Eur. Phys. J. D **13**, 261–269 (2001)

THE EUROPEAN PHYSICAL JOURNAL D

EDP Sciences

Two-species Coulomb chains for quantum information

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Received 19 May 2000

Abstract. We study from the point of view of quantum information the properties of the collective oscillations of a linear chain of ions trapped in a linear Paul trap and composed of two ion species. We discuss extensively sympathetic cooling of the chain and the effect of anharmonicity on laser-cooling and quantum-information processing.

PACS. 03.67.Lx Quantum computation – 32.80.Pj Optical cooling of atoms; trapping – 42.50.Vk Mechanical effects of light on atoms, molecules, electrons, and ions

1 Introduction

The rapid development of trapping techniques for neutral and charged particles has constituted a breakthrough in the investigation of quantum mechanical systems [1]. Among the many interesting experiments, ordered structures of charged ions have been achieved in Paul and Penning traps [2,3]. Such structures are composed from few up to thousands of particles, and they originate at low temperature from the combined effect of the Coulomb repulsive interaction among the ions and the trapping potential [4]. Therefore, their geometry depends intrinsically on the trap set-up.

The field of interest of these so-called "Coulomb crystals" is rather broad, and in quantum optics they find an application in the ion-trap quantum computer [5]. Here, a string of ions is proposed as a system for processing information, using two stable or metastable internal states of the ions for storing the quantum information and coherent interaction of the internal degrees of freedom of the single ions with the laser light for generating the unitary operations which process the information, while the coupling among ions is provided by the collective vibrational excitations of the chain. Present schemes for quantum information processing are based on the harmonicity of the ionic motion [6,7]. This regime can be achieved by laser cooling [8] the string of ions, and to a good extent the ions can be considered to vibrate harmonically around their equilibrium positions.

The coupling to the environment gives rise to phenomena which destroy the quantum coherence required for processing the information: decoherence affects both the internal and the motional quantum states. For motional states, decoherence can be inhibited by applying laser-cooling to the ion-chain on a regular rate or even continuously. Laser-cooling does not destroy the quantum information stored in the internal states, provided only some ions are addressed by the cooling laser (*cooling ions*), while the chain is sympathetically cooled *via* the Coulomb interaction. Furthermore it allows for simultaneous information processing on the other ions (*qu-bits*), provided the quantum gates do not require quantum coherence among the vibrational levels, as for the gate proposed in [7] and realized in [9]. In this respect, it is rather difficult to find a candidate ion which is, at the same time, a good qubit and cooling ion. In addition, some realizations of ion strings for quantum information do not rely on the spatial resolution of the ions with the laser [9]. Hence, one of the most recent issues in the ion-trap quantum computer is to use two different ionic species which compose the ion chain, one for quantum information processing, the other for laser-cooling [10–12]. This type of crystal, which we call here the *two-species Coulomb crystal*, has been already used for imaging the mechanical effect of radiation pressure on the crystallized ions and for sympathetic cooling of big ordered ionic structures [13].

In this work we study the mechanical motion in a two-species linear crystal from the point of view of quantum information, illustrating the general features and the differences from a linear crystal composed of ions of equal masses, and we discuss in some detail sympathetic cooling of the chain. The issue of decoherence is also discussed in connection to the mechanical properties of the system. In particular, in this paper we consider the decoherence due to the coupling of the ionic motion to the fluctuations of the electric field (which we assume to have an instantaneous value with zero spatial gradient) along the crystal, and thus couples with the center of mass motion. Finally, we discuss the harmonic approximation and the effect of the anharmonic corrections on laser cooling and quantum information processing. An analogous analysis has been presented in [11], where they studied one specific scheme for sympathetic cooling. Here, we study the

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more general system and its properties, and seek schemes which are more suitable for quantum information processing. In particular, we provide some examples calculated with $^{115}In^+$ and $^{25}Mg^+$ ions, which have been currently trapped and cooled in Garching [14,15].

The paper is organized as follows. In Section 2 the small oscillations formalism is introduced, and the mechanical properties of a chain of ions are discussed in detail. In particular, sympathetic cooling of the two-species linear chain is studied, and the rates of cooling for different crystal configurations are derived. In Section 3 the effect of the anharmonic corrections on cooling and quantum information processing is discussed. Summary and conclusions are presented in Section 4.

2 Small oscillations

In this section we investigate the collective vibrations around the equilibrium position of a chain of ions confined in a linear Paul trap, following the lines of the literature of small oscillations [16]. We assume the motion to be one-dimensional, *i.e.* confined along the trap axis of the linear Paul trap. This describes with good approximation the motion in a trap with very steep radial potential [17].

We consider a one-dimensional string of N ions with charge e and mass equal either to M or m, aligned along the $\hat{x}$-axis, which corresponds to the axis of the linear Paul trap. Indicating with i the position of the ion in the chain ($i = 1, ..., N$), the sequence of ionic masses is described by the array $\mathbf{m} = (m_1, ..., m_N)$ with $m_i = M, m$. The ions are confined by the electrostatic potential V_S and interact *via* the Coulomb repulsion [18]. Sufficiently far away from the electrodes, V_S can be considered harmonic and the total potential V has the form:

$$V = \sum_{i=1}^{N} \frac{1}{2} u_0 x_i^2 + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} \frac{e^2/4\pi\epsilon_0}{|x_i - x_j|}, \tag{1}$$

where x_i is the coordinate of the ion i and u_0 is a constant with the dimensions of an energy over a distance squared. If the ions are sufficiently cold [4], they crystallize around the classical equilibrium positions $x_i^{(0)}$, which are the solutions of the set of equations $\partial V/\partial x_i|_{x_i^{(0)}} = 0$. Those solutions are independent of the mass, as the potential of the electrodes interacts only with the ionic charges. A characteristic quantity is the equilibrium distance between two ions:

$$x_0 = x_2^{(0)} - x_1^{(0)} = \left(\frac{2e^2/4\pi\epsilon_0}{u_0} \right)^{1/3}, \tag{2}$$

where the ions are displaced symmetrically with respect to the center of the trap. This quantity scales the inter-ionic distance in the chain [19].

Assuming that the collective motion of the ions around the equilibrium position is harmonic, we approximate V with its Taylor expansion around $x_i^{(0)}$ truncated to second order. The dynamics of the system are described by the Lagrangian

$$L = \frac{1}{2} \left[\sum_{i=1}^{N} m_i \dot{q}_i^2 - \sum_{i=1}^{N} V_{ij} q_i q_j \right], \tag{3}$$

where $q_i = x_i - x_i^{(0)}$ are the displacements of the ions from the equilibrium positions, and V_{ij} are real coefficients which have the form:

$$\begin{aligned} V_{ij} &= \frac{\partial^2}{\partial x_i \partial x_j} V(x_1, ..., x_N)|_{\{x_i^{(0)}\}} \\ &= u_0 + 2 \sum_{k=1, k\neq i} \frac{e^2/4\pi\epsilon_0}{|x_i^{(0)} - x_k^{(0)}|^3} \quad \text{if } i = j \\ &= -2 \frac{e^2/4\pi\epsilon_0}{|x_i^{(0)} - x_j^{(0)}|^3} \quad \text{if } i \neq j. \end{aligned} \tag{4}$$

From (3) the equations for the normal modes of the motion are

$$\sum_{j=1}^{N} V_{ij} \beta_j^\alpha = \lambda_\alpha m_i \beta_i^\alpha \quad \text{with} \quad \alpha = 1, ..., N \tag{5}$$

where the eigenvalues λ_α are real given the hermiticity of V_{ij}, and where β^α is eigenvector at λ_α. Stable and harmonic oscillations exist if the condition $\lambda_\alpha > 0$ is fulfilled for any α, as it occurs in this case. Under this condition the frequency of the normal mode Ω_α is $\Omega_\alpha = \sqrt{\lambda_\alpha}$. The eigenvectors β_i^α are orthogonal in the Riemannian space with metric tensor $\mathbf{M}$, where $\mathbf{M}$ is a diagonal matrix whose diagonal corresponds to the array $\mathbf{m}$. For $\lambda_\alpha > 0$, introducing the mass-weighted coordinates $q_i' = \sqrt{m_i} q_i$ the eigenvalue problem can be rewritten as

$$\sum_j V_{ij}' \beta_j^{\alpha\prime} = \Omega_\alpha^2 \beta_i^{\alpha\prime} \quad \text{for} \quad \alpha = 1, ..., N, \tag{6}$$

where now $V_{ij}' = V_{ij}/\sqrt{m_i m_j}$, and the metric tensor is the identity matrix, as for Cartesian coordinates. The eigenvalue problem is now equivalent to the one of N identical ions of unitary mass. The matrix $\{\beta_i^{\alpha\prime}\}$ defines an orthogonal transformation, which reduces the system to the principal axes α of V_{ij} and of the kinetic term: $\pi_\alpha = \sum_i \beta_i^{\alpha\prime} q_i'$. In this representation the Lagrangian describes a set of N independent harmonic oscillators with frequencies Ω_α. We quantize the motion by associating a quantum mechanical oscillator with each mode. Then, denoting a_α, $a_\alpha^\dagger$ the annihilation, creation operators for the mode α, respectively, the coordinate π_α associated with the oscillator of frequency Ω_α is written as $\pi_\alpha = \sqrt{\hbar/2\Omega_\alpha} \left(a_\alpha + a_\alpha^\dagger \right)$. Going back to the original set of coordinates q_i, they have the quantized form

$$q_i = \frac{1}{\sqrt{m_i}} \sum_\alpha \left(\beta_i^{\alpha\prime} \right)^{-1} \sqrt{\frac{\hbar}{2\Omega_\alpha}} \left(a_\alpha + a_\alpha^\dagger \right). \tag{7}$$

Some general features can now be recognized. From equation (6) it is evident that the eigenmodes depend on the

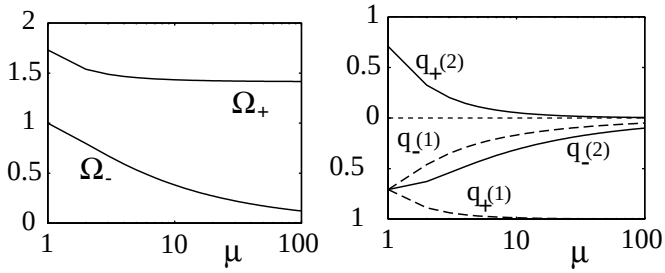


Fig. 1. (a) Eigenfrequencies of the two-ion crystal as a function of the mass ratio μ. The frequencies are rescaled by the factor $\sqrt{u_0/m}$. (b) Corresponding displacements in the original axes plotted as a function of μ. Solid line: particle of mass M. Dashed line: particle of mass m.

values of the ionic masses. Furthermore, since the matrix V_{ij} is symmetrical by exchange of any pair of ions, the properties of the motion will be mainly characterized by the symmetries of the sequence $\mathbf{m}$. These properties are reflected in the eigenmodes of the motion $\{\beta_\alpha\}$, and thus they affect the coupling of the crystal to radiation.

We discuss these points below. First, we consider the properties connected to two different values of the ionic masses, by analysing the case of two ions. Then, we discuss the ones connected to the symmetries of $\mathbf{m}$ by considering a three-ion crystal. Finally, on the basis of equation (7) we study the mechanical effect of radiation on the crystal, and in particular sympathetic cooling of the chain.

2.1 Two ions of different masses

We analyse here the two-ion crystal, where the ions have masses m and $M = \mu m$ with μ real parameter, $\mu > 1$. For this case the secular equation (6) can be solved analytically, and the eigenfrequencies of the motion have the form:

$$\Omega_\pm^2 = \frac{u_0}{m}\left(1 + \frac{1}{\mu} \pm \sqrt{1 + \frac{1}{\mu^2} - \frac{1}{\mu}}\right), \tag{8}$$

with corresponding displacements:

$$q_\pm = N_\pm \left(\frac{1 - \mu \mp \sqrt{1 + \mu^2 - \mu}}{\sqrt{\mu}}, \frac{1}{\sqrt{\mu}}\right), \tag{9}$$

where the first and second components refer to the particles of mass m and M, respectively. Here, $N_\pm$ are the normalization factor, according to the scalar product $q_i(1)q_j(1) + \mu q_i(2)q_j(2) = \delta_{ij}$ with $i, j = \pm$.

In Figures 1a and 1b we plot the eigenfrequencies and the eigenvectors $q_\pm$, respectively, as a function of μ. The ratio $\mu = 1$ corresponds to the the well-known case of two ions of equal masses in a linear trap, where the ratio of the eigenfrequencies are in the relation $1{:}\sqrt{3}$. For this value of μ, Ω_- and Ω_+ correspond to the center of mass (COM) and stretch mode frequencies, respectively, as it can also be verified from equation (9). As μ increases, the value of the eigenfrequencies decreases and tends asymptotically to the values $\Omega_- \to 0$ and $\Omega_+ \to \sqrt{2u_0/m}$. The limit $\Omega_- \to 0$ corresponds to the case where both ions stand still at their equilibrium position, as it can be seen in Figure 1b, while for the limit $\Omega_+ \to \sqrt{2u_0/m}$ the heavy ion does not move, and the light ion oscillates around its equilibrium position.

In the following we will concentrate on the case $\mu > 1$. As it is apparent from Figure 1b and equation (9) the two modes preserve some characteristics of the case of two ions with equal masses: in the mode of eigenfrequency Ω_- the ions oscillate in phase, whereas for Ω_+ they oscillate with opposite phases. The two modes, however, do not correspond to the COM and relative motion any longer. This can be understood by observing that, in absence of interactions, the trap frequency for an ion of mass m is proportional to $1/\sqrt{m}$. This argument applies to an N-ion chain of two (or more) species, and can be verified by substituting the vector $q^{\rm COM} = (1, 1, ..., 1)/\sqrt{N}$ describing the center of mass motion inside the secular equation (5); one obtains $\sum_j V_{ij} = u_0 = m_i \lambda^{\rm COM}$ for $i = 1, ..., N$, which cannot be fulfilled for any value of $\lambda^{\rm COM}$, unless all masses m_i are equal.

The non-separability of the modes into center of mass and relative motion has some consequences on the dynamics. For example, for two ions the anharmonicity (*i.e.* the corrections to the harmonic approximation of the potential in Eq. (3)) couples the two modes, whereas in the crystals of ions with equal masses the COM motion is an exact eigenmode of the problem. A further consequence is the coupling of both modes to the fluctuations of the electric field at the trap-electrodes, since none of the modes is orthogonal to the COM motion. The strength with which each mode couples to this source of decoherence is a function of the mass-ratio between the species μ, as has been discussed in [11].

2.2 N-ion crystal

As discussed above, the characteristic properties of the motion of a two-ion crystal are a function of the mass ratio μ. For crystals with $N > 2$ ions, some further parameters characterize the properties of the motion: the number of ions of each species and the sequence in which they are arranged. These two features are described through the array $\mathbf{m}$. In one dimension, the relevant symmetry property of the sequence $\mathbf{m}$ is the symmetry under reflections with respect to the center of the trap (which is also the center of the string). This corresponds to an invariance of the Hamiltonian under parity transformations. Be $\Pi^{(N)}$ the parity operator, defined on the wave functions $|\phi(x_1, x_2, ..., x_N)\rangle$ of the N-ion Hilbert space as $\Pi^{(N)}|\phi(x_1, x_2, ..., x_N)\rangle = |\phi(-x_N, -x_{N-1}, ..., -x_1)\rangle$. This operator has eigenvalues $p = +1$ (even), $p = -1$ (odd), corresponding to the states with even and odd parity, respectively. If the array $\mathbf{m}$ is symmetric under reflections, the Hamiltonian for the small oscillations commute with

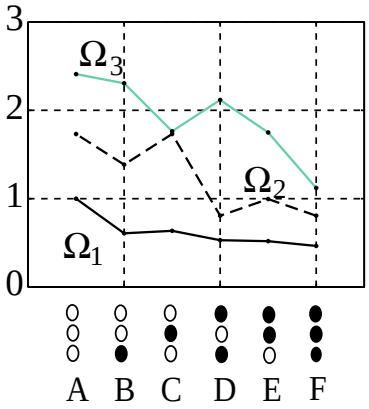


Fig. 2. Eigenfrequencies Ω_α *vs.* all possible configurations of a $N = 3$ ionic sequence made up of indium (black circles) and/or magnesium (white circles) ions. The eigenfrequencies are rescaled by the value of Ω_1 for a chain of magnesium ions.

$\Pi^{(N)}$ and the eigenmodes of equation (6) are also eigenvectors of $\Pi^{(N)}$ at the eigenvalue either $p = 1$ or $p = -1$. From a simple evaluation of the number of degrees of freedom, one can verify that the even modes are $N/2$ for an even number N of ions and $(N-1)/2$ for N odd. In particular, for symmetry reasons the central ion does not move in the modes of even parity of a chain with an odd number of ions. Thus, these modes are independent of the mass of the central ion, as it can be deduced from equation (5).

It is instructive to take a closer look at the eigenfrequencies of a chain of N ions as a function of all possible sequences $\mathbf{m}$. We discuss the case of 3 ions, since it shares some similarities with the normal modes of a triatomic molecule, as discussed in textbooks [16], and it exhibits features which can be extended to chains of large N.

In Figure 2 we plot the eigenfrequencies of a $N = 3$ chain as a function of all possible sequences of indium and magnesium ions, where the sequences have been ordered with increasing total mass $M_{\rm C}$ of the crystal. The mode of frequency Ω_1 (solid line) is characterized by the oscillation in phase of the three ions. For ions of equal mass it corresponds to the center of mass mode, but in all cases still represents the mechanical response of the whole crystal to excitations: in fact, $\Omega_1 \propto 1/\sqrt{M_{\rm C}}$ and in general it does not show an appreciable dependence on the order in which the ions are arranged.

The properties of the higher excitations depend on μ and on the sequence. In particular, the distance among the eigenenergies changes depending on where the heavy ions are placed in the sequence. In addition, symmetric sequences preserve some properties of a chain of three ions of equal masses. Thus, the eigenmode of frequency Ω_2 (dashed line) is characterized by the out-of-phase oscillation of the external ions, whereas the central ion stands still. Hence, Ω_2 takes the same value for the sequences A and C, and for the sequences D and F. On the contrary, in asymmetric sequences and for $\mu \neq 1$ the oscillation amplitude of the central ion is relatively large.

For the eigenmode Ω_3, in the symmetric sequences the external ions oscillate in phase, whereas the central ion oscillates out-of-phase, and its amplitude is a monotonic function of $1/\mu$. For the sequence C, in particular, $\Omega_2 > \Omega_3$. The two frequencies are almost degenerate since both modes correspond to the case where the outer ions move symmetrically with respect to the center, while the central ion in Ω_3 makes relatively small displacements (and in Ω_2 does not move). On the other hand, in asymmetric sequences (B, E) the light ions have large oscillation amplitudes, whereas the displacements of the heavy ions decrease as μ increases.

These properties have some immediate implications for quantum information processing with a two-component chain. For example, the eigenmodes of even parity of symmetric sequences are decoupled from the fluctuations of the electric field at the electrodes, and thus are good candidate for the quantum bus. This issue have been discussed quantitatively for a particular sequence in [11].

Furthermore, in symmetric sequences the parity operator $\Pi^{(N)}$ commutes with the one-dimensional Hamiltonian H: hence, the eigenstates with odd parity are not coupled *via* anharmonicity to the ones with even parity. The axial motion, however, is coupled to the radial motion by non-linearities, and in three-dimension there are no subset of states which are decoupled from the others. We discuss further this point in Section 3.

Another important implication regards the spacing between the eigenfrequencies. In fact, when choosing a mode for processing information, the distance in energy among the eigenfrequencies should be taken into account, since the presence of quasi-degeneracies will lower the efficiency of single mode addressing in quantum logic operations. Thus, *e.g.*, it is not convenient to use the sequence C and the mode Ω_3 as quantum bus, since the mode frequency is very close to the value of Ω_2.

Finally, from the mechanical properties of the chain we can infer in which position the cooling ions should be placed for optimal sympathetic cooling of the chain. We analyse this aspect in the next subsection.

2.3 Interaction of the crystal with light

In the dipole approximation the coupling of the external degrees of freedom of an atom with radiation is represented by the kick operator $\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r})$, where $\mathbf{k}$ is the wave vector of light and $\mathbf{r}$ the atomic position. In a Coulomb crystal of atomic ions, optical light couples to the internal degrees of freedom of a single ion, which we consider here a two-level dipole transition, and to the external degrees of freedom of the collective motion. Thus, assuming that the ion j scatters a photon and that $|\psi_{\rm i}\rangle$ is the motional state of the crystal before the scattering, after the scattering the motion of the crystal is described by the state $|\psi_{\rm f}\rangle$ given by:

$$\begin{aligned} |\psi_{\rm f}\rangle &= \exp(\mathrm{i}kx_j)|\psi_{\rm i}\rangle \\ &= \mathrm{e}^{\mathrm{i}\phi}\exp(\mathrm{i}kq_j)|\psi_{\rm i}\rangle, \end{aligned} \tag{10}$$

where $\phi = kx_j^{(0)}$ is a real scalar, and k is the projection of $\mathbf{k}$ on the axis of the crystal. The coupling of radiation to the collective modes of the crystal is visible by substituting equation (7) into (10). Thus, the kick operator can be written as

$$\exp(\mathrm{i}kq_j) = \Pi_{\alpha=1}^{N}\mathrm{e}^{\mathrm{i}\eta_j^\alpha(a_\alpha^+ + a_\alpha)}, \tag{11}$$

where η_j^α is the Lamb-Dicke parameter for the mode α and the ion j, and is defined as:

$$\eta_j^\alpha = k\beta_j^{\alpha\prime}\sqrt{\frac{\hbar}{2m_j\Omega_\alpha}}\,. \tag{12}$$

Through the Lamb-Dicke parameter we can infer the mechanical response of the crystal to the scattering of a photon. For one ion of mass m, it corresponds to the square root of the ratio between the recoil frequency $\omega_{\rm R} = \hbar k^2/2m$ and the trap frequency Ω: $\eta = \sqrt{\omega_{\rm R}/\Omega}$, and it determines how many motional levels are coupled by the scattering of one photon. The Lamb-Dicke regime corresponds to the case in which $\omega_{\rm R} \ll \Omega$, and mathematically to the condition $\eta\sqrt{n} \ll 1$, where n is the vibrational state number. In this limit the kick operator can be expanded in powers of η, and a change in the quantum motional state due to the incoherent scattering of one photon is of higher order in η [20]. In this regime an ion can be sideband cooled to the ground state of the vibrational motion [21].

In presence of more than one ion, the Lamb-Dicke parameter η_j^α describes how the displacement of the ion j couples to the mode α. In particular, it determines (i) the possibility of addressing a single motional sideband, which appears when scanning a probe beam through the resonance frequency (and thus of exciting one mode selectively) [22], and (ii) the possibility of laser-cooling a mode to its vibrational ground state, in analogy to the one-ion case.

Let us first consider the response to light of a two-ion crystal, and compare the case where the ions have equal masses, as discussed in [22], with the case where they have different masses. In the first case, due to the symmetry of the configuration the Lamb-Dicke parameters for each ion are equal (apart for some difference in the sign). In the second case, we can see in equation (12) that the Lamb-Dicke parameters depend on the mass of the ion, and given the asymmetry of the crystal the geometrical factor $\beta_j^{\alpha\prime}$ has different values for the two ions. One might be tempted to think that the Lamb-Dicke regime can be more easily accessed by addressing the heavier ions. This, however, is actually not true for all modes. This consideration is particularly applicable to the mode of lowest frequency, which shares some properties with the center of mass motion, and in general describes the response of the crystal as a whole to the mechanical excitation. For this mode, the displacements of the two ions are comparable, and actually the displacement of the heavier ion is slightly larger, as can be seen in Figure 1b. On the contrary, the eigenmode with frequency Ω_+ is characterized by smaller displacements of the heavy ion than of the lighter one. For this mode, the heavy ion might be well in the Lamb-Dicke regime, while the light ion is not.

This situation can be visualized by comparing the absorption spectra obtained by shining light on each ion separately. We define the absorption spectrum in a two-level transition with resonant frequency ω_0 and driven by a laser of frequency $\omega_{\rm L}$ through the function $I(\delta)$, where

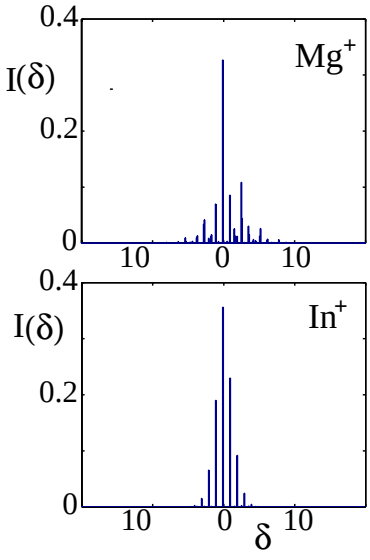


Fig. 3. Absorption spectrum $I(\delta)$ *vs.* the detuning δ for a crystal of an indium and magnesium ion obtained shining light on magnesium and indium, for a thermal distribution with average energy $5\hbar\Omega_-$. Here, $\eta_{\rm Mg}^- = 0.22$, $\eta_{\rm Mg}^+ = 0.5$, $\eta_{\rm In}^- = 0.38$, $\eta_{\rm In}^+ = -0.06$, as follows from (12).

$\delta = \omega_{\rm L} - \omega_0$ is the detuning, which is evaluated by summing all contributions to laser-excited transitions at frequency $\omega_{\rm L}$ [22]:

$$I(\delta) = \sum_{E_{\mathbf{n}} - E_{\mathbf{l}} = \delta} |\langle \mathbf{n}|\exp(\mathrm{i}kq_j)|\mathbf{l}\rangle|^2 P(\mathbf{n}). \tag{13}$$

Here $|\mathbf{n}\rangle = |(n_1, n_2)\rangle$ are the motional states of energy $E_{\mathbf{n}} = n_1\hbar\Omega_1 + n_2\hbar\Omega_2$, with n_α occupation of the mode Ω_α ($\alpha = 1, 2$), and $P(\mathbf{n})$ is a normalized distribution over the motional states $|\mathbf{n}\rangle$. The coordinate q_j characterizes the driven ion. In Figure 3 we plot $I(\delta)$ as a function of δ for a crystal composed of a magnesium and an indium ion. Figure 3 shows the absorption spectrum when driving separately the magnesium and the indium ion, for a thermal distribution over the motional states with average total energy $E = 5\hbar\Omega_-$, where for the chosen parameters $\Omega_- = 0.552$ MHz and $\Omega_+ = 1.456$ MHz. In both cases the motional sidebands of the mode with frequency Ω_- are visible, whereas when driving the In^+ ion the sidebands of Ω_+ almost disappear. In fact, as evaluated from (12) the Lamb-Dicke parameters for Ω_- are $\eta_{\rm Mg}^- = 0.22$, $\eta_{\rm In}^- = 0.38$, whereas the ones for Ω_+ are $\eta_{\rm Mg}^+ = 0.5$, $\eta_{\rm In}^+ = -0.06$, *i.e.* the weight of the motional sidebands for the mode Ω_+ in indium is two orders of magnitude smaller than the ones for the mode Ω_-. It is interesting to compare this result with the case of two ions of equal masses. In that case the absorption spectrum is the same independently of which ion of the chain is driven. Then, if the COM mode is in the Lamb-Dicke regime, the relative motion mode is also in the Lamb-Dicke regime, since in that case the Lamb-Dicke parameter scales simply as the inverse of the squared root of the eigenfrequency.

For crystals with $N > 2$ ions the factor β_j^α in (12) reflects the structure of the chain and consequently how the driven ion couples to the mode to cool. It thus contains some information on where the cooling ions should be placed in the sequence so as to achieve more efficient cooling. This can be theoretically illustrated by a rate

equation, which describes cooling of one mode in a chain in the Lamb-Dicke regime [23]. Here, we define the Lamb-Dicke regime with the condition:

$$\max_{\{j\}}|\eta_j^\alpha|^2 n_\alpha \ll 1 \quad \text{for} \quad \alpha = 1, ..., N \tag{14}$$

where n_α denotes the occupation of the mode α and where the set of ions $\{j\}$ represents the set of positions of the cooling ions in the chain. Assuming that the laser interacts with the internal two-level transition of the individual atom, in second order perturbation theory in the parameter g/γ, with g Rabi frequency and γ decay rate of the atomic transition, the excited state can be eliminated, and one obtains a set of equations projected on the electronic ground state, where populations and coherences between different motional states are coupled. In the Lamb-Dicke limit such coupling can be neglected, thus reducing the equation for the N-ion density matrix ρ in the low saturation limit to rate equations [22]. Furthermore, introducing the reduced density matrix ρ_α for the mode α defined by:

$$\rho_\alpha = \sum_{n_{\beta_1}} ... \sum_{n_{\beta_{N-1}}} \langle n_{\beta_1}, ..., n_{\beta_{N-1}}|\rho|n_{\beta_1}, ..., n_{\beta_{N-1}}\rangle, \tag{15}$$

with $\beta_1, ..., \beta_{N-1} \neq \alpha$, one can derive the rate equation for cooling of the mode α in one-dimension [24]:

$$\frac{\mathrm{d}}{\mathrm{d}t}P(n_\alpha) = \frac{g^2}{\gamma}\sum_{\{j\}}\eta_j^{\alpha 2}[(n_\alpha+1)A_-^\alpha P(n_\alpha+1) - ((n_\alpha+1)A_+^\alpha + n_\alpha A_-^\alpha)P(n_\alpha) + n_\alpha A_+^\alpha P(n_\alpha-1), \tag{16}$$

the coupling with the other modes being of higher order in the Lamb-Dicke parameter. Here, $P(n_\alpha) = \langle n_\alpha|\rho_\alpha|n_\alpha\rangle$ and the coefficients $A_\pm^\alpha$ are defined as

$$A_+^\alpha = \frac{1}{16\Omega_\alpha^2/\gamma^2+1} + \frac{2}{5}\frac{1}{4\Omega_\alpha^2/\gamma^2+1}, \tag{17}$$

$$A_-^\alpha = 1 + \frac{2}{5}\frac{1}{4\Omega_\alpha^2/\gamma^2+1}, \tag{18}$$

where we have assumed that the Rabi coupling is spatially constant over the whole crystal and equal to g, and that the laser is tuned on the first red sideband of the mode Ω_α. Equation (16) is the sum of all contributions to cooling of mode α from the coupling g of the cooling laser to the driven ions. It is fully equivalent to the equation for cooling of one ion in a harmonic trap of frequency Ω_α in the Lamb-Dicke regime [20], apart from the scaling factor multiplying the term on the RHS of (16):

$$W_\alpha = \sum_{\{j\}}|\eta_j^\alpha|^2. \tag{19}$$

Provided that (19) is different from zero, it does not affect the steady state, but scales the rate of cooling of the mode α. The factor W_α represents the contribution of the cooling ions in the array to the speed of the process. Obviously, the largest cooling rate is achieved when all ions are driven by the cooling laser. In that case, W_α has the form

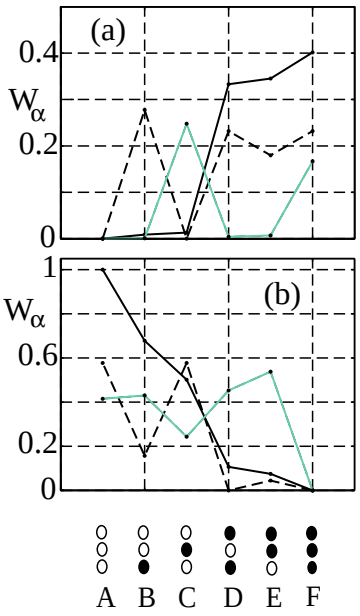


Fig. 4. Cooling rate W_α *vs.* all the possible configurations of a $N = 3$ ionic sequence made up of indium (black circles) and/or magnesium (white circles) ions, where W_α has been rescaled by the value of $W_\alpha^{\max}$ for a chain of magnesium ions. Solid line: eigenmode Ω_1; dashed line: eigenmode Ω_2; grey line: eigenmode Ω_3 (*cf.* Fig. 3).

$W_\alpha^{\max} = \sum_{j=1}^N |\eta_j^\alpha|^2 = \omega_{\mathrm{R}}/\Omega_\alpha$, where ω_{R} is the recoil frequency of the single ion. The rate of cooling of each mode scales according to the relation $W_\alpha^{\max} = W_{\alpha'}^{\max}\Omega_{\alpha'}/\Omega_\alpha$, and it scales with the mass m of the cooling ion as $W_\alpha^{\max} \propto \sqrt{1/m}$ since $\omega_{\mathrm{R}} \propto 1/m$ and $\Omega_\alpha \propto 1/\sqrt{m}$.

For quantum information processing we are interested in employing only some ions of the chain for cooling. We look thus for the best sequence and mode for cooling, where for "best sequence" we intend a compromise between the highest number of ions for quantum computation (*i.e.* the lowest number of cooling ions) and the largest cooling rate.

In Figure 4 we plot the factor W_α *vs* all possible sequences of $N = 3$ ions, made up of magnesium and/or indium ions, where the cooling ions are in (a) indium and (b) magnesium ions. Note that between the curves in (a) and (b) there is a scaling factor corresponding, as expected, to the squared root of the ratio of the ionic masses. The curves in Figure 4 can be easily interpreted by considering the properties of the modes, discussed in the previous subsection. Thus, as the mode of frequency Ω_1 is characterized by an oscillation in phase of all ions, and does not strongly depend on the sequence, the cooling rate increases as the number of cooling ions increases. On the other hand, the mode with frequency Ω_2 is mainly characterized by the oscillation of opposite phase of the ions placed externally. Thus, large rates of cooling are achieved when the cooling ions are placed in the external positions. In particular, the cooling rates of the sequences A and C, and of the sequences D and F are equal. In fact, these configurations are symmetric under reflection and the mode with eigenfrequency Ω_2 has even parity. Thus, the central ion does not contribute to cooling nor to quantum information processing with the mode. Finally, in symmetric configurations, the mode of frequency Ω_3 is characterized by large oscillations of the central ions, and a relatively large rate of cooling is obtained by simply placing the

cooling ion in the center, as can be noticed for sequence C in Figure 4a and sequence D in Figure 4b. In asymmetric sequences (B, E) the rate of cooling in (a) is small, whereas in (b) is large, as expected from the considerations made in the previous subsection.

In general, we can conclude that by preparing certain sequences one can have efficient sympathetic cooling of some modes using a relatively small number of cooling ions. This characteristic does not depend strongly on the mass-ratio μ between the qu-bit and the cooling ions. In a crystal with large total mass $M_{\rm C}$, however, the Lamb-Dicke regime condition can be accessed more easily. In this respect, it would be better to use heavier ions as qu-bits.

Finally, sequences with an even number N of ions are to be preferred over sequences with odd N, so that all positions in the chain contribute either to the quantum computer or to the cooling process.

3 Effects of the anharmonicity on cooling and quantum logic

The harmonic approximation of the mechanical potential in (1) relies on the assumption that V possesses strict local minima, around which the motion is well-localized. In that case, the higher orders of its Taylor expansion are a small correction. For two ions those terms have the form (for $x_2 > x_1$):

$$\delta V = \sum_{n=3}^{\infty} \delta V^{(n)} = \sum_{n=3}^{\infty} (-1)^n \frac{e^2/4\pi\epsilon_0}{x_0^{n+1}} \left[q_2 - q_1\right]^n , \qquad (20)$$

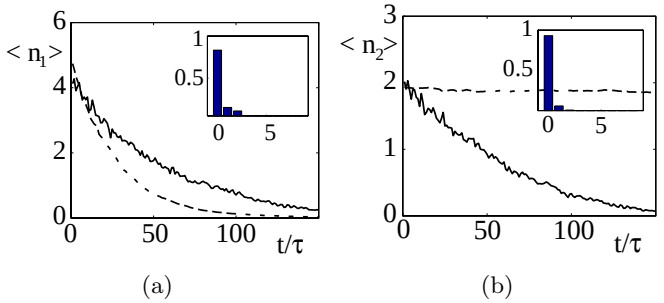
where $\delta V^{(n)}$ is the nth order correction. The effect of these terms, the so-called anharmonicity, consists in causing shifts to the motional energies, and mixing the eigenstates of the normal modes. Such mixing is in general a small correction to the eigenstates of the ideal case, but it may become particularly enhanced because of quasi degeneracies among the motional energies of the states. In fact, the density of motional states of an N-ion chain in the interval of energy $[E, E+\delta E]$ is approximately $D(E) \propto E^{N-1}$. Thus, as the number N of ions increases and/or for larger values of the motional energies, the dynamics of quasi-degenerate states are definitely affected by the anharmonicity. Here, we discuss the effects of the departures from the ideal harmonic system, first on sideband cooling and then on the efficiency of quantum logic gates.

In sideband cooling the laser addresses the motional sideband of the mode to be cooled. Thus, cooling will be efficient as long as the shift in energy caused by the anharmonicity is much smaller than the frequency of one phonon of the mode addressed. On the other hand, the mixing between the eigenstates will constitute a thermalization effect among the modes, and it will not constitute an obstacle to cooling as long as all modes are at sufficiently low temperatures, so that δV is a small correction to the whole system.

To obtain some estimates, we evaluate the order of magnitude of the shift to the energy in first order perturbation theory, and ask for which range of values of the vibrational numbers sideband cooling may still work. In [22] it has been shown that in the perturbative regime $\delta V \approx \delta V^{(3)}$ [25]. Thus:

$$\langle \delta V^{(3)} \rangle \approx \frac{e^2/4\pi\epsilon_0}{x_0} \left(\frac{a_{0\alpha}}{x_0}\right)^3 n_\alpha^{3/2}, \qquad (21)$$

where $a_{0\alpha} = \sqrt{\hbar/m_i\Omega_\alpha}$, n_α vibrational number of the mode α, and m_i mass of the lighter ion. In deriving (21) we have assumed $n_\alpha/\Omega_\alpha \geq n_\beta/\Omega_\beta$ $(\alpha, \beta = 1, 2, ..., N)$. Taking two ions, one indium and one magnesium, $\Omega_1 = 1$ MHz and the mass of magnesium $^{25}{\rm Mg}^+$, then $|\langle \delta V \rangle|/\hbar \approx 6 \times 10^{-3} n_1^{3/2} \Omega_1$, which implies that first order perturbation theory holds for $n_1 \ll 80$ $(n_2 \ll 30)$. In this limit, a laser tuned on the first sideband to the red of the mode Ω_1 cools the system to the ground state. We have verified this conjecture numerically: we have taken a two-ion chain composed of an indium and a magnesium ion, and considered sideband cooling in the Lamb-Dicke regime of one of the modes, comparing the case in which the mechanical potential is fully harmonic with the case where the third and fourth orders in the anharmonic expansion have been included. We have not noticed any significant difference between the two cases, and the system is cooled efficiently to the ground state. In particular, no visible effect could be interpreted as due to the anharmonic coupling between quasi-degenerate states. However, according to the above estimates, in the interval of states of the numerical calculation the spectrum of energy is not very "dense". Then, in order to verify numerically the effect of anharmonicities in presence of quasi-degeneracies we take a system with exact degeneracies, and more specifically with two modes of frequencies $\Omega_1 = \Omega$ and $\Omega_2 = 2\Omega$. Here, in the Lamb-Dicke regime a laser sideband-cools the mode of frequency Ω_1. We compare the harmonic with the anharmonic case, where here we simply substitute the chosen values Ω_1, Ω_2 in the quantized form of the displacements of equation (7). In Figure 5 the average occupation number for the modes (a) Ω_1 and (b) Ω_2 is plotted as a function of the time.



(a) (b)

Fig. 5. Average occupation of the mode (a) $\Omega_1 = \Omega$ and (2) $\Omega_2 = 2\Omega$ as a function of the time in unit of the optical pumping time τ, for the harmonic (dashed line) and anharmonic case (solid line). Here, $\Omega = 1$ MHz, $\eta_{1\Omega} = 0.1$, $\eta_{2\Omega} = 0.1/\sqrt{2}$, $\gamma = 0.1\Omega$, $\delta = \omega_{\rm L} - \omega_0 = -\Omega$, $g = 0.01\Omega$, $\tau = \gamma/g^2$. Insets: population of the modes (a) Ω_1 and (b) Ω_2 as a function of their vibrational number at time $t = 150\tau$ for the anharmonic case.

The dashed and solid lines correspond to the harmonic and anharmonic case, respectively. In the harmonic case the mode Ω_1 is cooled and Ω_2 is like "frozen", since it is coupled to radiation at higher orders in the Lamb-Dicke parameter [22]. In the anharmonic case the rate of cooling of the mode addressed is slowed down, whereas the mode Ω_2 is simultaneously cooled: the system is cooled as a whole, but on a relatively slower time-scale. Thus, the two modes thermalize on a time-scale which is faster than the cooling one.

With respect to quantum information processing, present quantum logic schemes with ions are based on the harmonic properties of the motion. Thus, they are affected both by the shift in energy and the mixing induced by the anharmonicity. Quantum gates which require the preparation of the system in the ground state of the motion will be very weakly affected, since in that part of the spectrum the anharmonic perturbation is extremely small, and there are no quasi-degeneracies. On the other hand, the perturbation may affect the efficiency of hot gates, since they operate on higher-lying motional states. Thus, the speed of hot gates must be faster than the rate of anharmonic coupling between quasi-degenerate states. We can define a time-scale $\tau_{\rm Anh}$ for the anharmonic perturbation $\tau_{\rm Anh} \approx \hbar/|\langle \delta V \rangle|$. The typical duration of a quantum gate must be shorter than $\tau_{\rm Anh}$. In presence of degenerate states which are coupled by three-phonon transitions (*i.e.* for $\Omega_\alpha \sim 2\Omega_\beta$), from (21) $\tau_{\rm Anh} \sim 10$ μs given $\Omega_\alpha = 1$ MHz and $n_\alpha \sim 10$. This estimate, which is rather worrying if compared with the duration of a quantum gate [7,26], reflects the worst case, which might occur for certain sequences, large number of ions and large excitations. Note that, if the degenerate states are coupled by a four-phonon transition (*i.e.* for $\Omega_\alpha \sim 3\Omega_\beta$), then $\tau_{\rm Anh} \sim 600$ μs. In general, we expect this problem to arise when working with a large number of ions and for high excitations. It could be minimized by choosing symmetric sequences: in that case the "effective density" of motional states which are coupled by the anharmonicity of the axial potential will decrease, since only states with the same parity will be coupled to each other, whereas the coupling with the radial degrees of freedom is of higher order.

As a general rule, however, one should avoid degeneracies among the radial and the axial frequencies.

4 Conclusions

We have studied the small oscillations behaviour of a two-component linear crystal, with particular emphasis on the applications to sympathetic cooling and quantum information with the ions, and have discussed the effect of anharmonicity on the operations of the ion-trap quantum computer. We have seen that higher efficiency in quantum information and sympathetic cooling are achieved by selecting the right ionic sequences. That raises the issue of how to prepare the desired sequence of ions. A rigorous investigation in this direction should take into account the full non-linear potential in the three-dimensional space and it is subject of on-going investigations.

We would like to thank P. Lambropoulos for many stimulating discussions and the critical reading of this manuscript, and W. Lange, S. Köhler, V. Ludsteck, E. Peik, who are involved in the experimental realization of the ion structure discussed here. This work is supported in parts by the European Commission within the TMR-networks ERB-FMRX-CT96-0087 and ERB-FMRX-CT96-0077.

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