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Phonon–phonon interactions due to non-linear effects in a linear ion trap

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ABSTRACT We examine in detail the theory of the intrinsic non-linearities in the dynamics of trapped ions due to the Coulomb interaction. In particular, the possibility of mode–mode coupling, which can be a source of decoherence in trapped ion quantum computation, or can be exploited for parametric down-conversion of phonons, is discussed and conditions under which such coupling is possible are derived.

PACS 32.80.Pj; 42.50.Vk; 03.67.Mn

1 Introduction

Cold ions confined in electromagnetic traps and cooled by means of lasers are very important experimental systems, both for the study of problems of fundamental physics, such as cold non-neutral plasmas or quantum dynamics, and for technological applications, such as optical frequency standards. In the past few years, systems of this kind have been the subject of intense study as a possible architecture for the realization of a quantum computer [1–3] (for reviews of progress towards this goal, see [4–7]). In comparison with other experimental systems used in the investigation of fundamental quantum phenomena, cold-trapped ions offer a number of advantages. In particular, it is a relatively "clean" system whose behavior is well characterized by theory; simplified models of interactions between two-level systems and quantum harmonic oscillators can be realized experimentally. Considerable achievements in the production of non-classical states of matter [8], and other fundamental physics problems such as high-efficiency measurements of Bell's inequalities [9] or tests of cavity quantum electrodynamics [10], have been made.

As is well known [11], it is impossible to confine charged particles by electrostatic forces alone. To overcome this problem, the radio-frequency Paul trap was developed: such devices create an effective binding potential in the x and y directions, while a weaker static potential is applied in the z direc-

tion [12]. When two or more ions are confined in such a trap, they will repel each other due to the Coulomb force, resulting in confined charged plasmas with very low densities. When sufficiently cold, the plasma will condense into a crystalline state. In the highly anisotropic traps used for some atomic clocks [13] and for quantum computing, this crystalline state is, for small enough numbers of ions, a simple chain of ions lying in a straight line along the axis of weak binding. In what follows, we shall examine the oscillatory behavior of ions confined in such a linear configuration.

The ions are assumed to be sufficiently cold that they undergo only small oscillations around their equilibrium positions. In this case, the Lagrangian of the motion can be expanded as a Taylor series around these equilibrium positions. As we shall see, the first term of this expansion is a constant (which has no effect on the motion), the second term vanishes (by virtue of the condition for equilibrium), the third term describes coupling of one ion's motion to all of the others (and can be easily resolved into a series of normal modes describing the collective oscillations of the ions), and the fourth term (whose consequences are the main theme of this paper) describes an intrinsic coupling between the different modes.

The effects of non-linearities in the coupling of harmonically bound particles is a problem with a long history: for example, Fermi, Pasta, and Ulam investigated such dynamics computationally in 1954–55, using the early Los Alamos MANIAC computer, with a view to explaining the equipartition of energy between modes as the system reaches thermal equilibrium [14]. In the quantum realm, the non-linearities lead to couplings between the normal modes of oscillation. In certain ways this coupling is analogous to $\chi^{(2)}$ non-linear optical effects [15], in that, provided certain conditions are met, quanta of one oscillatory mode can be down-converted into twinned pairs of quanta of other modes. Obviously, since the Taylor expansion is an infinite series, higher terms, describing more complex multi-mode couplings, will be present; we will, however, not consider them in this current work.

The paper is organized as follows. In Sect. 2 the Lagrangian of the ion motion is presented and the derivation of the normal modes of the ion oscillations is reprised; the classical description of mode–mode coupling in terms of the Hamiltonian, is formulated. In Sect. 3 the properties of the mode–mode coupling coefficients are discussed, and Sect. 4 discusses the quantum theory of this coupling and the pop-

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ulation transfers that it can cause. Section 5 summarizes our conclusions.

2   Lagrangian of the ion motion in the trap

Consider N identical ions of mass M and charge Q confined in an effective three-dimensional harmonic potential[1]. The position of the n-th ion will be denoted by (x_{n1}, x_{n2}, x_{n3}) (see Fig. 1), where the ions are numbered in order of increasing value of their axial positions x_{n3}, so that $n > m$ implies that $x_{n3} > x_{m3}$. Besides the trap potential, each ion experiences a Coulomb interaction with each of the other ions. Thus the total potential energy of the ions is given by

$$V = \frac{M}{2} \sum_{n=1}^{N} \sum_{i=1}^{3} \omega_i^2 x_{ni}^2 + \frac{Q^2}{8\pi\varepsilon_0} \sum_{\substack{n,m=1 \\ m\neq n}}^{N} \left[\sum_{i=1}^{3} (x_{ni} - x_{mi})^2 \right]^{-\frac{1}{2}},$$

(1)

where ω_1, ω_2, and ω_3 are the angular frequencies of the trap in the three directions. For simplicity, we will assume that the trapping potentials are equal in two transverse directions (1 and 2) and that the trapping potential in the axial direction 3 is much weaker, i.e.

$$\omega_1 = \omega_2 = \omega_3/\sqrt{\alpha},$$

(2)

where $\alpha \ll 1$ is a dimensionless parameter characterizing the anisotropy of the trap.

The equilibrium positions of the ions, denoted by $\bar{x}_{ni}$ $((n = 1, \ldots, N), (i = 1, 2, 3))$, are determined by the following equations:

$$\left. \frac{\partial V}{\partial x_{ni}} \right|_0 = 0 \quad (n = 1, \ldots, N) \quad (i = 1, 2, 3),$$

(3)

where the subscript 0 denotes that the partial derivatives are evaluated at $x_{ni} = \bar{x}_{ni}$. The solutions of these equilibrium equations in strongly anisotropic trapping conditions (so that the ions are aligned along the weak axial direction 3, i.e. $\bar{x}_{n1} = \bar{x}_{n2} = 0$) have been investigated by various authors [17–19] (see also [20, 21] for analysis of ion crystals with two different species of ion). It will be convenient to use the dimensionless equilibrium positions defined by $u_n = \bar{x}_{n3}/\ell$, where the length scale ℓ is defined by

$$\ell = \left(\frac{Q^2}{4\pi\varepsilon_0 M \omega_3^2} \right)^{1/3}.$$

(4)

The displacements of the ions from their equilibrium position are denoted by ξ_{ni}, i.e.

$$x_{ni}(t) = \bar{x}_{ni} + \xi_{ni}(t).$$

(5)

[1] In reality, the ions experience a time varying force whose effects can be modeled as an effective harmonic motion plus a high-frequency oscillation called micromotion. Experimental techniques for minimizing this effect are explained in [16]. Here we will assume that the amplitudes of transverse oscillations are sufficiently small that micromotion can be neglected in this paper.
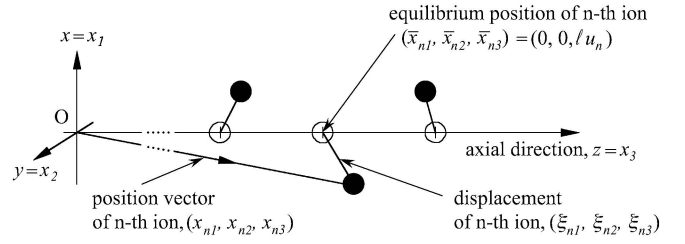

FIGURE 1   Illustration of the notation used in this paper

The Lagrangian describing the motion is then

$$L = T - V = \frac{M}{2} \sum_{n=1}^{N} \sum_{i=1}^{3} \dot{\xi}_{ni}^2 - \frac{M}{2} \sum_{n=1}^{N} \sum_{i=1}^{3} \omega_i^2 \left[\bar{x}_{ni} + \xi_{ni}(t) \right]^2$$

$$- \frac{Q^2}{8\pi\varepsilon_0} \sum_{\substack{n,m=1 \\ m\neq n}}^{N} \left\{ \sum_{i=1}^{3} \left[\bar{x}_{ni} + \xi_{ni}(t) - \bar{x}_{mi} - \xi_{mi}(t) \right]^2 \right\}^{-\frac{1}{2}}.$$

(6)

Making a Taylor expansion about the equilibrium positions, this may be approximated as

$$L = \frac{M}{2} \sum_{n=1}^{N} \sum_{i=1}^{3} \dot{\xi}_{ni}^2 - V_0 - \frac{1}{2} \sum_{m,n=1}^{N} \sum_{i,j=1}^{3} \left. \frac{\partial^2 V}{\partial x_{mi} \partial x_{nj}} \right|_0 \xi_{mi} \xi_{nj}$$

$$- \frac{1}{6} \sum_{m,n,p=1}^{N} \sum_{i,j,k=1}^{3} \left. \frac{\partial^3 V}{\partial x_{mi} \partial x_{nj} \partial x_{pk}} \right|_0 \xi_{mi} \xi_{nj} \xi_{pk} + O\left[\xi_{mi}^4 \right].$$

(7)

Neglecting both the constant V_0 (which has no effect on the dynamics) and the higher order terms, and evaluating the partial derivatives explicitly (see Appendix A), the Lagrangian may be approximated by

$$L \approx \frac{M}{2} \left[\sum_{n=1}^{N} \left(\dot{\xi}_{n3} \right)^2 - \omega_3^2 \sum_{m,n=1}^{N} A_{mn} \xi_{m3} \xi_{n3} \right]$$

$$+ \frac{M}{2} \sum_{i=1}^{2} \left[\sum_{n=1}^{N} \left(\dot{\xi}_{ni} \right)^2 - \omega_3^2 \sum_{m,n=1}^{N} B_{mn} \xi_{mi} \xi_{ni} \right]$$

$$- \frac{M\omega_3^2}{2l} \sum_{m,n,p=1}^{N} C_{mnp} \, \xi_{p3} \left(2\xi_{m3}\xi_{n3} - 3\xi_{m1}\xi_{n1} - 3\xi_{m2}\xi_{n2} \right).$$

(8)

The first term represents oscillations of the ions along the axial ($i = 3$) direction, the second term oscillations in the transverse directions ($i = 1, 2$), and the third term represents coupling between these oscillations which are a direct and unavoidable consequence of the Coulomb interaction between the ions.

The tensors A_{mn}, B_{mn}, and C_{mnp} are given by

$$
A_{mn} = \begin{cases} 1 + 2 \sum_{\substack{p=1 \\ p \neq m}}^{N} \dfrac{1}{|u_m - u_p|^3} & \text{if } m = n\,, \\[12pt] \dfrac{-2}{|u_m - u_n|^3} & \text{if } m \neq n\,, \end{cases} \tag{9}
$$

$$
B_{mn} = \left(\frac{1}{\alpha} + \frac{1}{2} \right) \delta_{mn} - \frac{1}{2} A_{mn}\,, \tag{10}
$$

$$
C_{mnp} = \begin{cases} \sum_{\substack{q=1 \\ q \neq m}}^{N} \dfrac{\text{sgn}(q - m)}{(u_q - u_m)^4} & \text{if } m = n = p\,, \\[14pt] \dfrac{-\,\text{sgn}(p - m)}{(u_p - u_m)^4} & \text{if } m = n \neq p\,, \\[12pt] 0 & \text{if } m \neq n \neq p\,, \end{cases} \tag{11}
$$

where sgn(x) stands for the sign of x and δ_{mn} is the Kronecker delta. The third rank tensor C_{mnp} is symmetric under any exchange of two subscripts; thus, for example, $C_{224} = C_{242} = C_{422} = -1/(u_2 - u_4)^4$, while $C_{442} = C_{244} = C_{424} = 1/(u_2 - u_4)^4$. All the elements of A_{mn} and C_{mnp} can be calculated numerically from the dimensionless equilibrium positions of the ions.

The matrix A_{mn} is real, symmetric, and positive definite. Thus its eigenvalues μ_p are non-negative. The eigenvectors $b_n^{(p)}$ ($p = 1, \dots, N$) are defined by

$$
\sum_{n=1}^{N} A_{mn} b_n^{(p)} = \mu_p b_m^{(p)} \quad (p = 1, \dots, N)\,, \tag{12}
$$

where the eigenvectors are numbered in order of increasing eigenvalue. The eigenvectors form a complete basis so that

$$
\sum_{p=1}^{N} b_m^{(p)} b_n^{(p)} = \delta_{mn}\,, \quad \sum_{m=1}^{N} b_m^{(p)} b_m^{(q)} = \delta_{pq}\,. \tag{13}
$$

For any value of N, the first two eigenvectors are the center of mass mode $b^{(1)} = 1/\sqrt{N}(1, 1, \dots, 1)$, ($\mu_1 = 1$) and the stretch mode $b^{(2)} = (1/\mathcal{N})(u_1, u_2, \dots, u_N)$ ($\mu_2 = 3$), where $\mathcal{N} = \sqrt{\sum_{n=1}^{N} u_n^2}$. All the eigenvalues and eigenvectors can be calculated numerically; their approximate values are given, for example, in [18] for two to ten ions. The dynamics of these modes have been confirmed directly in experiments [22]. From (10) we see that B_{mn} has the same eigenvectors as A_{mn} but different eigenvalues:

$$
\sum_{n=1}^{N} B_{mn} b_n^{(p)} = \gamma_p b_m^{(p)} \quad (p = 1, \dots, N)\,, \tag{14}
$$

where the eigenvalue γ_p is related to the longitudinal eigenvalue by the formula

$$
\gamma_p = \frac{1}{\alpha} + \frac{1}{2} - \frac{\mu_p}{2}\,. \tag{15}
$$

If $\alpha > \alpha_{\text{crit}} = 2/(\mu_N - 1)$ the matrix B_{nm} is not positive definite; this implies unstable transverse oscillation modes, and results in the formation of "zig-zag" crystal structures [23]. We shall assume however that α is kept sufficiently small that this situation does not arise. Note that, with this convention, the transverse oscillation modes are numbered in order of decreasing eigenvalue, so that the $p = 1$ center of mass mode has the largest eigenvalue.

Using these eigenvectors, the normal modes of the oscillations of the ions in the three directions are defined as follows:

$$
X_p(t) = \sum_{n=1}^{N} b_n^{(p)} \xi_{n1}(t)\,,
$$

$$
Y_p(t) = \sum_{n=1}^{N} b_n^{(p)} \xi_{n2}(t)\,,
$$

$$
Z_p(t) = \sum_{n=1}^{N} b_n^{(p)} \xi_{n3}(t)\,. \tag{16}
$$

The Lagrangian (8) can be rewritten in terms of these normal modes quite straightforwardly. Not surprisingly, one finds that, neglecting the fourth order term, the Lagrangian becomes a sum of Lagrangians of harmonic oscillators. The canonical momenta conjugate to X_n are $\Pi_n^x = \partial L / \partial \dot{X}_n$ (with analogous definitions for Π_n^y and Π_n^z). Using these momenta, the Hamiltonian for the ion motion is

$$
H = H_0 + H_{\text{I}}\,, \tag{17}
$$

where H_0 is the Hamiltonian for all of the uncoupled collective oscillations, i.e.

$$
H_0 = \sum_{n=1}^{N} \left[\frac{\Pi_n^{x2}}{2M} + \frac{M\Omega_n^2 X_n^2}{2} \right] + \sum_{n=1}^{N} \left[\frac{\Pi_n^{y2}}{2M} + \frac{M\Omega_n^2 Y_n^2}{2} \right]
$$

$$
+ \sum_{n=1}^{N} \left[\frac{\Pi_n^{z2}}{2M} + \frac{M\nu_n^2 Z_n^2}{2} \right]\,, \tag{18}
$$

with $\nu_n = \omega_3 \sqrt{\mu_n}$ being the angular frequency of the n-th mode in the z direction and $\Omega_n = \omega_3 \sqrt{\gamma_n}$ being the angular frequency of the n-th transverse mode. The Hamiltonian H_{I} describes the perturbation which, in certain circumstances, couples these various modes. It is given by

$$
H_{\text{I}} = \frac{M\omega_z^2}{2l} \sum_{m,n,p=1}^{N} D_{mnp} Z_p (2Z_m Z_n - 3X_m X_n - 3Y_m Y_n)\,, \tag{19}
$$

where the mode–mode coupling coefficients D_{pqr} are defined by

$$
D_{pqr} = \sum_{l,m,n=1}^{N} C_{lmn} b_l^{(p)} b_m^{(q)} b_n^{(r)}\,. \tag{20}
$$

Note that the sign of D_{pqr} depends on the sign of the eigenvector $\boldsymbol{b}^{(p)}$, which is undetermined. We will adopt the convention that the sign of the N-th component of $\boldsymbol{b}^{(p)}$ is always positive, for all modes and values of N.

We should mention that other mechanisms by which resonant interactions between ion motion in different directions are coupled have been studied. In particular Werth et al. at the University of Mainz have investigated experimentally the parametric coupling of different stable configurations of molecular ion clouds [24]. Cross-mode couplings due to static field imperfections, which can be a cause of heating or of decoherence, have also been discussed in Sect. 4.1.8 of [4].

3   Properties of the coupling coefficients

In this section we discuss some of the properties of the coefficients C_{mnp} and D_{mnp}, which are central to the subsequent development of phonon–phonon interactions in ion traps. The first important symmetry property stems directly from the definition of C_{mnp}, (11): the tensor C_{mnp} is symmetric under exchange of two subscripts; further, because of the definition (20), so is D_{mnp}. From (11), we also have the property $C_{mmn} = -C_{nnm}$ (provided that $m \neq n$). These properties imply that

$$\sum_{p=1}^{N} C_{mnp} = 0 \,. \tag{21}$$

This can be shown as follows: if $m \neq n$, we have $\sum_{p=1}^{N} C_{mnp} = C_{mnn} + C_{mnm}$, since C_{mnp} is always zero if all three indices are different. However, since $C_{mnm} = C_{mmn} = -C_{nnm} = -C_{mnn}$, the sum is zero. If $m = n$, $\sum_{p=1}^{N} C_{mmp} = C_{mmm} + \sum_{p=1, p \neq m}^{N} C_{mmp}$, which, by the definition of C_{mmm} from (11), must also be zero. The identity (21) implies that, since $b^{(1)} = (1/\sqrt{N})\{1, 1, \ldots 1\}$,

$$D_{mn1} \equiv \frac{1}{\sqrt{N}} \sum_{i,j=1}^{N} b_i^{(m)} b_j^{(n)} \sum_{k=1}^{N} C_{ijk} = 0 \,. \tag{22}$$

Thus, when considering the three-mode mixing described by (19), the center of mass ($p = 1$) mode has zero coupling strength to any other mode. Physically, this can be explained as follows. The $p = 1$ mode is special since it is the only mode in which the center of mass of the crystal is displaced: as can be seen from (13), $\sum_{m=1}^{N} b_m^{(p)} = 0$ if $p \neq 1$. Thus to excite or de-excite the $p = 1$ mode requires the application of an external force to change the momentum of the crystal as a whole, while no such force is required to transfer energy between any of the other modes.

This result has important consequences: firstly, if one wants to avoid mode–mode coupling entirely, for example when performing quantum logic operations between ions, it would behoove one to use the center of mass mode as the "quantum bus" as originally proposed by Cirac and Zoller [1]. However, in some experiments [25], it has been found that the quantum state of the center of mass mode is rapidly degraded by excitations from various extraneous sources. Our result, (22), tends to rule out coupling to other ion oscillation modes which may have been imperfectly cooled as a sources of such heating. Furthermore, when the center of mass mode is preferentially heated, it will not cause heating of the other modes.

A second interesting property of C_{mnp} can be expressed as

$$\sum_{p=1}^{N} u_p C_{mnp} = \frac{1}{2} [\delta_{mn} - A_{mn}] \,, \tag{23}$$

where A_{mn} is the ion coupling tensor defined by (9). This result can be demonstrated as follows: if $m \neq n$, then $\sum_{p=1}^{N} C_{mnp} u_p = C_{mnn} u_n + C_{mnm} u_m = (u_n - u_m) C_{mnn} = 1/|u_n - u_m|^3$, where the last step results from the definition of C_{mnn} in terms of the scaled equilibrium positions u_p. For the case $m = n$, $\sum_{p=1}^{N} C_{mmp} u_p = -u_m \sum_{p=1, p \neq m}^{N} C_{mmp} + \sum_{p=1, p \neq m}^{N} C_{mmp} u_p = -\sum_{p=1, p \neq m}^{N} /|u_p - u_m|^3$. Comparing these expressions involving the u_p's with the definition of A_{mn}, (9), we obtain (23). This result implies that

$$D_{mn2} = \sum_{i,j=1}^{N} b_i^{(m)} b_j^{(n)} \sum_{k=1}^{N} \frac{u_k}{\mathcal{N}} C_{ijk} = \frac{1 - \mu_m}{2\mathcal{N}} \delta_{mn} \,, \tag{24}$$

where, as before, $\mathcal{N} = \sqrt{\sum_{n=1}^{N} u_n^2}$. Thus the coupling of the first stretch mode ($p = 2$) is constrained so that it will only be coupled to a single other mode rather than to two distinct modes.

For $N = 2$ and $N = 3$, we can determine the coefficients D_{mnp} algebraically, using the exact expressions for the equilibrium positions and mode vectors which can be obtained in those two simple cases. We find that

$$N = 2 : D_{222} = -2^{\frac{1}{6}} \,,$$

$$N = 3 : D_{233} = -\frac{3}{\sqrt{2}} \left(\frac{4}{5}\right)^{\frac{4}{3}} \,, \quad D_{222} = -\frac{1}{\sqrt{2}} \left(\frac{4}{5}\right)^{\frac{1}{3}} \,. \tag{25}$$

All the other coefficients must be determined numerically, although this is a reasonably straightforward task. The approximate numerical values of the non-zero coefficients for two to ten ions are given in Tables 2 and Table 3.

4   Quantum motion of the ions

4.1   *Quantization of the Hamiltonian*

We can now consider the quantum motion of the ions by introducing the following position and momentum operators:

$$Z_n(t) \to \hat{Z}_n = \sqrt{\frac{\hbar}{2M\nu_n}} \left(\hat{a}_n + \hat{a}_n^\dagger\right)$$

$$\Pi_n^z(t) \to \hat{\Pi}_n^z = i\sqrt{\frac{M\hbar\,\nu_n}{2}} \left(\hat{a}_n^\dagger - \hat{a}_n\right) \,,$$

$$X_n(t) \rightarrow \hat{X}_n = \sqrt{\frac{\hbar}{2M\Omega_n}} \left(\hat{b}_n + \hat{b}_n^\dagger \right)$$

$$\Pi_n^x(t) \rightarrow \hat{\Pi}_n^x = i\sqrt{\frac{M\hbar\,\Omega_n}{2}} \left(\hat{b}_n^\dagger - \hat{b}_n \right) ,$$

$$Y_n(t) \rightarrow \hat{Y}_n = \sqrt{\frac{\hbar}{2M\Omega_n}} \left(\hat{c}_n + \hat{c}_n^\dagger \right)$$

$$\Pi_n^y(t) \rightarrow \hat{\Pi}_n^y = i\sqrt{\frac{M\hbar\,\Omega_n}{2}} \left(\hat{c}_n^\dagger - \hat{c}_n \right) , \quad (26)$$

where, as before, the Z-coordinate refers to motion along the axial direction of the trap, while the X- and Y-coordinates correspond to displacements in the transverse direction. These operators obey the canonical commutation relations

$$\left[\hat{X}_p, \hat{\Pi}_q^x \right] = \left[\hat{Y}_p, \hat{\Pi}_p^y \right] = \left[\hat{Z}_p, \hat{\Pi}_p^z \right] = i\hbar\delta_{pq} ,$$

$$\left[\hat{a}_p, \hat{a}_q^\dagger \right] = \left[\hat{b}_p, \hat{b}_q^\dagger \right] = \left[\hat{c}_p, \hat{c}_q^\dagger \right] = \delta_{pq} . \quad (27)$$

The Hamiltonian becomes

$$\hat{H} = \hat{H}_0 + \hat{H}_I , \quad (28)$$

where

$$\hat{H}_0 = \sum_{n=1}^N \hbar \left\{ v_n \hat{a}_n^\dagger \hat{a}_n + \Omega_n \left[\hat{b}_n^\dagger \hat{b}_n + \hat{c}_n^\dagger \hat{c}_n \right] \right\} ,$$

$$\hat{H}_I = \varepsilon\hbar\omega_3 \sum_{m,n,p=1}^N \frac{D_{mnp}}{\sqrt[4]{\mu_p}} \left(\hat{a}_p + \hat{a}_p^\dagger \right)$$

$$\times \left(\frac{2}{\sqrt[4]{\mu_m \mu_n}} \left(\hat{a}_m + \hat{a}_m^\dagger \right) \left(\hat{a}_n + \hat{a}_n^\dagger \right) \right.$$

$$- \frac{3}{\sqrt[4]{\gamma_m \gamma_n}} \Big[\left(\hat{b}_m + \hat{b}_m^\dagger \right) \left(\hat{b}_n + \hat{b}_n^\dagger \right)$$

$$\left. + \left(\hat{c}_m + \hat{c}_m^\dagger \right) \left(\hat{c}_n + \hat{c}_n^\dagger \right) \Big] \right) , \quad (29)$$

where ε is a dimensionless quantity which characterizes the strength of the non-linearity; it is given by

$$\varepsilon = \frac{1}{4\sqrt{2}} \left[\frac{\hbar\omega_3}{\alpha_{\text{fsc}}^2 Mc^2} \right]^{1/6} , \quad (30)$$

where α_{fsc} is the fine structure constant. Alternatively, $\varepsilon = \sigma/4\ell$, where $\sigma = \sqrt{\hbar/2M\omega_3}$ is the approximate width of the wavepackets of the individual ions, and ℓ, defined by (4), is the length scale on the order of the separation between ions. Since both D_{mnp} and μ_p are, at most, on the order of unity, while γ_p is assumed to be much larger than unity, we have

$$\left| \frac{\hat{H}_I}{\hat{H}_0} \right| \sim \varepsilon . \quad (31)$$

Values of ε for a variety of ions and traps are given in Table 1, which shows that this parameter tends to have a small value in experimental circumstances, implying that the treatment of $\hat{H}_I$ as a perturbation can be justified.

We will denote the eigenstates and eigenvalues of $\hat{H}_0$ by

$$|\Psi\rangle = \left| \left\{ n_1^x, \ldots, n_N^x \right\}, \left\{ n_1^y, \ldots, n_N^y \right\}, \left\{ n_1^z, \ldots, n_N^z \right\} \right\rangle \quad (32)$$

$$E_\Psi = \hbar \sum_{p=1}^N \Omega_p \left(n_p^x + n_p^y \right) + v_p n_p^z . \quad (33)$$

4.2 *Resonance conditions*

Fermi's golden rule [26] implies that population transfer between two eigenstates $|i\rangle$ and $|f\rangle$ of $\hat{H}_0$ induced by the interaction $\hat{H}_I$ can only occur if the matrix element $\langle f|\hat{H}_I|i\rangle$ is non-zero and if the energies of $|i\rangle$ and $|f\rangle$ are equal[2]. These conditions allow us to neglect a considerable number of the terms that occur when (29) is expanded. For example, because the square roots of the eigenvalues of A_{mn} are all irrational numbers (with the sole exception of μ_1), it follows that $\pm\left(\sqrt{\mu_p} \pm \sqrt{\mu_m} \pm \sqrt{\mu_n}\right) \neq 0$; hence we can neglect all the terms of the form $(\hat{a}_p + \hat{a}_p^\dagger)(\hat{a}_m + \hat{a}_m^\dagger)(\hat{a}_n + \hat{a}_n^\dagger)$. Similarly, terms involving three creation or three annihilation operators can be ignored. Making these approximations, and using the symmetry properties of D_{mnp} and the commutation relations (27), we obtain the following simplified expression for the interaction Hamiltonian (in the interaction picture):

$$\hat{H}_I \approx -3\varepsilon\hbar\omega_3$$

$$\times \sum_{m,n,p=1}^N \frac{D_{mnp}}{\sqrt[4]{\gamma_m \gamma_n \mu_p}} \left[2\hat{a}_p \left(\hat{b}_m^\dagger \hat{b}_n + \hat{c}_m^\dagger \hat{c}_n \right) e^{i\Delta_{mnp}^{(-)}\omega_z t} \right.$$

$$\left. + \hat{a}_p \left(\hat{b}_m^\dagger \hat{b}_n^\dagger + \hat{c}_m^\dagger \hat{c}_n^\dagger \right) e^{i\Delta_{mnp}^{(+)}\omega_z t} \right] + h.a., \quad (34)$$

where $h.a.$ stands for the hermitian adjoint of the preceding term, and $\Delta_{mnp}^{(\pm)} = \sqrt{\gamma_m} \pm \sqrt{\gamma_n} - \sqrt{\mu_p}$. We shall refer to the term proportional to $\exp(i\Delta_{mnp}^{(-)}\omega_z t)$, which involves the creation of a transverse phonon and simultaneous annihilation of both a longitudinal and a transverse phonon

Ion	ω_3	ε	$\varepsilon\omega_3$
$^9\text{Be}^+$	(2π) 5.0 MHz	1.06×10^{-3}	(2π) 5.30 kHz
$^{40}\text{Ca}^+$	(2π) 2.0 MHz	7.09×10^{-4}	(2π) 1.42 kHz
$^{88}\text{Sr}^+$	(2π) 200 kHz	4.24×10^{-4}	(2π) 85 Hz
$^{112}\text{Cd}^+$	(2π) 2.8 MHz	6.32×10^{-4}	(2π) 1.77 kHz

TABLE 1 Values of the parameter ε for various ions and trapping frequencies

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[2] This is equivalent to the energy matching condition in parametric down-conversion. Since the modes here do not represent travelling waves, there is no momentum conservation (or phase matching) condition as there is the non-linear optics.

(and the reverse process, contained within the hermitian adjoint part of (34)), as a resonance of the first kind; the term with $\exp(i\Delta_{mnp}^{(+)}\omega_z t)$, (which creates two transverse phonons in different modes by annihilating a longitudinal phonon) will be called a resonance of the second kind. Since the only experimentally controllable parameter in the definitions of $\Delta_{mnp}^{(\pm)}$ is the anisotropy parameter α, it is natural to ask at what values of α a resonance can occur. A necessary condition for resonance (i.e. for $\Delta_{mnp}^{(+)} = 0$ or $\Delta_{mnp}^{(-)} = 0$) is

$$\alpha = \frac{16\mu_p}{4\mu_p^2 + \mu_m^2 + \mu_n^2 - 8\mu_p + 4\mu_p\mu_m + 4\mu_p\mu_n - 2\mu_m\mu_n} .$$
(35)

Using the known values of the eigenvalues μ_p (see Table 2 of [18]), appropriate values for α can be found straightforwardly. However, not all of these values of α given by (35) correspond to a resonance, and one must determine whether or not the appropriate condition for either type of resonance is satisfied by direct substitution into the formulas for $\Delta_{mnp}^{(\pm)}$. Since $\sqrt{\mu_p} \neq 0$, resonances of the first kind are only possible when two distinct transverse modes are involved (i.e. $m \neq n$); resonances of the second kind can occur involving a single transverse mode (i.e. m can be equal to n). Resonances of the first kind tend to be very weak; the coupling coefficients do not exceed 1.6×10^{-3} for $L \leq 10$, and are always zero for $L \leq 6$. The values of α for the two types of resonance are given in Tables 2 and 3 (Appendix B) and are plotted for different numbers of ions in Fig. 2. Only those values less than the critical value α_{crit} are included, since our analysis is based on the assumption that the ions are in a linear configuration.

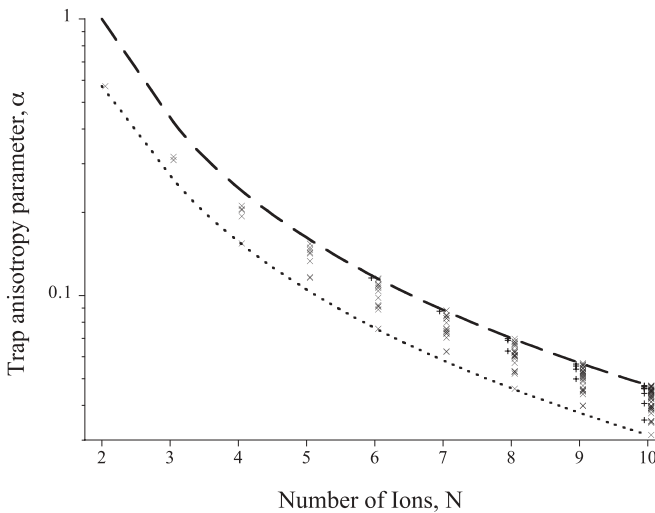One important result stems from this analysis. Resonance cannot occur for values of α below the minimum value given by

$$\alpha_{\min} = \begin{cases} \dfrac{16\mu_N}{\mu_N(9\mu_N + 2\mu_{N-1} - 8) + \mu_{N-1}^2} > \dfrac{4}{3\mu_N - 2} \\ \qquad\qquad\qquad\qquad\qquad \text{if } N \text{ is odd}, \\ \dfrac{4}{3\mu_N - 2} \qquad\qquad\quad\; \text{if } N \text{ is even}. \end{cases}$$
(36)

Thus, should one wish to avoid any form of mode–mode coupling due to the fourth order terms we consider in this paper, this can be ensured by using a trap with an anisotropy parameter smaller than $4/(3\mu_N - 2)$. This can also be expressed in terms of the critical anisotropy for the onset of zig-zag, α_{crit}: there will be no three-mode mixing if $\alpha < 4\alpha_{\mathrm{crit}}/(\alpha_{\mathrm{crit}} + 6)$.

4.3   *Example of mode–mode coupling*

As a specific example of the above general analysis, let us assume that we have six ions confined in a trap with an anisotropy factor of $\alpha = 0.09151$. For this value of α, a resonance of the second kind ($\Delta_{mnp}^{(+)} = 0$) occurs for the three modes $(m, n, p) = (5, 6, 5)$ and also for $(m, n, p) = (6, 5, 5)$ (since there is symmetry between m and n for resonances of the second kind).

The coupling Hamiltonian can be simplified by neglecting all off-resonant terms; for this case we get

$$\hat{H}_\mathrm{I} \simeq -3\varepsilon\hbar\omega_3 \frac{D_{565}}{\sqrt[4]{\mu_5\gamma_5\gamma_6}} \hat{a}_5 \left(\hat{b}_5^\dagger \hat{b}_6^\dagger + \hat{c}_5^\dagger \hat{c}_6^\dagger \right)$$

$$+ -3\varepsilon\hbar\omega_3 \frac{D_{655}}{\sqrt[4]{\mu_5\gamma_6\gamma_5}} \hat{a}_5 \left(\hat{b}_6^\dagger \hat{b}_5^\dagger + \hat{c}_6^\dagger \hat{c}_5^\dagger \right) + h.a.$$

$$= -\varepsilon\hbar\omega_3 \frac{6D_{565}}{\sqrt[4]{\mu_5\gamma_5\gamma_6}} \hat{a}_5 \left(\hat{b}_5^\dagger \hat{b}_6^\dagger + \hat{c}_5^\dagger \hat{c}_6^\dagger \right) + h.a. ,$$
(37)

where we have used the fact that $D_{655} = D_{565}$ and that $\left[\hat{b}_5^\dagger, \hat{b}_6^\dagger \right] = 0$ (and similarly for the $\hat{c}_m^\dagger$). From Table 3 we see that $D_{655} = 4.2528$ and $\alpha = 0.09151$; from Table 2 of [18] we find $\mu_5 = 13.51$; using (15) we find $\gamma_5 = 4.6709$ and $\gamma_6 = 2.2949$; thus $6D_{655}/\sqrt[4]{\mu_5\gamma_5\gamma_6} = 7.3556$.

As an example we will consider the case of coupling between three states defined by

$$|\Psi\rangle = |\,\{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 1, 0\}\rangle ,$$
$$|\Phi\rangle = |\,\{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 1, 1\}, \{0, 0, 0, 0, 0, 0\}\rangle ,$$
$$|\chi\rangle = |\,\{0, 0, 0, 0, 1, 1\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}\rangle ,$$
(38)

where we have used the notation for the motional quantum states of the ion modes defined in (32). Note that the coupling defined by (37) only involves the fifth longitudinal mode and the fifth and sixth transverse modes; the states of the other modes are unaffected; thus although we have set these other modes to have zero population in the definitions of $|\psi\rangle$, $|\phi\rangle$, and $|\chi\rangle$, they can be in arbitrary states without changing the analysis. The interaction picture state describing the system is given by

$$|\Psi(t)\rangle = \psi(t)|\Psi\rangle + \phi(t)|\Phi\rangle + \chi(t)|\chi\rangle .$$
(39)

FIGURE 2   Values of the anisotropy parameter α for which resonant three-mode mixing can occur. The *horizontal/vertical crosses* represent resonances of the first kind ($\Delta_{mnp}^{(-)} = 0$) and the *diagonal crosses* represent resonances of the second kind ($\Delta_{mnp}^{(+)} = 0$). The *upper limiting curve* represents the critical value α_{crit}, above which the linear configuration of the ions becomes unstable. The *lower curve* represents the highest value of α for which resonant mode–mode coupling cannot occur (see (36))

Axis labels: Trap anisotropy parameter, α (vertical); Number of Ions, N (horizontal)

Due to the resonance condition, $\left[\hat{H}_0, \hat{H}_I\right] = 0$ and the interaction picture coupling Hamiltonian is

$$e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_I e^{-\frac{i}{\hbar}\hat{H}_0 t} = \hat{H}_I. \tag{40}$$

Thus the Schrödinger equation describing the evolution of the system is given by

$$i\hbar\frac{d}{dt}|\Psi_I(t)\rangle = \hat{H}_I|\Psi_I(t)\rangle, \tag{41}$$

which implies that the probability amplitudes obey the following set of coupled equations:

$$i\dot{\psi}(t) = -\Gamma\left[\phi(t) + \chi(t)\right],$$
$$i\dot{\phi}(t) = -\Gamma\,\psi(t),$$
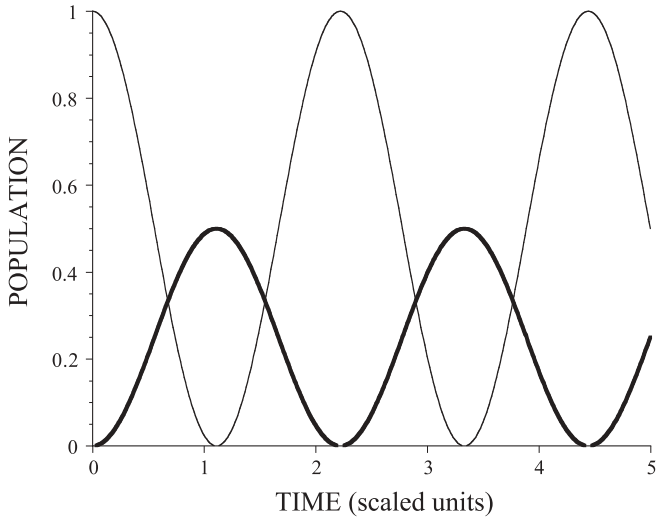$$i\dot{\chi}(t) = -\Gamma\,\psi(t), \tag{42}$$

FIGURE 3   The evolution of the populations when the initial state is $|\psi\rangle$. The *thin line* represents $|\psi(t)|^2$ and the *wide line* $|\phi(t)|^2 = |\chi(t)|^2$. Time is in units of $1/\Gamma$
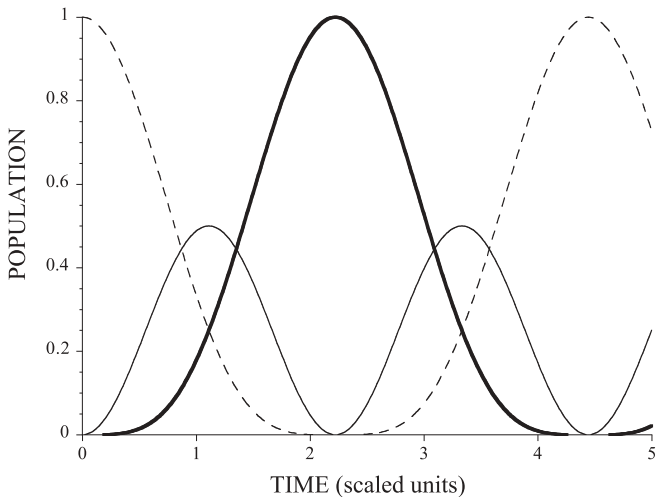

FIGURE 4   The evolution of the populations when the initial state is $|\phi\rangle$. The *thin line* represents $|\psi(t)|^2$, the *dashed line* $|\phi(t)|^2$, and the *wide line* $|\chi(t)|^2$. Time is in units of $1/\Gamma$

where $\Gamma = \varepsilon\omega_3(6D_{565}/\sqrt[4]{\mu_5\gamma_5\gamma_6})$. The solutions of these equations can be obtained straightforwardly using Laplace transforms:

$$\psi(t) = \psi(0)\cos\left(\sqrt{2}\Gamma t\right) + \frac{i\left(\phi(0) + \chi(0)\right)}{\sqrt{2}}\sin\left(\sqrt{2}\Gamma t\right),$$

$$\phi(t) = \frac{i\psi(0)}{\sqrt{2}}\sin\left(\sqrt{2}\Gamma t\right) + \phi(0)\cos^2\left(\frac{\Gamma t}{\sqrt{2}}\right)$$

$$- \chi(0)\sin^2\left(\frac{\Gamma t}{\sqrt{2}}\right),$$

$$\chi(t) = \frac{i\psi(0)}{\sqrt{2}}\sin\left(\sqrt{2}\Gamma t\right) - \phi(0)\sin^2\left(\frac{\Gamma t}{\sqrt{2}}\right)$$

$$+ \chi(0)\cos^2\left(\frac{\Gamma t}{\sqrt{2}}\right). \tag{43}$$

These solutions are plotted in Fig. 3 for the case $\psi(0) = 1$ (i.e. the longitudinal phonon mode initially excited) and in Fig. 4 for the case of $\phi(0) = 1$ (i.e. two transverse modes in the x direction initially excited).

4.4   *Entanglement*

Let us consider in detail the first example, shown in Fig. 3. The crystal of six ions was prepared with a single quanta in the fifth oscillatory mode, i.e. the state

$$|\Psi(0)\rangle$$
$$= |\{0,0,0,0,0,0\},\{0,0,0,0,0,0\},\{0,0,0,0,1,0\}\rangle. \tag{44}$$

After a time $t_1 = \pi/2\sqrt{2}\Gamma$ the crystal will have evolved into the state

$$|\Psi(t_1)\rangle$$
$$= \frac{i}{\sqrt{2}}(|\{0,0,0,0,0,0\},\{0,0,0,0,1,1\},\{0,0,0,0,0,0\}\rangle$$
$$+ |\{0,0,0,0,1,1\},\{0,0,0,0,0,0\},\{0,0,0,0,0,0\}\rangle). \tag{45}$$

This later state has the property of being entangled: it cannot be written as a product of the state of fifth and of the sixth oscillatory modes. This can be thought of as analogous to the type of polarization entangled states of photon pairs generated in optical down-conversion experiments [27]. The two transverse directions of oscillation are analogous to the photon polarizations, while the oscillatory mode is analogous to the spatial mode of the photons. The initially excited longitudinal oscillations play the role of the pump laser. Controlling this process in ion traps will be achieved by switching the trap anisotropy parameter α into the appropriate resonance parameter for the appropriate amount of

time, then rapidly switching it to a non-resonant value: this will have the effect of turning on the phonon–phonon interaction for a specific time. Furthermore, the technology for preparing oscillatory quantum states of trapped ions is, at the moment, more advanced than the current state of the art for preparing quantum states of the electromagnetic field. Specifically, one can hope to prepare the "pump" longitudinal mode in a single excitation Fock state, while creating single photons is still somewhat problematic. Thus, in principle, deterministic preparation of oscillatory entangled states may be attained, in contrast to the non-deterministic, post-selection state preparation in quantum optics experiments. Furthermore the method of entangled oscillatory state preparation described here, combined with the variety of techniques for creating entanglement of internal degrees of freedom raises the possibility of creating hyper-entangled states in ion traps [28].

5   Conclusion

In this paper we have analyzed the dynamics of ions confined in harmonic traps. The normal modes of the oscillations of the ions are intrinsically coupled by the Coulomb interaction. This "three-mode mixing" is in some ways analogous to non-linear optical effects. There are two important results that our analysis has revealed: first, if one wishes to avoid these effects altogether, the trap anisotropy, characterized by the parameter α defined by (2), must be less than a certain value given by (36); secondly, this effect in principle may be exploited to create entangled motional states of the ions, by carefully controlling the dynamics of the ions, as outlined in Sects. 4.3 and 4.4. How the resulting entangled states may be exploited for tasks in quantum information is a promising avenue for further investigation.

Appendices

Appendix A   Derivation of (9), (10), and (11)

In this Appendix, we show how to derive the Lagrangian (8) from (7). We will use the following notation:

$$R_i^{(mn)} = x_{mi} - x_{ni} \,, \tag{A.1}$$

$$R^{(mn)} = \left[\sum_{i=1}^{3} (x_{mi} - x_{ni})^2 \right]^{\frac{1}{2}} \,. \tag{A.2}$$

The potential energy of the ions is

$$V = \frac{M}{2} \sum_{n=1}^{N} \sum_{i=1}^{3} \omega_i^2 \, x_{ni}^2 + \frac{Z^2 e^2}{8\pi\varepsilon_0} \sum_{\substack{n,m=1 \\ m\neq n}}^{N} \frac{1}{R^{(mn)}} \,. \tag{A.3}$$

Thus we have

$$\frac{\partial V}{\partial x_{mi}} = M\omega_i^2 \left(x_{mi} - \frac{\ell^3 \omega_3^2}{\omega_i^2} \sum_{\substack{p=1 \\ p\neq m}}^{N} \frac{R_i^{(mp)}}{R^{(mp)3}} \right) \,, \tag{A.4}$$

$$\frac{\partial^2 V}{\partial x_{mi}\partial x_{nj}} = M\omega_i^2 \left[\delta_{mn}\delta_{ij} - \frac{\ell^3 \omega_3^2}{\omega_i^2} \sum_{\substack{p=1 \\ p\neq m}}^{N} \frac{\delta_{mn} - \delta_{pn}}{R^{(mp)3}} \right.$$
$$\left. \times \left(\delta_{ij} - 3\frac{R_i^{(mp)} R_j^{(mp)}}{R^{(mp)2}} \right) \right] \,, \tag{A.5}$$

$$\frac{\partial^3 V}{\partial x_{mi}\partial x_{nj}\partial x_{pk}} = 3M\ell^3\omega_3^2 \sum_{\substack{q=1 \\ q\neq m}}^{N} \left(\delta_{mn} - \delta_{qn} \right)\left(\delta_{mp} - \delta_{qp} \right)$$
$$\times \left(\frac{\delta_{ij}R_k^{(mq)} + \delta_{ik}R_j^{(mq)} + \delta_{jk}R_i^{(mq)}}{R^{(mq)5}} \right.$$
$$\left. -5\frac{R_i^{(mq)} R_j^{(mq)} R_k^{(mq)}}{R^{(mq)7}} \right) \,. \tag{A.6}$$

{m, n, p}	D_{mnp}	α_{res}	{m, n, p}	D_{mnp}	α_{res}	{m, n, p}	D_{mnp}	α_{res}
$N = 6$			$N = 7$					
{3, 6, 3}	2.8395×10^{-4}	0.11575	{4, 7, 3}	5.4794×10^{-4}	0.087700			
$N = 8$								
{3, 8, 3}	3.1152×10^{-6}	0.062943	{4, 8, 4}	1.0031×10^{-3}	0.069797	{5, 8, 3}	7.4469×10^{-4}	0.068879
$N = 9$								
{3, 9, 4}	5.7509×10^{-6}	0.054162	{4, 9, 3}	5.7509×10^{-6}	0.049960	{5, 9, 4}	1.2967×10^{-3}	0.056583
{6, 9, 3}	8.8502×10^{-4}	0.055637						
$N = 10$								
{3, 10, 3}	5.9416×10^{-8}	0.035465	{3, 10, 5}	7.3591×10^{-6}	0.046313	{4, 10, 4}	1.0248×10^{-5}	0.044211
{5, 10, 3}	7.3591×10^{-6}	0.040715	{5, 10, 5}	1.5984×10^{-3}	0.047291	{6, 10, 4}	1.4703×10^{-3}	0.046822
{7, 10, 3}	9.8451×10^{-4}	0.045964						

TABLE 2   Coupling constants for resonances of the first kind (in which a transverse phonon creates a longitudinal phonon and a transverse phonon), see Appendix B for notes

$\{m, n, p\}$	D_{mnp}	α_{res}	$\{m, n, p\}$	D_{mnp}	α_{res}	$\{m, n, p\}$	D_{mnp}	α_{res}
$N = 2$			**$N = 3$**					
$\{2, 2, 2\}$	-1.1225	0.57143	$\{3, 2, 3\}$	-1.5754	0.30917	$\{3, 3, 2\}$	-1.5754	0.31746
$N = 4$								
$\{3, 3, 4\}$	-1.8332	0.21132	$\{4, 2, 4\}$	-1.9493	0.19337	$\{4, 3, 3\}$	-1.8332	0.20560
$\{4, 4, 2\}$	-1.9493	0.20391	$\{4, 4, 4\}$	2.1084	0.15429			
$N = 5$								
$\{4, 3, 5\}$	-1.9683	0.14895	$\{4, 4, 4\}$	-0.89355	0.15387	$\{5, 2, 5\}$	-2.2887	0.13340
$\{5, 3, 4\}$	-1.9683	0.14187	$\{5, 4, 3\}$	-1.9683	0.14619	$\{5, 4, 5\}$	3.1611	0.11561
$\{5, 5, 2\}$	-2.2887	0.14311	$\{5, 5, 4\}$	3.1611	0.11668			
$N = 6$								
$\{4, 4, 6\}$	-1.8850	0.11439	$\{5, 3, 6\}$	-2.0625	0.10985	$\{5, 4, 5\}$	8.1287×10^{-2}	0.11527
$\{5, 5, 6\}$	4.2528	0.092393	$\{6, 2, 6\}$	-2.6084	0.098229	$\{6, 3, 5\}$	-2.0625	0.10398
$\{6, 4, 4\}$	-1.8850	0.10784	$\{6, 4, 6\}$	4.0185	0.088947	$\{6, 5, 3\}$	-2.0625	0.10937
$\{6, 5, 5\}$	4.2528	0.091510	$\{6, 6, 2\}$	-2.6084	0.10658	$\{6, 6, 4\}$	4.0185	0.091151
$\{6, 6, 6\}$	-2.3706	0.075762						
$N = 7$								
$\{6, 3, 7\}$	-2.1382	0.084291	$\{6, 5, 7\}$	4.9336	0.074398	$\{6, 6, 6\}$	4.3077	0.075526
$\{7, 2, 7\}$	-2.9149	0.075728	$\{7, 3, 4\}$	5.4794×10^{-4}	0.088234	$\{7, 3, 6\}$	-2.1382	0.079773
$\{7, 4, 5\}$	-1.7957	0.082749	$\{7, 4, 7\}$	4.7748	0.070376	$\{7, 5, 4\}$	-1.7957	0.084569
$\{7, 5, 6\}$	4.9336	0.072836	$\{7, 6, 3\}$	-2.1382	0.085059	$\{7, 6, 5\}$	4.9336	0.074000
$\{7, 6, 7\}$	-3.8751	0.062565	$\{7, 7, 2\}$	-2.9149	0.082796	$\{7, 7, 4\}$	4.7748	0.073152
$\{7, 7, 6\}$	-3.8751	0.062861						
$N = 8$								
$\{6, 6, 8\}$	5.2871	0.062147	$\{7, 3, 8\}$	-2.2035	0.066792	$\{7, 5, 8\}$	5.4173	0.060792
$\{7, 6, 7\}$	3.6190	0.062378	$\{7, 7, 6\}$	3.6190	0.062674	$\{7, 7, 8\}$	-5.8640	0.053277
$\{8, 2, 8\}$	-3.2119	0.060393	$\{8, 3, 5\}$	7.4469×10^{-4}	0.069615	$\{8, 3, 7\}$	-2.2035	0.063341
$\{8, 4, 6\}$	-1.7158	0.065623	$\{8, 4, 8\}$	5.4691	0.057068	$\{8, 5, 5\}$	-1.5767	0.067200
$\{8, 5, 7\}$	5.4173	0.059134	$\{8, 6, 4\}$	-1.7158	0.068081	$\{8, 6, 6\}$	5.2871	0.060526
$\{8, 6, 8\}$	-5.1946	0.052159	$\{8, 7, 3\}$	-2.2035	0.068170	$\{8, 7, 5\}$	5.4173	0.061000
$\{8, 7, 7\}$	-5.8640	0.053018	$\{8, 8, 2\}$	-3.2119	0.066389	$\{8, 8, 4\}$	5.4691	0.060029
$\{8, 8, 6\}$	-5.1946	0.052896	$\{8, 8, 8\}$	2.1526	0.046043			
$N = 9$								
$\{7, 6, 9\}$	5.4146	0.052246	$\{7, 7, 8\}$	1.6006	0.053125	$\{8, 3, 9\}$	-2.2623	0.054311
$\{8, 5, 9\}$	5.7898	0.050462	$\{8, 6, 8\}$	2.6715	0.052000	$\{8, 7, 7\}$	1.6006	0.052867
$\{8, 7, 9\}$	-7.3423	0.045500	$\{8, 8, 6\}$	2.6715	0.052744	$\{8, 8, 8\}$	-7.5531	0.045900
$\{9, 2, 9\}$	-3.5017	0.049433	$\{9, 3, 6\}$	8.8502×10^{-4}	0.056425	$\{9, 3, 8\}$	-2.2623	0.051650
$\{9, 4, 5\}$	1.2967×10^{-3}	0.056883	$\{9, 4, 7\}$	-1.6468	0.053425	$\{9, 4, 9\}$	6.1214	0.047245
$\{9, 5, 6\}$	-1.4030	0.054734	$\{9, 5, 8\}$	5.7898	0.048927	$\{9, 6, 5\}$	-1.4030	0.055586
$\{9, 6, 9\}$	-6.3927	0.044000	$\{9, 7, 4\}$	-1.6468	0.056011	$\{9, 7, 6\}$	5.4146	0.050996
$\{9, 7, 8\}$	-7.3423	0.044970	$\{9, 8, 3\}$	-2.2623	0.055954	$\{9, 8, 5\}$	5.7898	0.051126
$\{9, 8, 7\}$	-7.3423	0.045400	$\{9, 8, 9\}$	3.8083	0.039874	$\{9, 9, 2\}$	-3.5017	0.054558
$\{9, 9, 4\}$	6.1214	0.050180	$\{9, 9, 6\}$	-6.3927	0.045081	$\{9, 9, 8\}$	3.8083	0.039988
$N = 10$								
$\{7, 7, 10\}$	5.2107	0.044976	$\{8, 6, 10\}$	5.4385	0.044332	$\{8, 7, 9\}$	-0.42626	0.045380
$\{8, 8, 10\}$	-1.9896	0.045779	$\{8, 8, 10\}$	-8.6478	0.039673	$\{9, 3, 10\}$	-2.3165	0.045099
$\{9, 4, 9\}$	3.3150	0.047113	$\{9, 5, 10\}$	6.0930	0.042512	$\{9, 6, 9\}$	1.6336	0.043878
$\{9, 7, 8\}$	-0.42626	0.044846	$\{9, 7, 10\}$	-8.5012	0.039123	$\{9, 8, 7\}$	-0.42626	0.045279
$\{9, 8, 9\}$	-8.0166	0.039760	$\{9, 9, 6\}$	1.6336	0.044957	$\{9, 9, 8\}$	-8.0166	0.039874
$\{9, 9, 10\}$	6.3437	0.035161	$\{10, 2, 10\}$	-3.7855	0.041300	$\{10, 3, 7\}$	9.8451×10^{-4}	0.046733
$\{10, 3, 9\}$	-2.3165	0.043017	$\{10, 4, 6\}$	1.4703×10^{-3}	0.047276	$\{10, 4, 8\}$	-1.5874	0.044422
$\{10, 4, 10\}$	6.7435	0.039798	$\{10, 5, 7\}$	-1.2642	0.045500	$\{10, 5, 7\}$	-1.2642	0.045500
$\{10, 5, 9\}$	6.0930	0.041163	$\{10, 6, 6\}$	-1.1721	0.046259	$\{10, 6, 8\}$	5.4385	0.042265
$\{10, 6, 10\}$	-7.5034	0.037564	$\{10, 7, 5\}$	-1.2642	0.046721	$\{10, 7, 7\}$	5.2107	0.043067
$\{10, 7, 9\}$	-8.5012	0.038483	$\{10, 8, 4\}$	-1.5874	0.046923	$\{10, 8, 6\}$	5.4385	0.043500
$\{10, 8, 8\}$	-8.6478	0.039085	$\{10, 8, 10\}$	5.3952	0.034687	$\{10, 9, 3\}$	-2.3165	0.046823
$\{10, 9, 5\}$	6.0930	0.043468	$\{10, 9, 7\}$	-8.5012	0.039269	$\{10, 9, 9\}$	6.3437	0.035057
$\{10, 10, 2\}$	-3.7855	0.045724	$\{10, 10, 4\}$	6.7435	0.042604	$\{10, 10, 6\}$	-7.5034	0.038860
$\{10, 10, 8\}$	5.3952	0.035000	$\{10, 10, 10\}$	-1.7362	0.031318			

TABLE 3   Resonances of the second kind (in which a longitudinal phonon creates two transverse phonons), see Appendix B for notes

These terms can be evaluated at equilibrium by making the following substitutions:

$$\bar{R}_i^{(mn)} = \ell \, \delta_{i3}(u_m - u_n), \tag{A.7}$$

$$\bar{R}^{(mn)} = \ell \, |u_m - u_n|. \tag{A.8}$$

We thus obtain

$$\left.\frac{\partial V}{\partial x_{mi}}\right|_0 = M\omega_i^2 \delta_{i3}\left(u_m - \sum_{\substack{n=1 \\ n \neq m}}^{N} \frac{\text{sgn}\,(u_m - u_n)}{(u_m - u_n)^2}\right), \tag{A.9}$$

$$\frac{\partial^2 V}{\partial x_{mi} \partial x_{nj}}\bigg|_0$$

$$= M\omega_3^2 \left[\delta_{mn}\delta_{ij} \frac{\omega_i^2}{\omega_3^2} - \sum_{\substack{p=1 \\ p \neq m}}^{N} \frac{\delta_{mn} - \delta_{pn}}{|u_m - u_p|^3} \left(\delta_{ij} - 3\delta_{i3}\delta_{j3}\right) \right], \tag{A.10}$$

$$\frac{\partial^3 V}{\partial x_{mi} \partial x_{nj} \partial x_{pk}}\bigg|_0$$

$$= \frac{3M\omega_3^2}{\ell} \sum_{\substack{q=1 \\ q \neq m}}^{N} \frac{\text{sgn}\left(u_m - u_q\right)\left(\delta_{mn} - \delta_{qn}\right)\left(\delta_{mp} - \delta_{qp}\right)}{(u_m - u_q)^4}$$

$$\times \left(\delta_{ij}\delta_{k3} + \delta_{ik}\delta_{j3} + \delta_{jk}\delta_{i3} - 5\delta_{i3}\delta_{j3}\delta_{k3}\right). \tag{A.11}$$

The equations that determine the equilibrium positions u_m are given by (A.9)). From (A.10)) we can write

$$\frac{1}{2} \sum_{m,n=1}^{N} \sum_{i,j=1}^{3} \frac{\partial^2 V}{\partial x_{mi} \partial x_{nj}}\bigg|_0 \xi_{mi}\xi_{nj}$$

$$= \frac{M\omega_3^2}{2} \sum_{m,n=1}^{N} A_{mn}\xi_{m3}\xi_{n3} + B_{mn} \left(\xi_{m1}\xi_{n1} + \xi_{m2}\xi_{n2}\right), \tag{A.12}$$

with

$$A_{mn} = \delta_{mn} + 2 \sum_{\substack{p=1 \\ p \neq m}}^{N} \frac{\delta_{mn} - \delta_{pn}}{|u_m - u_p|^3} \tag{A.13}$$

and

$$B_{mn} = \frac{\delta_{mn}}{\alpha} - \sum_{\substack{p=1 \\ p \neq m}}^{N} \frac{\delta_{mn} - \delta_{pn}}{|u_m - u_p|^3}, \tag{A.14}$$

which are equivalent to the expressions given in Sect. 2. Finally,

$$\frac{1}{6} \sum_{m,n,p=1}^{N} \sum_{i,j,k=1}^{3} \frac{\partial^3 V}{\partial x_{mi} \partial x_{nj} \partial x_{pk}}\bigg|_0 \xi_{mi}\xi_{nj}\xi_{pk}$$

$$= \frac{M\omega_3^2}{2\ell} \sum_{mnp=1}^{N} C_{mnp} \,\xi_{p3} \left(2\xi_{m3}\xi_{n3} - 3\xi_{m1}\xi_{n1} - 3\xi_{m2}\xi_{n2}\right), \tag{A.15}$$

where

$$C_{mnp} = \sum_{\substack{q=1 \\ q \neq m}}^{N} \frac{\text{sgn}\left(u_q - u_m\right)\left(\delta_{mn} - \delta_{qn}\right)\left(\delta_{mp} - \delta_{qp}\right)}{(u_m - u_q)^4}. \tag{A.16}$$

Appendix B   Notes on Tables 2 and 3

Tables 2 and 3 list the non-zero values of the mode cross-coupling coefficients D_{mnp} defined by (20) for crystals of two to ten ions, together with the associated resonant anisotropy parameter α. Other values may be determined via the symmetry relation $D_{mnp} = D_{mpn} = D_{npm} = D_{nmp} = D_{pmn} = D_{pnm}$. Note however that the value of α is symmetric only under interchange of the first two indices.

REFERENCES

1 J.I. Cirac, P. Zoller: Phys. Rev. Lett. **74**, 4094 (1995)
2 C. Monroe, D.M. Meekhof, B.E. King, W.M. Itano, D.J. Wineland: Phys. Rev. Lett. **75**, 4714 (1995)
3 M.A. Nielsen, I.L. Chuang: *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000) Sect. 7.6
4 D.J. Wineland, C. Monroe, W.M. Itano, D. Leibfried, B. King, D.M. Meekhof: J. Res. Natl. Inst. Stand. Technol. **103**, 259 (1998)
5 D.F.V. James: Fort. d. Phys. **48**, 823 (2000)
6 D. Kielpinski, C. Monroe, D.J. Wineland: Nature **417**, 709 (2002)
7 M. Šašura, V. Bužek: J. Mod. Opt. **49**, 1593 (2002)
8 C.A. Sackett, D. Kielpinski, B.E. King, C. Langer, V. Meyer, C.J. Myatt, M. Rowe, Q.A. Turchette, W.M. Itano, D.J. Wineland, C. Monroe: Nature **404**, 256 (2000)
9 M.A. Rowe, D. Kielpinski, V. Meyer, C.A. Sackett, W.M. Itano, C. Monroe, D.J. Wineland: Nature **409**, 791 (2001)
10 J. Eschner, C. Raab, F. Schmidt-Kaler, R. Blatt: Nature **413**, 495 (2001)
11 S. Earnshaw: Trans. Cambridge Phil. Soc. **7**, 97 (1842); see also, for instance, J.A. Stratton: *Electromagnetic Theory* (McGraw–Hill, New York 1941) p. 116
12 P.K. Ghosh: *Ion Traps* (Clarendon Press, Oxford 1995)
13 D.J. Berkeland, J.D. Miller, J.C. Bergquist, W.M. Itano, D.J. Wineland: Phys. Rev. Lett. **80**, 2089 (1998)
14 E. Fermi, J. Pasta, S. Ulam: 'Studies of Nonlinear Problems I'. In Los Alamos Scientific Laboratory report # LA-1940 (May, 1955); reprinted in S. Ulam: *Stanislaw Ulam: Sets, Numbers and Universes; Selected Works*, ed. by W.A. Beyer, J. Mycielski, G.-C. Rota (MIT Press, Cambridge MA 1974) p. 490
15 See, for example, N. Gisin, J.G. Rarity, G. Weihs: In *The Physics of Quantum Information*, ed. by D. Bouwmeester, A. Ekert, A. Zeilinger (Springer, Berlin 2000) Sect. 3.4, p. 53
16 D.J. Berkeland, J.D. Miller, J.C. Berquist, W.M. Itano, D.J. Wineland: J. Appl. Phys. **83**, 5025 (1998)
17 A.M. Steane: Appl. Phys. B **64**, 623 (1997)
18 D.F.V. James: Appl. Phys. B **66**, 181 (1998)
19 T.P. Meyrath, D.F.V. James: Phys. Lett. A **240**, 37 (1998)
20 D. Kielpinski, B.E. King, C.J. Myatt, C.A. Sackett, Q.A. Turchette, W.M. Itano, C. Monroe, D.J. Wineland, W.H. Zurek: Phys. Rev. A **61**, 032310 (2000)
21 G. Morigi, H. Walther: Eur. Phys. J. D **13**, 261 (2000); erratum: Eur. Phys. J. D **15**, 137 (2000)
22 H.C. Nagerl, D. Leibfried, F. Schmidt-Kaler, J. Eschner, R. Blatt: Opt. Express **3**, 89 (1998)
23 D. Enzer, M.M. Schauer, J.J. Gomez, M.S. Gulley, M.H. Holzscheiter, P.G. Kwiat, S.K. Lamoreaux, C.G. Peterson, V.D. Sandberg, D. Tupa, A.G. White, R.J. Hughes, D.F.V. James: Phys. Rev. Lett. **85**, 2466 (2000)
24 X.Y. Chu, M. Holzki, R. Alheit, G. Werth: Int. J. Mass. Spectrom. Ion Processes **173**, 107 (1998); Note that these authors use the word "mode" in a different context to that used in this paper
25 Q.A. Turchette, D. Kielpinski, B.E. King, D. Leibfried, D.M. Meekhof, C.J. Myatt, M.A. Rowe, C.A. Sackett, C.S. Wood, W.M. Itano, C. Monroe, D.J. Wineland: Phys. Rev. A **61**, 063418 (2000)
26 L.I. Schiff, *Quantum Mechanics*, 2nd edn. (McGraw–Hill, New York 1968) Sect. 35
27 A.G. White, P.G. Kwiat, D.F.V. James, P.H. Eberhard: Phys. Rev. Lett. **83**, 3103 (1999)
28 P.G. Kwiat: J. Mod. Opt. **44**, 2173 (1997)