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Simulation of the Jahn–Teller–Dicke magnetic structural phase transition with trapped ions

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Abstract

We study theoretically the collective E $\otimes$ e Jahn–Teller–Dicke distortion in a system of trapped ions. In a previous work (Porras *et al* 2012 *Phys. Rev. Lett.* **108** 235701) we have focused on cooperative Jahn–Teller models consisting of an ensemble of effective spins coupled to a set of many vibrational modes. Here, we show that under suitable conditions the spin ensemble may interact only with a single vibrational mode in each radial direction with U(1) symmetric couplings. Our model is exactly solvable in the thermodynamical limit and it is amenable to be solved by exact numerical diagonalization for a moderate number of ions. We show that trapped ions are ideally suited to study the spontaneous breaking of a continuous symmetry as well as magnetic structural phase transitions in a mesoscopic spin–boson system.

(Some figures may appear in colour only in the online journal)

1. Introduction

Physical systems where bosonic modes interact with electronic or pseudospin degrees of freedom reveal a rich variety of phenomena in condensed matter and atomic physics. A prominent example is given by Jahn–Teller (JT) models [1, 2] which describe the interaction of electronic orbital degrees of freedom with vibrational modes either in molecules or solids. The JT effect is formulated as a structural instability of molecular configurations in electronically degenerate states. In particular, the electron–phonon coupling shifts the potential minima of the nuclei, which leads to position reordering and molecular distortion. Similar to molecular systems, the properties of some crystals are also strongly affected by the JT coupling that induces symmetry breaking and structural phase transitions [3]. Furthermore, the strong electron–phonon coupling in cooperative JT models is an important factor in the description of colossal magneto-resistance in manganites and high T_c -superconductivity [4, 5].

Atomic systems such as ultracold atoms and trapped ions allow experimentalists to implement JT models in a controllable way that is not possible in solid-state or molecular setups. This is a motivation to push the current quantum technology towards the realization of analogical quantum simulators (AQS). The latter are controllable systems where interactions between particles can be tuned and quantum states can be accurately prepared and measured with high efficiency. Recently, physical realizations of JT couplings have been discussed in terms of two-level systems coupled to a bimodal cavity [6] and Bose–Einstein condensates in the presence of spatially dependent laser fields [7]. These systems pave the way for studying quantum phenomena such as ground-state entanglement [8, 9] and the creation of artificial non-Abelian magnetic fields [10]. Quantum chaotic behaviour in the energy spectrum of multi-spin lattice JT model was discussed in [11].

Among the most promising physical systems for implementing AQS are linear ion crystals interacting with

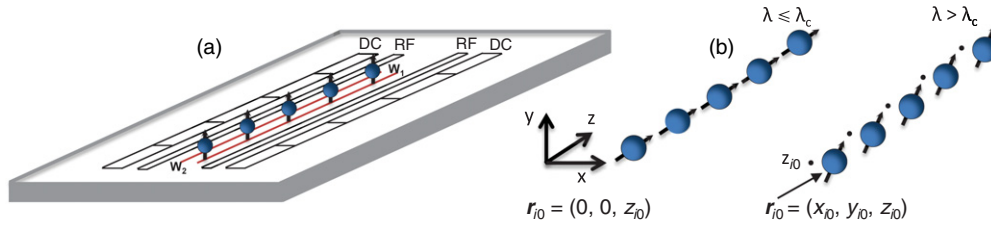


Figure 1. (a) Exemplary geometry for the realization of the collective Jahn-Teller-Dicke model with a time-varying magnetic field gradient produced by a surface-electrode trap. A linear ion crystal is oriented along the z axis. Oscillating currents in two wires W_1 and W_2 parallel to the linear ion crystal are used to provide the symmetric spin-phonon coupling. (b) A magnetic structural phase transition. For spin-phonon coupling $\lambda \leq \lambda_c$ the equilibrium positions of the ions, z_{i0} , are aligned along the z axis, i.e. $x_{i0} = y_{i0} = 0$ and the only non-zero projection of the total collective spin operator is $\langle \hat{J}_z \rangle / j = -1$. Increasing $\lambda > \lambda_c$ the system undergoes a magnetic structural phase transition, wherein the radial ions' equilibrium positions are displaced by $x_{i0} = q_0 \sqrt{2\alpha_x/j}$ and $y_{i0} = q_0 \sqrt{2\alpha_y/j}$, accompanied by a spin ordering with $\langle \hat{J}_{x,y}^2 \rangle \neq 0$.

external lasers or magnetic fields [12, 13]. The main advantages of trapped ions are their addressability, long coherence times and high fidelity readout. The current available ion trapping technology allows us to explore the physics of quantum phase transitions in complex spin systems [14–18], interacting bosons [19–23], relativistic effects, [24, 25] and quantum open systems [26].

In this work we propose an implementation of AQS of an infinite range E $\otimes$ e JT model based on a trapped ion crystal. The doublet of electronic states is replaced here by two internal metastable states of the ions. The pair of molecular vibrational modes is represented by the two degenerate orthogonal center-of-mass (c.m.) modes, respectively, in the two radial directions. We show that the U(1) symmetric JT spin-phonon coupling can be provided by applying a magnetic field with time-oscillating gradient, which couples the collective spin ensemble to the two orthogonal c.m. modes [27–29], figure 1(a). Such an oscillating magnetic field has been used to implement experimentally a single qubit rotation and multi-qubit quantum gates [30], which shows that our model could be realized with the current state-of-the-art ion trap setup. In a previous work [21] we have focused on cooperative JT models in which all vibrational modes are coupled to the effective spins, something that leads to the reordering of the ion positions and the formation of a spin-phonon quasi-condensate. In contrast, here we study the interactions between the spin ensemble and a single vibrational mode in each radial direction. We will use the denomination Jahn-Teller-Dicke (JTD) model for the single-mode Hamiltonian studied here, to distinguish it from the cooperative many-mode systems. The JTD model is quasi-exactly solvable in the sense that the ground state can be found exactly in the thermodynamical limit [31], or even studied by exact numerical diagonalization with a moderate number of ions. The experimental implementation of the JTD model can be used for the controlled study of quantum phenomena such as symmetry breaking, as well as to benchmark trapped ion quantum simulators in a numerically tractable limit.

The E $\otimes$ e JTD model possesses a continuous symmetry associated with rotation in the plane orthogonal to the trap axis. There is a critical spin-phonon coupling above which the U(1) symmetry is spontaneously broken and the system evolves into one particular ground state which does not respect the same symmetry as the Hamiltonian. That broken symmetry

is associated with a magnetic structural phase transition at zero temperature, where the equilibrium positions of the ions are displaced in an *arbitrary* direction within the radial x - y plane, together with the creation of macroscopic spin coherence, see figure 1(b). We show that the radial distortion of the ion crystal is accompanied with the creation of density of phonon excitations and macroscopic spin coherence, which is an analogue to the normal-to-super-radiance phase transition in the Dicke model [32, 33].

The paper is arranged as follows: in section 2 we describe the collective vibrational spectrum of the linear ion crystal. We show that an oscillating magnetic field gradient could select only one vibrational mode in each radial direction and thus to provide the symmetric JTD spin-phonon coupling. In section 3 we explore the spin-phonon interaction assuming a thermodynamical limit. By using the well known technique of the Holstein-Primakoff representation we derive an analytical result for the amount of distortion and the spin ordering of the system. The experimental requirements for the physical implementation and readout of the final state of our model are discussed in section 4. Finally, in section 5 we conclude our findings and present further interesting phenomena to be explored.

2. The trapped-ion E $\otimes$ e Jahn-Teller-Dicke model

2.1. Trapped-ion radial vibrational Hamiltonian

We consider a crystal of N identical ions with mass M and charge e confined in a linear Paul trap along the z axis. Each ion has two metastable internal levels with energy separation $\tilde{\omega}_0$. The system is described by the Hamiltonian ($\beta = x, y, z$ and $\hbar = 1$ from now on)

$$\hat{H}_0 = \hat{H}_{\text{spin}} + \hat{H}_{\text{vib}},$$

$$\hat{H}_{\text{spin}} = \sum_{i=1}^N \frac{\tilde{\omega}_0}{2} \sigma_i^z, \quad \hat{H}_{\text{vib}} = \sum_{\beta} \sum_{i=1}^N \frac{\hat{p}_{\beta,i}^2}{2M} + \hat{V}. \quad (1)$$

The first term in $\hat{H}_0$ describes the energy of the two-level systems with σ_i^β being the Pauli matrices for ion i . $\hat{H}_{\text{vib}}$ is the vibrational Hamiltonian, which contains the ions' kinetic energy and the potential energy of the ion crystal. The latter

consists of the effective harmonic potential and the mutual Coulomb repulsion [35]

$$\hat{V} = \frac{M}{2} \sum_{\beta} \sum_{i=1}^N \omega_{\beta}^2 \hat{r}_{\beta,i}^2 + \sum_{i>l}^N \frac{e^2}{|\hat{r}_i - \hat{r}_l|}, \quad (2)$$

where $\hat{r}_i$ is the position vector operator of ion i and ω_{β} denote the trapping frequencies. In this work we consider the symmetry condition $\omega_x = \omega_y = \omega_r$, which can be achieved by proper adjustment of the trapping voltages or by special design of the trap geometry [34]. For sufficiently strong radial confinement ($\omega_r \gg \omega_z$) ions occupied equilibrium positions $\vec{r}_{i0} = (0, 0, z_{i0})$ along the z axis. The latter are determined by the balance between the Coulomb repulsion and the harmonic trapping force, which yields $(\partial \hat{V} / \partial \vec{r}_i)_{\vec{r}_i = \vec{r}_{i0}} = 0$. At low temperature the ions undergo only small oscillations around the equilibrium positions, namely

$$\hat{r}_i = \delta \hat{r}_{x,i} \vec{e}_x + \delta \hat{r}_{y,i} \vec{e}_y + (z_{i0} + \delta \hat{r}_{z,i}) \vec{e}_z, \quad (3)$$

where $\delta \hat{r}_{\beta,i}$ are the displacement operators.

The radial vibrational spectrum is essential for the implementation of our idea. For that reason we discuss here its main characteristics, a more complete discussion can be found, for example in [35–37]. First we notice that a suitable length scale is given by $l_0^3 = e^2 / (M \omega_z^2)$. Accordingly, we define a dimensionless equilibrium position, $z'_{i0} = z_{i0} / l_0$. Making a Taylor expansion of the potential (2) around z'_{i0} and neglecting $\delta \hat{r}_{z,i} \delta \hat{r}_{\alpha,i}^2$, $\delta \hat{r}_{\alpha,i}^3$ and higher order terms, the radial vibration is described by the Hamiltonian ($\alpha = x, y$ from now on)

$$\hat{H}_{\text{rad}} = \sum_{\alpha} \sum_{i=1}^N \frac{\hat{p}_{\alpha,i}^2}{2M} + \frac{M \omega_r^2}{2} \sum_{\alpha} \sum_{i,l=1}^N \mathcal{K}_{il} \delta \hat{r}_{\alpha,i} \delta \hat{r}_{\alpha,l}. \quad (4)$$

Note that within harmonic approximation of the potential (2) the radial motion is decoupled from the axial motion. The collective vibrational frequencies $\omega_n = \omega_r \sqrt{\kappa_n}$ can be found by solving the eigenvalue problem,

$$\sum_{l=1}^N \mathcal{K}_{il} b_{l,n}^{\alpha} = \kappa_n b_{i,n}^{\alpha}, \quad (5)$$

where $b_{l,n}^{\alpha}$ are the normal mode eigenvectors and κ_n are the corresponding eigenvalues. The matrix $\mathcal{K}_{il}$ is given by

$$\mathcal{K}_{il} = \begin{cases} 1 - \sum_{l' \neq l}^N \frac{\omega_z^2}{\omega_r^2} \frac{1}{|z'_{l0} - z'_{l'0}|^3}, & (i = l), \\ \frac{\omega_z^2}{\omega_r^2} \frac{1}{|z'_{i0} - z'_{l0}|^3}, & (i \neq l). \end{cases} \quad (6)$$

The equilibrium positions for the ions in natural units depend on the number of ions N only, and thus, the radial vibrational modes are governed solely by the ratio ω_z / ω_r .

The vibrational Hamiltonian $\hat{H}_{\text{rad}}$ can be diagonalized by defining

$$\begin{aligned} \delta \hat{r}_{\alpha,i} &= \sum_{n=1}^N b_{i,n}^{\alpha} q_n^0 (\hat{a}_{\alpha,n}^{\dagger} + \hat{a}_{\alpha,n}), \\ \hat{p}_{\alpha,i} &= i \sum_{n=1}^N b_{i,n}^{\alpha} p_n^0 (\hat{a}_{\alpha,n}^{\dagger} - \hat{a}_{\alpha,n}), \end{aligned} \quad (7)$$

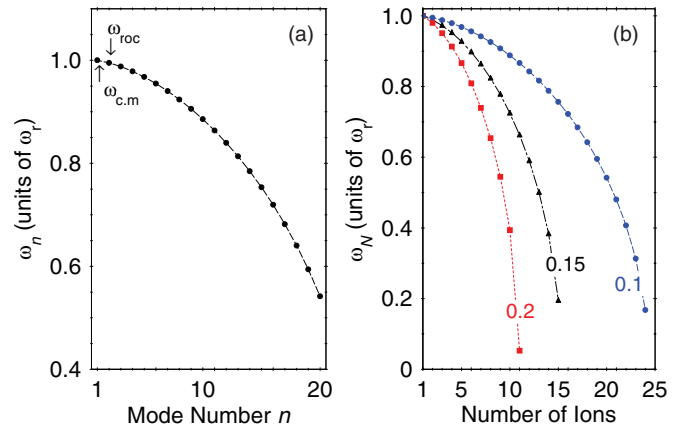


Figure 2. (a) Eigenfrequencies ω_n of the radial collective vibrational spectrum for a linear ion crystal with $N = 20$ ions and $\omega_z / \omega_r = 0.1$. The highest and second highest vibrational frequency is the $\omega_{c.m.}$ and the rocking mode ω_{roc} , respectively. (b) The lowest vibrational frequency, ω_N , as a function of the number of ions for various aspect ratios $\omega_z / \omega_r = 0.2, 0.15$ and 0.1 . Note that for a given aspect ratio, there is a maximum value for the number of ions above which the frequency ω_N becomes imaginary. The latter condition signals the transition from the linear into the zigzag structural phase. The critical N varies for different aspect ratio ω_z / ω_r .

with $q_n^0 = 1 / \sqrt{2M\omega_n}$, and $p_n^0 = \sqrt{M\omega_n/2}$. By substituting (7) in $\hat{H}_{\text{rad}}$ we obtain a set of uncoupled collective vibrational modes

$$\hat{H}_{\text{rad}} = \sum_{\alpha} \sum_{n=1}^N \omega_n \left(\hat{a}_{\alpha,n}^{\dagger} \hat{a}_{\alpha,n} + \frac{1}{2} \right). \quad (8)$$

Here $\hat{a}_{\alpha,n}^{\dagger}$ and $\hat{a}_{\alpha,n}$ are the creation and annihilation operators of phonon in the n th vibrational mode and direction α , respectively.

2.2. Scaling of the vibrational modes with N

In this work we will focus on a range of parameters such that internal states are coupled only to the c.m. mode and we can neglect all the other vibrational modes. To understand the validity of this approximation, it is essential to calculate the energy splitting from the c.m. mode to the energetically nearest vibrational mode, since that gap determines the time scales upon which the c.m. mode can be resolved. Obviously, the c.m. energy addressability imposes a restriction on N , since energy levels get energetically closer for longer ion chains.

For the radial modes considered in this work, the c.m. energy, $\omega_{c.m.}$ is the highest one. The next nearest vibrational energy, ω_{roc} corresponds to the rocking mode, see figure 2(a). The relevant energy for finding the regime of validity of the JTD Hamiltonian is thus the difference in energy between those radial modes, $\Delta_{c.m.} = \omega_{c.m.} - \omega_{roc}$. Remarkably, that difference can be exactly calculated, and it only depends on the ratio ω_z / ω_r (see [35]),

$$\Delta_{c.m.} = \omega_r - \omega_r \sqrt{1 - \left(\frac{\omega_z}{\omega_r} \right)^2}. \quad (9)$$

Apparently equation (9) suggests that the vibrational gap does not depend on the number of ions N . However, for a fixed ratio ω_z / ω_r , there is a maximum number of ions, N_{max} , for which the

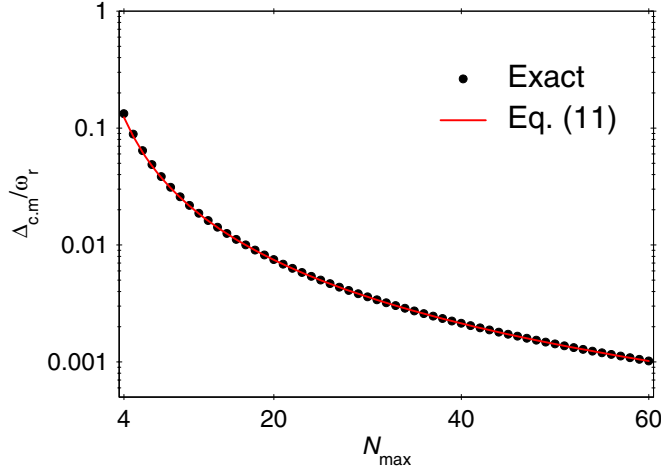


Figure 3. The scaling of the energy gap $\Delta_{c.m.}$ with N_{max} . The exact result (black circle) is compared with equation (11) (solid line).

ion chain undergoes a structural transition into a zigzag phase [38, 39], see figure 2(b). This effect is the main limitation for the scalability of our proposal. We estimate first the scaling of ω_z/ω_r with N_{max} . For this we follow the definitions in [40] and define $\beta_z = 2e^2/(M\omega_z^2 d_0^3)$, $\beta_r = e^2/(M\omega_r^2 d_0^3)$, where d_0 is the average distance between ions. For a value $\beta_r = \beta_{r,c} \approx 1$ the radial trapping energy becomes comparable to the Coulomb coupling between the radial ion displacements, and we expect the onset of the transition to a zigzag phase. Note that

$$\beta_r(N) = \frac{1}{2}\beta_z \left(\frac{\omega_z}{\omega_r}\right)^2 \approx \frac{1}{24} \frac{N^2}{\log(6N)} \left(\frac{\omega_z}{\omega_r}\right)^2, \quad (10)$$

being an approximate result for Coulomb chains [41]. Equation (10) allows us to determine N_{max} by the relation $\beta_{r,c} = \beta_r(N_{max})$. Together with equation (9), and considering the limit $(\omega_z/\omega_r)^2 \ll 1$, we arrive to

$$\frac{\Delta_{c.m.}}{\omega_r} \approx 12\beta_{r,c} \frac{\log(6N_{max})}{(N_{max})^2}. \quad (11)$$

That is, up to logarithmic corrections, the vibrational gap scales like the inverse of the maximum possible number of ions. In figure 3 we show a numerical exact calculation which confirms that scaling with a value $12\beta_{r,c} = 0.6228$. To find N_{max} we have calculated the number of ions at which the smallest vibrational energy becomes negative, which signals the onset of the transition to a zigzag phase.

The scaling imposed by equation (11) poses severe limitations for our proposal to be scaled up. For example, consider a moderate chain with $N = 15$, which leads to $\Delta_{c.m.} \approx 0.013\omega_r$. However, we note, that the limitation results in a trade-off between the length of the chain, and the speed of the quantum simulation, being mesoscopic systems with a high number of entangled ions is still possible.

2.3. Jahn–Teller $E \otimes e$ spin–phonon coupling

We describe the interaction of the trapped ion spin ensemble with the collective vibrational modes. Those interactions can be induced either by laser dipole forces or by magnetic field gradients. Here we focus on the latter technique since it naturally implements symmetric couplings in the x – y plane,

and it also avoids undesired effects like high-order terms in the Lamb–Dicke expansion and the spontaneous emission decoherence [28, 29]. Let us assume that the ion crystal interacts with an oscillating magnetic quadrupole of the form

$$\vec{B}(t; x, y) = Bf(t)(\vec{e}_x x - \vec{e}_y y). \quad (12)$$

Such a field can be created in a micro-structured planar ion trap, recently experimentally demonstrated [30], which contains two wires parallel to the linear ion crystal (figure 1(a)) [42]. The magnetic field affects only the radial motion of the ion crystal and thus the motion along the z axis can be safely neglected. We consider a time modulation $f(t) = (\cos \nu_b t + \cos \nu_r t)$ to control the couplings. The magnetic dipole interaction is described by the interaction Hamiltonian

$$\hat{H}_I = - \sum_{i=1}^N \hat{\vec{\mu}}_i \cdot \vec{B}(t; \delta r_{x,i}, \delta r_{y,i}), \quad (13)$$

where $\hat{\vec{\mu}}_i = \mu_x \sigma_i^x + \mu_y \sigma_i^y$ is the magnetic dipole moment operator of the ion i , and we assume the condition $\mu_x = \mu_y = \mu$. To control the spin–phonon couplings we choose driving frequencies

$$\nu_{b,r} = (\tilde{\omega}_0 - \omega_0) \pm (\omega_{c.m.} - \omega). \quad (14)$$

The goal is to drive spin-flip transitions with detuning ω_0 as well as blue- and red-sideband transitions of the c.m. mode $\omega_{c.m.}$ with detuning $\pm\omega$. The applied bichromatic magnetic field in x – y plane, establishes Jaynes–Cummings and anti-Jaynes–Cummings interactions, which couple the internal and the motional states of the ions [30, 43]. The Hamiltonian in the interaction picture with respect to $\hat{H}_0$ is given by

$$\begin{aligned} \hat{H}_I = & -\frac{\mu B}{2} \sum_{i=1}^N \delta \hat{r}_{x,i}(t) (\sigma_i^+ e^{i\tilde{\omega}_0 t} + \sigma_i^- e^{-i\tilde{\omega}_0 t}) f(t) \\ & -i \frac{\mu B}{2} \sum_{i=1}^N \delta \hat{r}_{y,i}(t) (\sigma_i^+ e^{i\tilde{\omega}_0 t} - \sigma_i^- e^{-i\tilde{\omega}_0 t}) f(t), \end{aligned} \quad (15)$$

where $\sigma_i^\pm$ are the Pauli spin-flip operators. The displacement operators $\delta \hat{r}_{\alpha,i}$ are recast in terms of collective operators by means of equation (7) such that we can in a controlled way choose the driving frequencies to pick the radial c.m. mode as the only resonant one. For this, the following set of conditions has to be satisfied,

$$\begin{aligned} \omega_n & \ll \tilde{\omega}_0, \\ \lambda, \omega, \omega_0 & \ll \Delta_{c.m.}, \end{aligned} \quad (16)$$

where $\lambda = -\mu q_0 B / \sqrt{2}$ is the spin–phonon coupling with $q_0 \equiv q_1^0$ being the size of the c.m. wave packet. The latter conditions ensures the approximation that any vibrational mode but the c.m. one can be neglected in a rotating wave approximation. Consider as an example Zeeman $^{40}\text{Ca}^+$ qubits with transition frequency $\tilde{\omega}_0 = 30$ MHz confined in a planar trap with radial trapping frequency $\omega_r/2\pi = 4$ MHz, the first condition in equation (16) is justified. Assuming crystal with $N = 10$ ions the frequency splitting is approximately $\Delta_{c.m.}/2\pi \approx 103$ kHz, see table 1. With current ion-trap technology a spin–phonon coupling of the order of $\lambda/2\pi \approx 5$ kHz is achieved by magnetic field gradient $b = 35 \text{ Tm}^{-1}$, which allowed the contribution

Table 1. The values of $\Delta_{\text{c.m.}}$, $\lambda = 5 \times 10^{-2} \Delta_{\text{c.m.}}$, ΔE_{JTD} and total interaction time T for various N_{max} . We choose $\omega_r/2\pi = 4$ MHz, $\omega = 1.29\lambda$ ($\omega = \omega_0$) and $T = 5\tau_{\text{JTD}}$.

N_{max}	$\Delta_{\text{c.m.}}/2\pi$ (kHz)	$\lambda/2\pi$ (kHz)	$\Delta E_{\text{JTD}}/2\pi$ (kHz)	T (ms)
10	103.3	5.2	0.9	5.5
20	29.9	1.5	0.2	28.4
30	14.4	0.7	0.1	74.9
40	8.5	0.4	0.03	149.8

of the off-resonant terms in equation (15) to be neglected. Under those assumptions we can approximate the interaction Hamiltonian by

$$\hat{H}_I = \frac{\lambda}{\sqrt{2N}} (\hat{a}_x^\dagger e^{i\omega t} + \hat{a}_x e^{-i\omega t}) (\hat{J}_+ e^{i\omega_0 t} + e^{-i\omega_0 t} \hat{J}_-) + i \frac{\lambda}{\sqrt{2N}} (\hat{a}_y^\dagger e^{i\omega t} + \hat{a}_y e^{-i\omega t}) (\hat{J}_+ e^{i\omega_0 t} - \hat{J}_- e^{-i\omega_0 t}). \quad (17)$$

Here $\hat{a}_\alpha$ and $\hat{a}_\alpha^\dagger$ correspond to the annihilation and creation operators of the c.m. phonon, respectively. Note that the factor $N^{-1/2}$ in (17) appears due to the excitation of the radial c.m. modes, wherein the spin–phonon coupling scales as $b_{j,1}^\alpha \sim N^{-1/2}$ [35]. Since the ions are equally coupled with the phonons we have introduced the collective spin operators $\hat{J}_+ = \sum_{i=1}^N \sigma_i^+$ ($\hat{J}_+^\dagger = \hat{J}_-$) and $\hat{J}_z = 1/2 \sum_{i=1}^N \sigma_i^z$, which describe the combined ionic pseudospin of length $j = N/2$. The collective spin basis is spanned by the Dicke states $|j, m\rangle$, which are eigenvectors of $\hat{J}^2 |j, m\rangle = j(j+1) |j, m\rangle$ and $\hat{J}_z |j, m\rangle = m |j, m\rangle$, respectively. The Hilbert space of the total system is spanned by the states $\{|j, m\rangle \otimes |n_x, n_y\rangle\}$, where $|n_{x,y}\rangle$ is the Fock state with $n_{x,y}$ phonons. After performing the time-dependent unitary transformation $\hat{F} = e^{i\omega t(\hat{n}_x + \hat{n}_y) + i\omega_0 t \hat{J}_z}$, such that $\hat{H}_{\text{JTD}} = \hat{F}^\dagger \hat{H}_I \hat{F} - i\hbar \hat{F}^\dagger \partial_t \hat{F}$, we express the Hamiltonian (17) as

$$\hat{H}_{\text{JTD}} = \omega(\hat{n}_x + \hat{n}_y) + \omega_0 \hat{J}_z + \frac{\lambda}{\sqrt{4j}} (\hat{J}_+ + \hat{J}_-) (\hat{a}_x^\dagger + \hat{a}_x) + i \frac{\lambda}{\sqrt{4j}} (\hat{J}_+ - \hat{J}_-) (\hat{a}_y^\dagger + \hat{a}_y). \quad (18)$$

Hence we arrive at the realization of the collective JTD model, which describes a two-degenerate vibrational modes coupled to the effective spin ensemble by the symmetric JT coupling. The Hamiltonian (18) is a multi-particle extension of the E $\otimes$ e model in molecular and solid-state physics. The trapped ion realization of the JTD model allows for easy tuning of the effective spin and phonon frequencies by adjusting the detuning and the spin–phonon coupling via the magnetic gradient.

It is convenient to rewrite the Hamiltonian (18) in terms of right and left chiral operators [24]

$$\hat{a}_r^\dagger = \frac{1}{\sqrt{2}} (\hat{a}_x^\dagger + i\hat{a}_y^\dagger), \quad \hat{a}_l = \frac{1}{\sqrt{2}} (\hat{a}_x + i\hat{a}_y), \quad (19)$$

which can be used to express the z component of the total angular momentum $\hat{L}_z = \sum_{j=1}^N \hat{L}_j^z = \hat{n}_r - \hat{n}_l$. Using (19), the Hamiltonian (18) is expressed in the form

$$\hat{H}_{\text{JTD}} = \omega(\hat{a}_r^\dagger \hat{a}_r + \hat{a}_l^\dagger \hat{a}_l) + \omega_0 \hat{J}_z + \frac{\lambda}{\sqrt{2j}} \hat{J}_+ (\hat{a}_r^\dagger + \hat{a}_l) + \frac{\lambda}{\sqrt{2j}} \hat{J}_- (\hat{a}_r + \hat{a}_l^\dagger), \quad (20)$$

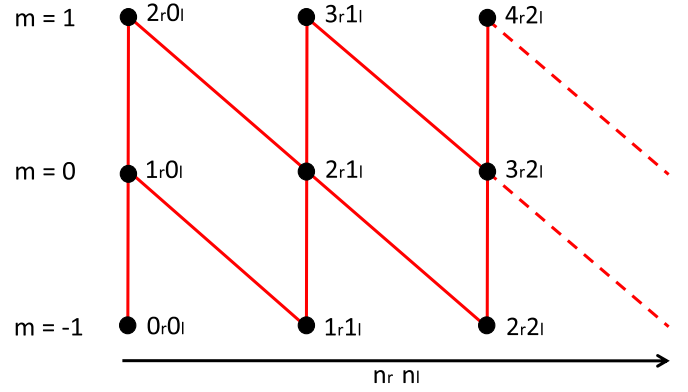


Figure 4. Coupling pattern of the relevant ionic and vibrational states $|j, m\rangle |n_r, n_l\rangle$ for $j = 1$. Due to the symmetries in spin–phonon coupling and parity of the Hamiltonian (18), the quantum number $n_r - n_l - m$ is preserved and the Hilbert space is decomposed into subspaces of positive (negative) parity. Here we show the non-vanishing couplings (solid lines) between states with $n_r - n_l - m = 1$ and positive parity.

which shows that in the JTD model the creation of collective atomic excitation is accompanied by the creation (annihilation) of right (left) quantum of angular momentum and vice versa.

2.4. Symmetries

Due to the symmetry in the spin–phonon interaction the JTD Hamiltonian (18) is invariant under the combined application of a rotation in the x – y plane

$$\begin{bmatrix} \hat{a}_x \\ \hat{a}_y \end{bmatrix} = \begin{bmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} \hat{a}_x' \\ \hat{a}_y' \end{bmatrix} \quad (21)$$

and a phase shift $\hat{J}_+ \rightarrow e^{-i\phi} \hat{J}_+$. Hence, the JTD model is U(1) invariant, with the charge $\hat{C} = \hat{L}_z - \hat{J}_z$ being the group generator, $[\hat{H}, \hat{C}] = 0$. This implies that the Hilbert space is decomposed into subspaces with a well-defined quantum number $n_r - n_l - m$, figure 4. Because the Hamiltonian (18) is quadratic in the spin and phonon operators, it is also invariant under the application of the parity operator $\hat{\Pi} = \exp[i\pi(\hat{n}_r + \hat{n}_l + \hat{J}_z + j)]$. The Hilbert space of the total system is thus additionally decomposed into two noninteracting subspaces with an even and odd number of total excitations [44].

2.5. Holstein–Primakoff representation

In order to study the critical behaviour of a collective JTD model (18) in the thermodynamical limit $j \rightarrow \infty$, we use the Holstein–Primakoff transformation [45], whereby the spin- $N/2$ degree of freedom is expressed in terms of single mode bosonic operators, namely $\hat{J}_+ = \hat{b}^\dagger \sqrt{2j - \hat{b}^\dagger \hat{b}}$, $\hat{J}_- = \sqrt{2j - \hat{b}^\dagger \hat{b}} \hat{b}$ and $\hat{J}_z = \hat{b}^\dagger \hat{b} - j$. This transformation preserves the spin algebra and allows the JTD Hamiltonian (18) to be converted into the Hamiltonian

$$\begin{aligned}\hat{H}_{\text{JTD}} = & \omega(\hat{n}_x + \hat{n}_y) + \omega_0(\hat{b}^\dagger \hat{b} - j) \\ & + \frac{\lambda}{\sqrt{2}} \left\{ \hat{b}^\dagger \sqrt{1 - \frac{\hat{b}^\dagger \hat{b}}{2j}} + \sqrt{1 - \frac{\hat{b}^\dagger \hat{b}}{2j}} \hat{b} \right\} (\hat{a}_x^\dagger + \hat{a}_x) \\ & + i \frac{\lambda}{\sqrt{2}} \left\{ \hat{b}^\dagger \sqrt{1 - \frac{\hat{b}^\dagger \hat{b}}{2j}} - \sqrt{1 - \frac{\hat{b}^\dagger \hat{b}}{2j}} \hat{b} \right\} (\hat{a}_y^\dagger + \hat{a}_y),\end{aligned}\quad (22)$$

which describes three coupled bosonic field modes. This approach is the basis for the theoretical discussion in the following section.

3. Magnetic structural phase transition

We make a Taylor expansion of the square roots in the Hamiltonian (22) and assume $\langle \hat{b}^\dagger \hat{b} \rangle / j \ll 1$, which yields

$$\begin{aligned}\hat{H}_{\text{JTD}}^{(1)} = & \omega(\hat{n}_x + \hat{n}_y) + \omega_0 \hat{b}^\dagger \hat{b} + \frac{\lambda}{\sqrt{2}} (\hat{b}^\dagger + \hat{b}) (\hat{a}_x^\dagger + \hat{a}_x) \\ & + i \frac{\lambda}{\sqrt{2}} (\hat{b}^\dagger - \hat{b}) (\hat{a}_y^\dagger + \hat{a}_y) + E_G^{(1)},\end{aligned}\quad (23)$$

where $E_G^{(1)} / j = -\omega_0$ in the ground-state energy in the limit $j \rightarrow \infty$. The validity of the condition $\langle \hat{b}^\dagger \hat{b} \rangle / j \ll 1$ will be checked self-consistently below. We diagonalize (23) by a Bogoliubov transformation, and get (see appendix A.1)

$$\hat{H}_{\text{JTD}}^{(1)} = \sum_{p=1}^3 \varepsilon'_p \left(\hat{c}_p^\dagger \hat{c}_p + \frac{1}{2} \right) - \left(\omega + \frac{\omega_0}{2} \right) + E_G^{(1)}. \quad (24)$$

The eigenfrequencies ε'_p can be found by solving the eigenvalue problem

$$\sum_{l=1}^3 \mathcal{B}'_{il} v_l^{(p)} = \varepsilon_p'^2 v_i^{(p)}, \quad (25)$$

with the matrix

$$\mathcal{B}'_{il} = \begin{bmatrix} \omega^2 & -\lambda \sqrt{\frac{\omega_0 \omega}{m_+}} & \lambda \sqrt{\frac{\omega_0 \omega}{m_-}} \\ -\lambda \sqrt{\frac{\omega_0 \omega}{m_+}} & \frac{\omega^2 + \omega_0^2}{2m_+} & \frac{\omega^2 - \omega_0^2}{2\sqrt{m_+ m_-}} \\ \lambda \sqrt{\frac{\omega_0 \omega}{m_-}} & \frac{\omega^2 - \omega_0^2}{2\sqrt{m_+ m_-}} & \frac{\omega^2 + \omega_0^2}{2m_-} \end{bmatrix}, \quad (26)$$

where $m_\pm = (1 \pm \lambda \sqrt{2/\omega_0 \omega})^{-1}$. We obtain a non-negative real ε'_p ($p = 1, 2, 3$) for $\lambda \leq \sqrt{\omega_0 \omega / 2}$, which allows us to define a critical coupling $\lambda_c = \sqrt{\omega_0 \omega / 2}$. We note that the condition for the matrix (26) to be Hermitian holds for $\lambda \leq \lambda_c$. The vacuum state $|0_1\rangle$ of Hamiltonian (24) is defined by the condition $\hat{c}_p |0_1\rangle = 0$.

In this phase the expectation values of the operators $\hat{a}_\alpha$ and $\hat{b}$ do not depend on the number of atoms and they grow as λ approach λ_c [46]. Thus, the mean value $\langle \hat{b}^\dagger \hat{b} \rangle$ is an intensive quantity, and in the thermodynamical limit we get $\langle \hat{b}^\dagger \hat{b} \rangle / j \rightarrow 0$, within the phase $\lambda < \lambda_c$. In that limit, the phase is characterized with vanishing density of phonon excitations $\langle \hat{a}_\alpha^\dagger \hat{a}_\alpha \rangle / j = 0$ and collective spin pointing along the z axis, $\langle \hat{J}_z \rangle / j = -1$.

We may find a simple physical interpretation of the critical spin–phonon coupling λ_c . Indeed, it is well known that in the presence of spin–orbit coupling, the minima of the lower adiabatic potential surface APS (effective nuclei potential in the molecular physics) for $\lambda \leq \lambda_c$ appears at the origin, while for $\lambda > \lambda_c$ APS has a sombrero shape. Increasing the spin–phonon coupling, the energy is minimized by breaking some spatial symmetry and thus leads to a JT distortion [2].

In order to quantify the amount of distortion and the spin ordering in the ion crystal above the critical coupling λ_c , we follow the general procedure introduced by Emary and Brandes in [31] for the quantum Dicke model. We displace each of the bosonic modes $\hat{a}_x^\dagger \rightarrow \hat{a}_x^\dagger + \sqrt{\alpha_x^*}$, $\hat{a}_y^\dagger \rightarrow \hat{a}_y^\dagger + \sqrt{\alpha_y^*}$ and $\hat{b}^\dagger \rightarrow \hat{b}^\dagger - \sqrt{\gamma^*}$, where α_x, α_y and γ are generally complex parameters in the order of j . By using the Holstein–Primakoff representation and by substituting the displaced operators, the Hamiltonian (22) becomes

$$\begin{aligned}\hat{H}_{\text{JTD}}^{(2)} = & \omega(\hat{a}_x^\dagger \hat{a}_x + \sqrt{\alpha_x^*} \hat{a}_x + \sqrt{\alpha_x} \hat{a}_x^\dagger + |\alpha_x|) \\ & + \omega(\hat{a}_y^\dagger \hat{a}_y + \sqrt{\alpha_y^*} \hat{a}_y + \sqrt{\alpha_y} \hat{a}_y^\dagger + |\alpha_y|) \\ & + \omega_0(\hat{b}^\dagger \hat{b} - \sqrt{\gamma^*} \hat{b} - \sqrt{\gamma} \hat{b}^\dagger + |\gamma| - j) \\ & + \frac{\lambda}{\sqrt{2}} \sqrt{\frac{k}{2j}} (\hat{a}_x^\dagger + \hat{a}_x + \sqrt{\alpha_x^*} \\ & + \sqrt{\alpha_x}) \{ \hat{b}^\dagger \sqrt{\xi} + \sqrt{\xi} \hat{b} - \sqrt{\xi} (\sqrt{\gamma^*} + \sqrt{\gamma}) \} \\ & + i \frac{\lambda}{\sqrt{2}} \sqrt{\frac{k}{2j}} (\hat{a}_y^\dagger + \hat{a}_y + \sqrt{\alpha_y^*} + \sqrt{\alpha_y}) \{ \hat{b}^\dagger \sqrt{\xi} \\ & - \sqrt{\xi} \hat{b} - \sqrt{\xi} (\sqrt{\gamma^*} - \sqrt{\gamma}) \},\end{aligned}\quad (27)$$

where

$$k = 2j - |\gamma|; \quad \sqrt{\xi} = \sqrt{1 - \frac{\hat{b}^\dagger \hat{b} - \hat{b}^\dagger \sqrt{\gamma} - \hat{b} \sqrt{\gamma^*}}{k}}. \quad (28)$$

The parameters $\alpha_{x,y}$ and γ can be found from the condition that all terms linear in the bosonic field operators in equation (27) are cancelled

$$\begin{aligned}\sqrt{\alpha_x} = & \frac{\lambda}{\omega} \sqrt{j(1-s^2)} \cos \phi, \quad \sqrt{\alpha_y} = \frac{\lambda}{\omega} \sqrt{j(1-s^2)} \sin \phi, \\ \sqrt{|\gamma|} = & \sqrt{j(1-s)},\end{aligned}\quad (29)$$

with $s = \lambda_c^2 / \lambda^2$. The phase $\phi = \arg(\sqrt{\gamma})$ remains undetermined which is a result of the arbitrariness in the choice of a direction in spontaneous symmetry breaking. Again, making a Taylor expansion of $\sqrt{\xi}$ and neglect the terms with j in the denominator the Hamiltonian (27) can be brought to the diagonal form (see appendix A.2)

$$\begin{aligned}\hat{H}_{\text{JTD}}^{(2)} = & \sum_{p=2}^3 \varepsilon_p'' \left(\hat{r}_p^\dagger \hat{r}_p + \frac{1}{2} \right) - \omega - \frac{\omega_0}{4s} (1+s) \\ & - \frac{\lambda^2}{2\omega} (1-s) + E_G^{(2)},\end{aligned}\quad (30)$$

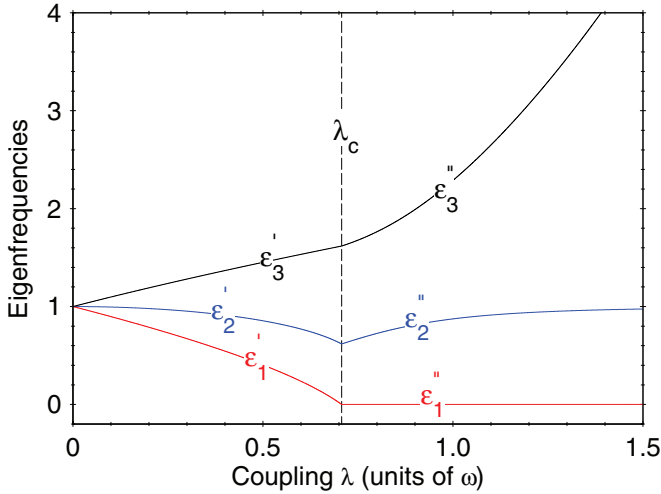


Figure 5. The excitation energy spectrum of the collective E⊗e JTD model in the limit $j \rightarrow \infty$ as a function of the spin–phonon coupling λ with $\omega = \omega_0$. For $\lambda \leq \lambda_c$ the eigenfrequencies ε_p are given as a solution of equation (25). At $\lambda = \lambda_c$ the system undergoes a magnetic structural phase transition with broken U(1) symmetry. The new eigenfrequencies ε'_p for $\lambda \geq \lambda_c$ are given by equation (31).

where $E_G^{(2)}/j = -(\frac{\lambda^2}{\omega} + \frac{\omega_0^2 \omega}{4\lambda^2})$ is the ground-state energy in the limit $j \rightarrow \infty$. The new excitation frequencies ε'_p are solution of the eigenvalue problem

$$\sum_{l=1}^3 B''_{il} v_l^{(p)} = \varepsilon_p'' v_i^{(p)}, \quad (31)$$

for the matrix

$$B''_{il} = \begin{bmatrix} \xi^2 M_- & \lambda^2 \sqrt{2M_-} & v \sqrt{M_+ M_-} \\ \lambda^2 \sqrt{2M_-} & \omega^2 & -\lambda^2 \sqrt{2M_+} \\ v \sqrt{M_+ M_-} & -\lambda^2 \sqrt{2M_+} & \xi^2 M_+ \end{bmatrix}, \quad (32)$$

with $\xi^2 = (\frac{\omega^2}{2} + \frac{\omega_0^2}{2s^2})$, $v = (\xi^2 - \frac{\omega_0^2}{s^2})$ and $M_{\pm} = (1 \pm s)$, respectively. In contrast to (25), now the frequencies ε'_p remain positively defined in the region $\lambda \geq \lambda_c$, figure 5.

The mean-value phonon number with respect to the new vacuum state $|0_2\rangle$ of the Hamiltonian (30) with $\hat{r}_p|0_2\rangle = 0$ is $\langle \hat{n}_x \rangle / j = (\lambda^2 / \omega^2)(1 - s^2) \cos^2 \phi$ and $\langle \hat{n}_y \rangle / j = (\lambda^2 / \omega^2)(1 - s^2) \sin^2 \phi$, indicating a non-zero radial phonon excitation, figure 6. The collective displacement of the c.m. mode implies a position reordering of the ions' equilibrium positions in the radial x – y plane. Indeed, from equations (3) and (7) it follows that the new radial equilibrium positions are $x_{i0} = q_0 \sqrt{2\alpha_x} / j$ and $y_{i0} = q_0 \sqrt{2\alpha_y} / j$. The structural transition also is accompanied with the ferromagnetic spin ordering, $\langle \hat{J}_x^2 \rangle / j^2 = (1 - s^2) \cos^2 \phi$, $\langle \hat{J}_y^2 \rangle / j^2 = (1 - s^2) \sin^2 \phi$, respectively, figure 7. We note that, the magnetic structural transition breaks the continuous U(1) symmetry of the JTD model, which reflects to the energy spectrum, namely one of the eigenfrequencies corresponds to the gapless Goldstone mode, $\varepsilon'_1 = 0$, see figure 5.

4. Preparation and detection of the magnetic structural phase transition

In the following we discuss the implementation of our model in a realistic trapped ion experiment. Consider an ion crystal

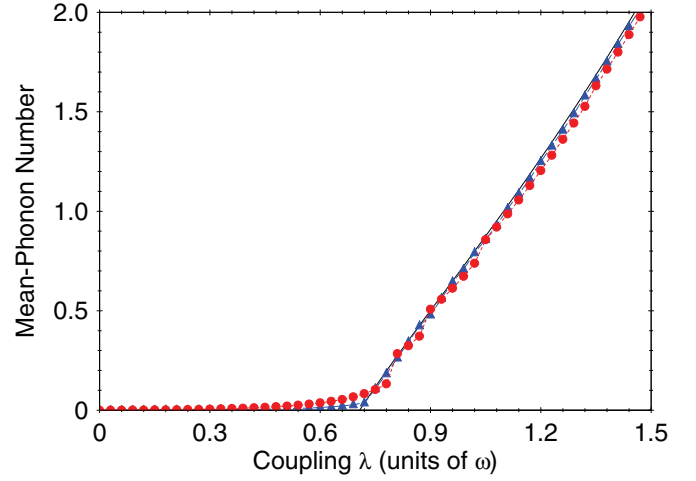


Figure 6. The mean-phonon number $(\langle \hat{n}_x \rangle + \langle \hat{n}_y \rangle) / j$ as a function of the spin–phonon coupling λ . The numerical results for 10 (red circles) and 20 (blue triangles) ions are plotted together with the mean-field solution (solid line). For $\lambda \leq \lambda_c$ the phase is characterized with zero mean-phonon number. A position reordering is observed for $\lambda > \lambda_c$ accompanied with non-zero mean-phonon number. The magnetic structural transition becomes sharper with increasing N .

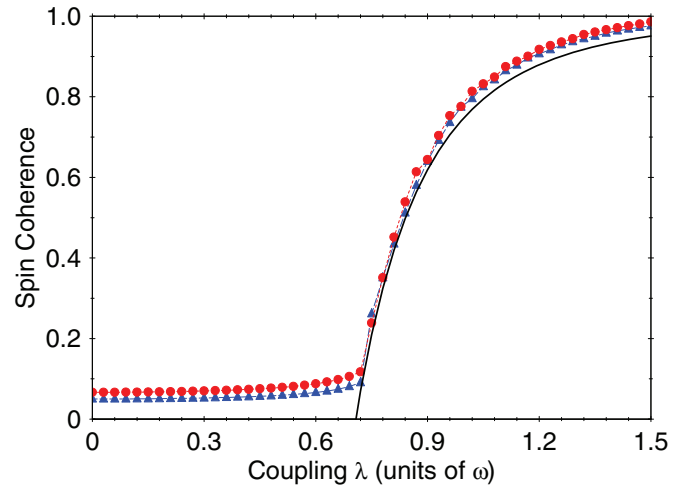


Figure 7. The mean-field result for $(\langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle) / j^2$ as a function of the spin–phonon coupling λ . The numerical results for 30 (red circles) and 40 (blue triangles) ions are compared with the mean-field solution (solid line). A creation of macroscopic spin-coherence is observed for $\lambda > \lambda_c$, which is an analogue to the super-radiance phase in the Dicke model.

which consists of $^{40}\text{Ca}^+$ ions with qubit states encoded at the Zeeman $S_{1/2}$ levels, $|\uparrow\rangle$ and $|\downarrow\rangle$. The experimental sequence is started by initializing the ion crystal in the ground state of the normal phase by laser cooling of the radial c.m. modes and pumping spins to $|-j\rangle = |\downarrow\downarrow\downarrow \dots \downarrow\rangle$. The proposed method for realization of the JTD model is based on magnetic field interaction, such that the spectator modes could be only Doppler cooled. This is a key advantage compared to the laser–ion interaction, where the spin–phonon coupling would depend on the spectator modes by the Debye–Waller factor, which is a significant source of decoherence [47]. After the preparation of the initial state, the coupling λ is slowly increased, relatively

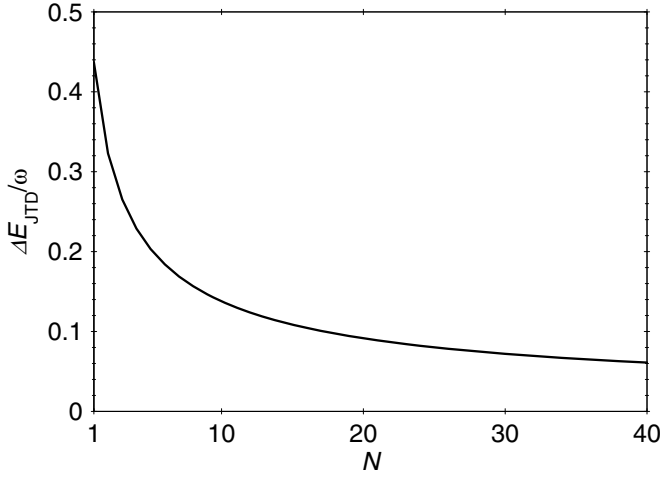


Figure 8. The numerical result for the energy splitting ΔE_{JTD} between the first excited state and ground state of Hamiltonian (20) at the critical coupling λ_c as a function of N for $\omega = \omega_0$.

to the energy gap ΔE_{JTD} between the first excited state and ground state. In figure 8 we show the numerical result for ΔE_{JTD} calculated at the critical coupling λ_c as a function of the number of atoms N . Defining $\tau_{\text{JTD}} = (\Delta E_{\text{JTD}}/2\pi)^{-1}$, the adiabaticity requires $T \gg \tau_{\text{JTD}}$, where T is the total interaction time. In table 1, we list the values of T together with other parameters for different values of N , such that all the approximations leading to the JTD Hamiltonian, and the adiabatic condition are satisfied.

The magnetic structural phase transition can be detected by measuring either the radial displacement or the spin population. Considering spin-phonon coupling $\lambda/2\pi = 5$ kHz at the end of the quantum simulation and direction of spontaneous symmetry breaking $\phi = \pi/4$, the equilibrium positions are displaced in the radial x - y directions by $x_0 = y_0 \approx q_0$. Such a structural transition can be detected by laser induced fluorescence, which is imaged on a CCD camera. The detection of the magnetic ordering can be performed by measuring the expectation value of the projection operator $\hat{P} = |\uparrow\uparrow \dots \uparrow\rangle\langle\uparrow\uparrow \dots \uparrow|$. We note that because $[\hat{H}_0, \hat{P}] = 0$, the projection operator is not affected under the rotating frame transformation and consequently of it the readout of the spin states does not introduce additional error. For particular ion species, an illumination of the crystal with resonant light near 397 and 866 nm would provide a spin-dependent laser fluorescence, namely all spins up emit light and appear bright while spins down remain dark.

5. Conclusion

We have presented a proposal for the physical realization of the collective JTD model based on a linear ion crystal. We have shown that the JTD model exhibits a magnetic structural phase transition in the thermodynamical limit. Beyond the critical coupling the continuous U(1) symmetry is spontaneously broken which leads to collective motional displacement of the radial coordinates and creation of macroscopic spin-coherence. The features of the magnetic structural transition

can be easily measured in the mesoscopic ion crystal by laser induced fluorescence. All parameters can be tuned by changing the detuning and the magnetic field gradient. In future we will investigate the JT effects in 2D ion crystals, which are relevant to orbital physics in solids. Furthermore, the ion crystal also can serve as a platform for studying non-equilibrium phenomena and effects of decoherence in such complex many-body systems, which are computationally intractable.

Acknowledgments

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Appendix A. Diagonalization of the mean-field Hamiltonian

A.1. Normal phase

We start with the diagonalization of the Hamiltonian (23). It is convenient to work in the position-momentum representation by introducing position and momentum operators for each of the bosonic modes,

$$\begin{aligned} \hat{a}_x &= \sqrt{\frac{\omega}{2}} \hat{x} + \frac{i}{\sqrt{2\omega}} \hat{p}_x, & \hat{a}_y &= i\sqrt{\frac{\omega}{2}} \hat{y} - \frac{1}{\sqrt{2\omega}} \hat{p}_y, \\ \hat{b} &= \sqrt{\frac{\omega_0}{2}} \hat{z} + \frac{i}{\sqrt{2\omega_0}} \hat{p}_z, \end{aligned} \quad (\text{A.1})$$

where the quantum oscillators have frequency ω in the x - y plane and ω_0 in the z direction. The transformation gives

$$\begin{aligned} \hat{H}_{\text{JTD}}^{(1)} &= \frac{\omega^2}{2} (\hat{x}^2 + \hat{y}^2) + \frac{\omega_0^2}{2} \hat{z}^2 + \frac{1}{2} (\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) \\ &\quad + \lambda\sqrt{2\omega_0\omega} \hat{z} \hat{x} - \lambda\sqrt{\frac{2}{\omega_0\omega}} \hat{p}_z \hat{p}_y - e_0, \end{aligned} \quad (\text{A.2})$$

with $e_0 = \omega_0(j + 1/2) + \omega$. The effective Hamiltonian (A.2) describes a system of three quantum harmonic oscillators which are coupled through position and momentum dependent couplings. To express (A.2) as a set of uncoupled oscillators we need first to eliminate the momentum dependent interaction term. To achieve that first we rotate the coordinate system along the x axis with the matrix

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}, \quad (\text{A.3})$$

such that $(\hat{x}, \hat{y}, \hat{z})^T = R_x(\hat{q}_1, \hat{q}_2, \hat{q}_3)^T$ and $(\hat{p}_x, \hat{p}_y, \hat{p}_z)^T = R_x(\hat{p}_1, \hat{p}_2, \hat{p}_3)^T$. The transformed Hamiltonian is given by

$$\begin{aligned} \hat{H}_{\text{JTD}}^{(1)} &= \frac{1}{2} (\omega^2 \hat{q}_1^2 + \hat{p}_1^2) + \frac{1}{2} \left(\epsilon^2 \hat{q}_2^2 + \frac{\hat{p}_2^2}{m_+} \right) + \frac{1}{2} \left(\epsilon^2 \hat{q}_3^2 + \frac{\hat{p}_3^2}{m_-} \right) \\ &\quad + \lambda\sqrt{\omega_0\omega} \hat{q}_1 (\hat{q}_3 - \hat{q}_2) + (\omega^2 - \epsilon^2) \hat{q}_2 \hat{q}_3 - e_0, \end{aligned} \quad (\text{A.4})$$

with $\epsilon^2 = (\omega^2 + \omega_0^2)/2$. Hence, the momentum dependent coupling vanishes but as a consequence two of the effective harmonic oscillators acquire different effective masses

$$m_+ = \left(1 + \lambda \sqrt{\frac{2}{\omega_0 \omega}}\right)^{-1}, \quad m_- = \left(1 - \lambda \sqrt{\frac{2}{\omega_0 \omega}}\right)^{-1}. \quad (\text{A.5})$$

The Hamiltonian (A.4) can be rewritten in a compact form as follows

$$\hat{H}_{\text{JTD}}^{(1)} = \frac{\hat{p}_1^2}{2} + \frac{\hat{p}_2^2}{2m_+} + \frac{\hat{p}_3^2}{2m_-} + \frac{1}{2} \sum_{i,l=1}^3 \mathcal{B}_{il}^{(1)} \hat{q}_i \hat{q}_l - e_0. \quad (\text{A.6})$$

Here $\mathcal{B}_{il}^{(1)}$ is (3×3) real and symmetric matrix, given by

$$\mathcal{B}_{il}^{(1)} = \begin{bmatrix} \omega^2 & -\lambda \sqrt{\omega_0 \omega} & \lambda \sqrt{\omega_0 \omega} \\ -\lambda \sqrt{\omega_0 \omega} & \epsilon^2 & \omega^2 - \epsilon^2 \\ \lambda \sqrt{\omega_0 \omega} & \omega^2 - \epsilon^2 & \epsilon^2 \end{bmatrix}. \quad (\text{A.7})$$

Still, Hamiltonian (A.6) is not in the desirable normal mode form, because the quantum oscillators have different effective masses. To overcome this problem we normalize the position operators $\hat{q}'_1 = \hat{q}_1$, $\hat{q}'_2 = \sqrt{m_+} \hat{q}_2$, $\hat{q}'_3 = \sqrt{m_-} \hat{q}_3$ and momentum operators $\hat{p}'_1 = \hat{p}_1$, $\hat{p}'_2 = \hat{p}_2 / \sqrt{m_+}$, $\hat{p}'_3 = \hat{p}_3 / \sqrt{m_-}$, respectively, to obtain

$$\hat{H}_{\text{JTD}}^{(1)} = \frac{1}{2} \sum_{i=1}^3 \hat{p}_i'^2 + \frac{1}{2} \sum_{i,l=1}^3 \mathcal{B}'_{il} \hat{q}_i' \hat{q}_l' - e_0, \quad (\text{A.8})$$

where

$$\mathcal{B}'_{il} = \begin{bmatrix} \omega^2 & -\lambda \sqrt{\frac{\omega_0 \omega}{m_+}} & \lambda \sqrt{\frac{\omega_0 \omega}{m_-}} \\ -\lambda \sqrt{\frac{\omega_0 \omega}{m_+}} & \frac{\omega^2 + \omega_0^2}{2m_+} & \frac{\omega^2 - \omega_0^2}{2\sqrt{m_+ m_-}} \\ \lambda \sqrt{\frac{\omega_0 \omega}{m_-}} & \frac{\omega^2 - \omega_0^2}{2\sqrt{m_+ m_-}} & \frac{\omega^2 + \omega_0^2}{2m_-} \end{bmatrix}. \quad (\text{A.9})$$

To find the collective spin-phonon modes, we solve the eigenvalue problem

$$\sum_{l=1}^3 \mathcal{B}'_{il} v_l'^{(p)} = \varepsilon_p'^2 v_i'^{(p)}, \quad (\text{A.10})$$

for the eigenfrequencies ε_p' and the eigenvectors $\vec{v}''^{(p)}$ with $p = 1, 2, 3$. Finally, we introduce a new set of bosonic field operators by the relation

$$\hat{q}_i' = \sum_{p=1}^3 \frac{v_i'^{(p)}}{\sqrt{2\varepsilon_p'}} (\hat{c}_p^\dagger + \hat{c}_p), \quad \hat{p}_i' = i \sum_{p=1}^3 \sqrt{\frac{\varepsilon_p'}{2}} v_i'^{(p)} (\hat{c}_p^\dagger - \hat{c}_p), \quad (\text{A.11})$$

and arrive at the diagonal Hamiltonian

$$\hat{H}_{\text{JTD}}^{(1)} = \sum_{p=1}^3 \varepsilon_p' \left(\hat{c}_p^\dagger \hat{c}_p + \frac{1}{2} \right) - \omega_0 \left(j + \frac{1}{2} \right) - \omega. \quad (\text{A.12})$$

A.2. Magnetic structural phase transition

In order to diagonalize Hamiltonian (27) in the limit $j \rightarrow \infty$ we perform the following two steps. (i) Expand the Hamiltonian (27) as a power series in $1/k$ and neglect the terms in order of j in the denominator. (ii) Eliminate the terms in (27) which are linear in the bosonic operators by the condition, equation (29). The resulting Hamiltonian becomes

$$\begin{aligned} \hat{H}_{\text{JTD}}^{(2)} = & \omega(\hat{n}_x + \hat{n}_y) + \frac{\omega_0}{2s} (1+s) \hat{b}^\dagger \hat{b} + \frac{\lambda}{2} \sqrt{1+s} \\ & \times (\hat{a}_x^\dagger + \hat{a}_x)(\hat{b}^\dagger + \hat{b}) + i \frac{\lambda}{2} \sqrt{1+s} s (\hat{a}_y^\dagger + \hat{a}_y)(\hat{b}^\dagger - \hat{b}) \\ & - \frac{\lambda}{2} \frac{1-s}{\sqrt{1+s}} (e^{i\phi} \hat{b}^\dagger + e^{-i\phi} \hat{b}) \{ \cos \phi (\hat{a}_x^\dagger \\ & + \hat{a}_x) + \sin \phi (\hat{a}_y^\dagger + \hat{a}_y) \} + \frac{\lambda^2}{4\omega} \frac{(1-s)(3+s)}{(1+s)} \\ & \times (e^{i\phi} \hat{b}^\dagger + e^{-i\phi} \hat{b})^2 - \tilde{e}_0, \end{aligned} \quad (\text{A.13})$$

with

$$\tilde{e}_0 = j \left\{ \frac{\lambda^2}{\omega} + \frac{\omega_0^2 \omega}{4\lambda^2} \right\} + \frac{\lambda^2}{2\omega} (1-s). \quad (\text{A.14})$$

We can further simplify (A.13) by applying the following transformations

$$\begin{aligned} \hat{a}_x &= \hat{d}_x \cos \phi - \hat{d}_y \sin \phi, \\ \hat{a}_y &= \hat{d}_x \sin \phi + \hat{d}_y \cos \phi, \end{aligned} \quad (\text{A.15})$$

and $e^{i\phi} \hat{b}^\dagger \rightarrow \hat{b}^\dagger$. Then, the Hamiltonian reads

$$\begin{aligned} \hat{H}_{\text{JTD}}^{(2)} = & \omega(\hat{d}_x^\dagger \hat{d}_x + \hat{d}_y^\dagger \hat{d}_y) + \frac{\omega_0}{2s} (1+s) \hat{b}^\dagger \hat{b} \\ & + \frac{\lambda s}{\sqrt{1+s}} (\hat{b}^\dagger + \hat{b})(\hat{d}_x^\dagger + \hat{d}_x) \\ & + i \frac{\lambda}{2} \sqrt{1+s} (\hat{b}^\dagger - \hat{b})(\hat{d}_y^\dagger + \hat{d}_y) \\ & + \frac{\lambda^2}{4\omega} \frac{(1-s)(3+s)}{(1+s)} (\hat{b}^\dagger + \hat{b})^2 - \tilde{e}_0. \end{aligned} \quad (\text{A.16})$$

Following the standard procedure, we introduce the position and momentum operators for each of the bosonic modes

$$\begin{aligned} \hat{d}_x &= -i \sqrt{\frac{\omega}{2}} \hat{X} + \frac{1}{\sqrt{2\omega}} \hat{P}_X, & \hat{d}_y &= \sqrt{\frac{\omega}{2}} \hat{Y} + \frac{i}{\sqrt{2\omega}} \hat{P}_Y, \\ \hat{b} &= -i \sqrt{\frac{\tilde{\omega}}{2}} \hat{Z} + \frac{1}{\sqrt{2\tilde{\omega}}} \hat{P}_Z, \end{aligned} \quad (\text{A.17})$$

with $\tilde{\omega} = (\omega_0/2s)(1+s)$. The Hamiltonian (A.16) in the position-momentum representation is given by

$$\begin{aligned} \hat{H}_{\text{JTD}}^{(2)} = & \frac{\omega^2}{2} (\hat{X}^2 + \hat{Y}^2) + \frac{\tilde{\omega}^2}{2} \hat{Z}^2 + \frac{1}{2} (\hat{P}_X^2 + \hat{P}_Y^2) + \frac{\hat{P}_Z^2}{2m} \\ & + \frac{2s}{1+s} \hat{P}_Z \hat{P}_X - \lambda^2 (1+s) \hat{Z} \hat{Y} - \omega - \frac{\tilde{\omega}}{2} - \tilde{e}_0, \end{aligned} \quad (\text{A.18})$$

with $m = (1+s)^2/4$. It is convenient to normalize the position and momentum operators in x and y directions as follows

$$\begin{aligned} \sqrt{m} \hat{P}_X &\rightarrow \hat{P}_X, & \frac{\hat{X}}{\sqrt{m}} &\rightarrow \hat{X}, \\ \sqrt{m} \hat{P}_Y &\rightarrow \hat{P}_Y, & \frac{\hat{Y}}{\sqrt{m}} &\rightarrow \hat{Y}. \end{aligned} \quad (\text{A.19})$$

Then the Hamiltonian reads

$$\begin{aligned}\hat{H}_{\text{JTD}}^{(2)} = & \frac{m\omega^2}{2}(\hat{X}^2 + \hat{Y}^2) + \frac{\tilde{\omega}^2}{2}\hat{Z}^2 \\ & + \frac{1}{2m}(\hat{P}_X^2 + \hat{P}_Y^2 + \hat{P}_Z^2) + \frac{s}{m}\hat{P}_Z\hat{P}_X - 2\lambda^2 m\hat{Z}\hat{Y} \\ & - \omega - \frac{\tilde{\omega}}{2} - \tilde{e}_0.\end{aligned}\quad (\text{A.20})$$

Similar as before, the diagonalization proceeds by nullifying the momentum dependent interaction term in (A.20), which is achieved by rotating the coordinate system along the y axis with the matrix

$$R_y = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}, \quad (\text{A.21})$$

such that $(\hat{X}, \hat{Y}, \hat{Z})^T = R_y(\hat{Q}_1, \hat{Q}_2, \hat{Q}_3)^T$ and $(\hat{P}_X, \hat{P}_Y, \hat{P}_Z)^T = R_y(\hat{P}_1, \hat{P}_2, \hat{P}_3)^T$. After performing the rotation we obtain

$$\begin{aligned}\hat{H}_{\text{JTD}}^{(2)} = & \frac{m\xi^2}{2}\hat{Q}_1^2 + \frac{m\omega^2}{2}\hat{Q}_2^2 + \frac{m\xi^2}{2}\hat{Q}_3^2 \\ & + \frac{\hat{P}_1^2}{2m_1} + \frac{\hat{P}_2^2}{2m} + \frac{\hat{P}_3^2}{2m_3} + mv\hat{Q}_1\hat{Q}_3 \\ & - \sqrt{2}m\lambda^2\hat{Q}_2(\hat{Q}_3 - \hat{Q}_1) - \omega - \frac{\tilde{\omega}}{2} - \tilde{e}_0,\end{aligned}\quad (\text{A.22})$$

with $\xi^2 = (\frac{\omega^2}{2} + \frac{\omega_0^2}{2s^2})$ and $v = (\xi^2 - \frac{\omega_0^2}{s^2})$, respectively. Two of the quantum oscillators acquire new effective masses

$$m_1 = \frac{m}{M_-}, \quad m_3 = \frac{m}{M_+}, \quad (\text{A.23})$$

with $M_{\pm} = (1 \pm s)$. Again as before to express the Hamiltonian (A.6) in normal mode form we normalize the position and momentum operators, namely: $\hat{Q}_1'' = \sqrt{m_1}\hat{Q}_1$, $\hat{Q}_2'' = \sqrt{m}\hat{Q}_2$ and $\hat{Q}_3'' = \sqrt{m_3}\hat{Q}_3$ and, respectively, $\hat{P}_1'' = \hat{P}_1/\sqrt{m_1}$, $\hat{P}_2'' = \hat{P}_2/\sqrt{m}$ and $\hat{P}_3'' = \hat{P}_3/\sqrt{m_3}$. Then the Hamiltonian becomes

$$\hat{H}_{\text{JTD}}^{(2)} = \frac{1}{2} \sum_{i=1}^3 \hat{P}_i''^2 + \frac{1}{2} \sum_{i,l=1}^3 \mathcal{B}_{il}'' \hat{Q}_i'' \hat{Q}_l'' - \omega - \frac{\tilde{\omega}}{2} - \tilde{e}_0, \quad (\text{A.24})$$

where

$$\mathcal{B}_{il}'' = \begin{bmatrix} \xi^2 M_- & \lambda^2 \sqrt{2M_-} & v\sqrt{M_+M_-} \\ \lambda^2 \sqrt{2M_-} & \omega^2 & -\lambda^2 \sqrt{2M_+} \\ v\sqrt{M_+M_-} & -\lambda^2 \sqrt{2M_+} & \xi^2 M_+ \end{bmatrix}. \quad (\text{A.25})$$

The new eigenfrequencies are obtained by solving the eigenvalue problem,

$$\sum_{l=1}^3 \mathcal{B}_{il}'' v_l''^{(p)} = \varepsilon_i'' v_i''^{(p)}. \quad (\text{A.26})$$

We find that one eigenvalue $\varepsilon_1'' = 0$ corresponds to a free mode. The latter is the Goldstone mode related to the breaking of the $U(1)$ symmetry. We may define bosonic creation $\hat{r}_p^\dagger$ and annihilation $\hat{r}_p$ operators for the nonzero energy modes $\varepsilon_{2,3}''$ by the relation

$$\hat{Q}_i'' = \sum_{p=2}^3 \frac{v_i''^{(p)}}{\sqrt{2\varepsilon_i''}} (\hat{r}_p^\dagger + \hat{r}_p), \quad \hat{P}_i'' = i \sum_{p=2}^3 \sqrt{\frac{\varepsilon_i''}{2}} v_i''^{(p)} (\hat{r}_p^\dagger - \hat{r}_p). \quad (\text{A.27})$$

Submitting (A.27) in (A.24) we obtain the following diagonal Hamiltonian, which refers to two decoupled oscillators,

$$\begin{aligned}\hat{H}_{\text{JTD}}^{(2)} = & \sum_{p=2}^3 \varepsilon_p'' \left(\hat{r}_p^\dagger \hat{r}_p + \frac{1}{2} \right) - \omega - \frac{\omega_0}{4s} (1 + s) \\ & - j \left(\frac{\lambda^2}{\omega} + \frac{\omega_0^2 \omega}{4\lambda^2} \right) - \frac{\lambda^2}{2\omega} (1 - s).\end{aligned}\quad (\text{A.28})$$

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