Evaporative Cooling in Electromagnetic Radio Frequency Traps

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Evaporative Cooling in Electromagnetic Radio Frequency Traps

by

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Abstract

Paul traps are used in many different fields of physics to contain ions for different purposes. Given the oscillating fields that this type of trap employs to trap an ensemble and the heating that the interactions of these fields with multiple ions can cause, cooling the system could be of great interest, and there are several methods of doing so. This study explores one of these methods, evaporative cooling, applied to a type of Paul trap, a Linear Paul Trap (LPT), using computer simulations.

This thesis will first describe a trapped ion ensemble and an evaporation event both physically and how it is computationally modeled. It then proceeds to discuss the conditions for which evaporative cooling applied to an LPT could be optimized to maximize the chances of achieving highest temperature drop per particle evaporated.
Acknowledgements

First and foremost, I would like to thank Rob Thompson for his intellectual, and financial support throughout this difficult process. Michael Cummings was both the friend and the encyclopedia everyone needs, Rachid Ouyed helped me when I was lost in the computer science and needed to find my way back into the physics, and Michael Wieser kept me sane through this long journey. I could have not done this without you all.

I would also like to both thank and apologize to WestGrid for providing me with ample computation time and the countless hours that was spent correcting my mistakes. Additionally, I would like to thank NSERC, for giving great researchers the opportunity to allow students like me chase their dreams.

And lastly, to my friends and family, you were all that kept me going when it all look so grim.
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5.1 The lowest-order stability regions in a-q parameter space based on the single-ion EOM (Equations (2.12–2.14)) in the x-y plane of a 3D LPT. Note that the diagram is symmetric about the y-axis, hence the stability of the x and y ion trajectories is constrained by the same set of a and q values.

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## List of Symbols, Abbreviations and Nomenclature

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<th>Definition</th>
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<td>ABM</td>
<td>Adams-Bashforth-Moulton.</td>
</tr>
<tr>
<td>AC</td>
<td>Alternating Current.</td>
</tr>
<tr>
<td>APRR</td>
<td>Axial Potential Reduction Rate.</td>
</tr>
<tr>
<td>DC</td>
<td>Direct Current.</td>
</tr>
<tr>
<td>EPT</td>
<td>Evaporative Paul Trap.</td>
</tr>
<tr>
<td>IC</td>
<td>Initial Condition.</td>
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<tr>
<td>LPT</td>
<td>Linear Paul Trap.</td>
</tr>
<tr>
<td>MC</td>
<td>Monte-Carlo.</td>
</tr>
<tr>
<td>MFV</td>
<td>Maximum Field Velocity.</td>
</tr>
<tr>
<td>RK4</td>
<td>Runge-Kutta of 4\textsuperscript{th} Order.</td>
</tr>
<tr>
<td>RF</td>
<td>Radio Frequency.</td>
</tr>
<tr>
<td>RPRR</td>
<td>Radial Potential Reduction Rate.</td>
</tr>
<tr>
<td>PRTC</td>
<td>Potential Reduction Time Constant.</td>
</tr>
<tr>
<td>U of C</td>
<td>University of Calgary.</td>
</tr>
<tr>
<td>(a)</td>
<td>Unitless parameter in the Mathieu equations of motion.</td>
</tr>
<tr>
<td>(a_{\text{initial}})</td>
<td>Initial value of unitless parameter (a).</td>
</tr>
<tr>
<td>(a_t)</td>
<td>Value of (a) at time (t).</td>
</tr>
<tr>
<td>(C_{2k})</td>
<td>Mathieu amplitude coefficients.</td>
</tr>
<tr>
<td>(dt)</td>
<td>Integration time step.</td>
</tr>
<tr>
<td>(e)</td>
<td>Elementry charge. Also mathematical constant (e).</td>
</tr>
<tr>
<td>(\langle E \rangle)</td>
<td>Average energy.</td>
</tr>
<tr>
<td>(E_{BE})</td>
<td>Energy of the system before evaporative cooling.</td>
</tr>
<tr>
<td>(\langle E_k \rangle)</td>
<td>Average Kinetic energy.</td>
</tr>
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</table>
$E_p$ Energy of a particle.

$E_{TP}$ Total energy of the evaporating particles.

$\Delta E$ The difference between the particle energy and the mean energy of the system.

$f$ Trap stability parameter equal to $\frac{q}{q_{th}}$.

$f_{initial}$ Initial value of unitless parameter $f$.

$f_t$ Value of $f$ at time $t$.

$h$ Integration time step.

$i$ Parameter to sum, or multiply over.

$j$ Parameter to sum, or multiply over.

$k$ Parameter to sum, or multiply over.

$k_B$ Boltzmann constant.

$K_1$ RK4 integration approximation.

$K_2$ RK4 integration approximation.

$K_3$ RK4 integration approximation.

$K_4$ RK4 integration approximation.

$m$ Ion mass.

$n$ Variable representing the number of particles escaping a system.

$N$ Number of ions.

$N_0$ Initial number of particles.

$N_{rf}$ Integration steps per rf-period.

$q$ Unitless parameter in the Mathieu equations of motion.

$q_{th}$ The highest value of $q$ when $a = 0$, for which a system trapped by an LPT would remain stable.

$r_o$ Radius of the trap.

$|r_{ij}|$ Distance between the $i^{th}$ and $j^{th}$ particle.
$r_{\text{max}}$ Approximate maximum radial distance an ion may have from the centre of the trap.

t$_0$ Initial time.

$T$ Period of oscillation. Also temperature.

$T_0$ Initial temperature.

$T_b$ Temperature of the system after a particle has evaporated.

$T_u$ Marginal temperature in the arbitrary direction $u$.

$\Delta T$ Drop in temperature.

$u_{m}(t)$ Micro motion amplitude as a function of time.

$u_{s}(t)$ Secular motion amplitude as a function of time.

$u_{s,n}$ $n^{\text{th}}$ particle’s secular motion amplitude.

$U_{dc}$ Amplitude of the static potential.

$U_{rf}$ Amplitude of the alternating potential.

$v_r$ Relative velocity of ions in the trapped system.

$\delta v_u$ Variance in velocity in the arbitrary direction $u$.

$\sigma_{v_u}$ Velocity variance in the arbitrary direction $u$.

$v_{u,i}$ $i^{\text{th}}$ particle’s velocity in the arbitrary direction $u$.

$v_{s,u,i}$ $i^{\text{th}}$ particle’s secular velocity in the arbitrary direction $u$.

$V_{u,n}$ $n^{\text{th}}$ particle’s high temperature velocity in the arbitrary direction $u$.

$x$ Cartesian coordinate. Also, an arbitrary independent variable.

$X$ Unitless position parameter used to describe the motion of an ion in an LPT.

$\delta x$ Variance in position, in the x direction.

$y$ Cartesian coordinate. Also, an arbitrary independent variable.

$Y$ Unitless position parameter used to describe the motion of an ion in an LPT.
$z$  Cartesian coordinate. Also, an arbitrary independent variable.

$z_0$  Axial length of the trap.

$z_{max}$  Approximate maximum axial distance an ion may have from the centre of the trap.

$Z$  Unitless position parameter used to describe the motion of an ion in an LPT.

$\alpha$  Trapped plasma aspect ratio.

$\epsilon_0$  The vacuum permittivity.

$\eta$  Constant depending on the geometry of the electrodes that make up the trap.

$\omega_z$  Axial oscillation frequency.

$\omega_{sec}$  True secular oscillation frequency.

$\omega_{sec,o}$  First order approximation of the secular oscillation frequency.

$\Omega$  Oscillation frequency.

$\rho$  Density of the trapped system.

$\sigma_o$  Ion-ion collision cross section.

$\sigma_{coll}$  Ion-ion collision rate.

$\tau$  Unitless time parameter used to describe the motion of an ion in an LPT.

$\alpha_0$  Initial aspect ratio of the trapped plasma.

$\Delta r$  Average ion distance in the radial direction.

$\Delta z$  Average ion distance in the axial direction.
Chapter 1

INTRODUCTION

The goal of this thesis is to computationally explore and optimize evaporative cooling in Linear Paul Traps (LPT). The process of evaporative cooling is well understood, however, applying it to Paul traps has not been extensively explored previously. The study is carried out by computationally modeling the trapped ion ensemble and the containing fields through direct solution of the differential equations of motion. An optimization is achieved by maximizing the reduction in temperature, while minimizing the loss in particles when evaporative cooling is applied with LPTs.

1.1 A Short History of Particle Trapping

Since the first demonstration of ion trapping in 1923 by Kingdon [2], trapping of ions, plasmas, and neutral particles has been one of the widely studied areas in physics. This was achieved by continuing the progress used in the development of particle accelerators such as the cyclotron [3] and betatron [4] which occurred around the end of 1940’s. Where accelerators trap particles in one direction and accelerate it in another, particle traps confine them in every direction. By taking advantage of the Coulomb force, the trapping of ions is made especially easy. This is done by applying selected voltages to specific electrode configurations that would create electromagnetic fields that would contain the desired species of charged particles. Since then, a wide array of different trapping geometries and electromagnetic field shapes have been used for commercial and scientific gain in different areas of interest, including atomic and molecular spectroscopy [5, 6], quantum information [7, 8, 9], quantum computing [10], time standards [11], and antimatter physics [12, 13].

One of these traps is the Paul trap which is the focus of this thesis and will be explored...
Another notable trapping system is the Penning trap, which was suggested and created by Hans Dehmelt based on the magnetic field gauge studies done by Frans Penning [14]. The Penning trap uses static quadrupole electric fields combined with a static axial magnetic field to confine ions.

Furthermore, the study of trapped systems can be taken one step further by applying a cooling method to lower the average energy of a charged or neutral ensemble (which is trapped using inhomogeneous magnetic fields interacting with the dipole moment of the neutral particles) so that it can be studied more accurately. One such example is the precision of the mass measurement of trapped charged particles is increased as their temperature is reduced [15]. Also, feats such as achieving Bose-Einstein condensates would not be possible without a combination of different types of cooling applied to a system of trapped neutral bosons [16]. While many studies have been done on the trapping and cooling of ions, there are still combinations of trapping and cooling that have not been explored thoroughly.

1.2 Paul Traps

Electromagnetic radio frequency traps, or Paul traps, named after it’s inventor Wolfgang Paul, were explained in detail in his Nobel Lecture [17] and by many other authors e.g. [18, 19, 20, 21]. This particular trap was a construct of previous mass selection studies of ions and achieves trapping using both static and time-dependent voltages applied to two sets of hyperbolic electrodes, one set for the axial direction and another for the radial direction. The electrode configuration of this trap can be seen in Figure 1.1. The central region created by this geometry would result in a confining force felt by an ion in all directions that increases linearly with displacement from trap center, and hence contains it.

In the 1950s, this newly invented trap interested researchers for three main reasons: i) The geometry of the electrodes was that previously used in mass spectrometry [18] and so it was not hard to achieve; ii) the resulting equation of motion of a single ion due to it’s trapping
Figure 1.1: The electrode configuration of the original Paul trap can be seen where the two sets of electrodes are labeled as end-cap electrodes and ring electrode. Different combination of AC and DC voltages can be applied to these electrodes to contain ions. In this figure, both AC and DC voltages are applied to the two sets of electrodes.

field was determined to take the form of the extensively studied and well understood Mathieu equation\cite{22, 23, 24}, which would allow for the stability and characteristics of the ion motion to be studied analytically; and finally iii) it allowed for the confinement of relatively low temperature systems, which presented the opportunity for high-resolution of spectroscopy and other atomic physics experiments\cite{19}.

The original or spherical style Paul trap shown in Figure 1.1 creates a spherical confining volume. To increase the number of stored ions, as well as to have a larger ion storage at zero field locations, as the field of trapping progressed, other geometries of Paul traps such as ring traps and later on, Linear Paul Traps \cite{25, 26} were developed. The ring-style traps were created by bending a linear quadruple mass filter into a closed loop \cite{27} which gave it the name "‘race-track’". Later, inspired by the race-track trap design, the linear trapping
geometry of LPTs were realized, which have the benefits of allowing a larger trapping volume compared to that of the spherical Paul trap, relative simplicity and ease of ion loading, and large spacing between electrodes permitting measurements and manipulations to be done to the system and thus presented more opportunities for researchers[18]. The LPTs are basically identical to the linear quadrupole mass filters except an additional static field is present along the longer axis of the trap which in addition to a time-dependent electric field in the transverse direction, would allow for three dimensional trapping. The electrode configuration of LPTs and the resulting oscillating field can be seen in Figure 1.2. Note that the fields in the axial direction create a simple harmonic well, and are not shown.

1.3 Cooling Trapped Systems

One of the most revolutionary uses of the Paul-style traps occurred following the invention of the laser by Theodore Maiman in 1960 [28], and the development of laser cooling theory which following it [29]. The laser cools the system by ensuring that the frequency and polarization of a laser pointed at a trapped system produces photons that would be absorbed by the trapped species when they are moving towards the photons, and hence reducing

Figure 1.2: On the left, the electrode configuration of an LPT can be seen. Note that the end-caps are not shown, but are the same as the end-caps shown in Figure 1.1. On the right the resulting oscillating field by applying an AC voltage to the electrodes is shown.
their kinetic energy and temperature. By applying this cooling method to atomic systems [30], the study of low temperature ion systems became possible for researchers, and the opportunities for high-resolution spectroscopy, and mass spectrometry became immediately apparent [30, 31, 15, 32]. Furthermore, by cooling trapped ionic systems, ordered arrays that are similar to crystalline solids [33], were observed in Paul [34] and Penning [35] traps which became known as Coulomb, Wigner, or ionic crystals.

The invention of laser cooling also allowed for the development of sympathetic cooling [31, 36], which can be applied to systems composed of two different species of ions, where one species is accessible to be cooled by the lasers, and the other is not. By cooling the accessible species, and allowing it to collide and interact with the other, the total temperature of the system can be reduced. The applications of sympathetic cooling and the theory behind it continues to be studied and explored [36, 37, 38, 39]. While this method was first developed to work in conjunction with laser cooling, it can also be applied with other methods such as evaporative cooling described below.

Evaporative cooling is a process that has natural occurrences every day, and can be illustrated by the example of the cooling of hot coffee. Even when the temperature of the coffee is below its boiling point, there are particles that have high enough energy to overcome the surface tension of the liquid and evaporate. These particles have an energy higher than that of the average particle in the fluid. Hence, when they leave and the system is allowed to re-equilibrate, the average energy and temperature of the coffee will be reduced.

In the beginning of 1990s, the possibility of applying evaporative cooling to trapped systems was studied. In 1995, by applying evaporative cooling to trapped neutral particles, the Bose-Einstein condensate state [16] was achieved for the first time. Later, applying the same cooling method was one of the key components in allowing the trapping and study of anti-hydrogen by the ALPHA group [40, 41].

In the case of a trapped ion ensemble, particles require sufficient energy to overcome
Figure 1.3: The energy distribution of a sample ensemble before and after evaporative cooling. On the left, the particle(s) with the highest energy which are shown by the arrow have enough energy to evaporate. In the middle, the particles have escaped the trap, however the system has not re-equilibrated yet. On the right, the system after it re-equilibrates is shown. The new energy distribution will have a lower mean and so the temperature of the system is reduced.

the trapping potentials to evaporate. However, for evaporation to cool the system, two conditions must be met: i) The system needs to interact and equilibrate to achieve a typical Maxwell-Boltzmann energy distribution such as that shown in Figure 1.3 and ii) one of the highest energy particles must escape so that the average energy is lowered after the evaporation. As the temperature of the system is reduced, the evaporation events become less frequent and the cooling rate is reduced. To counter this effect, the trap depth can be reduced to allow particles to continue escaping at similar rates and hence, for the system to reach lower temperatures. However, the rate at which this reduction occurs, must be set very carefully to optimize the balance between thermalisation of the ions and particle escape rates in order to (a) avoid the effects of too much ion heating and (b) take into account the fact that as the trap potential is lowered, the ion volume increases, which in turn reduces the ion collision rate, but on the other hand, as the ions lose energy, they grow closer together, increasing their collision rate. The definition and derivation of what is considered a collision between two ions in this study can be found in Chapter 2.

One of the advantages of evaporative cooling, is it being a non-invasive cooling method that can be applied to any type of trap without any extra cost, hence making it a very attractive options for different experimental groups. One such group is the TITAN group,\textsuperscript{1}

\textsuperscript{1}https://titan.triumf.ca/
which studies exotic isotopic species produced using the ISAC\(^2\) facility at TRIUMF, where evaporative cooling could potentially be applied to any of the three trapping stages present in their experimental apparatus ((1) the catching-cooling linear Paul Trap, (2) the charge-state-generating eBIT Trap \[^{42,43}\], or three (3) the high precision mass analysing Panning Trap), to reduce the temperature of the ions, and therefore increasing the precision of their measurements \[^{15}\]. The work in this thesis is motivated by the potential to carry out evaporative cooling to enhance TITAN’s capabilities, and as this is the first study of its nature for TRIUMF, it focuses on the potential for evaporative cooling in the first of TITAN’s trapping systems, its catching-cooling LPT.

1.4 Simulations of Trapped Ions

When more than two particles exist in the trap, the ion equations of motion become too complex to allow for exact solutions and hence, computer simulations need to be used to study the system. As such, molecular dynamics simulations \[^{44,45}\] have been previously used in studies of rf-heating \[^{38}\], where two or more trapped ions are forced close to each other by the oscillating potential, which in turns causes them to fly away from each other, increasing their energy and sympathetic cooling. Similarly, this study will utilize the trajectories of individual particles which are evolved numerically based on the Newtonian equations of motion to extract properties of interest such as the temperature of the system. The implementation of this type of simulation however, requires a specific integrator to numerically solve the equations of motion, which would determine the positions and velocities of particles at discrete points in time, where the separation between these time points is known as the integration step size or time-step.

Previous work done in this computational field contains examples that employ a variety of different methods such as the 4\(^{th}\)-order Runge-Kutta (RK4) algorithm for the study of shell

\(^{2}\)http://www.triumf.ca/research-program/research-facilities/isac-facilities
structure \cite{46} and phase transitions \cite{47}, the Euler-Picard routine for sympathetic cooling studies in Paul traps \cite{38}, and 5\textsuperscript{th}-order Gear technique to compute the rf-heating present in linear Paul trap confinement \cite{38}. On the other hand, there are studies that have utilized more than one integration method to be able to compare and contrast results \cite{49}. However, using analysis done previously to compare and contrast different integration methods in modeling trapped particles by LPTs \cite{1}, only the RK4 method of integration is used in this study and will be further explored in Section 3.

1.5 Thesis Goals

This Thesis seeks to determine the feasibility and effectiveness of applying evaporative cooling techniques in a linear Paul Trap (LPT), which would allow experiments that make use of cold ions in Paul traps, such as the TITAN experiment, to make use of this technique to reduce the temperature of the trapped species.

This is done by building up on accurate and extensive previous work \cite{1} done on simulating trapped ions in an LPT and by utilizing its results, will focus on performing evaporative cooling in LPTs. More specifically, it will outline the theory behind the conditions required for evaporations to first occur. From there, the intrinsic heating mechanism of the trap will be explained, and whether these evaporations are able to compete with these sources of heating to lower the average energy of the system. Then, it will outline the method used to measure the efficiency of this type of cooling using average temperature lost per particle evaporated, and finally will explain the searching method used to optimize the trapping and cooling parameters, what these parameters are, and why they are the most optimum way of cooling an ensemble of ions trapped in an LPT.

To better tie this computational study to the aforementioned TITAN experiment, the dimensions of the simulated LPT used in these simulations, are that of the TITAN experiment \cite{50}, located at TRIUMF.
Given the temperature regime that this trap operates in, throughout the thesis, it will be assumed that classical physics can accurately model the ion’s motional evolution in the system.

1.6 Thesis Structure

Given the goals of this thesis, the physical ion ensemble trapped by an LPT must first be understood, modeled computationally, and finally evolved using simulations so that the results could be analyzed. To achieve this, chapter 2 will outline and explore the theory behind Paul traps, specifically the LPT and how a trapped ensemble confined by it will behave. Furthermore, it will explore the theory behind evaporative cooling and how it can be achieved, as well as describing the heating mechanisms that naturally occur for ion ensembles in LPTs, which compete with any cooling techniques applied to such ensembles. From there, the method of temperature calculation is explained in chapter 3. The computational tools used to simulate and model the physical systems are discussed in chapter 4. Finally, chapter 5 presents the results of this study, chapter 6 discusses these results, and chapter 7 will summarize the thesis and its most significant results and limitations, while identifying avenues that require further study.
Chapter 2

ION TRAP THEORY: A BRIEF OUTLINE

To be able to model the system of interest computationally and understand the parameter space that affects evaporative cooling of the system, first the ion trap dynamics and intrinsic heating processes need to be understood. From there, the trap of interest will be mathematically introduced. Furthermore, evaporative cooling in general needs to be modeled. Finally, this type cooling can be applied to the specific trap studied, and the details explored.

2.1 Electric Potential of LPT

Trapping in general requires a three-dimensional electric field that would apply an increasing restoring force to a particle as it moves away from the center of the trap in any direction \[1\]. In principle, this can be achieved for charged particles by an electric potential of the form:

\[
\phi(x, y, z) = \alpha_o x^2 + \beta_o y^2 + \gamma_o z^2 \tag{2.1}
\]

where \(\alpha_o, \beta_o, \gamma_o > 0\). \[2\]

On the other hand, using Gauss's law, for physically permissible electric potentials, we have the restriction that

\[
\nabla^2 \phi = 0 \tag{2.3}
\]

which puts the additional constraint of

\[
\alpha_o + \beta_o + \gamma_o = 0 \tag{2.4}
\]
on the parameters. These two sets of constraints imposed on \( \alpha_o, \beta_o, \) and \( \gamma_o \) cannot be satisfied at the same time (other than with the non-useful null result \( \alpha_o = \beta_o = \gamma_o = 0 \)) if the trapping fields are to have a static configuration. However, if the constants are allowed to vary in time, then equations (2.2) and (2.4) can both be satisfied simultaneously, at least in a time-averaged sense, which is the case with an LPT. In creating the Paul Trapping potential, a field consisting of a combination of attractive and repulsive potentials could be utilized for particle trapping, as long as the field reversed before the ion escaped a trapping volume.

Figure 2.1: On the left, the electrode configuration of an LPT with the coordinate system that has been used to describe the potentials mathematically can be seen. Note that the end-caps are not shown. On the right, the resulting saddle shaped, oscillating field which is created by applying an AC voltage to the electrodes can be seen where the field is shown at times \( t_0 \) and half a period later, \( t_0 + \frac{T}{2} \).

The LPT electrodes and coordinate system used can be seen in Figure 2.1 where the potentials can be described mathematically by

\[
\phi(x, y, z, t) = \frac{U_{rf}}{r_o^2} (x^2 - y^2) \cos(\Omega t) + \eta \frac{U_{dc}}{z_o^2} \left[ z^2 - \frac{1}{2} (x^2 + y^2) \right].
\] (2.5)

Here, \( r_o \) and \( z_o \) are the radial radius and axial length of the trap that are subject to a time-varying potential of amplitude \( U_{rf} \) oscillating at the frequency of \( \Omega \) and a static potential.
of $U_{dc}$. The geometry of the trap electrodes determines the constant $\eta$, which for the sake of simplicity will be set to unity for the rest of this thesis \[1\]. This potential will create an oscillating field in the x-y plane referred to as a flapping potential and has a two-dimensional saddle shape shown in Figure 2.1 while the axial or z-direction potential is simply a static harmonic well. It should be mentioned that the form of the potential described above is not unique and Paul traps can also be created by application of time-varying fields of different geometries. However, this study will specifically focus on LPTs.

It should be mentioned that not all combinations of values of $r_o$, $z_o$, $U_{dc}$, $U_{ac}$, and $\Omega$ create a stable trapping system. For example, if the value of $\Omega$ is too small, an ion will start to escape from a direction with low potential amplitude, and the potential does not oscillate fast enough to force the ion back into the center of the trap. To determine whether or not an ion trajectory is bounded within the trap, one must study the equations of motion of an ion confined by these potentials, as has been done in the next section.

2.2 Equations of Motion

By applying Maxwell and Newton’s laws to a system of $N$ ions with charge ‘$e$’, confined to the potential described by Equation (2.5), the equation of motion for the $i^{th}$ ion can be written as

$$m \frac{d^2 x_i}{dt^2} = - \frac{2e}{r_o^2} [ -U_{DC} + U_{RF} \cos (\Omega t) ] x_i + \frac{e^2}{4\pi \epsilon_o} \sum_{j=1}^{N} \frac{x_i - x_j}{|r_{ij}|^3}$$

(2.6)

$$m \frac{d^2 y_i}{dt^2} = - \frac{2e}{r_o^2} [ +U_{DC} + U_{RF} \cos (\Omega t) ] y_i + \frac{e^2}{4\pi \epsilon_o} \sum_{j=1}^{N} \frac{y_i - y_j}{|r_{ij}|^3}$$

(2.7)

$$m \frac{d^2 z_i}{dt^2} = - \frac{2eU_{DC}}{z_o^2} z_i + \frac{e^2}{4\pi \epsilon_o} \sum_{j=1}^{N} \frac{z_i - z_j}{|r_{ij}|^3}.$$  

(2.8)

Here, $x_i - x_j$, $y_i - y_j$ and $z_i - z_j$ are the distance between the $i^{th}$ and $j^{th}$ particles in $x$, $y$ and $z$ direction respectively, $|r_{ij}|$ is the distance between the $i^{th}$ and $j^{th}$ particles, $m$ is the
ion mass and $e$ is the charge of the ions. The first and second terms in each of these three equations represents the ion-trap and the ion-ion interactions, respectively. By introducing the unitless time and position variables defined by

\[ \tau = \frac{\Omega t}{2}, \quad X = \frac{x}{r_o}, \quad Y = \frac{y}{r_o}, \quad Z = \frac{z}{r_o}, \] (2.9)

and unitless stability parameters

\[ q = \frac{4eU_{RF}}{mr_0^2\Omega^2}, \] (2.10)
\[ a = \frac{4eU_{DC}}{mz_0^2\Omega^2}, \] (2.11)

these equations can be further simplified for a single particle and written as

\[ \frac{d^2 X}{d\tau^2} = [a + 2q \cos (2\tau)]X \] (2.12)
\[ \frac{d^2 Y}{d\tau^2} = [a - 2q \sin (2\tau)]Y \] (2.13)
\[ \frac{d^2 Z}{d\tau^2} = -2aZ \] (2.14)

where the term due to the Coulomb interaction has vanished for a single ion and so Equations (5-7) becomes a set of decoupled differential equations. The $X$ and $Y$ equations of motion are then identified as Mathieu equations, who’s mathematical properties have been extensively studied [22, 23, 24] and have stable (bounded) solutions [51], among several regions of stability in a-q space, for $|q| < |q_{th}| = 0.90804 \ldots$ and $a = 0$. When $a \neq 0$, the system will be stable for specific range of $a$ and $q$ values which can be seen in the stability diagram shown in Figure 2.2. Note that this diagram is symmetric across its q-axis and hence, any sets of $a$ and $q$ that cause bound motion in the $x$ direction, would also do so in the $y$ direction. However, for the particle to be trapped in the $z$ direction as well, an additional constraint of $a > 0$ must be required [51].
Figure 2.2: The three lowest-order stability regions in a-q parameter space based on the single-ion EOM (Equations (2.12–2.14)) in the x-y plane of a 3D LPT. Note that the diagram is symmetric about the y-axis, hence the stability of the x and y ion trajectories is constrained by the same set of a and q values.

For multiple ions however, due to the complex nature of the pair interactions of ions, no closed form solution to these equations exists. Hence numerical techniques must be used to evolve the system in time.

The solution for the axial direction equation of motion is simply that of a harmonic oscillator. Hence, the axial oscillation frequency $\omega_z$ can be defined as

$$\omega_z = \frac{\Omega}{2} \sqrt{2a}$$  \hspace{1cm} (2.15)

which would indicate that the motion in the axial direction is purely harmonic with an amplitude that is solely dependent on stability parameter $a$.  

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2.3 Pseudopotential Approximation

Due to the full Mathieu solution being too problematic to handle analytically, different approximations have been developed [18, 52, 32] to better understand the trajectories and their periods of motion. The pseudopotential approximation that was developed by Kapitsa [53] and was later applied to trapping by Dehmelt [52], which applies to single-ion trajectories in LPTs will be the focus of this section.

The pseudopotential approximation has been long understood, and used extensively in literature [18, 32, 1], so it will only be briefly described here. The pseudopotential concept is based on the understanding that for a properly chosen set of trapping parameters \(a\) and \(q\) the oscillating fields create a time-averaged restoring or trapping potential in which the ion oscillates slowly. However, as the electric fields are oscillating to create this potential, a fast driving field is superimposed on the time-averaged restoring potential. Hence, the implementation of this approximation is that the motion of any single ion in an LPT can be decomposed into two distinct modes: the slow, large amplitude motion, known as secular motion \(u_s(t)\), and the rapid, small amplitude motion, known as micro-motion \(u_m(t)\) where \(u\) is an arbitrary direction. By averaging over an rf-period, the micro-motion contribution will disappear, and we are left with the secular equation of motion

\[
\frac{d^2 u_s}{dt^2} = -\left(\frac{q^2}{2} - a\right) \frac{\Omega^2}{4} u_s
\]  

(2.16)

where normal units of time are used. This would result in the equation of motion of a harmonic oscillator with an oscillation frequency of

\[
\omega_{\text{sec},o} = \frac{\Omega}{2} \sqrt{\frac{q^2}{2} - a}.
\]  

(2.17)

Here, \(\omega_{\text{sec},o}\), denotes the first-order approximation to the true secular frequency \(\omega_{\text{sec}}\). It has been shown however, that these approximations used to generate the secular frequency,
breakdown for $|q| > 0.4$ and hence, the more precise value of

$$\omega_{sec} \approx \frac{\Omega}{2} \left[ -a + \frac{(a + 1)q^2}{2(a + 1)^2 - q^2} + \frac{(5a - 7)q^4}{32(a + 1)^3(a + 4)} + \frac{(9a^2 - 58a + 29)q^6}{64(a + 1)^5(a + 4)(a + 9)} \right]^{1/2} \quad (2.18)$$

will be used in this work to calculate the secular frequency for $q > 0.4$.

It should be noted that the pseudopotential cannot exist without the presence of at least one ion inside the trap since it explicitly requires the separation of micro motion and secular motion. Hence, the pseudopotential is not a property of the trapping fields, but a concept that arises due to the behavior of the particle trapped in a time-varying potential. It should be further noted that the pseudopotential concept is introduced to aid in the understanding of ion evolution but all simulations used the full electric fields as described in Equations (2.6-2.8) to evolve the system, and not any form of approximation to these potentials and interactions.

For sake of computational simplicity and to avoid any confusion, a new stability parameter

$$f = \frac{q}{q_{th}} \quad (2.19)$$

is defined and used throughout this report, in which $|f| < 1$ corresponds to the $q < q_{th}$ stability regime. This would allow us to more easily compare future results generated for different trapping geometries or systems.

### 2.4 Plasma Aspect Ratio

To predict the shape of an ion ensemble, the secular and axial frequencies of the trap can be used to determine the plasma aspect ratio in high enough temperature regimes where the ion-ion interactions are relatively weak. Using the equipartition theorem, it can be derived that the harmonic potential in the axial direction, which has two degrees of freedom,
drives an ion of mass \( m \) to an approximate maximum distance of

\[
z_{\text{max}} = \frac{1}{\omega_z} \sqrt{\frac{2k_B T}{m}}
\]

from the trap center. Similarly, the mean maximum radial displacement using the pseudopotential approximation is

\[
r_{\text{max}} = \frac{1}{\omega_{\text{sec}}} \sqrt{\frac{2k_B T}{m}}.
\]

Thus, the aspect ratio of a trapped plasma in an LPT can be defined as

\[
\alpha = \frac{z_{\text{max}}}{r_{\text{max}}}
\]

or in terms of trapping parameters

\[
\alpha = \frac{\omega_{\text{sec}}}{\omega_z}.
\]

Note that this aspect ratio is a characteristic of the trap design rather than the ion ensemble, and thus depends on the trap parameters and not values such as ion number or ion temperature. The radial symmetry of the LPT implies that the system would take the geometry of a type of an ellipsoid of revolution, with the value of \( \alpha \) determining its exact shape. For \( \alpha > 1 \) the ensemble takes the form of an oblate spheroid, \( \alpha < 1 \) creates a prolate spheroid, and finally \( \alpha = 1 \) results in a spherical ensemble. The value of \( \alpha \) will be used throughout this thesis to explain physical processes as well as choosing different values of \( a \) for chosen values of \( f \).

2.5 Heating in Paul Traps

When ions are confined by any set of oscillating trapping potentials, they will generally undergo a mean ion kinetic energy increase. This increase can potentially be due to the collision of ions with background gases, ion-ion collisions, and imperfections in the trapping
Table 2.1: The median values of heating rate for $N = 256$ as previously published [1]. Note that the values of $f$ and $a$ are kept constant, and all units are K/sec

<table>
<thead>
<tr>
<th>$f$</th>
<th>$a$</th>
<th>$T$ [K]</th>
<th>Heating Rate [K/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.04</td>
<td>0.00002</td>
<td>3</td>
<td>0.2 ± 1.0</td>
</tr>
<tr>
<td>0.04</td>
<td>0.00002</td>
<td>30</td>
<td>0.43 ± 0.15</td>
</tr>
<tr>
<td>0.04</td>
<td>0.00022</td>
<td>3</td>
<td>0.1 ± 0.8</td>
</tr>
<tr>
<td>0.04</td>
<td>0.00022</td>
<td>30</td>
<td>0.26 ± 0.34</td>
</tr>
<tr>
<td>0.16</td>
<td>0.000322</td>
<td>3</td>
<td>3 ± 12</td>
</tr>
<tr>
<td>0.16</td>
<td>0.000322</td>
<td>30</td>
<td>120 ± 15</td>
</tr>
<tr>
<td>0.16</td>
<td>0.00353</td>
<td>3</td>
<td>56 ± 33</td>
</tr>
<tr>
<td>0.16</td>
<td>0.00353</td>
<td>30</td>
<td>240 ± 19</td>
</tr>
<tr>
<td>0.64</td>
<td>0.00595</td>
<td>30</td>
<td>640 ± 100</td>
</tr>
<tr>
<td>0.64</td>
<td>0.061</td>
<td>30</td>
<td>700 ± 210</td>
</tr>
</tbody>
</table>

fields. However, due to the non-conservative nature of the trapping potential of Paul traps, another heating effect called radio-frequency heating appears [36]. This process transfers energy from the oscillating part of field into the system during ion-ion collisions and the amount of energy added to the system depends on oscillation frequency, the trapping potential amplitude [1], and the trap geometry. This heating always occurs for systems of more than one ion, and would increase non-linearly as $f$, $a$, or $\frac{1}{T}$ is increased.

This is relevant to this study due to the competition of evaporative cooling with this heating to lower the total temperature of the ensemble. A detailed analysis of this heating has be done by Cummings [1], whose results were confirmed by the author where simulations were ran to measure heating rates as a function of $f$, $a$, and $T$.

A summary of the heating rates relevant to this study for $N = 256$ particles can be found in Table 2.1

2.6 Evaporative Cooling

The idea of evaporative cooling can be explained at its most basic level by how hot coffee cools: Even though the temperature of the coffee is below its boiling point, there are still
particles that have enough energy to overcome surface tension and evaporate, taking with them a disproportionate amount of kinetic energy. Their departure thus reduces the average kinetic energy of the coffee and cools it down.

To quantify the change in temperature based on the energy of the particle lost, assume a gaseous system of monatomic neutral particles that are at thermal equilibrium at the temperature $T_0$. Given the equipartition theorem, the total energy of the system before any evaporation is

$$E_{BE} = \frac{3}{2} N k_B T_0$$  \hspace{1cm} (2.24)

where $N$ is the number of particles in the system, and $k_B$ is the Boltzmann constant. It would follow that the average energy per particle is

$$\langle E_{BE} \rangle = \frac{E_{BE}}{N} = \frac{3}{2} k_B T_0.$$  \hspace{1cm} (2.25)

Now assume that a particle with energy $E_p = \langle E_{BE} \rangle + \Delta E$ escapes the system. Hence, after the equilibration of the system, the energy would become

$$E_{BE} - E_p = E_{BE} - (\langle E_{BE} \rangle + \Delta E) = \frac{3}{2} (N - 1) k_B T_b$$  \hspace{1cm} (2.26)

where $T_b$ is the temperature of the system after the particle has evaporated and the system re-equilibrates. Plugging in Equation (2.25) and Equation (2.24) into the above gives

$$\frac{3}{2} N k_B T_0 - \frac{3}{2} k_B T_0 - \Delta E = \frac{3}{2} (N - 1) k_B T_b$$  \hspace{1cm} (2.27)

$$\frac{3}{2} (N - 1) k_B T_0 - \Delta E = \frac{3}{2} (N - 1) k_B T_b$$  \hspace{1cm} (2.28)

$$T_0 - T_b = \frac{\Delta E}{\frac{2}{3(N-1)k_B}}$$  \hspace{1cm} (2.29)

$$\Delta T = \frac{\Delta E}{\frac{2}{3(N-1)k_B}}$$  \hspace{1cm} (2.30)
where in the last equation, $\Delta T = (T_0 - T_b)$, which shows that the temperature change is directly proportional to $\Delta E$, and inversely proportional on the number of particles $N$. Using the same method, the final temperature of the system can be calculated, as more particles escape the system, assuming the escape occurs after the equilibration of the ensemble each time.

On the other hand, one can calculate the drop in temperature when $n$ particles are lost between equilibrations of the system, taking with them a total energy of $E_{TP} = n \langle E_{BE} \rangle + \sum_{i=1}^{n} \Delta E_i$, where each $E_i$ is the difference between the $i$th particle’s energy and the mean energy of the system before evaporation, $\langle E_{BE} \rangle$. The temperature drop can then be calculated to be

$$\Delta T = \frac{2}{3(N-n)k_B} \sum_{i=1}^{n} \Delta E_i. \quad (2.31)$$

Note that the right hand side of Equation (2.31) might not always be positive. If the value of $\sum_{i=1}^{n} \Delta E_i$ is negative, it would mean that $\Delta T$ is negative, which would correspond to the rise in temperature. Such evaporations are possible, and are labeled as ”‘undesirable evaporations’”, and will be discussed further in the upcoming chapters.

The above general concept is completely relevant for ions trapped in an LPT. In general, to achieve evaporation in electromagnetic traps, the trapping potential is reduced to allow for highest energy particles in the system to escape. Consider a system of particles with a Boltzmann energy distribution, trapped by the potentials shown in Figure 2.3. When the height of the potential walls is reduced, the particles that make up the high energy tail of the distribution escape the system and after re-equilibration, the system will have an energy distribution that corresponds to a lower temperature. However as previously mentioned, not every evaporation would necessarily reduce the temperature of the system. For example if particles that make up the low end of the energy distribution manage to escape, after re-equilibration, the resulting system will have a distribution that would correspond to a
higher temperature.

To make sure that evaporating particles do in fact reduce the temperature of the system, two conditions must be met: (1) the ensemble is required to have a physically achievable (Boltzmann) energy distribution and (2) the escaping particles make up the high energy tail of said distribution. To achieve the first goal, the ions in the system are required to interact with each other sufficiently to create an equilibrated energy distribution. During this period, the trapping potential must remain sufficiently constant as to not allow additional particles to escape. The required time for this process will depend on the ion collision rate which will be discussed in the next section. When the conditions for the first goal is met, if the potentials are dropped sufficiently slowly, only the highest energy particles will have a chance to escape and so fulfilling the second condition. However, if too much time is spent waiting for the system to equilibrate, i.e. the potentials are dropped too slowly, RF heating could take over and hence reduce the effectiveness of the evaporative cooling.

Therefore, values such as trapping parameters $a$ and $f$, ion collision rate, the rate of reduction of the trapping potentials, and the period for which the potentials are kept constant
will all affect the average cooling of evaporations and will be explored further in the upcoming chapters.

2.7 Adiabatic Cooling

Adiabatic cooling in the context of the trapped ensembles, refers to the decrease in Coulomb potential energy when the average distance between ions is increased as a trapping volume is increased, typically due to a reduction in the trap depth. This is analogous to the adiabatic expansion and cooling of noble gasses. In the discussed LPT specifically, the average ion distance depends on the \( f \), \( a \), \( T \), and the ion charge. The trapping potentials try and force the ensemble into the center of the trap which would cause the ions to be closer to each other, while the Coulomb force between them drives them away from each other. This average distance between the particles has a corresponding Coulomb energy which would affect the velocities of the ions, and consequently, the temperature of the system.

For every evaporative cooling simulation that is run, due to the reduction of \( f \) and \( a \), when the temperature is plotted as a function of number of particles remaining in the trap, two distinct processes can be seen. The resulting plot from one such simulation can be seen in Figure 2.4. Here, there is a drop in temperature as the number of particles stays constant. This would point to the average distance of the particles and so the volume of the ensemble increasing, while no particles escape. With the continued increase of the volume, at some point the system expands enough so that the trajectory of particles collide with the position of the physical electrodes and escape the system.

This process can be seen in the Figure 2.4 where a semi-logarithmic graph of temperature as the number of particles is given, and the arrows show the direction of time evolution of the system. Here, the figure can be divided into two distinct parts, first being when the number of particles is constant while the temperature is dropping, which would point to adiabatic cooling since the only change to the system is its increase in volume, and when the particles
start escaping the system, and the temperature is further reduced.

Figure 2.4: The temperature as a function of particles for a random evaporative cooling simulation done, where the arrows indicate the direction of time evolution of the system. The temperature drop is separated by two distinct processes. First, there is a temperature drop without the loss of any particles due to the increase in average separation of the ions. When the system has expanded enough, the particles start evaporating and in this case cooling the system further.

A more detailed study and discussion of adiabatic cooling and the evaporative cooling that may follow the expansion is provided in chapter 6 of this thesis.

2.8 Collision Rate in LPT

As previously discussed, for evaporative cooling to take place, the system must first have a physical energy distribution such as the Boltzmann distribution. For this to occur, the ions must interact with each other. To understand how long this equilibration process will take,
the rate at which ions interact with each other inside an LPT must be explored.

Given the infinite range of interaction between charged particles by the Coulomb force, defining a collision rate is no trivial task. By obtaining the minimum scattering angle for which the error in the equation of motion calculation would be computationally manageable, \( \theta_{\text{min}} \approx 4\pi/7 \), derived by M. Cummings\[1\], one can integrate over the differential cross section

\[
\frac{d\sigma_o}{d\Omega_{\text{solidangle}}} = \left( \frac{e^2}{8\pi \epsilon_o k_B T} \right)^2 \frac{1}{\sin^4 \left( \frac{\theta}{2} \right)}
\]

over the bounds of \( \theta_{\text{min}} < \theta < \pi \) which would give the scattering cross section of

\[
\sigma_o = 2 \left( \frac{e^2}{4\pi \epsilon_o k_B T} \right)^2 .
\]

Multiplying this value with the mean relative velocity, \( \langle v_r \rangle \),

\[
\langle v_r \rangle = \frac{2}{\pi^{1/2}} \sqrt{\frac{k_B T}{m}}
\]

and density of the trapped particles, \( \rho \),

\[
\rho = \frac{3\pi^{1/2}}{32} \left( \frac{m}{k_B} \right)^{3/2} \frac{\omega_{\text{sec}}^2 \omega_z}{T^{3/2}}
\]

would determine the high temperature collision rate, \( \sigma_{\text{coll}} \) of

\[
\sigma_{\text{coll}} = \frac{3}{128\pi^2} \frac{m e^4}{e_o^2 k_B^3} \frac{\omega_{\text{sec}}^3}{\alpha T^3}
\]

where for convenience, \( \omega_z \) is written in terms of \( \alpha \) and \( \omega_{\text{sec}} \). A more detailed derivation can be found in Appendix F of \[1\]. This would indicate that a higher collision rate is achieved by reducing the plasma aspect ration \( \alpha \) and increasing \( \omega_{\text{sec}} \) and by extension, the unitless parameter \( f \). As the collision rate increases, the time required for equilibration of the system is reduced. Equation \(2.36\) cv will be used in later chapters to explain the range of effectiveness achieved by evaporative cooling, given specific sets of simulation parameters.
2.9 Conclusion

This section outlined and mathematically described the different elements that were modeled computationally. The fields created by an LPT, how these fields contain the ions, the heating processes involved in a trap with oscillating fields, approximations used to simplify the system, and the shape of ensemble were discussed. Furthermore, the ideas of evaporative and adiabatic cooling were introduced, and it was mathematically shown that evaporations can either cool or heat the trapped ions. Therefore, conditions for which cooling would be achieved were outlined. Adiabatic cooling was also discussed, and it was shown that the changes to the trapping potential that create adiabatic cooling, may also generate evaporations, depending on exactly how the field changes are generated. And lastly, given all the conditions set by previous sections, the collision rate of ions inside an LPT was discussed to be used as a tool to explain the results.

The upcoming chapter will discuss how the temperature of the ensemble is calculated which is crucial to measuring the effectiveness of the cooling processes involved.
Chapter 3

TEMPERATURE

When simulating trapped ion systems, the ensemble temperature is necessary to gain insight into the physical properties of the system. More specifically, the physics of any method of cooling applied, and ion heating can be related to the ensemble kinetic energy evolution, and hence its temperature, which is determined using the positions and velocities of ions. Furthermore, the determination of temperature would provide a means to connect theoretical study of trapped ion systems to its physical reality counterpart and specifically measurements that can be carried out in the laboratory. This chapter will discuss how temperature is generally calculated, and will outline the specific method used to calculate the temperature of a trapped ensemble of ions.

3.1 Temperature Calculation Background

In simulations of ions confined by time-varying or static potentials, the ion velocities are what is used to calculate system temperature\[52, 56, 46, 57\]. The reason is due to the complication that arises due to the Coulomb force between the ions. This force adds a non-quadratic position-dependent term to the Hamiltonian of the system, which would not allow for the extraction of temperature using the equipartition theorem following\[55\]

\[
\frac{1}{2}k_B T = \frac{1}{2}m\delta x^2
\]

where \(m\) is the mass of the particles and \(\delta x^2\) represents the variance of position.

However, the theorem stands when calculating temperature using the variance in velocity
and states that each quadratic term in the Hamiltonian would contribute $k_B T/2$ to the mean energy \[55\].

These equations assume a global thermal equilibrium and hence requires that the velocities in each coordinate to be of the Gaussian distribution with the same variance. However, this might not always be the case, and systems (for example, trapped ion distributions) exist that even though the velocity distributions are of Gaussian form in every direction, they do not have the same variance. Such a case was observed in laser cooling of ions in LPTs \[58\]. Therefore, in analogy to the global temperature of the system, one can define marginal temperature for the system in different coordinates which would simply represent the Gaussian variance of velocities in that direction, with the system temperature defined as the average of these marginal temperatures. More specifically, in LPTs, the use of the marginal temperatures is defined for both axial and radial directions.

In the simulation of a system of $N$ particles with mass $m$, the time dependent marginal temperature in the direction $u$, can be defined as \[1\]

$$T_u(t) = \frac{m}{k_B} \left[ \frac{1}{N} \sum_{j=1}^{N} \left[ v_{u,i}(t) \right]^2 - \left[ \frac{1}{N} \sum_{j=1}^{N} v_{u,i}(t) \right]^2 \right]$$  \hspace{1cm} (3.3)

where $v_{u,i}$ is the $i$th particle’s velocity in the $u$ direction, and the marginal temperature is calculated using the ensemble velocity variance in the direction of $u$. Equation (3.3) could easily be used to calculate the temperature in any conservative potential, such as the axial direction in the LPT. However, the problem is further complicated by the micro-motion of the fields in the radial direction of the LPT. This non-conservative potential poses the challenge of defining the velocity variance in the radial direction since the total velocity, will be a combination of the secular and micro motion velocities of each particle. While
the equipartition explicitly relies on randomness, the micro-motion of the trapped ions is the result of the driving field. Hence, its non-randomness would provide a non-Gaussian contribution to the ensemble, and any velocity caused by the micro-motion needs to be excluded from the calculation in order to extract an accurate temperature. For this reason, any accurate temperature calculation requires either measurements at times where the micro motion velocity is non-existent, or application of a technique to average out the micro motion velocity.

3.2 Temperature Calculation Assumptions

Many different methods of temperature calculation in Paul traps have been devised and tested in simulations [1]. From these different techniques, the Maximum Field Velocity (MFV) temperature calculation method was picked, due to its simplicity, speed, and accuracy and the large $f$ values used in some of the simulations ran. The next section will mathematically outline this method, where the characteristics and effectiveness of this method is derived under the following assumptions:

1. Large Number of Ions. For any statistical evaluation including the calculation of velocity variance, to be applicable, an approximate distribution is required.

2. Thermal Equilibrium. The system in one Cartesian direction, is assumed to have a thermal distribution in secular velocities and positions, while the micro-motion velocities and positions could be of any distribution. Furthermore, the velocity variances may not be identical to each other in each direction.

3. No Center of Mass Motion. Steps have been taken to remove any center of mass motion from the initial conditions of the system. If an ensemble has zero mean velocity, that would imply that the ensemble variance is equal to the
ensemble average mean square velocity in that direction or

\[ \delta v_u^2 = \langle v_u^2 \rangle \]  

(3.4)

These assumptions would allow for position and velocity distributions to be used to calculate the temperature.

3.3 Mathematical Derivation for Temperature Calculation Used

As previously mentioned, to calculate the temperature of a system of ions that is trapped in an rf-field, the micro-motion of the system complicates the matter greatly and must be extracted and removed from the calculation. The MFV method was first derived and determined to be the most efficient and accurate technique to calculate temperature by Cummings [1]. This method is labeled in this manner due to the amplitude of the field when the velocity is sampled, which simplifies this complication by averaging of the ensemble velocity variances at two adjacent field maxima (i.e, when \( t_j = j\pi/\Omega \) and \( t_{j+1} = (j+1)\pi/\Omega \) with \( j \) being an integer). This is done due to the micro-motion velocity being zero when the field is at its maximum and in doing so, the calculation of temperature is simplified.

To calculate the marginal temperatures using this methods, three steps are taken: i) First the velocity is found at the aforementioned two time points, \( t_j = j\pi/\Omega \) and \( t_{j+1} = (j+1)\pi/\Omega \) with \( j \) being an integer, ii) then the kinetic energy is calculated from each of these distributions using their velocity variance, and finally iii) the mean value of these energies is taken to produce the MFV marginal temperature. To begin lets consider the high temperature velocity of the \( n^{\text{th}} \) ion in the arbitrary direction \( u \) of the flapping potential at time \( t = j\pi/\Omega \)

\[
V_{u,n}(j\pi/\Omega) = \frac{qU_n\Omega}{2} \sin(jk\pi) + \frac{v_{s,u,n}(j\pi/\Omega)}{\omega_{sec}} \sum_{k=-\infty}^{\infty} C_{2k}(k\Omega + \omega_{sec}) \cos(jk\pi) \]  

(3.5)

\[
- u_{s,n}(j\pi/\Omega) \sum_{k=-\infty}^{\infty} C_{2k}(k\Omega + \omega_{sec}) \sin(jk\pi) \]  

(3.6)
where $U_n$ is the mean position of ion $n$ in direction $u$, $v_{s,u,n}$ is the secular velocity of ion $n$ in the $u$ direction, $C_{2k}$ are Mathieu amplitude coefficients \[23, 1\], and $u_{s,n}$ is the secular motion amplitude of ion $n$ in the $u$ direction. Due to the sinusoidal function, this can be simplified to

$$V_{u,n}(\frac{j\pi}{\Omega}) = \frac{v_{s,u,n}(\frac{j\pi}{\Omega})}{\omega_{sec}} \sum_{k=-\infty}^{\infty} (-1)^k C_{2k}(k\Omega + \omega_{sec})$$

and the velocity variance can be obtained as

$$\langle V_{u,n}(t_j)^2 \rangle = \sigma_{v_u}^2 \sum_{k,l=-\infty}^{\infty} C_{2k} C_{2l} \frac{(k\Omega + \omega_{sec})(l\Omega + \omega_{sec})}{\omega_{sec}^2 (-1)^{j(k+l)}} (-1)^j$$

which results in the mean kinetic energy

$$\langle E_{k,u}(t_j) \rangle = \frac{1}{2} m\sigma_{v_u}^2 \sum_{k,l=-\infty}^{\infty} C_{2k} C_{2l} \frac{(k\Omega + \omega_{sec})(l\Omega + \omega_{sec})}{\omega_{sec}^2} (-1)^j \left[ 1 + (-1)^{(k+l)} \right].$$

The MFV marginal temperature $T_u$ is then calculated from the average of the kinetic energies at times $t_j$ and $t_{j+1}$ to be

$$T_u = \frac{m\sigma_{v_u}^2}{k_B} \sum_{k,l=-\infty}^{\infty} C_{2k} C_{2l} \frac{(k\Omega + \omega_{sec})(l\Omega + \omega_{sec})}{\omega_{sec}^2} (-1)^j \left[ 1 + (-1)^{(k+l)} \right].$$

From here, the value of the average term, $\frac{1}{2}[1 + (-1)^{(k+l)}]$ either vanishes or becomes unity depending on whether $k + l$ is even or odd. Thus with the substitution $k \rightarrow 2k - l$ the temperature becomes

$$T_u = \frac{m\sigma_{v_u}^2}{k_B} \sum_{k,l=-\infty}^{\infty} C_{4k-2l} C_{2l} \frac{(2k - l)\Omega + \omega_{sec})(l\Omega + \omega_{sec})}{\omega_{sec}^2}.$$

And so the results from an MFV temperature calculation method should display no time variation, as is observed in many techniques that rely on imperfect removal of effects due to trapped ion velocity oscillation suppression through averaging techniques alone \[1\]. However for smaller number of particles, a secular period average may still be employed to
reduce the temperature variation at different times. To obtain the functional dependence of temperature on $q$, the Mathieu coefficients $C_{2k}$ and $\omega_{sec}$ can be evaluated to order $q^3$. This would yield the result

$$T_u \approx \frac{m\sigma_{v_u}^2}{k_B}(1 - \frac{q^2}{16}). \tag{3.12}$$

which is how the radial temperature is calculated.

Finally, we can expand this method to calculate the ion ensemble’s overall temperature in a linear Paul trap, taking into account each marginal temperature. The temperature in the direction that a static harmonic field is applied to would simply be

$$T_z = \sigma_{v_z}^2 \tag{3.13}$$

and so it would follow that the temperature for an LPT would be given by the average over the three marginal temperatures as

$$T = \frac{m}{3k_B} \left[ (\sigma_{v_x}^2 + \sigma_{v_y}^2) \sum_{k,l=-\infty}^{\infty} C_{4k-2l}C_{2l} \left( \frac{(2k-l)\Omega + \omega_{sec}}{\omega_{sec}^2} \right) \left( l\Omega + \omega_{sec} \right) + \sigma_{v_z}^2 \right]. \tag{3.14}$$

For equal velocity variances and applying the order $q^3$ approximation, the equation takes on the familiar form

$$T \approx \frac{m\sigma_{v_x}^2}{k_B} (1 - \frac{q^2}{24}) \tag{3.15}$$

which shows that the MFV method reproduces the true temperature in the LPT to a high degree of accuracy up to large $q$ values, with a 2\% underestimation\[1\] in the true temperature for the highest value of $q$ used in this thesis. Here the true temperature is the temperature of a weakly interacting ensemble confined in a harmonic well. In this situation, the secular motion can be defined to be the thermal component of the trajectory, and hence the marginal
temperature in an arbitrary direction $u$ can be defined as

$$T_u = \frac{m\sigma_u^2}{k_B}.$$  \hfill (3.16)

Furthermore, the true equilibrium temperature is the appropriately weighted average over the marginal temperatures in different directions.

3.4 Conclusion

This chapter explored how the temperature is generally calculated, and why calculation of temperature in an LPT is challenging and not a trivial task. It then set forth the assumptions used to calculate the temperature, and the method used in the simulations was mathematically described and linked to the trapping parameters of an LPT.

The next chapter will outline the computational methods, techniques, and considerations that have been used to model the system.
Chapter 4

NUMERICAL INTEGRATION AND TECHNIQUES CONSIDERATIONS

As discussed in Chapter 1, while some simpler physical systems can be completely described analytically, other systems that are governed by a more complex set of equations, such as rf-heating, require numerical solutions to be studied. Since the number of particle-particle interactions for an $N$-ion ensemble of order $N^2$, as the number of particles increase, the computation time required to model the system grows rapidly [59, 60]. Hence, simulations with a large number of particles may take days or weeks to complete. Furthermore, a vast number of different integration methods can be used to model the desired trapped ion system. This presents us with two questions: which integration method should be used and what integration time step should be set? This section will try to answer these two questions based on balancing the simultaneous needs for accurate results with efficient calculation tools to minimize calculation times.

4.1 Integration Method

The modeling of the evaporation of particles from the system, presents a unique numerical situation: particles that are still trapped at current time $t_a$, might evaporate and therefore not exist in the simulation at time $t_b = t_a + dt$ where $dt$ is the simulation time step. Hence, choosing the most efficient integration method will not solely be dependent on temperature and trapping potentials as considered in previous work [1]. Computational efficiency, in this specific case, would be decreased significantly for methods that require retaining the position and velocity values for too many steps in the past since they might not be needed at time
An example for such inefficiency is the Adams-Bashforth-Moulton method \[61, 62\] for which, depending on its order, requires the saving of a number of position and velocity values at times \( t < t_b \)[63]. On the other hand, every time a particle is lost, all arrays used in the simulation need to be re-sized. This re-sizing requires very high amounts of memory and so the fewer number of arrays used in the numerical integration process, the quicker the simulations would finish. Hence, it is desirable to find a technique that would work well and be efficient for the specific case of ion simulations where evaporation is present.

4.1.1 4th order Runge-Kutta Integration Method

A substantial and detailed analysis on 11 different integration methods for simulations of trapped ions using paul traps has been done[1]. One of these methods, the 4th order Runge-Kutta technique, is widely used in simulating physical problems \[61, 62\]. This technique, uses the weighted average of four linear approximations to generate a solution. Even though this causes 2 - 4 times more function evaluations compared to the other methods, no additional array needs to be created, re-sized, or saved. To use this approach, propagation of the equations of motion, \( f(y, x) \), at each integration step can be done in five stages

1. First extrapolation stage. The first approximation, \( K_1 \), is calculated using

\[
K_1 = hf(y_k, x_k)
\]  

(4.1)

where \( h \) is the integration step-size, and \( \frac{dy}{dx} = f(y, x) \).

2. Second extrapolation stage. A second approximation, \( K_2 \) is calculated using

\[
K_2 = hf(y_k + \frac{1}{2}K_1 + \frac{1}{2}h)
\]  

(4.2)
3. Third extrapolation stage. A third approximation, $K_3$ is calculated using

$$K_3 = hf(y_k + \frac{1}{2}K_2, x_k + \frac{1}{2}h)$$  \hspace{1cm} (4.3)

4. Fourth extrapolation stage. A final approximation, $K_4$ is calculated using

$$K_4 = hf(y_k + K_3, x_k + h)$$ \hspace{1cm} (4.4)

5. Averaging stage. These approximations are then averaged to calculate the value of the function at the next time-step using

$$y_{k+1} = y_k + \frac{K_1 + 2K_2 + 2K_3 + K_4}{6}$$ \hspace{1cm} (4.5)

Given the inefficiency problems discussed earlier, this method is more efficient than other analyzed algorithms such as the Gear4, Gear5, Gear6, ABM2, ABM3, ABM4, and ABM5 methods[61, 62], due to it not saving additional position and velocity arrays, not having to create or delete extra arrays other than the minimum needed, and applying minimum resizing to the arrays required.

Furthermore, it was shown in the same analysis that three other considered techniques, Velocity-Verlet, Euler-Picard, and Beeman require simulation step sizes orders of magnitude smaller than that of the RK4 to achieve the same accuracy. Hence, considering both the overall efficiency, and efficiency when particle evaporations are present, the RK4 method is picked over all other 10 methods considered here.
4.1.2 Integration Time-Step

One of the most crucial parts of any integration technique, is the integration time-step $dt$. Again, a detailed analysis on $dt$ has been done by Cummings in terms of integration steps per rf-period \[1\]

$$N_{rf} = \frac{2\pi}{\Omega dt}$$ \hspace{1cm} (4.6)

where $dt$ was varied in the form of

$$dt = \frac{2\pi}{\Omega} \left(\frac{2^k}{10}\right), k \in \mathbb{Z}$$ \hspace{1cm} (4.7)

and results were contrasted to determine at what point, reducing the step size would not be desired based on how much more precise the simulation would be, and how much longer the computation time would become. From the above equation, $N_{rf}$ can be written as

$$N_{rf} = \frac{10}{2^k}$$ \hspace{1cm} (4.8)

which would not depend on $\Omega$.

The analysis done by Cummings \[1\] suggests that the value of $N_{rf}$ for the RK4 method changes based on the trapping parameters $f$ and $a$, and the ensemble temperature. It also shows when using the RK4 technique, The highest value of $N_{rf}$ required to keep the error in temperature measures beneath 10% tolerance at $T = 30$ K, is 1280 steps for the highest values of $f$ and $a$ and any value below it that has been used in this thesis. This value, corresponds to the time step $dt = 3.125 \times 10^{-10}$ sec. Since the simulation might have to handle temperature calculations at values slightly above 30 K, the time-step was kept constant at a lower value, $dt = 2.5 \times 10^{-10}$ sec which would provide more precise results.

4.2 Modeling Evaporative Cooling

The two subjects that will be tackled in this section are (1) how to achieve the evaporation of a particle and (2) how the evaporated particle that has left the system will be computationally
modeled.

In its simplest form, from a computational aspect, a particle could escape the trap if there are simply defined boundaries for the trap in the radial and axial directions which would correspond to the physical size of the trap. However, even though these evaporations might cool down the system for a short period of time, since the system is intrinsically heated, after a while, if no further evaporations occur, the temperature will start to rise again. Furthermore, the cooling might not be enough to reduce the temperature of the ensemble to the desired levels.

This method, also requires us to follow and model the physical process that allows for increasingly lower energy particles to continue escaping the trap: the lowering of the trapping potential depth. To do this, parameters \( f \) and \( a \) that directly correspond to the depth of radial and axial trapping fields were reduced at rates that will be referred to as Radial Potential Reduction Rate, \( RPRR \), and Axial Potential Reduction Rate, \( APRR \), both of which have units of sec\(^{-1}\). Using these values, one can write

\[
f_{t_2} = f_{t_1} - RPRR(t_2 - t_1) \tag{4.9}
\]
\[
a_{t_2} = a_{t_1} - APRR(t_2 - t_1) \tag{4.10}
\]

where \( f_{t_1} \) and \( a_{t_1} \) are the \( f \) and \( a \) values at time \( t_1 \), and \( f_{t_2} \) and \( a_{t_2} \) are the values of \( f \) and \( a \) after the reduction. By rearranging these equations, one can solve for \( APRR \) and \( RPRR \) to get

\[
RPRR = \frac{f_{t_1} - f_{t_2}}{t_2 - t_1} \tag{4.11}
\]
\[
APRR = \frac{a_{t_1} - a_{t_2}}{t_2 - t_1}. \tag{4.12}
\]

By lowering either \( f \), \( a \), or both, particles are allowed to move farther out in the radial, axial, or both directions, and if they pass the boundaries set as mentioned above, the ions will
be considered to have left the system and are dropped from the simulation. However, even though potential reductions based on application of these two computational variables can achieve evaporations, evaporative cooling might not necessarily be achieved. The essential element missing from achieving the cooling, as mentioned in Chapter 2, is to allow the system to equilibrate. If the trap potential is lowered continuously, at sufficiently large rates, the equilibration process will not occur. On the other hand, if the values of $RPRR$ and $APRR$ are lowered to the point that this thermalisation could occur, not only could the heating of the system dominate, but it would greatly increase the computation time. To avoid these problems, another parameter referred to as Potential Reduction Time Constant, $PRTC$, with units of seconds was defined. This parameter would change how often the potentials would be reduced turning the potential function into a step function in time as shown in Figure [4.1].

The time in which the potentials are kept at a constant allows for the equilibration of the system and so that when the potential is stepped down, the particles escaping could actually cool the system.

Given the dependance of the results of cooling on the rates and time constants of potential reduction, all three values of $RPRR$, $APRR$, and $PRTC$ must be optimized. Due to the independence of these variables, and little theoretical information about which values would provide the best cooling results, a Monte-Carlo method was used to search for parameters that maximize temperature drop per particle lost. However, a Monte-Carlo search in three dimensions requires a very large number of simulations to be run, is very computationally costly, and could require orders of magnitude more time compared to a two dimensional Monte-Carlo search.

Hence, due to computational time restrictions, a three dimensional Monte-Carlo search of $RPRR$, $APRR$, and $PRTC$ was not possible, and the value of $PRTC$ was systematically varied while keeping trapping parameters $a$ and $q$ constant, to find the value that would best
Figure 4.1: The plot of the value of $f$ which directly corresponds to the radial potential depth, as time goes on. Here, $RPRR = 1000 \text{ sec}^{-1}$ and $PRTC = 10^{-6} \text{ sec}$. The length of the horizontal lines which allow the system to equilibrate represent the value of $PRTC$ and will change directly with it. The vertical drops in the value of $q$ which allow for evaporations to happen represent the magnitude of $RPRR \times PRTC$ and will change directly with it.
allow the system to equilibrate. A value between $PRTC = 5 \times 10^{-6}$ and $PRTC = 10^{-7}$ gave temperature values within 1% of each other and provided the highest temperature drop per particle. Since the micro-motion velocity is zero when the amplitude of the oscillating trapping field is at a maximum, if a particle escapes within a few time-steps of the time at which the potential was reduced, the velocity of the lost particle will have a negligible micro-motion component [1]. Therefore, the potential reduction time constant was kept constant at $PRTC = \frac{20}{5\pi \times 10^6} = \frac{20}{11}$. This indicates that whenever the potential is dropped, it would be at its maximum amplitude value and hence, particles are lost shortly after. In conclusion, the three variables $RPRR$, $APRR$, and $PRTC$ provide all necessary tools to physically model and achieve evaporative cooling.

The lack of a full MC search on the value of $PRTC$, brings with it the risk of missing a value of $PRTC$ for which the temperature drop per particle would be higher. However, the temperature drop is reduced rapidly at values of $PRTC < 10^{-7}$ and $PRTC > 5 \times 10^{-6}$, and so even though it is possible that a value of $PRTC$ outside the range mentioned above would provide better results, it would be improbable.

The second part to be discussed, is how the escaped particles are handled in the simulations. Again, since the basis of this computational study is to model everything as close to their physical counterpart as possible, the way in which particles are lost from the trap in a lab setting must first be considered. In reality, the particles are considered to have been lost from the trapping fields, which occurs physically when an ion is absorbed by one of the mentioned electrodes that create the trapping fields, or escapes between the electrodes. Given their charge, $e$, after absorption, these ions cause a small perturbation in the potential, denoted by $\delta$, for a short period of time, $t_\delta$, until they are grounded. The magnitude of the applied potentials points to both $U_{RF} >> \delta$ and $U_{DC} >> \delta$. This combined with the almost instantaneous nature of the absorption of the ion, and that $dt >> t_\delta$, all the effects of the absorption are computationally ignored, and instead, an evaporated particle is simply
removed from the simulation between time $t$ where the evaporation has occurred and time $t + dt$.

4.3 Monte-Carlo method

Given the large range of values the two cooling parameters $APRR$ and $RPRR$ can take on, a systematic search would be both computationally intensive and, depending on the fineness of the search, could miss important trends. A standard Monte-Carlo method\cite{64} can counteract both these challenges. Hence, a two stage Monte-Carlo process was implemented into the code to search for trends of temperature drop per particle at different $APRR$ and $RPRR$ values. The first stage was designed to assign random values to the $APRR$ and $RPRR$ variables independently, and determine general tendencies in temperature drop per particle. This allowed for a more efficient use of computation time by highlighting potential areas of interest for the cooling parameters.

The second stage of the MC followed the results of the first stage, by running more simulations at ranges of $APRR$ and $RPRR$ values that showed increase in cooling efficiency. This allowed for a more defined set of data at these areas of increased temperature drop per particle. This method however, focuses on finding the ranges that allow for the most efficient cooling.

To confirm the theoretical discussions made in Chapter 2 of this thesis about undesirable evaporations, more MC simulations were manually created in regions encompassing $APRR$ and $RPRR$ values that would result in very little or no cooling. More specifically, the two parameters were given values that were an order of magnitude larger, or smaller than the most efficient values found.
4.4 Initial Condition Generation

For the results of any computational study to be physically valid, the initial positions and velocities of the modeled particles must correspond to physically representative distributions as well. For example, for the temperature of a simulated system to be defined, a system must have an identifiable thermal distribution. Furthermore, due to the Coulomb interaction, an undesirable set of initial positions where ions are placed too close to each other, could cause a chaotic multi-ion system \[65, 66\]. Therefore, it is of great consequence to use an initial condition (IC) generation method that is well understood and would not cause the system to behave in an unphysical manner.

In previous publications, typically the method of acquiring the desired initial states has either been to draw the ICs from a ”random” distribution \[56\] or it has been less completely outlined \[47\]. In contrast, this thesis will use a method previously studied and used to explore different types of IC generation \[1\], which improves on the study done by Prestage \textit{et al.} \[46\].

The generation of initial positions and velocities were done in four steps:

1. An ensemble of ions was created by setting their positions and velocities from a thermal distribution with a temperature higher than that desired, and neglecting the Coulomb interaction.

2. The system was put in the trapping potentials, under the influence of the Coulomb interactions. A combination of simulated laser cooling and photon recoil heating was applied to the ensemble to adjust the temperature to near the target temperature value.

3. The simulated cooling and heating was slowly reduced over hundreds of secular periods, to remove any chance of creating discontinuities in the forces acting on the particles.
4. The ensemble was allowed to equilibrate over several hundred secular periods without the presence of the driven heating/cooling described in point 2 (above), but, under the influence of the trapping potentials and the ion-ion interactions.

A more detailed procedure of creating the initial conditions of the simulations, including its mathematical description, can be found in Chapter 10 of [1].

It should be noted that every result mentioned in this thesis is the product of assessing and averaging three simulations using the same trapping and cooling parameters, with a very small perturbation of the order of 1 part in $10^{10}$ applied to the ICs, as to avoid using results that are obtained by chaotic trajectories cause by undesirable ICs.

4.5 Conclusion

This chapter outlined and described the tools necessary to computationally model and evaluate, a system of ions trapped by an LPT, where evaporations may occur. It explained the reasoning behind the use of the RK4 method to integrate the equations of motion of the system, and the time step of $dt = 2.5 \times 10^{-10}$. It also introduced cooling variables $APRR$ and $RPRR$, and the tools necessary to model evaporative cooling in this system. Furthermore, it explored the MC method used to search over these cooling parameters. Finally, it described the method used to create the ICs of the simulations ran, to ensure that the results are physically valid.

The next chapter will present the possible values of $f$, $a$, $RPRR$, and $APRR$ that were used in the MC search, the simulation parameters used, and results of the simulation sets that were run.
Chapter 5

RESULTS

As mentioned in previous chapters, the goal of this thesis is to find the most optimal conditions that allow the highest temperature drop per particle evaporated and thus to determine what level of cooling is achievable under these conditions. This is done by varying the values for $RPRR$ and $APRR$ using the Monte-Carlo method. This chapter will discuss the physical constants of each simulation that was run, such as trap size and number of particles, the trapping parameters used, the results obtained by running the MC search, and finally the implications of these results.

5.1 Possible RPRR and APRR Values

As mentioned in the theory section of this thesis, for specific $q$ and $a$ values, the trapped particles become unstable. Here $q$ has been used to make the mathematical equations in this section simpler. Since the values of $q$ and $a$ are being reduced, only the gray area shown in Figure 5.1 is of interest. More specifically, if the condition

$$q^2 \geq 2a$$

is required [1], then the trap would be in its first stability zone and the particles will have bound trajectories. This can be written for any time $t \geq 0$ as

$$(q - RPRR \times t)^2 \geq 2(a - APRR \times t).$$

for the values of $APRR$ and $RPRR$ to never put $f$ and $a$ into an unstable zone, Equation (5.2) must have real values for all $t \geq 0$. Hence, this quadratic equation has either 1) no real roots, 2) one root, or 3) two roots where the larger one is located at $t = 0$. The third case
Figure 5.1: The lowest-order stability regions in a-q parameter space based on the single-ion EOM (Equations (2.12–2.14)) in the x-y plane of a 3D LPT. Note that the diagram is symmetric about the y-axis, hence the stability of the x and y ion trajectories is constrained by the same set of a and q values.

is immediately rejected since at $t = 0$, $q \neq a \neq 0$. The first and second conditions, suggest that

$$APRR^2 - 2APRR \times RPRR \times q + 2RPRR^2 \times a \leq 0 \quad (5.3)$$

and solving this for $APRR$ would give

$$RPRR \times q - \sqrt{RPRR^2 \times q^2 - 2RPRR^2 \times a} \leq APRR \leq RPRR \times q + \sqrt{RPRR^2 \times q^2 - 2RPRR^2 \times a}. \quad (5.4)$$

Since the $APRR$ will only be reducing the value of $a$, the higher bound on $APPR$ in the
above inequality can be ignored, and final restraining equation becomes

\[ R_{PRR} \times q - \sqrt{R_{PRR}^2 \times q^2 - 2R_{PRR}^2 \times a} \leq APRR. \]  \hspace{1cm} (5.5)

This means that for the mentioned Monte-Carlo, some randomized values of \( R_{PRR} \) and \( APRR \) will be rejected as simulation parameters, and only simulations that have parameter values following Equation (5.5) will be run.

Furthermore, since particles would not remain trapped in the axial direction for \( a \leq 0 \), a minimum value for \( a \) and consequently \( q \) must be set. The \( a_{\min} \) was set to be one percent of its initial value \( a_0 \) and hence, \( q_{\min} = \sqrt{2a_{\min}} = \sqrt{0.02a_0} \).

5.2 Simulation Parameters

Since the experimental model system for this study was chosen to be the radio frequency quadruple trap used by the TITAN group located at the TRIUMF facility, the physical dimensions of the simulated trap were set to follow theirs as closely as possible. Hence, the radius of the trap was set to be \( r_o = 10^{-2} \) m and the axial length of the trap was set to be \( z_o = 4 \times 10^{-2} \) m. Furthermore, the mass of the simulated ions were set to \( m = 4 \times 10^{-26} \) kg, corresponding to Sodium, with a one electron deficiency.

The number of particles that were simulated followed two rules. Firstly, the number of particles was required to be in the form of \( N = 2^i \) where \( i \) is any positive integer as to increase computational efficiency. Secondly, even though simulating a low number of ions would significantly reduce the computation time, it would not provide enough statistical data to draw any physical conclusions from the results. Hence, the number of particles was set to \( N = 256 \) which is a relatively high number that only takes a few hours to simulate, compared to the few days of computation time required to complete a simulation with \( N = 512 \).

The initial trapping parameter \( f \) was set to two values of \( f = 0.32 \) and \( f = 0.64 \). From there, the \( a \) was calculated for \( \alpha_{\text{initial}} = \frac{1}{16} \). It should be mentioned that test runs for plasma
shapes corresponding to $\alpha_{initial} = 16$ and $\alpha_{initial} = 1$ were both conducted and both cooling results were worse by at least an order of magnitude.

To reduce the total simulation time and to have results that can be contrasted with each other, the simulations were considered complete and the results were saved when the temperature of system was lower than 50 K, and one of following three conditions was met:

1. If the temperature of the system reached 2% of its initial value $T_0$, initially suggested by the TITAN group based on the requirements of the experiment. This would allow for significant cooling given the temperature regime. It should be noted that lower temperatures can be achieved, however it will come at the cost of losing many more particles.

2. When more than 90% of the particles were lost, meaning $N = 25$. Generally, in the TITAN experiment, it is desired to retain as many of particles as possible, and hence this would reduce the time spent on simulations that simply lose too many of the trapped ions.

3. The simulation time $t_b = 10^{-3}$ sec was reached. If the values of $APRR$ and $RPRR$ are low, the first two conditions may not be met and so this final constraint would assure the completion of all simulations. It should be noted that for $RPRR < 50$, the simulations time was increased to $t_b = 10$ sec.

Table 5.1 summarizes all the variables used in each simulation, whether they are constant or variable, and if they are constant, the values that have been used.

5.3 Evaporations

As previously mentioned, not all ion evaporations are desirable and depending on the energy of the particle that escapes the system, the ensemble can either heat up or cool down. This
Table 5.1: The list of trapping and cooling simulation parameters that are kept constant during the Monte-Carlo search done over the RPRR and APRR variables.

section of the thesis will cover specific examples of these two different classes and provide examples from simulations that were run.

5.3.1 Undesirable Evaporations

When a particle which has lower energy than the mean energy of the system is allowed to evaporate, the average energy of the remaining ensemble will shift to higher values, and hence, heat the ensemble. These evaporations can occur in two cases, first, if the system has not had enough time to equilibrate (the horizontal steps in Figure 4.1 are too small), but the trapping potential depth has been reduced far enough to still allow for particles to escape, particles that evaporate may heat the system. On the other hand, the system could have had enough time to equilibrate, but the potential drops too rapidly (the vertical steps in Figure 4.1 are too large) which allows for both low and high energy particles to escape and possibly heating the system overall. Example of these evaporations can be seen in Figure 5.2 where the energy distribution and mean energy of the system is shown, and the evaporated
ion at the time of the evaporation $t_{\text{evap}}$, is shown in red. These undesirable evaporations can take place for either very small values of $PRTC$, very large values of $APRR$ and $RPRR$, or both.

Figure 5.2: The energy distribution of the system right before an evaporation occurs with bin size of 20 meV. The vertical line represents the mean energy. The bin marked with the red color is the bin from which a particle is evaporated and has lower than mean energy in the ensemble. When this particle is evaporated, after re-equilibration, the mean energy is increased.

The effect of such evaporations can be seen in Figure 5.3 where after a temperature drop due to adiabatic cooling which will be discussed further in the next chapter, when the particles start escaping, the system heats up and eventually, when enough particles are lost, the system starts to cool down again due to the small number of particles the expansion of the system. In the system modeled, a temperature of 16 K is achieved, but only after losing about 90% of the trapped species.
5.3.2 Desirable Evaporations

If the conditions mentioned in the theory section are achieved for every evaporation, then particles that escape the system will lower the temperature of the system. An example of the energy distribution of the ensemble and the particle evaporated of such events can be seen in Figure 5.4.

The result of a simulation where desirable evaporations lower the temperature of the system can be seen in Figure 5.5 where after the temperature is lowered by adiabatic cooling, every evaporation lowers the temperature of the system. In the system modeled, a temperature of 16 K is achieved by losing less than 10% of the trapped species.
Figure 5.4: The energy distribution of the system right before an evaporation occurs with bin size of 20 meV. The vertical line represents the mean energy. The bin marked with the red color is the bin from which a particle is evaporated and is the highest energy particle in the ensemble. When this particle is evaporated, after re-equilibration, the mean energy is lowered.

5.4 Monte-Carlo Simulation Results

As mentioned in Table 5.1, simulation sets with different $f_{\text{initial}}$ and $\alpha_{\text{initial}}$ parameters were run. When $f_{\text{initial}} = 0.64$, values of $\alpha_{\text{initial}} = \{16, 1, \frac{1}{16}\}$ correspond to values of $a_{\text{initial}} = \{5.95 \times 10^{-3}, 6.1 \times 10^{-2}, 1.13 \times 10^{-1}\}$, respectively, which give the plasma a cigar, spherical, or cylindrical shape respectively. Thousands of MC simulations were run and the results are shown in Figures 5.6 - 5.10. Here, the temperature drop per particle lost, is calculated by dividing the total temperature drop by the total number of particles evaporated, as explained previously, and plotted against their corresponding $RPRR$ values.

In the entirety of this research, tens of thousands of simulations were run, which include
Figure 5.5: The evolution of temperature while desirable evaporations occur. After the rapid temperature drop due to the adiabatic cooling, every evaporation further reduces the temperature of the system, until a temperature of 16 K is achieved by evaporating less than 10% of the trapped system.

but are not limited to confirming the validity of the modeling of the trapped ensemble, confirming the validity of modeling ion evaporating from the trap, creating initial conditions, and finding trapping and cooling parameters for which cooling is optimized. In the next sections, only the final relevant results have been presented, which add up to thousands of simulations and are only a portion of the simulations run.

5.4.1 \( f_{\text{initial}} = 0.64 \) and \( \alpha_{\text{initial}} = \{16, 1, \frac{1}{16}\} \)

The following figures show the results of the MC search over \( APRR \) and \( RPRR \) when \( f_{\text{initial}} = 0.64 \). When \( \alpha_{\text{initial}} = 16 \) there are clear peaks and areas of interest where the average temperature drop per particle is maximized and minimized. However, for \( \alpha_{\text{initial}} = 1 \) and \( \alpha_{\text{initial}} = \frac{1}{16} \), there are no clear peaks or areas which point to cooling being optimized.
Figure 5.6: The temperature drop per particle of the MC search over RPRR when $f_{\text{initial}} = 0.64$ and $\alpha_{\text{initial}} = 16$. The figure can be separated into three sections: 1) when $RPRR > 2750$ which does not have any distinct peaks, 2) when $1000 < RPRR < 2750$ where the efficiency of evaporative cooling is at its highest and the highest value of temperature drop per particle can be reached, 3) when $RPRR < 1000$ where the temperature drop per particle is steadily reduced and reaches values less than 0. All three sections will be discussed in the chapter 5.4.2

5.4.2 $f_{\text{initial}} = 0.32$ and $\alpha_{\text{initial}} = \{16, 1\}$

For $f_{\text{initial}} = 0.32$, values of $\alpha_{\text{initial}} = \{16, 1\}$ correspond to values of $a_{\text{initial}} = \{1.32 \times 10^{-3}, 1.28 \times 10^{-2}\}$ which give the plasma a cigar and spherical shapes respectively. Simulations for when $\alpha_{\text{initial}} = \frac{1}{16}$ were not run due to the initial conditions having temperatures much higher than 900 K and evaporating within a few simulation time steps.

The results of these MC simulation sets can be seen in Figures 5.12 and 5.14. As for the case of $f_{\text{initial}} = 0.64$ and $\alpha_{\text{initial}} = \{1, \frac{1}{16}\}$, no clear peaks can be seen for which the temperature drop per particle lost is maximized.
Figure 5.7: The temperature drop per particle of the MC search over APRR when $f_{\text{initial}} = 0.64$ and $\alpha_{\text{initial}} = 16$. Here no distinct peaks can be seen. High values for temperature drop per particle can be found at a variety of different APRR values. Furthermore, both high and low values for temperature drop per particle can be found at the same values of APRR. This would suggest that the dependence of temperature drop per particle on APRR is negligible and instead, the efficiency of the evaporative cooling relies on the RPRR value it is paired with.

5.5 Conclusion

This section provided the constant and variable parameters used in this study, and presented the results of the MC search done over them. These results outline the cooling and trapping parameters that show the most promise for maximizing temperature drop per particle. The next chapter will move on to discussing these results, and explore the effects that the variations in cooling and trapping parameters have on the average temperature drop per particle and the possible reasons behind them.
Figure 5.8: The temperature drop per particle of the MC search over $RPRR$ when $f_{\text{initial}} = 0.64$ and $\alpha_{\text{initial}} = 1$. No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of $RPRR$. 
Figure 5.9: The temperature drop per particle of the MC search over $APRR$ when $f_{\text{initial}} = 0.64$ and $\alpha_{\text{initial}} = 1$. No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of $APRR$. 
Figure 5.10: The temperature drop per particle of the MC search over \( RPRR \) when \( f_{\text{initial}} = 0.64 \) and \( \alpha_{\text{initial}} = 1/16 \). No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of \( RPRR \).
Figure 5.11: The temperature drop per particle of the MC search over $APRR$ when $f_{initial} = 0.64$ and $\alpha_{initial} = 1/16$. No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of $APRR$. 
Figure 5.12: The temperature drop per particle of the MC search over RPRR when $f_{\text{initial}} = 0.32$ and $\alpha_{\text{initial}} = 16$. No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of RPRR.
Figure 5.13: The temperature drop per particle of the MC search over \( \text{APRR} \) when \( f_{\text{initial}} = 0.32 \) and \( \alpha_{\text{initial}} = 16 \). No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of \( \text{RP RR} \).
Figure 5.14: The temperature drop per particle of the MC search over $RPRR$ when $f_{\text{initial}} = 0.32$ and $\alpha_{\text{initial}} = 1$. No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of $RPRR$. 
Figure 5.15: The temperature drop per particle of the MC search over \( APRR \) when \( f_{\text{initial}} = 0.32 \) and \( \alpha_{\text{initial}} = 1 \). No distinct peaks can be found which suggests that using the simulation cutoff values and the trapping parameters, the system can only be adiabatically cooled and the evaporation of particles has no significant effects regardless of \( RPRR \).
Chapter 6

DISCUSSION

This chapter will discuss the results previously presented by analyzing first, the different types of cooling present while achieving evaporative cooling, and then, why the temperature drop per particle is optimized for specific cooling parameters and it does not efficiently cool the system for other parameters.

6.1 Adiabatic Cooling

When the values of $f$ and $a$ are reduced over time at the $RPRR$ and $APRR$, the average distance of the ions is increased. This increase, reduces the Coulomb energy and therefore causes a drop in temperature, without the loss of any particles. The effects of this can be seen in Figures 5.3 and 5.5 where at the beginning of both simulations, there is a temperature drop while the number of particles remain at their original value of $N_0 = 256$. Furthermore, the temperature drop due to adiabatic cooling far exceeds the cooling done by evaporations as can be seen in Figures 5.3 and 5.5. In fact, if the the trap had dimensions of $r_o \to \infty$ and $a_o \to \infty$, as $f \to 0$ and $a \to 0$, then $T \to 0$. However, since the trap has finite dimensions, the values of $RPRR$ and $APRR$ affect the rate at which the ensemble expands and when the average ion distance is high enough, particles will start escaping the system by hitting the trapping electrodes.

Even though the reduction of $f$ and $a$ would cause the system to expand and cool, as can be observed in Figure 5.3, the sets of evaporations that follow one another, might not be desirable. In Figure 5.5 after the adiabatic cooling, the evaporations further reduce the temperature of the system so that a temperature of less than 20 K is achieved by losing about 10% of $N_0$. In contrast, in Figure 5.3 after the adiabatic cooling, evaporations start
to heat up the system initially, and to achieve the same 20 K temperature, 90% of $N_0$ is lost. Therefore it is reasonable to claim that no matter the values of $RPRR$ and $APRR$, the adiabatic cooling will take place, however, depending on the rates of potential reduction, the evaporations that occur afterwards could either heat or cool the system.

Since adiabatic cooling has a significant role in reducing the temperature of the trapped ensemble, the initial shape of the system which is determined by the $\alpha_{initial}$ value, will have an intrinsic effect on how well the system can be cooled. When $\alpha_{initial} = 16$, the ensemble has the initial shape of an oblate spheroid which is denser compared to an ensemble that has an initial shape dictated by $\alpha_{initial} = 1/16$. This means that if two ensembles having $\alpha_{initial} = 16$ and $\alpha_{initial} = 1/16$ respectively have the same initial temperature, the system that is more compact, can expand further and therefore cool the system more using adiabatic cooling. This effect has a contributing factor to why there is a significant difference in temperature drop per particle between systems with $\alpha_{initial} = \{16, 1, \frac{1}{16}\}$ as can be seen in Figures 5.6-5.10 where the temperature drop per particle of the system with $\alpha_{initial} = 16$ is the highest, follow by the system with $\alpha_{initial} = 1$ and finally $\alpha_{initial} = 1/16$.

Given all the above factors, one can conclude that to achieve evaporative cooling LPTs, one will inevitably cool the particles adiabatically as well, and hence, these two processes go hand in hand when evaporating particles in an LPT. To avoid any confusion, the combination of these types of cooling in an LPT, will be referred to as Evaporative Paul Trap (EPT) cooling from here on in.

6.2 Trap Size

As mentioned in the previous section, using adiabatic cooling, as the trap dimensions $r_o \to \infty$ and $a_o \to \infty$, as $f \to 0$ and $a \to 0$, then $T \to 0$. However, since the dimensions of the trap must be finite, as the volume increases, the particles will eventually hit the electrodes and evaporate. Assuming the trapped ensemble in an LPT takes on the shape of an ellipsoid of
revolution, the density can be approximated by

$$\rho \propto \frac{1}{\frac{4\pi}{3} \Delta r^2 \Delta z}$$  \hspace{1cm} (6.1)

where $\Delta r$ and $\Delta z$ are the average ion separation in the radial and axial directions. Hence as the average separation is increased, the density of the system is reduced as a cubic function, which would make it increasingly hard for the ions to interact with each other and the system to equilibrate. So even though the EPT cooling has the ability to reduce to temperatures to lower levels, the equilibration time of the system is increased by orders of magnitude. In fact, to achieve desirable evaporative cooling with 10 times the trap sizes mentioned in 5.1, a single simulation would have to be run for weeks.

Therefore, the effects of the trap size was only briefly studied and the dimensions of the LPT trap used in the TITAN experiment was set, and kept as a constant for all simulations.

### 6.3 Temperature Drop Per Particle Optimization

This section will explore whether $APRR$, $RPRR$, or both can be optimized to allow for the largest temperature drop per particle lost due to EPT cooling, for the different trapping parameters.

#### 6.3.1 Dependence of $f_{\text{initial}}$

The dependance of the temperature drop per particle on the $f_{\text{initial}}$ value can be explored by comparing Figure 5.6 and Figure 5.12. The initial value of this trapping parameter will affect both methods of cooling.

First, a larger value for $f_{\text{initial}}$ would indicate a denser cloud of particles where the average distance $\Delta r$ is reduced. Hence, this would allow for the adiabatic cooling to be more effective. This is made possible since the average distance can be increased further compared to smaller values of $f_{\text{initial}}$ before evaporation will start to occur.
Furthermore, as can be seen in these two figures, the temperature drop per particle is an
order of magnitude higher for \( f = 0.64 \). This arises from the fact that the collision rate \( \sigma_{\text{coll}} \)
mentioned in Equation (2.36) has a dependance on \( f_{\text{initial}} \) as

\[
\sigma_{\text{coll}} \propto f^3
\]  

(6.2)

and so when \( f_{\text{initial}} \) is doubled, the collision rate is increased by 8 times. This higher collision
rate would allow for the system to equilibrate faster, and hence reach a physical Boltzmann
distribution sooner. Consequently, the highest energy tail can evaporate easily and not allow
for the intrinsic heating of the system to take over. Furthermore, a higher \( f \) would cause
the initial volume of the system to be lower, and would allow adiabatic cooling to be more
effective. Given all these effects, even though the intrinsic heating of the system increases as
well when \( f_{\text{initial}} \) is doubled, as it was shown in the figures, the increase in cooling exceeds
the increase in heating rate hence making the cooling more efficient overall. Therefore, given
a constant \( \alpha_{\text{initial}} \) and \( T_0 \), on average, every evaporation that occurs for a simulation with
trapping parameter \( f = 0.64 \) will be more efficient than the evaporations that occur for
simulations that have \( f = 0.32 \).

6.3.2 Dependance on \( \alpha_{\text{initial}} \)

As mentioned before and shown in Figures 5.6, 5.8 and 5.10, the temperature drop per
particle of the system with \( \alpha_{\text{initial}} = 16 \) is the highest, follow by the system with \( \alpha_{\text{initial}} = 1 \)
and finally \( \alpha_{\text{initial}} = 1/16 \). There are two dominating factors that cause this hierarchy. First,
as mentioned in the previous section, the adiabatic cooling can reduce the temperature to
lower levels for more condensed systems (\( \alpha_{\text{initial}} = 16 \)). Second, the collision rate \( \sigma_{\text{coll}} \)
mentioned in Equation (2.36) has a dependance on \( \alpha_{\text{initial}} \) and \( T \) as
\[ \sigma_{\text{coll}} \propto \frac{1}{\alpha} \]  \hspace{1cm} (6.3)

\[ \sigma_{\text{coll}} \propto \frac{1}{T^3}. \]  \hspace{1cm} (6.4)

This suggests that for \( f = 0.64 \) and \( \alpha_{\text{initial}} = 16 \), \( \sigma_{\text{coll}} \) is reduced linearly due to the increase in \( \alpha \), while at the same time, since the adiabatic cooling can reduce the temperature much more efficiently, \( \sigma_{\text{coll}} \) is increased as \( T^{-3} \). The combination of these two effects has a net increase in \( \sigma_{\text{coll}} \), and hence as previously mentioned, this would allow for more efficient evaporations. Therefore, given a constant \( f_{\text{initial}} \) and \( T_0 \), on average, every evaporation that occurs for a simulation with trapping parameter \( \alpha_{\text{initial}} = 16 \) will be more efficient than the evaporations that occur for simulations that have \( \alpha_{\text{initial}} = 1 \) and \( \alpha_{\text{initial}} = 1/16 \).

### 6.3.3 Dependence on APRR

The focus of the MC search was on traps that have \( f_{\text{initial}} = 0.64 \), since it provided much better cooling results than when \( f = 0.32 \). The results of the search over different APRR values constrained by the conditions previously mentioned, can be found in Figures 5.7, 5.9, and 5.11. The maximum temperature drop per particle values occur at different locations and do not seem to have a functional dependance on the APRR itself. This idea is reinforced since both high and low values for temperature drop per particle can be achieved for the same values of APRR. Therefore, the optimization does not directly depend on APRR, and in fact, depends on the RPRR value that it is paired up with.

Even though the best evaporations do not seem to depend on the value of APRR, the results show that for very low or very high values, efficient cooling cannot be achieved.

The trapped system will only be stable when the condition set by Equation (5.5) is met, and hence, very low values of APRR, have to be paired with very low values of RPRR. As it will be shown in the next section, very low values of RPRR do not provide the system with the conditions needed to optimize evaporative cooling.
On the other hand, very high values of $APRR$ will drop the trapping parameter $a$ to its lower limit within the first few potential drops. This could allow the particles to escape from the axial direction rapidly, without equilibration, which is not desirable.

6.3.4 Dependence on $RPRR$

Given all the previous discussions, the most detailed MC search was done on trapping parameters $f_{\text{initial}} = 0.64$ and $\alpha_{\text{initial}} = 16$. The result of this search can be found in Figure 5.6 where high values of temperature drop per particle can be achieved between the values of $RPRR = 1000 \text{ sec}^{-1}$ and $RPRR = 3000 \text{ sec}^{-1}$. As mentioned before, whether the system can be cooled or not is the result of the competition between the intrinsic heating of the system and the evaporative and adiabatic cooling. Hence, the study of RPRR can be split into three different subsections.

i) $RPRR > 2750 \text{ sec}^{-1}$

If we focus only on values of $RPRR > 2750 \text{ sec}^{-1}$ as shown in Figure 6.1, it can be seen that the temperature drop per particle does not vary by much and is kept at a constant minimum. This points to the fact that on average, the evaporating particles do not affect the temperature of the system, which is due to the potential being dropped too fast. When the potential is dropped too fast, the system is not allowed to equilibrate before particles escape the system and hence an undesirable evaporation occurs. Even though this undesirable event might not heat the system, it might not cool the system efficiently either and so the average drop in temperature will not be optimized.

The distribution of ions during an evaporation of a random simulation with cooling parameters $RPRR = 8022 \text{ sec}^{-1}$ and $APRR = 128 \text{ sec}^{-1}$ can be found in Figure 6.2 where even though the energy distribution of the particles somewhat resembles that of a Boltzmann distribution, and the particle escaping has a higher than mean energy, it does not come from a bin that is at the tail of the distribution.
Figure 6.1: Temperature drop per particle for $RPRR > 2750$. No significant peaks can be seen here due to the very fast potential drop. This high value of $RPRR$ does not give the system enough time to equilibrate before evaporation and hence, reducing the effectiveness of evaporative cooling.

ii) $1000 < RPRR < 2750$

Figure 6.3 focuses on the most interesting part of Figure 5.6. Here, very high values for temperature drop per particle can be achieved and the range of $RPRR$ values give the system enough time to equilibrate to achieve desirable evaporative cooling, while at the same time, do not reduce the potential too slowly to allow excessive heating.

However, for the same values of $RPRR$ that cooling seems to be optimized, simulations with the $APRR$ and $RPRR$ values that vary by less than 1%, give results that show temperature drop per particle reduced by up to 10 times. This points to the chaotic nature of trapped ion ensembles. For instance, if a bad evaporation occurs at any point during a simulation due to two low energy ions getting too close to each other, there is a possibility
Figure 6.2: The distribution of particles during an evaporation. The darker bin shows the energy of the particle that has evaporated. As can be seen, the distribution somewhat represents a physical Boltzmann distribution, however, the evaporated particle is not from the high energy tail of the distribution.

that the entire system will require orders of magnitude more time to achieve the cut-off temperature.

The other contributing factor to this discrepancy might arise from the perturbation applied to the initial conditions of every simulation. These perturbations combined with even the smallest changes in the values of the cooling parameters, have the potential to change the outcome of the simulations and reduce the effectiveness of EPT cooling.

Even though there is a possibility of not achieving very high temperature drop per particle, the range of $RPRR = 1000$ sec$^{-1}$ and $RPRR = 2750$ sec$^{-1}$ has the highest chance of achieving optimized evaporative cooling compared to the rest of the values of $RPRR$. This gives experiments a clear range of values to set the value of $RPRR$ at to maximize their
Figure 6.3: Temperature drop per particle for 1000 < $R_{PRR}$ < 2750. The highest values of temperature drop per particle can be found for this range of $R_{PRR}$ values. However, there are cases that two simulations with very similar $R_{PRR}$ and $A_{PRR}$ provide results that are a maximum of an order of magnitude different. This points to the chaotic nature of the trapped ensemble that there is chance that even if the cooling parameters are finely tuned, an undesirable evaporation could occur. However, this range has the highest chance of giving the best temperature drop per particle.

The chances of achieving the lowest temperature with the least number of particles lost, however, it would not guarantee it. On the other hand, the worst results in this range, are still equal or better than the temperature drop per particle lost achieved using other trapping, or cooling parameters.

iii) $R_{PRR}$ < 1000

As the value of RPRR becomes lower, the temperature drop per particle is lowered until it reaches negative values as can be seen in Figure 6.4 which focuses on values of $R_{PRR}$ < 1000. This reduction is due to the potential drop being too slow and allowing for the heating to
take over. If the value of $RPRR$ is low enough, the rate of heating will be much higher than
the rate of evaporative cooling, resulting in temperatures that are higher than the initial
temperature. The negative values of temperature drop per particle in Figure 6.4 show these
cases.

Relatively few number of simulations with very low values of $RPRR$ were run due to the
very high computation time of the order of days, or sometimes weeks.

Figure 6.4: Temperature drop per particle for $RPRR < 1000$. In this area the temperature
drop per particle starts to decrease and the heating in the system takes over. The heating
will increase, to the point where when $RPRR$ values are low enough, the system starts to
achieve temperatures that are higher than $T_0$. The points that have a negative temperature
drop per particle represent these simulations.
6.4 Applicability of Results to Experiments

The results of this research show that not only is it possible to evaporatively cool ionic systems in LPTs, but given the trapping parameters, the cooling can also be optimized. However, this study only optimized the results for a very narrow set of conditions which include trap size, initial number of particles, initial temperature, ion charge, and $PRTC$. Given the chaotic nature of the system, extrapolating the effects of a change in any of these parameters, on the temperature drop per particle is not a simple task.

Hence, if an experiment uses the same trapping parameters as those explored in the research, such as the TITAN experiment, the results indicate how EPT cooling can be optimized by setting $APRR$ and $RPRR$ in a specific range. On the other hand, if the trapping parameters are different, rather than there being a clear range of $APRR$ and $RPRR$ values to achieve the highest temperature drop per particle, there are general guidelines of how to move towards it. These guidelines, which have been discussed above, generally affect the initial density of the ion cloud, collision rate of ions, and rate of particle evaporations which are the key factors in EPT cooling.

6.5 Summary

Simulations have shown that EPT cooling which is a combination of evaporation of particles alongside adiabatic expansion can cool down systems from hundreds of Kelvins down to 1% of its initial temperature. Even though at first glance, adiabatic cooling seems to do the majority of the work, to ensure that the evaporations that follow it are not heating the system, several factors need to be considered:

1. Varying the value of the potential reduction time constant from $PRTC = 5 \times 10^{-6}$ to $PRTC = 10^{-7}$ only changes the final temperature lost per particle by less than 2%. Values lower than $10^{-7}$ do not allow the system to equilibrate
before the next potential drop. Values higher than $5 \times 10^{-6}$ were not explored due to time constraints.

2. Bigger trap size does not necessary mean lower final temperature. Even though bigger trap size would mean that adiabatic cooling on its own can achieve lower temperatures, the particles will take too long equilibrate with each other and evaporations will be random, hence losing particles without any decrease in temperature.

3. Shape of the ion cloud can change efficiency of the cooling by orders of magnitude. At temperature $T$, a more condensed system would be more efficiently cooled by evaporative cooling compared to another system at the same temperature, but with larger volume.

4. The trapping parameters can affect the collision rate greatly. By picking higher values of $f_{\text{initial}}$, the time spent by the system to equilibrate is lowered. This would consequently reduce the amount of heating done to the system. Even though the higher values of $f_{\text{initial}}$ would cause higher heating rates, the drastic drop in equilibration time more than makes up for this heating.

5. In an LPT, high efficiency evaporative cooling can occur for any value of $APRR$ as long as the value is not too low to take the system out of its stability region or too high to cause rapid particle loss without equilibration.

6. In an LPT, the rate at which the value of $f_{\text{initial}}$ is dropped, or $RPPR$, can change the temperature lost per particle by orders of magnitude. If the value of $RPPR$ is set too low, the trapping parameter $f_{\text{initial}}$ will remain large for extended periods of time, causing the ensemble to heat. However, if the value of $RPPR$ is too high, the system will expand too fast and not give the particles enough time to equilibrate. This would mean the previously mentioned
conditions for a desirable evaporation will not be met, and the escaping particle may heat the system. For $f_{\text{initial}} = 0.64$, any value between the values of $RPRR = 1000 \text{ sec}^{-1}$ and $RPRR = 2750 \text{ sec}^{-1}$ was found to achieve this delicate balance.
Chapter 7

CONCLUSION AND FUTURE PROSPECTS

7.1 Conclusion

LPTs are used in many different physics experiments by confining particles using radio frequency electromagnetic fields. The equations of motion of any trapped ensemble with more than 2 particles cannot be analytically solved and hence computer simulations are used to study the system.

Given the oscillating nature of the fields, the system is non-conservative and any ensemble with more than 2 ions will heat over time. To counteract this heating, there are many different ways to cool the trapped system. One of the least explored methods, is applying evaporative cooling to an ensemble trapped by an LPT, which in this specific case, cools the system using a combination of adiabatic expansion and evaporation of particles. This was achieved by lowering the trapping potential amplitudes using variable $RPRR$ and $APRR$ which depending on their values, would cause evaporations that could cool or heat the system. This thesis explored the values of $RPRR$ and $APRR$ at which the evaporations cooled the system, and optimized the cooling in terms of the average temperature drop divided by the number of particles evaporated.

It was shown that for evaporative cooling to be effective, the system must first have a physical energy distribution, and then the evaporated particle comes from the high energy tail of this distribution. For this to be achieved, the trapping potentials must remain constant long enough for the ions to interact with each other and the system to equilibrate. However, if the equilibration period is too long, the intrinsic heating of the system will take over. To study this delicate balance, large MC simulation sets of the order of tens of thousands of simulations, were run where different cooling parameters $RPRR$ and $APRR$ were picked at
It was found that the initial shape of the ensemble was of great importance. If two ensembles at the same temperature but with different shapes are used as the initial conditions of the simulations, an initially more condensed cloud could be cooled orders of magnitude better than an initially less dense ion ensemble. Furthermore, trapping parameters that enhance the interaction rate of the particles are preferred over those that hinder it.

Finally, it was shown that the optimization of evaporative cooling does not depend on \textit{APRR}, as long as it is not too low to force the trap into instability, or too high to allow undesirable evaporations to occur. On the other hand, the value of \textit{RPRR} can greatly enhance or reduce the effectiveness of evaporative cooling. It was shown that for very low values of \textit{RPRR}, the system will start heating to the point that it will surpass the systems initial temperature \( T_0 \). On the other hand, when the potential is dropped very fast, undesirable evaporations occur which could heat the system. The highest values for temperature drop per particle is achieved when the reduction rate is not too slow or too fast, or more specifically, when \( 1000 < \textit{RPRR} < 2750 \). However due to the chaotic nature of the trapped ion system, the value of temperature drop per particle can vary an order of magnitude for same \textit{APRR}s and \textit{RPRR}s varying less than 1%.

7.2 Future Prospects

While this research studied how the evaporative cooling changes with respect to the potential reduction rates, the simulations of trapped ions in an LPT have many different parameters that can be tweaked. This section will suggest the future work that can be done by trying to optimize other parameters and why they could be of interest to the results of evaporative cooling.
7.2.1 Trap Size

As mentioned in the previous chapter, the trap size can have a significant effect on how much the system can be cooled by adiabatic cooling. If the trap dimensions are too small, adiabatic cooling cannot cool the system enough before particles start to evaporate. On the other hand, as trap dimensions get larger, even though the evaporative cooling can cool the system very well, the ion-ion interactions would disappear and cause evaporations to not be desirable.

A potential area of study is the trap size and whether it can be optimized in terms of the number of particles present inside an ensemble and its initial temperature to maximize the efficiency of the delicate balance between evaporative cooling and achieving desirable evaporations.

7.2.2 Potential Reduction Time Constant

As previously discussed, it was found the value of $PRTC$ does not affect the resulting temperature at $f = 0.64$ and $f = 0.32$ when it was set within the range of $PRTC = 5 \times 10^{-6}$ and $PRTC = 10^{-7}$. However, this was tested for a limited set of $RPRR$ and $APRR$ values and does not rule out the possibility of a connection between the values of $RPRR$, $APRR$, and $PRTC$.

For instance, the temperature drop per particle could increase if the potential is dropped more often when the $RPRR$ is small enough that the system does not necessarily require the potential to remain constant for a long period of time to equilibrate. This idea would lead to the possibility of varying the value of $PRTC$ based on the collision rate of the ensemble, which dictates the period of time needed for the system to equilibrate.

Hence, more studies could be done on the possibility of optimizing the $PRTC$ for different trapping and cooling parameters.
7.2.3 Different Plasma Aspect Ratios

While it was found that the value of $\alpha$ could change the temperature lost per particle by an order of magnitude when it was set to its lowest value, there must be a lower limit on its value. This arises from the Coulomb force between ions tending towards infinity as they get closer to each other. Hence, as value of $\alpha$ is decreased, the temperature and the Coulomb energy will increase to the point that the system cannot be cooled to a desired temperature, i.e. $T_0 = 500$ K, or as soon as the system is evolved, the particle move away from each other with great acceleration and escape the trap.

A potential area of study is to determine how low the value of $\alpha$ can get before it would cause a chaotic system and whether given an initial temperature, there is an optimized value for $\alpha$ that would optimize evaporative cooling.

7.2.4 Different Temperature Regimes

The initial temperature regime of the system is another possible area of exploration. Applying evaporative cooling to ion ensembles at temperatures that differ by orders of magnitude would allow the comparing and contrasting the efficiency of this method with others such as laser cooling in different regimes. This would open the door to combining different methods of cooling to achieve very cold trapped ion systems faster. This could be specially of use when trying to reduce the energy of radioactive ions in an experiment like those carried out in TITAN at TRIUMF.

7.2.5 Different Temperature and Number of Particle Cutoffs

To allow for faster computation time and to be able to compare all results with each other, when the system reached a certain temperature or had about 90% of its particles evaporated, the simulation was considered to be completed and it was stopped.

When the cutoff temperature is set to $0.1 \times T_0$, there exist values of $RPRR$ and $APRR$ for which the system can be adiabatically cooled to $T = 0.1 \times T_0$ without the need to evaporate
any particles. This suggests that as the temperature cutoff is changed, the possible range of values for \( R_{PRR} \) and \( A_{PRR} \) could change.

Furthermore, the loss of 90\% of the trapped species might not be acceptable to some experiments. This value could be changed to match an experiments requirements and to allow the \( R_{PRR} \) and \( A_{PRR} \) to be tuned only in the regions that would be able to cool the system without losing too many particles.

Hence, a definite area of interest is the range of values of \( R_{PRR} \) and \( A_{PRR} \) for which the maximum cooling per particle that can be achieved given values of \( T_{cutoff} \) and \( N_{cutoff} \).

7.2.6 Moving Forward to TITAN: Buffer Gasses

This research marks the first steps towards fully modeling the radio frequency trap in the TITAN experiment and there are still many components that the code cannot model. One such component is the buffer gas that is injected into the radio frequency trap which is used as a means for initial ion cool down through collisions. If the gas is cooler than the ion cloud, on average, the collisions would reduce the temperature of the trapped ensemble.

There are currently no modules in the code that can model the collisions between ions and neutral particles and hence the next step could be to program these collisions to model the cooling done by buffer gases and combine them with evaporative cooling.

7.2.7 Applying Evaporative Cooling to Penning Traps

Another direction that can be taken using the program is to apply the evaporative cooling modules to another widely used trap, the Penning trap. Other than the radio frequency trap, the TITAN experiment makes use of two additional Penning traps [15]. To optimize the cooling across the experiment, simulations could be run where evaporative cooling is applied to each of these traps and the results compared to each other.

Modules to model a trapped ion system inside a Penning trap were added to the code, however, no large scale simulations on evaporative cooling in Penning traps were done.
Bibliography


