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Lieb-Robinson Bounds for Spin-Boson Lattice Models and Trapped Ions

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We derive a Lieb-Robinson bound for the propagation of spin correlations in a model of spins interacting through a bosonic lattice field, which satisfies a Lieb-Robinson bound in the absence of spin-boson couplings. We apply these bounds to a system of trapped ions and find that the propagation of spin correlations, as mediated by the phonons of the ion crystal, can be faster than the regimes currently explored in experiments. We propose a scheme to test the bounds by measuring retarded correlation functions via the crystal fluorescence.

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The possibility of designing or simulating many-body systems in quantum-optical setups, such as ultracold atoms [1–4] or large ion crystals [5], is stimulating considerable progress in our understanding of nonequilibrium quantum many-body phenomena. However, the interpretation of these experiments demands powerful theoretical tools, including the Lieb-Robinson bounds (LRBs) [6] developed in this work. On the surface, LRBs show that nonrelativistic quantum many-body systems, under certain conditions, display a causal structure analogous to relativistic quantum field theories. More deeply, LRBs are essential to prove fundamental quantum many-body properties, such as the exponential decay of correlations in the ground state of gapped local Hamiltonians-the so-called "clustering of correlations" [7], scaling laws for entanglement entropy [8]—the "area laws" [9], or the robustness of topological order under local perturbations [10].

Causality limits how local measurements and perturbations, described by an operator O_X in region X, affect later measurements of another operator O_Y in a separate region Y [11]. In analogy to Heisenberg's principle [12], this uncertainty is quantified by a commutator $C_{YX}(t) =$ $\langle [O_Y(t), O_X(0)] \rangle$. Lorentz invariance and the mathematical structure of relativistic theories guarantee causality [11]. Thus, $C_{YX}(t) = 0$ when the distance $d_{XY} > ct$ places both regions outside the light cone defined by the speed of light c. In nonrelativistic quantum mechanics, causality is violated at the few particle level [11]. Remarkably, in the many-body regime, an approximate light cone emerges, outside of which such correlations are vanishingly small. This phenomenon, first demonstrated by Lieb and Robinson [6] for a lattice of locally interacting spins, has been generalized to finite-dimensional models, anharmonic oscillators, and master equations [7,13-16].

In this Letter, we address the role of bosons as mediators of interactions between particles in the light of LRBs. This is done for a general model of finite-dimensional systems interacting through a bosonic field that satisfies a LRB itself. New bounds are derived, which are then applied to a crystal of trapped atomic ions, where the spins and the bosons map to the ions' internal states and the crystal's phonons, respectively. These LRBs work for all spin-boson lattice models of any dimensionality and geometry realized with state-of-the-art technology [5,17–19]. Comparing with LRBs for the effective spin models [20,21] in quantum simulations [5,17], we show that correlations can spread much faster in the nonperturbative regime. We note that the correlation spread in the perturbative regime has received considerable attention [22] and also remark that our results immediately extend to a variety of other fields, such as superconducting quantum circuits and quantum dots or NV centers interacting with coupled cavities or photonic crystals.

The model.—We consider a lattice model of bosons interacting locally with a collection of finite-dimensional quantum systems. The lattice is an undirected graph, where each of the N vertices forms a Hilbert space that groups a boson with a system of finite dimension d, i.e., "spin." The Hamiltonian is

$$H = \frac{1}{2} \sum_{i,j=1}^{N} \mathbf{R}_{i}^{T} \mathcal{Q}_{ij}(t) \mathbf{R}_{j} + \sum_{i=1}^{N} \mathbf{B}_{i}(t)^{T} \mathbf{S}_{i} + \sum_{i=1}^{N} \mathbf{R}_{i}^{T} G_{i}(t) \mathbf{S}_{i}.$$
(1)

Here, the bosons are represented by adimensionalized harmonic oscillators with positions and momenta $\mathbf{R}_i^T = (x_i, p_i)$ satisfying $[\mathbf{R}_i, \mathbf{R}_j^T] = -\delta_{i,j}\sigma^y$, with the Kronecker delta $\delta_{i,j}$ and the Pauli matrix σ^y . The spins $\mathbf{S}_i = (S_i^1, \ldots, S_i^m)$ are dimensionless operators forming a Lie algebra with structure constants $f^{\alpha\beta\gamma}$ [23]. The dynamics of this spin-boson lattice is given by Eq. (1), where bosons at different vertices are coupled by a matrix $Q_{ij}(t) = Q_{ji}(t) \in \mathbb{R}^{2\times 2}$, and spins precess under a general magnetic field $\mathbf{B}_i^T(t) = (B_i^1(t), B_i^2(t), B_i^3(t))$. Finally, the spin-boson coupling is strictly local, taking place exclusively at the vertices through matrices $G_i(t) \in \mathbb{R}^{2\times 3}$.

Whereas the first part of this Letter introduces the proof of the LRB for the very general spin-boson Hamiltonian of Eq. (1), the second part shows how this model applies to trapped ions. We estimate correlation speeds and time scales, suggesting concrete experimental protocols to assert these bounds. As an aid to the reader, in the Supplemental Material [24] we provide additional background material, a step-by-step version of the proof, and alternative experimental setups or considerations.

Spin-boson LRB.—Let us assume that the propagator W of the free bosonic lattice without spins ($G_i = 0$) satisfies a LRB

$$\|[\mathbf{R}_{j}(t), \mathbf{R}_{k}(0)]\| \le \|W_{jk}(t, 0)\| \le \alpha e^{\nu_{LR}t} f(d_{jk})$$
(2)

characterized by a LR speed v_{LR} , a normalization $\alpha > 0$, and a function of the lattice distance such that

$$a_0 := \max_{ik} \left[f(d_{ik})^{-1} \sum_j f(d_{ij}) f(d_{jk}) \right] < +\infty.$$
(3)

Under these conditions, assuming bounded interactions $||G_j(t)|| \le g$ and spins $||\mathbf{S}|| \le S$, a LRB emerges for the spin correlations $\mathbf{Z}_{ik}(t) := [\mathbf{S}_i(t), S_k^{\phi}(0)], \phi \in \{1, 2, 3\}$

$$\|\mathbf{Z}_{jk}(t)\| \le \alpha e^{\nu_{\mathrm{LR}}t} f(d_{jk}) \times \frac{2S^2}{a_0} (e^{(g^2/\nu_{\mathrm{LR}})2S\alpha a_0 t} - 1).$$
(4)

Intuitively, since bosons mediate interactions, the bosonic velocity v_{LR} limits the propagation speed of spin correlations. This is precisely the first term of the above expression, which duplicates the bosonic LRB. Additionally, the efficiency with which distant spins excite and reabsorb a propagating boson affects the LRB. This is the second term in Eq. (4), which depends on the rate $\sim g^2/v_{LR}$ at which bosons are emitted or absorbed by spins. This nonperturbative correction shows that the buildup of correlations is suppressed if bosons are much faster than spins $g \ll v_{LR}$, an adiabatic-type argument.

Note that Eqs. (2) and (3) include a very large family of bounds

$$e^{\nu_{\rm LR}t}f(d_{jk}) = e^{\nu_{\rm LR}t - \mu d_{jk}}(1 + d_{jk})^{-\eta},\tag{5}$$

with appropriate $\mu \ge 0$ and $\eta > 0$. For nearest-neighbor or short-range interactions $\mu > 0$ yields a light cone, $\mu d_{jk} - v_{LR}t \sim 0$, outside of which correlations are exponentially suppressed. For algebraically decaying interactions, $\mu = 0$, and the lines of constant correlation are only straight at short distances and times.

The proof.—We will sketch the technical steps to recover this result (see the Supplemental Material [24]). The Heisenberg equations of motion are $\dot{\mathbf{R}}_j = -\sum_k J Q_{jk}(t) \mathbf{R}_k - J G_j(t) \mathbf{S}_j$ and $\dot{\mathbf{S}}_j = i K_j(t) \mathbf{S}_j$, with a Hermitian matrix $K_j(t)$ that depends on the couplings, boson operators, and spin structure constants. The first equation is formally integrated $\mathbf{R}_j(t) = \sum_k W_{jk}(t, 0) \mathbf{R}_k(0) - \int_0^t d\tau \sum_k W_{jk}(t, \tau) J G_k(\tau) \mathbf{S}_k(\tau)$. In this

notation, the free boson propagator W is an $N \times N$ block matrix, where each block $W_{jk}(t_1, t_2) \in \mathbb{R}^{2 \times 2}$ spreads correlations between sites j and k.

The bosonic bound (2) influences the spin-spin correlations through the spin-boson correlators $\mathbf{C}_{jk}(t) := [\mathbf{R}_j(t), S_k^{\phi}(0)]$. This is seen in $\dot{\mathbf{Z}}_{jk} = i \sum_{n \in \{x,p\}} C_{jk}^n A_j^n(t) \mathbf{S}_j + i K_j(t) \mathbf{Z}_{jk}$, where the matrices $A_j^n(t)$ are defined in terms of the spin-boson couplings (Supplemental Material [24]). To eliminate the local precession of the spins, we change variables $\mathbf{D}_{jk}(t) := O_j^{-1}(t) \mathbf{Z}_{jk}(t)$ with a unitary $O_j(t)$ obtained by solving $\dot{O}_j(t) = i K_j(t) O_j(t)$. Thus,

$$\dot{\mathbf{C}}_{jk} = -\sum_{l} J Q_{jl}(t) \mathbf{C}_{lk} - J G_{j}(t) O_{j}(t) \mathbf{D}_{jk}, \qquad (6)$$

$$\dot{\mathbf{D}}_{jk} = iO_j^{-1}(t)\sum_n C_{jk}^n A_j^n(t) \mathbf{S}_j$$
(7)

describe the buildup of spin-boson correlations (6) and the conversion of spin-boson into spin-spin correlations (7). Some remarks are in order: (i) the equation for C_{jk} is solved formally in terms of D_{jk} , creating a recursion; (ii) the operator O_i absorbing the unbounded local rotations does not influence the LRB because (iii) D_{jk} and Z_{jk} have the same operator norms.

Equations (6) and (7), with the upper bounds $||G_j(t)||$, $||A_j^n(t)|| \le g$, $||\mathbf{S}_j(t)|| \le S$, the bosonic LRB (2), and the geometric factor a_0 , provide a Dyson-type recursion for the commutators norms

$$\|\mathbf{D}_{jk}(t)\| \le \|\mathbf{D}_{jk}(0)\| + 2g^2 S\alpha \sum_{l} \int_{0}^{t} d\tau_1$$
$$\times \int_{0}^{\tau_1} d\tau_2 f(d_{jl}, v_{\mathrm{LR}}(\tau_1 - \tau_2)) \|\mathbf{D}_{lk}(\tau_2)\|.$$
(8)

After summing this recursion to infinite order, the desired LRB (4) for the spin-boson lattice is recovered.

Bosonic LRB.—For the previous results to be useful, the bound of Eq. (2) must be sufficiently tight. Whereas the bosonic LR speed has been studied for nearest-neighbor [14] and algebraically decaying [15] time-independent couplings Q, we have developed a tighter bound for such models (Supplemental Material [24]). Our LR speed only relies on the off-diagonal couplings, using a recursion similar to that in Ref. [15], but eliminating the diagonal terms with unitary transformations. The case relevant for trapped ions involves long-range interactions

$$\|Q_{ik}(t)\|_{i\neq k} \le \kappa (1+d_{ik})^{-\eta} \tag{9}$$

with a strength κ that bounds the couplings and a decay power $\eta \ge 0$. We then recover Eq. (2) with $f(d) = (1+d)^{-\eta}$, $\alpha = (1+a_0)/a_0$, and a bosonic LR speed $v_{\text{LR}} = \kappa a_0$.

Trapped-ion implementation.—Equation (4) applies to a great variety of systems. In particular, we show below that

the case of trapped ions, a prominent architecture for quantum information [25], is an ideal setup to experimentally test our LRB.

Laser-cooled ions in radio-frequency or Penning traps form crystals of tunable dimensionality and geometry. The spin-boson model of Eq. (1) can be implemented on top of this state-of-the-art technology. The "bosonic lattice" describes the small transverse displacements **R** of the ions from their equilibrium positions in the crystal. The spins $\mathbf{S} = \vec{\sigma}$ are encoded in two levels of the atomic structure $\{|\uparrow\rangle, |\downarrow\rangle\}$ with long coherence times [26]. The spin-boson coupling is provided by dipole forces that push the atoms depending on their internal state [27]. Without loss of generality [28], we assume that near-field microwaves or lasers induce a uniform force in the σ^z basis. In Eq. (1) this maps to $G_i^{n\gamma}(t) = F_z(t)\delta_{n,x}\delta_{\gamma,3}$, where the strength $F_z = \sqrt{2}\tilde{\Omega}\gamma$ depends on the field intensity or Rabi frequency $\tilde{\Omega}(t)$ and the Lamb-Dicke parameter $\gamma \ll 1$.

For this trapped-ion implementation of the spin-boson lattice, we can evaluate the LRB (4), obtaining a power-law behavior (5). We start by considering the bosonic part of the evolution. The phonon coupling $Q_{ij} = \text{diag}\{\omega_t \delta_{i,j} + \mathbb{V}_{ij}(m\omega_t)^{-1}, \omega_t \delta_{i,j}\}$ contains the ions' mass *m*, the transverse trap frequency ω_t , and a dipolar interaction [29]. The off-diagonal couplings thus satisfy Eq. (9) with algebraic decay $\eta = 3$, d_{ij} being the lattice distance of the ions in the crystal. The interaction strength $\kappa = 4\beta\omega_t$ is defined in terms of the stiffness parameter [20], $\beta = e^2/4\pi\epsilon_0 m\omega_t^2 d_m^3$, which measures the ratio of the Coulomb repulsion to the trapping energy and depends on the minimal separation between two ions in the crystal d_m . Introducing the maximum force $g = \max_t |F_z(t)|$ and S = 1, the bound reads

$$\|[\sigma_{i}(t), \sigma_{j}^{\phi}(0)]\|_{\infty} \leq \frac{2}{a_{0}(1+d_{ij})^{3}} e^{\alpha_{1}(\beta\omega_{t})t} (e^{\alpha_{2}(\beta\omega_{t})t} - 1),$$
(10)

where we define $\alpha_1 = 8a_0$ and $\alpha_2 = (1/4)(1 + a_0^{-1}) \times (g/\beta\omega_t)^2$. As anticipated in the proof, the LRB depends fundamentally on the maximum group velocity of the phonon branch, given by $\beta\omega_t$, and on the efficiency of the force in exciting and absorbing a propagating phonon, $(g^2/\beta\omega_t)$.

To evaluate Eq. (10) in a realistic experimental situation, we focus on ⁹Be⁺ ions in a Penning trap [5] and refer the reader to the Supplemental Material [24] for other setups. These ions, confined with a transverse trap frequency of $\omega_t/2\pi \approx 0.8$ MHz, form a triangular crystal of $N \sim$ 100–300 lattice sites characterized by a minimal distance $d_m \sim 20 \ \mu$ m. In such experiments, the maximum phonon group velocity is currently $\beta \omega_t/2\pi \approx 60$ kHz, and oscillating state-dependent forces with $g/2\pi \approx 0.6$ kHz have been obtained from two noncopropagating laser beams in a Raman configuration. As discussed in the Supplemental Material [24], by employing larger angles of the incident beams and short pulses that relieve the need for compensating ac-Stark shifts and resolving sidebands, the strength of the forces can be increased to $g/2\pi \approx 0.3$ MHz. Still higher forces can be achieved with counterpropagating pairs of ultrafast laser pulses [30].

The last piece of information to evaluate (10) is the parameter a_0 . A crude approximation is to use an infinite lattice with uniform geometry (triangular or onedimensional) and obtain a_0 from the convolution defined above (3). This leads to $a_0 \approx 8.5$ and would set the correlation time scale at ~0.1-1 μ s.

Impulsive regime.—We will now discuss a regime where the correlation time scale can approach the optimal prediction of the LRB (10). The impulsive regime relies on strong forces $g \gg \beta \omega_t$ during a short lapse $\delta t \sim g^{-1}$. In particular, we assume that a pulsed force is applied at t = 0 to the *j*th ion to create a bosonic excitation correlated to the spin. After propagation of the bosonic field, another pulsed force is applied at the distant *i*th ion to create the spin-spin correlations. The evolution operator is obtained analytically (Supplemental Material [24]), without approximations

$$\|[\sigma_i^{x}(t), \sigma_j^{x}(0)]\|_{\infty} \le \frac{8(1+a_0)}{a_0(1+d_{ij})^3} e^{\alpha_1(\beta\omega_i)t} \times |\theta_i\theta_j|, \quad (11)$$

where $\alpha_1 = 8a_0$. The pulse area $\theta_l = \int_0^t d\tau F_{z,l}(\tau)$ gives a measure of the number of phonons excited $\bar{n}_t \sim |\theta_l|^2$. As argued above, forces can be as large as $g/2\pi \approx 0.3$ MHz for ⁹Be⁺ ions in a Penning trap so that $\beta \omega_l/g \approx 0.2$ and we achieve the impulsive regime. Note that the pulsed forces should be switched on-off in $\delta t \sim 0.1-1 \ \mu$ s. In Fig. 1, we numerically solve the impulsive time evolution (see Supplemental Material [24]). The spread of correlations is much faster ($\sim 10 \ \mu$ s) than experimental decoherence (without reaching the theoretical maximum).

Perturbative regime.—Whereas our LRB (10) gives the fastest time scale of correlation, many experiments for the simulation of quantum magnetism [5,17] are implemented in the so-called perturbative regime, which leads to significantly slower correlation speeds. The perturbative



FIG. 1 (color online). Spin correlation spread in the impulsive regime. In this regime, we evaluate numerically the bound $\|[\sigma_i^x(t), \sigma_j^x(0)]\|_{\infty} \le f(t)$, where $f(t) = \max_{\tau \le t} \{8|\sin(W_{ij}^{xp}(\tau, 0))|\} \times \theta_i \theta_j$ is obtained from the exact time evolution of the impulsive regime. We consider a crystal of N = 253 ⁹Be⁺ ions [5], assuming pulse areas of $\theta_l = 1$. The white circle corresponds to a wave front advancing at a speed of $3d_m\beta\omega_t$.



FIG. 2 (color online). Experimental sequence to test the LRB: (a) Always-on and (b) pulsed spin-phonon forces. We represent the initialization step in blue, which consists of laser cooling followed by optical pumping \mathcal{P} and leads to $|\downarrow\cdots\downarrow\rangle\langle\downarrow\cdots\downarrow|\otimes\rho_{\rm th}$, where $\rho_{\rm th}$ is a thermal state of the phonons after Doppler cooling. We then apply a $\pi/2$ pulse $U_i =$ $\exp\{i(\pi/2)\sigma_i^{y}\}$ by driving the carrier transition [25]. In the measurement step in red, one collects the state-dependent fluorescence \mathcal{M} during a continuous driving of the cycling transition [25]. At the beginning of the evolution step $t = t_0$, we apply the unitary U_V associated to the impulsive perturbation V(t) described in the main text. This is followed by the actual evolution under the state-dependent forces: (a) in the always-on regime, the forces should be switched on continuously during the evolution, or (b) in the impulsive regime, we apply two pulsed forces. Additionally, at the middle of the evolution, we apply the spin-echo sequence $U_{SE} \sigma_i^z \rightarrow -\sigma_i^z$ and $\tilde{\Omega} \rightarrow -\tilde{\Omega}$ to refocus uncompensated ac-Stark shifts. Before measuring, we apply another $\pi/2$ pulse $\tilde{U}_i = \exp\{-i(\pi/2)\sigma_i^y\}$.

regime is characterized by oscillating forces that are much weaker than their detuning from the trap frequency $g \ll \delta_t$. In this regime, phonons can be approximately traced out, leading to effective algebraically decaying spin-spin interactions [20,21], $H_{\text{eff}} = \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$. When $\beta \omega_t \ll 2\delta_t$, the effective interaction is dipolar $||J_{ij}|| \leq 8J_0/(1 + d_{ij})^3$, with $J_0 = (g/4\delta_t)^2 \beta \omega_t$. In this case, we can apply the existing LRBs for spin models [13], obtaining

$$\|[\sigma_i(t), \sigma_j^{\phi}(0)]\|_{\infty} \le \frac{2}{a_0(1+d_{ij})^3} (e^{\tilde{\alpha}_2(\beta\omega_i)t} - 1), \quad (12)$$

where $\tilde{\alpha}_2 = (a_0/8)(g/\delta_t)^2$. For the large detunings required to obtain the dipolar decay, $\delta_t/2\pi \approx 80$ kHz, the propagation of spin correlations (12) becomes very slow (~1 s). For this reason, experiments use smaller detunings [5], leading to stronger couplings at the expense of becoming truly long ranged where the paradigm of LRBs no longer applies [13]. Yet, one can still expect correlation propagation in time scales ~1 ms from the effective model, which are still much slower than the optimal LRB (10) [31].

Probing the LRB through fluorescence.—We discuss how to exploit the control or measurement tools of trapped-ion experiments [25] to probe LRBs. Note that single-time observables, e.g., $\langle \sigma_i^{\alpha}(t) \rangle$, $\langle \sigma_i^{\alpha}(t) \sigma_j^{\beta}(t) \rangle$, are already being measured with trapped ions [32] or atoms in optical lattices [1,33]. Our aim is to measure retarded correlation functions $\langle \sigma_i^{\alpha}(t) \sigma_i^{\beta}(0) \rangle$.

The experimental scheme to accomplish it, both for always-on [Fig. 2(a)] and pulsed [Fig. 2(b)] statedependent forces, is composed of three steps. (i) The initialization consists of preparing a localized spin excitation $|+\rangle = (\uparrow +\rangle |\downarrow\rangle)/\sqrt{2}$ by a $\pi/2$ pulse at the *j*th ion [34], while the phonon lattice is in a thermal state ρ_{th} (details in Fig. 2), such that $\rho_0 = |\downarrow \cdots +_i \cdots \downarrow\rangle \langle \downarrow \cdots +_i \cdots \downarrow| \otimes$ ρ_{th} . (ii) The *evolution* consists of letting the excitation propagate for $t \in (t_0, t_f)$, while switching on the statedependent forces continuously [Fig. 2(a)] or in two pulses [Fig. 2(b)]. To measure the retarded spin correlation functions to test the LRBs, we need to apply two unitaries in addition to the forces. First, we should apply an impulsive perturbation $V(t) = \lambda_B \sigma_i^x \delta(t - t_0)$ localized at the *j*th ion and $\lambda_B \ll 1$. Second, after letting the system evolve, we should apply a $\pi/2$ pulse at the distant *i*th ion. (iii) The measurement consists of collecting the state-dependent fluorescence of the ion crystal, which amounts to a measurement of $\langle \sigma_i^z(t_f) \rangle$. Using a linear-response-theory-type argument (Supplemental Material [24]), we have shown that $\partial_{\lambda_B} \langle \sigma_i^z(t_f) \rangle |_{\lambda_B=0} = -i \langle \sigma_i^x(t_f) \sigma_j^x(t_0) \rangle$. By modification of the unitaries (Supplemental Material [24]) [35], it is possible to recover any retarded spin correlation $\langle \sigma_i^{\alpha}(t_f) \sigma_i^{\beta}(t_0) \rangle$. We remark that the operations required in each step are performed individually with accuracies better than 99% in current experiments [25].

Conclusions.—We have derived a new LRB for a collection of models (1) involving spins and bosons in a lattice. Although the LRB applies to a variety of quantum-optical setups (e.g., superconducting circuits), we have focused on ion crystals, where it pinpoints that spin correlations can spread much faster than the experimental regimes currently considered. Regardless of the infinite dimensionality of Eq. (1), we conjecture that the LRB encloses further theoretical implications, such as the clustering of correlations or the efficiency of time-dependent density matrix renormalization group methods, which might be of interest to recent studies [37].

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Note added.—Upon completion of this manuscript, we became aware of the e-print of Ref. [33], figuring a similar measurement protocol for spin correlations.

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m = 3. However, our LRBs apply to any Lie algebra with fully antisymmetric $f^{\alpha\beta\gamma}$.

- [24] See Supplemental Material at http://link.aps.org/ supplemental/10.1103/PhysRevLett.111.230404 for a detailed account of the spin-boson proof, a proof of a tighter version of the existing bound for harmonic systems in Ref. [15], and details on the application of LRB and measurement schemes in trapped-ion setups.
- [25] See H. Haeffner, C. F. Roos, and R. Blatt, Phys. Rep. 469, 155 (2008) and references therein.
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- [27] See K.-A. Brickman Soderberg and C. Monroe, Rep. Prog. Phys. 73, 036401 (2010) and references therein.
- [28] Time-dependent forces in different bases and combinations thereof can also be obtained experimentally (see Supplemental Material [24]) and treated with our LRB (4).
- [29] The dipole-dipole couplings are $\mathbb{V}_{ij} = e_0^2/|\mathbf{r}_i^0 \mathbf{r}_j^0|^3$ for $i \neq j$ and $\mathbb{V}_{ii} = -\sum_{j \neq i} \mathbb{V}_{ij}$, where $e_0^2 = e^2/4\pi\epsilon_0$ is given in terms of the ion charge e and the vacuum permittivity ϵ_0 .
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