A mapping approach to synchronization in the ‘Zajfman trap’: II. The observed bunch

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Abstract
We extend a recently introduced mapping model, which explains the bunching phenomenon in an ion beam resonator for two ions (Geyer and Tannor 2004 J. Phys. B: At. Mol. Opt. Phys. 37 73), to describe the dynamics of the whole ion bunch. We calculate the time delay of the ions from a model of the bunch geometry and find that the bunch takes on a spherical form at the turning points in the electrostatic mirrors. From this condition we derive how the observed bunch length depends on the experimental parameters. We give an interpretation of the criteria for the existence of the bunch, which were derived from the experimental observations by Pedersen et al (2002 Phys. Rev. A 65 042704).

1. Introduction

Ions in an ion trap usually behave like a gas: they try to fill all the available volume, defined by the trap’s electromagnetic fields. It was only in storage rings and some carefully designed traps with dedicated steering electrodes where the ions could be forced into well-localized bunches. But even there the ions’ mutual repulsion and the inevitable spread in their kinetic energies tend to redistribute the ions throughout the whole accessible volume (see [1] and, e.g., [2]).

Recently a surprising cooperative behaviour of the ions was discovered in a Zajfman trap [3], an ion trap resonator built of only two opposite electrostatic mirrors and two focussing lenses [4]: the ions are injected into the trap from an ion beam and this injected bunch of ions bounces back and forth between the two mirrors but does not diffuse in the trap—without any time-dependent control fields! The ions, which all have the same charge and also slightly different energies and trajectories through the trap, seem to ‘stick together’; they are not only confined to the trap volume, but also seem to be trapped within the bunch, which oscillates back and forth like a single macroscopic ‘super particle’. This bunch works as a ‘dynamic inner trap’, itself moving between the static electric fields of the external trap.
As a first application of this ‘Zajfman trap’ operating in the bunching regime a high resolution Fourier transform mass spectrometer has been demonstrated with a resolution of $\Delta m/m \approx 7 \times 10^{-6}$ [5]. This value was until now only achieved in storage rings [6]. This high resolution is made possible by observing the oscillations of the macroscopic bunch through the trap over time intervals of several tenths of a second. The observation time is limited by the trapping time of the ions in the inner trap (the bunch), which is determined by the number of collisions between the ions and residual gas atoms in the vacuum chamber [7].

The operating regime of the trap and the stability conditions, under which this counter intuitive ‘self-bunching’, or synchronization, occurs, were first explained by Strasser et al [5] by relating the ion dynamics to the so-called negative mass instability [1]: due to the special dispersion of the trap the period of an ion increases with its energy. This can be described by a negative effective mass of the ions. Consequently, the ions have to repel each other in order to synchronize their motion.

A microscopic explanation of the observed synchronization for two identical ions was given by the authors in [8] which we refer to as ‘part I’ in the following. There the problem is described by a set of simple mappings for the evolution of the ions’ relative coordinate through the different parts of the trap. The ions’ interaction is incorporated phenomenologically as a time delay. With this approach we not only confirm the already known stability conditions but also describe the microscopic process taking place: synchronization is a continued alternation of energy and position exchange between the two ions.

In this paper we show how the model of two identical ions can be generalized to describe the dynamics of the whole bunch. For this we associate one of the ions with a ‘test ion’, which moves through the cloud of the other ions, and the other describes the motion of the bunch’s CM. With the two identical ions we did not need to specify the interaction to explain the mechanism, but now the interaction potential that the test ion feels is an important part of the effect: it is derived from the charge distribution in the bunch, i.e., the test ion’s average position in the bunch, which in turn is determined self-consistently from the motion of the test ion inside this bunch. This test ion case is a specialization as well as a generalization of the two identical ions description: by specifying the interaction we can describe the generalized behaviour of arbitrarily many ions through a mean field treatment.

This paper is organized as follows: section 2 reviews the mapping approach of part I. We show that the approach can be extended from the two-ion case to $N$ ions. The key issue left unresolved in section 2 is how to calculate the time delay of the test ion in the bunch. This question is taken up in section 3, where we show how this parameter can be obtained from a mean field treatment of the bunch potential. A central result of section 3 is the derivation of the spherical geometry of the bunch at the turning points. In section 4 the dependence of the bunch length on the various parameters of the trap and the ions is derived. In section 5 the momentum spread of the bunch is calculated. Then, in section 6 we show how the experimental criteria for bunching deduced from the observations by Pedersen et al [9], are connected to our explanations. The results are summarized and further developments are sketched in section 7.

2. Review of the mapping model

2.1. Coordinate system, transit times and the dispersion relation

In this section we briefly review the basics of the two-ion case. For information about the trap and the experimental findings the reader is referred to [9, 10]. For more details about the mapping model we refer the reader to ‘part I’ [8].
Consider two ions with the simplified trap potential:

\[
V(x) = \begin{cases} 
0 & \text{when } |x| \leq \frac{L}{2} \\
\left(|x| - \frac{L}{2}\right)F & \text{when } |x| > \frac{L}{2}.
\end{cases}
\] (1)

\(F\) is the constant gradient of the mirror fields, \(L\) is the field-free distance between the two mirrors.

In general the two ions have masses \(m_1\) and \(m_2\) and charges \(q_1\) and \(q_2\), respectively. As synchronization shows up in the distance between the ions, we use centre of mass (CM) and relative coordinates. With the total mass \(M = m_1 + m_2\) and the reduced mass \(\mu = \frac{m_1 m_2}{m_1 + m_2}\) we define

\[
R = \frac{m_1 x_1 + m_2 x_2}{M} \implies \begin{cases} 
x_1 = R + \frac{m_2}{M} x \\
x_2 = R - \frac{m_1}{M} x.
\end{cases}
\] (2)

The corresponding momenta are

\[
P = p_1 + p_2 \implies \begin{cases} 
p_1 = \frac{m_1}{M} p + p \\
p_2 = \frac{m_2}{M} p - p.
\end{cases}
\] (3)

\(R\) and \(P\) are the CM coordinate and momentum, respectively; the relative motion is described by \(x\) and \(p\). The ions’ positions and momenta are denoted by \(x_1, p_1\) and \(x_2, p_2\).

With the ion–ion interaction \(W(x)\) the Hamiltonian for these two ions reads

\[
H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + q_1 V(x_1) + q_2 V(x_2) + q_1 q_2 W(x_1 - x_2)
\]

\[
= \frac{p^2}{2M} + \frac{p^2}{2\mu} + q_1 V \left( R + \frac{m_2}{M} x \right) + q_2 V \left( R - \frac{m_1}{M} x \right) + q_1 q_2 W(x).
\] (4)

To separate CM and relative coordinates when both ions are in the same part of the trap potential we need that \(q_1 V(x_1) + q_2 V(x_2) = (q_1 + q_2) V(R)\). With the potential of equation (1) we get the condition that both ions must have the same charge to mass ratio:

\[
\frac{q_1 m_2 - q_2 m_1}{M} = 0 \iff \frac{q_1}{m_1} = \frac{q_2}{m_2}.
\] (5)

For two identical ions this condition is trivially fulfilled. Here we describe a bunch of \(N + 1\) identical ions; then the above condition is also fulfilled, if we take one of the ions to be a test ion of mass \(m\) and charge \(q\) and identify the other with the remaining \(N \geq 1\) identical ions of the bunch:

\[
m_1 = m \quad m_2 = Nm
\]

\[
q_1 = q \quad q_2 = Nq.
\] (6)

The number of ions \(N\) is consequently a positive integer, which can be \(N = 1\), too. Now, with \(M = (N + 1)m\) and \(\mu = \frac{N}{N + 1} m\), the CM and relative coordinates (equations (2) and (3)) become:

\[
R = \frac{x_1 + N x_2}{N + 1} \implies \begin{cases} 
x_1 = R + \frac{N}{N + 1} x \\
x_2 = R - \frac{1}{N + 1} x
\end{cases}
\] (8)
and
\[ P = p_1 + p_2 \]
\[ p = \frac{N}{N+1} p_1 - \frac{1}{N+1} p_2 \]  
\(\iff\)
\[ \begin{cases} p_1 = \frac{1}{N+1} (P + p) \\ p_2 = \frac{N}{N+1} (P - p) \end{cases} \]  
(9)

In part I [8] we combined the geometry of the trap and the ions’ mass and energy into two parameters, which are derived from the times that the ions spend in the mirror, i.e., at \(|x| > L/2\), and in the central part of the trap, respectively.

An ion with the laboratory energy \(E_0\) and the momentum \(p_0 = \sqrt{2mE_0}\) spends the time \(T_m\) inside the mirror:
\[ T_m = \frac{2p_0}{qF} = \frac{2P}{NqF} \]  
(10)

\(T_m\) is one of the two parameters mentioned above.

When the ion turns around at \(T_m/2\) it has penetrated into the mirror potential for the distance
\[ X_m = \frac{E_0}{qF} \]  
(11)

The ions have the velocity \(p_0/m \approx P/M\) and therefore need the time
\[ T_i = \frac{Lm}{p_0} = \frac{LM}{P} := \alpha T_m \]  
(12)
to pass through the central field free region of the trap.

It turns out that not the times themselves but their ratio \(\alpha\)—the second parameter—determines, if synchronization occurs. When we express \(\alpha\) in terms of the experimental parameters, where \(U\) is the acceleration voltage, i.e. \(E_0 = qU\), we get
\[ \alpha = \frac{LqF}{4E_0} = \frac{LF}{4U} \]  
(13)

With \(T_m\) and \(T_i\) we calculate the total time \(T\) for one period as
\[ T = 2T_m + 2T_i \]  
(14)
\[ = \sqrt{\frac{2m}{q}} \left( \frac{4\sqrt{U}}{F} + \frac{L}{\sqrt{U}} \right) \]  
(15)

This form highlights the importance of the bunching effect for mass spectrometry applications: the period of the bunch, i.e., the synchronized ions, which can be measured very precisely for a huge number of revolutions, is directly related to the ratio \(\frac{m}{q}\).

The factor \(\alpha\) also shows up in the dispersion \(\frac{\partial T}{\partial p_0}\) of the trap, i.e., in the dependence of the period of one ion on its momentum. With equations (11) and (13) the dispersion is a simple relation between the ‘geometric’ parameters:
\[ \frac{\partial T}{\partial p_0} = \frac{4}{F} (1 - \alpha) = \frac{1}{U} (4X_m - L) \]  
(16)

For \((1 - \alpha) > 0\) the period \(T\) increases with the ion’s momentum \(p_0 = \sqrt{2mE_0}\) and vice versa.
2.2. Independent ions: the momentum kick and the basic mapping structure

In our model potential the CM and the relative motion separate for nearly all the time, except for a short interval $\tau_k$. This is the time between when the first ion crosses the kink between the flat part and one of the mirrors at ± $\frac{L}{2}$ and when the second one passes that point, too. During that time the ions are accelerated relative to each other by the trap potential. For the case of ions going into the mirror at $\frac{L}{2}$ it is

$$\tau_k = \frac{x}{p_2/m}. \quad (17)$$

After this time the momentum $p_2$ of the second ion will be the same, $p'_2 = p_2$, but $p_1$ is slowed down to

$$p'_1 = p_1 + \tau_k \left( -\frac{\partial V}{\partial x_1} \right) = p_1 - \frac{x m_2}{p_2} q F. \quad (18)$$

The two ions have almost the same velocity, so $\frac{p_1}{m_2}$ is approximated by $\frac{p_0}{m}$. The relative momentum $p = \frac{N}{N+1} p_1 - \frac{1}{N+1} p_2$ (9) now changes with equation (10) as

$$p' = p - \frac{N m}{N+1} q F \frac{p_0}{m} x = p - \frac{2 \mu}{T_m} x. \quad (19)$$

As $\tau_k$ is short, the relative distance $x$ does not change during this time in our approximation; also the ions’ very weak interaction can be neglected [8]. This sudden change of the momentum (19) can be formulated as a mapping $K$ of the relative distance and momentum $x$ and $p$ just before this kick onto the values $x'$ and $p'$ right after the kick:

$$K: \left( \frac{x}{p} \right) \mapsto \left( \frac{x'}{p'} \right) = \left( \frac{x}{p - \frac{2 \mu}{T_m} x} \right). \quad (20)$$

Without the ions’ interaction the relative coordinate evolves freely in the central part and inside the mirrors, leading to the two mappings $F$ and $M$, respectively, which differ only in the length of their time interval:

$$F: \left( \frac{x}{p} \right) \mapsto \left( \frac{x'}{p'} \right) = \left( \frac{x + \frac{T_m}{\mu} p}{p} \right) \quad (21)$$

$$M: \left( \frac{x}{p} \right) \mapsto \left( \frac{x'}{p'} \right) = \left( \frac{x + T_m p}{p} \right). \quad (22)$$

The complete dynamics of two noninteracting ions in their CM system can be described by these three mappings $K$, $F$ and $M$. They consequently form the foundation of our mapping model. With the ions’ interaction incorporated into this picture we are able to determine the stability conditions for bunching and, as we will show in this paper, also describe the extension of the whole bunch with respect to the external parameters.

2.3. Including the ion–ion interaction: the time delay and the stability condition

As shown in part I [8], the ions’ motion is synchronized by their repulsion when the ions interact in the mirror. Without further specifying the form of the interaction potential we can model its effect by a time delay $\tau_m$ that affects the relative motion when the ions’ paths cross each other. We include this delay $\tau_m$ into the mirror mapping as

$$M': \left( \frac{x}{p} \right) \mapsto \left( \frac{x'}{p'} \right) = \left( \frac{x + \frac{T_m}{\mu} \tau_m p}{p} \right). \quad (23)$$
Now we can determine the stability of the motion by calculating the eigenvalues of the linearized mapping

$$P'_{1/2} = F_{1/2} \otimes K \otimes M' \otimes K \otimes F_{1/2}$$

(24)
of a half period. They have the form

$$\lambda_{1/2} = -1 + 2\gamma \pm 2\sqrt{\gamma^2 - \gamma},$$

(25)

where we applied the abbreviation

$$\gamma = \epsilon (1 - \alpha) \quad \text{with} \quad \epsilon = \frac{\tau_m}{T_m}.$$  

(26)

Equation (25) was one of the central equations of part I. Analysing the two-ion case in this paper it will take on a new significance in describing the stability of the $N$-ion bunch.

The three mappings $K, M'$ and $F$ are independent of the ratio of the two masses $m_1$ and $m_2$; consequently, the behaviour of the relative coordinate and the stability criterion are the same here in the test ion case ($m_1 \ll m_2$) as for the two identical ions, which was discussed extensively in part I [8].

The eigenvalues $\lambda_{1/2}$ (25) are complex for $0 < \gamma < 1$. Then the test ion is stably synchronized with the bunch [11]—which then will be stable, as the test ion describes the motion of all the other ions in the bunch, too. This requires that the dispersion be positive, i.e., $\alpha < 1$, and the delay in the mirror be positive, $\tau_m > 0$. For a negative delay, $\tau_m < 0$, which would lead to synchronization for $\alpha > 1$, in general an attractive interaction is necessary, which does not occur for equally charged ions. We will in the following only consider the case of $\alpha < 1$ and $\tau_m > 0$, i.e. the interaction between the test ion and the other ions of the bunch is repulsive and it takes place around the bunch’s turning point in the mirror.

To explain the observed synchronization in the two-ion model of part I [8] it was sufficient that the ions experience a time delay, when their paths cross in the mirror. The magnitude of this delay did not matter, only its sign. However, for understanding the geometry of the $N$-ion case the magnitude is important as well. In section 3 we will show that the time delay can be obtained once one knows the bunch geometry, while the bunch geometry in turn determines the delay. Thus, these two quantities are determined self-consistently.

2.4. Incorporating the effect of off-axis motion

There is yet another difference between our one-dimensional model and the real trap that we need to include: in the real trap even two ions with exactly the same energy may have different periods, as the length of their orbits varies with the radial distance off the trap’s central axis. Pedersen et al characterized this spread of isoenergetic periods by a time difference $\Delta T_i$ [3]. If this spread is too big, synchronization is suppressed in the experiment.

As our one-dimensional model does not allow for off-axis orbits, we include this spread as an externally given parameter in the following way, explained for two identical ions: in the central part $T_i$ is effectively independent of whether a given trajectory lies on or off the trap’s central axis. So this difference in the period is accumulated in the mirrors. There a delay $\tau_i$ of one of the two ions with respect to the other due to the spatial dispersion leads to a bigger separation between the ions, which is equal to extending the time that the CM spends inside the mirror by $\frac{\Delta T_i}{2}$; if the total spread after one period is $\Delta T_1 = 2\tau_i$ we consequently have to replace the time interval $T_m$ in $M'$ (23) by $T_m + \frac{\Delta T_1}{4}$. This is valid for a test ion and the bunch, too. The mirror’s mapping then takes on the following form:

$$M' : \left( \begin{array}{c} x \\ p \end{array} \right) \mapsto \left( \begin{array}{c} x' \\ p' \end{array} \right) = \left( \begin{array}{c} x + \frac{1}{\mu} \left( T_m - \left( \tau_m - \frac{\Delta T_1}{4} \right) p \right) \\ p' \end{array} \right).$$

(27)
Figure 1. The phase-space positions of the ions in the injected bunch (a) serve as starting points for the ions’ oscillations around the centre of the bunch in the stable regime (b): no matter how small the energy (momentum) spread of the ion source is (a), the bunch’s internal energy in the trap depends on its length.

This form reduces to equation (23) when we define an effective delay
\[ \tau_m' = \tau_m - \frac{\Delta T_0}{4}. \]
Consequently the stability criterion \( \tau_m > 0 \) for \( \alpha < 1 \) has to be replaced by
\[ \tau_m' > 0 \iff \tau_m > \frac{\Delta T_0}{4}. \] (28)

The stability of the bunch is independent of the time spread \( \Delta T_0 \) (see [3]) caused by the finite energy resolution of the ion source: when the two ions are in the synchronized mode they oscillate around each other, exchanging momentum all the time. Therefore, even a beam which had been injected without any energy spread is ‘heated up’ corresponding to its length, as explained in [8] and figure 1. The energy spread of the initial injected bunch can be seen as a snapshot of the different ions somewhere on their orbit around the bunch’s CM.

This heating is related to the time delay \( \tau_m \), which we will determine in the following section. When we have actual numbers for \( \tau_m \) we will calculate the momentum and energy spread of the bunch.

3. Calculating the time delay and the bunch length

From the explanations of section 2.4 on the off-axis motion we conclude that the bunching phenomenon is more stable against perturbations when the time delay is larger: the observed bunch consequently will be the configuration that maximizes the delay for the given experimental parameters.

Thus, the key to understanding the properties of the \( N \)-ion bunch is to quantify the size of the time delay \( \tau_m \). This time delay depends on the bunch geometry, while the bunch geometry and stability in turn depend on the time delay. Thus these two quantities have to be determined self-consistently.

To do so we use the modified two-ion model introduced in the previous section: one of the ions with a mass \( m_1 = m \) is the test ion. It moves relative to the other ion with \( m_2 = Nm \), describing the CM of the other \( N \) ions of the bunch. The ions’ interaction, and therewith the time delay, which we did not have to specify in the two-ion case, is now derived from the bunch geometry.

3.1. Modified three-stage process

Consider first the case of non-interacting ions. Then we can divide the bunch’s behaviour in the mirror into three distinct steps (see figure 2): (i) at the first stage, the bunch enters the mirror. At this stage the ions get a compressing momentum kick, which for each ion is proportional to its distance from the CM (see equation (19)). Given the macroscopic length of the bunch, the momentum kick is much bigger than the spread of the ions’ momenta in the
central part of the trap. Therefore, to a very good approximation, the ions do not change their relative order, while the bunch contracts to some minimal length, shortly before the CM turns around in the mirror. (ii) At the second stage the CM turns around and the ions move through the now (stationary) bunch to the other side. (iii) At the third stage the bunch expands again on its way out of the mirror, until the second kick at the exit of the mirror undoes the first momentum kick and stops the expansion.

Now we have to incorporate the ions’ interaction into this process. When their interaction is weak compared to the momentum kick, this three-stage process will pertain. Since the effect of the ions’ interactions scales with their density their repulsion is most effective when the density is the highest, i.e., when the bunch is compressed to its minimal length at the turning point during the second stage. We incorporate the ions’ interaction into this stage only and arrive at a modified three-stage description: the first and last stages, where the bunch is compressed and expanded, respectively, remain unchanged. The modification is to the second stage only, during which the ions feel the potential of the compressed bunch and accumulate a time delay while they move to the other side of the bunch. Consequently the time delay and, therefore, all properties of the stable bunch are determined by its geometry at the turning point.

3.2. Transformation between the bunch lengths in the central part of the trap and at the turning points

As discussed in the previous paragraph, the motion of the ions during the second stage is determined by the momentum kick that they got at the entrance to the mirror. The magnitude of this momentum kick is in turn determined by the ions’ respective distances from the bunch centre when the bunch enters the mirror. We, therefore, have to derive a transformation for the first and third stages relating the bunch geometry in the central part of the trap to its extension at the turning point.

For noninteracting ions the length of the bunch in time is the same both at the observed length \( L_b \) and at the minimal length \( A \). It is identical to the time interval \( \tau_k \), which defines the momentum kick (17), expressed here with the average momentum \( p_0 \):

\[
\tau_k = \frac{L_b}{p_0/m}. \tag{29}
\]

The minimal length of the bunch occurs when the CM turns around in the mirror. Then the first ion, being in front by \( \tau_k \), has already returned from the turning point by the distance

\[
2A = q \left( -\frac{\partial V}{\partial X} \right)_{X_m} \frac{\tau_k^2}{2m}, \tag{30}
\]
while the last ion is still the same distance before \( X_m \) (11). Here we assume that the mirror potential at the turning point is linear over the (small) length \( 2A \) of the bunch.

In the two-ion case \([8]\) there was no need for some minimal bunch length, as the crossing time of two ions is always well defined, but for many ions the spatial extension of the continuous bunch translates into a length in time, during which the ions cross the bunch.

With the above form of \( \tau_k \) (29) and \( E_0 = \frac{p_0^2}{2m} \) we get

\[
A = \frac{q}{2E_0} \left( -\frac{\partial V}{\partial X} \right)_{X_m} L_b^2. \tag{31}
\]

Note that the form of the trap potential between the kink and the turning point does not influence the minimal bunch length: seen in the laboratory frame all ions ‘climb up’ the same potential ridge with essentially the same initial energy \( E_0 \); therefore, in our approximation their spacing in time remains constant all the way up to the turning point independent of the actual form of the mirror potential. We only require a linear potential right around the turning point.

For the following we nevertheless use the special form of our model potential (1) and come back to the general form only after we have analysed the behaviour of the observed bunch in our model potential. Then equation (31) becomes

\[
A = \frac{m}{2p_0 T_m} L_b^2. \tag{32}
\]

With the values of the initial experiment \([3]\), i.e., Ar ions with \( E_0 = 4.2 \) keV and \( F = 80 \text{kV m}^{-1} \), a bunch of, e.g., \( L_b = 2 \text{ cm} \) is compressed to \( A = 0.95 \text{ mm} \).

With the linear slopes at the turning point the bunch is contracted linearly during the first stage. Therefore, an arbitrary position \( x \) inside the uncompressed bunch of length \( L_b \) is transformed into \( x_i \) in the contracted bunch, i.e., when it has the length \( A \), as

\[
x_i = \frac{A}{L_b} x \quad \Rightarrow \quad x_i = \frac{mL_b}{2p_0 T_m} x. \tag{33}
\]

### 3.3. Calculating the time delay

According to the three-stage description explained above we have to deal with the following process: (i) the linear contraction translates an ion from a position \( x \) in the expanded bunch to the position \( x_i \) in the contracted bunch (33). (ii) From this position the ion starts to cross over the now stationary bunch potential to the other side until it reaches \( -x_i \). (iii) Finally, the linear interaction free expansion picks it up again.

Consequently, the time delay \( \tau_m \) due to the repulsive bunch potential is defined as the difference between the time \( T \) that the test ion needs to cross over the bunch of minimal length \( A \), starting from an initial position \( x_i \) up to the symmetric distance \( -x_i \), and \( T_0 \), the time needed for the same distance \( 2x_i \) without any potential:

\[
\tau_m = T - T_0 = \int_{x_i}^{-x_i} \frac{dz}{p(z)/m} - \frac{2x_i}{p(x_i)/m}. \tag{34}
\]

Note that with the interaction the spatially symmetric positions \( x_i \) and \( -x_i \) are not reached at times symmetric to \( T_m/2 \); all ions are delayed in the central stage, consequently they all reach their symmetric position on the other side of the bunch later than without interaction. The third, expanding stage only starts when all ions have changed to their respective side of the
bunch. Of course, this separation into three successive stages is an idealization, which will not be observed strictly in the experiment.

To calculate the times $T$ and $T_0$ we need the momentum of the ion at the end of the first stage, i.e., at $x_i$. In addition, to determine $T$ we need the explicit form of the bunch potential. These quantities will be calculated in the next two subsections.

### 3.3.1. Calculation of the momentum of the test ion

To evaluate equation (34) we start with the momentum $p(x_i)$: it is the sum of the ion’s initial momentum relative to the CM in the central part of the trap plus the momentum kick at the position $x$. For a macroscopic bunch the kick is much bigger than the momentum spread: an energy spread of 10 eV in the central part at an ion energy of 4.2 keV corresponds to a momentum spread of about 5.7 au for Ar$^+$ ions; during the time $T_m$ this momentum difference widens the bunch by about 0.25 mm, much less than the distance $2L_b$ of a few cm, which is traversed during the same time due to the momentum kick. We consequently neglect the momentum spread and calculate the ions’ energy relative to the CM from the kick alone.

The momentum change of one ion relative to the bunch at the position $x$ due to the kick was shown to be (equation (19) with $\mu = m$)

$$\Delta p = r_q q F = \frac{2m}{T_m} x.$$  \hspace{1cm} (35)

The corresponding energy relative to the bunch is $\epsilon = \frac{\Delta p^2}{2m} = \frac{2mx^2}{T_m}$. With the transformation $x = \frac{2p_0 T_m}{mL_b} x_i$ (33) we calculate the energy at the contracted position $x_i$ as

$$\epsilon(x_i) = \epsilon(x(x_i)) = \frac{8p_0^2}{mL_b} x_i^2.$$  \hspace{1cm} (36)

With $\epsilon(x_i)$ we can now determine $T_0$ (cf (34)):

$$T_0 = \frac{2x_i m}{\sqrt{2m\epsilon(x_i)}} = \frac{L_b m}{2p_0}.$$  \hspace{1cm} (37)

$T_0$ is independent of $x_i$ because due to the linear contraction of the bunch the momentum kick is proportional to the starting distance $x_i$.

### 3.3.2. Approximating the bunch potential

To calculate the time $T$ that the test ion needs to pass over the bunch we need the ions’ distribution in the bunch. From this we calculate the bunch potential and then the delay, which in turn determines if this specific bunch is stable. But if it is not stable for all $x_i$, the ions will redistribute, modifying the bunch potential. In a more exact treatment the bunch potential would have to be iterated so that for all ions in all parts of the bunch the stability criterion is fulfilled.

To keep the description simple we will not allow for an arbitrary bunch form but explicitly make the (mean field) ansatz that the ions are spread in a Gaussian distribution around the CM all of the time, i.e., in the central part of the trap and during the whole evolution through the mirror. With this assumption we only need one parameter to describe the width of the bunch. The charge density $\rho(x)$ of the contracted bunch will then be, with the total number of ions $N$ in the bunch and its length $A$ at the turning point:

$$\rho(x) = \frac{Nq}{\sqrt{2\pi}A} \exp(-x^2/2A^2).$$  \hspace{1cm} (38)
The ions interact via a repulsive Coulomb potential $\frac{q}{|x|}$. To allow them to pass by each other in our one dimensional model this singular potential is replaced by a so-called softcore Coulomb potential [12]:

$$W(x) = \frac{q}{\sqrt{x^2 + d^2}}.$$  (39)

The ‘softcore parameter’ or ‘impact parameter’ $d$ is a measure for how close the ions have to come when passing each other; it describes the radius of the ion beam in the trap potential.

With this ansatz and the Gaussian density profile (38) we calculate the bunch potential $W_b$ as

$$W_b(x_i) = \int \frac{dz q\rho(z - x_i)}{\sqrt{z^2 + d^2}}.$$  (40)

We could now insert this potential into (34), but then the delay for a specific ion depends on where it is located in the bunch. Therefore, we concentrate for the following on the ions around the centre of the bunch. Introducing $V(x_i)$ as the quadratic expansion of $W_b$ around the centre of the bunch, we have

$$W_b(x_i) \approx V(x_i) \equiv W_b(0) - \frac{m\omega^2}{2} x_i^2.$$  (41)

Clearly, we have

$$-\frac{\partial^2}{\partial x^2} W_b(x) \bigg|_{x=0} = m\omega^2,$$  (42)

a relation which will be needed below.

With this harmonic approximation we get for the energy $E_i = E(x_i)$ of the ion above the top of the bunch potential:

$$E_i = \epsilon(x_i) + V(x_i) - W_b(0) = \left(\frac{8p_0^2}{mL_b^2} - \frac{m\omega^2}{2}\right) x_i^2.$$  (43)

From this energy we may calculate the position-dependent momentum as

$$p(z) = m\omega \sqrt{\frac{2E_i}{m\omega^2} + z^2}.$$  (44)

Remember that $x_i$ denotes the starting position of the ion at the end of the first compressing stage, just as it starts to cross the bunch during the second stage, while the integration variable $z$ denotes the (time-dependent) position during the second, the crossing stage.

Using equations (34) and (44) the time $T$ that the ion needs to cross over the approximated bunch potential $V(x_i)$ (41) evaluates as

$$T = \frac{2}{\omega} \text{arsinh} \left[ \frac{L_p m \omega}{\sqrt{16 p_0^2 - L_b^2 m^2 \omega^2}} \right].$$  (45)

Here we reinserted the initial energy of the ion $E_i$ (43) into the time-dependent momentum $p(z)$ (44). Again, as for $T_0$, $T$, and therefore $\tau_m$, is independent of $x_i$ due to the harmonic approximation (41). This approximation allows us to focus on how the delay depends on the parameters of the trap and the bunch without having to deal with a whole range of initial conditions $x_i$. Remember that we already had neglected the ions’ momentum against the momentum kick.
The second derivative in $m\omega^2$ (42) and the integration in $W_b$ (40) can be interchanged to further evaluate the curvature of the bunch potential’s top:

$$m\omega^2 = \frac{q^2 N}{\sqrt{2\pi A^5}} \int \frac{dz}{\sqrt{z^2 + d^2}} e^{-z^2/2A^2} \left(1 - \frac{z^2}{A^2}\right)$$

$$= \frac{q^2 N}{\sqrt{2\pi A^5}} \int dy e^{-y^2/2} \frac{1 - y^2}{\sqrt{(d/A)^2 + y^2}}. \quad (46)$$

By changing the integration variable to $y = z/A$ the integral depends only on the fraction $\delta = d/A$, i.e., the ratio between the beam diameter $2d$ and the (total) length $2A$ of the bunch. In the following we will abbreviate the integral as

$$I(d/A) = I(\delta) = \int dy e^{-y^2/2} \frac{1 - y^2}{\sqrt{\delta^2 + y^2}}. \quad (47)$$

From the expressions for $\tau_m$ according to (34), (37), (45) and (46) we could now calculate the time delay numerically and learn about its behaviour. But these expressions are too complex to easily ‘see’ the dependences on the various parameters. We will therefore derive a simplified form thereof in the following section.

3.3.3. Linearizing $\tau_m$. In the previous section we derived the equations necessary to calculate the time delay numerically for a given trap configuration. However, these equations can be simplified so that the central stability criteria become much more obvious.

We can linearize the above set of equations by expanding both the Arsinh and the square root in equation (45). This approximation is valid for $L_b m\omega \ll 4 p_0$, i.e., when the ions’ energy from the momentum kick is much higher than necessary to cross the bunch (cf equation (43)). Then the resulting delay is small. From equations (38), (40) and (42) we see that $W_b$, and therefore $m\omega^2$, scales linearly with $N$. When $N$ is kept small enough this condition is fulfilled even for a short bunch or a thin beam.

We first set $(1 - x)^{-1/2} \approx 1 + x/2$ and then $\text{Arsinh}(x) \approx x - x^3/6$ to approximate equation (45) as

$$T \approx \frac{2}{\omega} \text{Arsinh} \left[ \frac{L_b m\omega}{4 p_0} \left(1 + \frac{L_b^2 m^2 \omega^2}{32 p_0^3}\right) \right] \approx \frac{L_b m}{2 p_0} \left( \frac{L_b m}{2 p_0} \right)^3 \frac{\omega^2}{12} + O(\omega^4). \quad (49)$$

The first summand in the second line equals $T_0$ (37). With equations (10), (32), (46) and (47) we finally arrive at an expression for $\tau_m$, which depends only on parameters that describe the bunch at the turning point in the mirror:

$$\tau_m = \frac{\sqrt{m}}{12} \left( \frac{A}{q F} \right)^{3/2} m\omega^3 \quad (50)$$

$$= \frac{\sqrt{mq}}{12 \sqrt{2\pi F^{3/2}}} \frac{N}{A^{1/2}} I(\delta). \quad (51)$$

Finally two degrees of freedom are left, which the bunch can adjust to achieve the most stable configuration, i.e., the biggest $\tau_m$: the number of ions $N$ and the ratio $\delta = d/A$ between the beam width and the bunch length at the turning point. All other quantities are fixed in the experiment.
From (51) it is readily seen that the delay is proportional to the number of ions $N$ in the bunch:

$$\tau_m \propto N.$$ \hspace{1cm} (52)

The bunch can consequently stabilize itself by taking up more ions; or, put the other way, the bunch has the tendency to keep all ions together. It is stable with respect to the number of ions.

### 3.4. Spherical bunch geometry

The dependence of $\tau_m$ on the beam diameter $d$ and the bunch length $A$ at the turning point in the mirror is less obvious, but if there is a ‘most efficient’ value of $A$, i.e., one for which the delay is maximal for a given $d$, then for this configuration the derivative $\frac{\partial \tau_m}{\partial A}$ vanishes.

Combining all the prefactors which are not related to $d$ or $A$ into one constant $C = \frac{Nq\gamma m}{12\sqrt{2\pi}\Gamma(3/2)}$ we get from (51) and (47):

$$\frac{\partial \tau_m}{\partial A} = \frac{C}{2A^{3/2}} \int dy e^{-y^2/2} (y^2 - 1) \frac{3y^2 + \delta^2}{\sqrt{\delta^2 + y^2}}.$$ \hspace{1cm} (53)

It will be shown later that the extremum at $\frac{\partial \tau_m}{\partial A} = 0$ is in fact a maximum. Since $C$ and $A$ always have a finite value, the maximum of $\tau_m$ is consequently determined by that value of $\delta$, for which the integral vanishes. This happens for $\delta = 1.01689\ldots$, which is about unity. Consequently, $\tau_m$ is maximal for $A \approx d$, i.e., when the bunch at the turning point has a spherical form. With $A = d$ the integral (47) in (51) takes on a constant value of $I(1) = 0.5778\ldots$.

This value of $\delta$ of nearly unity becomes more clear when we artificially replace for a moment the softcore interaction in the convolution of $W_b$ (40) by a Gaussian with a width $d$, i.e.,

$$W_b(x_i) \simeq \frac{Nq}{2\pi A d} \int dz e^{-z^2/2} e^{dz-x_i^2/2A^2}.$$ \hspace{1cm} (54)

With equation (42) this gives

$$m\omega^2 = \sqrt{\frac{2}{\pi}} \frac{Nq}{d^3(1+(A/d)^2)^{3/2}}.$$ \hspace{1cm} (55)

Plugging equation (55) into (50) we find with the same $C$ as above that

$$\tau_m = 2C \left( \frac{A}{d^2 + A^2} \right)^{3/2}.$$ \hspace{1cm} (56)

Now $\tau_m$ has its maximum where

$$\frac{\partial \tau_m}{\partial A} = \frac{3CA^{1/2}}{(d^2 + A^2)^{3/2}} (d^2 - A^2) = 0.$$ \hspace{1cm} (57)

In other words, given exactly the same functional form for both the longitudinal bunch form and the transverse bunch potential the delay $\tau_m$ has its maximum at exactly $A = d$. This result is not surprising as now both ingredients of the longitudinal bunch potential enter in a symmetric fashion, i.e., with the same functional form and on equal footing. Then the symmetric case of their width parameters being equal is clearly a special point; here the delay is maximal.

The slight offset to unity of the result obtained using the softcore potential can consequently be attributed to the fact that there were two different functional forms used.
for the longitudinal bunch profile and the transverse potential. Actually, these two quantities have different physically origins.

This result that a spherical bunch with \( A = d \) leads to the biggest delay can be understood in the following way: when the bunch is prolate, i.e., \( A > d \), the potential is flatter and slows down the ions less, whereas in a shorter, oblate bunch the distance \( 2x_i \), over which the delay is accumulated, shrinks faster than the increasing effect of the steeper potential barrier. Of course, somewhere in between these two extremal cases there has to be a maximum, apparently when the bunch is spherical at the turning point.

One might argue that for very short bunches the potential barrier should finally become so high that the ions come to a stop on top of the barrier. Then the delay would be high, too. But it is not only the length \( A \) of the bunch, which determines the potential’s form, but also its width \( d \): the curvature \( m \omega^2 \) at the potential top is limited by the wider of the two functions contributing to \( W_b \) (see equation (40)), be this the Gaussian ion distribution or the softcore Coulomb interaction.

With the more realistic softened Coulomb potential we obtained an optimal bunch form of \( A \) slightly less than \( d \), but for simplicity we will use \( A = d \) in the following. As this paper focuses on the general behaviour of the bunch and not on highly accurate numbers this small difference of a few per cent is clearly negligible.

Using \( A = d \), i.e., a fixed \( I(\delta) \), we see from equation (51) that the maximum delay for an otherwise fixed trap configuration scales with the adjustable parameters \( N \) and \( A \) as

\[
\tau_m \propto \frac{N}{A^{3/2}} \propto \frac{N}{d^{3/2}}.
\]

The result obtained above, that the most stable configuration is a bunch which is spherical at the turning point, is of central importance. As shown in part I [8] synchronization is an interplay between the dispersion of the trap and the delay that the ions experience when the bunch turns around at the turning point. The trap dispersion is fixed by the mechanical and electrical set-up of the trap. Only the delay, which is the other central ingredient of synchronization, can adapt. It is striking that in its most stable configuration the bunch has a spherical form at the turning point. The bunch observed in the central part of the trap is then the ‘projection’ of this spherical bunch out of the mirrors.

To arrive at equation (51), which is independent of the ions’ initial conditions and is ‘local in the turning point’, it was important that both the top of the bunch potential and the ions’ energy relative to the CM had the same quadratic dependence on the distance from the bunch’s centre. This is a consequence of the constant slopes of the mirror fields. But if the mirror is not linear, the bunch’s potential at the turning point can still be expanded as in equation (41). If the bunch is not contracted linearly from \( L_b \) into \( A \) in the real experiment’s mirror field, then the energy \( \epsilon(x_i) \) of the ions will not be quadratic in \( x_i \), but in any case it is a symmetric function of the distance from the CM. It can therefore at least be approximated by a quadratic dependence. Then \( \tau_m \) depends on \( x_i \), but the delay is still maximal for \( A \approx d \).

### 3.5. The bunch length in the central part of the trap

With the above result, i.e., by setting \( A = d \), we can use the transformation (31) to predict the observed bunch length \( L_b \) as

\[
L_b = \sqrt{\frac{8E_0d}{q}} \left( -\frac{\partial V}{\partial X} \right)^{-1} x_n.
\]
With the model potential of equation (1) we have \((-\frac{\partial V}{\partial X}) = F\) and, by expressing the ions’ energy through the acceleration voltage \(U\) as \(E_0 = qU\), the observed bunch length becomes

\[
L_b = \sqrt{\frac{8U}{F}}d = \sqrt{8X_md}. \tag{60}
\]

For the definition of \(X_m\) see (11). In our model trap \(L_b\) is determined solely by the geometric trap parameters at the bunch’s turning point: the penetration depth \(X_m\) of the ions into the mirror and the beam width \(d\) at this point. There a spherical bunch is formed, which is then ‘projected out’ into the trap’s central region. The position \(X_m\) of the turning point itself is of course determined by the ions’ energy.

Note that the observed bunch length does not depend on either the mass \(m\) of the ions or on their number \(N\), though the time delay \(\tau_m\) does (see equations (51) and (58)): the reason for this unexpected behaviour is that the condition for maximal delay is that the integral in the derivative \(\frac{\partial \tau_m}{\partial A}\) (53) be zero—a condition which only depends on the geometric properties \(d\) and \(A\) at the turning point. More or heavier ions lead to a higher delay, but do not change the bunch length of maximal delay.

This independence of the observed \(L_b\) on both \(m\) and \(N\) in our model is fully consistent with the experiments of Pedersen et al. They observe that after an initial thermalization stage ‘[…] the width is essentially constant, although the number of ions in the bunch decreases exponentially with time […]’ (see section B.1 of [9]). By comparing the asymptotic bunchlength from Ar\(^+\) and Xe\(^+\) ions of both 4.2 keV energy they find that the length in space is independent of the ion mass \(m\) (see section B.3 and figure 9 of [9]).

That the turning point is of central importance for the bunching could already be seen from the transformation (31); the form of the potential between the field free region and the turning point has no effect on the relation between \(A\) and \(L_b\); what matters is the slope at the turning point.

With the numerical values of the experiment, i.e., \(E_0 = 4.2\) keV, \(q = +1\) and an average \(F = 80\) kV m\(^{-1}\) we get \(X_m = 5.25\) cm. In [9] a beam radius of \(d = 0.5\) mm was derived from trajectory calculations. These trajectory calculations also had predicted a spherical bunch at the turning point. With this value of \(d\) we predict an observed bunch length in the central part of the trap of \(L_b = 1.45\) cm. Ar\(^+\) ions with the above \(E_0 = 4.2\) keV have a velocity of \(v_0 = 14.2\) cm µs\(^{-1}\), our \(L_b\) therefore corresponds to a length in the time domain of \(W_b = 0.1\) µs. For comparison Pedersen et al measured a value of \(W_b \approx 150\) ns (figure 9(a) of [9]) for \(V_1 \geq 4.5\) kV.

The greatest uncertainty in comparing our results to the measurements stems from the greatly simplified form of our model potential. In the experiment only the voltage on the last of the five electrodes was varied, we can therefore not expect that the resulting field is linear. Due to geometrical limitations, i.e., the length \(L\) of the trap is fixed and the maximal \(X_m\) is limited in the experiment, it will be difficult to check the validity of equations (59) or (60) over a wide range of parameters. Also the beam width \(d\) and the slope of the mirror potential \((-\frac{\partial V}{\partial X})\) at the turning point have to be determined from trajectory simulations for each field configuration.

With (11) and (13) the kinematic regime \(\alpha < 1\) in which the trap has to be operated is described by the following condition (see also equation (16)):

\[
E_0 > \frac{LqF}{4} \quad \text{or} \quad X_m = \frac{E_0}{qF} > \frac{L}{4}. \tag{61}
\]
The second form is a requirement on the trap’s geometry: the mirrors have to be ‘long’ enough, otherwise bunching cannot be observed.

From this condition—which is another way of expressing the bunching criterion $\alpha < 1$—we see that there is a minimal bunch length determined by the length $L$ of the field free region and the beam diameter $2d$ at the turning point:

$$L_b = \sqrt{\frac{2Ld}{\alpha}}.$$ (62)

Note that though the delay increases with the number of ions in the bunch (58), the observed $L_b$ itself is independent of $N$ in this approximation and is determined by external parameters only.

### 4. Numerical illustration of the behaviour of the time delay

In section 3 we set up and determined $\tau_m$ with the quadratic approximation to the bunch potential. The result is described by equations (37) and (45). Then we linearized $T$ (45) and found our central result that the time delay is maximal for $A = d$. Now we go back to equations (37) and (45) and numerically calculate the time delay from them. This will both confirm our findings with the linearized $T$ and illustrate the behaviour of the bunch with respect to the most important parameters.

The delay depends on a number of parameters, some of which are ‘externally given’, i.e., fixed for the given experimental set-up, while others describe how the bunch ‘reacts’ to this environment. For instance, the size $L$ of the trap, the energy $E_0$, the charge $q$ and the mass $m$ of the ions and the slope of the mirror fields $F$ are fixed. Derived from those are the momentum $p_0 = \sqrt{2mE_0}$, the time $T_m$ (10) and the dispersion parameter $\alpha$ (13), which we consider fixed, too. In the following these quantities will be set to their respective experimental values of $E_0 = 4.2 \text{ keV}$, $F = 80 \text{ kV m}^{-1}$, $q = +1 \text{ e}$ and $m = 40 \text{ amu}$, which were used in the initial experimental discovery of the bunching effect [3]. With these values we get $T_m = 1.48 \mu s$ and $\alpha = 0.956$.

On the other hand we have the number of ions in the bunch $N$, the observed length $L_b$ and the length $A$ in the mirror. There is no constraint on these quantities, so the bunch will try to adjust them to achieve the most stable configuration possible in the given trap regime. The two lengths, $L_b$ and $A$, are not independent, though. They are connected to each other by the transformation (31), determined by the slope of the mirror potential at the turning point. We view the minimal length in the mirror, $A$, as the more fundamental of these quantities, characterizing the minimal width in the mirror region where the ions cross the bunch; the experimentally observable $L_b$ is merely the projection of this contracted length out of the mirror. We do not expect the absolute values which we predict for the observed $L_b$ to be exact, but we expect that the important dependences, governed by $A$, will be reproduced.

The parameters we mentioned up to now are easily classified as fixed or variable. The beam radius $d$ has a special role: it belongs to the fixed quantities, as it is determined by the electrostatic potentials on the mirror electrodes, but in our treatment it appears as a constituent of the bunch potential $W_b$ (40) and it is closely intertwined with $A$, as we have seen above. We already know from equation (53) that the delay is maximal for $A \approx d$. Nevertheless, we will treat $d$ as a variable parameter in the following numerical illustrations—just to see our results of the previous section confirmed.

We will now in turn vary each of these three parameters, $A$, $d$ and $N$, while the other two remain fixed. This will give three different views on the behaviour of the bunch.
Figure 3. Time delay that the ions experience when they cross the bunch at the turning point with respect to the length of the bunch \( A \) at the turning point. The delay is calculated from (37), (45) and (46) for a constant number of ions \( N = 10^6 \) and three different externally given beam diameters of \( d = 0.2 \) mm ( - - - ), \( 0.5 \) mm ( — - — ) and \( 1 \) mm (——). The arrows indicate for each curve where the bunch length is equal to the beam diameter, i.e., \( A = d \). The thin broken curve plots for \( d = 0.5 \) mm the weighted average of the delay from the equations of motion with the full bunch potential, i.e., without the harmonic approximation (41) (see the text).

4.1. Time delay versus bunch length \( A \) and validity of the approximations

First we look at the time delay as a function of the bunch length \( A \) for fixed \( N \) and \( d \). We evaluate equations (37), (45) and (46) with \( N = 10^6 \) for three values of \( d \)—0.2 mm, 0.5 mm and 1 mm—and plot the results in figure 3. For short bunches, i.e., small \( A \), and for long bunches the delay is small with a maximum in between. This maximum of \( \tau_m \) occurs around \( A = d \), where the length and the width of the bunch are equal. This is exactly the behaviour predicted in the previous section.

The linearized result (51), from which we derived the condition \( A = d \), is indistinguishable from the full solution in figure 3; it differs by less than one per cent for small \( A \) and coincides for larger \( A \). This highlights the fact that with these parameters the delay of the ions through the bunch is a small perturbation compared to the momentum kick from the mirror potential.

To check the validity of our harmonic approximation of the bunch potential (41) we numerically evaluated \( \tau_m \) from equation (34). This means that we still keep the modified three-stage model of section 3.1, where the interaction between the test ion and the bunch is confined to the second stage, during which the bunch is static. The position-dependent momentum \( p(z) \) in equation (34) is calculated from its energy from the momentum kick \( \epsilon(x_i) \) (36) and the bunch potential \( W_b(x_i) \) of equation (40) as

\[
p(z) = \sqrt{2E(z)m} \quad \text{with} \quad E(z) = \epsilon(x_i) - (W_b(0) - W_b(z)).
\]

\( E(z) \) is the energy of the ion above the bunch potential. The resulting delay \( \tau_m = \tau_m(x_i) \) now depends on the ion’s position in the bunch \( x_i \) (33) at the end of the first stage, during which the bunch was compressed.

In figure 4 the delay \( \tau_m \) is plotted against the starting position \( x_i \) for \( A = d = 1 \) mm. For comparison also the contracted longitudinal bunch profile \( \rho(x_i) \) is shown. We see that \( \tau_m \) decays much slower with increasing distance \( x_i \) from the bunch’s centre than \( \rho(x_i) \); at \( x_i = 2.5 \) mm, where the bunch density becomes negligible, \( \tau_m \) is still half of the maximal value close to the centre. Thus most of the ions have a \( \tau_m \) of about the same magnitude. Consequently,
Figure 4. Time delay $\tau_m(x_i)$ computed from the equations of motion (solid line) and the ion density $\rho(x_i)$ of the bunch at the turning point (broken curve) against the initial distance $x_i$ (33), both for $A = d = 1$ mm (cf equation (38)). The solid horizontal line denotes the weighted average $\langle \tau \rangle$ of $\tau_m$, while the two vertical broken lines at $x_i = \pm A$ mark the width of the ion bunch.

Figure 5. Time delay as a function of the beam diameter for $N = 10^6$ and various fixed bunch lengths of $A = 0.5$ mm (- - -), 2 mm (— —) and 8 mm (— - —). The enveloping solid line marks the time delay for $A = d$ according to (58); the dots indicate the diameters, which correspond to the three bunch lengths shown. These correspond to values of $L_b$ of 14, 29 and 58 mm, respectively.

The density averaged delay $\langle \tau \rangle$ for $d = 0.5$ mm is given in figure 3 as a thin broken curve. It is quite close to the result with the harmonic approximation to the bunch potential. Thus, both the approximation to $W_b$ (41) and the subsequent linearization of $T$ ((48) and (49)) are justified. For the following illustrations we will therefore continue to evaluate equations (37), (45) and (46).

### 4.2. Time delay versus beam diameter $d$

When we now keep the bunch length fixed and vary the beam diameter the maximum of the delay for a spherical bunch shows up again. In figure 5 the delay is plotted for three different bunch lengths. It decreases with increasing beam diameter, but for fixed $d$ the maximum is at $A = d$. This configuration is indicated by the solid enveloping line with a slope of $-3/2$ according to equation (58).
Figure 6. (a) Maximal time delay achievable at a given beam diameter and (b) the observed bunch length $L_b$, for which this maximal $\tau_m$ is reached, as a function of the number of ions $N$. For further explanations please see text. The thin solid lines indicate in (a) the linear relation between $\tau_m$ and $N$ (52) and in (b) the constant $A = d$ according to the linearized solution of section 3.3.3.

From this plot it can be seen, too, that when the spatial dispersion requires a minimal delay of, e.g., $\Delta T_i/4 \approx 0.025$ ns (see (28)) then the beam has to be focussed to a radius of not more than 1 mm.

The necessary radial focussing can also be determined by inserting $A = d$ and $4\tau_m > \Delta T_i$ (28) into equation (51). The beam radius in millimeters has to be smaller than

$$d[\text{mm}] < 5.02 \times 10^{-4} \frac{(mq)^{1/3}N^{2/3}}{F\Delta T_i^{2/3}},$$

when the mass $m$ is given in atomic mass units (amu), the charge $q$ in elementary charges, the slope $F$ in kV m$^{-1}$ and the dispersion $\Delta T_i$ in nanoseconds.

4.3. Time delay versus ion number $N$

Another view of the behaviour of the time delay is presented in figure 6. Now for given $N$ and $d$ the bunch length $A$ is optimized to maximize the time delay. Panel (a) plots the maximal delay according to the optimized $A$. Panel (b) gives the corresponding observed bunch length $L_b$. Both the maximal $\tau_m$ and $L_b$ are plotted versus $N$ for two different values of $d$.

For small $N$ the delay grows linearly with $N$, as already derived in equation (58). This behaviour is depicted by the thin solid lines of slope 1 in panel (a). In this linear regime the bunch is spherical, as can be seen in panel (b): $L_b$ is constant, which implies that $A$ is constant, too (see (32)). The thin solid lines in panel (b) mark the values of $L_b$, which result from inserting the two beam radii $d = 0.5$ mm and $d = 0.2$ mm into (32).

For higher ion numbers, however, the maximal achievable delay increases (panel (a)) and is reached for shorter and shorter bunches (panel (b)). Finally, the ion number, and therefore
the density of the bunch, will become so high that the ions cannot pass over the bunch any more with the energy from the momentum kick. The ions then bounce back from the bunch and do not reach the other side any more. This is where \( 4p_0 \leq L_b m \omega \), consequently our formulation for the crossing time \( T \) (45) breaks down.

Inserting equations (46), (32) and (10) into this condition \( 4p_0 \geq L_b m \omega \) for (45) to be valid we see that this determines the maximal number \( N \) as

\[
N_{\text{max}} = \frac{4\sqrt{2\pi}}{T(1)} \frac{d^2 F}{q}.
\]  

(66)

Note that \( N_{\text{max}} \) is proportional to the beam area via \( d^2 \); this is consistent with our previous explanation that there is a maximal potential barrier from the contracted bunch that the ions can overcome with the energy from the momentum kick.

Consequently there are—for a given \( d \)—two limits for the number of ions in a bunch: the lower limit is determined by the minimal delay necessary to compensate for the spatial dispersion \( \Delta T \), and the maximal \( N \) stems from the requirement that the ions have to be able to pass over the contracted bunch’s potential.

Equation (65) in the previous section can be solved for the minimal number of ions necessary to support a given spatial dispersion \( \Delta T \):

\[
N_{\text{min}} = \frac{3\sqrt{2\pi}}{T(1)} \frac{d^{3/2} F^{3/2}}{\sqrt{m q}} \Delta T.
\]  

(67)

With the numbers from the experiment we calculate from (66) and (67) that for a beam radius of \( d = 0.5 \text{ mm} \) and a dispersion of \( \Delta T = 0.1 \text{ ns} \) [3] the number of ions may vary in the range of \( N = 3 \times 10^5 \text{ to } 2 \times 10^8 \), i.e., over nearly three orders of magnitude. Within this range the bunch length is independent of the number of ions.

This is consistent with the experimental observation that the bunch length is essentially independent of the density of the injected ion beam over at least three orders of magnitude [3]. Our estimate is more restrictive, especially \( N_{\text{max}} \) is bigger in the experiment. The reason lies in our harmonic approximation for \( \tau_m \): as we see from figure 4 the delay is smaller for ions in the wings of the bunch, which means that for them the momentum kick increases faster than the height of the potential barrier. These ions will be able to pass over a bunch, which already reflects the ions close to its centre. These will move away from the centre of the bunch. Consequently the form of the bunch changes, allowing the bunch to be stable for higher ion densities at the turning point than we estimated here. In order to find the ‘true’ \( N_{\text{max}} \) a dynamical model with a truly self-consistent bunch potential has to be used; our fixed Gaussian form of the density is too simplified to give accurate numbers in this extreme regime.

5. Momentum spread of the bunch

In section 2.4 we stated that the bunch is heated up to a specific energy spread in the trap by the momentum kicks from the trap potential, no matter how small the initial energy spread at injection time had been.

In ‘part I’ we derived a relation between the maximal distance between the two ions \( x_{\text{max}} \) and their maximal relative momentum \( p_{\text{max}} \) in the central part of the trap. As explained in section 2.4 in the real trap the effective delay \( \tau'_m = \tau_m - \Delta T/4 \) has to be used, and therefore equation (37) of [8] becomes

\[
p_{\text{max}} = \frac{x_{\text{max}}}{\beta} \quad \text{with} \quad \beta = \frac{T_m}{2m} \sqrt{\frac{T_m(1 - \alpha)}{\tau'_m}} \left( 1 - \alpha \right)^2.
\]  

(68)
This relation is valid for a constant $\tau'_m$. Our harmonic approximation to the bunch potential leads to the same constant delay for all ions of the bunch; consequently, we can use this relation to relate the longitudinal momentum spread of the bunch $\Delta p$ to its extension in the central part of the trap $L_b$, as $\Delta p = L_b/\beta$.

With the parameters of the original experiment, i.e., $T_m = 1.48 \mu s$, $\alpha = 0.956$ and $\tau'_m \lesssim 0.1$ ns, the second term in the square root in the above equation (68) is smaller than the first by six orders of magnitude and can therefore be neglected. We see then that $\Delta p$ scales with the square root of the effective time delay $\tau'_m$ and is proportional to the bunch length $L_b$:

$$\Delta p = \frac{2m}{T_m} \sqrt{\frac{\tau'_m}{T_m(1 - \alpha)}} L_b. \quad (69)$$

This form highlights that there are two different routes from the stable regime to the stability limit. One route is to increase the slope of the mirror potential to change the dispersion of the trap so that $\alpha \to 1$. In this case the momentum spread grows only slowly as long as the trap is ‘far’ in the stable regime, but as the mirror slope $F \to F_{max}$ (equation (13) with $\alpha = 1$) $\Delta p$ increases sharply and the bunch becomes drastically ‘hotter’. Right at the stability limit $\alpha = 1$ we get $\Delta p = \infty$. The bunch is ‘blown apart’ by its internal energy. Correspondingly the notion of a ‘momentum spread of the bunch’ loses its meaning, because the bunch itself ceases to exist. This ‘heating’ of the bunch is a collective effect of all ions together.

The other route, which was discussed less extensively, is to relax the radial focussing of the beam to allow for stronger off-axis motion of the ions. This increases $\Delta T_i$, and therefore decreases $\tau'_m$. Then $\Delta p$ decreases with $\Delta T_i/4 \to \tau_m$, i.e., the bunch becomes ‘cooler’ closer to the stability limit. This happens because a stronger off-axis motion increases the spread of the periods of the individual ions through the trap, which effectively stretches the bunch in time and consequently decreases the interaction between the ions at the turning point. In contrast to the first collective route to instability via the longitudinal trap dispersion this second effect stems from the transverse dispersion due to different off-axis orbits of the individual ions. On the first route the bunch is ‘blown apart’ because the bunching mechanism cannot confine the internal energy anymore, while on the second route the bunch ‘boils off’ ions that stray away too far from the bunch. Only those ions that have similar orbits through the trap stay together, thus reducing the internal momentum spread of the remaining bunch.

We once again can insert the numbers from the original experiment, i.e., $T_m = 1.48 \mu s$, $F = 80$ kV m$^{-1}$, $q = +1$ and $\alpha = 0.956$ and find from figure 3 that $\tau_m = 0.07$ ns at $d = 0.5$ mm for $N = 10^6$ ions. With a realistic $\Delta T_i = 0.18$ ns [3] and $x_{max} = L_b = 1.44$ cm we calculate a momentum spread of $\Delta p = 13.5$ au. With $m = 40$ amu this translates into an energy spread in the laboratory frame of $\Delta E = \frac{\Delta p}{m} = 0.87$ au = 24 eV at a beam energy of $E_0 = 4.2$ keV.

6. Comparing to the empirical criteria for bunching

In [9] three empirical criteria were given by Pedersen et al for synchronization to occur. We now show how these criteria are related to the results derived from our mapping approach about how and when synchronization occurs and about the size and behaviour of the bunch.

(i) The first criterion is the so-called kinematical criterion which in [9] is given as $\frac{\partial T}{\partial E} > 0$. This criterion is obviously the same as our stability criterion of $\alpha < 1$ for $\tau_m > 0$ (see equations (16) and (25)). Both expressions state that the dispersion of the trap has to be positive, i.e., that a faster ion has a longer period.
(ii) The second criterion of Pedersen et al., the ‘focussing criterion’, states that the interaction of the ions is important only in the mirror regions and that the beam diameter has to be compressed to about the same width as its length. We have shown in part I [8] that collisions in the central part are far more unlikely than collisions in the mirror and that only collisions in the mirror can synchronize the ions. We found the requirement of comparable longitudinal and transverse dimensions at the turning point when we estimated the bunch length in sections 3 and 4: a spherical bunch is most efficient in delaying the ions and therefore most stable against external perturbations. With this result, i.e., $A = d$, and the transformation (31) between $A$ and $L_b$ we then derived an estimate for the observed bunch length (59), which agrees with the prediction of Pedersen et al (see equation (29) of [9]).

(iii) The third criterion of Pedersen et al, the ‘collision criterion’, states ‘[... ] the collision probability at the turning point must ensure that the ions indeed lock their motion [...]’ and ‘[... ] too few collisions and too many lead to diffusion [...]’. In our treatment the ‘number of collisions’ corresponds to the magnitude of the effective time delay $\tau_m = \tau_m - \Delta T_4 > 0$ (see equation (28)). As discussed in sections 4.2 and 4.3 the delay $\tau_m$ due to the collisions has to be bigger than the intrinsic dispersion $\Delta T_4/4$ for synchronization to survive this perturbation, corresponding to the observation that too few collisions lead to diffusion. We want to emphasize again that the time spread $\Delta T_4$ of [9] due to the ions’ different energies is not a perturbation but a part of the ion dynamics.

The upper limit of too many collisions was illustrated in figure 6: if the bunch contains too many ions or is focussed too tightly, the ions bounce off the bunch potential, experience a negative delay and diffuse out of the bunch. In the framework of our approximations this upper limit is described by equation (66).

7. Summary and conclusions

In this paper we extended a recently proposed description of the synchronization effect in the ‘Zajfman trap’ [8] from describing the motion of two identical ions to the behaviour of a macroscopic ion bunch: the motion of the two identical ions through the trap field was described in their CM system by three mappings, one for each of the different parts of the trap. When the paths of the ions cross in the mirror their repulsive interaction slows them down temporarily and the resulting time delay, together with the dispersion of the trap, is responsible for coupling their motion. Here we generalize this two-ion approach to describe the motion of a (representative) test ion in a macroscopic bunch. The same stability condition applies as in the two-ion case. The interaction between the ions is now specified through the size and form of the bunch. Together with a relation between the observed bunch length in the central part of the trap and its size at the turning point in the mirror the time delay can be calculated explicitly.

We show that the time delay is maximal for a bunch which is spherical at the turning point and we calculate how the observed bunch length derived from this most stable configuration depends on the various parameters of the system.

Not only does our prediction of the observed bunch length match the experimental results within the level of approximation of our model, but we also confirm that the bunch length is essentially independent of the number of ions. The lower and the upper limits to this number are identified: the lower limit is connected to the spread of the ions’ periods due to off-axis motion, as the time delay that the ions experience when they cross the bunch has to be big enough to compensate for it. At the upper limit the repulsive bunch potential of the compressed bunch at the turning point becomes too high and the ions cannot cross the bunch any more.
Then they bounce back from the bunch, the resulting time delay changes its sign, the ions do not synchronize any more and consequently the bunch loses ions.

The numerical evaluation of the time delay for various parameters illustrates the behaviour of the bunch and confirms the validity of the approximations employed in our description. We make several new predictions that we hope will be tested experimentally:

(i) To directly observe our central result of \( A = d \) at the turning point some kind of imaging technique has to be used. This would allow one to capture the form of the bunch at that moment when it comes to rest without having to resort to trajectory calculations.

(ii) Much easier than the direct visualization of the turning bunch is to check the validity of equation (60), which is based on \( A = d \). For a constant mirror slope \( F \) at the turning point we predict that the bunch length observed in the central part of the trap \( L_b \) scales with the square root of the beam diameter \( 2d \) at the turning point. For a fixed \( d \), \( L_b \) would be inversely proportional to the square root of the slope \( F \). However, \( L_b \) cannot become shorter than a minimal value, which depends on the total length \( L \) of the field free region of the trap according to (62).

(iii) We found that the bunch length is determined by the mirror slope at the turning point only and not by the dispersion, see (59). This can be verified with a nonlinear mirror potential, which keeps the slope at the turning point constant for different trap dispersions.

(iv) The observed bunch length is independent of the number of ions in the bunch within certain limits, which are given by equations (66) and (67). The two limits scale differently with the parameters of the trap and the ions.

(v) With equation (69) we derived a relation between the bunch size and its longitudinal momentum spread. According to this equation there are two ways that a bunch can become unstable, either via the longitudinal or via the transverse dispersion of the trap. The two routes, depending on the mirror slope and the beam diameter, respectively, have opposite effects on the momentum spread.

Finally we explain the empirical conditions for synchronization given by Pedersen et al in the framework of our model.

In this paper we considered only a static bunch, i.e., the bunch exists initially and is either stable or not. Future work therefore has to focus on the dynamical properties of the synchronization effect, as, e.g., how and at which rate the bunch acquires additional ions from which parts of phase space. Other open questions are related to the issues of ions of different masses: what is the mass resolution of a ‘Zajfman trap’ operated as a mass spectrometer? Do bunches of different ions ‘stick together’ or can one have more than one bunch in the trap independently?

Another set of questions is connected to the internal dynamics of the bunch and whether there is an application for this ‘inner trap’ moving through the outer macroscopic trap.

It is not clear at the moment if our simple model can be used to answer these questions or if a more detailed description of the many-ion dynamics has to be used. Nevertheless, our simple model can explain the underlying mechanism and the stability criteria and provide insight into how the macroscopic bunch reacts to the externally given conditions and parameters.

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