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Fast dynamic exchange cooling of trapped ions

Master's Thesis

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Abstract

Ion recooling is currently a necessary but time-consuming task in trapped-ion quantum information processing experiments. This thesis proposes a way of cooling an ion from its Doppler limit back to the ground state in time-scales about an order of magnitude faster than current laser-cooling methods.

This is done by taking a ground-state cooled ion and performing a cooling motion that brings the coolant ion and the heated ion close together for a short time. The energy is then exchanged by a motional exchange mechanism due to the Coulomb coupling between the two charged particles, given that this cooling motion is timed such that the energy is swapped exactly.

In the case of cooling an ion with one of equal mass, shortcuts to adiabaticity methods are applied to design this cooling motion in a way that does not induce additional motional excitations of the ions and also robustness towards experimental imperfections is designed into the scheme. Here, linear tilts of the trapping potential are considered, as these are a major source of error in trapped-ion experiments, due to stray charges and imperfect calibration. This results in a scheme that can swap the energy of the two ions in a minimal time of about 10 cycles of the ion motion. Also the maximally tolerable potential tilt for the exchange mechanism is determined. Using a given experimental apparatus, this maximal tilt is found to increase with parameter choices that speed up the cooling.

In the case of cooling an ion with one of different mass, the shortcut to adiabaticity method is derived and cooling demonstrated to be possible as well. Here, additional care has to be taken to make sure that the motional frequencies of the two ions are equal, such that the motional exchange mechanism is possible.

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Introduction

In the early 1980s it was first realised that simulating a general quantum system requires an exponentially growing number of classical objects. The first to state this fact was Yuri Manin [1, 2], only to then propose a “quantum automaton” that implements general quantum computation as unitary rotations in Hilbert space, without being bound to a particular physical implementation. Such quantum computers have been proposed or demonstrated in various systems such as superconducting qubits [3], NV centres [4], topological Majorana qubits [5] and trapped ions [6].

In the quest for a trapped ion quantum computer, two main avenues for progress lie in improving qubit quality by reducing noise and increasing the number of logical operations within the given coherence times. Several experimental building blocks have recently seen significant speed-ups. As a natural time scale in trapped-ion QIP is given by the periodicity of the ion motion, these efforts attempt to increase the logic speed of quantum information processing (QIP) by achieving run-times of as few motional cycles as possible. Two-qubit gates and ion transport operations have already been achieved in only a few motional cycles or less [7, 8, 9]. Ion separation on the other hand is currently only possible at adiabatic speeds taking more than 100 motional cycles [10, 11]. However, a scheme using shortcuts to adiabaticity (STA) methods has been proposed in [12] that promises to reduce this run-time to below 10 motional cycles.

Another necessary operation in trapped ion QIP experiments is recooling. As trapped ions need to be close to their motional ground state to yield good quantum gates, periodic recooling is necessary [13, 14]. Recooling from the Doppler limit (around 6 quanta for $^{40}\text{Ca}^+$ [15]) to the ground state takes several hundred motional cycles using current methods such as electromagnetically-induced transparency cooling and resolved sideband cooling. This time scale is dictated by atomic properties [16] and cannot easily be improved by orders of magnitude.

As recooling is slow compared to all operations except ion separation, it is rapidly becoming a bottleneck in trapped-ion QIP experiments. To close this gap, this thesis adapts the STA methods presented in [12] and proposes a new way to cool an ion close to the ground state while doing so about one order of magnitude faster than current methods.

A proposal for fast dynamic exchange cooling

To cool an information-carrying ion in a QIP experiment, we propose an energy exchange with a cold ion. Due to the Coulomb interaction, the motions of the two ions around their respective equilibrium positions are coupled. Much in the same way as two spring-coupled pendulums swap their motional energy back and forth, the ions exchange their motional energy. This effect is covered in detail in chapter 1. Most notably, the energy exchange speeds up cubically with decreasing ion distance.

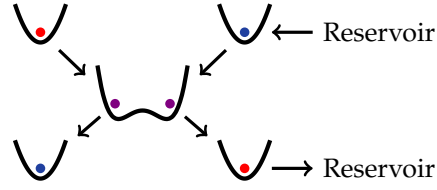


Figure 0.1: Schematic depiction of the overall cooling scheme. The coolant ion is initially cold (top, blue circle) and the information ion hot (top, red circle). After the cooling scheme, the ion energy has been swapped.

To implement this exchange cooling, a reservoir is supposed to exist, where a number of ions are constantly kept close to their motional ground state. Once the need to cool an information ion arises, for example after a resonant readout, a long computation or background gas collisions, the procedure schematically depicted in Fig. 0.1 is executed. First, a coolant ion is transported to the information ion from this reservoir. At this intermediate outer distance, the motional exchange should still be negligible. A cooling motion is then performed, bringing the ions to a close inner distance, before returning them to their starting positions. The inner distance must be chosen small enough such that the motional exchange takes just a few motional cycles. If timed right, this dynamic procedure can swap the ion energies, leaving the information ion with an energy close to its motional ground state while the coolant ion now carries all the energy and is transported back to the reservoir for laser recooling, without further interrupting the QIP experiment.

The challenging aspect of this scheme is designing the ion transport from outer to inner distance and back out. A transport protocol that excites two initially unexcited ions with a final energy above the target level for the information ion (as depicted in Fig. 0.2a) can not achieve cooling successfully. Therefore it is a prerequisite to solve this transport problem as presented in Fig. 0.2b, where the excitations due to the transport are negligible.

We thus separate the design of such a cooling scheme into two distinct tasks. The first part consists of designing the ion transport such that it induces no motional excitation. The second part of the cooling scheme is then straightforward: given a well-designed transport, the motional energy can be swapped simply by finding the right timing. We will call parameter sets found in this way cooling solutions, even though the energy is in fact only exchanged from ion to ion.

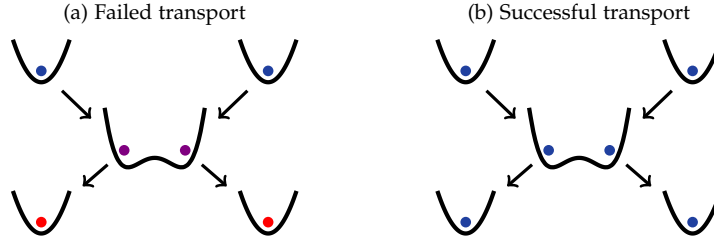


Figure 0.2: Schematic depiction of the transport problem. (a) shows a failed transport where the ions are excited at the final time despite being cold initially, while (b) shows the desired transport result, leaving unexcited ions.

While implementing such a cooling motion at adiabatic speeds is easy, this is not the case for the run-times targeted in this thesis. The desired ion transport is similar to the procedure used in ion separation/merging, only that here, the ions are not necessarily merged into a single trapping well. The splitting performed in [10] with an adiabatic run-time of 112 motional cycles still leaves the ions with a final excitation of 4.16 quanta. Since the information ion is to be cooled to a motional occupation close to the ground state ($\ll 1$ quanta), this shows insufficient control of the ion transport despite the long run-time.

Better methods are thus needed to design the desired ion transport. Following the path laid out by Palmero in [12], we find these in the form of shortcuts to adiabaticity (STA) methods. These promise to retain the results of an adiabatic execution, even at non-adiabatic run-times. Such schemes have been proposed for various applications such as transport of single trapped ions and ion chains [17, 18, 19, 20], ion separation [12], atom launching [21] and atom cooling [22]. It has also been demonstrated that STA methods can be designed for optimal robustness towards experimental imperfections and noise [23, 24, 25, 26, 18, 27, 28, 29]. It seems thus alluring to add robustness to typical error sources of trapped ion QIP experiments to the design of the transport scheme.

The thesis is subdivided into the following parts:

Chapter 1 explains the theoretical foundations of the Coulomb motional exchange that is the basis of this proposal.

Chapter 2 introduces the STA formalism in a general way. This knowledge is then applied in **Chapter 3** to solve the transport problem for ions of equal mass as depicted in Fig. 0.2b and introduce robustness towards experimental errors. Several optimisation methods are compared and numerical results presented.

Chapter 4 then employs the gained transport capability and varies its parameters of the transport scheme to find cooling solutions at various timings. Furthermore, the influences of experimental capabilities and limitations on the achievable quality and speed of the cooling are discussed.

Chapter 5 generalises the STA formalism for the case where the two ions are

of unequal mass.

Chapter 6 concludes the proposal and offers an outlook for future work.

Motional exchange mechanism

The motional exchange induced by the Coulomb interaction lays the groundwork for the cooling proposal of this thesis. It is thus important to understand the principles of this phenomenon in order to design cooling solutions and predict experimental requirements. The effect is analogous to the motional exchange between two spring-coupled pendulums, that takes place when one pendulum is initially set in motion while the other is at rest. The motion of the first pendulum is exchanged to the second pendulum via the spring. After a certain amount of time the first pendulum comes to rest, while all kinetic energy has been swapped to the second. The analogy to our ion cooling scheme is completed by pointing out that the Coulomb coupling plays the role of the spring and the pendulum motions correspond to the ions oscillating in their trapping potential wells.

Such a motional exchange between two trapped ions has first been demonstrated by Brown et al. in [30], where two $^9\text{Be}^+$ ions are held $40\text{ }\mu\text{m}$ apart in a Paul trap while their motional frequencies are tuned into resonance. The ions then swap their motional energies back and forth at a frequency of 3 kHz. This exchange frequency, depending on the ion masses, motional frequencies and distance, can be learned from a simple Taylor expansion of the Coulomb potential, a derivation that we shall now reiterate from [30].

Suppose two singly charged ions of mass m_1 and m_2 are trapped in a general electrical potential $V_{\text{el}}(x)$. Note that the ion confinement in the radial directions y and z is assumed to be much stronger than in the axial direction x , allowing us to neglect the radial components of the motion and treating the system in a one-dimensional way. This notion is retained throughout this thesis. The total potential is then given by

$$V_{\text{tot}}(x_1, x_2) = V_{\text{el}}(x_1) + V_{\text{el}}(x_2) + \underbrace{\frac{C_C}{|x_2 - x_1|}}_{V_C}, \quad (1.1)$$

where $x_1 < x_2$ are the position coordinates of the two ions, V_C is the Coulomb potential and $C_C = \frac{e^2}{4\pi\epsilon_0}$ the Coulomb constant. The ions oscillate around their equilibrium positions $x_1^{(0)}$ and $x_2^{(0)}$, which depend on the explicit shape

1. MOTIONAL EXCHANGE MECHANISM

of V_{el} . The motional frequencies are determined by the potential curvature at $x_i^{(0)}$ as

$$\omega_i = \sqrt{\left. \frac{1}{m_i} \frac{\partial^2 V_{\text{tot}}}{\partial x_i^2} \right|_{x_i=x_i^{(0)}}}. \quad (1.2)$$

The Coulomb term V_C in eq. 1.1 can then be written in terms of the equilibrium distance $d = x_2^{(0)} - x_1^{(0)}$ and the motional displacements $\delta_i = x_i - x_i^{(0)}$ as

$$V_C(x_1, x_2) = \frac{C_C}{d + \delta_2 - \delta_1}. \quad (1.3)$$

Assuming the ion motion is small compared to the equilibrium distance, a second order Taylor expansion yields

$$V_C(x_1, x_2) \approx \frac{C_C}{d} \left(1 + \frac{\delta_1 - \delta_2}{d} + \frac{\delta_1^2}{d^2} + \frac{\delta_2^2}{d^2} - \frac{2\delta_1\delta_2}{d^2} \right). \quad (1.4)$$

Upon quantising this expression, the last term becomes a coupling between the ions motion. Using the harmonic oscillator ladder operators $a, a^\dagger, b$ and $b^\dagger$ to describe the coordinates $\delta_1 = \sqrt{\frac{2\hbar}{m_1\omega_1}}(a + a^\dagger)$ and $\delta_2 = \sqrt{\frac{2\hbar}{m_2\omega_2}}(b + b^\dagger)$, it becomes

$$\frac{-2C_C}{d^3} \delta_1 \delta_2 = -\hbar \Omega_{\text{ex}} (a + a^\dagger)(b + b^\dagger) \approx -\hbar \Omega_{\text{ex}} (ab^\dagger + a^\dagger b) \quad (1.5)$$

and if the ion frequencies are resonant $\omega_1 = \omega_2$ and fast-rotating terms are neglected, the motional exchange frequency is given by

$$\Omega_{\text{ex}} = \frac{C_C}{\sqrt{m_1 m_2} \sqrt{\omega_1 \omega_2} d^3}. \quad (1.6)$$

The exchange frequency means that the ions have exchanged their motional energy after a time of $\tau_{\text{ex}} = \frac{\pi}{2} \frac{1}{\Omega_{\text{ex}}}$. Note that Ω_{ex} has an inverse cubic dependence on the ion distance. This motivates the transport protocol described in the introduction, as bringing the ions close together speeds up the exchange considerably.

It is also important to note that this exchange is a resonant effect. If the ion frequencies ω_i are detuned from each other, the actual exchange frequency drops below the maximal Ω_{ex} . This insight implies that the condition $\omega_1 = \omega_2$ has to be fulfilled sufficiently well in cooling schemes, placing constraints on experimental accuracy that will be quantified in later chapters.

As an illustration, we numerically simulate this motional exchange by placing two $^{40}\text{Ca}^+$ ions at a constant distance of $17.5 \mu\text{m}$. The ions are placed in wells

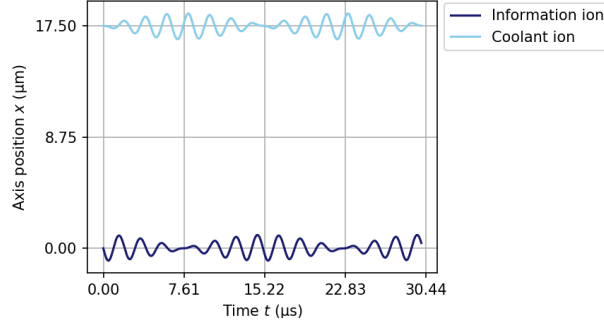


Figure 1.1: A simple demonstration of the energy exchange mechanism through the example of two $^{40}\text{Ca}^+$ ions exchanging energy with an exchange time of $\tau_{\text{ex}} = 7.61 \mu\text{s}$.

of $\omega_i = 2\pi \times 0.5 \text{ MHz}$, resulting in an expected exchange time of $\tau_{\text{ex}} = 7.61 \mu\text{s}$ or 3.8 motional cycles.

To obtain the classical trajectories in this example, the equations of motion $m_i \ddot{x}_i = -\frac{\partial V}{\partial x_i}$ are solved, with the initial kinetic energy of the information ion being equivalent to a coherent state of 1000 motional quanta ($E_{i,0} = 1000\hbar\omega_1$), while the coolant ion starts at rest. The results, depicted in Fig. 1.1 show the two ions exchanging motional energy with the predicted period.

Rapidly bringing the ions to an inner distance as in this example would thus enable cooling in just a few motional cycles, given that the ion transport to this distance can be designed reliably. This will be the content of the following two chapters. Later on, these example parameters will turn out to be realistic for a cooling solution.

Shortcuts to adiabaticity for trapped ions

Designing the desired ion cooling motion to cause negligible excitations despite a target run-time of just a few motional cycles is not a straightforward task, due the non-adiabaticity of the problem. A possible solution is to apply shortcuts to adiabaticity (STA), a set of methods to design protocols for quantum systems that can be executed in arbitrarily short times while yielding the same final result as an adiabatic evolution. STA methods have been proposed for many applications in trapped-ion QIP [17, 18, 19, 20, 12, 21, 22, 23].

Of the various STA methods, we chose to use invariant-based inverse engineering as detailed in [31]. This is an approach that allows the construction of a Hamiltonian $H(t)$ such that the populations in the instantaneous basis of $H(t_0)$ at starting time $t_0 = 0$ match the populations of $H(t_f)$, t_f being the final time. For the example of a single ion in a harmonic well with movable centre, suppose that the system is in a quantum state $|n\rangle$ for $t < t_0$. The Hamiltonian can be designed such that the well is moved to another position during the run-time and the system is still in the state $|n\rangle$ of the now displaced well at $t > t_f$. This can be done in arbitrarily short run-times, allowing fast ion transport.

In this chapter, we will state the general steps needed for the STA treatment of a two-ion system using the two-ion cooling transport with equal mass ions for illustration. The extension to an N -ion system is straightforward. The next chapter then carries out the procedure explicitly for two ions.

For the cooling motion needed in this thesis, the goal is engineering the explicit time-dependence of a Hamiltonian that describes the transport of two ions from an outer distance d_{out} to an inner distance d_{in} and back out. This should be done such that the initial motional states of the ions are retained at final time. Contrary to the single-ion transport example above, this will only be possible approximately and the achievable run-times are in general not arbitrarily short.

A useful potential parametrisation is the quartic double-well potential

$$V_{\text{el}}(t, x) = \alpha(t)x^2 + \beta(t)x^4, \quad (2.1)$$

defined along the axial direction x of the trap. This allows to have two ions in separate wells and move these wells in and out.

The parameters $\{\alpha(t), \beta(t)\}$ describe the harmonic and quartic parts of the potential given in units of N m^{-1} and N m^{-3} , respectively. As long as $\alpha(t) < 0$, V_{el} is a double-well potential, which is illustrated in Fig. 2.1. The goal of the STA treatment is to design the time-dependence of $\{\alpha(t), \beta(t)\}$ explicitly.

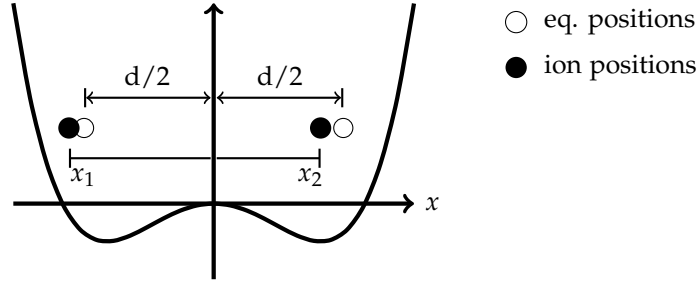


Figure 2.1: Position coordinates for two ions trapped in a quartic double-well potential.

The total Hamiltonian is given by

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_{\text{tot}}(x_1, x_2, t) \quad (2.2)$$

$$V_{\text{tot}}(x_1, x_2, t) = \alpha(t) (x_1^2 + x_2^2) + \beta(t) (x_1^4 + x_2^4) + \frac{C_C}{x_2 - x_1}$$

where $\{p_i, x_i\}$ are canonical position and momentum coordinates of the ions and we assume that $x_2 > x_1$, as shown in Fig. 2.1.

The STA treatment of the Hamiltonian eq. 2.2 is schematically shown in Fig. 2.2. Depicted are the major mathematical objects relevant to each step and the variables and functions which describe them. The various parts of the treatment are described below and can be found described in greater detail in [32, 31, 33, 34, 12, 35]:

- **Dynamical normal modes:** No inverse-engineering approach is known for the exact Hamiltonian eq. 2.2. It has to be brought into the form of two time-dependent harmonic oscillators (HO) $H_{\text{HO}}^{(-)}(t) + H_{\text{HO}}^{(+)}(t)$ by way of a technique called “dynamical normal mode approximation”, derived in detail in [35].

The time-dependent HO frequencies are denoted by $\Omega_{\pm}(t)$ (later corresponding to the stretch and centre-of-mass-mode (CoM) frequencies). Note that the normal mode procedure gives a correspondence between the potential parametrisation (here $\{\alpha(t), \beta(t)\}$) and the HO frequencies $\Omega_{\pm}(t)$, as indicated in Fig. 2.2.

In the case of an N -ion system, this step is easily generalised by decomposing the system into N HO Hamiltonians.

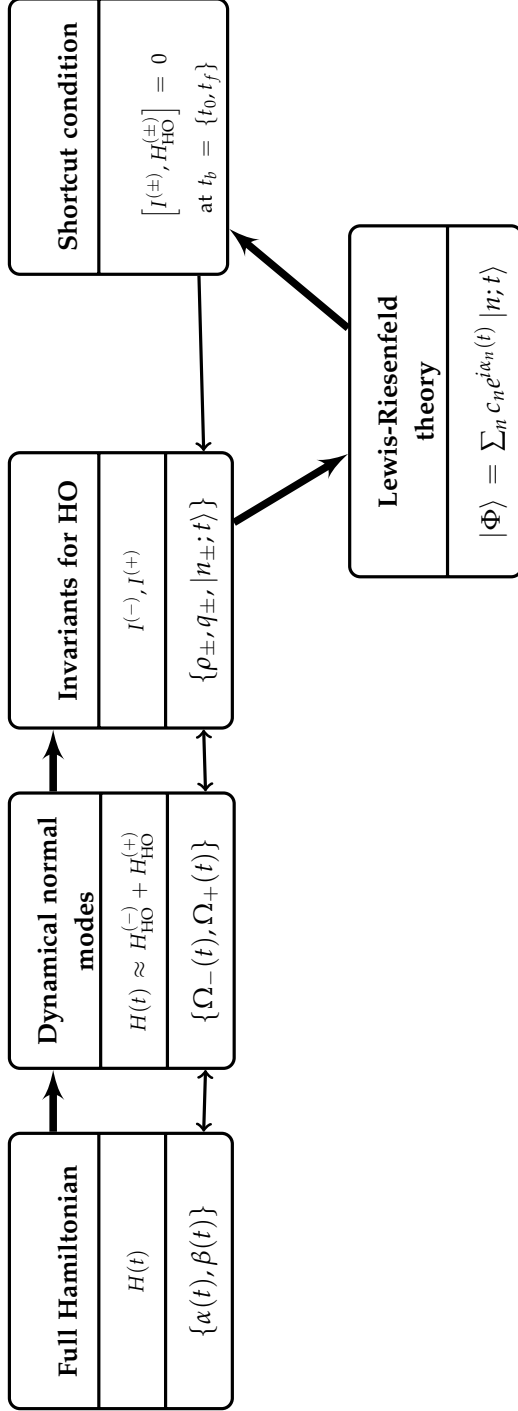


Figure 2.2: Flowchart illustrating the steps needed for invariant-based inverse engineering methods, illustrated using the example of the cooling motion as used in this thesis.

- **Dynamical invariants:** The inverse-engineering technique makes use of dynamical invariants $I(t)$. Invariants $I(t)$ are operators with constant expectation values:

$$\frac{\partial}{\partial t} \langle \Psi | I(t) | \Psi \rangle = 0 \quad (2.3)$$

where $|\Psi\rangle$ are solutions to the Schrödinger eq. for $H(t)$.

For a Hamiltonian $H_{\text{HO}}^{(\pm)}(t)$ with HO form, such invariants are known explicitly, but not for the general form (2.2). Thus the dynamical normal mode step is necessary to find an approximation $H \approx H_{\text{HO}}^{(-)} + H_{\text{HO}}^{(+)}$ for which explicit invariants exist. They are defined by two auxiliary functions $\rho_{\pm}(t)$ and $q_{\pm}(t)$, which will turn out to correspond to the curvature and centre position of the harmonic well. Note that a correspondence between the variable sets $\{\Omega_{\pm}(t)\}$ and $\{\rho_{\pm}(t), q_{\pm}\}$ exists again.

For the following steps, it is necessary to explicitly know the eigenvectors $|n_{\pm}; t\rangle$ of $I(t)$, where $n_{\pm}$ is the eigenvalue and t denotes the time-dependence.

- **Lewis-Riesenfeld theory:** According to Lewis and Riesenfeld [32], if the two Hamiltonians $H^{(\pm)}(t)$ and corresponding invariants $I^{(\pm)}(t)$ are known, the individual solutions $|\Psi_{\pm}\rangle$ to the Schrödinger equation are given as a superposition of eigenvectors $|n_{\pm}; t\rangle$ of $I^{(\pm)}(t)$:

$$|\Psi_{\pm}\rangle = |\Psi_{\pm}(t)\rangle = \sum_{n_{\pm}} c_{n_{\pm}} e^{i\alpha_{n_{\pm}}(t)} |n_{\pm}; t\rangle \quad (2.4)$$

where the coefficients $c_{n_{\pm}}$ are constant and the phases $\alpha_{n_{\pm}}(t)$ are known explicitly.

- **Shortcut condition:** If the invariant commutes with the Hamiltonian $([H_{\text{HO}}^{(\pm)}(t_b), I^{(\pm)}(t_b)] = 0)$ at boundary times $t_b = \{t_0, t_f\}$, they share an eigenbasis at t_0 . This means that the initial populations in the eigenbasis of $H_{\text{HO}}^{(\pm)}(t_0)$ are also the populations of the invariant eigenvectors $|n_{\pm}; t_0\rangle$. Since Lewis-Riesenfeld theory yields that the population numbers $c_{n_{\pm}}$ are constant, the system is still in the superposition $\sum_{n_{\pm}} c_{n_{\pm}} e^{i\alpha_{n_{\pm}}(t_f)} |n_{\pm}; t_f\rangle$ at final time, only that the invariant eigenvectors $|n_{\pm}; t_f\rangle$ have evolved. But since Hamiltonian and invariant commute again at t_f , they share again an eigenbasis, meaning that the populations in the initial instantaneous basis of $H_{\text{HO}}^{(\pm)}(t_0)$ have been carried over to the new basis of $H_{\text{HO}}^{(\pm)}(t_f)$. This yields an evolution that recovers the initial instantaneous populations at final time. Note that at intermediate times, the system may generally not follow the adiabatic evolution, but reaches the same final state nonetheless.

An alternative STA method that follows the adiabatic evolution at all times is given by the counterdiabatic driving method as demonstrated in [36].

- **Inverse-engineering:** The aforementioned steps produce a condition that ensures adiabatic transfer at arbitrary time scales. To infer the full Hamiltonian $H(t)$ (here in the form of $\{\alpha(t), \beta(t)\}$) from this, an inverse-engineering technique is used. Since the invariants $I^{(\pm)}(t)$ are defined through auxiliary functions $\{\rho_{\pm}(t), q_{\pm}(t)\}$, these are designed first to always satisfy the shortcut condition on the commutator. From there, the Hamiltonian can be inferred through the chain of correspondences $\{\rho_{\pm}(t), q_{\pm}\} \leftrightarrow \{\Omega_{\pm}(t)\} \leftrightarrow \{\alpha(t), \beta(t)\}$.

Note that this procedure is not exact due to the dynamical normal modes step being approximate. Arbitrarily low run-times are therefore only possible in general when the Hamiltonian is in fact a harmonic oscillator, for example in ion transport.

The procedure for treating an N -ion system is very similar, only that N HO Hamiltonians have to be found, leading to N invariants, N pairs $\{\rho_i, q_i\}$ and N shortcut conditions.

The steps for this treatment shall now be given in detail so that it can later be applied to the Hamiltonian eq. 2.2 for ions of equal mass and for a similar Hamiltonian in the unequal mass case.

2.1 Dynamical normal modes for two-dimensional systems

For the shortcuts-to-adiabaticity treatment to be feasible, we need to bring the full Hamiltonian eq. 2.2 into the form of two time-dependent harmonic oscillators. This can be done by decomposing the motion into uncoupled dynamical normal modes (NM). A detailed treatment of this general procedure is given by Lizuain in [35] and we shall now reiterate the relevant parts in the following.

Assume we want to bring a two-particle Hamiltonian (for example eq. 2.2)

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_{\text{tot}}(x_1, x_2, t) \quad (2.5)$$

into the double harmonic oscillator form

$$H_{2\text{HO}} = \sum_{i=1}^2 \left[\frac{P_i^2}{2} + \frac{1}{2} \Omega_i^2(t) \left(X_i - \frac{F_i(t)}{\Omega_i^2(t)} \right)^2 \right]. \quad (2.6)$$

Here $\{P_i, X_i\}$ denote canonical momentum and position coordinates which will turn out to be mass-weighted normal mode coordinates, $\Omega_i(t)$ are the harmonic oscillator frequencies and $\frac{F_i(t)}{\Omega_i^2(t)}$ are the oscillator centres.

For this we need to take a second-order approximation to H and diagonalise the mass-weighted¹ Hessian matrix K of the potential V_{tot} in eq. 2.5 around the equilibrium positions $x_1^{(0)}(t)$ and $x_2^{(0)}(t)$.

¹The mass weighting is due to the full derivation actually diagonalising the complete Hamiltonian eq. 2.5, including the mass-dependent momentum terms, and not only the position-dependent potential V_{tot} .

$$K_{ij} = \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 V_{\text{tot}}}{\partial x_i \partial x_j} \Big|_{\{x_1^{(0)}, x_2^{(0)}\}}$$

$$K = \begin{pmatrix} \frac{k_1+k}{m_1} & \frac{-k(t)}{\sqrt{m_1 m_2}} \\ \frac{-k(t)}{\sqrt{m_1 m_2}} & \frac{k_2(t)+k(t)}{m_2} \end{pmatrix}. \quad (2.7)$$

Since the Hessian has to be symmetric, the parametrisation $\{k_1, k_2, k\}$ is justified. Later, in the case of trapped ions coupled by the Coulomb interaction, k will turn out to be the Coulomb coupling term.

Note that the variables $x_i^{(0)}(t), k(t), k_1(t), k_2(t), \lambda_i(t), \Omega_i(t), \theta(t), P_{0,i}(t)$ that will appear throughout this section are generally time-dependent, but for clarity of notation, this is suppressed.

Due to K being a symmetric matrix, it can be diagonalised orthogonally by the rotation matrix O

$$O = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \quad (2.8)$$

such that

$$O^T K O = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \quad (2.9)$$

where the $\lambda_i = \Omega_i^2$ are the positive eigenvalues of K corresponding to the frequencies of the normal modes.

The angle θ of the eigenvectors is given by

$$\tan(2\theta) = \frac{2k\sqrt{m_1 m_2}}{m_1(k_2 + k) - m_2(k_1 + k)}. \quad (2.10)$$

The change-of-coordinates matrix²

$$A(t) = O^T \text{diag}(\sqrt{m_1}, \sqrt{m_2}) = \begin{pmatrix} \sqrt{m_1} \cos \theta & \sqrt{m_2} \sin \theta \\ -\sqrt{m_1} \sin \theta & \sqrt{m_2} \cos \theta \end{pmatrix} \quad (2.11)$$

defines new canonical coordinates $\{X'_-, X'_+, P'_-, P'_+\}$ via

$$\begin{pmatrix} X'_- \\ X'_+ \end{pmatrix} = A(t) \begin{pmatrix} x_1 - x_1^{(0)} \\ x_2 - x_2^{(0)} \end{pmatrix}$$

$$\begin{pmatrix} P'_- \\ P'_+ \end{pmatrix} = \left(A^T(t)\right)^{-1} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}. \quad (2.12)$$

²As with the mass-weighting of K , the actual coordinate transformation $A(t)$ is not identical to the matrix O due to the complete Hamiltonian eq. 2.5 being diagonalised, including its mass-dependent momentum terms. Refer to [35] for the full derivation.

2.1. Dynamical normal modes for two-dimensional systems

The momentum transformation $(A^T(t))^{-1}$ is given by

$$(A^T(t))^{-1} = O^{-1} \text{diag}\left(\frac{1}{\sqrt{m_1}}, \frac{1}{\sqrt{m_2}}\right) = \begin{pmatrix} \frac{\cos \theta}{\sqrt{m_1}} & \frac{\sin \theta}{\sqrt{m_2}} \\ -\frac{\sin \theta}{\sqrt{m_1}} & \frac{\cos \theta}{\sqrt{m_2}} \end{pmatrix}. \quad (2.13)$$

In these coordinates, after truncating the expansion of the potential V_{tot} in eq. 2.5 in x_1 and x_2 around $x_1^{(0)}$ and $x_2^{(0)}$ after the second order and correcting for inertial effects, the Hamiltonian takes the intermediate form

$$H' = \frac{1}{2} \sum_{i=-,+} \left(P_i'^2 + \Omega_i^2 X_i'^2 \right) - \underbrace{(P'_-, P'_+) A(t) \begin{pmatrix} \dot{x}_1^{(0)} \\ \dot{x}_2^{(0)} \end{pmatrix} - \dot{\theta} (X'_- P'_+ - X'_+ P'_-)}_{\text{Inertial corrections}}. \quad (2.14)$$

The terms in the derivatives of the equilibrium positions and the angle θ are corrections due to inertial effects, as the coordinate transformation $A(t)$ may not result in an inertial frame.

It already becomes apparent at this stage that given a time-independent eigenvector angle ($\dot{\theta} = 0$), the initial Hamiltonian separates into two independent parts, even if those do not yet have the form of a harmonic oscillator. Thus only systems that satisfy $\dot{\theta} = 0$ are of interest to us and we will assume this to be the case going forward. An example is a system with the Hamiltonian eq. 2.2, as this leads to $k_1 = k_2$ and $m_1 = m_2$ (see following chapter). For this, $\theta = \frac{\pi}{4}$ is constant and the Hamiltonian separates exactly. The same Hamiltonian with two unequal masses already does not show this property, foreshadowing the need to choose a different Hamiltonian for unequal mass systems.

To finally reach the desired form eq. 2.6, we use a further coordinate transformation to shift the momenta

$$\begin{aligned} X_i &= X'_i \\ P_i &= P'_i - P_{0,i} \end{aligned} \quad (2.15)$$

where

$$\begin{pmatrix} P_{0,-} \\ P_{0,+} \end{pmatrix} = A(t) \begin{pmatrix} \dot{x}_1^{(0)} \\ \dot{x}_2^{(0)} \end{pmatrix} \quad (2.16)$$

and $i = \{-, +\}$.

In these coordinates and assuming that we are working with a Hamiltonian that fulfils $\dot{\theta} = 0$, the Hamiltonian H' takes the final HO form

$$H_{2\text{HO}} = H_{\text{HO}}^{(1)} + H_{\text{HO}}^{(2)} = \sum_{i=-,+} \left[\frac{P_i^2}{2} + \frac{1}{2} \Omega_i^2 \left(X_i + \frac{\dot{P}_{0,i}}{\Omega_i^2} \right)^2 \right]. \quad (2.17)$$

Upon comparing with eq. 2.6, it becomes apparent that we have constructed the desired form of two harmonic oscillators. The HO frequencies are given by the NM frequencies $\Omega_{\pm}(t)$ and the mode centres by $-\frac{p_{0,\pm}(t)}{\Omega_{\pm}^2(t)}$. For an explicit form of V_{tot} , this procedure yields the needed correspondence between the NM frequencies $\Omega_{\pm}(t)$ and the parametrisation of V_{tot} ($\{\alpha(t), \beta(t)\}$ in the cooling transport) and we can go on to find the invariants that accompany such harmonic oscillators.

2.2 Dynamical invariants for the harmonic oscillator

After decomposing the full Hamiltonian into two (or N) harmonic oscillators, we go on to fulfil the second prerequisite of the STA treatment, finding accompanying dynamical invariants. We reiterate the treatment summarised in [17].

Originally developed by Lewis and Leach [37] and Dhara and Lawande [38], the Lewis-Riesenfeld invariant $I(t)$ for a one-dimensional Hamiltonian of the form

$$H = \frac{p^2}{2M} - F(t)x + \frac{M}{2}\Omega^2(t)x^2, \quad (2.18)$$

can be stated explicitly. The following discussion is reiterated from Torrontegui [17].

Here $\{p, x\}$ are the canonical coordinates, M is the particle mass, $\Omega(t)$ the oscillation frequency (will later be the NM frequency) and $F(t)$ a force term.

By completing the square and adding a purely time-dependent and thus physically irrelevant term, eq. 2.18 becomes

$$H_{\text{HO}} = \frac{p^2}{2M} + \frac{M}{2}\Omega^2(t) \left(x - \frac{F(t)}{M\Omega^2(t)} \right)^2, \quad (2.19)$$

and we see that this Hamiltonian is equivalent to one of the time-dependent HO as obtained in eq. 2.6 by the dynamical normal mode treatment

Note that in eq. 2.6, the mass M has been set to 1 as the Hamiltonian is given in mass-weighted NM coordinates.

The invariant for H_{HO} is defined through the two auxiliary functions $\rho(t)$ and $q(t)$ and is given by [17]

$$I = \frac{1}{2M} [\rho(p - M\dot{q}) - M\dot{\rho}(x - q)]^2 + \frac{1}{2}M\Omega_0^2 \left(\frac{x - q}{\rho} \right)^2. \quad (2.20)$$

The auxiliary functions $\rho(t)$ and $q(t)$ need to fulfil the following ordinary differential equations (ODE):

$$\begin{aligned} \ddot{\rho} + \Omega^2\rho &= \frac{\Omega_0^2}{\rho^3} \\ \ddot{q} + \Omega^2q &= \frac{F(t)}{M}, \end{aligned} \quad (2.21)$$

but can be freely chosen otherwise. $\Omega_0 = \Omega(t_0)$ is the initial frequency. Note that we neglect to denote the time-dependence of $\Omega(t)$, $\rho(t)$ and $q(t)$ if not needed.

Referring back to the STA flowchart in Fig. 2.2, these equations give the correspondence between the descriptions $\{\rho_{\pm}, q_{\pm}\} \leftrightarrow \{\alpha(t), \beta(t)\}$, making this a key result that allows us to find the HO frequencies from the auxiliary functions when performing the inverse-engineering step.

The function q will later turn out to correspond to the NM centre and ρ to the NM state width [12]. When for example treating the case of a single ion in a rigid harmonic well, $\rho(t) = 1$ is constant as the HO keeps a constant frequency but the centre can be moved in space which is described by q .

The eigenvectors $|n; t\rangle$ of the invariant, as needed for Lewis-Riesenfeld theory, are known and their position-space wave functions $\Phi_n(x, t)$ are given by

$$\Phi_n(x, t) = \langle x | n; t \rangle = \frac{1}{\rho^{1/2}} e^{\frac{iM}{\hbar} [\dot{\rho}x^2/2\rho + (\dot{q}\rho - q\dot{\rho})x/\rho]} \mathfrak{H}_n\left(\underbrace{\frac{x - q}{\rho}}_{:=\sigma}\right) \quad (2.22)$$

where the $\mathfrak{H}_n(\sigma)$ are solutions of the instantaneous initial Schrödinger equation with quantum number n

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \sigma^2} + \frac{1}{2} M \Omega_0^2 \sigma^2 \right] \mathfrak{H}_n(\sigma) = \hbar \Omega_0 (n + 1/2) \mathfrak{H}_n(\sigma). \quad (2.23)$$

This is just the Schrödinger equation for a static HO in the normalised coordinate σ , for which the solutions are given by the Hermite functions

$$\mathfrak{H}_n(q) = \frac{1}{\sqrt{2^n n!}} \left(\frac{M \Omega_0}{\pi \hbar} \right)^{1/4} e^{-\frac{M \Omega_0 q^2}{2\hbar}} H_n \left(\sqrt{\frac{M \Omega_0}{\hbar}} q \right) \quad (2.24)$$

where H_n are the Hermite polynomials.

The phases $\alpha_n(t)$ for the transport modes $|n; t\rangle_{\alpha} = e^{i\alpha_n(t)} |n; t\rangle$ are then given as derived in section 2.3 by

$$\alpha_n = -\frac{1}{\hbar} \int_0^t dt' \left(\frac{\hbar \Omega_0 (n + 1/2)}{\rho^2} + \frac{M(\dot{q}\rho - q\dot{\rho})^2}{2\rho^2} \right). \quad (2.25)$$

Now that the complete transport modes $|n; t\rangle_{\alpha}$ are known explicitly, the instantaneous energies $\langle n; t |_{\alpha} H_{\text{HO}} |n; t\rangle_{\alpha}$ can be calculated.

A lengthy calculation gives the instantaneous energies depending on the auxiliary functions ρ and q [12, 17]

$$E_n(t) = \langle n; t |_\alpha H_{\text{HO}} | n; t \rangle_\alpha = \frac{\hbar(2n+1)}{4\Omega_0} \left(\dot{\rho}^2 + \Omega(t)^2 \rho^2 + \frac{\Omega_0^2}{\rho^2} \right) + \frac{M}{2} \dot{q}^2 + \frac{M}{2} \Omega(t)^2 \left(q - \frac{F(t)}{M\Omega^2(t)} \right)^2. \quad (2.26)$$

Note that the phases $\alpha_n(t)$ are irrelevant in obtaining the energies.

These energies are a key result as they allow finding forms of the auxiliary functions that retain the initial energy at final time, thus constructing a shortcut.

In the case of two trapped ions as depicted in Fig. 2.2, there are two HO Hamiltonians $H_{\text{HO}}^{(\pm)}$ and thus two invariants $I^{(\pm)}$ as well as four functions $\{\rho_\pm, q_\pm\}$.

The Lewis-Riesenfeld theory that yields the shortcut condition on ρ and q as shown in Fig. 2.2 is derived next.

2.3 Lewis-Riesenfeld theory

Lewis and Riesenfeld in their 1969 paper [32] used dynamical invariants of explicitly time-dependent Hamiltonians $H(t)$ to solve the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H(t) |\Psi\rangle. \quad (2.27)$$

In the following, we reiterate the treatment given in [32, 33].

Suppose the Hamiltonian $H(t)$ has a known Hermitian invariant $I(t)$ that fulfills

$$i\hbar \frac{\partial I}{\partial t} - [H(t), I(t)] = 0. \quad (2.28)$$

This equation is the condition for the expectation values of the invariant to be constant:

$$\frac{\partial}{\partial t} \langle \Psi | I(t) | \Psi \rangle = 0. \quad (2.29)$$

It can then be shown that the solutions $|\Psi\rangle$ of the Schrödinger equation (2.27) are constant superpositions of eigenvectors $|n; t\rangle$ of the invariant $I(t)$, together with a time-dependent phase $\alpha_n(t)$.

This result can be derived from the eigenequation

$$I(t) |n; t\rangle = n(t) |n; t\rangle \quad (2.30)$$

and eq. 2.28 by calculating the following steps:

1. If $|\Psi\rangle$ is a solution of the Schrödinger equation, then $I(t)|\Psi\rangle$ is as well. This can be seen by acting on $|\Psi\rangle$ with eq. 2.28 and using the Schrödinger equation to obtain

$$i\hbar \frac{\partial}{\partial t} [I(t)|\Psi\rangle] = H(t)[I(t)|\Psi\rangle]. \quad (2.31)$$

2. When acting on eq. 2.28 with eigenvectors $\langle m;t|$ and $|n;t\rangle$, we find the relation

$$i\hbar \langle m;t| \left(\frac{\partial I}{\partial t} \right) |n;t\rangle = (n - m) \langle m;t| H(t) |n;t\rangle \quad (2.32)$$

3. The eigenvalues $n(t)$ of the invariant $I(t)$ are constant: $n(t) = n$. This is easily derived by taking the time-derivative of eq. 2.30 and acting on it with $\langle n;t|$. This leads to $\frac{\partial n}{\partial t} = \langle n;t| \frac{\partial I}{\partial t} |n;t\rangle = 0$ with eq. 2.32. Note that the eigenvectors are in general time-dependent.
4. For all n, m with $n \neq m$ it holds that

$$\langle m;t| i\hbar \frac{\partial}{\partial t} |n;t\rangle = \langle m;t| H(t) |n;t\rangle. \quad (2.33)$$

This is obtained by deriving the eigen-equation (2.30) w.r.t. time and multiplying the result with $\langle m;t|$. The relation (2.33) is obtained upon inserting eq. 2.32.

Note that if this property would hold for all n, m , then already the eigenstates $|n;t\rangle$ would be solutions to the Schrödinger equation. Instead we now also need to treat the case $n = m$.

5. This is done by modifying the eigenvectors to $|n;t\rangle_\alpha = e^{i\alpha_n(t)} |n;t\rangle$, where

$$\alpha_n(t) = \frac{1}{\hbar} \int_0^t \langle n;t'| i\hbar \frac{\partial}{\partial t'} - H(t') |n;t'\rangle dt', \quad (2.34)$$

which now do solve the Schrödinger equation.

This can be seen from the fact that the $|n;t\rangle_\alpha$ are still eigenvectors to $I(t)$ (assuming it does not contain the time-derivative operator), so eq. 2.33 stays valid. Inserting the Ansatz $|n;t\rangle_\alpha$ into eq. 2.33 for $n = m$ yields the condition (2.34).

Thus we see that the modified invariant eigenvectors $|n;t\rangle_\alpha$ solve the Schrödinger equation and we are able to write the solutions $|\Psi\rangle$ as superpositions

$$|\Psi(t)\rangle = \sum_n c_n |n;t\rangle_\alpha \quad (2.35)$$

of the "transport modes" $|n;t\rangle_\alpha$ where the populations c_n are constant throughout time and are therefore determined by initial conditions. The time dependence of the solution $|\Psi(t)\rangle$ is thus entirely confined to the modified eigenvectors $|n;t\rangle_\alpha$. This result can now be used to find a shortcut condition, as suggested in Fig. 2.2.

2.4 Shortcut condition and inverse engineering approach

We have now stated all relevant parts needed to formulate the inverse-engineering STA method as detailed in [22, 31].

The goal is to take a Hamiltonian $H(t)$ and design it in such a way that the populations in the instantaneous bases at $t = 0$ and $t = t_f$ are the same. In the case of the two-ion Hamiltonian eq. 2.2, we can gain the insight that the condition for the populations to match up at initial and final times is that the HO Hamiltonians $H_{\text{HO}}^{(\pm)}$ and their invariants $I^{(\pm)}$ need to commute at these times:

$$[H_{\text{HO}}^{(\pm)}(t_0), I^{(\pm)}(t_0)] = [H_{\text{HO}}^{(\pm)}(t_f), I^{(\pm)}(t_f)] = 0. \quad (2.36)$$

If the operators commute initially, they have a shared eigenbasis. Thus if the system is in an eigenstate of $H_{\text{HO}}^{(\pm)}(t_0)$, this must be some eigenstate $|n_{\pm}; t_0\rangle$ of the invariant. Since *section 2.3* tells us that the solutions to the Schrödinger equation can be written in terms of the eigenstates $|n_{\pm}; t\rangle$ of $I^{(\pm)}$ and that their coefficients $c_{n_{\pm}}$ are constant, we conclude that the system will be in the evolved eigenstate $|n_{\pm}; t_f\rangle$ at final time t_f . If the commutation holds again at t_f , Hamiltonian and invariant will share an eigenbasis again and $|n_{\pm}; t_f\rangle$ must be an eigenstate of the Hamiltonian, thus having retained the quantum number $n_{\pm}$. For example, if the system was in the ground state initially, it will be in the ground state again at t_f , but the ground state may now be described by a different wave function, for example if it describes an ion that was spatially displaced.

As depicted in Fig. 2.2, the invariant-based inverse engineering approach then consists of leaving the Hamiltonian undetermined at first and instead designing the invariant such that eq. 2.36 holds. Since the dynamical normal mode Hamiltonian eq. 2.17 consists of two HO parts, two invariants are needed and this means designing two sets of functions $\{\rho_{\pm}, q_{\pm}\}$. These can be chosen freely, as long as the ODEs in eq. 2.21 are fulfilled and necessary physical constraints are met (such as setting inner and outer distances d_{in} and d_{out}). The HO Hamiltonian can then be learned from the auxiliary differential equations (2.21), specifically by solving for $\Omega_{\pm}$. From this in turn, the time dependence of the full Hamiltonian can be inferred. In the case of the double well potential eq. 2.2, this means inverting the correspondence between $\{\alpha, \beta\}$ and the HO frequencies $\Omega_{\pm}$ that was gained from the dynamical normal mode treatment.

Despite this treatment not being exact due to the dynamical normal mode approximation, the freedom in designing $\rho_{\pm}$ and $q_{\pm}$ can be used to minimise the effect this discrepancy and obtain an acceptable shortcut even for the exact system, even though this will break down for short run-times. This freedom can also be used to mitigate the effect of experimental imperfections.

In the following chapter we will now go on to apply the described procedure explicitly first to a system of two trapped ions of equal mass in a quartic

2.4. Shortcut condition and inverse engineering approach

double well potential eq. 2.1 in order to design the cooling motion of Fig. 0.2b and then generalise this for a system of two ions of unequal mass.

Designing the cooling motion for two ions of equal mass

In this chapter we want to apply the formalism stated in chapter 2 to design the two-ion cooling motion as depicted in Fig. 0.2b. This in-out transport must leave the ions unexcited and would ideally be robust towards experimental error sources. Thus we stabilise the cooling scheme against a linear error term in the trapping potential, a term which is a major error source in many trapped ion experiments [10, 12, 39].

Suppose we trap two ions of equal mass m in a harmonic-quartic potential V_{el}

$$V_{\text{el}}(t, x) = \alpha(t)x^2 + \beta(t)x^4. \quad (3.1)$$

The total Hamiltonian is given by

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_{\text{tot}}(x_1, x_2, t) \quad (3.2)$$

$$V_{\text{tot}} = \alpha(t) (x_1^2 + x_2^2) + \beta(t) (x_1^4 + x_2^4) + \frac{C_C}{x_2 - x_1}$$

where $\{p_1, x_1\}$ and $\{p_2, x_2\}$ are the position and momentum coordinates of the two ions.

The steps needed for STA schemes shown in Fig. 2.2 are carried out explicitly. To this end, we first explicitly calculate the dynamical normal modes according to section 2.1. From this we will obtain a harmonic approximation of the Hamiltonian and the corresponding wave functions and instantaneous energies according to Lewis-Riesenfeld invariant theory in section 2.3. Then, as described in section 2.4, we can inverse-engineer the Hamiltonian by enforcing the commutation condition (2.36) and obtain the potential trajectory $\{\alpha(t), \beta(t)\}$.

As the dynamical normal mode decomposition is only a second order approximation, further optimisation will also be needed to eliminate the effect of the

higher order terms. This will be done by introducing and then numerically optimising a number of free parameters in the engineered invariant.

3.1 Dynamical normal modes for two trapped ions of equal mass

To find the dynamical normal modes for the full Hamiltonian eq. 3.2, we apply the theory from section 2.1 and follow the discussion in [12]. We take the harmonic approximation of H at the equilibrium positions $x_1^{(0)}$ and $x_2^{(0)}$ that are found via $\partial V_{\text{tot}}/\partial x_1|_{x_1^{(0)}} = \partial V_{\text{tot}}/\partial x_2|_{x_2^{(0)}} = 0$.

The variable d denotes the equilibrium distance of the two ions, as is illustrated in Fig. 3.1. Since the potential is spatially symmetric, the equilibrium positions are also symmetric and given by $x_1^{(0)} = -\frac{d}{2}$ and $x_2^{(0)} = \frac{d}{2}$.

Note that we again neglect to explicitly denote the time dependence of the variables $d, \alpha, \beta, \Omega_{\pm}(t)$ and $P_{0,\pm}$.

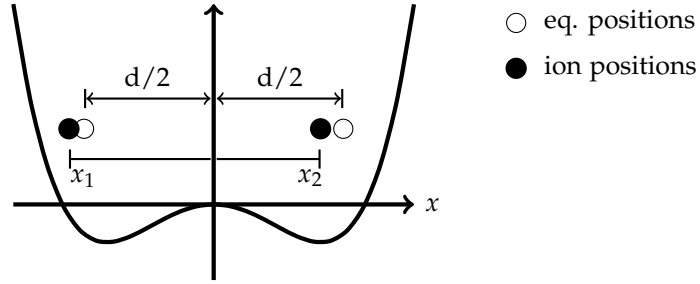


Figure 3.1: Schematic depiction of position and equilibrium coordinates for two ions trapped in a quartic double-well potential. Note that the Coulomb potential has been neglected from the potential shape.

The mass-weighted Hessian K then becomes

$$K = \frac{1}{m} \begin{pmatrix} 2\alpha + 3\beta d^2 + \frac{2C_C}{d^3} & -\frac{2C_C}{d^3} \\ -\frac{2C_C}{d^3} & 2\alpha + 3\beta d^2 + \frac{2C_C}{d^3} \end{pmatrix}. \quad (3.3)$$

As K has the simple structure $\begin{pmatrix} A & B \\ B & A \end{pmatrix}$, it is easily diagonalised by the constant eigenvectors

$$\begin{aligned} v_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ v_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \end{aligned} \quad (3.4)$$

giving an angle $\theta = \frac{\pi}{4}$.

3.1. Dynamical normal modes for two trapped ions of equal mass

Variables with a $(-)$ -subscript will be associated with the centre-of-mass mode while $(+)$ -subscripts will denote stretch mode variables.

The eigenvalues $\lambda_{\pm}$ of K are the squared normal mode frequencies and are given by

$$\begin{aligned}\lambda_- &= \Omega_-^2 = \frac{1}{m}(2\alpha + 3\beta d^2), \\ \lambda_+ &= \Omega_+^2 = \frac{1}{m}(2\alpha + 3\beta d^2 + \frac{4C_C}{d^3}).\end{aligned}\tag{3.5}$$

According to eq. 2.12, the intermediate normal mode coordinates are then given by

$$\begin{aligned}\begin{pmatrix} X'_- \\ X'_+ \end{pmatrix} &= \sqrt{\frac{m}{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 + \frac{d(t)}{2} \\ x_2 - \frac{d(t)}{2} \end{pmatrix} = \sqrt{\frac{m}{2}} \begin{pmatrix} x_2 + x_1 \\ (x_2 - x_1) - d(t) \end{pmatrix} \\ \begin{pmatrix} P'_- \\ P'_+ \end{pmatrix} &= \sqrt{\frac{1}{2m}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \sqrt{\frac{1}{2m}} \begin{pmatrix} p_2 + p_1 \\ p_2 - p_1 \end{pmatrix}\end{aligned}\tag{3.6}$$

The second and final coordinate transformation is defined by eq. 2.16 and eq. 2.15

$$\begin{aligned}\begin{pmatrix} X_- \\ X_+ \end{pmatrix} &= \begin{pmatrix} X'_- \\ X'_+ \end{pmatrix} \\ \begin{pmatrix} P_- \\ P_+ \end{pmatrix} &= \begin{pmatrix} P'_- - P_{0,-} \\ P'_+ - P_{0,+} \end{pmatrix} \\ \begin{pmatrix} P_{0,-} \\ P_{0,+} \end{pmatrix} &= \sqrt{\frac{m}{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} -\frac{\dot{d}}{2} \\ \frac{\dot{d}}{2} \end{pmatrix} = \sqrt{\frac{m}{2}} \begin{pmatrix} 0 \\ \dot{d}(t) \end{pmatrix}\end{aligned}\tag{3.7}$$

This finally yields the normal mode Hamiltonian eq. 2.17 in the explicit form

$$H_{2\text{HO}} = H_{\text{HO}}^{(+)} + H_{\text{HO}}^{(-)} = \underbrace{\frac{P_+^2}{2} + \frac{1}{2}\Omega_+^2 \left(X_+ + \sqrt{\frac{m}{2}} \frac{\ddot{d}}{\Omega_+^2} \right)^2}_{H_{\text{HO}}^{(+)}} + \underbrace{\frac{P_-^2}{2} + \frac{1}{2}\Omega_-^2 X_-^2}_{H_{\text{HO}}^{(-)}}\tag{3.8}$$

The corresponding Lewis-Riesenfeld invariants for $H_{\text{HO}}^{(-)}$ and $H_{\text{HO}}^{(+)}$ are then according to eq. 2.20

$$I^{(\pm)} = \frac{1}{2} [\rho_{\pm}(P_{\pm} - \dot{q}_{\pm}) - \dot{\rho}_{\pm}(X_{\pm} - q_{\pm})]^2 + \frac{1}{2}\Omega_{0\pm}^2 \left(\frac{X_{\pm} - q_{\pm}}{\rho_{\pm}} \right)^2\tag{3.9}$$

with the auxiliary functions $\rho_{\pm}$ and $q_{\pm}$ defined according to eq. 2.21 as

$$\ddot{\rho}_{\pm} + \Omega_{\pm}^2 \rho_{\pm} = \frac{\Omega_{0\pm}^2}{\rho_{\pm}^3} \quad (3.10a)$$

$$\ddot{q}_+ + \Omega_+^2 q_+ = -\sqrt{\frac{m}{2}} \ddot{d} \quad (3.10b)$$

$$q_- = 0. \quad (3.10c)$$

The initial NM frequencies $\Omega_{0\pm}$ are later deduced from physical boundary conditions such as the desired starting distance.

The physical meaning of the auxiliary variables $q_{\pm}$ can be understood as the NM centre, while $\rho_{\pm}$ corresponds to the oscillator curvature. For example in the case of transport of one ion in a constant trapping well the variable ρ can be set to 1, as the ion experiences the same potential curvature at all times, while the spatial translation is described by q .

The fact that q_- is zero at all times can then be understood intuitively as a consequence of the spatial symmetry of the potential. Since the equilibrium positions are always symmetric, the CoM-mode centre is exactly zero at all times.

The instantaneous energies of the stretch and CoM mode states are known from eq. 2.26 as

$$\begin{aligned} E_{n-}(t) &= \langle n_-; t |_{\alpha} H_{\text{HO}}^{(-)} | n_-; t \rangle_{\alpha} = \frac{(2n+1)\hbar}{4\Omega_{0-}} \left(\dot{\rho}_{-}^2 + \Omega_{-}^2 \rho_{-}^2 + \frac{\Omega_{0-}^2}{\rho_{-}^2} \right) \\ E_{n+}(t) &= \langle n_+; t |_{\alpha} H_{\text{HO}}^{(+)} | n_+; t \rangle_{\alpha} = \frac{(2n+1)\hbar}{4\Omega_{0+}} \left(\dot{\rho}_{+}^2 + \Omega_{+}^2 \rho_{+}^2 + \frac{\Omega_{0+}^2}{\rho_{+}^2} \right) \\ &\quad + \frac{1}{2} \dot{q}_{+}^2 + \frac{1}{2} \Omega_{+}^2 \left(q_{+} + \frac{\sqrt{m} \ddot{d}}{\sqrt{2}\Omega_{+}^2} \right)^2. \end{aligned} \quad (3.11)$$

Note that the stretch mode energy includes additional terms in q_{+} due to the non-stationary mode centre.

Before going over to the inverse-engineering step, we need a correspondence between the normal mode frequencies $\Omega_{\pm}$ and the potential parametrisation given by $\{\alpha, \beta\}$ as depicted in Fig. 2.2. This can be gained from the expressions for the normal mode frequencies eq. 3.5 and from the condition on the equilibrium distance [12]

$$\beta d^5 + 2\alpha d^3 - 2C_C = 0. \quad (3.12)$$

Inverting these relations leads to the expressions

$$d(t) = \sqrt[3]{\frac{4C_C}{m(\Omega_+^2 - \Omega_-^2)}}, \quad (3.13a)$$

$$\alpha(t) = \frac{1}{8}m(3\Omega_+^2 - 5\Omega_-^2), \quad (3.13b)$$

$$\beta(t) = \frac{2C_C}{d^5} - \frac{2\alpha}{d^2(t)} \quad (3.13c)$$

The instantaneous motional frequencies ω_1 and ω_2 of the two ions are equal and are given by the diagonal entries of the Hessian K (compare to eq. 1.2)

$$\begin{aligned} \omega^2 = \omega_1^2 = \omega_2^2 = K_{11} = K_{22} &= \frac{\Omega_+^2 + \Omega_-^2}{2} \\ &= \frac{1}{m}(2\alpha + 3\beta d^2 + \frac{2C_C}{d^3}) = \frac{1}{m}(2\beta d^2 + \frac{4C_C}{d^3}), \end{aligned} \quad (3.14)$$

where eq. 3.12 was used in the last step.

Now we proceed to discuss the shortcut condition for the two HO Hamiltonians $H_{\text{HO}}^{(\pm)}$ and the invariant $I^{(\pm)}$ and inverse-engineer the potential V_{el} .

3.2 Inverse engineering the cooling motion

3.2.1 Ensuring the commutation condition

As detailed in section 2.4, we now want to inverse-engineer the invariants $I^{(\pm)}$ from eq. 3.9 to commute with the Hamiltonians $H_{\text{HO}}^{(\pm)}$ from eq. 3.8 at boundary times $t_b = \{t_0, t_f\}$ and follow the approach in [12].

Satisfying this commutation condition is achieved by setting a number of conditions on the auxiliary functions $\rho_{\pm}$ and $q_{\pm}$. After this step, we see that by rewriting eq. 3.10 as

$$\Omega_{\pm} = \sqrt{\frac{\Omega_{0\pm}^2}{\rho_{\pm}^4} - \frac{\ddot{\rho}_{\pm}}{\rho_{\pm}}}, \quad (3.15)$$

choosing the starting values $\Omega_{0\pm}$ and the functions for $\rho_{\pm}$, the protocol $\{\alpha(t), \beta(t)\}$ is determined by eq. 3.13.

The commutation can be ensured by setting the boundary conditions (BC)

$$\rho_{\pm}(t_b) = 1, \quad (3.16a)$$

$$\dot{\rho}_{\pm}(t_b) = \ddot{\rho}_{\pm}(t_b) = \rho_{\pm}^{(3)}(t_b) = \rho_{\pm}^{(4)}(t_b) = 0 \quad (3.16b)$$

$$q_{+}(t_b) = \dot{q}_{+}(t_b) = \ddot{q}_{+}(t_b) = 0, \quad (3.16c)$$

on the auxiliary functions, where $t_b = \{t_0 = 0, t_f\}$.

The conditions on the zeroth and first derivatives can be learned from inserting the BC into the wave functions (2.22) and requiring that they coincide with the instantaneous solutions eq. 2.24. The first two derivatives of the distance $\dot{d}(t_b)$ and $\ddot{d}(t_b)$ should also be zero, so that the scheme starts and ends with stationary ions and to minimise the energy $E_{n+}(t_f)$ in eq. 3.11. This together with the auxiliary ODEs leads to the remaining conditions.

Any choice of $\{\rho_{\pm}, q_{\pm}\}$ satisfying the BC eq. 3.16b and eq. 3.16c leads to a shortcut to adiabaticity, leaving flexibility to optimise the scheme for various purposes, such as cancellation of residual excitations or robustness to experimental imperfections.

Since choosing $\{\rho_{\pm}, q_{\pm}\}$ to simultaneously fulfil the ODEs eq. 3.10b and the BC eq. 3.16 is hard, we take the approach as in [12] and design only $\rho_{\pm}$, but leave a number of free parameters. Since choosing $\rho_{\pm}$ already completely determines the scheme via eq. 3.15, these parameters can be optimised numerically so that the BC on $q_{\pm}$ are fulfilled as well. One way of doing so is minimising the final stretch mode energy $E_{n+}(t_f)$ from eq. 3.11, thus finding parameters that result in $q_{+}(t_f) = \dot{q}_{+}(t_f) = 0$.

But most importantly, $\rho_{\pm}$ must be chosen to implement the desired physical action, namely to bring the ions from a starting distance d_{out} to a minimal distance d_{in} at $t = t_f/2$ and back. This is achieved by computing the boundary values $\rho_{\pm}(t_f/2)$ from physical constraints and then polynomially interpolating to set the time-dependence of $\rho_{\pm}$.

3.2.2 Physical constraints

In order to perform the interpolation of $\rho_{\pm}$, the boundary values of $\Omega_{\pm}$ at times $\{t_0 = 0, t_f/2, t_f\}$ and the intermediate value $\rho_{\pm}(t_f/2)$ need to be found and the following physical constraints shall be enforced.

In what follows, the subscript "in" denotes variables at time $t_f/2$ and the subscript "0" variables at times t_b .

- The ions start and end at the same distance $d(t_0) = d(t_f) = d_{out}$.
- The ions reach their closest point after half the run-time $d(t_f/2) = d_{in}$, $d_{in} < d_{out}$.
Note that the minimal reachable distance d_{in} without merging the two ions into a single-well potential is given by the relation (3.12) at the critical point $\alpha = 0$ as

$$d_c = \left(\frac{2C_C}{\beta_{max}} \right)^{\frac{1}{5}}. \quad (3.17)$$

Thus the maximal strength of the quartic confinement in a given trap alone determines d_c .

- The quartic confinement β must be strongest after half the run-time: $\beta(t_f/2) = \beta_{max}$.
This is to ensure the strongest possible confinement when the ions are

closest to each other and thus to the critical point $\alpha = 0$. In splitting/merging schemes, this critical point has to be crossed to take the ions from single-well to double-well confinement and vice versa. Typically this is the most error-prone moment in these procedures [39], as the potential curvatures are at their lowest at this point, leading to a maximal susceptibility to voltage fluctuations. This is therefore the optimal condition to reduce the effects of such experimental problems.

- The CoM-mode frequency is chosen to be the same $\Omega_-(t_0) = \Omega_-(t_f/2) = \Omega_-(t_f) = \Omega_{0-}$. In the polynomial interpolation that follows in subsection 3.2.3, this leads to Ω_- and ρ_- becoming constant. This is a reasonable choice as then the CoM mode does not need to be considered anymore and we only optimise ρ_+ . Other choices are possible such as a constant stretch mode frequency or constant ion frequencies. The latter choice would be motivated by the fact that it would minimise quantum squeezing effects. However, as the ions are not brought together closer than d_c , the ions frequencies change only by a few percent over the course of the scheme. As the cooling procedure will take several motional cycles and squeezing is negligible at such run-times, not much is to be gained from making the ion frequencies constant over the CoM mode frequency.¹

Using eq. 3.13 we first find

$$\begin{aligned}\beta_{\text{in}} &= \beta_{\text{max}} \\ \alpha_{\text{in}} &= \frac{C_C}{d_{\text{in}}^3} - \frac{\beta_{\text{max}} d_{\text{in}}^2}{2}.\end{aligned}\tag{3.18}$$

Through eq. 3.5, the NM frequencies $\Omega_{\text{in}-}$ and $\Omega_{\text{in}+}$ are uniquely determined.

From this and using $\Omega_{0-} = \Omega_{\text{in}-}$, inverting eq. 3.13a gives

$$\Omega_{0+}^2 = \frac{4C_C}{md_0^3} - \Omega_{\text{in}}^2\tag{3.19}$$

from which in turn α_0 and β_0 can be found using eq. 3.13.

Finally, by evaluating eq. 3.15 at $t_f/2$, the values of $\rho_{\pm}(t_f/2)$ can be determined. Neglecting the term $\frac{\ddot{\rho}_{\pm}}{\rho_{\pm}}$, $\rho_{\pm}(t_f/2)$ turns out to be

$$\rho_{\text{in}\pm} = \sqrt{\frac{\Omega_{0\pm}}{\Omega_{\text{in}\pm}}}.\tag{3.20}$$

¹As it is well known [30] that anomalous trap heating effects increase with decreasing ion motional frequencies, it would be generally helpful to develop a scheme where the initial ion frequencies can be chosen arbitrarily high. However when doing this, the simple polynomial interpolation performed in subsection 3.2.3 starts breaking down and the Ansatz for $\rho_{\pm}$ would need to be chosen more carefully.

This is reasonable since $\ddot{\rho}_{\pm} \propto t_f^{-2}$ due to the double time derivative and $\rho_{\pm}$ is on the order of 1. As $\Omega_{0\pm}$ is closely related to the motional frequencies ω_i , neglecting $\ddot{\rho}_{\pm}$ is justified as long as the cooling scheme takes several motional cycles, which will be the case in this work². If run-times are achieved where this assumption is problematic, one can add a further condition $\ddot{\rho}_{\pm}(t_f/2) = 0$ to the BC eq. 3.16.

Now a $\rho_{\pm}$ can be found that obeys the BC eq. 3.16 and interpolates between $\Omega_{0\pm}$ and $\Omega_{in\pm}$.

3.2.3 Polynomial Ansatz

To find a scheme that is precisely defined for all time $t_0 < t < t_f$, we interpolate $\rho_{\pm}$ between $\rho_{0\pm} = 1$ and $\rho_{in\pm}$ and choose a polynomial with exclusively even orders, such that it is symmetric around $\frac{t_f}{2}$. This is motivated by the fact that the ion motion starts and ends in the same state and should thus be time-symmetric. The simplest choice fulfilling this is a 10th-order polynomial in $\frac{t}{t_f} - \frac{1}{2}$ with only even orders

$$\sum_{i=0}^5 a_i \left(\frac{t}{t_f} - \frac{1}{2} \right)^{2i}. \quad (3.21)$$

After plugging this Ansatz into the BC conditions eq. 3.16 and solving the resulting system of equations for the coefficients a_i , we obtain

$$\begin{aligned} \rho_{\pm}(s) = & \rho_{in\pm} - 20(\rho_{in\pm} - 1) \left(s - \frac{1}{2} \right)^2 + 160(\rho_{in\pm} - 1) \left(s - \frac{1}{2} \right)^4 \\ & - 640(\rho_{in\pm} - 1) \left(s - \frac{1}{2} \right)^6 + 1280(\rho_{in\pm} - 1) \left(s - \frac{1}{2} \right)^8 \\ & - 1024(\rho_{in\pm} - 1) \left(s - \frac{1}{2} \right)^{10} \end{aligned} \quad (3.22)$$

where $s = \frac{t}{t_f}$ is the normalised time.

Note that since $\rho_{in-} = 1, \rho_{-}(t) = 1$.

Since such an Ansatz leaves no degrees of freedom to optimise different aspects of the scheme (such as fulfilment of BC for q_{+} , minimal final excitations due to the harmonic approximation breaking down or sensitivity to experimental imperfections), we follow the treatment in [12] and introduce up to two free parameters into ρ_{+} . This necessitates a 14th-order polynomial fulfilling the same BC conditions as before. One free parameter is defined to be the curvature of ρ_{+} at $s = 1/2$, $c = \frac{d^2 \rho_{+}}{ds^2} |_{s=1/2}$, whereas the second parameter a_7 is defined as the coefficient of the 14th-order term.

²Later, the lower limit of cooling is found to be around 10 motional cycles, validating neglecting $\ddot{\rho}_{\pm}$

Plugging this Ansatz into eq. 3.16 again we obtain

$$\begin{aligned}
 \rho_+(s) = & \rho_{in\pm} + \frac{c}{2} \left(s - \frac{1}{2}\right)^2 \\
 & + \frac{1}{1024} (245760 - 10240c - 245760\rho_{in\pm} - a_7) \left(s - \frac{1}{2}\right)^4 \\
 & - \frac{5}{256} (131072 - 4096c - 131072\rho_{in\pm} - a_7) \left(s - \frac{1}{2}\right)^6 \\
 & + \frac{5}{32} (73728 - 2048c - 73728\rho_{in\pm} - a_7) \left(s - \frac{1}{2}\right)^8 \\
 & - \frac{1}{8} (196608 - 5120c + 196608\rho_{in\pm} - 5a_7) \left(s - \frac{1}{2}\right)^{10} \\
 & + \frac{1}{4} (81920 - 2048c - 81920\rho_{in\pm} - 5a_7) \left(s - \frac{1}{2}\right)^{12} \\
 & + a_7 \left(s - \frac{1}{2}\right)^{14}.
 \end{aligned} \tag{3.23}$$

If a scheme with just one parameter is desired, the parameter a_7 can simply be set to zero.

To give an example of an STA scheme designed in this way, we apply the described inverse-engineering approach to a system of two $^{40}\text{Ca}^+$ ions in a trap that can reach a quartic confinement corresponding to the trap strength of the Sandia HOA2 trap when used with electronics equipment with a voltage range of $\pm 10\text{V}$, as found in Appendix B. The set of physical constraints is given in Table 3.1 as default set A.

Label	$\beta_{\max} (\text{N m}^{-3})$	$d_c (\mu\text{m})$	$d_{\text{out}} (\mu\text{m})$	$d_{\text{in}} (\mu\text{m})$	$m (\text{u})$
A (default)	$1 \cdot \beta_{\text{HOA}} = 0.85$	14.0	$5d_c = 70.1$	$1.25d_c = 17.5$	39.96 ($^{40}\text{Ca}^+$)

Table 3.1: List of the default set of physical constraints that will be used throughout this work. It is determined by the maximal quartic confinement β_{HOA} in the Sandia HOA2 trap when using electronics with a voltage range of $\pm 10\text{V}$ [15]. The critical distance is $d_c = 14.02 \mu\text{m}$ and the starting distance is set to be $d_{\text{out}} = 5d_c = 70.1 \mu\text{m}$, chosen such that the ions are almost decoupled ($\Omega_{0+}/\Omega_{0-} \approx 1.002$). This choice of inner distance will yield a good cooling solution later.

The resulting functions $\rho_{\pm}$ (using the parameter-less Ansatz eq. 3.22 for both), $\Omega_{\pm}$, α , β and d after applying the algorithm given before are shown in Fig. 3.2. The CoM mode frequency stays constant at about 0.48 MHz and the value of β reaches $\beta_{\max}$ after half the run-time. The harmonic potential part α stays negative throughout the scheme, signifying that the potential always has a double-well shape. As desired, the ions move from $70.1 \mu\text{m}$ to $17.5 \mu\text{m}$ and back out, never falling below the critical distance d_c .

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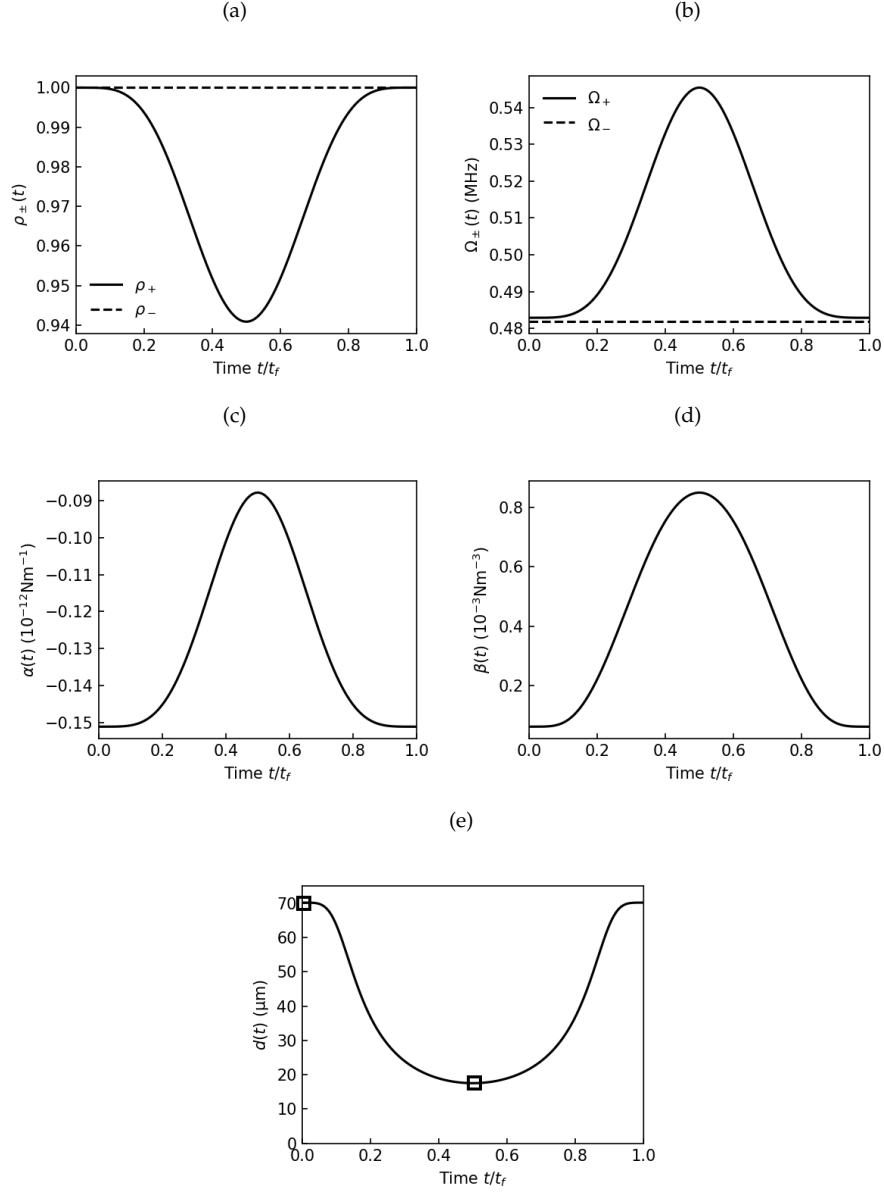


Figure 3.2: An overview of a basic inverse-engineered STA scheme using the physical constraints given in Table 3.1. (a) shows the auxiliary functions $\rho_{\pm}$ according to the Ansatz eq. 3.22, (b) shows the resulting NM frequencies according to eq. 3.15, (c) shows the harmonic confinement $\alpha(t)$, (d) shows the quartic confinement $\beta(t)$ and (e) shows the distance $d(t)$.

The markers in Fig. 3.2e designate the temporal positions at which Fig. 3.3 shows the shape of the potential V_{el} in eq. 3.1. In Fig. 3.3a the starting potential shows minima consistent with the distance $d_{\text{out}} = 70.1 \mu\text{m}$. The potential shape in Fig. 3.3b is still quartic, but the scale has changed such that the ions

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would now find an equilibrium distance $d_{\text{in}} = 17.5 \mu\text{m}$.

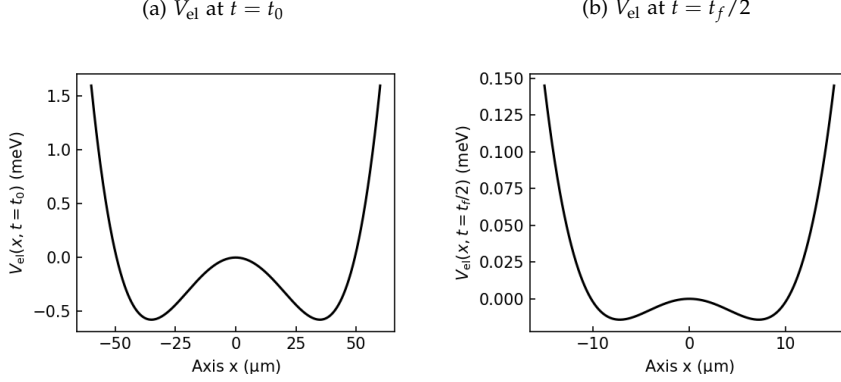


Figure 3.3: Shape of the potential V_{el} of the scheme shown in Fig. 3.2 at two points in time. (a) shows the initial potential at $t = t_0$ and (b) shows the potential after half the run-time $t = t_f/2$.

The task that is left now is to use the more flexible Ansatz eq. 3.23 and optimise the free parameters c , a_7 towards goals like minimal final excitations or maximal robustness. The results to this are presented in the following section.

3.3 Optimising the cooling motion for minimal excitations

The free parameters in Ansatz ρ_+ should now be optimised such that the cooling motion does not excite initially cold ions. We shall refer to this configuration as a “cold run”, as opposed to the coolant ion initially being in the ground state and the information ion in some excited state (a “hot run”).

If the dynamical normal mode decomposition in section 3.1 would be exact, simply ensuring the BC on q_+ would yield a perfect shortcut and the energies $E_{n\pm}$ in eq. 3.11 would be an exact description. This would hold no matter the initial energy in the normal modes, allowing us to find a timing at which the motion has swapped from one ion to the other. Since the dynamical normal mode approximation neglects higher order Coulomb terms and terms due to the quartic potential part as described in Appendix A, this result starts breaking down as faster run-times are approached. For the best results, we thus optimise ρ_+ to give a near-perfect shortcut for cold runs, hoping that this still holds approximately for small initial excitations. Optimising on the hot runs instead would lead to the result being dependent on the chosen initial energy.

3.3.1 Numerical prerequisites

Throughout this thesis, the final energies of the full Hamiltonian are simulated by solving the classical equations of motion

$$m\ddot{x}_i = -\frac{\partial V_{\text{tot}}}{\partial x_i} \quad (3.24)$$

where the potential $V(x_1, x_2, t)$ is given by eq. 3.2 and the trajectory $\{\alpha(t), \beta(t)\}$ is acquired from any choice of $\{m, d_{\text{out}}, d_{\text{in}}, \beta_{\text{max}}, \rho_+\}$ by the inverse engineering algorithm stated in section 3.2. Let the final energies of the two ions, computed with the full Hamiltonian, be denoted by $E_{f,i}$ for the information ion and $E_{f,c}$ for the coolant ion. The subscript "i" denotes the information ion, "c" the coolant ion and "f" the final time. The total energy is then $E_f = E_{f,i} + E_{f,c}$. These can be measured by analysing the state of the ions (potential and kinetic energy) at the final time when simulating eq. 3.24. Analogously, the initial energies are given by $E_{0,i}$, $E_{0,c}$. In calculating these values, quantum effects such as squeezing are expected to play a negligible role at the used run-times as was found in [40, 39, 41, 12]. However, it might still prove beneficial to design the ion curvature to be constant instead of the CoM-mode frequency Ω_- in subsection 3.2.2 to minimise squeezing.

Note that all energies are stated in terms of the energy of a single motional quantum $\bar{n} = \hbar\omega_0$ of the ions at their initial frequency $\omega_0 = \omega_1(t_0) = \omega_2(t_0)$.

3.3.2 Performance of the parameter-free scheme

To obtain a baseline for the performance of the constructed STA scheme, we first determine the time scale at which even a non-optimised ρ_+ performs well. When operating at long enough run-times, a cold run of a cooling scheme will behave almost adiabatically and return ground state ions. As run-times are decreased, anharmonicities and the non-optimised auxiliary function q_+ will lead to increasing excitations after a cold run.

To find the separation between the two different regimes, we first use the parameter-free polynomial eq. 3.22 for ρ_+ , thus disregarding the fact that the adiabatic shortcut is not complete until the BC on q_+ are satisfied. We use the default constraint set A from Table 3.1 and plot in Fig. 3.4 the total final energy E_f after cold runs, while sweeping the run-time t_f and the inner distance d_{in} .

To determine a minimal run-time T_{min} above which the transport scheme works well, we define the excitations to become negligible below a level of $\bar{n} = 0.1$. The upper part of Fig. 3.4 shows the final excitations E_f , stated in $\bar{n}$, for an inner distance of $1.25d_c$. Note that the energy decreases exponentially, while also showing periodic minima. The logarithmic excitations are then fitted with the function $f(t) = \log[a \exp(-bt) \sin^2(ct + d)]$. The non-periodic part $\log[a \exp\{-bt\}]$ can then be interpreted as an envelope functions, as shown in the upper part of Fig. 3.4. The intersection time of this envelope with an energy level of $\bar{n} = 0.1$ is then used as T_{min} .

In the bottom part of Fig. 3.4, the inner distance d_{in} is varied from $1 \cdot d_c = 14 \mu\text{m}$ to $1.5 \cdot d_c = 21 \mu\text{m}$ and the final energy is shown by the colour. Note that the periodic minima are visible as valleys of minimal excitations across d_{in} . For each inner distance, the determination of T_{min} is repeated and these

3.3. Optimising the cooling motion for minimal excitations

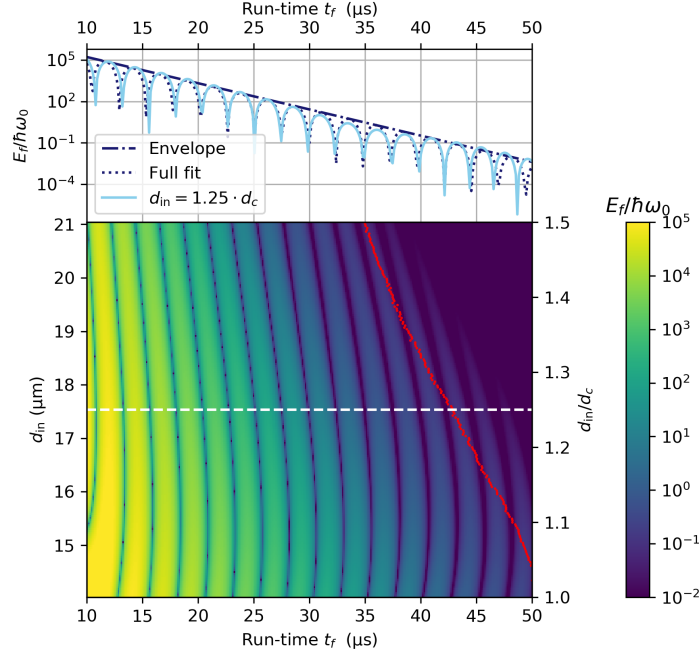


Figure 3.4: Final excitations E_f of cold runs vs. run-time t_f for an inner distance of $1.25d_c$ (upper part) and on a grid of run-times and minimal distances (lower part). The determined minimal run-times $T_{\min}$ are marked by red dots.

times are marked by a red dot. The resulting red line represents the “speed limit” until which this non-optimised transport scheme results in low enough excitations. Note that larger inner distances allow shorter run-times. This is due to the ions being accelerated less when the cooling motion extends over a shorter distance and thus produces less excitations.

Note that the initial ion frequency $\omega_0 = \omega_1(t_0) =$ depends on d_{in} due to the inverse engineering procedure and is between $2\pi \times 0.439 \text{ MHz}$ and $2\pi \times 0.532 \text{ MHz}$.

We thus conclude from Fig. 3.4 that to access run-times below the red line in Fig. 3.4, it becomes necessary to construct proper shortcuts, a task that will be accomplished in the next section by optimising the shape of ρ_+ .

3.3.3 Comparison of optimisation methods for ρ_+

To generate a near-perfect shortcut in the proposed approach, a number of free parameters in ρ_+ need to be numerically optimised as demonstrated in [12]. Assuming that the dynamical normal mode approximation holds, minimising the energy $E_{n=0,+}$ in eq. 3.11 is a natural way of making sure ρ_+ satisfies the BC on q_+ . Note that the ground state $n = 0$ is chosen here to reflect the fact that the cooling motion should not excite cold ions. As the

dynamical normal mode approximation eq. 3.8 is not exact and the approximate energies $E_{n\pm}$ do not provide a complete description, this method will yield solutions that excite the ions on cold runs when evaluated with the full Hamiltonian eq. 3.2. Ideally, the exact energy E_f is minimised instead (exact method), which will not necessarily lead to satisfied BC for q_+ , but to a shortcut for the exact system instead.

Both methods are applied and compared in Fig. 3.5. The polynomial eq. 3.23 with $a_7 = 0$ is used as an Ansatz for ρ_+ , leaving the single free parameter c to be optimised, for which the Nelder-Mead algorithm in SciPy's "optimize.minimize"³ routine is used. The default physical constraint set A (Table 3.1) is used.

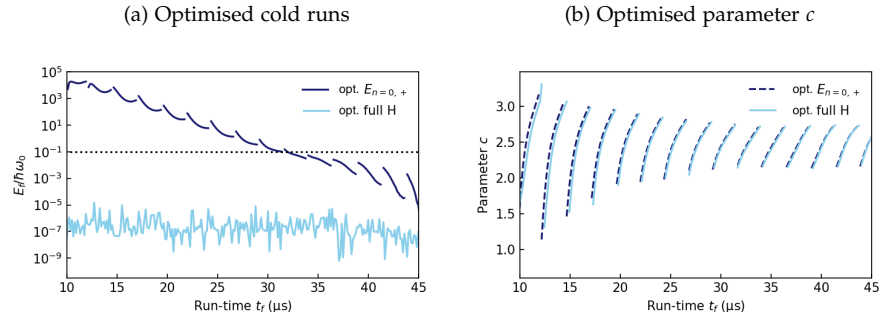


Figure 3.5: Comparison of optimisation methods to obtain a shortcut to adiabaticity. Shown are the results of minimising the approximate energy $E_{n=0,+}$ (dashed lines) and the full Hamiltonian (solid lines) for the default parameter set A. Dotted lines mark an energy level of $\bar{n} = 0.1$. (a) Excitation E_f after a cold run depending on the run-time. (b) Values of the optimised free parameter c .

Fig. 3.5a shows the exact final excitations E_f after the parameter c was optimised for each run-time t_f . The method where the approximated energy E_{n+} was optimised gives a much worse result than the exact method, which consistently yields negligible excitations. When setting the energy level below which excitations are to be considered negligible to $\bar{n} = 0.1$ (as shown in 3.5a), optimising $E_{n=0,+}$ leads to a minimal run-time of around $32 \mu s$, while the exact method shows no minimal time at all in the considered range. Note that the fluctuations of E_f for the exact method are due to the results dropping below the selected target accuracy of the optimisation.

A near-perfect shortcut is then possible if one is willing to expend the computational power on optimising the exact Hamiltonian. However numerical cost might not be an issue when considering that the approach in [12] optimised the approximate energy $E_{n=0,+}$ with up to three free parameters while still

³As the free parameter c is defined to be the curvature of ρ_+ at $t = t_f/2$, the initial values are chosen to be the curvature of the parameter-free Ansatz eq. 3.22, which is $c = 2.38$. This also explains that the minimisation algorithm jumps between valleys in Fig. 3.6 when departing too far from this initial value. No initial simplex is used.

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not obtaining results comparable to the exact minimisation⁴. This realisation makes improving the HO description by calculating perturbations to $E_{n\pm}$ as attempted in Appendix A and [12] seem especially futile.

The optimised parameters c for both methods, depending on run-time t_f , are shown in 3.5b. Despite giving vastly differing final energies, the two methods arrive at closely related optimal parameters. Also the optimal c exhibit periodic discontinuities. These results can be better understood when considering the grid plots of run-times t_f and parameter values c in Fig. 3.6.

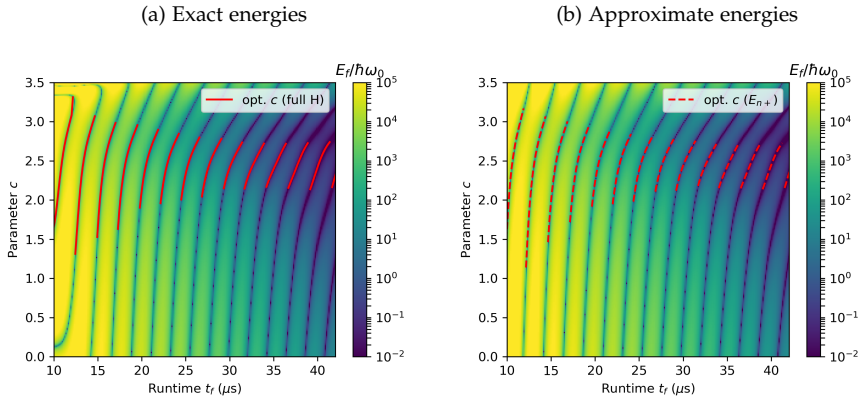


Figure 3.6: Final excitations of cold runs on a grid of run-times and the free parameter c for ρ_+ . Overlaid are the optimised values of c as in Fig. 3.5. The target values are the same as in Fig. 3.5. (a) Grid of exact final excitations E_f after cold runs. (b) Grid of exact approximate final excitations E_{n+} after cold runs.

Shown are both the exact and approximate final excitations E_f and $E_{n=0,+}$ after cold runs on a grid of run-times and values for c , otherwise using the same target value set as in Fig. 3.5. There are periodic “valleys” of minima and the overlaid values of c from Fig. 3.5b make clear that the minimisation algorithm simply follows these. This plot also assures us that the approximation E_{n+} gives very similar minima structures as the full calculation. The difference, most easily visible at low run-times, leads to the discrepancy between minimising E_f and $E_{n=0,+}$. As the excitations become exponentially larger at short run-times, even a small difference in c leads to a large energy difference.

Note that it is not feasible to stay in a single valley of minima. For negative c , the scheme would transiently bring the ions closer together than d_{in} and for too large c , the ions are initially moved to distances larger than d_{out} , hence the optimisation jumps between valleys.

Optimising the cooling motion also allows the first observation of a full swap of motional energy. Fig. 3.7 shows the final energy of the information ion

⁴Using the code written for this thesis, optimising the approximate energies was only faster by roughly a factor of two.

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$E_{f,i}$ of a hot run where the initial excitation of the information ion⁵ was $\bar{n} = 10$. The same target values and optimised parameters c as in Fig. 3.5 are used. For run-times around $15\ \mu\text{s}$ to $20\ \mu\text{s}$, the energy $E_{f,i}$ of the initially hot ion repeatedly decreases below the $\bar{n} = 0.1$, yielding near-perfect motional exchange. For run-times around two times longer, the energy is exchanged back again and the final energy approaches the initial $\bar{n} = 10$.

Note that no cooling effect could be observed when optimising the cooling motion with the approximate method, as E_f reaches levels above $\bar{n} = 100$ in the targeted time range in Fig. 3.5.

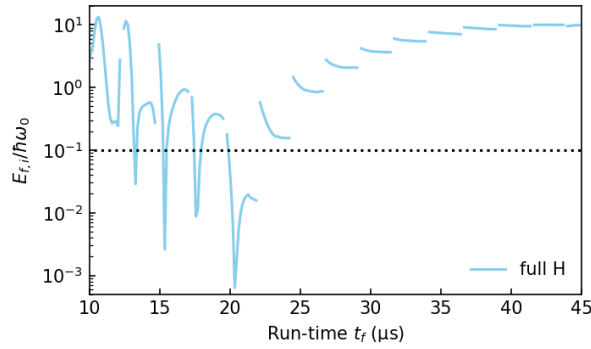


Figure 3.7: Final energy of the information ion after a hot run depending on the run-time t_f . The target value set and the optimised parameters c (using the exact method) as in Fig. 3.5 are used.

The parameter c influences the distance function $d(t)$ and thus the exchange frequency. Due to the optimal c being discontinuous in time, the final energy $E_{f,i}$ also shows jumps and multiple minima below $\bar{n} = 0.1$ can be observed.

In optimising on cold runs, we have assumed that the constructed shortcut holds for a range of non-zero excitations as well. This assumption is shown to start breaking down at the low run-time end of Fig. 3.7, where the final energy of the ion rises above the initial level of $\bar{n} = 10$. If even shorter run-times are to be achieved, some more work would be needed to ensure a valid shortcut at interesting energy levels. However due to the robustness considerations that are to follow, this run-time regime is not of interest in this work.

We have demonstrated that the cooling motion can be optimised to yield no excitations even at run-times where the dynamical normal mode approximation breaks down. This result may however still be useless if it is very sensitive to experimental inaccuracies. The next section develops a way to make this STA scheme more robust to such perturbations.

⁵The value of $\bar{n} = 10$ is chosen to be the same order of magnitude as the Doppler limit, which is $\bar{n} = 6$ for Calcium and $\bar{n} = 3$ for Beryllium [15].

3.4 Robustness to potential tilts

STA schemes can be optimised to be as insensitive to experimental imperfections as possible, as has been worked out for many cases in [23, 24, 25, 26, 18, 27, 28, 29]. A common source of errors in trapped-ion QIP, especially in splitting experiments [39, 10] is a linear tilt in the potential, for example due to stray charges in the trap or inaccuracies in the applied trap voltages, leading to a perturbed potential

$$\tilde{V}_{el}(t, x) = \gamma \tilde{x} + \alpha(t) \tilde{x}^2 + \beta(t) \tilde{x}^4, \quad (3.25)$$

where a linear term γ was added. Requiring robustness of the cooling motion against a linear term also seems sensible when regarding the linear term as the first order expansion of a general perturbation potential. This can be done by redoing the STA derivations given in section 3.1 and section 3.2 with the perturbed potential. This will lead to perturbed energies $\tilde{E}_{n\pm}$ which can then be used to numerically optimise the robustness, much in the same way as excitations were minimised in the previous section. This approach is inspired by Lu [25, 18].

Note that as the dynamical normal mode description of the two ion system is shown to break down at short run-times in subsection 3.3.3, we expect this approach to be limited in the same way.

Since such a linear perturbation shifts the ion motional frequencies, the resonance condition needed for motional exchange will not be perfectly fulfilled anymore. This effect is dealt with in section 4.2 as it is irrelevant to the cooling transport under consideration in this chapter.

3.4.1 Perturbative condition for error stability

The derivations of dynamical normal modes and the inverse engineering procedure are reiterated for a constant linear perturbation γ as in eq. 3.25 and only first-order effects of γ are included. This will yield perturbed normal-mode Hamiltonians, perturbed auxiliary ODEs and a way to minimise the influence of γ .

Let variables superposed with a tilde be those of the perturbed scheme, while the notation for unperturbed variables is carried over from section 3.1 and section 3.2.

The equilibrium positions $\tilde{x}_i^{(0)}$ are then given by $\frac{\partial \tilde{V}}{\partial \tilde{x}_i} = \gamma + 2\alpha \tilde{x}_i + 4\beta \tilde{x}_i^3 + \frac{(-1)^i C_C}{\tilde{d}^2}$ and we introduce the asymmetric position shift $\tilde{s}$ to denote $\tilde{x}_1^{(0)} = \tilde{s} - \frac{\tilde{d}}{2}$ and $\tilde{x}_2^{(0)} = \tilde{s} + \frac{\tilde{d}}{2}$ as demonstrated in Fig. 3.8. The assumption for a first-order treatment to hold is then that the shift be much smaller than the equilibrium distance: $\tilde{s} \ll \tilde{d}$.

When only considering linear terms in $\tilde{s}$, rewriting the equilibrium conditions yields

$$\tilde{d} \approx d \quad (3.26)$$

3. DESIGNING THE COOLING MOTION FOR TWO IONS OF EQUAL MASS

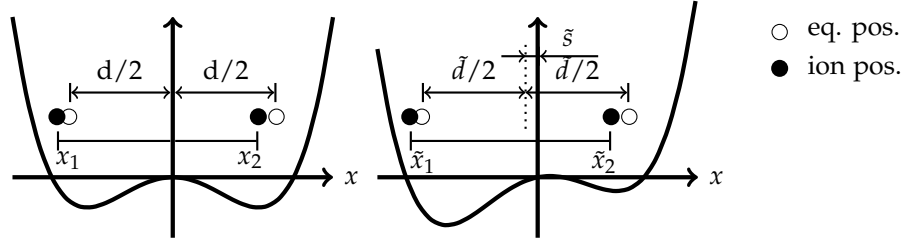


Figure 3.8: Schematic depiction of position and equilibrium coordinates for two ions trapped in a quartic double-well potential (left) and in a linearly perturbed potential eq. 3.25 (right). Note that the Coulomb potential has been neglected from the potential shape.

and

$$\tilde{s} \approx -\frac{\gamma}{2\alpha + 3\beta d^2} = -\frac{\gamma}{m\Omega_-^2}. \quad (3.27)$$

A dimensionless perturbation parameter η can then be defined as

$$\eta \equiv \frac{\tilde{s}}{d_{in}} = \frac{\gamma}{m\Omega_-^2 d_{in}}, \quad (3.28)$$

turning the linear approximation condition $\tilde{s} \ll \tilde{d}$ into

$$\eta = \frac{\tilde{s}}{d_{in}} \ll 1, \quad (3.29)$$

where d_{in} was chosen since it is the minimal distance between ions and thus the worst case.

The perturbed mass-weighted Hessian $\tilde{K}$ is then

$$\begin{aligned} \tilde{K} &= \frac{1}{m} \begin{pmatrix} 2\alpha + 12\beta (\tilde{x}_1^{(0)})^2 + \frac{2C_C}{\tilde{d}^3} & -\frac{2C_C}{\tilde{d}^3} \\ -\frac{2C_C}{\tilde{d}^3} & 2\alpha + 12\beta (\tilde{x}_2^{(0)})^2 + \frac{2C_C}{\tilde{d}^3} \end{pmatrix} \\ &\approx \frac{1}{m} \begin{pmatrix} 2\alpha + 3\beta d^2 + \frac{2C_C}{d^3} - 12\beta d\tilde{s} & -\frac{2C_C}{d^3} \\ -\frac{2C_C}{d^3} & 2\alpha + 3\beta d^2 + \frac{2C_C}{d^3} + 12\beta d\tilde{s} \end{pmatrix}. \end{aligned} \quad (3.30)$$

Diagonalising this, the normal mode frequencies stay the same to first order

$$\tilde{\Omega}_{\pm} = \Omega_{\pm} \quad (3.31)$$

but the eigenvectors change to

$$\begin{aligned}\tilde{v}_- &\approx \left(1 + \frac{6}{C_C} \beta d^4 \tilde{s}\right) \\ \tilde{v}_+ &\approx \left(-1 + \frac{6}{C_C} \beta d^4 \tilde{s}\right),\end{aligned}\tag{3.32}$$

corresponding to an angle $\tilde{\theta}$ given by $\text{atan}\left(1 + \underbrace{\frac{6}{C_C} \beta d^4 \tilde{s}}_{2\text{III}}\right) \approx \frac{\pi}{4} + \text{III}.$

The first coordinate change eq. 3.6

$$\begin{aligned}\begin{pmatrix} \tilde{X}'_- \\ \tilde{X}'_+ \end{pmatrix} &= \tilde{A}(t) \begin{pmatrix} \tilde{x}_1 - (\tilde{s} - \frac{d}{2}) \\ \tilde{x}_2 - (\tilde{s} + \frac{d}{2}) \end{pmatrix} \\ \begin{pmatrix} \tilde{P}'_- \\ \tilde{P}'_+ \end{pmatrix} &= (\tilde{A}^T)^{-1}(t) \begin{pmatrix} \tilde{p}_1 \\ \tilde{p}_2 \end{pmatrix}\end{aligned}\tag{3.33}$$

is then given by $\tilde{A}(t)$

$$\tilde{A}(t) \approx \sqrt{\frac{m}{2}} \begin{pmatrix} 1 - \text{III} & 1 + \text{III} \\ -(1 + \text{III}) & 1 - \text{III} \end{pmatrix}\tag{3.34}$$

The second and final coordinate transform as in eq. 3.7 is given by

$$\begin{aligned}\begin{pmatrix} \tilde{X}_- \\ \tilde{X}_+ \end{pmatrix} &= \begin{pmatrix} \tilde{X}'_- \\ \tilde{X}'_+ \end{pmatrix} \\ \begin{pmatrix} \tilde{P}_- \\ \tilde{P}_+ \end{pmatrix} &= \begin{pmatrix} \tilde{P}'_- - \tilde{P}_{0,-} \\ \tilde{P}'_+ - \tilde{P}_{0,+} \end{pmatrix} \\ \begin{pmatrix} \tilde{P}_{0,-} \\ \tilde{P}_{0,+} \end{pmatrix} &\approx \sqrt{\frac{m}{2}} \begin{pmatrix} 1 - \text{III} & 1 + \text{III} \\ -(1 + \text{III}) & 1 - \text{III} \end{pmatrix} \begin{pmatrix} \dot{\tilde{s}} - \frac{\dot{d}}{2} \\ \dot{\tilde{s}} + \frac{\dot{d}}{2} \end{pmatrix} \\ &= \sqrt{\frac{m}{2^3}} \begin{pmatrix} \dot{d}\text{III} \\ \dot{d} \end{pmatrix}\end{aligned}\tag{3.35}$$

when considering that $\dot{\tilde{s}} = 0$ due to Ω_- being chosen constant.

The intermediate normal mode Hamiltonians then become according to eq. 2.17

$$\tilde{H}_{\text{2HO}} = \sum_{i \in \{+, -\}} \frac{\tilde{P}_i^2}{2} + \frac{1}{2} \tilde{\Omega}_i^2(t) \left(\tilde{X}_i + \frac{\dot{\tilde{P}}_{0,i}(t)}{\tilde{\Omega}_i^2(t)} \right)^2 - \dot{\tilde{\theta}} (\tilde{X}'_+ \tilde{P}'_- - \tilde{X}'_- \tilde{P}'_+).\tag{3.36}$$

Note that due to $\text{III} \neq 0$, the eigenvectors and the angle $\tilde{\theta}$ are not constant, leading to mode coupling with the term in $\ddot{\theta}$. A part of this term can still be incorporated into the harmonic oscillator.

Upon calculating $\tilde{X}'_+ \tilde{P}'_- - \tilde{X}_- \tilde{P}_+ = (\tilde{X}_+ \tilde{P}_{0,-} - \tilde{X}_2 \tilde{P}_{0,+}) + (\tilde{X}_+ \tilde{P}_- - \tilde{X}_- \tilde{P}_+)$, the terms containing $\tilde{P}_{0,-}$ can be added to the harmonic oscillator by completing the square. This requires adding a purely time-dependent term with no physical significance. The remaining coupling term $H_c = \dot{\tilde{\theta}} (\tilde{X}_+ \tilde{P}_- - \tilde{X}_- \tilde{P}_+)$ is left away from now on, as STA theory cannot deal with terms of this form. It is thus to be expected that after optimising robustness, this will be the leading source of remaining perturbation effects.

After taking these steps, the final HO Hamiltonian turns out as

$$\tilde{H}_{2\text{HO}} = \tilde{H}_{\text{HO}}^{(+)} + \tilde{H}_{\text{HO}}^{(-)} = \sum_{i \in \{+, -\}} \frac{\tilde{P}_i^2}{2} + \frac{1}{2} \tilde{\Omega}_i^2(t) \left(\tilde{X}_i + \frac{\dot{\tilde{P}}_{0,i}(t) + i\dot{\tilde{\theta}} \tilde{P}_{0,-i}}{\tilde{\Omega}_i^2(t)} \right)^2. \quad (3.37)$$

After inserting eq. 3.35, realising that $\dot{\tilde{\theta}} = \text{III}$ and leaving away terms quadratic in η , the $\tilde{H}_{\pm}$ turn out to be

$$\begin{aligned} \tilde{H}_{\text{HO}}^{(-)} &= \frac{\tilde{P}_-^2}{2} + \frac{1}{2} \tilde{\Omega}_-^2(t) \left(\tilde{X}_- + \sqrt{\frac{m}{2}} \frac{\ddot{d}}{\tilde{\Omega}_-^2(t)} \text{III} \right)^2 \\ \tilde{H}_{\text{HO}}^{(+)} &= \frac{\tilde{P}_+^2}{2} + \frac{1}{2} \tilde{\Omega}_+^2(t) \left(\tilde{X}_+ + \sqrt{\frac{m}{2}} \frac{\ddot{d}}{\tilde{\Omega}_+^2(t)} \right)^2 \end{aligned} \quad (3.38)$$

The Hamiltonian $\tilde{H}_{\text{HO}}^{(+)} = H_{\text{HO}}^{(+)}$ has remained unchanged from the unperturbed results, while $\tilde{H}_{\text{HO}}^{(-)}$ now has a moving mode centre as well (compare eq. 3.8), invalidating the result $q_- = 0$. Finding the energies of these Hamiltonians leads to a way of minimising the perturbative effects and finding optimally robust schemes.

The auxiliary ODE for q_- is perturbed as well and turns out to be $\ddot{q}_- + \tilde{\Omega}_-^2 \tilde{q}_- = -\sqrt{\frac{m}{2}} \ddot{d} \text{III}$. This then yields the energy $\tilde{E}_{n-}$, which changes from E_{n-} to

$$\begin{aligned} \tilde{E}_{n-} &= \frac{(2n+1)\hbar}{4\tilde{\Omega}_{0-}} \left(\dot{\tilde{\rho}}_-^2 + \tilde{\Omega}_-^2 \tilde{\rho}_-^2 + \frac{\tilde{\Omega}_{0-}^2}{\tilde{\rho}_-^2} \right) \\ &\quad + \frac{1}{2} \dot{\tilde{q}}_-^2 + \frac{1}{2} \tilde{\Omega}_-^2 \left(\tilde{q}_- + \frac{\sqrt{m} \ddot{d}}{\sqrt{2} \tilde{\Omega}_-^2} \text{III} \right)^2. \end{aligned} \quad (3.39)$$

Note that as $H_{\text{HO}}^{(+)}$ remains unperturbed, the energies E_{n+} also don't change.

As desired, this yields a way to obtain optimally stable solutions (in a first-order picture) by minimising $\tilde{E}_{n,-}$ together with the unperturbed energy $E_{n,+}$, using the additional free parameter a_7 in ρ_+ .

3.4.2 Optimal robustness in a numerical example

To demonstrate the usefulness of the robustness condition derived just before, we once more pick our default example given by the physical constraints Table 3.1, making the example realistic for the HOA2 trap. The results of optimising the perturbed energy $\tilde{E}_{n,-}$ are to be compared to the non-robust results from section 3.3.

Similar to subsection 3.3.3, the two-parameter polynomial eq. 3.23 is chosen as an Ansatz for ρ_+ , but this time with both free parameters c and a_7 optimised. This allows the simultaneous minimisation of both the unperturbed excitations $E_{n=0,+}$ and the error sensitivity term $\tilde{E}_{n=0,-}$, which is done by choosing the cost function

$$\text{Perturbative cost} = E_{n=0,+} + \tilde{E}_{n=0,-} \Big|_{\eta=0.03} \quad (3.40)$$

The value of $\eta = 0.03$ was chosen since it corresponds to a reasonable tilt value of about 2.5 V m^{-1} (compare [10], where a potential tilt could be calibrated in steps of 0.1 V m^{-1}). Again we want to optimise the cold runs first, expecting the hot runs to work equally well for small enough energy levels. The same Nelder-Mead minimum search algorithm⁶ is then used to find optimal values of $\{c, a_7\}$.

To see whether using the full Hamiltonian instead of the dynamical normal mode approximation leads to similar discrepancies as in subsection 3.3.3, a method using exact energies is also applied for comparison. The cost function is

$$\text{Exact cost} = E_f \Big|_{\eta=0} + E_f \Big|_{\eta=0.03} + E_f \Big|_{\eta=-0.03} \quad (3.41)$$

thus minimising the final excitations for ideal potentials together with the exact excitations for two values of η , thus optimising for a flat response to a perturbation. As the harmonic oscillator approximation yielding $E_{n\pm}$ is shown to break down for short run-times in Fig. 3.5 but the exact minimisation does not, it would be expected that this exact robustness method also yields better results at short run-times.

The results are displayed in Fig. 3.9, showing the exact energies E_f on a grid of tilt parameters η and run-times t_f . The E_f are again normalised by the single phonon energy $\hbar\omega_0$, where ω_0 is the initial ion frequency as in subsection 3.3.2. Overlaid over the plots are contour lines at a level of $\bar{n} = 0.1$, marking the areas where excitations become negligible and the scheme is

⁶The values of $\{c, a_7\}$ are optimised for a sequence of run-times t_f . For each run-time, the results of the previous optimisation are used as initial values. For the first considered run-time t_f , a grid of different initial values $\{c, a_7\}$ is tested and the optimisation algorithm is shown to always converge to the same optimum.

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thus usable. To compare with the non-robust schemes of section 3.3, Fig. 3.9a shows the results of the single-parameter optimisation in subsection 3.3.3. The two robustness optimisation methods are shown in Fig. 3.9b (perturbative method using $\tilde{E}_{n-}$) and Fig. 3.9c which uses the exact method. Note that the perturbation is also shown in terms of the potential tilt γ , which is found from η using eq. 3.28.

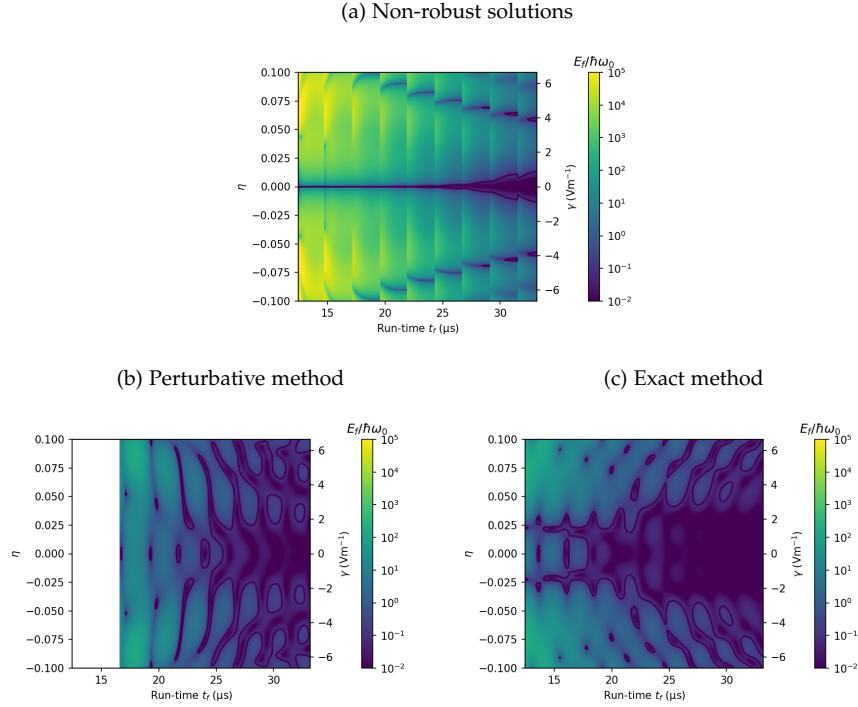


Figure 3.9: Comparison of error stabilisation methods in a grid of run-times and tilt parameters η . (a) Robustness grid for the non-robust results from section 3.3. (b) Robustness grid for the approximate method. (c) Robustness grid for the exact method.

The comparison between the non-robust and robust methods in Fig. 3.9 shows a clear improvement for the run-times considered. Even though the non-robust solutions in Fig. 3.9a show a nearly perfect shortcut for unperturbed potentials, this breaks down on much smaller scales of the perturbation parameter η than in both robust methods. However, the two robustness methods do not produce negligible excitations at all run-times. The perturbative method decreases below $\bar{n} = 0.1$ at roughly $25 \mu s$ (12.5 motional cycles), while the exact method does so slightly earlier at roughly $18 \mu s$ (9 motional cycles). Another interesting feature of both robust methods is the existence of vertical stripes with low excitations, marking run-times where the scheme is ultra-robust even against strong perturbations.

The fact that the exact method works well despite the simple choice of its cost function is encouraging, as it is plausible that it can be improved in similarly

simple ways. One could for example optimise more free parameters and choose more than two values of η in eq. 3.41, such that the robust range is increased. One could also change the cost function to include higher order perturbations.

Thus we conclude that the presented robustness optimisation methods are useful tools to make this STA scheme able to withstand experimental imperfections, even at the cost of introducing a lower bound to the achievable run-times. Having gained sufficient control over the cooling motion to perform it in below 10 motional without final excitations, we apply this to find timings where the motional states are swapped completely.

Exchange cooling with two trapped ions of equal mass

After gaining the ability to generate a near-perfect shortcut for ground-state ions and stabilise it against experimental imperfections, we now seek to use this to find cooling solutions. To this end, the exact robustness method of subsection 3.4.2 is applied to optimise the developed STA scheme as in the previous chapter and these optimised schemes are then used to find the right timing for a complete exchange of motional energy.

As suggested in the discussion in section 3.4, a linear potential tilt can shift the ion frequencies ω_i to be out of resonance. To predict the width of this effect and thus the necessary experimental accuracy, the resonance behaviour of the cooling solutions is discussed in this chapter.

The exchange frequency Ω_{ex} from eq. 1.6 depends by an inverse cubic power on the distance between the ions. It is therefore expected that reducing the inner distance d_{in} should generate faster aggregated exchange. As the ions should not be merged into a single well, the closest distance d_{in} is solely dependent on the critical distance d_c and thus the maximal quartic confinement β_{max} . It is therefore useful to examine how the cooling speed scales when changing this parameter, which is done in this chapter.

4.1 Cooling solutions

We demonstrate the existence and properties of cooling solutions using the usual example given in Table 3.1, but the inner distance d_{in} is varied from $1.15d_c$ to $1.35d_c$. As in Fig. 3.7, the initial energy of the information ion is chosen to be $\bar{n} = 10$.

The resulting final energy $E_{f,i}$ of the initially hot information ion depending on the run-time t_f is shown in Fig. 4.1. Note that the ions in the classical simulation were initially started at their equilibrium position, with all their energy thus being kinetic.

As expected, the resulting curves show that the hot ion reaches a minimal energy below $\bar{n} = 0.1$ at increasingly short run-times as d_{in} is decreased. At the shortest run-times plotted, the adiabatic shortcut breaks down in a similar

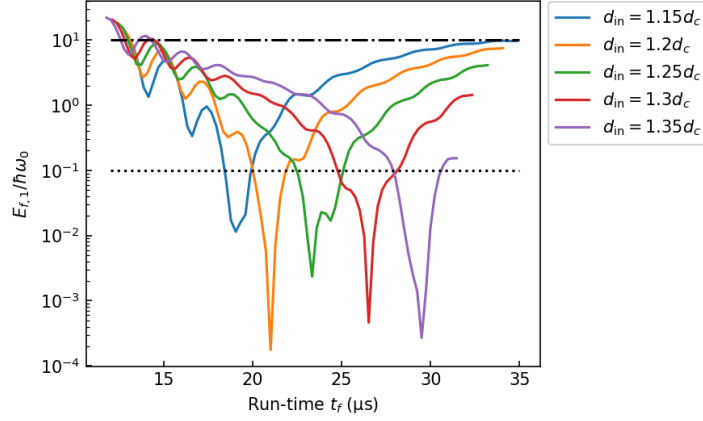


Figure 4.1: Final energies of hot runs with $\bar{n} = 10$, parametrised by the inner distance d_{in} .

fashion as in Fig. 3.7, as the procedure returns the ion with an increased energy.

Some further properties of the cooling minima shown in Fig. 4.1 are of interest, such as dependence on the initial motional phase, dependence of the final energy on the initial energy and robustness towards potential tilts. To demonstrate that these are not issues to worry about, we pick the example at $d_{\text{in}} = 1.25d_c$ from Fig. 4.1 which yields a cooling solution at $23.3\mu\text{s}$ and examine the described properties in Fig. 4.2.

As the robustness optimisation always starts with ions at rest, the influence of the initial motional phase on the exchange when one ion is excited is of interest. Ideally, there is no dependence at all, but since the motional phase slightly influences the ion distance at the start of the scheme, this is not expected to be the case in practice.

The motional phase ϕ is defined to be zero when the ion is at its equilibrium position, with all energy in the motion. The case $\phi = \pi/2$ is defined as the ion being at rest with only potential energy. The scheme is then run at motional phases 0 to 2π to determine the influence on the final energy. The result is shown in 4.2a. There is a periodic dependence of the final energy on the initial phase, but on a negligible scale below $\bar{n} = 0.1$.

In fig. 4.2b, the initial energy level was scanned over a range of $\bar{n} = 0$ to $\bar{n} = 100$. As the optimised parameters do not give a perfect shortcut for all $\bar{n}$, the final energy is lowest for $\bar{n} = 0$, only to then increase with rising initial energy. However, the final energy stays well in the negligible range, showing no signs of the solution breaking down.

As the solutions in Fig. 4.1 were optimised using the exact robustness method, the stability against potential tilts is shown in 4.2c. As desired, the excitations stay below $\bar{n} = 0.1$ for small perturbations η . In this example, the scheme is robust in a range of $\eta = -0.035$ to $\eta = 0.035$. Note that the minima

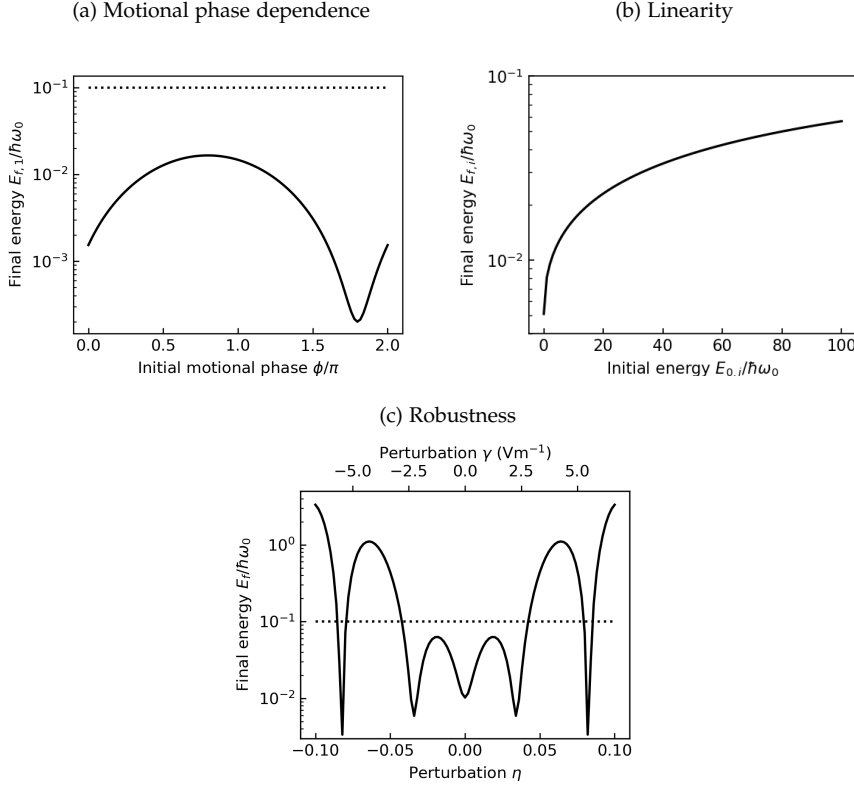


Figure 4.2: (a) Motional phase dependence, (b) initial energy dependence (c) and robustness behaviour plots for the example cooling solution found at $23.3 \mu\text{s}$ for $d_{\text{in}} = 1.25d_c$ in Fig. 4.1.

at $\eta = \pm 0.03$ are due to the design of the cost function in subsection 3.4.2, where these values of η were chosen.

We have thus demonstrated the existence of robust cooling solutions at around $20 \mu\text{s}$, corresponding to roughly 10 motional cycles, using parameters of a realistic trap and while keeping the ions in separate wells.

4.2 Exchange resonance condition

As noted in chapter 1, the motional exchange is a resonance effect with respect to the motional ion frequencies. Since a tilted potential shifts the ions frequencies, it is to be expected that the perturbation η does not only destroy the adiabatic shortcut when simply transporting the two ions as analysed in section 3.4, but also affects the exchange mechanism itself. This effect determines the needed experimental accuracy to perform this cooling scheme successfully. Note that contrary to the robustness of the cooling motion to such potential tilts, no shaping of ρ_+ can mitigate this off-resonance effect.

Using the results from section 3.4, we now go on to roughly predict the width of this resonance.

4.2.1 Lorentzian approximation

As the exchange interaction is a resonance effect, it is reasonable to assume that the final energy of the initially hot ion has a Lorentzian shape with respect to the perturbation parameter η .

Let $\omega = \omega_1 = \omega_2$ be the unperturbed motional frequencies of the two ions as in eq. 3.14 and $\{\omega_{1\eta}, \omega_{2\eta}\}$ the values after applying some linear perturbation η . The ion with index 1 is understood to be the information ion, whereas the index 2 denotes the coolant ion. The unperturbed ion frequency at t_0 is denoted by ω_0 .

The Lorentzian shape of the final energy can then be written as

$$E_{f,i} = E_{0,i} \left(1 - \frac{1}{1 + \left(k \frac{\delta\omega}{\Omega_{\text{ex}}} \right)^2} \right), \quad (4.1)$$

where $E_{0,i}$ is the initial energy of the information ion, $\delta\omega = \omega_{2\eta} - \omega_{1\eta}$ is the ion frequency mismatch due to a perturbation and k is a constant factor that is to be determined. We want to rewrite $\frac{\delta\omega}{\Omega_{\text{ex}}}$ in terms of η and the physical constraints β_{max} , d_{in} and d_{out} , allowing us to predict the resonance width independently of the precise trajectory $d(t)$. For this, two crude approximations are taken: (i) The term in $\frac{C_C}{d^3}$ in the ion frequency eq. 3.14 is neglected, as it only contributes a few percent to the total frequency. (ii) The motional exchange only takes place when the ions are closest together, leading to $d = d_{\text{in}}$.

Together with eq. 3.28 and the perturbed mass-weighted Hessian eq. 3.30, this allows to write the perturbed ion frequencies as

$$m\omega_{i\eta}^2 \approx 2\beta d^2 + \frac{4C_C}{d^3} \mp 12\beta d\tilde{s} \approx 2\beta d_{\text{in}}^2 \mp 12\beta d_{\text{in}}^2 \eta = \underbrace{2\beta d_{\text{in}}^2}_{\approx m\omega_0^2} [1 \mp 6\eta] \quad (4.2)$$

$$\omega_{i\eta} \approx \omega_0 \sqrt{1 \mp 6\eta} \approx \omega_0 (1 \mp 3\eta),$$

where $i = \{1, 2\}$.

The frequency mismatch $\delta\omega$ is then given by

$$\delta\omega = \omega_{2\eta} - \omega_{1\eta} = 6\eta\omega_0 \quad (4.3)$$

and the Lorentzian becomes, again using the approximations described above:

$$E_{f,i} = E_{0,i} \left(1 - \frac{1}{1 + \left(k \frac{\delta\omega}{\Omega_{\text{ex}}} \right)^2} \right) \approx E_{i,1} \left(1 - \frac{1}{1 + \left(\eta \frac{6km\omega_0^2 d_{\text{in}}^3}{C_C} \right)^2} \right). \quad (4.4)$$

This result allows to predict the maximal perturbation η such that the final energy after cooling is still below a certain threshold.

The resonance width $\eta_{1/2}$ with respect to the perturbation parameter η , given by the Lorentzian half-width (HWHM), is

$$\eta_{1/2} = \frac{C_C}{6km\omega_0^2 d_{\text{in}}^3}. \quad (4.5)$$

Note that the width increases with decreasing d_{in} . This is useful as it means the objectives of fast cooling and having a broad resonance are compatible with each other. In other words, for a given trap strength, the most insensitive configuration against potential tilts is also the fastest cooling solution.

As an example of this resonance effect, Fig. 4.3 recreates the robustness plots of Fig. 3.9, but this time for hot runs. The same parameters and optimised values of c and a_7 are used as in results of the exact optimisation in 3.9c. This time however, the information ion is excited by 10 quanta and its final energy $E_{f,i}$ is plotted on the grid of perturbations η and run-times t_f . For unperturbed potentials corresponding to $\eta = 0$, this yields the familiar cooling solution at 23.3 μs . However, for increasingly perturbed potentials, the exchange mechanism breaks down and the final energy is close to the initial $\bar{n} = 10$.

Note that Fig. 4.3 is not symmetric anymore with respect to η . This is due to the fact that the initial energy allocation is also not symmetric anymore.

The right part of the plot shows the shape of this breakdown at the cooling minimum (cut marked by the white dotted line). On top of the simulated resonance shape, the result of fitting the Lorentzian eq. 4.4 to the central part of it is shown. This is obtained by finding the optimal value¹ of the fit parameter k which is found to be $k = 0.52$ in this case. For small η , the fit matches the data well, leading to the conclusion that eq. 4.4 is a reasonable approximation.

So far, this result tells us that to achieve the broadest and thus most insensitive resonance, one should use as close an inner distance d_{in} as possible. To further mitigate the effect of tilts on the cooling, the intuitive approach is to increase the motional frequency ω , such that the ions are more strongly confined and thus less sensitive. To vary the confinement throughout the scheme, different values of β_{max} are needed. The dependence of the Lorentzian width $\eta_{1/2}$ on β_{max} is thus of interest.

4.2.2 Resonance width scaling with quartic confinement

To determine the behaviour of the resonance width $\eta_{1/2}$ with β_{max} , the relevant terms of 4.5 are examined. As the only terms in $\eta_{1/2}$ that can depend on β_{max} are ω_0 and d_{in} , the scaling of the distance $d(t)$ is examined first.

¹This is done using a least-squares method. As the Lorentzian is only expected to be a good approximation close to the resonance, only the data where $E_{f,i}/\hbar\omega_0 < 2$ is used, ensuring that the fit is not distorted by the behaviour far away from $\eta = 0$.

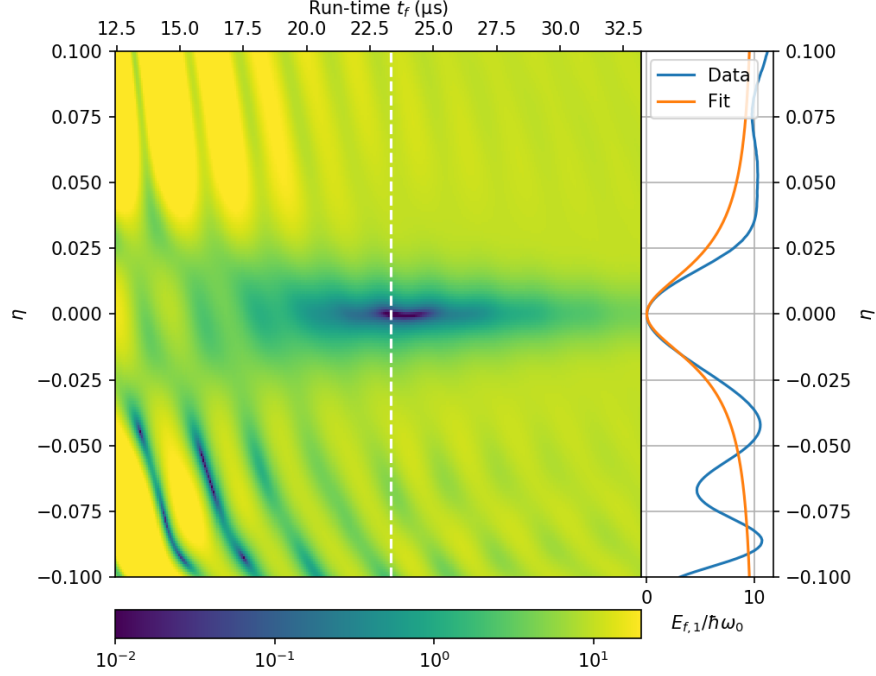


Figure 4.3: Final energy of the information ion after a hot run on a grid of perturbations η and run-times t_f , showing the cooling resonance.

The dependence of the distance trajectory $d(t)$ on $\beta_{\max}$ is simply given by the critical distance d_c . If only $\beta_{\max}$ is scaled, but the inner and outer distances are kept the same in dimensionless variables (for example, the ions are always brought from $5d_c$ to $1.25d_c$ no matter the value of $\beta_{\max}$), then $d(t)$ can be written as

$$d(t) = \underbrace{\frac{d(t)}{d_c}}_{:=D(t)} d_c = D(t) \left(\frac{2C_C}{\beta_{\max}} \right)^{\frac{1}{5}}, \quad (4.6)$$

where $D(t)$ is the dimensionless distance trajectory. Therefore, the distance scales as $d \propto \beta_{\max}^{-\frac{1}{5}}$.

Next, the scaling of the ion frequencies $\omega_1 = \omega_2$ can be found from eq. 3.14:

$$\begin{aligned}
 m\omega_i^2(t) &= \underbrace{2\alpha + 3\beta d^2}_{m\Omega_-^2 = \text{const.}} + \frac{2C_C}{d^3} \\
 &= 2\alpha(t_f/2) + 3 \underbrace{\beta(t_f/2)}_{\beta_{\max}} d_{\text{in}}^2 + \frac{2C_C}{d^3(t)} \\
 &= \frac{2C_C}{d_{\text{in}}^3} + 2\beta_{\max} d_{\text{in}}^2 + \frac{2C_C}{d^3(t)}.
 \end{aligned} \tag{4.7}$$

For the second equality, the fact that Ω_- is constant in time is used to replace the function values with those at time $t_f/2$. In the third equality, the equilibrium distance relation (3.12) was applied to replace α .

Using the knowledge from eq. 4.6, this can then be rewritten as

$$\begin{aligned}
 m\omega_i^2(t) &= \frac{2C_C}{d_{\text{in}}^3} + 2\beta_{\max} d_{\text{in}}^2 + \frac{2C_C}{d^3} \\
 &= \left[\frac{2C_C}{D^3(t_f/2)} + 2D^2(t_f/2) + \frac{2C_C}{D^3(t)} \right] \cdot \beta_{\max}^{\frac{3}{5}}.
 \end{aligned} \tag{4.8}$$

The ion frequencies therefore scale as $\omega_i \propto \beta_{\max}^{\frac{3}{10}}$.

Finally, the scaling of the resonance width $\eta_{1/2}$ can be found by putting the two results together and rewriting

$$\eta_{1/2} \propto \omega_0^{-2} d_{\text{in}}^{-3} \propto \beta_{\max}^{-\frac{3}{5}} \beta_{\max}^{\frac{3}{5}} \propto \beta_{\max}^0. \tag{4.9}$$

The resonance width is therefore not expected to depend on the maximal quartic confinement. Note that this result does not rely on any approximations and is therefore exact.

Label	$\beta_{\max}$ (N m ⁻³)	d_c (μm)	d_{out} (μm)	m (u)
A (default)	$1 \cdot \beta_{\text{HOA}} = 0.85$	14.0	$5d_c = 70.1$	39.96 (⁴⁰ Ca ⁺)
B	$3 \cdot \beta_{\text{HOA}} = 2.55$	11.3	$5d_c = 56.3$	39.96 (⁴⁰ Ca ⁺)
C	$9 \cdot \beta_{\text{HOA}} = 7.65$	9.04	$5d_c = 45.2$	39.96 (⁴⁰ Ca ⁺)
D	$27 \cdot \beta_{\text{HOA}} = 22.95$	7.26	$5d_c = 36.3$	39.96 (⁴⁰ Ca ⁺)

Table 4.1: List of several sets of physical constraints. Each set corresponds to choosing a different maximal quartic confinement $\beta_{\max}$.

To demonstrate that this is in fact the case, we calculate the cooling resonance for four values of $\beta_{\max}$. Table 4.1 shows the chosen values, ranging from one to 27 times the HOA2 trap strength. As in all examples before, the outer distance is always chosen to be five times the critical distance, which is also

given in Table 4.1. For each $\beta_{\max}$, the inner distance d_{in} is varied from $1.1d_c$ to $1.4d_c$. The scheme is optimised using the exact robustness method, such that the run-time giving a cooling solution can be found for each value of $\{\beta_{\max}, d_{\text{in}}\}$. For each cooling solution, the resonance width with respect to a perturbation η is calculated and the Lorentzian eq. 4.4 is fitted to it in the same way as in Fig. 4.3, yielding the dimensionless fit parameter k .

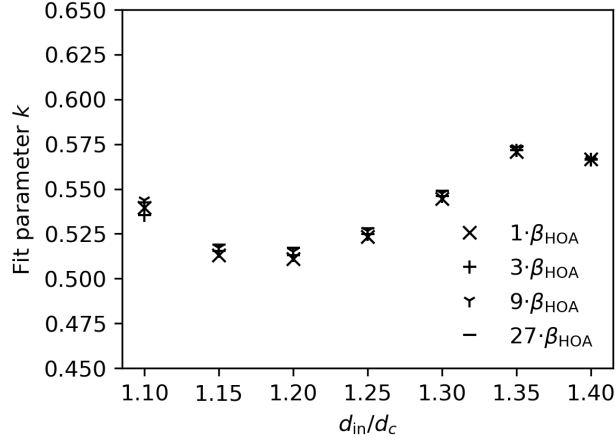


Figure 4.4: The values of the fit parameter k in the Lorentzian Ansatz eq. 4.4, shown for a range of inner distances d_{in} from $1.1d_c$ to $1.4d_c$ and for four parameter sets in Table 4.1.

If the derivation of this scaling behaviour is accurate, the resulting values of k should be the same for all values of $\beta_{\max}$. This is confirmed in Fig. 4.4, where the values of k are consistent with being independent of $\beta_{\max}^2$. Furthermore, Fig. 4.4 does also not show a strong dependence of k on d_{in} , as all k are around 0.55. Thus we conclude that the estimation eq. 4.4 yields a good guess of the resonance width for all parameters $\{\beta_{\max}, d_{\text{in}}\}$ when using this value of k , despite the crude approximations that were taken.

From the preceding discussion, one could erroneously come to the conclusion that using a trap with a higher quartic confinement is not advantageous as the resonance width stays the same. But since the perturbation parameter η corresponds to a potential tilt γ as $\gamma = m\Omega_-^2 d_{\text{in}} \eta$ (see eq. 3.28), the tolerable tilt still increases as $\beta_{\max}$ and with it the frequency Ω_- grows.

The resonance width can therefore be predicted independently of the exact distance trajectory $d(t)$, thus setting the necessary precision of the apparatus. For a desired final energy level (for example $\bar{n} = 0.1$) to which an ion should be cooled, eq. 4.4 immediately gives the maximal tolerable perturbation, telling an experimenter how precise the potential-generating electronics need to be, how well potential tilts have to be calibrated and how well the potentials generated by the trap electrodes have to be known.

²This is equivalent to being independent of d_{in} , due to $d \equiv \beta_{\max}^{-\frac{1}{2}}$ from 4.6.

In the example cooling solution shown in Fig. 4.3, the perturbation must not be larger than $|\eta| = 0.002$ (or $|\gamma| < 0.12 \text{ V m}^{-1}$), otherwise the information ion stays above its target value of $\bar{n} = 0.1$ after the cooling procedure. This range is small but not entirely unrealistic, as a tilt compensation resolution of 0.1 V m^{-1} was achieved in the ion separation experiment of [10].

Comparing this range to fig. 4.2c, it becomes apparent that the perturbation range in which the cooling motion alone works well is much larger than the cooling resonance width. This could be exploited experimentally by scanning the value of a compensating tilt in the range allowed by the transport. Doing this until the cooling resonance is found immediately yields the ideal calibration.

After having found ways to optimise the cooling resonance by varying the maximal quartic confinement $\beta_{\max}$, the next section explores the dependence of the cooling solution timing on $\beta_{\max}$.

4.3 Trap strength scaling behaviour

As a larger quartic confinement leads to a smaller critical distance d_c , it is expected that faster cooling solutions are found when using larger values of $\beta_{\max}$. This motivates an analysis of the STA scheme behaviour when scaling the trap strength.

To predict the results for scaled values of $\beta_{\max}$, we go over to express all parameters in a dimensionless way. As before, all distances are expressed in terms of d_c and all energies on a scale of $\hbar\omega_0$. Values denoting time can be made dimensionless by multiplying with a frequency such as ω_0 , such that all times are expressed as motional cycles of the ions. Rewritten as such, the scheme only depends on $\beta_{\max}$ and the dimensionless distance trajectory between $d_{\text{out}}/d_c = D(t_0)$ and $d_{\text{in}}/d_c = D(t_f/2)$ as in eq. 4.6.

Reusing the scaling results of subsection 4.2.2, the $\beta_{\max}$ -dependence of the exchange frequency can be calculated. The exchange frequency Ω_{ex} is also written in a dimensionless way by dividing it with the initial ion frequency ω_0 :

$$\frac{\Omega_{\text{ex}}}{\omega_0} = \frac{C_C}{m\omega_0 \sqrt{\omega_1(t)\omega_2(t)} d^3(t)}. \quad (4.10)$$

Using the scaling laws of the distance $d(t)$ and the ion frequencies ω_i as obtained in subsection 4.2.2, as well as the fact that both ions have the same motional frequency $\omega_1 = \omega_2$ in the unperturbed case, we find

$$\frac{\Omega_{\text{ex}}}{\omega_0} \propto \omega_0^{-1} \omega_i^{-1}(t) d^{-3}(t) \propto \beta_{\max}^{-\frac{3}{10}} \cdot \beta_{\max}^{-\frac{3}{10}} \cdot \beta_{\max}^{\frac{3}{5}} = \beta_{\max}^0. \quad (4.11)$$

In dimensionless variables, the exchange frequency is therefore independent of the quartic confinement $\beta_{\max}$. Thus we expect to always find the cooling solutions at the same number of motional cycles, given that the dimensionless distance trajectory $D(t)$ has remained the same.

To demonstrate this scaling behaviour, we perform a similar analysis as in Fig. 4.4 and again use the sets of constraints shown in Table 4.1. The inner distance d_{in} is varied between $1.1d_c$ and $1.4d_c$ and we calculate the following results for all combinations $\{\beta_{\text{max}}, d_{\text{in}}\}$, which are shown in Fig. 4.5:

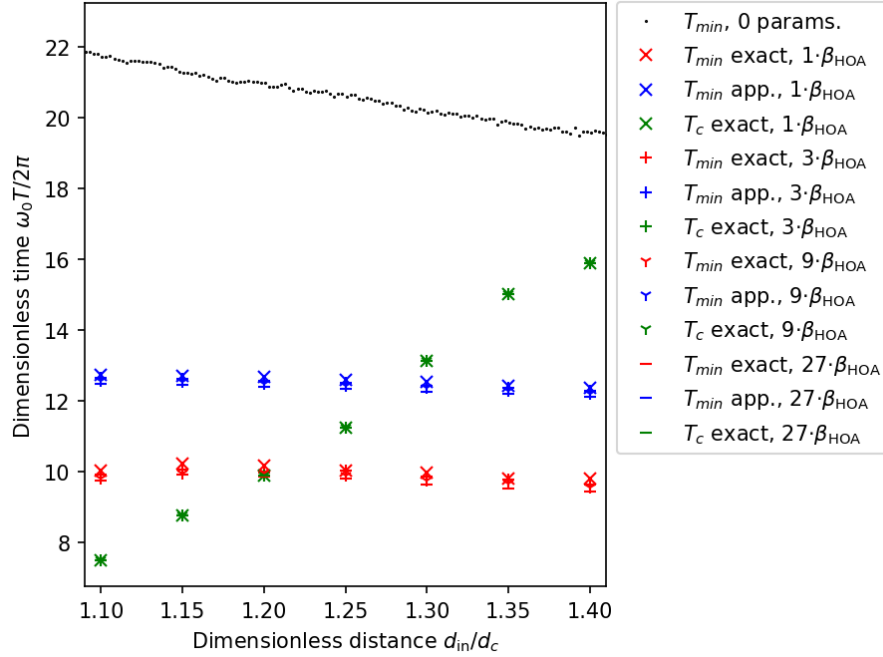


Figure 4.5: Scaling plot showing the cooling solutions (green symbols), the transport speed limit of the approximate method (blue symbols) and of the exact method (red symbols). For comparison, the speed limit of the parameter-free scheme from Fig. 3.4 is also shown (black dots).

- Cooling solutions:** For each combination of $\{\beta_{\text{max}}, d_{\text{in}}/d_c\}$, the exact cost function eq. 3.41 is used to optimise the STA cooling motion. Then the run-time T_c resulting in a cooling solution is found in the same way as in section 4.1. All results are plotted in Fig. 4.5 as green symbols, each symbol denoting a different value of β_{max} . Note that the cooling time T_c is made dimensionless by multiplying with the initial ion frequency ω_0 , which depends on the value of β_{max} . As expected, all values of β_{max} result in a cooling solution in the same number of motional cycles, given the same choice of the dimensionless inner distance d_{in}/d_c . Furthermore, the number of cycles needed to cool decreases with the inner distance.
- Transport speed limit of the perturbative method:** The STA transport scheme is optimised using the perturbative cost function eq. 3.40 for each combination of $\{\beta_{\text{max}}, d_{\text{in}}/d_c\}$. The total final excitations E_f have the same periodic shape with the run-time t_f as the result shown for the parameterless STA scheme in subsection 3.3.2. The same fit as in

Fig. 3.4 is applied to find an exponential envelope, such that the minimal run-time $T_{\min}$ can be found, below which the transport cannot be realised with less excitations than 0.1 quanta.

These times $T_{\min}$ are shown in Fig. 4.5 as blue symbols. Note that again, $\beta_{\max}$ does not influence the result. In conclusion, the perturbative optimisation method generates cooling motions that work well above about 12.5 motional cycles, which is the speed limit for cooling solutions using this method.

- **Transport speed limit of the exact method:** The same analysis is carried out again, but this time using the exact cost function eq. 3.41. The results are shown in Fig. 4.5 as red symbols. Note that the speed limit of the exact method is again independent of $\beta_{\max}$, but the transport now works down to 10 motional cycles, resulting in a reduction of 2.5 motional cycles over the approximate method.
- **Transport speed limit of the parameter-free scheme:** For comparison, we also show the speed limit of the parameter-free STA scheme discussed in subsection 3.3.2. The black dots represent the same data as the red line in Fig. 3.4, obtained by constraint set A (Table 4.1). This then shows that this unoptimised transport scheme is around two times slower than the best optimised version, even without being designed for robustness.

Summarising, Fig. 4.5 shows that in terms of motional cycles, the proposed STA scheme gives the same results independent of the choice of $\beta_{\max}$. The best method of optimising the transport for minimal excitations and robustness, the exact cost function eq. 3.41, yields usable results down to 10 motional cycles. The inner distance d_{in} can then be chosen such that a cooling solution is found exactly at this limit. Fig. 4.5 shows that this can be done by choosing $d_{\text{in}} \approx 1.2d_c$, resulting in the fastest possible cooling solution at 10 motional cycles.

Fig. 4.5 also shows that to speed up the cooling solutions, one would first and foremost need to improve the transport optimisation method. The inner distance d_{in} could in principle be chosen below $1.2d_c$ for faster cooling. However, the current design of the adiabatic shortcut prevents this due to the speed limit at 10 motional cycles. If the transport can be optimised such that it works beyond this limit, one immediately finds faster cooling solutions at lower d_{in} , but still without merging the ions at the critical distance. As discussed in subsection 3.4.2, the optimisation method could be improved by using even more free parameters to shape the form of ρ_+ and choosing a more involved cost function in place of eq. 3.41.

Note that the results of Fig. 4.5 also depend on the choice of outer distance d_{out} . If d_{out} is chosen larger than $5d_c$ in Table 4.1, the ions are accelerated more strongly. Thus one would expect the transport excitations to become stronger and the speed limits in Fig. 4.5 to be shifted towards slower run-times.

Cooling two ions of unequal mass

So far, we have only considered the case where both the information ion and the coolant ion are of equal mass. When trying to extend the cooling scheme to ions of unequal masses $m_1 \neq m_2$, a fundamental problem arises: if we keep using a symmetric potential such as the harmonic-quartic double well potential of eq. 3.1, then the ions will always sit at symmetric equilibrium positions. The motional ion frequencies, given by eq. 1.2, can then not be equal anymore, as the potential curvature is the same for both ions, but the mass is not. The resonance condition $\omega_1 = \omega_2$ on the motional exchange is thus violated and no or only incomplete cooling can be achieved.

This is mitigated in this chapter by introducing an asymmetric term to the potential V_{el} , which can be used to force the motional frequencies to be equal throughout the scheme. The simplest choice is to add a linear term¹ leading to the trapping potential

$$V_{\text{el}}(x, t) = \gamma(t)x + \alpha(t)x^2 + \beta(t)x^4 \quad (5.1)$$

and corresponding full Hamiltonian

$$\begin{aligned} H &= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V_{\text{tot}}(x_1, x_2, t) \\ V_{\text{tot}}(x_1, x_2, t) &= V_{\text{el}}(x_1, t) + V_{\text{el}}(x_2, t) + \frac{C_C}{x_2 - x_1} \\ &= \gamma(t)(x_1 + x_2) + \alpha(t)(x_1^2 + x_2^2) + \beta(t)(x_1^4 + x_2^4) + \frac{C_C}{x_2 - x_1}, \end{aligned} \quad (5.2)$$

where $\{p_1, p_2, x_1, x_2\}$ are the position and momentum coordinates of the two ions and we assume that $x_2 > x_1$.

This is reminiscent of section 3.4, where such a linear term was treated as an undesirable perturbation. Here in contrast, the potential tilt is intentional.

¹Another choice is to add a cubic term. The dynamical normal mode calculations for this are given in Appendix C.

Note that in this chapter, the variables $\alpha, \beta, \gamma, d, s, \lambda_{\pm}, \Omega_{\pm}, x_i^{(0)}, P_{0,\pm}, \rho_{\pm}, q_{\pm}$ are in general time-dependent, but we omit this in the notation.

This chapter then performs the familiar STA steps given in chapter 2 to arrive at a cooling motion that fulfills the same purpose as in the equal-mass case. The main difference to the derivations before lies in the fact that the potential is now parametrised by three functions $\{\alpha(t), \beta(t), \gamma(t)\}$. The dynamical normal mode treatment decomposes the full Hamiltonian eq. 5.2 into two harmonic oscillators as before, but the correspondence $\{\Omega_{\pm}\} \leftrightarrow \{\alpha(t), \beta(t), \gamma(t)\}$ between the HO frequencies and the potential parametrisation now includes the term γ . It is at this step in the derivation where $\omega_1 = \omega_2$ is enforced.

In the following, we will again proceed as in chapter 3, perform the dynamical normal mode decomposition, then inverse-engineer the Hamiltonian eq. 5.2 and optimise a number of free parameters to correct for perturbations.

5.1 Dynamical normal modes for two trapped ions of unequal mass

We again follow the theory of section 2.1 and take a harmonic approximation of H at the equilibrium positions, which are now not symmetric anymore.

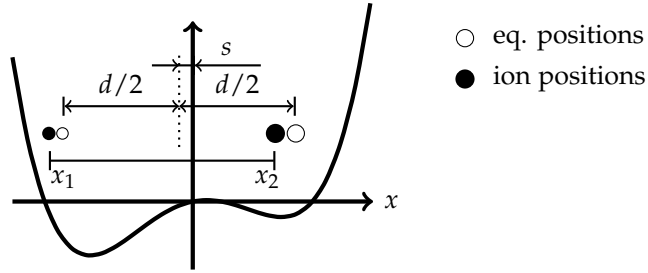


Figure 5.1: Schematic depiction of position and equilibrium coordinates for two ions of unequal mass trapped in a quartic double-well potential with a linear tilt. Note that the Coulomb potential has been neglected from the potential shape.

The equilibrium positions fulfil

$$\left. \frac{\partial V}{\partial x_i} \right|_{x_i^{(0)}} = \gamma + 2\alpha x_i^{(0)} + 4\beta \left(x_i^{(0)} \right)^3 - \frac{(-1)^i C_C}{x_2^{(0)} - x_1^{(0)}} = 0, \quad (5.3)$$

where $i = \{1, 2\}$. We introduce the shifted parametrisation

$$\begin{aligned} x_1^{(0)} &= s - \frac{d}{2} \\ x_2^{(0)} &= s + \frac{d}{2} \end{aligned} \quad (5.4)$$

5.1. Dynamical normal modes for two trapped ions of unequal mass

as in section 3.4.

The mass-weighted Hessian K that needs to be diagonalised is given by

$$K = \begin{pmatrix} \frac{2\alpha + 12\beta (x_1^{(0)})^2 + \frac{2C_C}{d^3}}{m_1} & -\frac{2C_C}{\sqrt{m_1 m_2} d^3} \\ -\frac{2C_C}{\sqrt{m_1 m_2} d^3} & \frac{2\alpha + 12\beta (x_2^{(0)})^2 + \frac{2C_C}{d^3}}{m_2} \end{pmatrix} \quad (5.5)$$

Note then that having equal ion frequencies at all times is an equivalent condition to having equal diagonal entries $K_{11} \stackrel{!}{=} K_{22}$. This conditions shall be enforced from now on and the matrix K takes again the simple form $\begin{pmatrix} A & B \\ B & A \end{pmatrix}$ and is thus easily diagonalised with same constant eigenvectors as in section 3.1

$$\begin{aligned} v_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ v_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned} \quad (5.6)$$

again with an angle $\theta = \frac{\pi}{4}$.

Note that when not enforcing equal diagonal entries of K , the angle θ is not constant in general and the dynamical normal modes stay coupled (see eq. 2.14).

The eigenvalues are

$$\begin{aligned} \lambda_{\pm} &= \Omega_{\pm}^2 = \frac{1}{m_1} \left[2\alpha + 12\beta (x_1^{(0)})^2 + \frac{2C_C}{d^3} \left[1 \pm \sqrt{\frac{m_1}{m_2}} \right] \right] \\ &= \frac{1}{m_2} \left[2\alpha + 12\beta (x_2^{(0)})^2 + \frac{2C_C}{d^3} \left[1 \pm \sqrt{\frac{m_2}{m_1}} \right] \right]. \end{aligned} \quad (5.7)$$

The change of variables to NM coordinates is given according to eq. 2.11 as

$$A(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{m_1} & \sqrt{m_2} \\ -\sqrt{m_1} & \sqrt{m_2} \end{pmatrix} \quad (5.8)$$

and the momentum shifts eq. 2.16 as

$$\begin{aligned} \begin{pmatrix} P_{0,-} \\ P_{0,+} \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{m_1} & \sqrt{m_2} \\ -\sqrt{m_1} & \sqrt{m_2} \end{pmatrix} \begin{pmatrix} \dot{s} - \frac{d}{2} \\ \dot{s} + \frac{d}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\sqrt{m_2} + \sqrt{m_1}}{\sqrt{2}} \dot{s} + \frac{\sqrt{m_2} - \sqrt{m_1}}{2\sqrt{2}} d \\ \frac{\sqrt{m_2} - \sqrt{m_1}}{\sqrt{2}} \dot{s} - \frac{\sqrt{m_2} + \sqrt{m_1}}{2\sqrt{2}} d \end{pmatrix}. \end{aligned} \quad (5.9)$$

5. COOLING TWO IONS OF UNEQUAL MASS

This finally gives us the normal mode Hamiltonian eq. 2.17 in the explicit form

$$H_{2\text{HO}} = H_{\text{HO}}^{(+)} + H_{\text{HO}}^{(-)}$$

$$H_{\text{HO}}^{(\pm)} = \frac{P_{\pm}^2}{2} + \frac{1}{2}\Omega_{\pm}^2 \left(X_{\pm} + \frac{\sqrt{m_2} \mp \sqrt{m_1}}{\sqrt{2}} \frac{\ddot{s}}{\Omega_{\pm}^2} + \frac{\sqrt{m_2} \pm \sqrt{m_1}}{2\sqrt{2}} \frac{\ddot{d}}{\Omega_{\pm}^2} \right)^2. \quad (5.10)$$

The corresponding Lewis-Riesenfeld invariants for $H_{\text{HO}}^{(-)}$ and $H_{\text{HO}}^{(+)}$ are then according to eq. 2.20

$$I_{\text{HO}}^{(\pm)} = \frac{1}{2} [\rho_{\pm}(P_{\pm} - \dot{q}_{\pm}) - \dot{\rho}_{\pm}(X_{\pm} - q_{\pm})]^2 + \frac{1}{2}\Omega_{0\pm}^2 \left(\frac{X_{\pm} - q_{\pm}}{\rho_{\pm}} \right)^2 \quad (5.11)$$

with the auxiliary functions $\rho_{\pm}$ and $q_{\pm}$ defined according to eq. 2.21 by

$$\begin{aligned} \ddot{\rho}_{\pm} + \Omega_{\pm}^2 \rho_{\pm} &= \frac{\Omega_{0\pm}^2}{\rho_{\pm}^3} \\ \ddot{q}_{\pm} + \Omega_{\pm}^2 q_{\pm} &= -\frac{\sqrt{m_2} \mp \sqrt{m_1}}{\sqrt{2}} \ddot{s} - \frac{\sqrt{m_2} \pm \sqrt{m_1}}{2\sqrt{2}} \ddot{d}. \end{aligned} \quad (5.12)$$

Note that q_{-} cannot be set to zero anymore in the unequal mass case, meaning that COM-mode centre is not static anymore. This was to be expected as the potential is not symmetric anymore.

The instantaneous energies are known from eq. 2.26 as

$$\begin{aligned} E_{n\pm} = \langle n_{\pm}; t |_{\alpha} H_{\text{HO}}^{(\pm)} | n_{\pm}; t \rangle_{\alpha} &= \frac{(2n_{\pm} + 1)\hbar}{4\Omega_{0\pm}} \left(\dot{\rho}_{\pm}^2 + \Omega_{\pm}^2 \rho_{\pm}^2 + \frac{\Omega_{0\pm}^2}{\rho_{\pm}^2} \right) \\ &+ \frac{1}{2}\dot{q}_{\pm}^2 + \frac{1}{2}\Omega_{\pm}^2 \left(q_{\pm} + \frac{\sqrt{m_2} \mp \sqrt{m_1}}{\sqrt{2}} \frac{\ddot{s}}{\Omega_{\pm}^2} + \frac{\sqrt{m_2} \pm \sqrt{m_1}}{2\sqrt{2}} \frac{\ddot{d}}{\Omega_{\pm}^2} \right)^2. \end{aligned} \quad (5.13)$$

As before in the equal mass case, we now want to engineer the auxiliary functions $q_{\pm}$ and $\rho_{\pm}$ such that the Hamiltonians $H_{\text{HO}}^{(\pm)}$ and invariants $I_{\text{HO}}^{(\pm)}$ commute at boundary times $t_b = \{0, t_f\}$. After doing so, the normal mode frequencies $\Omega_{\pm}$ will be known from the auxiliary ODEs eq. 5.12. Since one experimentally can only implement the potential eq. 3.2 given by $\{\alpha, \beta, \gamma\}$ and not the NM frequencies, a correspondence is needed between the two sets of variables.

This can be gained from the expressions for the normal mode frequencies eq. 5.7 by inverting these relations and using the resonance condition $K_{11} \stackrel{!}{=} K_{22}$. A lengthy but straightforward calculation leads to the expressions

$$\begin{aligned}
 d(t) &= \sqrt[3]{\frac{4C_C}{\sqrt{m_1 m_2}(\Omega_+^2 - \Omega_-^2)}} \\
 \beta(t) &= \frac{m_1 + m_2}{8d^2} (\Omega_+^2 + \Omega_-^2) - \frac{2C_C}{d^5} \\
 s(t) &= \frac{m_2 - m_1}{48\beta d} (\Omega_+^2 + \Omega_-^2) \\
 \alpha(t) &= \frac{C_C}{d^3} - \frac{\beta d^2}{2} - 6\beta s^2 \\
 \gamma(t) &= -2\alpha s - 2\beta \left(\frac{3}{2}d^2 s + 2s^3 \right).
 \end{aligned} \tag{5.14}$$

This concludes the dynamical normal mode derivations and allows to find the physical potential from the normal modes. These are now to be inverse-engineered by shaping the auxiliary functions $\rho_{\pm}$.

5.2 Inverse engineering the unequal-mass cooling scheme

5.2.1 Ensuring the commutation condition

As the full Hamiltonian was brought into the usual harmonic oscillator form in the preceding section, we can retain the commutation condition from section 3.2 and obtain the same boundary conditions

$$\rho_{\pm}(t_b) = 1, \tag{5.15a}$$

$$\dot{\rho}_{\pm}(t_b) = \ddot{\rho}_{\pm}(t_b) = \rho_{\pm}^{(3)}(t_b) = \rho_{\pm}^{(4)}(t_b) = 0 \tag{5.15b}$$

$$q_+(t_b) = \dot{q}_+(t_b) = \ddot{q}_+(t_b) = 0 \tag{5.15c}$$

for the auxiliary functions.

As in the equal mass case, after choosing functions $\rho_{\pm}$ that satisfy their BC and setting the initial frequencies $\Omega_{0\pm}$, the scheme can be reverse-engineered by finding the NM frequencies via

$$\Omega_{\pm} = \sqrt{\frac{\Omega_{0\pm}^2}{\rho_{\pm}^4} - \frac{\ddot{\rho}_{\pm}}{\rho_{\pm}}}. \tag{5.16}$$

This also determines $q_{\pm}$ through the auxiliary ODE eq. 5.12 and some free parameters in $\rho_{\pm}$ need to be chosen such that the BC on $q_{\pm}$ are also fulfilled.

And again, $\rho_{\pm}$ must be chosen according to physical constraints to implement the desired action, which is again to bring the ions from a starting distance d_{out} to a minimal distance d_{in} at $t = t_f/2$ and back.

5.2.2 Physical constraints

The desired physical target values are the same as before:

- The ions start and end at the same distance $d(t_0) = d(t_f) = d_{\text{out}}$.
- The ions reach their closest point after half the run-time $d(t_f/2) = d_{\text{in}}$, $d_{\text{in}} < d_{\text{out}}$.
- The quartic confinement β must be strongest after half the run-time: $\beta(t_f/2) = \beta_{\text{max}}$.
- The CoM-mode frequency is again chosen to be constant: $\Omega_{-}(t_0) = \Omega_{-}(t_f/2) = \Omega_{-}(t_f) = \Omega_{0-}$. In the polynomial interpolation that follows in subsection 3.2.3, this leads to Ω_{-} and ρ_{-} becoming constant at all times.

The value of $\rho_{\pm}$ after half the run time is defined as before as

$$\rho_{\text{in}\pm} = \sqrt{\frac{\Omega_{0\pm}}{\Omega_{\text{in}\pm}}} \quad (5.17)$$

and for that the NM frequencies at time t_0 and t_f need to be known.

The NM frequency $\Omega_{\text{in}+}$ can be found by setting d_{in} and β_{max} and inverting the relations (5.14). Then, knowing Ω_{-} and d_{out} , the remaining open variable Ω_{0+} is found by inverting the relation for $d(t)$ in eq. 5.14.

Now again a $\rho_{\pm}$ can be found that interpolates between $\Omega_{0\pm}$ and $\Omega_{\text{in}\pm}$ and obeys the BC eq. 3.16. Since the boundary conditions remain unchanged, the same polynomials eq. 3.22 and eq. 3.23, the latter containing two free parameters, can be reused.

To give an example of an STA scheme designed in this way, we recreate Fig. 3.2 and apply the described approach to a system of a $^{40}\text{Ca}^{+}$ ion and a $^9\text{Be}^{+}$ ion in a trap that can reach the quartic confinement of the HOA2 trap, $\beta_{\text{max}} = 0.85 \times 10^{-3} \text{ N m}^{-3}$. The auxiliary ρ_{+} is chosen to be the parameter-free Ansatz eq. 3.22. The outer and inner distances are also chosen as in target value set A in Table 3.1.

The resulting functions $\Omega_{\pm}$, α , β , γ , s and d are shown in Fig. 5.2. The CoM mode frequency stays constant at about 0.60 MHz and α stays negative throughout the scheme, due to never bringing the ions closer than the critical distance d_c . The value of β reaches β_{max} after half the run-time as before. The tilt γ given by eq. 5.14 is minimal when the ions are closest together, mirroring the centre shift s . The distance function d looks similar as in Fig. 3.2, bringing the ions from 70.1 μm to 17.5 μm as desired.

Note the scale of the required tilt γ in Fig. 5.2d is about an order of magnitude larger than the tolerable linear perturbations in the equal-mass scheme in Fig. 3.9. This is encouraging as the unequal-mass scheme then not very sensitive to erroneous tilts of the same scale as before. Furthermore, it should be possible to also design the unequal-mass scheme to be robust in the same way as before in section 3.4.

5.2. Inverse engineering the unequal-mass cooling scheme

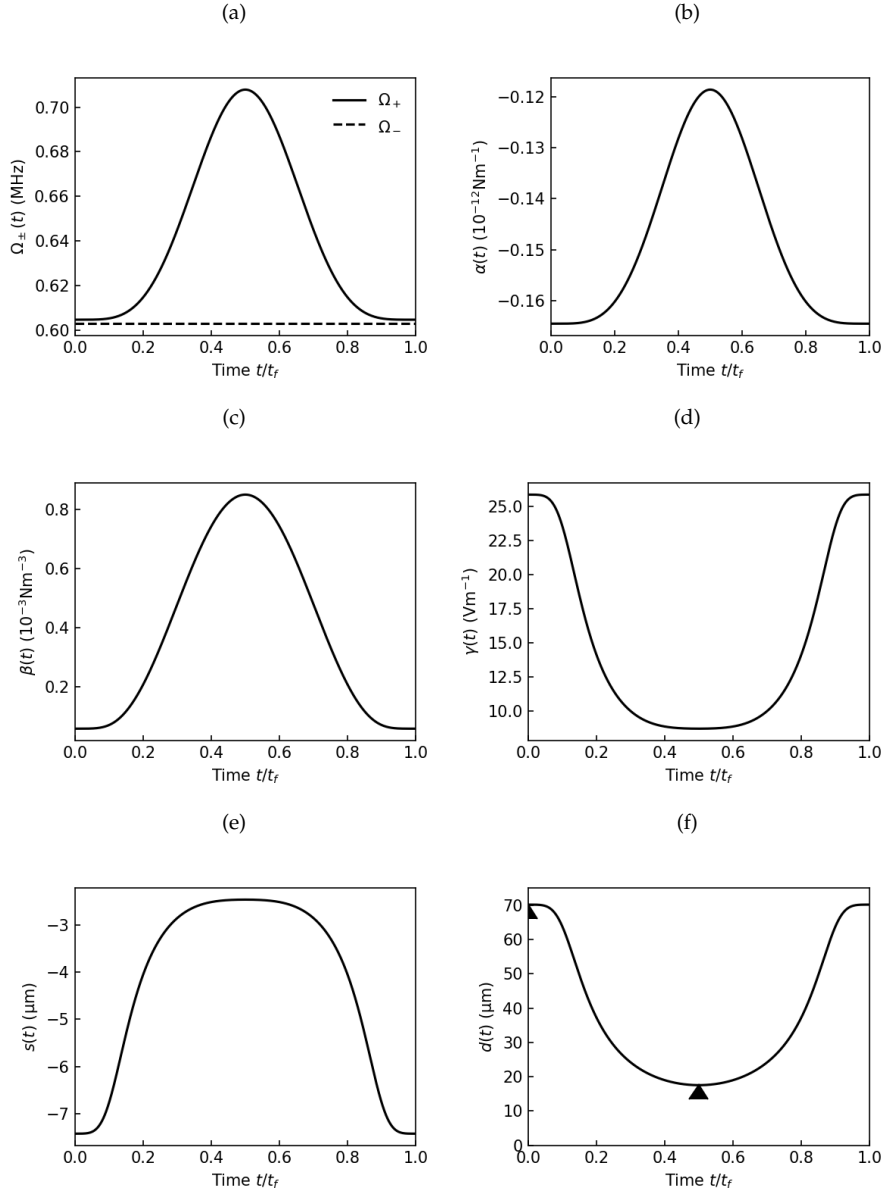


Figure 5.2: An overview of a basic inverse-engineered unequal-mass STA scheme involving a Calcium ion and a Beryllium ion. Shown are the resulting NM frequencies (a), the harmonic confinement $\alpha(t)$ (b), the quartic confinement $\beta(t)$ (c), the linear term γ (d), the asymmetric shift $s(t)$ (e) and the distance function $d(t)$ (f).

The markers in Fig. 5.2f designate the positions in time at which Fig. 5.3 shows the shape of the potential eq. 5.1. In Fig. 5.3a the starting potential at t_0 shows minima consistent with the distance $d_{\text{out}} = 70.1 \mu\text{m}$, but shifted the left according to s . The potential shape in Fig. 5.3b has equilibrium positions

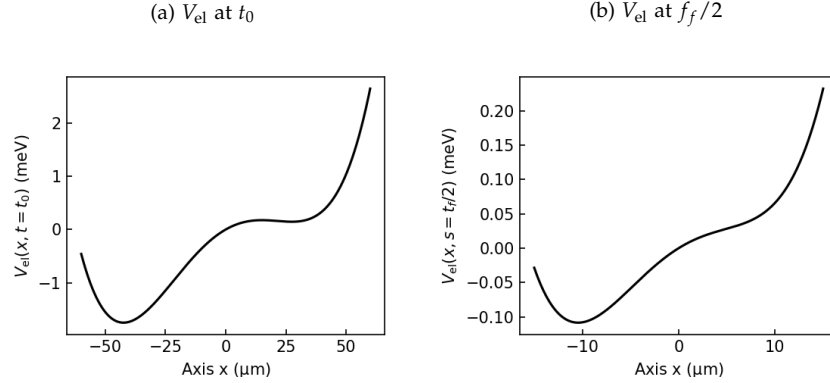


Figure 5.3: Potential shapes V_{el} of the scheme shown in Fig. 5.2 at time t_0 (a) and $t_f/2$ (b).

that are $17.5\mu\text{m}$ apart. Note that this is not a double-well potential anymore, despite the inner distance being larger than d_c . Due to the additional term γ , the point where the potential changes to a single-well shape is not simply given by d_c anymore². If the potential is required to have a double-well shape at all times, then the inner distance d_{in} has to be chosen increasingly larger than d_c as the masses diverge.

The unequal-mass scheme can now be optimised for minimal excitations by shaping the auxiliary function ρ_+ in the same way as before. Designing optimal robustness towards experimental imperfections should be straightforward by reproducing the discussion in section 3.4, but is beyond the scope of this thesis.

5.3 Transport scheme optimisation and cooling solutions

Much in the same way as in section 3.3, the Ansatz for ρ_+ needs to be optimised to result in a shortcut. We take the Ansatz eq. 3.23 and optimise up to two free parameters, such that the total final energy E_f , calculated with the full Hamiltonian, is minimal after performing a cold run. For this we use the Nelder-Mead algorithm as before.

After optimising the cooling motion in this way, Fig. 5.4a shows the excitations after cold runs when optimising with one vs. two parameters. The physical constraints are chosen to be the default set A (Table 3.1), but with the coolant ion being only half the mass of the information ion, which is chosen to be a $^{40}\text{Ca}^+$ ion. When only using one parameter (c), the excitations increase exponentially despite using the exact Hamiltonian. This is due to both NM centres being excited (see eq. 5.13) and we cannot further set

²The condition could be found by calculating the number of minima of the potential. For this, the first derivative $\partial V_{el}/\partial x$ is taken and set to zero, resulting in a cubic equation. If it has three real solutions, then the potential has double-well shape. This is determined by calculating the discriminant of the equation, which is omitted here due to the calculation being very cumbersome.

$q_- = 0$. A single parameter is then not enough anymore to optimise the scheme. The Ansatz of ρ_+ using two parameters c and a_7 on the other hand reaches negligible energy levels for any run-time, recovering the result found in the equal-mass case, albeit with two free parameters instead of only one.

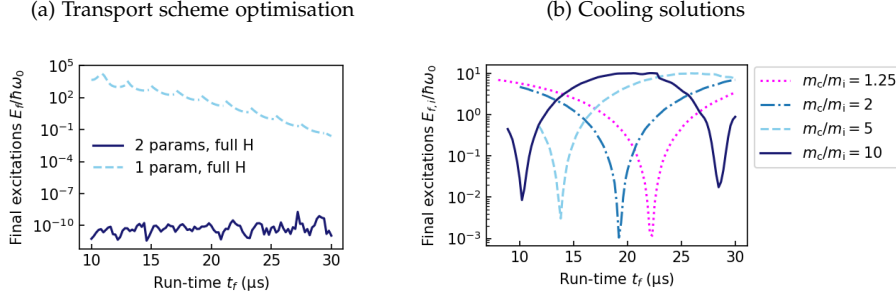


Figure 5.4: (a) Excitations E_f after optimising the unequal-mass cooling motion for a mass ratio of 2. (b) The cooling solutions for mass ratios m_c/m_i of 2, 5 and 10 when optimising two free parameters.

As in the equal-mass case before, one can apply the optimised cooling motion to find cooling solutions. Note that the mass notation is changed from m_1 and m_2 to m_c , denoting the mass of the coolant ion, and m_i for the information ion, which is always chosen to be a $^{40}\text{Ca}^+$ ion in this example. It does not matter whether the lighter or heavier ion is chosen to be the information ion, as the cooling scheme swaps the motional states in both cases.

The two-parameter optimisation is run for a wide range of mass ratios of $m_c/m_i = \{1.25, 2, 5, 10\}$, corresponding to ever lighter coolant ions, and the results are used to scan the run-time t_f and obtain cooling solutions. The results are then shown in Fig. 5.4b by plotting the final energy $E_{f,i}$. The information ion was initially excited by 10 quanta. Note that the energy of a single quanta $\hbar\omega_0$ is the same for both ions, since their frequency is equal despite the unequal masses.

The cooling solutions are shifted to faster run-times with increasing mass ratio. This is explained by the mass dependence of the exchange frequency Ω_{ex} , which is proportional to $\frac{1}{\sqrt{m_1 m_2}}$. As the mass ratio is increased by decreasing the coolant ion mass m_c , Ω_{ex} increases. However, consider that if the ions are to be in a double-well potential at all times, the inner distance d_{in} has to be increased with the mass ratio as discussed for Fig. 5.3b. The increase in exchange frequency might therefore be cancelled out.

Nonetheless, this chapter demonstrates the successful generalisation of the cooling scheme for two ions of unequal mass. The key point is keeping the ion frequencies equal at all times, allowing the motional exchange to take place as in the equal-mass case. This comes at the cost of requiring a more complicated potential shape, which has been expanded by a linear term. Designing the scheme to be robust to experimental imperfections is a natural extension of the work presented in this thesis.

Conclusion & Outlook

Conclusion

Recooling of ions is an experimental necessity in trapped-ion QIP experiments, currently taking more than one hundred motional cycles of the ions. In this thesis, I have proposed a way to cool an ion about an order of magnitude faster by coupling it to a ground-state cooled ion by the Coulomb force. Much in the same way as two spring-coupled pendulums exchange their motion, the two ions exchange their motional energy. As this exchange increases in speed with decreasing ion distance, a cooling motion was designed that brings moves the ions from a large initial distance to a distance where the exchange is fast, only to move them back to their starting position. For this, the ions are trapped in a harmonic-quartic double-well potential. Cooling is then achieved by timing this motion correctly, such that the motional energies have been exactly swapped afterwards.

I have designed this cooling motion for two ions of equal mass in such a way that it does not additionally excite the ions. This is challenging, as the targeted cooling times of just a few motional cycles are beyond the adiabatic limit. To this end, shortcut to adiabaticity methods were applied, which allowed me to design the trapping potentials for the cooling motion such that minimal final excitations are produced even at arbitrarily short run-times. However, as this method can only be applied to an approximation of the two-ion system, the achievable run-times are limited. A further limitation is given by the minimal distance between the ions if they are not to be merged into a single-well potential. This mainly depends on the achievable quartic potential term in a given Paul trap.

The shortcut to adiabaticity methods are well-suited to design such schemes to be optimally robust to experimental imperfections. For the case of two ions of equal mass, I have therefore devised the cooling motion to be robust towards linear potential tilts, which are a major source of errors in trapped-ion experiments due to stray charges and imperfect calibration. The final result is found in the form of cooling solutions at a minimal cooling time of 10 motional cycles. As the motional frequencies are mainly increased by using a trap with a stronger quartic confinement, this is the main factor in setting the speed of the cooling scheme.

As the motional exchange requires the ion motional frequencies to be res-

onant, such potential tilts reduce the cooling effect by shifting the ion frequencies to be off-resonant. The maximal tolerable tilt is stated in terms of experimental parameters, yielding a prediction of the necessary experimental accuracy.

Furthermore, in the case of two ions of unequal mass, the shortcut to adiabaticity approach is derived and applied to design the cooling motion in a way that does not excite the ions additionally. However, implementing the robustness towards experimental errors in analogy to the equal-mass case is deferred to future work.

Outlook

The future outlook of this topic should be divided into further theoretical work and a first experimental demonstration of the proposal presented in this thesis.

On the theory side, the robustness towards potential tilts could be improved and higher order perturbations might be considered as well. In the case of two ions of unequal mass, robustness should be reproduced in analogy to the equal-mass case. An interesting generalisation of this work would be to consider cooling strings of N ions with a single cooling ion. This might prove challenging as possibly only a single mode of the N -ion string can be cooled at a time. Furthermore, the extension of the cooling scheme to the radial modes as considered in Appendix D could be of interest.

Experimentally, this cooling scheme should be demonstrated. For this, the implementation of the designed trapping potentials needs to be accurate enough such that cooling can be achieved. This places stringent constraints on the electronics equipment, the calibration methods and the knowledge of the actual potential generated by a certain voltage in the trap. A more easily achievable target might be to adapt the cooling motion to perform an ion separation, as this operation has still not been implemented at non-adiabatic speeds. For ion separation, the cooling resonance effect plays no role, thus relaxing the needed experimental accuracy.

Appendix A

Perturbative corrections to the dynamical normal modes

The dynamical normal modes are calculated in a second order approximation of the full Hamiltonian at hand. Since eq. 3.2 contains a Coulomb term and a quartic electric potential, it is natural to consider some perturbations to the solutions of the two Harmonic oscillators eq. 3.8.

When the third order terms in the expansion of the Hamiltonian eq. 3.2 are considered, there are corrections due to the Coulomb term $\frac{C_C}{x_2 - x_1}$ and due to the quartic part of V_{el} .

The higher order Coulomb terms are given in [42, 12] as

$$\delta V^{(j)} = (-1)^{j+1} \frac{C_C}{d^{j+1}} \left(\sqrt{\frac{2}{m}} X_+ \right)^j, \quad (\text{A.1})$$

where X_+ is the stretch-mode position coordinate.

Note that the Coulomb force only affects the stretch-mode motion and does not couple the normal modes.

The third order Coulomb correction to the instantaneous energies is thus given after a lengthy calculation that is similar to the one leading to eq. 2.26 by

$$\begin{aligned} \delta E_{n_+,C}^{(3)}(t) &= \langle n_+; t |_\alpha \delta V^{(3)} | n_+; t \rangle_\alpha \\ &= \frac{C_C}{d^4} \left(\frac{2}{m} \right)^{3/2} \left[q_+^3 + 3\rho_+^2 q_+ \left[\frac{\hbar}{\Omega_{0+}} \left(n_+ + \frac{1}{2} \right) \right] \right]. \end{aligned} \quad (\text{A.2})$$

The third order corrections due to the quartic part of the potential are given by writing down the third term of the Taylor expansion of eq. 3.2 without the Coulomb term.

$$\begin{aligned}
\delta V^{(3)} &= \frac{1}{3!} \frac{\partial^3 V}{\partial x_1^3} \left(x_1 - x_1^{(0)} \right)^3 + \frac{1}{3!} \frac{\partial^3 V}{\partial x_2^3} \left(x_2 - x_2^{(0)} \right)^3 \\
&= \frac{1}{4} \beta d \left(\frac{2}{m} \right)^{3/2} \left[2X_+^3 + 6X_+ X_-^2 \right].
\end{aligned} \tag{A.3}$$

The correction of the instantaneous energies are then given by

$$\begin{aligned}
\delta E_V^{(3)}(t) &= \left[\langle n_+; t |_\alpha \otimes \langle n_-; t |_\alpha \right] \delta V^{(3)} \left[| n_-; t \rangle_\alpha \otimes | n_+; t \rangle_\alpha \right] \\
&= \frac{1}{2} \beta d \left(\frac{2}{m} \right)^{3/2} \left[q_+^3 + 3\rho_+^2 q_+ \frac{\hbar}{\Omega_{0+}} \left(n_+ + \frac{1}{2} \right) \right. \\
&\quad \left. + \frac{3\hbar}{\Omega_{0-}} q_+ \rho_-^2 \left(n_- + \frac{1}{2} \right) + 3q_+ q_-^2 \right].
\end{aligned} \tag{A.4}$$

Note that for an adiabatic shortcut, the mode centres $q_\pm$ return to 0 at final time t_f and all third order contributions vanish. However, these matrix elements might be used in time-dependent perturbation theory as for example done in [27] by calculating then minimising the time-averaged energy of these perturbations.

Appendix B

The Sandia HOA2 trap

To determine realistic experimental boundaries of a cooling scheme such as the one proposed in this thesis, we analyse a trap that is available in the TIQI group, the High Optical Access (HOA) Trap 2.0 designed and fabricated by Sandia National Laboratories [43].

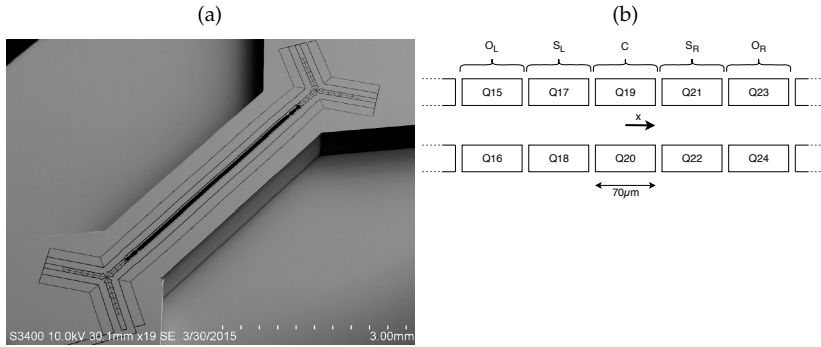
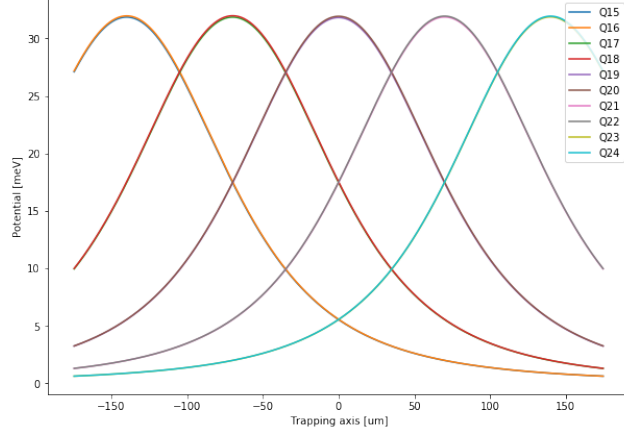


Figure B.1: (a) The HOA2 trap. Image taken from [43]. (b) Schematic depiction of the central quantum region.

It is a surface Paul trap with a slit for optical access in the central region. In this “quantum region” designed for the most precise control, each electrode is addressed individually and extends over 70 μm. Further away from the trap centre, control signals are reused periodically. The ions are trapped 68 μm over the surface. Fig. B.1a shows a scanning electrode image of the trap.

A detailed scheme of the quantum region is shown in Fig. B.1b. To this thesis, only the five central electrode pairs along the axial trap direction x will be relevant. The central pair C is made up by electrodes Q19/Q20, the while the left and right outermost pairs O_L/O_R consist of electrodes Q15/Q16 and Q23/Q24 respectively. The two pairs that are sandwiched in between are

Figure B.2: The potentials in the trapping axis $68\mu m$ above the trap surface generated by applying $1V$ to each of the ten central electrodes in the HOA2 trap. Simulation data provided by Sandia National Laboratories.



referred to as S_L/S_R and consist of the electrodes Q17/Q18 and Q21/Q22.

When applying a voltage U_i to electrode i ($i = Q15, \dots, Q24$), the electrode generates an electrical potential, depending on electrode geometry. These potentials are known from simulation data, which are provided by the trap manufacturer in the case of the HOA2 trap. Fig. B.2 shows the potentials in the trap axis $68\mu m$ above the surface for all considered electrodes, assuming a voltage of $U_i = 1V$ has been applied. Note that both electrodes of a pair generate almost, but not exactly, equal potentials.

We shall now take a brief look at methods to utilise these electrode potentials and generate the quartic double well potentials needed for the implementation of the cooling proposal in this thesis.

B.1 Generating quartic potentials

For the cooling scheme presented herein, the ability to generate quartic potentials

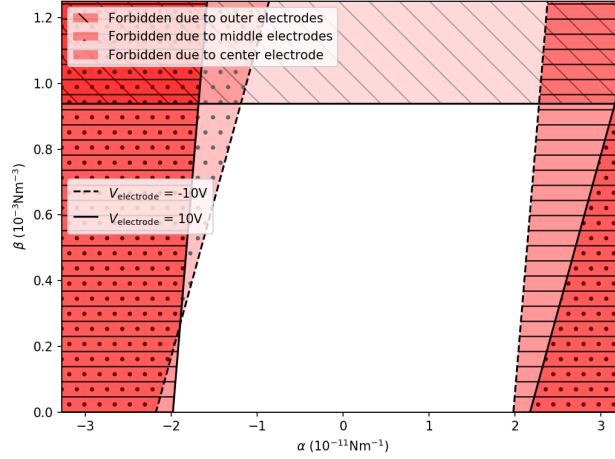
$$V_{el}(t, x) = \alpha(t)x^2 + \beta(t)x^4.$$

along the trap axis x is a prerequisite. This is doable using five electrodes as in [10] and we thus restrict ourselves to the five central electrode pairs of the HOA2 trap, Q15-Q24 as shown in Fig. B.1b.

When applying a set of voltages U_i (measured in V) to the considered electrodes, the overall potential along the trapping axis is then given by the superposition of the trap potentials V_i

$$V_{el}(t, x) = \sum_{i=Q15}^{Q24} V_i(x) \cdot U_i(t), \quad (B.1)$$

Figure B.3: $\alpha - \beta$ -confinements that are allowed by the maximal electrode voltage of ± 10 V. Since this constraint needs to be true for all electrode pairs, each electrode excludes a different area of the $\alpha - \beta$ -plane.



where the voltages $U_i(t)$ can change with time.

The problem of generating a desired potential $V_{\text{el}}(t, x)$ is then solved by using an optimisation algorithm on the voltages $U_i(t)$ to minimise the potential error $V_{\text{el}}(t, x) - \sum_{i=Q15}^{Q24} V_i(x) \cdot U_i(t)$. Similar to the approach in [15], this is done using the software package Gurobi [44], designed for solving convex optimisation problems.

This procedure can also be used to determine what range of potentials V_{el} can be implemented given a certain trap and voltage-generating electronics. This is done for the HOA2 trap in the next section.

B.2 Trap constraints

The major constraint on achievable potential shapes is given by the trap potentials V_i of the HOA2 trap and the fact that the used electronics in the TIQI group generate voltages of up to ± 10 V. To find the achievable potentials V_{el} , we determine the necessary voltages for purely harmonic and quartic potentials. The results are shown in Fig. B.3, where contour lines of each electrode pair reaching the limit of ± 10 V are shown on a grid of α and β -terms. The regions where one electrode pair violates this constraint are shaded and the region left white corresponds to combinations of α and β that can be achieved in the HOA2 trap.

To generate a high β -confinement, the constraint mainly lies in the need for a high voltage on the outermost electrodes O_L and O_R , which are not used at all to generate purely harmonic potentials. The cutoff due to the outer electrodes is therefore independent of α and lies at a value of $\beta_{\text{max}} = 0.92 \times 10^{-3} \text{ N m}^{-3}$.

To be sure that the voltage generation algorithm never comes too close to this boundary, the used value of the maximal quartic confinement of the HOA2 trap has been reduced slightly to $0.85 \times 10^{-3} \text{ N m}^{-3}$ in this thesis.

The constraints on the electrodes S , O_L and O_R depend on both α and β . This is due to the fact that the needed voltages for a term in α might be of opposite sign than those needed for β , thus leading a lower total voltage on that electrode and extending the achievable area in the $\alpha - \beta$ -plane. Note that the needed values of α , for example shown in Fig. 3.2c, are not an issue in this thesis as they are much lower than the achievable values shown in Fig. B.3.

Cooling two ions of unequal mass with a cubic-quartic potential

The cooling scheme for ions of unequal mass presented in chapter 5 relies on a linear term in the potential to enforce equal ion motional frequencies. Alternatively, a cubic term can be chosen for the same purpose. As a cubic function is "flatter" around zero than a linear function, such a potential might retain a double-well shape at short ion distances where the linearly tilted potential eq. 5.1 already yields a single well.

The potential is then given by adding a cubic term with prefactor $\delta(t)$ to the familiar quartic potential:

$$V_{\text{el}} = \alpha(t)x^2 + \beta(t)x^4 + \delta(t)x^3. \quad (\text{C.1})$$

In this chapter, parts of the dynamical normal mode decomposition will be given, namely the correspondence between the potential parametrisation $\{\alpha, \beta, \delta\}$ and the normal mode frequencies $\{\Omega_{\pm}\}$. This is the most lengthy and cumbersome step of the dynamical normal mode treatment.

The full Hamiltonian is given by

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V_{\text{tot}}(x_1, x_2, t)$$

$$V_{\text{tot}}(x_1, x_2, t) = \delta(t) (x_1^3 + x_2^3) + \alpha(t) (x_1^2 + x_2^2) + \beta(t) (x_1^4 + x_2^4) + \frac{C_C}{x_2 - x_1}. \quad (\text{C.2})$$

Note that in this chapter, the variables $\alpha, \beta, \delta, s, d, \lambda_{\pm}, \Omega_{\pm}, x_i^{(0)}$, are in general time-dependent, but we omit this in the notation.

As before, the Hamiltonian is reduced to a second-order approximation around the equilibrium positions of the ions. For this, the mass-weighted Hessian matrix K is diagonalised, yielding the normal mode frequencies.

The equilibrium positions of the ions fulfil

$$\left. \frac{\partial V_{\text{tot}}}{\partial x_i} \right|_{x_i^{(0)}} = 2\alpha x_i^{(0)} + 4\beta \left(x_i^{(0)}\right)^3 + 3\delta \left(x_i^{(0)}\right)^2 - \frac{(-1)^i C_C}{x_2^{(0)} - x_1^{(0)}} = 0, \quad (\text{C.3})$$

where $i = \{1, 2\}$. We introduce the familiar shifted parametrisation

$$\begin{aligned} x_1^{(0)} &= s - \frac{d}{2} \\ x_2^{(0)} &= s + \frac{d}{2}. \end{aligned} \quad (\text{C.4})$$

The mass-weighted Hessian K that needs to be diagonalised is given by

$$K = \begin{pmatrix} \frac{2\alpha + 6\delta x_1^{(0)} + 12\beta \left(x_1^{(0)}\right)^2 + \frac{2C_C}{d^3}}{m_1} & -\frac{2C_C}{\sqrt{m_1 m_2} d^3} \\ -\frac{2C_C}{\sqrt{m_1 m_2} d^3} & \frac{2\alpha + 6\delta x_2^{(0)} + 12\beta \left(x_2^{(0)}\right)^2 + \frac{2C_C}{d^3}}{m_2} \end{pmatrix} \quad (\text{C.5})$$

As in chapter 5, the condition that enforces equal ion frequencies is that the diagonal entries of this K need to be equal, as they correspond to the squared ion frequencies. Setting $K_{11} \stackrel{!}{=} K_{22}$ then again leads K to take the simple form $\begin{pmatrix} A & B \\ B & A \end{pmatrix}$, which is diagonalised by the same equal eigenvectors again as in chapter 5.

The eigenvalues of K are

$$\begin{aligned} \lambda_{\pm} = \Omega_{\pm}^2 &= \frac{1}{m_1} \left[2\alpha + 6\delta x_1^{(0)} + 12\beta \left(x_1^{(0)}\right)^2 + \frac{2C_C}{d^3} \right] \left[1 \pm \sqrt{\frac{m_1}{m_2}} \right] \\ &= \frac{1}{m_2} \left[2\alpha + 6\delta x_2^{(0)} + 12\beta \left(x_2^{(0)}\right)^2 + \frac{2C_C}{d^3} \right] \left[1 \pm \sqrt{\frac{m_2}{m_1}} \right]. \end{aligned} \quad (\text{C.6})$$

We now want to obtain the correspondence $\{\Omega_{\pm}\} \rightarrow \{\alpha, \beta, \delta\}$ between the potential parametrisation and the normal mode frequencies.

By building the difference of the eigenvalues $\Omega_{\pm}^2$, the distance d is easily obtained as

$$d = \sqrt[3]{\frac{4C_C}{\sqrt{m_1 m_2}} \frac{1}{\Omega_+^2 - \Omega_-^2}}. \quad (\text{C.7})$$

By utilising the expressions for the equilibrium position together with the sum of the eigenvalues, one obtains the following relations between α, β, δ and s :

$$\begin{aligned}
\beta &= \frac{m_1 + m_2}{8d^2} (\Omega_+^2 + \Omega_-^2) - \frac{2C_C}{d^5} \\
\delta &= \frac{m_2 - m_1}{12d} (\Omega_+^2 + \Omega_-^2) - 4\beta s \\
\alpha &= \frac{C_C}{d^3} - 6\beta s^2 + \frac{\beta d^2}{2} - 3\delta s.
\end{aligned} \tag{C.8}$$

Note that so far, we have obtained the formula eq. C.7 for d that only depends on the NM frequencies. From the above relations, only the one for β is thus complete, while the formulas for α and δ still depend on each other and on the centre shift s . For s , the following equation can be found after a lengthy calculation that involves adding the two equilibrium conditions eq. C.3:

$$\begin{aligned}
0 &= [8\beta] s^3 - \left[\frac{m_2 - m_1}{2d} (\Omega_+^2 + \Omega_-^2) \right] s^2 + \left[\frac{4C_C}{d^3} - 2\beta d^2 \right] s \\
&\quad + \left[\frac{m_2 - m_1}{8} d (\Omega_+^2 + \Omega_-^2) \right].
\end{aligned} \tag{C.9}$$

This is a cubic equation in s with coefficients that only depend on d and β , both of which already can be calculated from the NM frequencies $\Omega_{\pm}$. Solving this equation for s , one can then go on to resolve δ and from that α in the relations eq. C.8. The correspondence between NM frequencies and potential parametrisation is thus complete.

Now the usual STA approach could be continued by finding the auxiliary functions $\rho_{\pm}$ to fulfil the shortcut condition, calculating the NM frequencies and from there the time-dependence of the potential using the results of this chapter. This is however beyond the scope of this work.

Note that introducing a cubic term in the potential V_{el} necessitated solving a cubic equation later in the derivation. Should more complicated potential shapes involving terms with orders above four ever be necessary, for example when trying to find a cooling scheme for 1-to- n ions, this would probably mean that quintic or higher equations have to be solved when deriving the normal modes. As these equations have no analytic solution, designing the STA scheme will be challenging.

Appendix D

Motional exchange in the radial modes

Simultaneously cooling the radial modes along with the axial mode would make this cooling scheme more interesting. To find the strength of the exchange coupling of the radial modes, we thus generalise the derivation of the motional exchange frequency given in chapter 1 to include the motion in the radial directions y and z . We follow again the derivation by Brown in [30].

Consider two singly charged particles with coordinates $\vec{r}_1 = (x_1, y_1, z_1)$ and $\vec{r}_2 = (x_2, y_2, z_2)$ that are trapped in a potential with an axial equilibrium distance $x_0 > 0$ and radial equilibrium positions of $y_0 = 0$ and $z_0 = 0$. The Coulomb potential of this system is then given by

$$V_C(\vec{r}_1, \vec{r}_2) = V_C(\Delta x, \Delta y, \Delta z) = \frac{1}{\|\vec{r}_2 - \vec{r}_1\|} = \frac{1}{\sqrt{\underbrace{\Delta x^2 + \Delta y^2 + (\Delta z + d_0)^2}_{(\Delta r)^2}}} \quad (\text{D.1})$$

where we changed to coordinates $\Delta x = x_2 - x_1$, $\Delta y = y_2 - y_1$ and $\Delta z = (z_2 - z_1) - d_0$.

Again, this potential is to be expanded to second order by a Taylor series around the equilibrium coordinates $\Delta r = (d_0, 0, 0)$.

Firstly, the gradient is calculated as

$$\nabla V_C(\Delta x, \Delta y, \Delta z) = \begin{pmatrix} -\frac{\Delta x}{\|\Delta r\|^3} \\ -\frac{\Delta y}{\|\Delta r\|^3} \\ -\frac{\Delta z + d_0}{\|\Delta r\|^3} \end{pmatrix}. \quad (\text{D.2})$$

Secondly, the elements of the Hessian matrix are calculated. The off-diagonal elements are given by

$$\begin{aligned}
 \frac{\partial^2 V_C}{\partial \Delta x \partial \Delta y} &= \frac{\partial^2 U}{\partial \Delta y \partial \Delta x} = \frac{\partial}{\partial \Delta y} \left(-\frac{\Delta x}{\|\Delta r\|^3} \right) = \frac{3\Delta x \Delta y}{\|\Delta r\|^5} \\
 \frac{\partial^2 V_C}{\partial \Delta x \partial \Delta z} &= \frac{\partial^2 U}{\partial \Delta z \partial \Delta x} = \frac{\partial}{\partial \Delta z} \left(-\frac{\Delta x}{\|\Delta r\|^3} \right) = \frac{3\Delta x (\Delta z + d_0)}{\|\Delta r\|^5} \\
 \frac{\partial^2 V_C}{\partial \Delta y \partial \Delta z} &= \frac{\partial^2 U}{\partial \Delta z \partial \Delta y} = \frac{\partial}{\partial \Delta z} \left(-\frac{\Delta y}{\|\Delta r\|^3} \right) = \frac{3\Delta y (\Delta z + d_0)}{\|\Delta r\|^5}.
 \end{aligned} \tag{D.3}$$

The same calculations for the diagonal elements:

$$\begin{aligned}
 \frac{\partial^2 V_C}{\partial \Delta x^2} &= \frac{\partial}{\partial \Delta x} \left(-\frac{\Delta x}{\|\Delta r\|^3} \right) = \left[-\frac{1}{\|\Delta r\|^3} + \frac{3\Delta x^2}{\|\Delta r\|^5} \right] \\
 \frac{\partial^2 V_C}{\partial \Delta y^2} &= \frac{\partial}{\partial \Delta y} \left(-\frac{\Delta y}{\|\Delta r\|^3} \right) = \left[-\frac{1}{\|\Delta r\|^3} + \frac{3\Delta y^2}{\|\Delta r\|^5} \right] \\
 \frac{\partial^2 V_C}{\partial \Delta z^2} &= \frac{\partial}{\partial \Delta z} \left(-\frac{\Delta z + d_0}{\|\Delta r\|^3} \right) = \left[-\frac{1}{\|\Delta r\|^3} + \frac{3(\Delta z + d_0)^2}{\|\Delta r\|^5} \right].
 \end{aligned} \tag{D.4}$$

Evaluated at $\Delta r = (\Delta x, \Delta y, \Delta z) = (d_0, 0, 0)$, the Hessian becomes

$$H_{\Delta r=0} = \begin{pmatrix} -\frac{1}{\|\Delta r\|^3} & 0 & 0 \\ 0 & -\frac{1}{\|\Delta r\|^3} & 0 \\ 0 & 0 & -\frac{1}{\|\Delta r\|^3} + \frac{3d_0^2}{\|\Delta r\|^5} \end{pmatrix} = \begin{pmatrix} -\frac{1}{d_0^3} & 0 & 0 \\ 0 & -\frac{1}{d_0^3} & 0 \\ 0 & 0 & \frac{2}{d_0^3} \end{pmatrix}. \tag{D.5}$$

This yields the Taylor expansion of V_C

$$\begin{aligned}
 V_C(\Delta r) &\approx V_C(0) + (\nabla V_C)^T \Big|_{\Delta r=0} \cdot \Delta r + \frac{1}{2} \Delta r^T \cdot H_{\Delta r=0} \cdot \Delta r \\
 &= \frac{1}{d_0} + \frac{1}{d_0^2} \Delta z + \frac{1}{d_0^3} \Delta z^2 - \frac{1}{2d_0^3} \Delta x^2 - \frac{1}{2d_0^3} \Delta y^2.
 \end{aligned} \tag{D.6}$$

To check for consistency with chapter 1, one can set the radial variables to zero and expand the terms in Δz to obtain the same result as for the one-dimensional case in eq. 1.4. Since the motional exchange terms are generated by the quadratic terms Δx^2 , Δy^2 and Δz^2 , the exchange frequency ends up being the same for the radial directions x and y as for the axial direction z , only that it is multiplied by a prefactor of $\frac{1}{2}$. Also the radial terms are of opposite sign, giving the motional exchange an opposite phase.

We thus conclude that the exchange frequency for the radial modes is given by the same formula as for the axial mode, only that it is slower by a factor of 2. This means that the cooling scheme presented in this thesis is also feasible for the radial modes, only at increased cooling times. Simultaneous cooling of all modes is challenging as the radial and axial trapping frequencies usually differ, but also influence the exchange frequency.

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