectral properties, such as when the quench is across the phase transition linear-zigzag. Nevertheless, the visibility exhibits revivals as a function of the time after the quench. These revivals occur at the frequency of the lowest normal mode of the zigzag structure, which becomes unstable at the instability and corresponds to the zigzag mode of the linear chain. This mode is in fact the one which has the largest overlap with the difference between zigzag and linear structures. This feature of the visibility is scalable, the periodicity of the revival remains in fact finite as the size of the chain is increased. The height of the peaks, however, decays as \( N \) is scaled up, consistently with the fact that the amplitude of excitation of the zigzag mode by a displacement of the central ion decreases as the size of the chain is increased. In the thermodynamic limit, hence, the surviving feature is the decay of the visibility signal at short times, corresponding to the fact that the quantum superposition of the spin irreversibly dephases. When instead the quench is between two linear chains, there is a quasiperiodic rephasing of the system, corresponding to the creation of squeezing by sudden changing the trap frequency and thus the normal mode frequencies. The amplitude of the oscillations decays to zero while the visibility reaches a constant value which approaches unity as \( g \) is increased.

**V. CONCLUSIONS**

The dynamical properties of an ion crystal after a quench have been theoretically investigated, when the quench is performed by creating coherent superpositions of motional states close to and across the linear-zigzag structural transition. These dynamics have been related to the visibility of the signal when Ramsey interferometry is performed on one ion of the chain. The visibil-
ity decays at short times as the internal state becomes entangled with the motional state of the crystal, but exhibits periodic revivals at longer times, determined by the frequency of the zigzag mode. Further periodic signals appear at multiples of the zigzag mode and at sums of different motional excitations, suggesting squeezing and entanglement in the vibrational motion generated by the quench of the trap frequency. These spectral properties persist as the number of ions increases, even though the heights of the revivals decrease. These results are based on a theoretical model which we report in detail and which allows one to calculate the visibility for different parameter regimes. This model is valid as long as the harmonic theory of the crystal is applicable and is thus reliable for the parameters we consider in this paper.

Our analysis shows that, if the crystal is initially in the motional ground state, these features can be observed for parameters that are consistent with ongoing experimental work (a discussion can be found for instance in [1]). We remark that ground state cooling of ion chains composed to up to 4 ions have been successfully demonstrated in [27]. We conclude by observing that the visibility signal allows one to study the behaviour of the soft mode across the classical phase transition. Extensions of these studies to the parameter regime where quantum effects at the phase transition are relevant [28, 29] would allow one to extract the corresponding quantum fidelity, in the spirit of the work performed in [30], and will be subject of future studies.

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Appendix A: Multimode Squeezing Operator and disentanglement theorem

In order to obtain Eq. (3.21) from Eq. (3.20) we follow the method of Bogoliubov and Shirkov [31]. The basic idea is best understood by first considering operator $e^{\lambda (\sigma_+ + \sigma_-)}$, with $\lambda$ scalar, $\sigma_+$ the Pauli matrix and $\sigma_\pm$ the raising and lowering operators for a spin 1/2, such that $[\sigma_+, \sigma_-] = \sigma_z, [\sigma_-, \sigma_\pm] = \pm \sigma_\pm$. The disentangling formula reads:

$$e^{\lambda (\sigma_+ + \sigma_-)} = e^{\sigma_+ \tanh(\lambda)} e^{-\sigma_- \ln[\cosh(\lambda)]} e^{\sigma_- \tanh(\lambda)},$$

(A1)

and can be obtained using the procedure sketched in Ref. [32]. Assuming $\lambda$ to be a continuous parameter, one makes the ansatz $e^{\lambda (\sigma_+ + \sigma_-)} = e^{F(\lambda) \sigma_+} F(\lambda) e^{g(\lambda) \sigma_-}$ with $F(\lambda)$ an operator such that $F(0) = 1$, while $f(\lambda)$ and $g(\lambda)$ are analytic functions of $\lambda$ with $f(0) = 0$ and $g(0) = 0$. Under these assumptions $F(\lambda)$ can be written as

$$F(\lambda) = e^{-f(\lambda)\sigma_+} e^{\lambda (\sigma_+ + \sigma_-)} e^{-g(\lambda)\sigma_-}.$$  

(A2)

We take the derivative of $F(\lambda)$ and obtain a first-order differential equation which contains all operators.

The contributions from $\sigma_+$ and $\sigma_-$ cancel out by choosing $f(\lambda) = g(\lambda) = \tanh(\lambda)$, so that $F(\lambda) = \exp[-\sigma_+ \ln(\cosh\lambda)]$, hence demonstrating Eq. (A1).

This procedure can be generalized to show the equality

$$e^{\frac{1}{2}(a^2 - a^2)} = e^{\tanh(\lambda) a^2} - (a^+ a + \frac{1}{2}) \ln[\cosh\lambda] e^{-\tanh(\lambda) a^2},$$

(A3)

where $a, a^\dagger$ are the annihilation and creation operators of a harmonic oscillator.

Moreover, we can use the procedure sketched above in order to disentangle the multimode squeezing operator:

$$\exp\left\{\frac{1}{2} \sum_{j,k} (\xi_{jk} a_j^\dagger a_k^\dagger - \xi_{jk}^* a_j a_k)\right\}$$

$$= Z e^{\frac{1}{2} \sum_j A_{jk} a_j a_j^\dagger} e^{-\sum_{j,k} B_{jk} a_j^\dagger a_k} e^{-\frac{1}{2} \sum_{j,k} C_{jk} a_j a_k},$$

(A4)

with

$$A_{jk} = \frac{\tanh(\lambda_j) \lambda_j \lambda_k}{\sum_j \tanh(\lambda_j) \lambda_j \lambda_k},$$

(A5)

$$B_{jk} = \frac{\ln[\cosh(\lambda_j)] \lambda_j^* \lambda_k}{\sum_j \ln[\cosh(\lambda_j)] \lambda_j^* \lambda_k},$$

(A6)

$$C_{jk} = \frac{\tanh(\lambda_j) \lambda_j^* \lambda_k}{\sum_j \tanh(\lambda_j) \lambda_j^* \lambda_k} = A_{jk}^*,$$

(A7)

$$Z = \exp\left\{-\sum_j \frac{1}{2} \ln[\cosh(\lambda_j)]\right\}.$$  

(A8)

This can be done after observing that, since $\xi$ is complex symmetric, we can perform Takagi’s factorization $\xi = \Lambda \Lambda^T$, where $\Lambda$ is unitary and $\chi = \text{diag}\{\chi_1, \chi_2, \ldots\}$ is diagonal with $\chi_j \geq 0$ real and non-negative (this factorization exists for any complex symmetric matrix). This defines the transformation $b_j^\dagger = \sum_k \Lambda_{kj} a_k^\dagger, b_j = \sum_k \Lambda_{kj}^* a_k$ for a new set of operators for which the squeezing operator is in diagonal form, $\exp\left\{\frac{1}{2} \sum_j \chi_j (b_j^2 - b_j^2)\right\}$. These new operators have bosonic commutation relations, $[b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0$, and $[b_j^\dagger, b_k] = \sum_k \Lambda_{kj} \Lambda_{jk}^*$ since $\Lambda$ is unitary. Therefore, operators of different modes factorize as $\prod_j \exp\left\{\frac{1}{2} \chi_j (b_j^2 - b_j^2)\right\}$, and one finally obtains

$$\exp\left\{\frac{1}{2} \sum_{j,k} (\xi_{jk} a_j^\dagger a_k^\dagger - \xi_{jk}^* a_j a_k)\right\}$$

$$= \prod_j e^{\tanh(\chi_j) b_j^2} e^{-\ln[\cosh(\chi_j)] e^{-\tanh(\chi_j) b_j^2}}.$$  

(A9)
The terms belonging to different modes commute now, so bringing factors with operators $b_j^{(m)}$ to the left and factors with $b_j^{(b)}$ to the right and writing them as a function of operators $a_k$ and $a_k^\dagger$, one obtains Eq. \ref{A4}.

**Appendix B: Calculation of the Normalization Constant**

In order to calculate the constant $Z$ we use the normalization condition of the states as stated in Eq. (3.32),

$$1 = Z^2 \langle 0 \left| \left( \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A^{(n)} A^{(m)} \right) |0\rangle .$$

Since $A$ contains only creation operators, only the summands with $m = n$ give a contribution:

$$Z^{-2} = \langle 0 \left| \left( \sum_{n=0}^{\infty} A^{(n)} A^{(n)} \right) |0\rangle = \sum_{n=0}^{\infty} W_n ,$$

where $W_n$ is defined as

$$W_n = \frac{1}{(2^n n!)^2} \sum_{j_1 \cdots j_{2n}} A_{j_1 j_2} \cdots A_{j_{2n-1} j_{2n}} A_{k_1 k_2} \cdots$$

$$\cdots A_{k_{2n-1} k_{2n}} |0\rangle b_{j_1} b_{j_2} b_{k_1}^\dagger \cdots b_{k_{2n}}^\dagger |0\rangle . \quad (B2)$$

The sum contains $(2n)!$ summands (which contain $2n$ Kronecker-delta symbols) which do not vanish, corresponding to the number of all pairs of sets of indices \{$j_1 \cdots j_{2n}$\} and \{$k_1 \cdots k_{2n}$\} which are identical (apart for a permutation within the same set). For example,

$$W_1 = \frac{1}{2^2} \sum_{j_1 j_2 k_1 k_2} A_{j_1 j_2} A_{k_1 k_2} \left\{ \delta_{j_1 k_1} \delta_{j_2 k_2} + \delta_{j_1 k_2} \delta_{j_2 k_1} \right\} .$$

while $W_2$ has already 24 summands, we write only two of them exemplarily:

$$\sum_{j_1 j_2 j_3 j_4} A_{j_1 j_2} A_{j_3 j_4} A_{k_1 k_2} A_{k_3 k_4} \cdot \delta_{j_1 k_1} \delta_{j_2 k_2} \delta_{j_3 k_3} \delta_{j_4 k_4} ,$$

$$\sum_{j_1 j_2 j_3 j_4} A_{j_1 j_2} A_{j_3 j_4} A_{k_1 k_2} A_{k_3 k_4} \cdot \delta_{j_1 k_1} \delta_{j_2 k_2} \delta_{j_3 k_3} \delta_{j_4 k_4} \quad (B3)$$

We now associate with each summand in $W_n$ a graph, which we call a $n$-graph. For this, let the first $n$ coefficients be represented by $n$ pairs of adjacent circles in an upper row, while the second $n$ coefficients are represented by the same number of pairs of circles in the lower row. The indices \{$j_1 \cdots j_{2n}$\} and \{$k_1 \cdots k_{2n}$\} are filled in in correct ordering into the circles such that there are only $j$’s in the upper and only $k$’s in the lower row.

Then for each Kronecker-$\delta$ we need to connect the corresponding two circles by a line. We find easily that each circle must be connected with another, and that there is a total of $2n$ lines. Thus each circle has exactly one line. For instance, the graphs for \[B3\] and \[B4\] are given by:

\[
\begin{bmatrix}
1 & 2 & 3 & 4 \\
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
1 & 2 & 3 & 4 \\
2 & 3 & 4 \\
\end{bmatrix}
\]

respectively. If we evaluate \[B3\], we find that it yields $\text{Tr}(A^4)$, while \[B4\] can be factorized into two terms

$$\sum_{j_1 j_2} A_{j_1 j_2} A_{k_1 k_2} \delta_{j_1 k_1} \delta_{j_2 k_2} \cdot \sum_{j_3 j_4} A_{j_3 j_4} A_{k_3 k_4} \delta_{j_3 k_3} \delta_{j_4 k_4} ,$$

which give $[\text{Tr}(A^2)]^2$. This factorization can also be shown graphically,

\[
\begin{bmatrix}
1 & 2 & 3 & 4 \\
1 & 2 & 3 & 4 \\
\end{bmatrix}
\equiv
\begin{bmatrix}
1 & 2 \\
3 & 4 \\
\end{bmatrix}
\cdot
\begin{bmatrix}
1 & 2 \\
3 & 4 \\
\end{bmatrix}
\]

Thus, a graph may be decomposed into a product of fully connected subgraphs or clusters. An $n$-graph can be decomposed into a product of $m_1$ 1-clusters, $m_2$ 2-clusters, $\ldots$, and $m_n$ $n$-clusters, where the $m_l$ fulfill

$$\sum_{l=1}^{n} m_l l = n . \quad (B5)$$

The evaluation of an $l$-cluster always yields $\text{Tr}(A^{2l})$, and there are $2^l l! 2^{l-1}(l-1)!$ ways to draw an $l$-cluster. So we are motivated to define the $l$-cluster integral by the sum of all possible clusters for $l$ pairs of circles in each row, which after evaluation is given by:

$$b_l = 2^l l! 2^{l-1}(l-1)! \text{Tr}(A^{2l}) . \quad (B6)$$

We have $b_0 = 1$ and $b_1 = 2 \text{Tr}(A^2)$, which finds its graphical representation by

\[
\begin{bmatrix}
\begin{array}{c}
\text{ } \text{ } \text{ } \text{ } + \\
\text{ } \text{ } \text{ } \text{ } \\
\end{array}
\end{bmatrix}
\]
 Accordingly one can draw the cluster-integrals for the higher orders. Here we have not filled out the circles, since the cluster integral is independent of the indices which are assigned to it. It is clear that for a given set of indices \( \{i_1, i_2, \ldots \} \) the circles have to be filled in the same ordering in each summand, and without loss of generality one can fill the circles in the natural ordering \((j_1, j_2, \ldots)\) and \((k_1, k_2, \ldots)\) where \(i_1 < i_2 < \cdots\). The total set of indices cannot be split arbitrarily in between the clusters, since pairs of indices of the form \((j_{2l-1}, j_{2l})\) always belong to the same cluster.

To resume the calculation, we note that

\[
W_n = \frac{1}{(2n!)^2} \sum_{\{m_i\}} \mathcal{S}\{m_i\}, \quad (B7)
\]

where \(\mathcal{S}\{m_i\}\) is the sum over all possible graphs described by the set of integers \(\{m_i\}\), and the primed sum denotes a restricted summation over all sets \(\{m_i\}\) which fulfill equation \(B5\). We see that

\[
\mathcal{S}\{m_i\} = \sum_{\mathcal{P}} b_1^{m_1} b_2^{m_2} \cdots, \quad (B8)
\]

where the summation over \(\mathcal{P}\) extends over all possible ways of distributing the two times \(n\) pairs of indices \(\{(j_1; j_2), \ldots, (j_{2n-1}; j_{2n})\}\) and \(\{(k_1; k_2), \ldots, (k_{2n-1}; k_{2n})\}\) into the circles obtaining only distinct graphs. Since there are \(n!\) ways of distributing these pairs (the ordering of a pair is already contained inside the cluster integral). A permutation of two \(l\)-clusters with the same \(l\) does not give a new graph, therefore we get a factor \(\prod_i (m_i!)^{-1}\). Moreover, a permutation of pairs inside a cluster integral does not give a new graph either. Thus we get a factor \(\prod_i (l!)^{-2 m_i}\).

Equation \(B8\) is then given by

\[
\mathcal{S}\{m_i\} = (n!)^2 \prod_{i=1}^n \frac{b_i^{m_i}}{m_i! (l!)^{2 m_i}}, \quad (B9)
\]

Replacing in \(B7\) one gets:

\[
W_n = \frac{1}{(2n!)^2} \sum_{\{m_i\}} (n!)^2 \prod_{i=1}^n \frac{b_i^{m_i}}{m_i! (l!)^{2 m_i}}
\]

\[
= \frac{1}{2^{2n}} \sum_{\{m_i\}} \prod_{i=1}^n \frac{1}{m_i!} \left( \frac{b_i}{(l!)^2} \right)^{m_i}
\]

\[
= \sum_{\{m_i\}} \prod_{i=1}^n \frac{1}{m_i!} \left( \frac{b_i}{(2l!)^2} \right)^{m_i}
\]

\[
= \sum_{\{m_i\}} \prod_{i=1}^n \frac{1}{m_i!} \left( \frac{b_i}{(2l!)^2} \right)^{m_i}, \quad (B10)
\]

We can now insert this result in Eq. \(B1\) and obtain:

\[
Z^{-2} = \sum_{n=0}^{\infty} \sum_{\{m_i\}} \prod_{i=1}^n \frac{1}{m_i!} \left( \frac{b_i}{(2l!)^2} \right)^{m_i}. \quad (B11)
\]

Summing over all \(\{m_i\}\) followed by summation over all \(n\) is equivalent to summing over all \(m_1, m_2, \ldots\) from 0 to \(\infty\) separately, so we can replace the restricted sum:

\[
Z^{-2} = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \prod_{i=1}^n \frac{1}{m_i!} \left( \frac{b_i}{(2l!)^2} \right)^{m_i}
\]

\[
= \prod_{i=1}^n \left[ \sum_{m_i=0}^{\infty} \frac{1}{m_i!} \left( \frac{b_i}{(2l!)^2} \right)^{m_i} \right]
\]

\[
= \prod_{i=1}^n \exp \left[ \frac{b_i}{(2l!)^2} \right] = \exp \left[ \sum_{i=1}^n \frac{b_i}{(2l!)^2} \right]. \quad (B12)
\]

Using equation \(B6\), we finally get

\[
Z^{-2} = \exp \left[ \sum_{l=1}^{\infty} \frac{\text{Tr}(A^2)}{2l} \right] = \exp \left( \frac{1}{2} \text{Tr} \left[ \ln \frac{1}{1-A^2} \right] \right), \quad (B13)
\]

which is valid if \(1 - A^2\) is non-singular. To show that this is true it is sufficient to show that any matrix norm of \(\text{A}\) is smaller than one. Using the spectral norm \(\|\cdot\|\), the form of Eq. \(A7\), and the submultiplicativity of the matrix norm, we have \(\|A\|_2 \leq \|A\|_2 \|\text{tanh} \chi\|_2 \|\text{tanh} \chi\|_2 = \|\text{tanh} \chi\|_2\). Using the fact that \(\chi\) is diagonal, real and positive, the spectral norm is equal to tangent hyperbolicus of the largest eigenvalue of \(\chi\). Thus \(\|\text{A}\|_2 < 1\) as the tangent hyperbolicus is smaller than 1 in its full domain.

Equation \(B13\) can thus be cast in the compact form:

\[
Z = \exp \left( -\frac{1}{4} \text{Tr} \left[ \ln \frac{1}{1-A^2} \right] \right) = \text{det} \left[ (1-A^2)^{\frac{1}{2}} \right]. \quad (B14)
\]

**Appendix C: Calculation of the Overlap Integral**

We consider the integral \((3.41)\) and first remove the time-dependent phase factors \(e^{-i\omega_j t}\) from the integration variables \(\alpha_j\) in \(a^* (\alpha(t) - \beta)\) by shifting it to the coefficients \(A_{jk}\) by defining \(A_{jk}(t) = A_{jk} e^{-i(\omega_j + \omega_k)t}\). We merge all terms into a single exponential whose exponent reads

\[
\frac{1}{2} \sum_{jk} \left( \frac{\alpha_j}{\alpha_j^*} \right)^T \left( \begin{array}{c} -A_{jk}(t) - -\delta_{jk} A_{jk}^* \\ \frac{\alpha_k}{\alpha_k^*} \end{array} \right)
\]

\[
- \sum_j S_j[\beta^*] \alpha_j^* - \sum_j S_j[\beta] e^{-i\omega_j t} \alpha_j + G^*(\beta) + G(\beta),
\]

with

\[
S_j[\beta] = \sum_k A_{jk} \beta_k - \beta_j^* \quad (C1)
\]

and

\[
G(\beta) = \sum_{jk} \frac{A_{jk}}{2} \beta_j^* \beta_k - \sum_j |\beta_j|^2. \quad (C2)
\]
We now express the integration variables by their real and imaginary parts, \( \alpha_j = u_j + i v_j \) and \( \alpha_j^* = u_j - i v_j \). The quadratic term is written as

\[
-\sum_{jk} (u_j)^T \left( \delta_{jk} - \Lambda_{jk}^+ - i \Lambda_{jk}^- \right) (v_k)
\]

with complex symmetric matrices

\[
\Lambda_{jk}^\pm = \frac{1}{2} \left( A_{jk}(t) \pm A_{jk}(0) \right).
\]

The linear term in the exponent takes the form

\[-\sum_j \left( S_j^+ u_j - i S_j^- v_j \right) \]

with

\[
S_j^\pm = S_j [\beta^*] \pm S_j [\beta] e^{-i \omega_j t}.
\]

Introducing the vector \( w = (u,v)^T \) where \( u = (u_1, \ldots, u_{2N}) \), \( v = (v_1, \ldots, v_{2N}) \), we can write the overlap as

\[
\mathcal{O}(t) = \frac{Z^2}{\pi^{2N}} e^{G^*(\beta)} e^{G(\beta)} \int dw e^{-w^T \Omega^{-1} w}.
\]

The result of the integral in Eq. (C5) is

\[
\mathcal{O}(t) = \frac{Z^2}{\sqrt{\det \Omega}} e^{2 \text{Re} \{G_0\} + \frac{1}{2} w^T \Omega^{-1} w},
\]

with

\[
G_0 = \sum_{jk} \frac{A_{jk}}{2} \beta_j^* \beta_k^* - \sum_j \frac{|\beta_j|^2}{2}.
\]

Using Eq. (3.35) in Eq. (C7), the visibility can then be cast in the form of Eq. (3.44).

The convergence of the integral in Eq. (C5) is verified by showing that the matrix \( \Omega = 1 - B \), with

\[
B = \begin{pmatrix}
\Lambda^+ & i \Lambda^- \\
- i \Lambda^- & - \Lambda^+
\end{pmatrix},
\]

has only eigenvalues whose real parts are greater than zero. For this purpose we consider the spectral radius of \( B \), \( \rho(B) = \max(|\lambda_B|) \), where \( \lambda_B \) is an eigenvalue of \( B \) and which fulfills \( \rho(B) \leq \|B\| \) for any matrix norm \( \| \) . If \( \|B\| < 1 \), it follows that all eigenvalues of \( B \) lie within a circle with radius \( \rho(B) < 1 \) centered around 1. Then, all the real parts of all eigenvalues of \( \Omega = (1 - B) \) are greater than zero. \( B \) can be brought to block-diagonal form \( D_B \) by a similarity transformation with an orthogonal matrix \( M_B \):

\[
B = \frac{1}{2} \begin{pmatrix}
1 & 1 \\
i & -i
\end{pmatrix} \begin{pmatrix}
A(t) & 0 \\
0 & A
\end{pmatrix} \begin{pmatrix}
1 & i \\
1 & -i
\end{pmatrix}.
\]

Thus \( \|B\| = \|M_B D_B M_B^*\| \leq \|M_B\| \|D_B\| \|M_B\| \) by the submultiplicativity of the matrix norm. The spectral norm of the orthogonal matrices is 1, and the spectral norm of \( D_B \), \( \|D_B\|_2 = \max\{\|A(t)\|_2, \|A\|_2\} \), but since \( \|A(t)\|_2 = \|A\|_2 \) we have \( \|D_B\|_2 = \|A\|_2 \).

We now proceed to perform a Taylor expansion of Eq. (3.44) for short times. For this purpose we first bring expression (3.44) into a more convenient form, using

\[
\Omega = \begin{pmatrix}
\mathbb{I} & -i \Lambda^- \\
i \Lambda^- & - \mathbb{I}
\end{pmatrix}
\]

where

\[
\mathbb{I} = 1 + \Lambda^+, \quad \mathbb{T} = 1 - \Lambda^+
\]

and which fulfills

\[
\det \Omega = \det \Xi \cdot \det \Theta.
\]

The determinant and the inverse matrix can be calculated with the help of the corresponding identities for a partitioned matrix [33],

\[
\det \Omega = \det \Xi \cdot \det \Theta,
\]

and

\[
\Omega^{-1} = \begin{pmatrix}
\Theta^{-1} & i \Theta^{-1} \Lambda^- \Xi^{-1} \\
i \Xi^{-1} \Lambda^- \Theta^{-1} & - \Xi^{-1} \Lambda^- \Theta^{-1} \Lambda^- \Xi^{-1}
\end{pmatrix}
\]

where \( \Theta \) is the Schur complement of \( \Xi \) given by

\[
\Theta = \mathbb{T} + \Lambda^- \Xi^{-1} \Lambda^-.
\]

The equations hold provided that \( \Xi \) and \( \Theta \) are nonsingular, which is true as shown in Appendix A.

Expanding the overlap for coherent states around \( t = 0 \), we find

\[
\mathcal{O}(t) \approx 1 - i \mathcal{O}_1 t - \frac{1}{2} \mathcal{O}_2 t^2,
\]

with \( \mathcal{O}_1 = \mathcal{O}(0) \) and \( \mathcal{O}_2 = \mathcal{O}'(0) \), which leads to the expression of the visibility in Eq. (3.48), where \( v = - (\mathcal{O}_2 - \mathcal{O}_2^2) \).

Chopped random basis quantum optimization

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In this work we describe in detail the Chopped RAn- don Basis (CRAB) optimal control technique recently introduced to optimize t-DMRG simulations [1]. Here we study the efficiency of this control technique in optimizing different quantum processes and we show that in the considered cases we obtain results equivalent to those obtained via different optimal control methods while using less resources. We propose the CRAB optimization as a general and versatile optimal control technique.

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Realizing artificial, controllable quantum systems has represented one of the most promising challenges in physics for the last thirty years [2]. On one side such systems could unveil unexplored features of Nature, when employed as universal quantum simulators [3]; on the other side this technology could be exploited to realize a new generation of extremely powerful devices, like quantum computers [4]. Along with the impressive progress marked recently in the construction of tunable quantum systems [2, 6], there is a renewed and increasing interest in quantum optimal control (OC) theory, the study of the optimization techniques aimed at improving the outcome of a quantum process [2]. Indeed OC can prove to be crucial under several respects for the development of quantum devices: first, it can be generally employed to speed up a quantum process to make it less prone to decoherence or noise effects induced by the unavoidable interaction with the external environment. Second, considering a realistic experimental setup in which just few parameters are tunable or, in the most difficult situations, only partially tunable, OC can provide an answer about the optimal use of the available resources.

Traditionally OC has been exploited in atomic and molecular physics [2, 3]. More recently, with the advent of quantum information, the requirement of accurate control of quantum systems has become unavoidable to build quantum information processors [10, 11]. However, the above mentioned methods often result in optimal driving fields that require a level of tunability incompatible with current experimental capabilities and in general, the calculation of the optimal fields requires an exact description of the system (either analytical or numerical). The field of application of these methods is severely limited also by the need to have access to huge amount of information about the system, e.g., computing gradients of the control fields, expectation values of observables as a function of time. Moreover, standard OC algorithms define a set of Euler-Lagrange equations that have to be solved to find the optimal control pulse [2], where the equation for the correction to the driving field is highly dependent on the constraints imposed on the system and on the figures of merit considered. This implies that considering different figures of merit and/or constraints on the system needs a redefinition of the corresponding Euler-Lagrange equations, hindering a straightforward adaptation of the optimization procedure to different situations.

In this work we discuss in detail the Chopped RAndom Basis (CRAB) technique, an optimization method directed to overcome these difficulties and already introduced in [1]. The CRAB optimization is based on the definition of a truncated randomized basis of functions for the control fields that recast the problem from a functional minimization to a multi-variable function minimization that can be performed, for example, via a direct-search method. As shown in the following, the CRAB optimization flexibility allows to construct OC pulses just exploiting the available resources. Indeed, different figures of merit and constraints can be easily considered without any complications. Another appealing characteristic of CRAB is its compatibility with t-DMRG techniques: this feature indeed significantly enlarges the class of controllable systems [1], from few-body or exactly solvable to general many-body quantum systems with “moderate” degree of entanglement generated during the dynamics [17]. This is, to the best of our knowledge, the unique OC algorithm that can be applied in such vast setting. Finally, it can be straightforwardly applied also in a closed-loop optimization experiment, where the simulation of the system under study is replaced with the experiments itself.

Here we analyze the CRAB optimization as a possible general OC algorithm to be used also in a standard context (solvable and/or few body systems) as a valid alternative tool with respect to standard OC methods to find optimal control fields. Indeed, recently optimization methods based on the expansion over a particular function basis have shown to be effective [18, 21]. In particular, a similar approach has been proved to be mathematically convergent and consistent [22, 23]. On top of that, some theoretical analysis over control landscapes suggests that, at least in the absence of constraints, the figure of merit landscape might be smooth enough to allow for simple optimization procedures to work [24, 25]. Here, we show that indeed a convenient choice of the function basis driven by physical or geometrical arguments is enough to obtain optimal driving fields. However, in the cases where no physical intuition drives the choice of the function basis, the CRAB algorithm allows to find the optimal driving fields where a simple ansatz would fail. Moreover, a comparison between the results...
of CRAB with and without a physically driven choice of the basis, as well as previous results obtained using different optimal control algorithms (Krotov’s algorithm), show comparable performances.

The structure of the paper is the following: in Sec. III the CRAB optimization is described; in Sec. IV it is applied to a paradigmatic quantum control problem, the state transformation of two coupled qubits, to show its potential. Then we compare the results obtained via CRAB optimization in more complex cases already present in the literature [26, 27]: in Sec. III the method is employed on the LMG model; and in Sec. IV we optimize the transfer of a state along a spin chain. Finally, in Sec. V the optimization is exploited to maximize the final entanglement entropy of the final state in the LMG model; and in Sec. VI a comparison between adiabatic and optimized processes is proposed.

I. CRAB OPTIMIZATION

The optimization problem we are dealing with is defined as follows: given a Hamiltonian $H$ acting on a Hilbert space $\mathcal{H} = \mathbb{C}^N$, depending on a set of time-dependent driving fields $\Gamma(t)$, we search for the optimal transformation to drive, in time $T$, an initial state $|\psi_0\rangle \in \mathcal{H}$ into a different one (target state) $|\psi_G\rangle \in \mathcal{H}$ with some desired properties expressed by a cost function $f(|\psi_G\rangle)$ we want to minimize. In addition, constraints might be present on the driving fields, e.g. to match experimental conditions: They can be expressed usually as a function of the driving fields $C_i(\Gamma(t))$. Typical scenarios and corresponding cost functions and constraints are:

1. The goal is the preparation of a well-defined quantum state $|\psi_G\rangle$ with high accuracy for which a convenient cost function is the infidelity,

$$f_1(|\psi(T)\rangle) \equiv I(T) = 1 - |\langle \psi(T)|\psi_G\rangle|^2.$$  

2. The target state is the unknown ground state of a Hamiltonian $H_p$. The cost function is then given by the final system energy,

$$f_2(|\psi(T)\rangle) \equiv E_f(T) = \langle \psi(T)|H_p|\psi(T)\rangle.$$  

3. The target is some property or condition that many states can satisfy, like for example, in the production of highly entangled states. In this case the cost function is simply defined as

$$f_3(|\psi(T)\rangle) \equiv -S(|\psi(T)\rangle),$$  

where $S(|\psi\rangle)$ is a convenient measure of the entanglement of the state $|\psi\rangle$.

4. A constraint is present on the power of the driving fields, that is, the solution should minimize also the fluences

$$C_i = \int |\Gamma_i(t)|^2 dt$$  

5. A limited bandwidth is allowed for the driving fields: below we show how this is already embedded in the algorithm and is not necessary to consider it as an additional explicit constraint.

6. The initial state or the driving fields are known within a given uncertainty $\epsilon$. In this case, the cost function can be defined as an average other all possible outcomes compatible with that uncertainty, as for example:

$$f_4 = \int f(\langle \psi(T, \epsilon)\rangle) d\epsilon.$$  

All of the aforementioned optimization problems are then recast in the problem of solving the Schrödinger equation (from now on we assume $\hbar = 1$)

$$i \frac{d}{dt} |\psi(t)\rangle = H(\Gamma(t))|\psi(t)\rangle,$$  

with boundary condition $|\psi_i\rangle = |\psi(0)\rangle$, while minimizing the cost function

$$F = \alpha_f + \sum_i \beta_i C_i(\Gamma(t)),$$  

where the coefficients $\alpha$ and $\beta_i$ allow for a proper weighting of the different contributions (the $\beta$s play the role of Lagrange multipliers) and $f$ is the chosen cost function.

To perform such an optimization, the CRAB algorithm starts from an initial pulse guess $\Gamma^0_j(t)$ and then looks for the best correction of the form

$$\Gamma^{\text{CRAB}}_j(t) = \Gamma^0_j(t) \cdot g_j(t).$$  

The functions $g_j(t)$ are expanded in a simple form in some function basis characterized by some parameters $\Omega_k$ (Fourier space, Lagrange polynomials, etc.): $g_j = \sum_k c_k^j \tilde{g}_j^k(\Omega_j^k)$. The two key ingredients of the CRAB optimization are that the function space is truncated to some finite number of components $N_c$ ($k = 1, \ldots, N_c$) and that the corresponding basis functions are “randomized” to enhance the algorithm convergence, i.e. $g_j^k \rightarrow \tilde{g}_j^k(\Omega_j^k(1+r^k_j))$ where $r^k_j$ is a random number. Indeed, this last choice breaks the orthonormalization of the functions $g_j^k$, however as we show in the following, it allows for an improved convergence of the algorithm as it enlarge the subspace of functions explored by the algorithm while keeping constant the number of optimization parameters.

The optimization problem is then reformulated as the extremization of the multivariable cost function $F(T, \tilde{c}^j)$, which can be numerically approached with a suitable
The optimization problem is reduced to the minimization just with respect to \(\vec{A}, \vec{B}\) and \(\vec{\omega}\), with \(N_c\) the dimension of each vector. In conclusion, given a fixed total evolution time \(T\), the cost function is clearly just a function of the control parameters,

\[
\mathcal{F} = \mathcal{F}^{\text{CRAB}}(\vec{A}, \vec{B}, \vec{\omega}).
\]  

The optimization problem is reduced to the minimization of \(\mathcal{F}^{\text{CRAB}}(\vec{A}, \vec{B}, \vec{\omega})\) as a function of \(3 \times N_c\) variables. As mentioned before, however, the space of the variables can be reduced even more: although in principle the frequencies \(\vec{\omega}\) can be considered free variables it is often convenient to keep them fixed and to perform the minimization just with respect to \(\vec{A}\) and \(\vec{B}\). Indeed as shown in our analysis this is sufficient to obtain good results. In this approach we need then a criterion to select the \(\vec{\omega}\)'s. When we have no available information about the typical energy scales of the system under consideration, the frequencies are picked randomly around principal harmonics: \(\omega_k = 2\pi k (1 + r_k)/T\), with \(r_k\) random numbers with flat distribution in the interval \([-0.5, 0.5]\) and \(k = 1, ..., N_c\). Viceversa when the physical details of the model are known, clearly one can exploit this information to select the relevant frequencies, as shown in the following sections.

II. TWO-QUBITS OPTIMIZATION

In this section we apply the CRAB optimization to a paradigmatic problem in quantum information theory and control: we search for the optimal way to perform a state transformation of a two-qubit system, in particular we consider two capacitively coupled Josephson charge qubits, even though the following analysis can be easily adapted to different qubit implementations. The Hamiltonian of the \(i\)-th qubit is defined as \([29, 30]\)

\[
\mathcal{H}_i = E_C \sigma_i^z + E_J \sigma_i^+ \sigma_{i+1}^-,
\]

where the \(\sigma\)s are Pauli matrices, \(E_C\) is the charging energy and \(E_J\) is the Josephson energy and \(i = 1, 2\). For capacitive coupled qubits, the interaction Hamiltonian reads

\[
\mathcal{H}_I = E_{cc} \sigma_2^z \sigma_1^2,
\]

where \(E_{cc}\) is the charging energy associated to the Coulomb interaction between the qubits. Hereafter we set \(E_J/E_C = -1\), while the coupling will be the driving field \(E_{cc}(t)/E_C = \Gamma(t)\) we use to optimize the transformation. We will consider as initial state the state with

---

**FIG. 1:** Infidelity \(f_1\) of the final state as a function of number of calls to the optimization algorithm \(N_f\) for two capacitively Josephson charge qubits with principal harmonics (dark grey [blue] line) and randomized frequencies (light grey [green] line), for the goal state \(|\psi_{G}^1\rangle\) and \(N_c = 2\) for thirty different random instances.

**FIG. 2:** Optimized infidelity \(f\) as a function of the number of optimization parameters \(N_c\) with principal harmonics (dark grey [blue], full symbols) and randomized frequencies (light grey [green], empty symbols) for different target states \(|\psi_{G}^1\rangle\) (circle), \(|\psi_{G}^2\rangle\) (squares), \(|\psi_{G}^3\rangle\) (diamonds).
no excess Cooper pairs $|\psi_0\rangle = |00\rangle$, and our goal states will be three different state with different properties: the reversed separable state $|\psi_{11}^C\rangle = |11\rangle$, the homogeneous superposition state $|\psi_{G}^2\rangle = \frac{1}{2} \sum_{i,j} |i,j\rangle$, and the maximally entangled Bell state $|\psi_{G}^3\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Note that due to the fact that only the coupling is controlled, all three states are not trivial to achieve. We set the total time of the transformation to the somehow arbitrary time scale $T = \pi / E_J$ and we perform a CRAB optimization using the truncated expansion of the function $q(t)$ given in Eq. (4), with a constant initial guess for the driving field $\Gamma(t) = \Gamma(0) = 1$. We considered an additional constraint on the fluence of the control field, thus the resulting cost function is defined as

$$F = f_1 + 0.1 C_1(\Gamma(t)),$$

where $f_1$ and $C_1$ are given by equations 11 and 4 respectively. Here we are interested in studying the effect of the randomness introduced in the frequencies of the expansion 3, thus we optimize both in the case of random $r_k$ and with $r_k = 0$. To perform a fair comparison, we ran the optimization in both cases with the same maximum number of calls $N_f \sim 30,000$ to the function $F$, which fixes the simulation complexity. Indeed, in the first case we repeated the optimization for thirty different $r_k$ random configurations (with a single $A_k, B_k$ random starting point), while in the second case the optimization was repeated over thirty initial random $A_k, B_k$ configurations. A typical result is shown in Fig. 4 for $N_c = 2$ and $|\psi_{G}^3\rangle$: it clearly shows that for the case of randomized $\omega_k$ the optimization is highly improved (notice the logarithmic scale). A more systematic comparison is shown in Fig. 2 where the best results are plotted against the number of optimization parameters $N_r$ for the three target states $|\psi_{G}^i\rangle$: in all cases the randomization of the frequencies improves the convergences to higher fidelities up to the simulation error. In particular, in one case, the final result without randomization is very far from being satisfactory as the final fidelity is of the order of ten percent, resulting in a very poor state transformation. On the contrary, using the randomized frequencies we were able to find optimal pulses to obtain fidelities below one percent – values that are comparable, in most cases, with experimental errors.

III. LIPKIN-MESHKOV-GLICK MODEL

The Lipkin-Meshkov-Glick (LMG) model is the paradigm of a system with long range interaction (infinite in the thermodynamical limit). The Hamiltonian is written as 31,32:

$$H = -\frac{J}{N} \sum_{i<j} (\sigma_i^x \sigma_j^x + \gamma \sigma_i^y \sigma_j^y) - \Gamma(t) \sum_i \sigma_i^z,$$

where $J$ is the uniform spin-spin interaction (we set $J = 1$ in the following), $N$ is the number of spins in the system, $\Gamma$ is the transverse field and $\sigma_i^\alpha$ are the Pauli matrices. By introducing the total spin operator $S_\alpha = \sum_i \sigma_i^\alpha / 2$, Eq. (12) can be rewritten, apart from an additive constant, as $H = -\frac{1}{N} [S_x^2 + \gamma S_y^2] - \Gamma S_z$. The Hamiltonian hence commutes with $S^2$ and does not couple states having a different parity in the number of spins pointing in the magnetic field direction: $[H, S^2] = 0$ and $[H, \prod_i \sigma_i^z] = 0$. In the isotropic case $\gamma = 1$, also the $z$-component of $\vec{S}$ is conserved, $[H, S_z] = 0$. In the thermodynamical limit the LMG model undergoes a second order quantum phase transition at $\Gamma_c = 1$ from a paramagnet ($\Gamma > 1$) to a ferromagnet ($\Gamma < 1$). The phase transition is characterized by mean-field critical exponents 32. The phase transitions dramatically affects...
the dynamical behavior of quantum systems: As discussed in more detail in Sec. [VI] the gap closure at the critical point promotes dynamical excitations, preventing adiabatic evolutions whenever the adiabaticity condition $T \gg \Delta^{-1}$ is not fulfilled, where $T$ is the total evolution time and $\Delta$ the minimum spectral gap.\cite{26,44} Following Ref. [26], we employ the CRAB optimization to drastically reduce the residual density of defects present in the system in a strongly non adiabatic dynamics, drastically reducing the time needed to connect the ground state in one phase with the ground state of the other phase with respect to adiabatic non-optimized strategies. We chose as initial state the ground state (gs) of $H[\Gamma(t)]$ at $\Gamma_i \gg 1$, i.e. the state in which all the spins are polarized along the positive z-axis (paramagnetic phase). As target state we chose the gs of $H[\Gamma = 0]$ (ferromagnetic phase). We focused our attention on the case $\gamma = 0$, representative of the class $\gamma < 1$ (for $\gamma = 1$ the dynamics is trivial due to the symmetry of $H$).\footnote{For this model indeed a lot of physical information is available: the gap between the ground state and the first excited state closes polynomially with the size at the critical point $\Delta \sim N^{-1/3}$. Furthermore it has been recently demonstrated that the minimum time required to obtain a perfect conversion between the initial and the final state here considered, the so called quantum speed limit, is given by $T_{\text{QSL}} = \pi/\Delta$.\cite{26,44}} In order to test the performance of CRAB, we fixed the total evolution time above this threshold, at $T = 2T_{\text{QSL}}$, in a regime in which in principle it is possible to produce an arbitrarily small infidelity with optimized evolutions.

The results of our simulations for the LMG model are summarized in Fig. [3] and Fig. [4] the data shown in the two pictures (with the only exception of the inset of Fig. [4] as explained in the following) have been produced assuming $\Gamma_0(t)$ as control field and the infidelity as cost function to minimize. In Fig. [5] we plotted the infidelity as a function of the size $N$, before the optimization for a linear driving field $\Gamma_0(t) \propto t/T$ (squares), and after the optimization with CRAB (circles): for each size we have been able to produce an infidelity below $10^{-6}$ starting from an infidelity of order $O(1)$. In particular the data have been produced by minimizing Eq. (10) with respect to $\vec{A}$ and $\vec{B}$, while keeping $\vec{\omega}$ fixed, for a total of $2 \times N_c = 16$ parameters. In this case the frequencies $\vec{\omega}$ have been chosen by exploiting the physical information available. We chose the frequencies equal to the minimum spectral gap $\omega_1 = 2\pi/T = 2\pi/2T_{\text{QSL}} = \Delta$ and we considered the main harmonics $\omega_k = k\omega_1$ for $k$ up to $N_c$. In Fig. [4] we plot the infidelity as a function of number of parameters employed to build the optimal field of Eq. (9) – adding a frequency $\omega_k$ corresponds to add two parameters, $A_k$ and $B_k$. First it can be noticed that 5 harmonics are sufficient to reach the best optimization result, $I \sim 10^{-6}$; however with only 3 harmonics the infidelity is already of order $10^{-4}$, of the order of the required threshold for fault-tolerant quantum computation. Considering the implementation of an optimal pulse in an NMR or quantum optics experiment, the gain with respect to other OC methods providing a totally arbitrary $\Gamma_{\text{opt}}(t)$ is evident. The second interesting feature is that the behavior of the infidelity in Fig. [4] is approximately independent of the size (for the smallest system considered, $N = 10$, finite size effects are more evident): this confirms the intuition that the most relevant energy scale for the LMG model is given by the minimum spectral gap.

Finally, in order to verify the independence of the optimization from the knowledge of the target state, we repeated the simulations assuming as a cost function the final energy $E_f(T)$ of Eq. (2). In the inset of Fig. [4] we compare the infidelity of the data optimized using as cost function the infidelity itself (empty circles) and the final energy (full circles), for a specific size of the system.
is the tunable magnetic field along the minimum, the spins are forced by the magnetic field to be aligned along the $z$-axis irrespective of their mutual interaction; instead close to the minimum, the n.n. coupling prevails and can be exploited to transfer the information (i.e. the state) from one site to the next. The Hamiltonian commutes with the total magnetic field along the $z$-direction, $[H(t), \sum_{n=1}^{N} \sigma_n^z] = 0$, so that the dynamics occurs in a subspace whose dimension grows just linearly with the size $N$ of the system. We chose to work in the subspace $\langle \sum_{n=1}^{N} \sigma_n^z = 1 \rangle$: in particular we aimed at transferring a spin-up state from one end of the chain to the opposite end, or in other words to transform the state $|\psi_i\rangle = |0\ldots0\rangle$ into the state $|\psi_f\rangle = |0\ldots01\rangle$, with 0 (1) corresponding to the $n$th spin pointing in the down (up) direction along the $z$-axis. We employed CRAB to optimize the two control parameters, $\Gamma_1(t) = d(t)$ and $\Gamma_2(t) = C(t)$; as in the previous section, we set the total evolution time above the quantum speed limit threshold at the value $T = 2T_{QSL}$, where for the latter we used the estimate made in Refs [27, 45]. The optimization has been performed by keeping $\vec{\omega}_1, \vec{\omega}_2$ fixed (in particular $\omega_{1k} = \omega_{2k} = 2k\pi/T$ for $k = 1, \ldots, N$) and minimizing the infidelity with respect to $\vec{A}_1, \vec{B}_1, \vec{A}_2, \vec{B}_2$, where the index 1 and 2 refer to $d(t)$ and $C(t)$ respectively.

The results of our simulations for the state transfer along the chain are summarized in Fig. 5 and Fig. 6. In Fig. 5 we show the infidelity as a function of the size before the optimization (squares), for a constant $C(t)$ and $d(t) = t/T$, and after the optimization with CRAB (circles): for each size considered we were able to reach an infidelity below the value $10^{-4}$ starting from an initial infidelity of order 1. In Fig. 6 we plot the infidelity as a function of the number of parameters employed in the minimization procedure; in this case, unlike for the LMG model in Fig. 4, the data show a strong dependence on the size. We interpreted this behavior as a consequence of the structure of the problem. Considering the particular transfer mechanism, in which the information moves step by step from one site to the next one, we ex-
pect the optimal pulse to be able to modulate the magnetic field around each spin; this occurs only when the spectrum of the pulse involves frequencies of the order of the inverse of the time spent on a generic site $n$, i.e., $\omega \sim 2\pi/(T/N) = N\omega_1$. As a test, in the inset of Fig. 4 we plotted the infidelity as a function of the number of parameters divided by the size; the good agreement of the rescaled data confirms our expectation.

V. ENTANGLEMENT ENTROPY MAXIMIZATION

Among its various applications, QC can be exploited for entanglement production \[37, 38\]. Here we employ the CRAB technique in the LMG model to maximize the von Neumann entropy $S_{L,N} = -\text{Tr}(\rho_{L,N} \log_2 \rho_{L,N})$ associated to the reduced density matrix $\rho_{L,N}$ of a block of $L$ spins out of the total number $N$ at a given final time $T$, which gives a measure of the entanglement present between two bipartitions of a quantum systems. As shown in Sec. \[39\] due to the symmetry of the Hamiltonian $[H, S^2] = 0$, the dynamics is restricted to subspaces with fixed total angular momentum; in particular assuming as initial state the ground state of the system, we have $S = N/2$. The Dicke states $|S = N/2, S^z\rangle$ with $S^z = -N/2, ..., N/2$ provide a convenient basis spanning the subspace accessible through the dynamics. Indeed the entanglement entropy $S_{L,N}$ can be easily evaluated noticing that, since the maximum value of the total spin can be achieved only with maximum value of the spin in each bipartition, the following decomposition holds \[40\]:

$$|N/2, n\rangle = \sum_{l=0}^{L} p_{l,n}^{1/2} |L/2, l - L/2\rangle \otimes |(N - L)/2, n - l - (N - L)/2\rangle,$$

where $n$ and $l$ correspond respectively to the number of up spins in the whole system and in the block of size $L$, and $p_{l,n} = L !(N - L)! n! (N - n)! / [[(L - l)! (n - l)!] (N - n - l)! N!].$ Expressing the evolved state $|\psi(T)\rangle$ in the Dicke state basis and using the previous decomposition, it is immediate to evaluate $S_{L,N}(T)$. In our simulations we considered a system equally bipartite, i.e. $L = N/2$, and we took as starting state the ground state of the LMG Hamiltonian at $\Gamma \gg 1$, in which all the spins are polarized along the positive $z$ direction, so that the state factorizes and the entanglement entropy vanishes, see Fig. 5. Then we performed the optimization with CRAB, modulating the field according to Eq. \[39\] and using as a cost function Eq. \[39\]. The behavior of entanglement entropy after the optimization $S_{opt}(T)$ for different values of the total evolution time $T$ is shown in Fig. 6 after a short transient of linear growth, $S_{opt}(T)$ reaches a saturation value growing with the size, as expected. It is interesting to notice that such a behavior closely resembles the features observed in one-dimensional systems after a sudden quench \[51\], although here we are dealing with a fully connected model \[51, 52\]. In Fig. 8 we plotted the saturation value reached with the optimization as a function of the size $N$; comparing our data with the maximum possible value of the von Neumann entropy for a subsystem of $L = N/2$ spins (described by a Hilbert space of dimension $N/2 + 1$), we obtain almost the maximal possible amount of entanglement, $S_{opt}/S_{max} \sim 0.95$.

VI. LINEAR VS OPTIMAL DRIVING

In this section we analyze in more detail the features characterizing the optimal dynamics induced by CRAB. In order to better understand the matter, we draw a comparison with a simpler non-optimized dynamics, in which the driving field is linearly dependent on time; in particular we focus the attention on the LMG model. An important point in the study of the dynamics of a quantum system is usually represented by the *adiabatic theorem* \[53\]. The latter establishes that a system initially prepared in its ground state can be driven by a time dependent Hamiltonian adiabatically (i.e. without introducing excitations), if the time scale of the evolution is much larger than the minimum spectral gap, i.e. $T \gg \Delta^{-1}$. In critical systems the spectral gap closes at the phase transition, so that the system gets excited from the instantaneous gs while crossing the critical point for any finite-time evolution \[54\]. For finite-size systems, the critical gap is not completely closed, but it presents a pronounced minimum where the excitation appears,
as shown in Fig. 9, an estimate of the excitations induced by a linear driving can be obtained by Kibble-Zurek theory [35, 37, 41, 43, 53]. In the picture we monitored the instantaneous total excitation probability $P_{tot}$ (dashed line), and the populations of lowest levels (different style [color] lines) during the dynamics. The evolution starts at large negative times (left) and ends at the time $t = 0$ (right); the critical point is crossed around the time $t = 11$ when $\Gamma(t) \sim 1$, see section III. Far from the critical point the system evolves adiabatically as demonstrated by the low total instantaneous excitation probability; notice that before reaching the critical point the total excitation probability coincides with the small excitation of only the first level (red continuous line). In a restricted region around the critical point ($-15 < t < -10$) the total excitation probability jumps to values of order 1 and does not change significantly any more. Notice that in the final part of the evolution more levels get populated, as shown by the difference between the instantaneous infidelity and the excitation probability of the first level. At the final time $t = T$ the excitation probability is equal to the infidelity of the process, i.e. $P_{tot}(T) = f_1$.

We then optimize the final infidelity, and the correspondent plot for the optimal evolution is reported in Fig. 10. The scenario in this case is completely different: the system is excited at the very beginning of the dynamics and remains excited for the most part of the evolution until close to the end, when the infidelity drops abruptly to zero. It is interesting to notice that just a few levels are excited, as demonstrated by the small difference between the total excitation probability (dashed line) and the excitation probability of the first level (red continuous line). This result is in agreement with previous findings where the authors showed that this kind of dynamics can be approximated by a two-level system dynamics [26]. The abrupt jump in the probabilities around the time 20 is due to an abrupt (double) change of sign in $\Gamma_{CRAB}(t)$, reversing suddenly the order of the levels and transforming the gs in the most excited state (dash-dash-dotted [cyan] line), thus this signature is not due to a collective involvement of all the levels but simply to a reshuffling of their order. Indeed as shown in the picture for $-18 < t < 0$, with the subsequent change of sign the previous order is reestablished. We can then summarize the main features of the optimal evolution induced by CRAB in three points: it is strongly non adiabatic; it involves just a restricted number of levels although not necessarily close to the nominal instantaneous ground state and it is such that at the very end all populations constructively interfere to obtain the desired goal state.

VII. CONCLUSIONS

In this paper we studied in detail the performance of quantum optimal control through the CRAB optimization [1]. In particular we focused the attention on three different systems and different figures of merit, in order to outline the versatility of the method. We first studied the optimization of state transformations of two qubits via a controlled coupling. We have shown that the CRAB optimization is very effective already using only a few optimization parameters and the fundamental role that the randomization of the function basis plays in increasing the process convergence. We then analyzed two many-body quantum systems: the first one, the LMG model, is the prototype of many-body system with long range interaction undergoing a quantum phase transition. The success of CRAB in this context confirms the possibility of controlling complex systems typically studied in condensed matter, with relatively small resources: due to CRAB unique features, only few parameters (3 frequencies) are indeed sufficient to obtain excellent results. The second many-body quantum system studied, the transfer of information along a spin chain, is a typical problem studied in quantum information theory: the high accuracy achievable through CRAB optimization makes it a valuable tool for this kind of applications. Moreover, due to the simple structure of the optimal pulses, they may be used to extract information on the typical timescales involved on the system dynamics, as we did for the information transfer in spin chains. We stress also that the exponential dependence of the figures of merit as a function of the number of parameters found in all cases (see Figs. 2, 4, 6) suggests that in general already a moderate number of optimization parameters will be sufficient to get huge improvements in the desired processes.

Finally, we have shown that with a simple change of the cost function, the CRAB optimization can be used to optimize the search of the unknown ground state of a Hamiltonian or to generate quantum states satisfying desired properties, i.e. high entangled states. Monitoring the instantaneous excitation probabilities generated by the optimized process, we have demonstrated the highly non adiabatic character of the dynamics and the fact
that, despite the complexity of the system under study, just a restricted number of excited levels are really populated during the evolution. The latter fact justifies the compatibility of CRAB with DMRG-like techniques. We mention that the CRAB optimization has been applied also to open quantum systems obtaining interesting results and thus increasing its possible applications [54].

In conclusion, the main features of the CRAB optimization—versatility (different constraints, compatibility with approximate simulation methods and experiments), fast convergence (the final error scales exponentially with the number of optimization parameters while the number of algorithm iterations linearly) and simplicity (small modification to existing numerical codes for quantum system simulations)– demonstrate that the CRAB optimization is not only an unique solution for many body quantum systems optimal control but it is a valid alternative also in many different settings where other optimal control tools exist [2].

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[34] S. Sachdev, Quantum Phase Transition (Cambridge University Press, 1999).
[55] The generalization of the problem to the optimization of an overall unitary transformation is straightforward, averaging over the contributions of a complete set of basis of the Hilbert space $\mathcal{H}$. 

Entanglement Storage Units

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We introduce a protocol to drive many body quantum systems into long-lived entangled states, protected from decoherence by big energy gaps. With this approach it is possible to implement scalable entanglement-storage units. We test the protocol in the Lipkin-Meshkov-Glick model, a prototype many-body quantum system that describes different experimental setups.

PACS numbers:

Entanglement represents the manifestation of correlations without a classical counterpart and it is regarded as the necessary ingredient at the basis of the power of quantum information processing. Indeed quantum information applications as teleportation, quantum cryptography or quantum computers rely on entanglement as a crucial resource\textsuperscript{1}. Within the current state-of-art, promising candidates for truly scalable quantum information processors are considered architectures that interface hardware components playing different roles like for example solid-state systems as stationary qubits combined in hybrid architectures with optical devices\textsuperscript{3}. In this scenario, the stationary qubits are a collection of engineered qubits with desired properties, as decoupled as possible from one another to prevent errors. However, this architecture is somehow unfavorable to the creation and the conservation of entanglement. Indeed, it would be desirable to have a hardware where “naturally” entanglement is present and that can be prepared in a highly entangled state that persists without any external control: the closest quantum entanglement analogue of a classical information memory support, i.e. an entanglement-storage unit (ESU). Such hardware once prepared can be used at later times (alone or with duplicates) – once the desired kind of entanglement has been distilled – to perform quantum information protocols\textsuperscript{1}.

The biggest challenge in the development of an ESU is entanglement frailty: it is strongly affected by the detrimental presence of decoherence\textsuperscript{1}. Furthermore the search for a proper system to build an ESU is undermined by the increasing complexity of quantum systems with a growing number of components, which makes entanglement more frail, more difficult to characterize, to create and to control\textsuperscript{2}. Moreover, given a many body quantum system, the search for a state with the desired properties might be very difficult. Indeed, a direct and comprehensive study of a many body quantum system is an exponentially hard task in the system size. Nevertheless, in many-body quantum systems entanglement naturally arises: for example —when undergoing a quantum phase transition — in proximity of a critical point the amount of entanglement possessed by the ground state scales with the size\textsuperscript{2}.\textsuperscript{4}. Unfortunately, due to the closure of the energy gap at the critical point, the ground state is an extremely frail state: even very little perturbations might destroy it, inducing excitations towards other states. Very recently, the entanglement properties of the eigenstates of many-body Hamiltonians have been investigated, and it has been shown that in some cases they are characterized by entanglement growing with the system size\textsuperscript{2}.\textsuperscript{13}.

In this letter we show that by means of recently developed optimal control technique\textsuperscript{7} it is possible to identify and prepare a many body quantum system in robust, long-lived entangled states (ESU states). More importantly, we drive the system towards ESU states without the need of any apriori information on the system, either about the eigenstates or about the energy spectrum. Finally, we show that properly prepared systems can be effectively used as ESU exploiting the fact that ESU states are well protected by large energy gaps.

Recently, optimal control has been used to drive quantum systems in entangled states or to improve the generation of entanglement\textsuperscript{8}. However, here we have in mind a different scenario: to exploit the control to steer a system into a highly entangled state that is stable and robust even after switching off the control (see Fig.1). In the following we show that ESU states are gap-protected entangled eigenstates of the system Hamiltonian in the absence of the control. Here we show that for an experimentally relevant model this is indeed possible, and that it is possible to drive the system in gap-protected

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{(Color online) Entanglement Storage Units protocol: a system is initially in a reference state \(\psi(-T)\), e.g. the ground state, and is optimally driven via a control field \(\Gamma(t)\) in an entangled eigenstate \(\psi(0)\), protected from decoherence by an energy gap.}
\end{figure}
states. We show that the ESU states, although not being characterized by the maximal entanglement sustainable by the system, are characterized by entanglement that grows with the system size. Once a good ESU state has been detected, due to its robustness it can be stored, characterized, and thus used for later quantum information processing.

Protocol - As depicted in Fig. 1 we consider the general scenario of a system represented by a Hamiltonian \( H_0 \) with an additional tunable term \( H_1[\Gamma] \), where \( \Gamma(t) \) is the driving field, starting in an initial state \( |\psi_0\rangle \), not necessarily entangled, in which the system can be easily prepared. The Hamiltonian is then \( H = H_0 + H_1[\Gamma] \), where the control parameter is initially set at a constant value (in particular it can vanish, \( \Gamma(0) = 0 \)). The control field is modulated \( \Gamma(t) \) for \(-T < t < 0\) with the condition that at time \( t = 0 \) the control field is \( \Gamma(-T) = \Gamma(0) \) (absence of control). A CRAB optimization is then performed –in the time interval \([-T, 0]– with the goal of minimizing the cost function \( \mathcal{F} \) (see [2] for details of the method):

\[
\mathcal{F}(\lambda)|\psi(T)\rangle = -S + \lambda \frac{\Delta E_0}{E_0},
\]

where \( S \) represents a measure of entanglement, \( \Delta E_0 = \sqrt{\langle \psi|H_0^2 - (H_0)^2|\psi\rangle} \) and \( E_0 = \langle \psi|H_0|\psi\rangle \) correspond respectively to the energy fluctuations and the energy computed with respect to \( H|\Gamma_0\rangle \), \( \lambda \) is a Lagrange multiplier, and the cost function is evaluated on the optimized evolved state \( |\psi(0)\rangle \). As shown in the following, the inclusion in \( \mathcal{F} \) of the constraint on the energy fluctuations is the crucial ingredient to stabilize the result of the optimization and possibly to steer the system into an ESU state.

Model - Here we provide an important example of this approach, based on the Lipkin-Meshkov-Glick (LMG) model [3]: we prepare an ESU maximizing the Von Neumann entropy of a bipartition of the system and we model the action of the surrounding environment with noise terms in the Hamiltonian. However, our protocol is compatible with different entanglement measures and different models, and with a straightforward generalization it can adapted to a full description of open quantum systems [15]. The LMG model represents a prototype of the challenge we address: it describes different experimental setups [3, 10], and the entanglement properties of the eigenstates are in general not known. Indeed, the entanglement properties of the eigenstates of one-dimensional many-body quantum systems have been related with the corresponding conformal field theories [3]; however for the LMG model, to our knowledge, this study has never been performed and a conformal theory is not available [2]. Finally, the optimal control problem we address is highly non-trivial as the control field is global and space-independent with no single-site addressability [2].

The LMG Hamiltonian describes an ensemble of spins with infinite-range interaction and is written as:

\[
H_{\text{LMG}} = -\sum_{i<j} J_{ij} \sigma_i^x \sigma_j^x - \Gamma(t) \sum_i \sigma_i^z, \quad \text{where } N \text{ is the total number of spins, } \sigma_i^{\alpha}'s (\alpha = x, y, z) \text{ are the Pauli matrices on the } i\text{th site and } J_{ij} = J/N \text{ (infinite range interaction). By introducing the total spin operator } \vec{J} = \sum_i \vec{\sigma}_i, \text{ the Hamiltonian can be rewritten, apart from an additive constant, as}
\]

\[
H = -\frac{1}{N} J_x^2 - \Gamma J_z,
\]

(from now on we set \( J = 1 \) and \( \hbar = 1 \)). The Hamiltonian hence commutes with \( J_z^2 \) and does not couple states having a different parity of the number of spins pointing in the magnetic field direction: \([H, J_z^2] = 0\) and \([H, \prod \sigma_i^z] = 0\). The symmetries of the Hamiltonian imply that the dynamics is restricted to subspaces of fixed total magnetization \( J \): a convenient basis for such subspaces is represented by the Dicke states \( |J, J_z\rangle \) with \(-J < J_z < J\) [11]. In the thermodynamical limit the system undergoes a 2nd order QPT from a quantum paramagnet to a quantum ferromagnet at a critical value of the transverse field \( |\Gamma_c| = 1 \). There is no restriction to the initial value of \( \Gamma_0 \) (in the implementation of Ref. [3] it goes to infinity when the control lasers are switched off) and to the initial state \( |\psi_0\rangle \): we choose \( \Gamma_0 \gg 1 \), corresponding to the paramagnetic phase and as initial state \( |\psi_0\rangle \), the ground state of \( H|\Gamma_0\rangle \), i.e. the separable state in which all the spins are polarized along the positive \( z\)-axis, A convenient measure of the entanglement in the LMG model is given by the von Neumann entropy \( S_{L,N} = -\text{Tr}(\rho_{L,N} \log_2 \rho_{L,N}) \) associated to the reduced density matrix \( \rho_{L,N} \) of a block of \( L \) spins out of the total number \( N \), which gives a measure of the entanglement present between two bipartitions of a quantum system [12]. In our analysis we consider two equal bipar-
the interval \( -2^N = 64 \); the control is active for negative times, i.e., in the inset of Fig. 3 for different values of the weighing factor \( \lambda \). The behavior of the entanglement is shown in the left panel of Fig. 3: the state prepared with \( \lambda = 1.8 \) and \( N = 64 \) (time unit \( J^{-1} \)) decays over very fast timescales \( \tau_0 \), while for \( \lambda \neq 0 \) it remains close to the unity for very long times \( \tau \gg \tau_0 \). The small residual oscillations for \( N = 64 \) and \( \lambda = 1.2 \) are due to the fact that in this case the optimization leads to a state corresponding to an eigenstate up to 98%. We repeated the optimal preparation for different system sizes and initial states, and show the entanglement of the optimized states for \( \lambda = 0 \) (empty green triangles) and \( \lambda \neq 0 \) (\( \Delta E_0/E_0 < 0.05 \), \( P > 95\% \) empty red circles) for different system sizes in Fig. 2. In all cases a logarithmic scaling with the size is achieved.

**Dynamics.**— We prepare the system in the ground state of the Hamiltonian \( H = H_0 + H_1(\Gamma_0) \) so that in the absence of control, i.e., \( \Gamma = \Gamma_0 \) independent from the time, the state does not evolve apart from a phase factor. After the action of the CRAB-optimized driving field \( \Gamma(t) \) for a time \( T \) the state is prepared in \( |\psi(0)\rangle \) (a typical optimal pulse is shown in the inset of Fig. 2). We observe the evolution of the state over times \( t > 0 \). The behavior of the entanglement is shown in the left panel of Fig. 3 for different values of the weighing factor \( \lambda \) and \( N = 64 \); the control is active for negative times, i.e., in the interval \( [-T,0] \). For \( \lambda = 0 \) highly entangled states are produced, however the entanglement \( S(t) \) oscillates indefinitely with the time, reflecting the fact that the system state is changing over time. On the contrary, if the energy fluctuations are included in the cost function (\( \lambda \neq 0 \)), the optimal driving field steers the system into entangled eigenstates, as confirmed by the absence of the oscillations in the entanglement and by the entanglement eigenstate reference values (empty blue circles). These results are confirmed by the survival probability in the initial state \( P(t) = |\langle \psi(0)|\psi(t)\rangle|^2 \) reported in the right panel of Fig. 3: the state prepared with \( \lambda = 0 \) decays...
(full diamonds) the effect of the noise is reduced; however, around a resonant frequency \( \nu_R \) (dashed line with crosses) its effect is enhanced and the state is quickly destroyed. We checked that the resonant frequency is the same for different eigenvalues, different sizes, and different noise strengths (data not shown), reflecting the fact that in the paramagnetic phase (\( \Gamma \gg 0 \)) the gap separating the eigenstates is proportional to \( \Gamma \), independently of the size of the system and of the state itself, see Eq. (2). Therefore we analyze this worst case scenario, setting \( \nu = \nu_R \) from now on. The results of this analysis, show that ESU states – differently from the states produced optimizing only entanglement – are extremely robust to noise at the resonant frequency. This is shown in Fig. 3 where we compare the survival probability \( P(t) \) for three instances of the disorder at the resonant frequency with an intensity of the disorder \( I_\alpha = I_\beta = 0.01 \). The noise-induce dynamics of the states obtained optimizing only with respect to the entanglement (i.e. setting \( \lambda = 0 \)) drastically depends on the (in general unknown) details of the noise affecting the system, as shown by the different evolutions induced by different instances of the noise. Thus, such states cannot be used as ESU, unlike those prepared with \( \lambda \neq 0 \) that are stable, noise-independent long-living entanglement states. Finally, in Fig. 4 we study the decay times of the survival probability \( P(t) \) studying the time \( T_{0.8} \) needed to drop below a given threshold \( P_{\text{min}} = 0.8 \) as a function of the system size \( N \) and of the intensity of the disorder \( I = I_\alpha = I_\beta \) (inset). These results clearly show that \( T_{0.8} \) for ESU states is almost independent from the system size, reflecting the fact that the energy gaps in this region of the spectrum are mostly size independent. Notice that, on the contrary, \( T_{0.8} \) for maximally entangled states decays linearly with the system size and that there are more than four orders of magnitude of difference in the decay times \( \tau_\chi \) and \( \tau_0 \). Finally, the inset of Fig. 5 shows that the scaling of \( T_{0.8} \) with the noise strength for ESU states is approximately linear and again depends very weakly on the system size \( N \).

Conclusions. Exploiting optimal control we proposed a method to steer a system into apriori unknown eigenstates satisfying desired properties. We demonstrated, on a particular system, that this protocol can be effectively used to build long-lived entangled states with many-body systems, indicating a possible implementations of an Entanglement Storage Unit scalable with the system size. The presented method is compatible with different measures of entanglement and it can be extended to any other property one is interested in, as for example the squeezing of the target state. It can be applied to different systems with apriori unknown properties: optimal control will select the states (if any) satisfying the desired property and robust to system perturbations. We underscore that an adiabatic strategy is absolutely ineffective for this purpose, as transitions between different eigenstates are forbidden. Applying this protocol to the full open-dynamics description of the system, e.g. via a CRAB optimization of the Lindblad dynamics as done in \[17\], will result in an optimal search of a Decoherence Free Subspace (DFS) with desired properties \[17\]. If no DFS exists, the optimization would lead the system in an eigenstate of the superoperator with longest lifetime and desired properties \[17\]. Although the state so prepared may be unstable over long times, it represents the best and most robust state attainable, and additional (weak) control might be used to preserve its stability. Finally, working with excited states would reduce finite temperature effects, relaxing low temperatures working-point conditions, simplifying the experimental requirements to build a reliable ESU.

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