Regular and Chaotic Dynamics in the Paul Trap: 
Fixed Points, Bifurcations, and Crystal Morphologies

by

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Abstract

The dynamics of multiple particles in a Paul-trap may often be modeled classically, leading to a system of non-linear equations describing the particles’ evolution. The non-linearity allows for the emergence of chaotic phenomena in the trap. Still, via damping, we may sometimes achieve an ordered, low-energy state of the particles, referred to as a crystal. In such a state, the particles stay nearly still, undergoing small-amplitude oscillations at the frequency of the trap’s driving force.

In this Thesis, we explore, for an isolated particle species, these low-energy states. For various particle numbers, we numerically determine which regions of parameter space allow for such crystallization, and also report parameter settings where crystallization is never observed. Through observation of bifurcations and unstable fixed points, we conclude that these latter regions are areas of global chaos. We also investigate the morphologies of observed crystals, both analytically and numerically. Specifically, we report predictions of the allowable crystalline morphologies for the three, four, and five-particle systems. Generalizing methods previously used for two-particle system, we predict morphology boundaries in parameter space. By four particles, we observe the emergence of double-wells, i.e. distinct crystalline states at a fixed parameter setting.
I would like to thank everyone who has assisted and supported me over my last year of research. This includes all the faculty and staff of the physics department, as well as the fellow members of my research group. In particular I would like to acknowledge my faculty advisor, Reinhold Blümel, and my research collaborator, YunSeong Nam, for their invaluable guidance throughout this graduate experience. I would also like to thank my parents and grandparents for helping me to reach to this point in my life. I am grateful for all I have learned, and feel truly blessed. Thank you all very much!
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Chapter 1

Introduction

The Paul trap\cite{1} is a device designed to stably confine microscopic particles without material contact. Via periodic electrical driving forces, the trap suspends the particles (e.g., Helium ions\cite{2}) at the hollow center of the trap. This engineered phenomenon is a testament to human ingenuity; the achievement is so remarkable, in fact, that the inventor, Wolfgang Paul, shared the 1989 Nobel Prize in Physics\cite{1} for this important contribution. Even today, as the Paul trap is actively researched, scientists and engineers are excited about its extraordinary capabilities. The trap’s possible applications are wide ranging; they include improving frequency standards\cite{2}, exploring chaotic phenomena\cite{3,4} investigating a single, isolated particle’s statistical mechanics (rather than an ensemble average)\cite{5}, and constructing a quantum computer\cite{6}. Understanding the dynamics of the trapped particles is, thus, essential to exploiting the Paul trap as a powerful experimental tool.

In addition, much of the material covered in the following chapters is relevant to other physical systems. For example, the equations of motion describing Paul trap
dynamics are nearly identical to the equations for the Penning trap\cite{1}, which uses both electric and magnetic fields to achieve three-dimensional trapping of ions. More broadly, the Paul trap is just one of many devices for focusing or confining particles. Many of these systems are examples of periodically driven systems. Later we will introduce the pseudo-potential approximation, which is applicable to a broad class of driven systems.

Chapter 1 is organized as follows. First, in Sec. 1.1, we give an account of the experimental and theoretical results published about the Paul trap since its advent in the late 1950’s. Then, in Sec. 1.2, we specify the physical setup of the Paul trap. Finally, in Sec. 1.3, we briefly describe the qualitative features of particle dynamics in the trap and outline the structure of the Thesis.

1.1 Historical Overview

In the late 1950’s in Bonn, Germany, Wolfgang Paul and his team were the first to construct a quadrupole ion trap, now called a Paul trap. Throughout the decade leading up this invention, Paul et al. \cite{7, 8} were investigating multi-pole electric fields (the quadrupole field being the simplest) as a means of tightening beams of neutral particles via dipole interactions. The question arose: what are the effects of such fields on charged particles (i.e. electrons, ions, etc.).

It had been realized since Maxwell that no static quadrupole field could simultaneously confine ions in all three dimensions. As we shall see, only a dynamic field can possibly accomplish such a task. Around this time, the strong focusing force was being proposed as a means of focusing high energy particle beams in accelerators (see, for example, \cite{9}). In this case, the focusing alternates between
two spatial dimensions while the beam propagates along the third spatial axis. This stable localization of particles was accomplished by passing them through a periodic sequence of converging and diverging electromagnetic lenses. Paul, drawing on these techniques, generalized the stable two-dimensional confinement of charged particles, to a three-dimensional focusing (i.e. trapping). Thus, the Paul trap was born.

Initially, the Paul trap was developed for application to mass spectrometry. This utilization was possible since, the Paul trap will, in general, fail to simultaneously trap two particles of the same charge, but different mass. Thus, the trap serves as a means of filtering out a particular species of particle. The first experiments using the Paul trap as a spectrometry tool were reported in 1962[10]. For this specific apparatus, trapped ⁴He⁺ atoms were spin-polarized via collisions with a polarized Cs atomic beam. This allowed for the observation of magnetic resonances in the free ⁴He⁺, determined by the nuclear magnetic moment and gyromagnetic ratio. Hence, data from these experiments led to an empirically determined value of the ground-state $g$-factor of the ions[11]. Around the same time, the Paul trap was being used for similar experiments involving ³He⁺[12] and other particles.

A decade later, in 1973, was the first report of the high-resolution microwave spectrum of trapped ions (specifically, the heavy ion ¹⁹⁹Hg⁺), via optical fluorescence pumping of the ground-state hyperfine structure sub-levels[13]. This work established a new frequency standard for spacecraft atomic clocks[2]. With laser capabilities still developing, it was five more years until the first publications of lasers used for resonance fluorescence experiment of ions stored in the Paul trap[14]. This new technique of using lasers in optical interactions with trapped ions entirely changed the scope of experimental possibilities by vastly increasing the signal-to-noise ratio, in comparison to UV lamps used in earlier
In 1978, Toschek et al.\cite{15} reported a landmark experiment involving laser cooling. Via high-intensity laser resonant scattering, the team was able to detect individual cooled ions. This remarkable optical observation of a single particle opened the field to a new world of precision measurements on an isolated, free particle. Now the evolution of a single ion could be traced, rather than merely statistically averaging the behavior of a collection of particles. For instance, this extreme resolution allows for a technique known as *ion shelving*\cite{5}, in which a single ion is placed in a particular state via laser excitation. Then, the life-time of the state is observed by detecting photons emitted as the particle transitions out of the state.

A decade later in 1988, the fundamental limit of laser cooling had been reached\cite{16}. It was reported\cite{17} that via sufficient laser cooling, the oscillatory motion of trapped particles may be damped until the mean Coulomb energy is larger than the ion kinetic energy. In such a case, the motion of the ions is spatially ordered, and a *crystalline* state of the particles is observed. The particles make tiny driven vibrations (at the trapping frequency $\Omega$) about a fixed center. Later, we will see that we may separate the particle’s motion into the slow-varying *macro-motion* which determines the guiding center, and a forced, rapid *micro-motion* at frequency $\Omega$. Through a method of averaging the *pseudo-potential* approximation was introduced\cite{19} as a means of predicting the evolution of the secular (i.e. macro-) motion. Crystalline states correspond to minima of the pseudo-potential, for which the guiding center of remains fixed. To lowest order, this confining potential is harmonic (with secular frequency $\omega_e$) as expected since the potential is confining.

Although this is a semi-classical description, by clever optical means\cite{21}, we may
form crystalline states in the Paul trap such that the quantum wavefunction is described by some coherent states of the harmonically bound particle. For such a state, the expectation value of the individual ion’s position and momentum simply oscillate at the trap frequency, just like a classical particle. Thus, the above classical reasoning may be extended to a quantum description of the crystalline states. In fact, laser cooling is a fundamentally quantum mechanical technique. Consider the simplest case of an atom with two internal quantum states: a ground state and an excited state, with resonant transition frequency $\omega_0$. A light beam (of frequency $\omega_L$) incident along the direction of the atomic motion, will have an absorption spectrum composed of a carrier frequency at $\omega_0$ and resolved sidebands at $\omega_0 \pm \hbar \omega_v$ due to the Doppler effect. When $\omega_L = \omega_0 - \omega_v$, spontaneously emitted photons of average energy $\hbar \omega_0$ reduce the kinetic energy of the atom by $\hbar \omega_v$ per scattering event. The natural energy scale is given by the energy levels of the harmonic potential, namely $E_n = \frac{\hbar^2}{2m}(2n + 1)$, and the cooling limit, called the zero-point energy, is then $E_0 = \frac{\hbar^2}{2m}$. Thus, in addition to the internal quantum numbers of each atom, the system is described by the translational quantum number, $n$, corresponding to kinetic motion of the particles. Via this technique of resolved sideband cooling, Monroe et al. [22] reported in 1994 the successful cooling of a single beryllium ion to the 3D ground-state. Such a super-cooled atom allows us to approach the ideal of a cooled quantum particle at rest. Cirac and Zoller have proposed a realization of a quantum computer, based on cooling of many particles to the quantum zero-state and achieving Jaynes-Cummings coupling via optically stimulated emission [6].

However, this technique of cooling stably trapped particles into a crystalline state only works at certain combinations of ac and dc applied voltages. In other words, at certain ac/dc voltage settings, the particles remain stably trapped, but are only
ever observed with chaotic secular motion. In 1992, Blümel et al. [3] predicted these crystal-free regions of parameter space for the specific case of the two-particle system. In numerical simulations, period-doubling bifurcations were observed, indicating that the crystal-free zones are in fact globally stochastic regions of parameter space.

Having given a brief historical overview, we are now ready to explore trap dynamics in the hopes of, for example, understanding more clearly the crystalline states of trapped particles. In order to proceed, we now turn to fully specifying the Paul trap apparatus.

1.2 The Paul Trap Apparatus

We begin by specifying the goal of the system, which is to exert a restoring force[23] on the particles, always accelerating them back to the center of the trap. By considering the force that we wish to exert on the particles, we can understand the Paul trap’s architecture. Denoting \( \vec{r} \) as the displacement vector measured from the center of the trap, the simplest possible focusing force is

\[
\vec{F} = -c \vec{r}, \tag{1.1}
\]

where \( c > 0 \) is a constant. In other words, the magnitude of the force grows linearly with distance from the origin. In Cartesian coordinates, and in the general, non-isotropic case, we may rewrite (1.1) as

\[
F_x = -\alpha x, \quad F_y = -\beta y, \quad F_z = -\gamma z, \tag{1.2}
\]

where \( F_x, F_y, \) and \( F_z \) denote the restoring forces in \( x, y, \) and \( z \) directions, respectively and \( \alpha, \beta, \) and \( \gamma \) are constants representing the strength of the restoring
forces in the $x, y,$ and $z$ directions, respectively. The component of the force in each direction shown in (1.2) is analogous to the restoring force experienced by a mass on an ideal spring. The corresponding scalar potential $\Phi$ producing such a force field then reads

$$\Phi \sim (\alpha x^2 + \beta y^2 + \gamma z^2).$$

(1.3)

Now, we would like to trap a charged particle without material contact, but only via electric fields. Assuming free space inside the Paul trap, the potential $\Phi$ in (1.3) must satisfy Laplace’s equation[24], i.e.,

$$\nabla^2 \Phi = 0.$$  

(1.4)

Inserting (1.3) into (1.4) we obtain

$$\alpha + \beta + \gamma = 0,$$

(1.5)

which implies we cannot simultaneously satisfy $\alpha, \beta, \gamma > 0,$ unlike with the spring system. At first glance, such a restriction seems to kill all hope of successfully trapping particles. After all, this requirement means that the trap cannot simultaneously produce a restoring force in the $x, y,$ and $z$ directions. At any time, the particle is being accelerated away from the origin in at least one direction. This is because, at any given moment, either $F_x, F_y,$ or $F_z,$ derived from the electric potential in (1.3) satisfying (1.4) must be positive. Indeed, if the electric potential is static, then after a short time the particle will have escaped the trap.

We therefore conclude that $\Phi$ must be dynamic, switching sign periodically, to have any hope of trapping particles. For the specific case of the Paul trap, this is accomplished as follows. To begin, we note that cylindrical symmetry, i.e. rotational symmetry about the $z$-axis, is achieved exactly when $\alpha = \beta.$ Thus, for a cylindrically symmetric system such as the Paul trap, in order to satisfy
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Figure 1.1: Paul Trap Apparatus

(1.5), we require \( \gamma = -2\alpha \). Then, in such a case, an equivalent condition to (1.3) is

\[
\Phi \sim \rho^2 - 2z^2,
\]

where \( \rho = (x^2 + y^2)^{1/2} \) denotes distance from the \( z \)-axis. As shown in Fig. 1.1 such a potential is generated by a rotationally-symmetric hyperbolic ring electrode (orange), equidistant between two identical, rotationally-symmetric hyperbolic cap electrodes (blue). Letting \( \Phi_0(t) \) denote the voltage applied to the trap, we may therefore denote the potential as

\[
\Phi = \Phi_0 \left( \frac{r_0^2 + 2z_0^2}{r_0^2 + 2z_0^2} \right) \left[ \rho^2 - 2z^2 \right],
\]

where, \( r_0 \) and \( z_0 \) are scaling constants representing the size and dimensions of the trap. More specifically \( 2z_0 \) is the distance between end-cap electrodes, and \( 2r_0 \) is the width of the ring electrode at its thinnest point (the middle). Now, in order for the electric potential \( \Phi \) to be periodic, we require that the voltage \( \Phi_0 \) is periodic. Hence, for the Paul trap, voltage is usually chosen to be sinusoidal\[1\], i.e. given by

\[
\Phi_0(t) = U_0 + V_0 \cos(\Omega t),
\]

where \( U_0 \) is the dc voltage, \( V_0 \) is the amplitude of the ac voltage, and \( \Omega \) is the ac frequency. In what follows, we assume the applied voltage is of the form (1.8),
although investigations of other periodic potentials (such as a delta function or square wave\cite{25}) exist in the literature. Also explored are deviations from the ideal hyperbolic geometry of the trap. Still, for inquiry about pure sinusoidal drive, \eqref{1.7} and \eqref{1.8} entirely describe the electric potential, and thus the force, induced by the trap on the particles.

1.3 Outline

With the physical apparatus now fully specified, the goal of this Thesis is to investigate the dynamics of one or more charged particle in such an ideal Paul trap. More specifically, for given initial conditions, we would like a description of each particle’s evolution. Of particular interest are the low-energy crystalline states first described in Sec. 1.1. In general, we say that trapped particles undergoing periodic motion are in a solid phase since snapshot of the system (taken with the frequency of the periodic motion) show each particle’s position and velocity unchanged. In the lowest-energy solid-states, the stroboscopic snapshots will show that the particles have a clear order and symmetry. This is why we call such a state a Coulomb crystal\cite{27}. These energy minima are expected, according to Wigner, who postulated that the ground state of a collection of electrons should have a crystalline form\cite{28}. For the two-particle system, three distinct morphologies were predicted in the early 1990’s\cite{3}. However, for this simple system, only one distinct morphology can exist at fixed parameter settings. We will see that by four particles, this is no longer the case. A single \((q,a)\) set will allow multiple solid-state configurations. Correspondingly, as we shall see, there are multiple minima of the time-averaged potential.

In general, when we load particles into the trap, they do not form a crystal.
Rather, they energetically float around in an unorganized motion, mutually repelling each other while never straying too far from the origin. The suspended particles form a more-or-less evenly dispersed cloud, centered at the origin. Just as in the solid-phase, the particles never sink to the bottom of the trap (unless they are heavy and gravity becomes non-negligible). Particles undergoing non-periodic motion are said to be a Coulomb gas, or in a gaseous phase, and will not be stroboscopically fixed.

Due to the complexity of the system, analytical methods quickly become futile as we increase in the number of particles. Consider one of the simplest non-trivial examples: a modeling of two charged particles in the trap. Such a system is non-linear, due to the Coulomb interactions; there are six coupled differential equations of motion that fully specify the dynamics. Therefore, we largely rely on numerical methods to explore our system theoretically.

One, two or even a few thousand trapped particles is an extremely small sample, compared to a macroscopic collection of particles ($\sim 10^{23}$). Still, low particle numbers is the regime of many important applications of the trap, and is, therefore, the focus of this Thesis. Furthermore, we assume that all particles are of the same species, i.e., that they have the same mass, charge, and other measurable features. For example, we may consider trapped electrons or trapped sodium ions, but not some mixture of the two. Additionally, we model the electrons or ions as point particles, which is an excellent approximation given the length scale of the system ($\sim 5\mu\text{m}$) compared to a typical atom size ($\sim 1\text{Å}$).

We note, however, that to model something as light as an electron, for which quantum mechanical effects are non-negligible, we would have to start from Schrödinger’s equation for a fully rigorous description of the system. Still, in most cases, the particle densities are low; in such a case, the quantum effects are in fact insignif-
icant and our classical model is valid. Furthermore, as discussed in Sec. 1.1, the low-energy states of the harmonically bound atoms may be described in terms of their normal modes, with the expectation values of a particle’s momentum and velocity harmonically oscillating like a classical particle. In such a state, the atoms may be referred to collectively as an exotic molecule or a pseudo-molecule [26], and again a semi-classical analysis is fruitful.

This Thesis is organized as follows. In Chapter 2, we review three textbook non-linear systems, as an introduction to many of the important techniques and ideas presented in this Thesis. We will frequently draw analogy between these simpler systems and the Paul trap system. Chapter 3 reviews the physics of a single charged particle in the trap, culminating in a description of which combinations of ac and dc voltages will stably trapped the particle. Chapter 4 discusses trapping multiple particles, and describes the numerical methods used to carry out our investigation. In Chapters 5-7 we present our results. More specifically, Chapter 5 formally distinguishes two phases in the trap (solid and gas) and investigates the phase dependence on voltage settings. In Chapter 6 we formalize these results by relating the observed phenomena to chaos. We then turn in, Chapter 7, to studying the solid phase, and investigating crystalline morphologies’ dependence on voltage settings. Finally, we give a summary and outlook in Chapter 8.
2.1 The Double Pendulum

The double pendulum\cite{29} is one of the simplest systems exhibiting chaos. As depicted in Fig. 2.1, the system consists of one ball of mass $m_1$ attached to a fixed pivot point by a massless rod of length $l_1$, and a second ball, of mass $m_2$, attached to the first ball, by a massless rod of length $l_2$. As shown, there are two generalized coordinates, namely $\theta_1$ and $\theta_2$, corresponding to the angle each rod
makes with the vertical $z$-axis. We denote the angular velocity of either angle by $\dot{\theta} = d\theta/dt$. We know from Lagrangian mechanics and the principle of least action that the initial conditions $\theta_1(t = 0), \theta_2(t = 0), \dot{\theta}_1(t = 0), \text{ and } \dot{\theta}_2(t = 0)$ uniquely determine the ensuing motion, for all time. In the language of dynamical systems, we define the phase-space vector

$$\vec{X}(t) = (\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2),$$

and say that the initial state $\vec{X}_0 = \vec{X}(0)$ determines all future motion. In other words, there is no randomness; the system has no choice but to move in one particular way, according to the equations of motion. Equivalently, we say that the double pendulum is a deterministic system.

The double pendulum is also an autonomous system. In general, an autonomous system is one that does not depend explicitly on time; for this reason, such systems are also called time-invariant. More precisely, the phase-space vector $\vec{X}$ of an autonomous system satisfies

$$\frac{d}{dt} \vec{X} = \vec{F}(\vec{X})$$

\[ (2.2) \]
for some vector-function $\vec{F}(\vec{X})$. On the other hand, for a non-autonomous system, $\vec{X}$ satisfies

$$\frac{d}{dt} \vec{X} = \vec{G}(\vec{X}, t)$$

(2.3)

for some function $\vec{G}(\vec{X}, t)$.

Comparing $\vec{F}$ and $\vec{G}$, we see that while the former depends only on the phase-space position $\vec{X}$, the latter is an explicit function of time. Therefore, for an autonomous system, we may write

$$\frac{\partial}{\partial t} \vec{F} = 0,$$

(2.4)

which implies

$$\frac{\partial}{\partial t} \mathcal{H} = 0,$$

(2.5)

where $\mathcal{H}$ is the Hamiltonian of the system. For such systems, energy is well-defined, and is equal to the Hamiltonian. For instance, even if we add damping to the double-pendulum system, the position and velocity at any given moment uniquely determine the Hamiltonian. Hence, the damped pendulum is an autonomous system, even though energy is lost to the surroundings via the frictional force. On the other hand, energy is, in general, not well-defined for a non-autonomous system.

For completeness, we now compute the energy of the (undamped) double pendulum system. First, we note that the potential energy $\mathcal{U}$ of the system is determined according to

$$\mathcal{U} = -m_1 g l_1 \cos \theta_1 - m_2 g (l_1 \cos \theta_1 + l_2 \cos \theta_2),$$

(2.6)

and the kinetic energy $\mathcal{K}$ is determined according to

$$\mathcal{K} = \frac{1}{2} m_1 (l_1 \dot{\theta}_1)^2 + \frac{1}{2} m_2 [(l_1 \dot{\theta}_1)^2 + (l_2 \dot{\theta}_2)^2 + 2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)].$$

(2.7)
Thus, combining (2.6) and (2.7), we see that the total energy of the system is

\[ \mathcal{H} = \mathcal{U} + \mathcal{K}. \]  

(2.8)

From equations (2.6)-(2.8), it is clear that the Hamiltonian is not explicitly time-dependent, and therefore the condition (2.5) is satisfied.

For the double pendulum system, kinetic energy transfers to potential energy, and vice-versa, while the total energy remains fixed. We may compute the lowest energy state of the system by setting \( \mathcal{K} = 0 \) and minimizing \( \mathcal{U} \). This state corresponds to the mass \( m_1 \) and \( m_2 \) stationary, aligned on the \( z \)-axis below the origin. In other words, the system is described by a point in phase-space given by the vector

\[ (\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2) = (0, 0, 0, 0). \]  

(2.9)

This lowest-energy state is called an \textit{equilibrium point}, or \textit{fixed point}. This particular fixed point is \textit{stable}, since, for example, if we perturb the initial condition (2.9) by giving the lower mass \( m_2 \) some tiny, non-zero angle with the \( z \)-axis, the system will not move very far away from the equilibrium point. In fact, if we add the slightest damping, the system will again be pulled onto this low-energy configuration. Alternatively, the configuration with both masses stacked vertically \textit{above} the origin corresponds to a maximum of the potential function. This arrangement is given by the phase-space vector

\[ (\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2) = (\pi, \pi, 0, 0) \]  

(2.10)
and is an unstable equilibrium point since upon perturbation, the system will quickly move away from this initial configuration.

In certain high-energy regions of phase-space, the motion of the double pendulum exhibits an extraordinary sensitivity to initial conditions. In Fig 2.2(i) we first plot the trajectory of some lower-energy initial conditions by tracing the motion of $m_2$ as time progresses. Fig 2.2(ii) shows the trajectory when the conditions in part (i) are slightly perturbed. The trajectories are visually identical. On the other hand, Fig. 2.3(i) shows the trajectory for some higher-energy initial conditions, while Fig. 2.3(ii) shows the trajectory when the conditions are slightly perturbed. Now the results are visibly different. The motion of the masses changed dramatically with a changing of the angle of $m_2$ by less than a tenth of a degree. This rapid divergence of initially close trajectories is a hallmark of chaos.

Figure 2.3: Chaotic Double Pendulum Trajectories
2.2 The Kicked Rotor

The double pendulum gives us a first glimpse at chaos. However, it is an autonomous system, which, as will be shown in Chapter 3, is not the case for the Paul trap. For this reason, we introduce another pendulum system, namely, the kicked rotor [31], or kicked pendulum, depicted in Fig. 2.4. The pendulum consists of a mass $m$ with charge $Q$, attached to a massless rod of length $l$. The rod is free to rotate, forming angle $\theta$ as shown. The system is assumed to be in outer space, in the absence of gravitational and frictional forces. Relative to the pivot point, the moment of inertia is $I = ml^2$. Denoting $\dot{\theta}$ as the angular velocity, the angular momentum at any point in time is

$$L = I\dot{\theta} = ml^2\dot{\theta} \quad (2.11)$$

and the kinetic energy is

$$K = \frac{L^2}{2I} = \frac{ml^2}{2}\dot{\theta}^2. \quad (2.12)$$

We now apply a driving force (with period $T$) by placing the pendulum equidistant between two long parallel electric plates. Whenever the time is an integer multiple of $T$, we instantaneously apply a voltage difference between the two plates. This is accomplished, for instance, by setting one plate to a positive voltage, while keeping the other plate grounded. At all other times, both plates are grounded, and there is no voltage difference. For the briefest moment, every $T$ units of time, the mass is immersed in an electric field. Correspondingly, the charged mass repeatedly feels an instantaneous driving force toward the grounded plate. This periodic driving force makes the potential explicitly time-dependent. Hence, the kicked-rotor system is non-autonomous.

When the extent of the parallel plates is much greater than, say, the rod length
$l$, the strength of the electric force is independent of the angle $\theta$; it is entirely determined by the distance between the plates and the magnitude of the potential difference. Denoting $K$ as the amplitude of the driving force and defining the $T$-periodic delta function as

$$\delta_T(t) = \sum_{m=-\infty}^{\infty} \delta(t - mT),$$

we can write down the potential energy

$$U(t) = K\delta_T(t) \cos \theta.$$  

Combining equations (2.13) and (2.14) we see that the time-dependent Hamiltonian of this system is given by

$$\mathcal{H} = U + K = \frac{m}{2}r^2\dot{\theta}^2 + K\delta_T \cos \theta.$$  

Invoking Hamilton’s equations\[^{[29]}\], we obtain

$$\dot{\theta} = \frac{L}{I}, \quad \dot{L} = K\delta_T \sin \theta.$$  

---

Figure 2.4: Kicked Rotor Apparatus
The first equation in (2.16) is just a trivial rearrangement of (2.11). The second equation, however, reveals important physics, namely that the angular momentum is constant whenever the electrical pulses are switched off. This means that if the position and angular momentum just before the \( n \)th pulse are given by \( \theta = \theta_n \) and \( L = L_n \), respectively, then we can calculate the angular momentum just after the pulse. This is so because the change in angular momentum resulting from the \( n \)th pulse may be obtained by integrating in (2.16) over some time interval \( (nT - \epsilon, nT + \epsilon) \), where \( \epsilon < T/2 \) is an arbitrarily small constant. In fact, in the limit of \( \epsilon \to 0 \), the position \( \theta_n \) remains unchanged, while the angular momentum is altered by the instantaneous driving force. In other words, while the position is constant throughout this infinitely short time interval, the angular momentum experiences a discontinuity of magnitude

\[
\Delta L_n = \int_{nT-\epsilon}^{nT+\epsilon} \dot{L}dt = K \sin \theta_n \int_{nT-\epsilon}^{nT+\epsilon} \delta_T(t)dt = K \sin \theta_n. \tag{2.17}
\]

This discontinuity is the source of an instantaneous change in energy. Recognizing that the angular momentum, according to (2.16), will remain constant until the next pulse, we can evaluate \( \theta_{n+1}, L_{n+1} \) from \( \theta_n, L_n \). In particular,

\[
L_{n+1} = L_n + \Delta L_n = L_n + K \sin \theta_n \tag{2.18}
\]

and

\[
\theta_{n+1} = \theta_n + \Delta \theta_n,
\]

\[
= \theta_n + \frac{T}{mr^2}L_{n+1}. \tag{2.19}
\]

since the change in position \( \Delta \theta_n \) between pulse \( n \) and pulse \( n + 1 \) according to (2.16) is

\[
\Delta \theta_n = \int_{nT}^{(n+1)T} \frac{L_{n+1}}{I}dt = \frac{1}{mr^2} \int_{nT}^{(n+1)T} L_{n+1}dt = \frac{T}{mr^2}L_{n+1}. \tag{2.20}
\]
Thus, by setting $T/mr^2$ to unity, we can express the recursion relations (2.18) and (2.19) as

$$L_{n+1} = L_n + K \sin \theta_n,$$

$$\theta_{n+1} = \theta_n + L_{n+1}. \quad (2.21)$$

In the case where (2.21) is computed modulo $2\pi$, the mapping becomes the well-known Chirikov-Taylor map, also known as the standard map.

In reaching (2.21) we have discretized the continuous variable $t$ into $t_n = nT$. We accomplished this by restricting inquiry about the system’s dynamical evolution to stroboscopic snapshots (of period $T$). Given an initial phase-space vector $\vec{X}_0 = (\theta_0, L_0)$ just before the first pulse, we can calculate the phase-space vector just before any future pulse using (2.21). In summary, we have arrived at a mapping, which describes the kicked rotor’s stroboscopic evolution.

However, just as with the double-pendulum, this mapping is extremely sensitive to initial conditions, especially for large $K$. Thus, due to inevitable imprecision in real-life experiments, (2.21) will often fail to have any predictive power. Again, in the language of dynamical systems, we say that the kicked rotor exhibits chaos.

Figs. 2.5(a)-(c) show this transition to chaos, by showing the evolution of many initial conditions with three different values of $K$. The green, which corresponds to chaotic trajectories, increasingly overwhelms the phase-space as $K$ increases.

Already mentioned in Sec. 2.1, and of interest throughout this Thesis, is the notion of fixed points, also called equilibrium points. In general, for a discrete map $\mathcal{M}$, defined according to

$$\vec{X}_{\nu+1} = \mathcal{M}(\vec{X}_\nu), \quad (2.22)$$

a period-$p$ fixed point satisfies

$$\vec{X}_{\nu+p} = \mathcal{M}^p(\vec{X}_\nu) = \vec{X}_\nu,$$
where $\mathcal{M}^p$ denotes the composition of $\mathcal{M}$ with itself $p$ times. A period-1 fixed point of the standard map satisfies [see (2.21)]

$$
\begin{pmatrix}
\theta_{n+1} \\
L_{n+1}
\end{pmatrix} = \begin{pmatrix}
\theta_n + L_n + K \sin \theta_n \\
L_n + K \sin \theta_n
\end{pmatrix} = \mathcal{M} \begin{pmatrix}
\theta_n \\
L_n
\end{pmatrix}.
$$

(2.23)

From equation (2.23), in modulo $2\pi$ space for $\theta$, it is clear that period-1 fixed points are

$$
\theta \in \{0, \pi\}, \quad L \in \{0, 2\pi, 4\pi, \ldots \}.
$$

(2.24)

We deliberately do not consider the angular momentum modulo $2\pi$, since each integer multiple of $2\pi$ corresponds physically to a distinct energy level. We note that whenever (2.24) is satisfied, the pendulum is not truly driven, since the driving force is always parallel with the rod, and thus exerts no torque. While these points are stroboscopically stationary, they still correspond physically to the dynamical system of the kicked rotor. For all cases except $L = 0$, the time-discrete fixed points correspond to periodic motion of the corresponding time-continuous system. The rotor spins, always coming back to the same place, with a frequency that is an integer multiple of the driving frequency. For the special case of $L = 0$, the rotor is truly stationary at angle $\theta = 0$ or $\pi$, not just stroboscopically. In other words, the points $(0, 0)$ and $(\pi, 0)$ are fixed points of the original, continuous
differential equation of motion, not just of the discretized mapping.

As discussed, the fixed points described in (2.24) are not, in fact, driven. Still, we can never have infinite precision (in a lab or with a computer) and thus we must consider initial conditions very close to a fixed point. These perturbed arrangements now feel torque from the electric plates, which makes establishing stability, i.e. resistance to perturbation, a difficult task for the standard map. In the next section, we formalize the notion of stability for the specific case of a period-1 fixed point of a one-dimensional map.

2.3 The Logistic Map

In connection with the standard map in Sec. 2.2 and the notion of fixed point stability, we introduce in this section the notion of attractors and repellers within the framework of the logistic map. This recursive mapping is used, among other things, to model population growth[30], and is defined by

\[
x_{\nu+1} = f(x_{\nu}) = \lambda x_{\nu} (1 - x_{\nu}).
\] (2.25)

We shall see that, for this one-dimensional, non-linear transformation, large values of the parameter \(\lambda\) lead to chaos, just as large values of the parameter \(K\) lead to chaos in the standard map.

To begin, we consider the condition for a period-1 fixed point. For the logistic map in (2.25), we have

\[
\bar{x} = \lambda \bar{x} (1 - \bar{x}),
\] (2.26)

where \(\bar{x}\) denotes the period-1 fixed point. From (2.26) we obtain

\[
\bar{x} = 0, \quad \text{or} \quad \bar{x} = 1 - 1/\lambda.
\] (2.27)
For now we consider the solution $\bar{x} = 0$. Later we will consider other fixed points, such as the period-1 fixed point at $1 - 1/\lambda$.

We consider some infinitesimal displacement $\epsilon$ from the origin as the initial condition for the logistic map, where $|\epsilon| \ll 1$. By iteratively applying the mapping logistic function, $f$, we construct the sequence $\{x_0, x_1, x_2, \ldots\}$. If this sequence converges to the origin, then the fixed point is *attractive*. If it stays $\epsilon$ close to the origin, but does not converge, the fixed point is *neutral*. If the sequence diverges from the origin exponentially in the number of iterations, the fixed point is *repulsive*.

We can formally determine the stability of the fixed point using a *linearization* technique\[32\]. We do this by expanding the mapping function around the fixed point, i.e.,

$$ f(\epsilon) = f(0) + f'(0)\epsilon + \frac{f''(0)}{2}\epsilon^2 + O(\epsilon^3). \quad (2.28) $$

Here, the function $f'$ denotes the spatial derivative of the mapping function, defined according to

$$ f'(x) = \frac{d}{dx} f(x) = \lambda(1 - 2x). \quad (2.29) $$

In the limit $\epsilon \to 0$, we can truncate the expansion in (2.28) at linear order in $\epsilon$. Thus, we obtain

$$ f(\epsilon) \approx \lambda \epsilon. \quad (2.30) $$

This means, after $n$ iterations of the mapping function, we have

$$ x_n = f^n(\epsilon) = \lambda^n \epsilon. \quad (2.31) $$

From (2.31) it is clear that if $|\lambda| < 1$, the sequence $\{x_0, x_1, x_2, \ldots\}$ converges to origin. In this case, we see that

$$ \lim_{n \to \infty} f^n(\epsilon) = 0, \quad (2.32) $$
yielding an attractive fixed point. On the other hand, if $|\lambda| > 1$, 

$$\lim_{n \to \infty} f^n(\epsilon) = \infty,$$  \hspace{1cm} (2.33)

and a repulsive fixed point is observed. In the special case of $\lambda = \pm 1$, we have 

$$\lim_{n \to \infty} |f^n(\epsilon)| = \epsilon,$$  \hspace{1cm} (2.34)

which results in a neutral fixed point.

In summary, a fixed point can be attracting, repelling, neutral. Attracting fixed points are stable; repelling fixed are unstable. Neutral fixed points are neither stable nor unstable. For the above mapping, if $|\lambda| < 1$ then the origin is an attracting fixed point; if $|\lambda| > 1$ it is a repulsive fixed point; and if $|\lambda| = 1$ then the origin is a neutral fixed point. By similar analysis we find that the period-1 fixed point at $\bar{x} = 1 - 1/\lambda$ is attractive when $\lambda$ is on the interval $L_0 = (1, 3)$, and repulsive otherwise.
Chapter 3

Single-Particle Paul Trap

Physics

In this chapter, we analyze the dynamics for the simplest case of a single particle stored in the Paul trap. Our classical model of the Paul trap is a \textit{deterministic} system, as are the kicked rotor and the double pendulum, discussed in Sec. 2.1 and Sec. 2.2, respectively. Therefore, we expect that in our deterministic single-particle Paul trap system, the initial phase-space vector

\[ \vec{X}_0 = (x_0, y_0, z_0, \dot{x}_0, \dot{y}_0, \dot{z}_0), \] 

\( \text{(3.1)} \)

together with the time-derivative,

\[ \frac{d}{dt} \vec{X} = \vec{F}(\vec{X}, t), \]

\( \text{(3.2)} \)

uniquely determines the particle’s evolution. In addition, for the current case of a single particle, the equations of motion are \textit{linear}, as we will show. Thus, the system will never exhibit chaos. In fact, we are able to obtain an analytic expression for particle’s phase-space vector \( \vec{X} \) at any time \( t \). In other words, given
the ion’s initial position and velocity, we can predict the position and velocity at any future time.

Provided with an analytic expression for $\vec{X}(t)$, the first question we now ask ourselves is whether the particle of interest will indeed be trapped in the Paul trap. To answer this question, we distinguish the two categories of possible phase-space trajectories:

(i) *Bounded*: Even in the limit of $t \to \infty$, the particle never goes further than some arbitrary distance $d$ from the origin (the center of the trap).

(ii) *Unbounded*: For any distance $d$, the particle will eventually move further than $d$ from the origin.

Clearly, bounded trajectories correspond to configurations such that the particle is stably trapped. On the other hand, unbounded trajectories correspond to configurations such that the particle has an escape route, and can travel infinitely far from the trap. The main investigation of this Chapter is then to determine if a given trap configuration and voltage settings will yield bounded (i.e. stable) or unbounded (i.e. unstable) trajectories for a given species of particle.

In Sec. 3.1 we derive the equation of motion, starting from the electric potential (see Sec. 1.2). These equations amount to three uncoupled Mathieu equations, which we introduce in Sec. 3.2. By finding solutions to the resulting Mathieu equations, we may determine which choices of parameter combinations lead to stable trapping. This defines in parameter space the *stable trapping zone*, discussed in Sec. 3.3. Finally, in Sec. 3.4, we consider the effect of adding a damping term to the equation of motion.
3.1 Equation of Motion for Undamped System

We start from the electric potential generated by the Paul trap. As discussed in Chapter 1, this potential is given by

$$\Phi(x, y, z, t) = \frac{U_0 + V_0 \cos(\Omega t)}{r_0^2 + 2z_0^2} (x^2 + y^2 - 2z^2), \quad (3.3)$$

where $U_0$ and $V_0$ denote the dc and ac voltage strengths, respectively, $\Omega$ is the frequency of the ac drive, and $r_0, z_0$ set the spatial scale of the trap (see Sec. 1.2).

Corresponding to this potential, the particle experiences electric force

$$\vec{F}_{\text{trap}}(x, y, z, t) = -Q\vec{\nabla}\Phi(x, y, z, t), \quad (3.4)$$

where $\vec{\nabla}$ denotes the gradient and $Q$ is the charge of the particle. Thus, using (3.4) together with Newton’s second law, we can immediately write down the equation of motion of a single particle in the Paul trap

$$m\frac{d^2}{dt^2} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + 2Q \left( \frac{U_0 + V_0 \cos \Omega t}{r_0^2 + 2z_0^2} \right) \begin{bmatrix} x \\ y \\ -2z \end{bmatrix} = 0, \quad (3.5)$$

where $m$ denotes the mass of the particle. Defining the dimensionless parameters $a$ and $q$ by

$$a = \frac{8QU_0}{m\Omega^2(r_0^2 + 2z_0^2)}, \quad q = \frac{4QV_0}{m\Omega^2(r_0^2 + 2z_0^2)}, \quad (3.6)$$

and dimensionless time unit $\tau$ by

$$\tau = \frac{\Omega t}{2}, \quad (3.7)$$

we obtain, by inserting (3.6) and (3.7) into (3.5) results in the dimensionless equation of motion of a single particle stored in the Paul trap

$$\frac{d^2}{d\tau^2} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + [a + 2q \cos(2\tau)] \begin{bmatrix} x \\ y \\ -2z \end{bmatrix} = 0. \quad (3.8)$$
Inspecting (3.8), we see the advantages of the non-dimensionalization are threefold. Firstly, dimensionless quantities are preferable for any mathematical analysis, since, for example, they are independent of scale. Secondly, we have reduced the parameter space from six dimensions (i.e. \( U_0, V_0, r_0, z_0, m, \) and \( Q \)) to two dimensions (i.e. \( q \) and \( a \)). All the information about the applied voltages, the mass of the particle, the charge of the particle, and the size of the trap is encoded into the ratios \( q, a \). In this sense, a single \((q, a)\) parameter setting corresponds to many physical systems, simultaneously. For example, doubling \( m \) and \( Q \) leaves both \( q \) and \( a \) unchanged; hence, the equation of motion is also unchanged, and the same physical behavior will be observed as long as these ratios remain fixed.

Finally, we recognize that each row of equation (3.8) is a version of Mathieu’s Equation[36]. The \( x \) and \( y \) rows are already in canonical form; the \( z \) row requires a simple transformation \( a \rightarrow -2a \) and \( q \rightarrow -2q \). Thus, the evolution of our single particle system is determined by a well-known differential equation.

The differential equation (3.8) yields an exact description the driven particle’s motion. To approximate the particle as moving through a time-invariant force-field, we first rewrite (3.8) as

\[
\ddot{\vec{q}} - \vec{F}_{trap} = 0, 
\]

(3.9)

where \( \vec{q} = (x, y, z) \) (distinct from the scalar-valued parameter \( q \)) and

\[
\vec{F}_{trap}(\vec{q}, \tau) = [a + 2q \cos(2\tau)] \begin{bmatrix} x \\ y \\ -2z \end{bmatrix}.
\]

(3.10)

Then, we may separate \( \vec{F}_{trap} \) into two components: a constant force \( \vec{F}_c \) corresponding the dc voltage, and an temporally periodic force \( \vec{F}_{osc} \) corresponding to
the ac voltage. More specifically, we define

$$\vec{F}_c(x, y, z) = -a \begin{bmatrix} x \\ y \\ -2z \end{bmatrix}, \quad \vec{F}_{osc}(x, y, z, \tau) = -2q \cos(2\tau) \begin{bmatrix} x \\ y \\ -2z \end{bmatrix}$$

(3.11)

and recognize that the $\vec{F}_{osc}$ now carries the time-dependent component of the trap force.

In an effort to lift this time-dependence, and arrive at an autonomous description of the single-particle system, we may compute the time-averaged force $\vec{F}_{avg}$ exerted on the particle by the ac force $\vec{F}_{osc}$. More precisely, we may write $\vec{F}_{avg}(x, y, z) = -\vec{\nabla}U_{\text{avg}}$, where $U_{\text{avg}}$ is given by

$$U_{\text{avg}}(x, y, z) = \frac{1}{8} \langle \vec{F}_{osc}^2 \rangle = \frac{q^2}{4} (x^2 + y^2 + 4z^2).$$

(3.12)

and is called a pseudo-oscillator potential$^{[35]}$. As we will detail in Sec. 7.3, when we explicitly compute the total time-averaged force exerted on a particle, that this approximated potential is only valid assuming that the amplitude of driven vibrations are small. For now, we may simply replace $\vec{F}_{osc}$ with $\vec{F}_{avg}$ in (3.8) to obtain the approximation

$$\ddot{\vec{q}} - \vec{F}_c(\vec{q}) + \vec{\nabla}U_{\text{avg}}(\vec{q}) = 0.$$  

(3.13)

In reaching (3.13) we have modeled the trapped particle as an autonomous system. In doing so, we have lost all information about the movements and vibrations that occur on the time-scale of $\pi$, the period of a single-trap cycle. This so-called micro-motion, caused by the ac voltage, has been averaged out, and thus the position vector $\vec{q}$ only traces the long-term guiding motion of the particle, called the macro-motion or secular motion. In other words, when restricting measurements to the beginning of each trap cycle, the macro-motion will dominate the observed
dynamics. In accordance with this reasoning, we may visualize the micro-motion by plotting a particle’s position continuously in time, as in Fig. 3.1(i); we notice that the particle repeatedly wiggles and snakes its way along some guiding oval. We trace this guiding macro-motion by only plotting the position of the particle at integer multiples of \( \pi \), as in Fig. 3.1(ii).

Finally, we note that plugging (3.12) into (3.13) we obtain

\[
\frac{d^2}{d\tau^2} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = - \begin{bmatrix} \mu_{\rho}^2 x \\ \mu_{\rho}^2 y \\ \mu_{z}^2 z \end{bmatrix},
\]

(3.14)

where

\[
\mu_{\rho} = \sqrt{a + \frac{q^2}{2}}, \quad \mu_{z} = \sqrt{2(q^2 - a)}.
\]

Thus, in this approximation, the particle is undergoing three-dimensional simple-harmonic motion, at radial frequency \( \mu_{\rho} \) and axial frequency \( \mu_{z} \). Thus, \( \mu_{\rho} \) and \( \mu_{z} \) correspond to the frequency of motion around the oval depicted in Fig. 3.1(ii), and are therefore referred to as the secular frequencies.
3.2 Solving the Mathieu Equation

The Mathieu equation is a second-order, linear differential equation of the form

\[ \ddot{u} + (a + 2q \cos 2\tau)u = 0. \]  

(3.16)

As we can see, a particular Mathieu equation is fully specified by fixing the parameters \( q \) and \( a \), which may be represented as a point in our two-dimensional \((q, a)\) parameter space. Thus, the choice of \( q \) and \( a \) determines the exact form of the solution. We note that for our physical application we need only consider the case where \( q \) and \( a \) are both real numbers. We also note that the general solution to (3.16) is unchanged by the transformation \( q \rightarrow -q \) since at time \( \tau = \pi/2 \) we arrive back at the original equation. Thus, we need only consider \( q > 0 \).

In order to derive the general solution to (3.16), we recognize that the driving term is periodic. This motivates us to invoke Floquet theory[36]. In general, Floquet theory is the study of differential equations of the form

\[ \dot{x} = A(\tau)x, \]  

(3.17)

where the matrix \( A \) is periodic in time. For the specific case of (3.16), the vector \( x \) is given by

\[ x(\tau) = \begin{bmatrix} u(\tau) \\ \dot{u}(\tau) \end{bmatrix}, \]  

(3.18)

and the \( \pi \)-periodic transformation \( A \) is given by

\[ A(\tau) = \begin{pmatrix} 0 & 1 \\ -2q \cos 2\tau - a & 0 \end{pmatrix}. \]  

(3.19)

Following Floquet theory, we conclude that there must exist a Floquet solution to (3.16) of the form

\[ u_1(\tau) = e^{i\nu\tau} \phi(\tau), \]  

(3.20)
where $\nu = \alpha + i\beta$ is a complex number for $\alpha, \beta \in \mathbb{R}$ and $\phi$ is a $\pi$-periodic function, since this is the periodicity of $A$. Since the function $\phi$ is periodic and therefore bounded, the exponential term $e^{i\nu \tau}$ of (3.20) determines the stability of a given Floquet solution. In particular, the exact form of $\nu$, sometimes referred to as the Floquet exponent, determines whether the solution is bounded or unbounded.

We have seen that one solution to the differential equation (3.16) may be obtained via Floquet Theory. Still, we require a second solution, linearly independent from the first, to obtain the general solution\[37\]. In the following, we distinguish the three possible categories of a given Floquet solution. In each case, we determine a second, linearly independent solution. In this way we construct, case by case, the general solution, and assess its stability.

1. If $\nu$ is not real (i.e. $\beta \neq 0$), the second solution $u_2(t)$, linearly independent from $u_1(\tau)$, is found to be\[36\]

$$u_2(\tau) = u_1(-\tau) = e^{-i\nu \tau} \phi(-\tau).$$

(3.21)

Thus, the general solution to the Mathieu equation (3.16) is

$$u(\tau) = Ae^{i\nu \tau} \phi(\tau) + Be^{-i\nu \tau} \phi(-\tau),$$

(3.22)

where $A$ and $B$ are constants of integration determined by initial conditions $u(0)$ and $\dot{u}(0)$, and the phase of the applied ac voltage. Since $\beta \neq 0$, we see that as $\tau \to \infty$ one of the two terms on the right-hand side of (3.22) will go to infinity, while the other goes to zero. Hence, the general solution is unstable when $\nu$ is non-real.

2. If $\nu$ is real (i.e. $\beta = 0$), but non-integer, then $u_2(\tau) = u_1(-\tau)$ is still a second, linearly-independent solution\[36\]. However, in this case, the general solution is stable since $\beta = 0$. In the special case where $\nu$ is a rational
number, i.e. \( \nu = m_1/m_2 \) where the integer \( m_2 \) does not divide the integer \( m_1 \), the general solution is

\[
\begin{align*}
    u(\tau) &= Ae^{\frac{m_1}{m_2}\tau}\phi(\tau) + Be^{-\frac{m_1}{m_2}\tau}\phi(-\tau).
\end{align*}
\]  

(3.23)

Recalling that \( \phi \) is \( \pi \)-periodic, we see that when \( \nu \) is rational, the general solution (3.23) has period no greater than \( 2m_2\pi \).

3. If \( \nu = n \) is an integer, we have that

\[
\begin{align*}
    u_1(\tau) &= e^{in\tau}\phi(\tau) = e^{in\tau}\phi(\tau) = [\cos(n\tau) + i\sin(n\tau)]\phi(\tau). 
\end{align*}
\]  

(3.24)

Since, \( \phi \) is \( \pi \)-periodic, the Floquet solution \( u_1 \) given in [3.20] has period \( \pi \) when \( n \) is even, and period \( 2\pi \) when \( n \) is odd. Note, in either case, the solution \( u_1(-\tau) \) is not linearly independent from \( u_1(\tau) \) [36]. Thus, we cannot arrive at the general solution by simple linear superposition of \( u_1(\tau) \) and \( u_1(-\tau) \). The second, linearly independent solution must have the form

\[
\begin{align*}
    u_2(\tau) &= C\tau u_1(\tau) + f(\tau), 
\end{align*}
\]  

(3.25)

where \( C \) is a constant, and \( f \) has same period as \( u_1 \). However, \( u_2 \) is clearly unbounded as \( \tau \to \infty \), and is, thus, unstable. Therefore, for all integer values of \( \nu \), the corresponding general solutions, the so-called Mathieu functions of integral order [36], are unstable.

We note that the Floquet exponent \( \nu \) is not unique. This is so because for any integer \( k \), we may define

\[
\begin{align*}
    \mu_k &= \nu - 2k, 
\end{align*}
\]  

(3.26)

such that

\[
\begin{align*}
    \psi_k(\tau) &= e^{2ik\tau}\phi(\tau), 
\end{align*}
\]  

(3.27)
which, together with (3.20), results in

\[ u_1(\tau) = e^{i(\mu_k+2k)\tau} \phi(\tau) = e^{i\mu_k\tau} e^{2ik\tau} \phi(\tau) = e^{i\mu_k\tau} \psi_k(\tau). \quad (3.28) \]

Thus, for every integer \( k \), the complex number \( \mu_k \) is also a characteristic exponent. Still, such a shift will have no bearing on the above classification. Thus, in general, we need only consider \( \nu \) modulo 2. From such reasoning, we conclude that whenever the Floquet exponent \( \nu \) is an even integer, we may set \( \nu = 0 \). Similarly, whenever \( \nu \) is an odd integer, we may set \( \nu = 1 \). When \( \nu = 0 \), the Floquet solution is period \( \pi \). When \( \nu = 1 \), the solution is period \( 2\pi \).

In summary, we have described how each \((q,a)\) site (or, equivalently, the Mathieu equation to which it corresponds) may be classified according to the form and stability of the general solution. Furthermore, we have seen how the exponent \( \nu \) can be used to classify a \((q,a)\) site according to stability.

### 3.3 Stability Diagram

We now relate the results of Sec. 3.2 back to our Paul-trap system. We will determine the combinations of trap parameters for which stable trapping is achieved. We require both radial and axial stability. Denoting \( \rho = (x^2 + y^2)^{1/2} \) as the radial distance from the z-axis, then from (3.8) we know that the radial motion is determined by

\[ \ddot{\rho} + [a + 2q \cos(2\tau)] \rho = 0. \quad (3.29) \]

Equation (3.29) also describes the axial motion when we replace \( \rho \) with \( z \), and \( a, q \) with \(-2a, -2q\), respectively. Therefore, to proceed, we must determine which regions of parameter space yield bounded (i.e. stable) general solutions to
the Mathieu equation (3.29). In other words, we want to determine which \((q, a)\) combinations have characteristic exponent as in case 2 of Sec. 3.2.

As a first step, we consider, for fixed value of \(q\), a Floquet solution \(f_a\) to (3.29) given by

\[
f_a(\tau) = e^{i\nu_a \tau} \phi_a(\tau),
\]

where the exact form of the \(\pi\)-periodic, complex-valued function \(\phi_a\), and of the complex number \(\nu_a\), are dependent on the \(a\) parameter setting. Next, we introduce two \textit{real}-valued solutions to (3.29), namely the Mathieu cosine \(C(\tau)\) and Mathieu sine \(S(\tau)\), defined by

\[
C_a(\tau) = \frac{1}{2}[f_a(\tau) + f_a(-\tau)]
\]

\[
S_a(\tau) = \frac{1}{2i}[f_a(\tau) - f_a(-\tau)].
\]

We have shown that when \(\nu_a = n\) is an integer (i.e., case 3 of Sec 3.2) the Floquet solution \(f_a\) is either \(\pi\) or \(2\pi\) period. Thus, in such a case we may write

\[
f_a(\tau) = \sum_{k=-\infty}^{\infty} c_{2k+n} e^{i(2k+n)\tau},
\]

where \(n = 0\) if \(f_a\) is \(\pi\) periodic and \(n = 1\) if \(f_a\) is \(2\pi\) periodic. Then, plugging (3.32) into (3.31) we find \textit{periodic} Mathieu cosine and sine functions, defined by

\[
CP_a(\tau) = \frac{1}{2} \sum_{k=-\infty}^{\infty} c_{2k+n} e^{i(2k+n)\tau} + e^{-i(2k+n)\tau} = \sum_{k=-\infty}^{\infty} c_{2k+n} \cos[(2k + n)\tau] \tag{3.33}
\]

and

\[
SP_a(\tau) = \sum_{k=-\infty}^{\infty} c_{2k+n} \sin[(2k + n)\tau], \tag{3.34}
\]

respectively. For fixed value of \(q\), there is a discrete (infinite) set of \(a\)-values yielding non-trivial solution of the form \(CP\). We index these special \(a\)-values, called
characteristic values of the Mathieu cosine, as \( a = a_i(q) \), for \( i \in \{0, 1, 2, \ldots \} \). Additionally we may consider the \( a \)-values yielding non-trivial periodic Mathieu sine functions \( \mathcal{SP} \), and indexed them as \( b_i(q) \), for \( i \in \{1, 2, 3, \ldots \} \). In Fig. 3.2 we show that the set \( \{a_0, b_1, a_1, b_2, \ldots \} \) varies continuously through the \((q, a)\) parameter space, defining the so-called characteristic curves \( a_0(q), b_1(q), a_1(q), b_2(q), \ldots \) \[36\]. We note that one may obtain analytic expressions for Mathieu cosine characteristic curves by plugging \((3.33)\) into the differential equation \((3.29)\) and thus reaching recursion relations among the coefficients. Similarly, we may reach expressions for the characteristic sine curve.

As it turns out, these characteristic curves are the boundary between stable and unstable regions of the parameter space \[36\]. To see this, first note that for \((q, a)\) values sandwiched between the line \( a_n(q) \) and the line \( b_{n+1}(q) \), the corresponding Floquet solution will always satisfy \( \nu \) is non-integer, real number (i.e., case 2 in Sec. 3.2). Therefore, these regions, shaded in Fig. 3.2, yield stable solutions.
As \( q \to \infty \), the function \( a_n(q) \) and \( b_{n+1}(q) \) converge on a single value; thus the width of that stability region shrinks to zero. On the other hand, the regions marked unstable on the graph are those areas sandwiched between some \( b_n \) and \( a_n \). In these parts of parameter space, \( \nu \) is non-real (i.e., case 1 in Sec. 3.2). As \( q \to \infty \), these regions fill the space [36]. The strictly periodic solutions (i.e., case 3 in Sec. 3.2) permitted along the characteristic curves in parameter space are the transition between cases 1 and 2.

From the lines determining stability of solutions to the Mathieu equation, we can immediately determine which \((q, a)\) settings will achieve both radial and axial confinement. Radial confinement is achieved at exactly the regions already displayed in Fig. 3.2. For axial focusing we require \((-2q, -2a)\) to be in the shaded, stable regions of Fig. 3.2. This corresponds to flipping the shaded regions about the
Chapter 3. Single-Particle Paul Trap Physics

3.4 Adding Damping

So far, we considered an ideal case of single-particle dynamics in a Paul trap. However, many laboratories using Paul traps have cooling devices (see Sec. 1.1) which our theory is still lacking. Therefore, we now introduce damping into our theory.

We begin with two important examples: buffer gas and laser cooling. Buffer
gas cooling is achieved by introducing low temperature neutral particles to the trap. Through collisions, energy is transferred from the hot ions to the neutral particles. Laser cooling is achieved by immersing the ions in a laser field. The lasers are tuned to frequencies that encourage the valence electron to transition to a lower energy state. Both of these methods are extensively covered in the literature\cite{38}.

In both of these examples the damping may very well be spatially dependent. With buffer gas cooling, if the density of gas is non-uniform, then there will be more cooling in certain regions than others. With laser cooling, the situation is similar if the beam profile of the laser is not uniform throughout the trap. As a first and simplest case, we assume that the cooling is not spatially dependent however. Furthermore, we assume, as usual, that the damping is proportional to the velocity of the particle, which in the case of laser cooling, for instance, is an excellent model. This also holds for buffer-gas cooling, assuming laminar flow. With these conditions, we may write down the equation of motion for the damped ion

\[
\frac{d^2}{dt^2} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \gamma \frac{d}{dt} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + (a + 2q \cos 2\tau) \begin{bmatrix} x \\ y \\ -2z \end{bmatrix} = 0, \tag{3.35}
\]

where \(\gamma\) is the damping coefficient. We note that, if the spatial dependence of \(\gamma\) needs to be modeled, a function \(\gamma(x, y, z, \tau)\) may be introduced\cite{39}.

Adding damping warps the stable trapping zone. Analytic predictions of these effects are available in \cite{39}. As it turns out, the damping serves to compress in the stability border in \(a\) direction, and elongate it in the \(q\) direction. This can, for instance, be used to induce the paradoxical notion of cooling induced
explosions, whereby we increase the damping at a fixed \((q, a)\) until the particles are no longer trapped.
Chapter 4

Multiple-Particle Paul Trap

Physics

Once there are two or more particles in the trap, the total system is described by a phase-space vector evolving according to a non-linear differential equation due to the Coulomb interactions between particles. Floquet theory is thus no longer applicable and finding general analytic solutions becomes impossible. Chaos may emerge from the non-linear Coulomb coupling, and therefore extensive numerical investigations are in order.

This chapter is organized as follows. In Sec. 4.1 we arrive at the differential equations of motion for $n$ particles in the Paul-trap. In Sec. 4.2, we discuss the computational means by which we may accurately simulate the Paul-trap dynamics.
Chapter 4. Multiple-Particle Paul Trap Physics

4.1 Equations of Motion

We start by noting that in comparison to the single-particle case discussed in Chapter 3, where we had three coupled differential equations determining the evolution of six variables, for \( n \) particles, we now have \( 3n \) coupled differential equations that determine the evolution of \( 6n \) variables. In addition, in the multi-particle case, there is an additional term in each equation of motion, representing the Coulomb interactions. Denoting the magnitude of the distance between particles \( i \) and \( j \) as \( R_{ij} = \left[ (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \right]^{1/2} \), and choosing the appropriate length scale, we may write the Coulomb force that particle \( j \) exerts on \( i \) to be

\[
\vec{F}_{\text{coul}}^{(i,j)} = \frac{1}{R_{ij}^3} \begin{bmatrix} x_i - x_j \\ y_i - y_j \\ z_i - z_j \end{bmatrix}.
\]  

(4.1)

Using (4.1) together with the single-particle equation of motion (3.8), the equation of motion for one of the trapped particles reads

\[
\frac{d^2}{dt^2} \begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix} + \left[ a + 2q \cos(2\tau) \right] \begin{bmatrix} x_i \\ y_i \\ -2z_i \end{bmatrix} = \sum_{j \neq i} \vec{F}_{\text{coul}}^{(i,j)}.
\]  

(4.2)

Although the stable trapping zone was derived analytically for the case of a single particle (see Sec. 3.3), it is still a valid boundary as we start adding more particles. Hence, even with Coulomb repulsion, stable trapping is possible. This is so because since the repulsive Coulomb forces between particles falls off quickly according to the inverse square law [29], while the focusing force exerted on the particle by the trap increase with distance from the center of the trap. Thus, we may load as many particles as we would like into the trap.
In Sec. 3.1 we introduced the average force exerted on a particle by the trap, and arrived at an approximate equation of motion (3.14). Analogously, by replacing the trap force represented in (4.2) with this averaged force, we reach the approximation

$$\frac{d^2}{d\tau^2} \begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix} + \begin{bmatrix} \mu^2_{\rho}x \\ \mu^2_{\rho}y \\ \mu^2_zz \end{bmatrix} = \sum_{j \neq i} \vec{F}^{(i,j)}_{\text{coul}},$$

(4.3)

where

$$\mu_{\rho} = \sqrt{a + \frac{q^2}{2}}, \quad \mu_z = \sqrt{2(q^2 - a)}.$$  (4.4)

This above equation determines the macro-motion of multiple trapped particles. We will use such an approximation in Chapter 7 as a means of predicting crystalline morphologies. We shall see that crystalline states correspond to minima of the time-invariant effective potential from which (4.3) may be derived.

Finally, we note that according to (4.2), even for two particles, there are six coupled, non-linear differential equations determining the evolution of \( \vec{X} \), the twelve-dimensional phase-space vector, making fully analytical approach difficult. In fact, the Coulomb coupling represented by the right-hand side of equation (4.2) prevents us from solving these equations analytically, in contrast to the single-particle case. This non-linearity in the multiple-particle case, however, leads to the emergence of rich chaotic dynamics. In order to investigate this chaos observed in our system, then, we now devise a numerical tool in the following section.

### 4.2 Numerical Methods

Since the Paul-trap system is non-autonomous (see Sec. 2.1), the time derivative of the phase-space vector will, in general, be non-zero. In other words, the phase-
space vector $\vec{X}$ satisfies

$$\dot{\vec{X}} = \frac{d}{d\tau} \vec{X} = \vec{F}(\vec{X}, \tau),$$  \hspace{1cm} (4.5)$$

where the time-dependent function $\vec{F}(\vec{X}, \tau)$ is the means by which we may simulate our system. To this end, we must first obtain an analytic expression for the function $\vec{F}(\vec{X}, \tau)$, which we accomplish in the following. Denoting the spatial part of the phase-space vector by

$$\vec{q}(\tau) = (q_1, \ldots, q_{3n}) = (x_1, y_1, z_1, \ldots, x_n, y_n, z_n),$$  \hspace{1cm} (4.6)$$

and the velocity component by

$$\vec{p}(\tau) = (p_1, \ldots, p_{3n}) = (\dot{q}_1, \ldots, \dot{q}_{3n}) = \dot{\vec{q}}(\tau),$$  \hspace{1cm} (4.7)$$

we may write

$$\vec{X}(\tau) = (\vec{q}, \vec{p}).$$  \hspace{1cm} (4.8)$$

In this notation, we can express the time derivative of $\vec{X}$ by

$$\dot{\vec{X}}(\tau) = (\vec{p}, \dot{\vec{p}}).$$  \hspace{1cm} (4.9)$$

Rearranging equation (4.2), we may write

$$\begin{bmatrix}
\ddot{x}_i \\
\ddot{y}_i \\
\ddot{z}_i
\end{bmatrix} = \sum_{j \neq i} F^{(i,j)}_{\text{coul}} + (2q \cos 2\tau - a) \begin{bmatrix}
x_i \\
y_i \\
-2z_i
\end{bmatrix} = \begin{bmatrix}
g_{3i-2}(\vec{X}, \tau) \\
g_{3i-1}(\vec{X}, \tau) \\
g_{3i}(\vec{X}, \tau)
\end{bmatrix}. $$  \hspace{1cm} (4.10)$$

By comparing the left-most term and right-most term in (4.10), together with the equality (4.7), we obtain

$$\dot{\vec{p}} = (g_1(\vec{q}, \tau), \ldots, g_{3n}(\vec{q}, \tau)).$$  \hspace{1cm} (4.11)$$

Plugging (4.7) and (4.11) into (4.9), we arrive at the function $\vec{F}(\vec{X}, \tau)$ satisfying (4.5). We define this function in terms of $6n$ component scalar functions, i.e.,

$$\vec{F}(\vec{X}, \tau) = (f_1(\vec{X}, \tau), \ldots, f_{6n}(\vec{X}, \tau)), $$  \hspace{1cm} (4.12)$$
where
\[ f_l(\vec{X}, \tau) = p_l(\tau), \quad f_{l+3n}(\vec{X}, \tau) = g_l(\vec{X}, \tau), \quad (4.13) \]
for \( l \in \{1, \ldots, 3n\} \). Note that if we add a damping term to the equation of motion, the functional form of the scalar functions \( g_l \) in (4.10) will change correspondingly, according to
\[
\begin{bmatrix}
    g_{3i-2}(\vec{X}, \tau) \\
    g_{3i-1}(\vec{X}, \tau) \\
    g_{3i}(\vec{X}, \tau)
\end{bmatrix}
\rightarrow
\begin{bmatrix}
    g_{3i-2}(\vec{X}, \tau) - \gamma x_i \\
    g_{3i-1}(\vec{X}, \tau) - \gamma y_i \\
    g_{3i}(\vec{X}, \tau) - \gamma z_i
\end{bmatrix}.
\]
We still arrive at a vector function \( \vec{F} \) satisfying (4.5) under this transformation, and this is all we require.

Provided with an analytic expression for the time-derivative, we now Taylor expand \( \vec{X}(\tau) \) with respect to the time variable. Denoting \( h \) as an infinitesimal time scale and using (4.5) we obtain
\[
\vec{X}(h) = \vec{X}_0 + h \cdot \vec{F}(\vec{X}_0, 0) + \frac{h^2}{2} \cdot \dot{\vec{F}}(\vec{X}_0, 0) + O(h^3), \quad (4.14)
\]
where \( \vec{X}_0 \) denotes the initial conditions. Thus, in the limit of small \( h \), we can approximate
\[
\vec{X}(h) \approx \vec{X}_0 + h \cdot \vec{F}(\vec{X}_0, 0). \quad (4.15)
\]
The above equation is, in fact, a canonical approximation known as Euler’s Method\[40\]. Since this discrete mapping is linear, it will fail to display any chaotic dynamics. Still, this method is the basis of more accurate, non-linear approximating techniques. Formally, Euler’s method is defined by the transformation
\[
\begin{align*}
\vec{X}_{\nu+1} &= \vec{X}_\nu + h \cdot \vec{F}(\vec{X}_\nu, t_\nu), \\
t_{\nu+1} &= t_\nu + h,
\end{align*} \quad (4.16)
\]
where \( \vec{X}_\nu = \vec{X}(t_\nu) \) and \( \nu \) is the index of the temporal mapping iteration.
Iteratively applying the mapping \((4.16)\), we can evolve the vector \(\vec{X}\) forward in time, thus approximating the phase space trajectory determined by our initial-value problem. This approximation, of course, can only be valid for small \(h\).

Subtracting \((4.15)\) from \((4.14)\), we see that the difference between the exact solution at time \(\tau = h\) and the approximate solution is

\[
\frac{h^2}{2} \cdot \vec{F}(\vec{X}_0, 0) + \mathcal{O}(h^3).
\]

Equivalently, we see that the error from a single iteration scales (approximately) proportional to \(h^2\). To evolve the system from time \(\tau = 0\) to time \(\tau = T\) requires \(m = T/h\) iterations of the mapping and, hence, the difference between the exact result \(\vec{X}(T)\) and the approximate result \(\vec{X}_m\) scales linearly in \(h\) to lowest order.

These considerations verify the importance of finely discretizing the time in our simulations (i.e. \(h \ll 1\)). The numerical error grows with the number of iterations\(^{10}\). The step-size required for accurate results, along with number of iterations for which a simulation remains accurate, will vary from system to system. Sometimes Euler’s method performs excellently; other times it fails\(^ {10}\). We want to trust that our numerical simulations remain accurate over millions of iterations, so that we can confidently use the computed data to make theoretical predictions about Paul-trap dynamics.

We note that there are better numerical tools than Euler’s method, detailed thoroughly in the literature\(^ {10}\). Giving a detailed description of such algorithms, and proving bounds on computational error are, however, beyond the scope of this Thesis. It is sufficient to note that for our simulations, we use the fourth-order Runge-Kutta method\(^ {10}\). This mapping has been shown to be extremely accurate for a variety of initial-value problems, including our Paul-trap system.
In addition to this quantitative reassurance, we can say a few qualitative things to reassure us about our simulation: First, that our system is periodically driven should only help to make the numerical results more accurate. This is because half of the time the phase-space vector will have positive curvature, the other half negative. Correspondingly the computation will over and under estimate with equal frequency. Second, in any chaotic regime of our phase-space, we would need infinite precision in $\vec{X}_0$ to calculate the corresponding trajectory of evolution. However, infinite precision is not only unavailable computationally, but is also unfeasible empirically. In other words, errors in the numerical simulation qualitatively reflect the experimental reality.

In summary, we identified the the only two sources of error in our simulations, namely, the Runge-Kutta approximation and the lack of infinite computer precision. As discussed above, these sources of error are of little significance. In short, we account for all of the physics taking place. Thus, we expect our simulations to give us reliable data that do indeed correspond to Paul-trap dynamics. The computer performs computations equivalent to the mapping in (4.16) and reports phase-space positions as a function of time. We are free to set $(q,a)$ values, as well as the initial phase-space conditions. With the correct flow of commands, we can design and carry out entire experiments: adding particles, adiabatically switching on and off the cooling, recording positions and velocities of the particles at any time, adding noise, and more; all these tools are at our fingertips. By examining these results, we have a perfect window into the world of the trapped particles.
Chapter 5

Crystal-Free Regions in Parameter Space

Using the numerical tools developed in Chapter 4, we are now able to trap particles in our virtual Paul-trap by exploring the voltage settings such that \((q, a)\) lies in the stable trapping zone (see Sec. 3.3). The first observation is that, at some parameter settings, there exist two possible phases of trapped particles: solid and gaseous. These categories are broad, and may contain subcategories. In fact, in Chapter 7, we will see that certain \((q, a)\) sets allow for multiple, distinct solid states. Recent results from our research group indicate that there may be a third, unique phase, namely a fluid phase. For now, we simply note that, by definition, particles in any solid phase undergo periodic motion. These periodic orbits correspond to fixed points of the time-discretized mapping which propagates the system forward by a single trap cycle. In fact, we shall see that a solid state is exactly an attractor in phase space (see Sec. 2.3). On the other hand, repelling fixed points correspond to energy maxima; the particles never achieve such an
orientation. Our numerical results indicate that certain combinations of $a$ and $q$ only support the gaseous phase, and that all fixed points are unstable at such parameter settings.

This Chapter is organized as follows. In Sec. 5.1 we generalize the notion of fixed points to multiple dimensions and relate these ideas to periodic orbits in the Paul-trap. Then, in Sec. 5.2 we address stability, and introduce the Liapunov Exponents, as a means of distinguishing attractors from repellers. Finally, in Sec. 5.3, we report computational results and relate them back to ideas discussed in Sec. 5.1 and Sec. 5.2. We will show that there are certain regions within the stable trapping zone where all fixed points are unstable (i.e. repellers).

5.1 Mapping and Fixed Points

We may easily distinguish the two classes of phase space trajectories by considering snapshots taken at the frequency of the motion. For particles undergoing periodic motion, such stroboscopic observation of the the particles shows them at rest. In contrast, the gaseous phase will not be stroboscopically still, nor will it have a clear organization. In general, we mathematically distinguish these two phases as follows:

(i) If there exists time $T > 0$ satisfying $\vec{X}(0) = \vec{X}(T)$, then the particles are on a periodic trajectory. If there is no earlier time $T' < T$ also fitting this description, then the trajectory has period $T$.

(ii) If no such time $T$ exists, than the trajectory is non-periodic.

Shown in Fig. 5.1 is a Poincaré surface of $(x, y)$ space, from a five-particle system observed in our virtual lab. Every $\pi$ units of time, we plot the $(x, y)$
coordinates of the particles, each represented by a unique plot symbol. We notice that, even though we plot over many trap cycles, Fig. 5.1 shows only five distinct dots, each produced by a single symbol. Furthermore, the particles have a clear organization and axial symmetry. They form a regular pentagon in the \((x, y)\)-plane. We therefore conclude that the system shown in Fig. 5.1 is in an ordered, solid state.

We also confirm the system’s periodicity by observing the system \textit{continuously}, not just stroboscopically. Fig. 5.2 plots the \((x, y)\) coordinates of the particles over one trap cycle. The motion of each particle forms a loop, moving radially in and out. This periodic phase space orbit shows each particle undergoing tiny vibrations at the trap frequency, about a fixed center, which is the particle’s time-averaged position. It makes sense that the orbit is of period-\(\pi\) since this is the driving-period of the trap [see, for instance, (4.2)]. Thus, \(\pi\) is the expected fundamental period of particle oscillations in the solid phase. We expect all oscillations of the particles in the solid phase to have periods that are integer multiples of \(\pi\). Orbits of period \(\pi\), like the one just depicted, are called period-1 orbits. In general, orbits of period \(n\pi\) are called period-\(n\) orbits.
Having convinced ourselves that the Poincaré surfaces are indeed a good means of visualizing distinct phases in our system, we can relate these plots back to the notion of fixed points, first discussed in Chapter 2. First, we let $\mathcal{M}$ denote the mapping function that propagates the phase-space vector $\vec{X}$ forward by one trap cycle. For initial conditions $\vec{X}(0) = \vec{X}_0$,  

$$\mathcal{M}\vec{X}_0 = \vec{X}(\pi) = \vec{X}_1,$$  

(5.1)  

where the subscript $j$ of $\vec{X}_j$ denotes the time step $j$ of time-propagation $j\pi$. In this notation, we can denote multiple iterations of the mapping by  

$$\mathcal{M}^n\vec{X}_0 = \vec{X}(n\pi) = \vec{X}_n,$$  

(5.2)  

where $\mathcal{M}^n$ is $\mathcal{M}$ composed with itself $n$ times and evolves the system over $n$ trap cycles. The above Poincaré sections plot two-dimensional projections of the phase-space vector $\vec{X}_j$ [i.e. each particle’s $(x, y)$ coordinate] over many iterations of the mapping. Periodic orbits are fixed points of this mapping. Explicitly, for a positive integer $\nu$, the vector $\vec{X}_0$ is on a period-$\nu$ orbit if  

$$\vec{X}_\nu = \vec{X}(\nu\pi) = \vec{X}(0) = \vec{X}_0,$$  

(5.3)
so that the system comes back to the same state every $\nu \pi$ units of times, and $\nu$ distinct plot symbols appears on the Poincaré plot.

### 5.2 Fixed Point Stability

For a given fixed point, we would like to determine its stability, i.e., resistance to perturbation. Note that this is a different sense of stability than stable trapping. We want to distinguish if a given fixed point vector $\vec{X}_{eq}$ is repelling, neutral, or attracting, in analogy to the one-dimensional case of the logistic map (Sec. 2.3). In order to do so, we consider an initial phase-space vector $\vec{X}_0$, nearly identical to $\vec{X}_{eq}$. More precisely, we define

$$\vec{X}_0 = \vec{X}_{eq} + \vec{w}_0, \quad (5.4)$$

where $\vec{w}_0$ is some tiny displacement with magnitude $||\vec{w}_0|| = \epsilon \ll 1$. On the Poincare map Fig. 5.1, $\vec{X}_0$ corresponds to each initial dot being randomly shifted by a small amount, according to the corresponding components in $\vec{w}_0$. In the limit $\epsilon \to 0$, the displacements are indiscernible and the particles form the same pentagon as in 5.1. We can think of $\vec{X}_0$ as an approximation of our fixed point, which is the best we can ever achieve, whether in our virtual lab (due to finite numerical precision) or with a physical Paul-trap (due to defects in the electrodes or deviations from a purely sinusoidal applied voltage).

We define three classes of fixed points on the basis of stability, as follows:

(a) The fixed point is a repeller, if the particles move exponentially away from their periodic orbits. In other words, as the phase-space vector $\vec{X}$ evolves in time, the distance $|\vec{X} - \vec{X}_{eq}|$ grows, until eventually the particles have fallen off the periodic orbits and return to the gaseous phase.
(b) The fixed point is *neutral* if the phase-space vector $\vec{X}(\tau)$ stays $\epsilon$-close to $\vec{X}_{eq}$ (i.e. $|\vec{X} - \vec{X}_{eq}| = \epsilon$), but does not converge. Visually, this corresponds to quasi-periodic motion.

(c) If the particles are pulled onto the attracting fixed point, and eventually $\vec{Y}$ converges to $\vec{X}_{eq}$, then we say that the fixed point is *attractive*.

We can understand qualitatively the difference between these three cases by drawing an analogy to a particle in one-dimensional harmonic potentials, such as $V_a = -x^2, V_b = 0, V_c = x^2$, shown in Fig. 5.3. For all three potentials, the point $x_0 = 0$ is an equilibrium point. However, upon perturbation, the particle in potential $V_a, V_b$ or $V_c$ will exhibit behavior (a), (b), or (c), respectively.

Equipped with the classification scheme, we are now ready to determine the stability of a fixed point $\vec{X}_{eq}$. First, expanding the non-linear transformation $\mathcal{M}$ about the equilibrium point $\vec{X}_{eq} = 0$, we reach

$$\vec{X}_1 = \mathcal{M}\vec{X}_0 = \mathcal{M}\vec{X}_{eq} + \mathcal{J}_\mathcal{M}(\vec{X}_0 - \vec{X}_{eq}) \cdot (\vec{X}_0 - \vec{X}_{eq}) + \ldots,$$

(5.5)

where $\mathcal{J}_\mathcal{M}(\vec{X}_{eq})$ denotes the Jacobian matrix of $\mathcal{M}$ evaluated at the equilibrium point. We now assume $\vec{X}_{eq} = \vec{0}$, since this may always be achieved by the simple linear transformation $\vec{X} \mapsto \vec{X} - \vec{X}_{eq}$. In this case, the initial condition $\vec{X}_0$ is equal to the perturbation (i.e. $\vec{X}_0 = \vec{w}_0$) and in general

$$\vec{X}_n = \vec{X}_{eq} + \vec{w}_n = \vec{w}_n.$$

(5.6)
In this case, the first term of equation (5.5) is zero. Thus, dropping higher order terms in (5.5), and using (5.6), we reach the approximation
\[
\vec{w}_{n+1} \approx \mathbb{J}_M \cdot \vec{w}_n, \tag{5.7}
\]
or, equivalently,
\[
\frac{d}{dn} \vec{w}_n = (\mathbb{J}_M - 1) \vec{w}_n. \tag{5.8}
\]
The matrix \( \mathbb{J}_M \) will have complex eigenvalues \( \lambda_1, \ldots, \lambda_m \), which we order according to size of the modulus (i.e. absolute value of the complex number):
\[
||\lambda_1|| \geq ||\lambda_2|| \geq \cdots \geq ||\lambda_m||. \tag{5.9}
\]
Corresponding to these are the eigenvectors \( \vec{e}_1, \ldots, \vec{e}_m \), respectively. In other words, for all \( i \in \{1, \ldots, m\} \), we have
\[
\mathbb{J}_M \vec{e}_i = \lambda_i \vec{e}_i. \tag{5.10}
\]
We now assume that the perturbation \( \vec{w}_0 \) is along the direction of some eigenvector, i.e. \( \vec{w}_0 \in \{\vec{e}_1, \ldots, \vec{e}_m\} \). Then, using (5.7) together with (5.10) we obtain
\[
\vec{w}_n = \mathbb{J}_M^n \vec{w}_0 = \lambda^n \vec{w}_0, \tag{5.11}
\]
where \( \lambda \in \{\lambda_1, \ldots, \lambda_m\} \) is the eigenvalue corresponding to \( \vec{w}_0 \). This means that if \( ||\lambda|| < 1 \), the system is stable in the \( \vec{w}_0 \) direction; the system is drawn back onto the fixed point. On the other hand, if \( ||\lambda|| > 1 \), the system will exponentially diverge from the fixed point upon perturbation in the \( \vec{w}_0 \) direction.

In general, \( \vec{w}_0 \) will not be an eigenvector of the Jacobian, and thus we have
\[
\vec{w}_0 = c_1 \vec{e}_1 + \cdots + c_m \vec{e}_m \tag{5.12}
\]
for appropriate choice of constants \( c_1, \ldots, c_m \). Since we have ordered the eigenvectors according to the magnitude of their corresponding eigenvalues, we can see
that the first term with non-zero coefficient in (5.12) will dominate the motion in
the limit $n \to \infty$. However, for a random perturbation (or with finite-precision)
there is a zero probability that $c_1 = 0$. Therefore, we conclude that if $||\lambda_1|| < 1,
the fixed point is an attractor. On the other hand, if $||\lambda_1|| > 1$, the fixed point is
a repeller. In the special case of $||\lambda_1|| = 1$, the fixed point is neutral.

In order to quantify the stability of a given fixed point we also introduce the
Liapunov exponent $\sigma_i$, also called the rate of divergence along the $\vec{e}_i$ direction,
and defined by

\[
\sigma_i = \sigma(\vec{e}_i) = \frac{1}{\pi} \log || \lambda_i ||. \tag{5.13}
\]

Once again, we may order the exponents by size:

\[
\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m. \tag{5.14}
\]

As before we may consider only the maximal Liapunov exponent (i.e. $\sigma_1$). We
see that the fixed-point is stable if $\sigma_1 < 0$. For $\sigma_1 > 0$, we have an unstable fixed
point. The boundary $\sigma_1 = 0$ yields a neutrally stable fixed point.

In the next chapter, we report the observation, in our virtual lab, of both attractors
and repellers, even for fixed $(q,a)$. Neutral fixed points, in general, often have zero-
measure (i.e. form infinitely thin ribbons) in parameter space, and thus are not
observed. For any equilibrium point, there is inevitable numerical deviation from
the exact (irrational) values of the periodic coordinates in phase space. Such error
can be viewed as a tiny displacement $\vec{w}_0$ from equilibrium and this perturbation
can even serve to computationally probe stability. In fact, we characterize the
response of the system by considering not only $\vec{w}_0$, but also a second perturbation
$\vec{v}_0$ of the same order of magnitude. We denote $\delta Z_0 = |\vec{v}_0 - \vec{w}_0|$ as the initial
magnitude of separation between these two trajectories. Then, in general, $\delta Z_n =
|\vec{v}_n - \vec{w}_n|$ denotes the separation magnitude after $n$ trap cycles. In this notation,
the rate of divergence of these trajectories is given by

$$\sigma_0 = \lim_{n \to \infty} \lim_{\delta \to 0} \frac{1}{n\pi} \ln \frac{\delta Z_n}{\delta Z_0}$$

(5.15)

and is approximately equal to the maximal Liapunov exponent of the fixed point (this equality is exact in the limit $\vec{v}_0 \to \vec{0}$). Thus, plotting $\delta Z_n$ as a function of $n$ over many trap cycles, we can visualize clearly the difference between stable and unstable fixed points. Figure 5.4(i) shows the case of a stable fixed point, i.e. an attractor. The two initial conditions are very close to a crystalline configuration, and fall onto the periodic orbit with the help of a small damping term. On the other hand, Fig. 5.4(ii) shows a repeller. As we increment through $n$, the separation of our trajectories $\delta Z_n$ increases exponentially, until it reaches its limit, corresponding to the fact that the particles are trapped. We note that in fewer than one hundred trap cycles, the particles, initially configured near a repeller, reach a non-periodic, gaseous state.
5.3 Computational Results

Having shown that a stable fixed point of the propagation matrix corresponds to a solid phase, we now attempt to form a solid phase at a particular \((q, a)\) site in the stable trapping zone. We do this by first generating random initial conditions and then incrementing the damping term \(\gamma\) over time. Essentially, by adding damping we are taking energy out of the system and forcing it into a low-energy state. From Liouville’s Theorem\(^{29}\), we expect that as we increase damping, the phase space will shrink onto some periodic orbit. Therefore, for fixed \((q, a)\), we may (mathematically) always achieve a periodic orbit; we simply require a sufficient (sometimes unphysical) damping coefficients in our equation of motion.

In other words, while the fixed point is clearly attractive when the damping is turned on, this may very well be due to the presence of the damping itself. Thus, we must confirm if the potential minimum the system has reached, still exists in the original, undamped system. We do this by adiabatically switching off the damping. The potential well is deforming continuously as the damping coefficient slowly decreases. If, after the cooling is removed, the particles remain near a periodic orbit, and are more-or-less stroboscopically fixed, then we know that we have indeed formed a damping-free solid phase. We refer to this state as a crystal phase, since, as we shall see in Chapter 7, the structure of the resulting solid appears very orderly. The crystal is resistant to perturbation and the particles in the crystal phase, if perturbed, maintain their orderly configuration without the aid of a damping term. On the other hand, if, while removing damping, the particles are no longer found on a periodic orbit, we know that at some point as we decrease the damping, the fixed point lost stability, and the corresponding potential well disappeared, by switching curvature. Thus, by looping over many
Figure 5.5: Crystal Free Regions in Parameter Space for (a) two-particle, (b) three-particles, and (c) four-particle systems.

(q,a) sites, we may see which regions of the stable trapping zone this method successfully finds crystal states, and in which regions it fails. Figures 5.5(a)-(c) show these results for particle numbers two through four, respectively.

We note that as we increase the particle number, the gaseous, non-crystal, region starts to occupy more of the stable trapping zone. The question now is whether the gaseous region will grow in particle number so quickly that the entire parameter space would not permit a crystal phase. We can answer this question by plotting the fractions of the stability zone corresponding to the crystalline region as a function of particle number. In Fig. 5.6, we can see that as the number of particles increases, the line does not tend to zero. From this we deduce that the crystal-phase region will not shrink to zero quickly.
Figure 5.6: Crystallization Area vs. Number of Particles
Chapter 6

Analyzing Chaos

In the previous chapter, we have seen that at certain \((q,a)\) combinations, the method of laser cooling was unable to form crystals. Thus, in certain regions of parameter space it seems that all fixed points are unstable and the dynamics are chaotic no matter the initial conditions. In other words, the system seems *globally chaotic*. While we have not eliminated theoretically the possibility of stable periodic orbits at these \((q,a)\) sites, we’ve observed that the area of phase space falling onto such attractive fixed points is negligible. By considering the notion of period-doubling *bifurcations*, we offer further evidence that the region of high \(q\) where crystals fail to form is indeed a chaotic regime. To begin, in Sec. 6.1, we will introduce bifurcations as they apply to the logistic map. Then, in Sec 6.2, we will present the observation of period-doubling bifurcations in our virtual lab.
6.1 Bifurcations in the Logistic Map

Recall from Sec. 2.3 that the logistic map is defined by

$$x_{\nu+1} = f(x_{\nu}) = \lambda x_{\nu}(1 - x_{\nu}). \quad (6.1)$$

and that the only non-trivial period-1 fixed point is at $\bar{x} = 1 - 1/\lambda$. Furthermore, we have shown that $\bar{x}$ is attractive on the interval $L_0 = (\lambda_0, \lambda_1) = (1, 3)$ and repelling for $\lambda > 3$. For this mapping, there is only one parameter, namely $\lambda$. Thus, the parameter-space is just the one-dimensional $\lambda$ axis.

Now consider a new mapping function $g_1(x)$, which is $f(x)$ composed with itself once. Explicitly,

$$g_1(x) = f(f(x)) = \lambda f(x)(1 - f(x))$$

$$= \lambda \left( \lambda x(1 - x) \right) \left( 1 - \lambda x(1 - x) \right)$$

$$= \lambda^2 x(1 - x)(1 - \lambda x + \lambda x^2). \quad (6.2)$$

For a period-2 fixed point $x$ of the original function $f$, we require

$$0 = g_1(x) - x$$

$$= -\lambda^3 x \left[ x - (1 - \frac{1}{\lambda}) \right] \left[ x^2 - (1 + \frac{1}{\lambda})x + \frac{1}{\lambda} \left( 1 + \frac{1}{\lambda} \right) \right]. \quad (6.3)$$

Thus, we see that $g_1$ has four distinct equilibrium points: the trivial solution at $x = 0$, the period-1 solution at $\bar{x} = 1 - 1/\lambda$, and two new solutions, $\bar{x}_+$ and $\bar{x}_-$, which are truly period-2 under the original mapping (6.1). We may compute these new fixed points immediately from (6.3), reaching

$$\bar{x}_\pm = \frac{1}{2} \left[ (1 + \frac{1}{\lambda}) \pm \frac{1}{\lambda} \sqrt{(\lambda - 3)(\lambda + 1)} \right]. \quad (6.4)$$
Since $\bar{x}_\pm$ have period-one under the mapping $g_1$, we may test for fixed point stability as we have done previously (see Sec. 2.3). More precisely, we need only consider derivatives of the mapping function $g_1(x)$. From such analysis we will find that these period-2 fixed points are stable on the interval $\lambda \in (3, \sqrt{6})$. Notice that, increasing through $\lambda$, the period-1 equilibrium point $\bar{x}$ loses stability exactly as $\bar{x}_+$ and $\bar{x}_-$ gain stability, namely at $\lambda_1 = 3)$. Thus, defining $\lambda_2 = \sqrt{6}$, we may write that the two new equilibrium points are stable on the interval $L_1 = (\lambda_1, \lambda_2)$.

In general, we compute $g_n$ (i.e. $f$ compose with itself $n$ times) and find $\sum_{i=0}^{n} 2^i$ equilibrium points: the trivial solution, $\sum_{i=0}^{n-1} 2^i$ solutions of lower periodicity, and $2^n$ solutions that are truly period-$n$. We will find that interval of the $\lambda$-axis supporting stable, non-trivial period-$n$ fixed points, and the region supporting stable period-$(n+1)$, will be exactly adjacent. In other words, the period-$n$ fixed point will be stable on $L_n = (\lambda_n, \lambda_{n+1})$, while the period-$(n+1)$ fixed point will be stable on $L_{n+1} = (\lambda_{n+1}, \lambda_{n+2})$. The sizes of the intervals shrink fast enough (with increasing $n$) that the sequence $(\lambda_1, \lambda_2, \lambda_3, \ldots)$ converges to $\lambda^* \approx 3.56995\ldots$. Beyond $\lambda^*$, most fixed points are unstable, except on tiny $\lambda$-intervals called islands of stability.

This period-doubling leading up to a non-periodic regime is exactly the transition to chaos, and may be visualized as follows. First, we recognize that in the one-dimensional example, the system has no choice but to fall onto an attractive fixed point, if one exists. Thus, setting $\lambda < \lambda^*$, and letting the system evolve according to (6.1), we will find that the limit of $\nu \to \infty$, the system has reached a periodic orbit, known as a limit cycle. For example, if $\lambda \in L_1$ then the sequence converges to the limit cycle $(\bar{x})$ consisting of the single, period-1 fixed point $\bar{x} = 1 - 1/\lambda$. In general, if $\lambda \in L_n$, then when we feed the initial condition $x_0$ into the mapping,
we generate the sequence

\[ (x_0, x_1, x_2, \ldots) = (x_0, g_1(x_0), g_2(x_0), \ldots). \quad (6.5) \]

Initially, we will observe non-periodic, irregular fluctuations in the sequence. However, with continued iterations of \( f \), this transient motion eventually subsides, and the sequence converges to the limit cycle \((\bar{x}_1, \ldots, \bar{x}_2^n)\), consisting of \(2^n\) period-\(2^n\) fixed points of \( f \). In Fig. 6.1 we plot limit cycles as a function of \( \lambda \). This splintering, as we increase \( \lambda \), is exactly what we mean by period-doubling bifurcation. The word bifurcation comes from the Latin two-forked.

### 6.2 Period-Doubling in the Paul Trap

In our Paul-trap system, we have observed period-1 orbits corresponding to crystalline states (see Sec. 5.3). We now consider higher-order periodic motion in the trap. In other words, we consider a period-\(n\) fixed point \( \vec{X}_{eq} \) of the mapping \( \mathcal{M} \), which evolves the phase space vector forward in time by one trap cycle (see Sec. 5.1). With initial conditions, \( \vec{X}_0 = \vec{X}_{eq} \), we will (stroboscopically) observe \( n \)
distinct fixed points

\[ \bar{X}_{eq}, \mathcal{M}\bar{X}_{eq}, \ldots, \mathcal{M}^{n-1}\bar{X}_{eq} \]  \hspace{1cm} (6.6)

as we propagate forward by \( \mathcal{M} \), until the system returns to its original arrangement

\[ \mathcal{M}^n\bar{X}_{eq} = \bar{X}_{eq}. \]  \hspace{1cm} (6.7)

Thus, \( \bar{X}_{eq} \) is a period-\( n \) under the mapping \( \mathcal{M} \), and period-1 under the mapping \( \mathcal{M}^n \). So, we may test for linear stability of the period-\( n \) motion by considering the Jacobian of \( \mathcal{M}^n \) (Sec. 5.2).

If \( \bar{X}_{eq} \) is attractive, then we may consider the set \( \mathcal{B} \) of all initial conditions which are eventually pulled on the limit cycle consisting of the points in (6.6). In other words, all \( \bar{X} \) such that the sequence

\[ (\bar{X}, \mathcal{M}\bar{X}, \mathcal{M}^2\bar{X}, \ldots) \]  \hspace{1cm} (6.8)

converges to the repeating fixed points \( (\bar{X}_{eq}, \mathcal{M}\bar{X}_{eq}, \ldots, \mathcal{M}^{n-1}\bar{X}_{eq}) \). The set \( \mathcal{B} \) is the so-called basin of attraction \cite{32}. If the fixed point is a repeller, the set \( \mathcal{B} \) is empty. Non-linear systems may have multiple attractors, each with a distinct basin of attraction; they also permit initial conditions which do not fall onto any attractor as time passes. For example, in the logistic map, we have seen that for most \( \lambda > \lambda^* \), any initial condition fed into the mapping leads to chaotic motion; in other words, all basins are empty, and all fixed points are, therefore, repellers.

Thus, at such \( \lambda \) values the system is globally chaotic. Similarly, Fig. 2.5 depicts basins of attraction and chaotic regimes for the standard mapping. In each image, green represents the chaotic, irregular motion, while all other colors correspond to distinct basins of attraction.

If the crystal-free regions of parameter space are indeed areas of global chaos, we expect that leading up to the chaos boarder, the crystalline state should undergo
a period-doubling cascade. More precisely, as we increase $q$ (by increasing the amplitude of the radio-frequency drive) we expect that eventually the period-1, breathing motion is broken, and the particles, moving on some more complicated loop, come back to their original positions after two trap cycles. Incrementing $q$ adiabatically, the initially period-1 crystalline orbit should lose stability just as the period-2 orbit gains stability. More generally, the period-$n$ orbit should lose stability just as the period-$(2n)$ orbit. Then, past some critical value $q^*$, all fixed points are unstable, and the dynamics are chaotic throughout the entire phase space. Indeed, using a dragging technique\cite{3}, we may observe such bifurcations. Such a phenomenon was first predicted in 1993\cite{3}, based on numerical results for the two-particle system. We now give a description of the experiment, and present a bifurcation from our virtual lab. We also report our new result: the expected observation of unstable fixed points in the crystal-free region.

First, at fixed $a$, we may consider, as we increase $q$, the first value $q^*$ at which the cooling method described Sec. 5.2 failed to form a crystalline state. Then, the setting, $(q_0, a) = (q^* - 10^{-5}, a)$ is near (but not in) the chaotic region, and we may damp to form a period-1 crystal. As usual, in this solid state, the particles will have some (stroboscopically) fixed positions encoded in the phase-space equilibrium point $\vec{X}_{eq}^{(0)}$. Next, we increase $q$ by some small step-size $\Delta q \ll 10^{-5}$ to the new (very similar) parameter setting $q_1 = q_0 + \Delta q$. After the transient motion dies down, we will find the system at some new (strobed) position in phase-space $\vec{X}_{eq}^{(1)}$, very close to $\vec{X}_{eq}^{(0)}$, corresponding to the crystalline state at this nearly identical parameter setting. In other words, at $(q_1, a)$ the initial condition $\vec{X}_{eq}^{(0)}$ is a perturbation to the attractive fixed-point $\vec{X}_{eq}^{(1)}$, and the system is quickly sucked onto the attractor with the help of moderate damping.

However, as we continue to increase $q$, we will eventually observe that at some
$q$-value the system no longer converges to a period-1 orbit. Instead, the system is now in the basin of a period-2 attractor, and with damping, the system will be pulled onto a period-2 orbit. Thus, we observe a period-doubling bifurcation as we increment $q$. Figure 6.2 displays a three-particle system undergoing such a bifurcation, as seen in our virtual lab. At each $q_i$, after waiting for the transient motion to pass, we plot one of the particle’s (strobed) $x$-position over multiple trap cycles. Originally, at lower $q$ values, there is only a single point since the system is in a crystalline state, and the particles are stroboscopically stationary. Eventually at higher $q$, we see that the traced particle has two limiting $x$-values, corresponding to the fact that the system is now undergoing period-2 motion. Although the period doubles over such a small range of $q$, we are able to resolve the step-size $\Delta q$ small enough that we observe the second bifurcation to period-4 motion. We may visualize this period-4 motion by plotting one of the particle’s $(x, y)$ position continuously over four trap cycles. This Poincaré surface of section, shown in Fig. 6.3 presents the closed orbit, coming back to its original position after $4\pi$ units of time. More precisely, supposing we start from the tip of the W, when the $y$-value is maximal, it will take the particle time $2\pi$ to travel along the
As we further increment, we see that by $q = q^*$ the system no longer displays periodic limiting behavior. In other words, by dragging through $q$, we have melted the crystal originally formed at $(q_0, a)$, and observe a gaseous phase at parameter setting $(q^*, a)$. We may perform this same analysis at many different values of $a$, finding the value $q^*_a$ at which the periodic orbits melt into the gaseous phase. This chaos boundary, made up of the points $(q^*_a, a)$ has been computed numerically for the two-particle case[3] and confirms the boundary presented in Chapter 5, between the crystal and crystal-free regions shown in 5.5.

In our simulations, we have observed the expected unstable fixed points, which had not yet been reported. For example, at some fixed $(q, a)$ where we have formed a stable period-2 system via dragging, we may also observe unstable period-1 orbits. Similarly, in the crystal-free regions (Chapter 5), we observe unstable equilibria points of various periodicities, as expected since we expect global chaos. Computational observation of these expected energy maxima is straightforward: we need only initialize the system such that, in phase space, it is $\epsilon$-close to the
repeller. Then, we may observe the exponential rate of divergence (see Sec. 5.2). Experimental verification of these unstable equilibria is not so simple, since the repeller is not accessible from anywhere in phase space.

In summary, we conclude that the crystal-free regions of parameter space presented in Chapter 5 are globally chaotic regimes. All fixed points (of any order) are repellers, and no periodic motion is observed.
Chapter 7

Crystal Morphologies

Having offered evidence toward our explanation of the chaotic regime of parameter space, we now return to the regions where solid state configurations are observed. Up until now, we have distinguished solid states (from gaseous states) by noting that they are exactly the phase space attractors, and thus, may be represented as fixed points of the corresponding time-discretized mapping. This has been a very effective technique, but it is still limited, in the sense that the analysis is insensitive to the actual arrangement of the particles. More specifically, by merely checking for periodicity, we will not notice any symmetries (or lack of symmetries) in the solid state morphology. Thus, even once the system has fallen into some solid state, we still have some unanswered questions. For example, is there a clear spatial symmetry to the particles? To be called a *crystal* we require such organization; a crystal will have no defects and will be the lowest-energy state of the system. In general, some snapshot of a higher-energy *glass* phase will show the particles with less organization, or in some semi-ordered lattice. On the other hand, Fig. 7.1 shows a snapshot of a twenty-five particle crystal, displaying a clear
Thus, a single \((q, a)\) set may support multiple distinct solid state morphologies. Indeed, by four particles, we observe bistability for certain parameter settings. At the same time, a specific \((q, a)\) still determines the morphologies are stable. How the \((q, a)\) settings affect the structure of the Coulomb crystals at low particle numbers is the main investigation of this Chapter. In Sec. 7.1 we will, for particle numbers two through five, detail the solid state morphologies observed in our lab, and show the dependence on the \((q, a)\) setting. Then in Sec 7.2, we will derive a general analytic means by which to predict which morphology is stable for a given \((q, a)\) set. Finally, in Sec. 7.3, we apply this technique to the specific case of the three-particle system.

### 7.1 Computational Results

In all that follows, we report only period-1 fixed points. Higher order orbits have been observed, for example via the dragging method described in Sec. 6.2. Frequency-locking\(^{[41]}\) can also produce higher-order orbits. Still, the low-energy,
crystalline states are of particular interest (see Sec. 1.1) and thus, we primarily investigate such states. We analyze each particle number individually. As discussed in Sec. 4.2, these numerical results truly represent the dynamics of trapped particles. Even with finite-precision error (on the order of $\sim 10^{-15}$) the simulated dynamics of the particles near fixed points will reveal whether or not the equilibrium position is stable. In non-chaotic regions of phase-space, such slight deviations in initial conditions are irrelevant.

Since angular momentum about $z$ has been damped out, we are free to align our coordinate system relative to the morphology for all time. Furthermore, due to the trap symmetry, a morphology and its reflection across the $(x, y)$ plane will have the same stability properties. In some cases, the morphology is unchanged under such inversion. A morphology and its planar reflection are therefore represented as a single class.

**Two-Particle System**

There are three distinct morphologies observed in the two-particle system, as predicted by Blümel *et al.* in the early 1990’s. This simplest system was the motivation behind our investigation into higher-particle numbers. We note that at a given $(q, a)$ setting, only one possible morphology is observed, i.e. there are no indications of multiple potential wells. These three phases are distinguished as follows:

1. **Rod phase:** The particles are confined to the $z$-axis and have no $r$ dimensionality. The stroboscopic images at period $\pi$ show one particle with
coordinates

\[(x_1, y_1, z_1) = (0, 0, A),\]

for some non-zero \(A\) value. At this same moment, the other particle is located at

\[(x_2, y_2, z_2) = (0, 0, -A).\]

That is, the particles are vertically stacked, equidistant from the origin.

2. **Tilted phase:** The snapshots show one particle at

\[(x_1, y_1, z_1) = (A, B, C),\]

for \(A\), \(B\), and \(C\) all non-zero. Correspondingly, the other particle is found at

\[(x_1, y_1, z_1) = (-A, -B, -C).\]

The line connecting the particles is no longer parallel with the \(z\)-axis.

3. **Planar phase:** The particles are confined to the \(x-y\) plane. Now one particle is found at

\[(x_1, y_1, z_1) = (A, B, 0),\]

while the other is found at

\[(x_1, y_1, z_1) = (-A, -B, 0).\]

Notice that always \(\vec{r}_1 + \vec{r}_2 = \vec{0}\) and \(z_1 + z_2 = 0\). In other words, all of these solid state configurations have a clear symmetry, and, thus correspond to two-particle crystalline states. Figure 7.2 shows the morphologies observed at different regions of parameter space. At a particular \((q, a)\), the final morphology of the solid-state does not change when we vary initial conditions. That is, by adding damping, we always fall onto the same attractor, no matter what the initial conditions. This
indicates that there is only one stable fixed point at fixed \((q, a)\), or that the basin of attraction for this fixed point consumes most of the phase-space.

By running dragging experiments similar to those in Chapter 6, we can see the morphology of the crystal change, and thus visualize the configuration’s dependence on the parameter settings. Now, rather than adiabatically changing the \((q, a)\) setting until the crystal explodes, we adiabatically change the setting and see the morphology of the change correspondingly. As we decrease \(a\), the morphology moves from the rod phase, to the tilted phase, and finally to the planar phase. This dragging experiment confirms that there is only a single well, which visits all three morphologies by varying the parameters.

Three Particle System

For three particles we report four distinct morphologies. Still, no bistability is observed. We distinguish the phases as follows.

1. **Rod Phase**: In this phase, the particles are confined to the \(z\) axis. One
particle is found at
\[(x_1, y_1, z_1) = (0, 0, A),\]
for non-zero \(A\); a second particle at
\[(x_2, y_2, z_2) = (0, 0, -A).\]
The final particle is located at the origin.

2. **Pop-out Phase:** In this phase, the particles now have non-zero radial components. The particle at the origin pops out, but still remains in the plane. The two particles symmetrically above and below pop in the other direction to compensate. Still, the normal vector of the plane containing the three particles lies in the \((x, y)\) plane. In this sense, the configuration is not tilted; it is aligned with the \(z\)-axis. By simply realigning the \(x\)-axis, we may always express the position of one particle as
\[(x_1, x_2, x_3) = (A, 0, B)\]
while a second will have position
\[(x_4, x_5, x_6) = (A, 0, -B)\]
The final particle will be found at
\[(x_7, x_8, x_9) = (C, 0, 0).\]

3. **Tilted Phase:** Now the particle’s configuration is no longer aligned with the \(z\) axis. In other words, the normal vector of the plane containing the particles does not lie in the \((x, y)\) plane. The particle positions will be given by
\[(x_1, x_2, x_3) = (A, B, C)\]
Figure 7.3: 3-Particle Crystalline Morphology Map in Parameter Space

\[(x_4, x_5, x_6) = (A, -B, -C),\]
\[(x_7, x_8, x_9) = (D, 0, 0).\]

4. **Planar Phase:** Finally, all three particles come to lie in the \((x, y)\) plane. In other words, the normal vector of the plane containing the particles is parallel to the \(z\)-axis. The particles form an equilateral triangle in the plane. Figure 7.3 details which morphology was observed throughout parameter space. Just as for two particles, we can start in the rod configuration at high \(a\), and by dragging down through \(a\), observe the morphologies smoothly deform: popping out, tilting, and the eventually flattening into the plane.

**Four Particle System**

For the four-particle system there are seven distinct morphologies. Rather than describe the configurations in words, we simply display them graphically. Figure 7.4 indicates the seven distinct morphologies. Figure 7.5 shows which configuration was observed in what regions of stable trapping zone. The black morphology,
Figure 7.4: Observed 4-Particle Morphologies
which appears fuzzy and speckled on the map, in fact corresponds to a second, distinct potential well, from the other six morphologies. Thus, an adiabatic dragging experiment starting from one of these other six morphologies will never enter in the higher-energy well of the black configuration. The results in Fig. 7.5 show the results, not from dragging along a single well, but from simply trying to form a solid, separately at each \((q,a)\) combination. Therefore, sometimes the system enters the black state by getting trapped in the corresponding potential well during cooling. Other times, the system falls into the well corresponding to the green phase. The probability of achieving black (vs. green) by cooling is determined by the relative size of the wells’ basins of attraction (see, Sec.6.2). We note also that two of the morphologies disappear at higher \(q\) values. Thus, if did a dragging experiment at higher \(q\), starting from the rod phase, we would only observe five of the seven morphologies. Still, the geometry of the two morphologies which now abut each other in this region of \((q,a)\) space are such that the deformation under such adiabatic dragging is still smooth.
Five Particle System

In the five-particle system, there is an even large region of parameter space allowing for bistability. For now, we simply list the ten distinct observed configurations. In Chapter 8, we will discuss and depict the five-particle morphology map.

1. **Vertical Rod:** All particles lie on the $z$-axis, and thus have no $x$ or $y$ dimensionality. One particle is at the origin; two are above the origin, at $z$ coordinates $A$ and $B$; two are below at $z$ coordinates $-A$ and $-B$. Without loss of generality, $A < B$. All observed rod crystals obey the relation $2A < B$, just as for a one-dimensional harmonic oscillator potential. Below is a tabular representation of the particle coordinates.

<table>
<thead>
<tr>
<th>Particle</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>A</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>-A</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>B</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>-B</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

2. **Vertical Zigzag:**

Now, all five particles have non-trivial projection onto the $x$-$y$ plane. However, the particles all lie in a single two-dimensional plane, which is vertically aligned. In other words, $\vec{n}$, the normal vector to the plane of the particles, lies the $x$-$y$ plane. There are two pairs of particles stacked vertically on top of each other, and a fifth particle with no $z$ dimensionality. Below is a tabular representation of the particle coordinates.
3. **Tilted Zigzag:** The pairs of particles from the previous morphology are no longer stacked; the line connecting a given pair has tilted and now forms a non-trivial angle with the $z$-axis. Below is a tabular representation of the particle coordinates.

<table>
<thead>
<tr>
<th>Particle</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$A$</td>
<td>$B$</td>
<td>$C$</td>
</tr>
<tr>
<td>2</td>
<td>$A$</td>
<td>$B$</td>
<td>$-C$</td>
</tr>
<tr>
<td>3</td>
<td>$D$</td>
<td>$E$</td>
<td>$F$</td>
</tr>
<tr>
<td>4</td>
<td>$D$</td>
<td>$E$</td>
<td>$-F$</td>
</tr>
<tr>
<td>5</td>
<td>$G$</td>
<td>$H$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

4. **Regular Triangular Dipyramid:** Three particles are arranged as an equilateral triangle in the $x$-$y$ plane. The other two are stacked symmetrically above and below the origin. Below is a tabular representation of the particle coordinates. The $\hat{x}, \hat{y}$ directions are chosen to exploit the symmetry of the triangle.

<table>
<thead>
<tr>
<th>Particle</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$A + J_1 \sin \theta_1$</td>
<td>$B + J_1 \cos \theta_1$</td>
<td>$C$</td>
</tr>
<tr>
<td>2</td>
<td>$A - J_1 \sin \theta_1$</td>
<td>$B - J_1 \cos \theta_1$</td>
<td>$-C$</td>
</tr>
<tr>
<td>3</td>
<td>$D + J_2 \sin \theta_2$</td>
<td>$E + J_2 \cos \theta_2$</td>
<td>$F$</td>
</tr>
<tr>
<td>4</td>
<td>$D - J_2 \sin \theta_2$</td>
<td>$E - J_2 \cos \theta_2$</td>
<td>$-F$</td>
</tr>
<tr>
<td>5</td>
<td>$G$</td>
<td>$H$</td>
<td>$0$</td>
</tr>
</tbody>
</table>
5. **Tetrahedron Counterbalancing a Point:** Four particles, forming a tetrahedron, have negative z values. The fifth particle has zero x and y coordinate; it is located on the positive z axis. Thus, projected onto the x-y plane, the fifth particle is at the origin, while the other four form a rectangle centered at the origin. Particles on opposite sides of the rectangle’s diagonal have the same z-value, and opposite x and y values. Below is a tabular representation of the particle coordinates. The variables always satisfy the relation $2C + 2F + G = 0$, hence the name of the morphology. Note also that if this morphology is stable, then sending $z \to -z$ for all particles, produces a configuration that is also stable.

<table>
<thead>
<tr>
<th>Particle</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>B</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>-A</td>
<td>B</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>C</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>D</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>0</td>
<td>-D</td>
</tr>
</tbody>
</table>

6. **Square Counterbalancing a Point:** This morphology is very similar to the previous morphology. Now, however, the four particles all have the same z value, and thus lie in a single plane. When projected onto the x-y plane,
the rectangle from the previous morphology is now, in fact, a square. Below is a tabular representation of the particle coordinates.

<table>
<thead>
<tr>
<th>Particle</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>2</td>
<td>-A</td>
<td>-B</td>
<td>C</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>-B</td>
<td>C</td>
</tr>
<tr>
<td>4</td>
<td>-A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>0</td>
<td>D</td>
</tr>
</tbody>
</table>

7. **Regular Pop-out Pentagon:** All particles have non-zero \( z \) values. Projected onto the \( x-y \) plane, the particles form an irregular pentagon. We can number the particles, around the perimeter of the pentagon, as shown below.

With this labeling, particles one and three have the same (positive) \( z \) value; particles four and five have the same (negative) \( z \) value; particle two has the most negative \( z \) value. Below is a tabular representation of the particle coordinates, matching the labeling of the pentagon above. The \( \hat{x} \) and \( \hat{y} \) directions have been chosen for convenience. Note that \( C > 0 \) and \( F, H < 0 \) satisfy \( 2C + 2F + H = 0 \)
8. **Deformed Pop-out Pentagon:** This morphology is very similar to the previous phase, but pairs of particles are no longer at the same \( z \)-value. The line connecting, for example, particles 1 and 3, has now been rotated about the line bisecting the two particles. Thus, one particle’s \( z \)-coordinate increases, while the other particle’s decreases equally. Similarly, the pair of particles 4 and 5 also rotates, but with the angle of rotation now having the opposite sign, so that the center of mass of the system remains at the origin.

9. **Planar Regular Pentagon** All particles lie in the \( x-y \) plane, and form a regular pentagon centered at the origin.

10. **Planar Centered Square** All particles lie in the \( x-y \) plane. One particle is at the origin; the other four form a square, centered at the origin.

With these results from our simulations, we now know what physics to expect. Eventually, experimentalists may be able to confirm these predictions.

### 7.2 Deriving Pseudo-Potential Approximation

In the previous section we have observed how the morphology of the crystalline state depends on the \((q, a)\) setting. These numerical techniques are informative,
but we would like an analytic means of confirming these results. To this end, in this section, we derive a general form of the so-called pseudo-potential approximation (see Sec. 4.1) in a crystalline state.

First, we introduce the notion of the quasi-energy[35], i.e. the Hamiltonian $\mathcal{H}$ of the system evaluated at the beginning of each cycle when the ac voltage reads zero. This stroboscopically evaluated Hamiltonian is time-independent, i.e. autonomous. Without loss of generality we may always decompose $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{K} + U_{\text{eff}}, \quad (7.1)$$

where

$$\mathcal{K} = \frac{1}{2} \sum_{i=1}^{n} \dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2 \quad (7.2)$$

denotes kinetic energy of the particles and $U_{\text{eff}}(\bar{X})$ is a time-independent potential, determined by both the focusing force and the Coulombic interactions over one trap cycle. The crystalline state has a (stroboscopically) fixed energy corresponding to the minimum of the time-independent Hamiltonian. Thus, we expect the effective potential near a stable fixed point to be approximately harmonic. More precisely, expanding the $U_{\text{eff}}$ about the equilibrium point $\bar{X}_{eq}$, we reach

$$U_{\text{eff}}(\bar{X}) = U_{\text{eff}}(\bar{X}_{eq}) + \bar{\nabla}U_{\text{eff}} \cdot (\bar{X} - \bar{X}_{eq}) + \frac{1}{2} (\bar{X} - \bar{X}_{eq}) H^T (\bar{X} - \bar{X}_{eq}) + \ldots, \quad (7.3)$$

where $\bar{\nabla}U_{\text{eff}}$ and $H^T$ denote the gradient and the transpose of the Hessian matrix, respectively, both evaluated at $\bar{X}_{eq}$. Note that for a minimum, we require $\bar{\nabla}U_{\text{eff}} = 0$. Thus, dropping higher-order terms, we reach

$$U_{\text{eff}}(\bar{X}) \approx U_{\text{eff}}(\bar{X}_{eq}) + \frac{1}{2} (\bar{X} - \bar{X}_{eq}) H^T (\bar{X} - \bar{X}_{eq}). \quad (7.4)$$
From (7.4) it is clear that near a fixed point each component of $\vec{X}_0$ is experiencing a harmonic potential to lowest order.

We now approximate a single particle’s effective potential in the crystalline state by using the averaging technique first mentioned in Sec. 3.1. To begin, we rewrite the equation of motion (4.2) for one of the trapped particles as

$$\begin{bmatrix} \ddot{x}_i \\ \ddot{y}_i \\ \ddot{z}_i \end{bmatrix} = -a \begin{bmatrix} x_i \\ y_i \\ -2z_i \end{bmatrix} + \sum_{j \neq i} F_{coul}^{(i,j)} - 2q \cos 2\tau \begin{bmatrix} x_i \\ y_i \\ -2z_i \end{bmatrix}. \quad (7.5)$$

Then, denoting $\vec{q}_i = (x_i, y_i, z_i)$ as the particle’s position vector, we may define

$$\vec{F}_1(\vec{q}_i) = -2q \begin{bmatrix} x_i \\ y_i \\ -2z_i \end{bmatrix}, \quad \vec{F}_2(\vec{q}) = -a \begin{bmatrix} x_i \\ y_i \\ -2z_i \end{bmatrix} + \sum_{j \neq i} F_{coul}^{(i,j)}, \quad (7.6)$$

where $\vec{q} = (\vec{q}_1, \ldots, \vec{q}_n)$. Since $\vec{F}_2$ is only a function of the particles’ positions, it is the gradient of some scalar potential $U(\vec{q})$. In other words, $\vec{F}_2(\vec{q}) = -\nabla U(\vec{q})$.

With this notation, plugging (7.6) into (7.5), we reach

$$\ddot{\vec{q}}_i = -\nabla U(\vec{q}_i) + \cos 2\tau \vec{F}_1(\vec{q}_i). \quad (7.7)$$

Next we impose the spatial organization expected in the crystalline state. In the next section, we will use such a position ansatz to compute the potential $U$ from only the $i$th particle’s coordinates. In general, such a technique allows us to write

$$U(\vec{q}) = U(\vec{q}_i). \quad (7.8)$$

Leaving the specifics to the next section, for now we simply plug (7.8) into (7.7) and reach

$$\ddot{\vec{q}}_i = -\nabla U(\vec{q}_i) + \cos 2\tau \vec{F}_1(\vec{q}_i). \quad (7.9)$$
In reaching (7.9) we have reduced the phase-space to three dimensions. In fact (7.9) is a special case of the more general equation

\[
\begin{bmatrix}
\mu_x \ddot{X} \\
\mu_y \ddot{Y} \\
\mu_z \ddot{Z}
\end{bmatrix} = -\nabla U(X, Y, Z) + \cos(\omega t) \begin{bmatrix} k_x X \\ k_y Y \\ k_z Z \end{bmatrix},
\]

(7.10)

which we will now address instead of the specific form (7.9).

Now, we assume that the position vector in (7.10) may be separated into two components: the macro motion corresponding to a slow-varying, large-scale guiding dynamics, and the micro-motion corresponding to high-frequency, tiny vibrations from the driving term. More specifically, we write

\[
\begin{bmatrix}
X(t) \\
Y(t) \\
Z(t)
\end{bmatrix} = \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} + \cos(\omega t) \begin{bmatrix} \epsilon \\ \eta \\ \zeta \end{bmatrix},
\]

(7.11)

where \(X, Y,\) and \(Z\) denote the macro-motion and \(\epsilon, \eta\) and \(\zeta\) represent the micro-motion amplitudes. Since the micro-motion vibrations have a much higher frequency, we assume that \(x, y, z\) are constant over the time scale \(2\pi/\omega\). Furthermore, we we assume \(\epsilon \ll x, \eta \ll y,\) and \(\zeta \ll z\) corresponding to the assumption that the micro-motion amplitudes are much less than inter-particle distances. Such an approximation is only valid at low \(q\) values, when the driving force is relatively weak. As the strength of the driving force increases, the amplitudes \(\epsilon, \eta, \zeta,\) will grow correspondingly.

Expanding \(U\) around \((x, y, z)\) yields

\[
U(X, Y, Z) = U(x, y, z) + \left[U_x \epsilon + U_y \eta + U_z \zeta\right] \cos \omega t
\]

\[
+ \left[\frac{1}{2} \left(U_{xx} \epsilon^2 + U_{yy} \eta^2 + U_{zz} \zeta^2\right) + U_{xy} \epsilon \eta + U_{xz} \epsilon \zeta + U_{yz} \eta \zeta\right] \cos^2 \omega t + \mathcal{O}(\cos^3 \omega t).
\]

(7.12)
for
\[ U_i = \frac{d}{dt} U|_{x,y,z}, \quad U_{ij} = \frac{d}{dtdj} U|_{x,y,z}, \quad i, j \in \{x, y, z\}. \] (7.13)

Dropping higher order terms in (7.12) and plugging in (7.11), we may rewrite the left-hand side of (7.10) as
\[
\begin{bmatrix}
\mu \dddot{x} \\
\mu \dddot{y} \\
\mu \dddot{z}
\end{bmatrix} - \omega^2 \cos \omega t \begin{bmatrix}
\mu x \\
\mu y \\
\mu z
\end{bmatrix}. \tag{7.14}
\]

Similarly, the right-hand side may be written as
\[
\cos \omega t \begin{bmatrix}
U_{xx} \\
U_{xy} \\
U_{xz}
\end{bmatrix} + \cos^2 \omega t \begin{bmatrix}
\mu_k x \\
\mu_k y \\
\mu_k z
\end{bmatrix} - \vec{\nabla} \left\{ U(x, y, z) + \left( U_{xx} + U_{yy} + U_{zz} \right) \right\} \cos \omega t
\]
\[ + \left( \frac{1}{2} \left( U_{xx} \epsilon^2 + U_{yy} \eta^2 + U_{zz} \zeta^2 \right) + U_{xy} \epsilon \eta + U_{xz} \epsilon \zeta + U_{yz} \eta \zeta \right) \cos^2 \omega t \right\}. \tag{7.15}
\]

Now we average over a single trap cycle. Recalling that, we have assumed \( z, y \) and \( z \) are constant on such a time-scale, we reach
\[
\begin{bmatrix}
\mu \dddot{x} \\
\mu \dddot{y} \\
\mu \dddot{z}
\end{bmatrix} = -\vec{\nabla} \left\{ U(x, y, z) \right\} - \frac{1}{2} \left( U_{xx} \epsilon^2 + U_{yy} \eta^2 + U_{zz} \zeta^2 \right) + U_{xy} \epsilon \eta + U_{xz} \epsilon \zeta + U_{yz} \eta \zeta \right\}. \tag{7.16}
\]

Using the three equations represented in (7.16), we may solve for the micro-motion amplitudes \( \epsilon, \eta \) and \( \zeta \) in terms of the variables \( x, y, z \). From such a process, we reach the expression
\[
\begin{bmatrix}
\mu \dddot{x} \\
\mu \dddot{y} \\
\mu \dddot{z}
\end{bmatrix} = -\vec{\nabla} U_{eff}(x, y, z), \tag{7.17}
\]
where
\[ U_{\text{eff}} = U(x, y, z) + \frac{1}{4} k_x x \epsilon + \frac{1}{4} k_y y \eta + \frac{1}{4} z \zeta. \]  \hspace{1cm} (7.18)

Thus, we have transformed out initially time-dependent equation of motion (7.10) of the variable \(X, Y, Z\), into a time-independent equation of motion (7.17) of the variables \(x, y, z\), describing the secular dynamics of the particles. This potential \(U_{\text{eff}}\), called the pseudo potential will not be sensitive to tiny vibrations of the micro motion.

### 7.3 Applying the Pseudo Potential Approximation

In this section, we use the results of Sec. 7.2 to predict morphology dependence on parameter settings. As a first example we consider the three-particle system. As discussed in Sec. 7.1, we observe four distinct three-particle morphologies. In all of these four cases, we may choose the coordinate system as shown in Fig. 7.6.

In other words, once the position of particle \(A\) has been set, so are the positions of the particles \(B\) and \(C\). To see this, we define \(R_{AB} = [(X_A - X_B)^2 + (Y_A - Y_B)^2 + (Z_A - Z_B)^2]^{\frac{1}{2}}\) as the distance between particles \(A\) and \(B\). Then, we are free to choose units such that the Coulomb force \(\vec{F}_{\text{coul}}^{AB}\) exerted on \(A\) by \(B\) is given by

\[ F_{\text{coul}}^{(A,B)} = \frac{1}{R_{AB}^3} \begin{bmatrix} X_A - X_B \\ Y_A - Y_B \\ Z_A - Z_B \end{bmatrix}. \]  \hspace{1cm} (7.19)

According to our coordinate scheme shown in Fig. 7.6 particle \(B\) has coordinates \((X_A, -Y_A, -Z_A)\). Thus, dropping the subscript \(A\) and plugging \((X, Y, Z) =\)
Chapter 7. Crystal Morphologies

Figure 7.6: 3-Particle Crystalline Coordinate Scheme

$(X_A, Y_A, Z_A)$ into (7.19), we reach

$$F_{coul}^{(A,B)} = \frac{1}{[(X - X)^2 + (Y + Y)^2 + (Z + Z)^2]^{3/2}} \begin{bmatrix} X - X \\ Y + Y \\ Z + Z \end{bmatrix}$$

(7.20)

$$= \frac{1}{[4Y^2 + 4Z^2]^{3/2}} \begin{bmatrix} 0 \\ 2Y \\ 2Z \end{bmatrix}.$$  

Similarly, the particle C has coordinates $(-2X, 0, 0)$ and exerts force $F_{coul}^{(A,C)}$ given by

$$F_{coul}^{(A,C)} = \frac{1}{[(X + 2X)^2 + (Y)^2 + (Z)^2]^{3/2}} \begin{bmatrix} X + 2X \\ Y \\ Z \end{bmatrix}$$

(7.21)

$$= \frac{1}{[9X^2 + Y^2 + Z^2]^{3/2}} \begin{bmatrix} 3X \\ Y \\ Z \end{bmatrix}.$$  

Then, plugging (7.20) and (7.21) into the equation of motion (7.5) we reach the
three equations

\[ 6 \ddot{X} = -6X[a + 2q \cos(2\tau)] + \frac{18X}{[9X^2 + Y^2 + Z^2]^{3/2}}, \]
\[ 2 \ddot{Y} = -2Y[a + 2q \cos(2\tau)] + \frac{4Y}{[4Y^2 + 4Z^2]^{3/2}} + \frac{2Y}{[9X^2 + Y^2 + Z^2]^{3/2}}, \] (7.22)
\[ 2 \ddot{Z} = 4Z[a + 2q \cos(2\tau)] + \frac{4Z}{[4Y^2 + 4Z^2]^{3/2}} + \frac{2Z}{[9X^2 + Y^2 + Z^2]^{3/2}}. \]

Upon setting \( \mu_x = 6, \mu_y = \mu_z = 2, \omega = 2, k_x = -12q, k_y = -4q, k_z = 8q, \) and

\[ U(X, Y, Z) = \frac{2}{[9X^2 + Y^2 + Z^2]^{1/2}} + \frac{1}{2Y^2 + Z^2]^{1/2}} + a[3x^2 + Y^2 - 2Z^2], \] (7.23)

we see that (7.22) is of the general form (7.10) in Sec. 7.2, Thus, we may immediately use the results of the previous section to reach an effective potential \( U_{eff}(\vec{x}) \) where \( \vec{q}_a = (x_a, y_a, z_a) \) describes the secular motion of particle A. We note that this potential is only valid near a crystalline state fitting the description of our ansatz. However, this is exactly the regime of interest since we are attempting to computing the stability boundary between morphologies. By computing appropriate derivatives at the correct choice of \( \vec{q}_a \), we may compute the stability boundaries between morphologies, as numerically predicted in Sec. 7.2. As an example, for the rod-phase, \( \vec{q}_a = (0, 0, z_a) \), and the second partial derivative of \( U_{eff} \) with respect to \( x_a \) is

\[ \left. \frac{\partial^2 U_{eff}(x_a, y = 0, z_a)}{dx^2} \right|_{x_a=0}. \] (7.24)

As numerically observed, the particle loses stability in the \( x \) direction (transitioning to the pop-out phase). Correspondingly, when the rod configurations loses stability, the curvature of the potential along \( x \) switches sign from positive to negative. Thus, we set the second derivative in (7.24) to zero to compute the
transition. We must also consider the pop-out phase position-ansatz to arrive at a sufficient number of equations, and solve for \( a \) as a function of \( q \). Figure 7.7 shows the morphology boundaries predicted by such analytic means, overlaid on the numerical results. As shown, the results are remarkable, especially for low \( q \), where the micro-motion approximation is valid. We can repeat the above procedure for other particle numbers using the general form (7.10) as a starting point. Figure 7.8 show the predictions for two-particle system. For the four-particle system, we observed similarly effective results when computing boundaries between morphologies in a given well.
Figure 7.8: Pseudo-Potential Prediction of Morphology Boundaries in 2-Particle System
Chapter 8

Discussion

In the previous Chapters we have investigated the dynamics of an isolated species of trapped particles, modeled classically. Numerical methods lead us to observe two broad phases of particles (solid and gas) defined stroboscopically. We recognized that the solid states correspond to attractive fixed points of the non-linear time-propagation mapping, which is fully specified by the parameters $q$ and $a$. Furthermore, we saw that for each particle number, only a limited percentage of the stable trapping zone allows for the formation of ordered solids (crystals) via cooling. Period-doubling leading up to the crystal-free regions of parameter space indicates that dynamics in the crystal-free regions are globally chaotic. This conclusion is reinforced by our report of repulsive fixed points in the crystal-free regions. Since bifurcation theory displays universality, we may even try to observe some two-dimensional Feigenbaum constants. More precisely, letting $Q_n$ denote the length of the $q$ interval leading to period-$n$ motion in a dragging experiment, then we must compute the ratio $Q_n/Q_{2n}$ in the limit of $n \to \infty$, and similarly for $a.$
Since the system is periodically driven, we were able to use the technique of time-averaging to arrive at a pseudo-potential which approximates the secular dynamics of trapped particles. We were even able to predict morphology boundaries by invoking the organization of the fixed, time-averaged particle positions. We report the emergence of *bistability* by four particles. In other words, for fixed \((q, a)\), multiple four-particle solid states exist, corresponding distinct minima of the pseudo-potential. Figure 8.1 shows that the five-particle pseudo-potential has two wells through much of the parameter space. To see this, we first note that this figure is generated by, independently at each \((q, a)\), starting from random initial conditions, and damping the system to form a crystal. The disjoint flecks depicted in the graph are expected whenever the system may settle into one of several possible wells.

To instead trace (for a specific well) the morphology dependence on parameter setting, we turn again to dragging experiments. For example, we can start in the planar pentagon phase (dark blue), adiabatically increase \(a\) until the system reaches the rod configuration (orange), and then decrease again to the original parameter setting. Slowly stepping through parameter space, the morphology moves smoothly from one color to a next; there is hoping back and forth between colors as we drag, since the system cannot not hop from one well to the other. Thus, the fuzziness of 8.1 is avoided. Eventually, the wells merge when the \(a\) value is high enough. Via techniques similar to those used in Sec.7.3 to compute morphology boundaries, we may even predict the line \(L_s\) marking the boundary between single and double-well potential. When \(a\) is then decreased, and crosses \(L_s\) a second time, and the wells again separate. However, we observe that the system has switched wells. Correspondingly, the morphology when we return to the initial parameter setting is no longer a planar pentagon; instead, the particles
form a centered planar square, i.e. four particles form a planar square, and the fifth is at the origin.

Furthermore, in the five-particle system, there are two different globally chaotic regimes (red), one for each well. Again, we may confirm these results by dragging simulations. For example, if we start in the black state and slowly increase $q$ towards the chaotic regime, the crystal survives through first red buffer that curls out, but shatters at the second, entirely filled red region. On the other hand, if instead we initialize the system in the lavender or white morphology (corresponding to the second well) and again adiabatically increase $q$, then the crystal shatters when $q$ reaches the first bits of red.

From these considerations, we conclude that for the five-particle system, there are two distinct morphology maps, one for each well. These two sheets are glued together to the left side of the line $L_s$. As we continue to increase in particle number (as we must for many practical implementations of these Coulomb crystals), the number of solid states and the number of potential wells only increases. It quickly becomes unmanageable to map all the branching sheets in parameter space, not to mention the distinct morphologies on each branch. Thus, to continue classifying different solid-state configurations, we must develop new techniques (inspired, for example, by statistical averaging, time-averaged energy, normal modes, or a generalized structure factor).

Although we formalized our understanding of the bifurcations using the notions of fixed points and linearized stability, we still were unable to make any analytic prediction of chaos. Therefore, we still have not eliminated (theoretically) the possibility that crystals exists at $(q,a)$ settings where we failed to form crystals via cooling; we have only shown these crystals are very difficult to access via simply cooling. In other words, we have only shown that the basin of attraction
for such a fixed point is very small, not that it is empty. To prove the all basins are empty in the (red) chaotic zones would involve, for example, showing analytically that a solid state corresponds to a fixed point of the propagation matrix, and that all fixed points in the red region are unstable. Hence, to proceed, we would need an analytic expression for the propagation matrix. For the specific case of a single particle with a square-pulse drive, this transformation matrix may be computed exactly. To start, following [35], we change the driving term in the equation of motion (4.2) from \( \cos(2t) \) to \( \theta(2t) \) defined by

\[
\theta(2t) = \begin{cases} 
1 & 0 \leq y < \frac{\pi}{4} \\
-1 & \frac{\pi}{4} \leq y < \frac{3\pi}{4} \\
1 & \frac{3\pi}{4} \leq y < \pi
\end{cases}
\]  

(8.1)

where \( y = \text{mod} \ (2t, \pi) \). Since there is only one particle in the trap, each equation of motion is uncoupled and thus, for example, the future \( x \)-position and momentum depend only on the \( x \)-dimension’s initial conditions. Furthermore, since the three changes in the potential happen instantaneously, we can directly integrate the system forward in time. More precisely, on each sub-interval in (8.1) the potential is constant, and the equation of motion yields simple harmonic or expo-
ential motion. Hence, the system is piece-wise autonomous, allowing us to solve for the propagation similarly to the case of the kicked rotor (Sec. 2.2). Explicitly, given initial $x$-position and momentum $x_0$ and $p_0$, we may calculate the position and momentum $x_1$ and $p_1$ at time $\pi$ according to

$$
\begin{pmatrix}
  x_1 \\
  p_1
\end{pmatrix} =
\begin{pmatrix}
  \frac{1}{m\omega_0}(\gamma s + \sigma) & \gamma c \\
  -m\omega_0(\gamma s - \sigma) & \gamma c
\end{pmatrix}
\begin{pmatrix}
  x_0 \\
  p_0
\end{pmatrix},
$$

(8.2)

where, defining $\nu = \pi\sqrt{q/2}$, we may express the constants in (8.2) as $\gamma = \cosh(\nu)$, $\sigma = \sinh(\nu)$, $c = \cos(\nu)$, $s = \sin(\nu)$, and $\omega_0 = \Omega(q/2)^{1/2}$.

Still, this is a one-particle system, and no chaos will be exhibited in the dynamics. If we may arrive at a similar matrix which propagates, for example, the two-particle system forwards, then we may analyze the eigenvalues and test for stability near a fixed point. For example, at certain fixed $a$ values, we expect to see a transition to instability as we increase $q$. To make the mathematics more manageable, we may want to start by considering a delta-function radio-frequency drive. Just as with the kicked rotor, this discontinuous driving makes integration easier for the two-particle Paul-trap system. We expect that (at certain $a$ settings) as we increase $q$, the period-one fixed point should lose stability just as the period-two fixed point becomes stable. One possible means of arriving at such a time-independent mapping is by invoking the pseudo-potential approximation, and the corresponding approximate equation of motion given in (4.3). We may even attempt to improve this potential approximation by considering higher-order harmonics in the micro-motion ansatz (7.11).

While there are many remaining questions, the results presented are very informative. For example, our results reported on low particle numbers are relevant to quantum cryptography, which only requires a few qubits. As we have stated, application of the Paul-trap as quantum computing hardware requires more than
Chapter 8. Discussion

just a handful of trapped ions (at least a few thousand) laser cooled to their quantum ground state. Still, by simulating higher numbers of particles, we may extend the results presented in Fig. 5.6. Thus, we have a means of predicting, as we add more particles, how the area of parameter space with easily accessible crystals changes and shrinks. In this sense our presented results are foundational, and exemplify general methodologies which may be used to investigate particle-numbers we have not yet considered. Similarly, throughout this Thesis, we draw connections between our system and other physical systems. For example, we have frequently made reference to periodically-driven and chaotic systems throughout. We note that our Paul trap system also has many of the features of a colloidal system. Conventionally, in chemistry, a colloid is achieved by suspending one, dispersed (i.e. low density), insoluble substance throughout another, continuous (i.e. high density) substance. The main distinction between the Paul trap system and a typical colloid, is that we must observe trapped particles scroboscopically in order to clearly distinguish phases. In conclusion, the Paul trap is a fascinating system with much to be discovered. Studying the system is informative to other specialized fields (through applications as an experimental tool) and to general theories (such as the theory of periodically driven systems or the theory of colloids). Thus, Paul trap research will continue simultaneously to inform and be informed by other areas of physics.
Bibliography


