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An Investigation of Traveling-Wave Electrophoresis using a Trigonometric Potential

James Vopal
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An Investigation of Traveling-Wave Electrophoresis using a Trigonometric Potential

James Vopal

Dissertation submitted to the
College of Arts and Sciences
at West Virginia University
in partial fulfilment of the requirements
for the degree of

Doctor of Philosophy
in
Physics

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Morgantown, West Virginia
2013

Keywords: Electrophoresis, Trigonometric Potential, Chaos, Devil's Staircase
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Abstract

An Investigation of Traveling-Wave Electrophoresis using a Trigonometric Potential

by

James Vopal

Traveling-wave electrophoresis, a technique for microfluidic separations in lab-on-a-chip devices, is investigated using a trigonometric model that naturally incorporates the spatial periodicity of the device. Traveling-wave electrophoresis can be used to separate high-mobility ions from low-mobility ions in forensic and medical applications, with a separation threshold that can be tuned for specific applications by simply choosing the traveling wave frequency. Our simulations predict plateaus in the average ion velocity verses the mobility, plateaus that correspond to Farey fractions and yield Devil's staircases for non-zero discreteness values. The plateaus indicate that ions with different mobilities can travel with the same average velocity. To determine the conditions for chaos, Lyapunov exponents and contact maps are employed. Through the use of contact maps, the chaotic trajectories are determined to be either narrowband or broadband. Narrowband chaotic trajectories are exhibited in the plateaus of the average velocity, while broadband chaotic trajectories are exhibited where the average velocity varies nonmonotonically with the mobility. Narrowband chaos will be investigated in future work incorporating the role of diffusion. The results of this and future work can be used to develop new tools for electrophoretic separation.

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Chapter 1

Introduction

1.1 Electrophoresis

Electrophoresis is the movement of ions in a stationary fluid by an external electric potential. The external electric potential traditionally has a constant gradient in one direction, and zero gradients in all other directions, resulting in a constant electric field with one directional component according to $\mathbf{E} = -\nabla\phi$. The constant velocity of the ions, when the short transients are ignored for the static electric field, is proportional to the electric field. This can be seen by analysing the forces on the ions, $\mathbf{F} = m\mathbf{a} = 0 = \mathbf{F}_E + \mathbf{F}_D$, where $\mathbf{F}_E$ is the force on the ion due to the electric field and $\mathbf{F}_D$ is the resistive force due to drag. The force due to the electric field is $\mathbf{F}_E = q\mathbf{E}$ where q is the charge of an ion. The force due to drag $\mathbf{F}_D$ is proportional to the velocity of the ion and is given by $\mathbf{F}_D = -6\pi\eta r\mathbf{v}$, where η is the fluid viscosity and r is the Stokes radius. This assumes that the Reynolds number is much less than one so that Stokes drag is applicable. Since $\mathbf{F}_E = -\mathbf{F}_D$, this results in $\mathbf{v} = \mu\mathbf{E}$ where $\mu = q/6\pi\eta r$. This proportionality constant μ is known as the electrophoretic mobility of the ion and is based upon its charge to size ratio.

One application of electrophoresis is capillary electrophoresis. This is where the ends of a capillary are held at different potentials resulting in a uniform electric field aligned with the axis of the capillary. Historically, capillary electrophoresis has been the standard for high-resolution separation of charged particles in solution.[10] Another application of electrophoresis is gel electrophoresis. This is essentially the same as capillary electrophoresis except the capillary is replaced with a channel of gel. Gel electrophoresis is historically used for the separation of DNA, RNA, or proteins.[9]

1.2 Previous Model

A simplified model of a spatio-temporal potential is developed for a repeating pattern of four interdigitated electrode arrays along the length of a microchannel.[6, 5] These electrodes are held at time-dependent sinusoidal potentials $\phi_1(t)$, $\phi_2(t)$, $\phi_3(t)$, and $\phi_4(t)$ that are phase shifted by a quarter period from one to the next as we move along the microchannel. The four-electrode pattern has two electrode arrays on the top of the channel and two on the bottom, with adjacent electrodes separated by a quarter wavelength along the length of the channel as seen in Fig. 1.1. Here, the wavelength is the distance in the x direction between electrodes of the same potential; therefore, this is the wavelength of the resulting electric potential wave. The wavelength of the electrode pattern is $80\mu\text{m}$. The electrode potential are driven at a frequency of $1 - 32\text{Hz}$. This results in a maximum possible velocity for an ion of $80 - 2560\mu\text{m/s}$. The four electrodes per wavelength meets the Nyquist-Shannon requirement of more than two electrodes per wavelength needed to represent a wave.[23, 25]

This pattern was designed for microfluidic separation of charged particles by traveling-wave electrophoresis (TWE). The traveling wave traps high-mobility ions

Figure 1.1: The four-node pattern that is repeated along the axis of the microchannel. The nodes alternate from top to bottom and are separated by a quarter wavelength in the x direction. The ratio of the electrode pattern wavelength λ to the microchannel height h gives the aspect ratio Γ .

and leaves lower mobility ions behind. The separation of charged substances is important in the fields of proteomics, molecular biology, cell biology, genetics, and bioengineering. Microfluidic lab-on-a-chip devices are being developed for rapid clinical and forensic analysis.[28] This technique uses a static, uniform electric field for ion separation. Both TWE and capillary electrophoresis separate ions depending upon their electrophoretic mobility, but TWE has the potential advantage of tunability, the ability to use the frequency of the wave to tune the separation threshold. Others have used interdigitated electrodes for charge transport by electrophoresis.[21, 22, 11, 12, 16, 15] In these cases, the electrode array was applied to a single surface and a static electric or gravitational field was used to move the ions to this surface. Single surface designs have also been developed to move charged particles via AC electroosmotic pumping [24, 8] and neutral bioparticles via dielectrophoresis.[4, 18]

The electric potential due to two of the electrodes of radius a along the upper wall

of the microchannel is given by

$$\phi = \Phi_0 \frac{\ln(r_3/r_1)}{\ln(\lambda/2a)}. \quad (1.2.1)$$

The values r_1 and r_3 are the distances to the electrodes with potentials ϕ_1 and ϕ_3 respectively. Similarly, the electric potential due to two of the long electrodes of the same radius along the lower wall of the channel is given by

$$\phi = \Phi_1 \frac{\ln(r_4/r_2)}{\ln(\lambda/2a)}, \quad (1.2.2)$$

where r_2 and r_4 are the distances to the electrodes with potentials ϕ_2 and ϕ_4 respectively. The walls of the channel are insulated requiring the use of image charges so that the gradient of the potential is zero in the z direction. The superposition of the potentials due to the electrodes along the microchannel and the required image charges result in

$$\phi(\mathbf{r}, t) = \frac{\Phi_0(t)}{\ln(\lambda/2a)} \sum_{l,m=-\infty}^{\infty} \ln \frac{|\mathbf{r} - \mathbf{r}_3^{(l,m)}|}{|\mathbf{r} - \mathbf{r}_1^{(l,m)}|} + \frac{\Phi_1(t)}{\ln(\lambda/2a)} \sum_{l,m=-\infty}^{\infty} \ln \frac{|\mathbf{r} - \mathbf{r}_4^{(l,m)}|}{|\mathbf{r} - \mathbf{r}_2^{(l,m)}|} \quad (1.2.3)$$

where $\mathbf{r}_i^{(l,m)}$ for $i = 1, 2, 3, 4$ are the positions of the electrodes and image charges associated with the potentials ϕ_i .

The need for a simplified model stems from the fact that the potential produced by this four-electrode pattern is described by equations requiring infinite sums and natural logarithms, which require long computing time for simulations.[6, 5] The simplified model is constructed from trigonometric functions with no infinite sums. The objective of this work is to study the nonlinear dynamics of the trigonometric model in order to understand how changes in the electrode spacing might affect performance, and to explore a wide range of conditions including a continuum of conditions ranging from discrete electrodes to a continuous 1-D potential.

The model predicts mode locking, otherwise known as phase locking or frequency locking. Mode locking occurs when the system behavior does not change as some external driving amplitude is varied. This has been seen in semiconductor lasers, [2] Van der Pol circuits, [13] the angular velocity of a ferrofluid droplet in a rotating elliptically polarized magnetic field, [14] and the Belousov-Zhabotinsky reaction. [19, 20] Our model equations involve two first-order equations governing the velocities in two spatial dimensions. The dimensionality of the phase space of the system allows for different possibly types of trajectories. The phase space of the system is a space that can be used to plot all the primary variables in the governing differential equations. This space may be different from the physical space involved in the system. Since these velocities depend explicitly on the time, the system is nonautonomous and can be described using a three-dimensional phase space (x, z, t) , the minimum dimensionality required for chaos. As will be seen, the model predicts chaos in certain regimes.

The trajectory and average velocity of an ion as a function of its electrophoretic mobility is investigated. This is done to determine under what criteria the ion will experience a chaotic trajectory. Criteria will also be varied to determined when ions with differing electrophoretic mobility experience the same average velocity.

1.3 Nonlinear Dynamics and Chaos

Chaos is defined as aperiodic long-term behaviour in a deterministic system that exhibits sensitive dependence on initial conditions.[27] Aperiodic long-term behaviour is indicative of a system that does not settle down onto a fixed point or a periodic trajectory as $t \rightarrow \infty$. To analyse the aperiodic long-term behaviour in the system,

contact maps will be employed. A contact map is a combination of the concepts behind a Poincaré map and an orbit diagram. A Poincaré map is a mapping of a trajectory through a surface of section from one intersection of the trajectory with the surface of section to the next. In this case a surface of section is a surface that has dimensionality one less than the space containing the trajectory. Since our trajectory is confined to two dimensions, the surface of section will be one dimensional. In the system that is being investigated, the surface of section may be the axis of the microchannel, the surface of an electrode,[6] or the wall of the microchannel. The intersections of the trajectory with the surface of section are then plotted with respect to a parameter in the system to create an orbit map. Traditionally, an orbit map is a map of all the relative extrema in one dimension of the phase space for a trajectory with respect to a parameter in the governing differential equations. The orbit map is then used to determine the periodicity (or aperiodicity) of a trajectory.

The second aspect of chaotic behaviour is that the system must be deterministic. A system is deterministic if there are no random inputs or parameters. Any irregular behaviour is the result of the nonlinearity of the system itself.

To determine the sensitivity to initial conditions the separation $\varepsilon(t)$ between two trajectories is tracked when they are started very close ε_0 to each other. It is said that there is extreme sensitivity to the initial conditions when the separation increases exponentially. If the separation increases exponentially then $|\varepsilon(t)| \propto |\varepsilon_0|e^{\Lambda t}$, where $\Lambda > 0$. In the cases where $\Lambda \leq 0$ then there is no sensitivity to initial conditions. When $\Lambda = 0$, the initial separation is maintained and when $\Lambda < 0$, the separation is decreasing indicating that the two trajectories are settling onto the same path. If $|\varepsilon(t)| \propto |\varepsilon_0|e^{\Lambda t}$, then Λ is average initial slope of the graph of $\ln |\varepsilon|$ with respect to

time t as seen in Fig. 1.2. The value Λ is known as the largest Lyapunov exponent.

Figure 1.2: An example of a plot of the natural logarithm of the separation of trajectories ε with respect to time. This plot is used to estimate the largest Lyapunov exponent Λ for a non-linear system. The blue line is the best linear fit to the initial portion of the plot and has a slope of Λ . Since $\Lambda > 0$, this indicates the system exhibits chaotic trajectories.

Chapter 2

Model for Traveling-Wave Electrophoresis

2.1 Chapter Introduction

The potential used in the previous model given in Eq. 1.2.3 requires infinite sums of natural logarithms. In order to avoid the infinite sums and natural logarithms, a model has been developed that has the qualitative characteristics. The infinite sums and natural logarithms that appear in the previous model require long computing time. In developing a new model, it has been decided to use trigonometric functions since their inherent periodic nature matches up well with the periodic nature of the electrode array. The insulated boundaries that lead to the infinite sums in the previous model can also be dealt with using trigonometric functions. In order to deal with the insulated boundaries, the squares of the sine and cosine functions are used since their derivatives are zero at the same respective values. These functions are adjusted so that the zero derivatives occur at the walls of the microchannel. The potentials of the electrodes are also varied sinusoidally with a phase shift of a quarter period from one electrode to the next. This leads to the use of the sine and cosine functions when it

comes to the time component of the new model. The result is a model where the three primary variables in the potential x , z , and t are incorporated using trigonometric functions.

2.2 Trigonometric Model

The dimensionless trigonometric potential is

$$\begin{aligned} \phi(x, z, t) = & \hspace{15em} (2.2.1) \\ & \cos(2\pi t) \cos(2\pi x) \left[\delta \sin^2 \frac{\pi \Gamma z}{2} + (1 - \delta) \cos^2(2\pi t) \right] + \\ & \sin(2\pi t) \sin(2\pi x) \left[\delta \cos^2 \frac{\pi \Gamma z}{2} + (1 - \delta) \sin^2(2\pi t) \right]. \end{aligned}$$

The two spatial coordinates are the position x along the axis of the channel and the position z measured transverse to this axis, both scaled by the electrode wavelength λ . The time is scaled by the period T of the potential, and the potential is scaled by its amplitude. The aspect ratio $\Gamma = \lambda/h$ is the nodal wavelength divided by the height of the channel, with the channel walls located at $z = 0$ and $z = h/\lambda = 1/\Gamma$. For our simulations, we use an aspect ratio of $\Gamma = 4$. A discreteness parameter $0 \leq \delta \leq 1$ is included to allow us to explore a range of behaviors. For $\delta = 0$, the potential is uniform in the z direction at all times; the model is spatially one-dimensional. Because of this, the phase space is two-dimensional in (x, t) and chaos is impossible. The $\delta = 0$ limit gives $\phi(x, t) = \cos^3(2\pi t) \cos(2\pi x) + \sin^3(2\pi t) \sin(2\pi x)$. For $\delta > 0$, we see variation in the z direction. At $t = 0$, the potential goes from a magnitude of 1 at the nodes along the upper wall to a smaller magnitude along the lower wall for equal x values. This smaller magnitude is still greater than zero. For $\delta = 1$, the potential goes to zero at the walls at times $t = nT/4$ where $n = 0, 1, 2, \dots$. For $\delta = 1$,

we reach the limiting case where, at $t = 0$, the potential goes from a magnitude of 1 at the nodes along the upper wall to zero along the lower wall. Figures 2.1-2.3 show the potential for $\delta = 0$, $\delta = 0.5$, and $\delta = 1$ at times $t = 0, 1/16, 1/8$, and $3/16$. Here we see not only how δ influences the potential at $t = 0$, but also how δ affects the potential when t is not an integer value. The $\delta = 1$ limit gives the four-electrode pattern and replicates the electrode potentials that we studied previously [6, 5]

$$\phi_i = \phi(\mathbf{r}_i^l, t) = \sin(i\pi/2 - 2\pi t), \quad i = 1, 2, 3, 4 \quad (2.2.2)$$

with electrode positions given by

$$\mathbf{r}_1^l = (l, 1/\Gamma) \quad (2.2.3a)$$

$$\mathbf{r}_2^l = (l + 1/4, 0) \quad (2.2.3b)$$

$$\mathbf{r}_3^l = (l + 1/2, 1/\Gamma) \quad (2.2.3c)$$

$$\mathbf{r}_4^l = (l + 3/4, 0), \quad (2.2.3d)$$

where $l = 0, \pm 1, \pm 2, \dots$ specifies the wavelength of the electrode pattern along the (infinite) channel. The motion of the ion is determined by the dimensionless electric field associated with the potential, $\mathbf{E} = -\nabla\phi$. The components of the electric field are

$$E_x(x, z, t) = \quad (2.2.4)$$

$$2\pi \cos(2\pi t) \sin(2\pi x) \left[\delta \sin^2 \frac{\pi\Gamma z}{2} + (1 - \delta) \cos^2(2\pi t) \right] -$$

$$2\pi \sin(2\pi t) \cos(2\pi x) \left[\delta \cos^2 \frac{\pi\Gamma z}{2} + (1 - \delta) \sin^2(2\pi t) \right]$$

$$E_z(x, z, t) = -(\delta\pi\Gamma/2) \sin(\pi\Gamma z) \cos[2\pi(x + t)]. \quad (2.2.5)$$

The current generated by the motion of the ions is on the order of $10\mu\text{A}$. This allows for an estimate of the strength of the magnetic field $B = \mu_0 I / 2\pi r$, where r

is taken to be the dimensional width of the microchannel of $20\mu\text{m}$. The result is a magnetic field strength of $B \approx 10^{-7}\text{T}$. The force on a moving particle due to a magnetic field is given by $\mathbf{F}_B = q\tilde{\mathbf{v}} \times \mathbf{B}$, where $\tilde{\mathbf{v}}$ is the dimensional velocity. If we assume the directions $\tilde{\mathbf{v}}$ and $\mathbf{B}$ are perpendicular, then $F_B = q\tilde{v}B$. Using the $q = -3.2 \times 10^{-19}\text{C}$ for flourescein used in experiments [6] and $\tilde{v} \approx 1\text{mm/s}$ results in $F_B \approx 10^{-29}\text{N}$. The magnetic force will cause a curvature in the path of the ion subject to $F_B = m\tilde{v}^2/r_C$, where r_C is the radius of curvature. Still working with a flourescein ion, we have $m = 5.5 \times 10^{-25}\text{kg}$. The resulting radius of curvature is approximately $1.7 \times 10^{-2}\text{m}$. Since $r_C \gg 80\mu\text{m}$, where $80\mu\text{m}$ is the dimensional wavelength of the microchannel, the affects of the magnetic field can be neglected.

In this model, we consider two forces exerted on the ion, an electric force $\mathbf{F}_E = q\phi_0/\lambda\mathbf{E}$ and a Stokes drag force $\mathbf{F}_D = -6\pi\eta r\lambda/T\mathbf{v}$, where q is the charge of the ion, ϕ_0 is the amplitude of the potential, λ is the nodal wavelength, η is the bulk viscosity, r is the hydrodynamic radius, and T is the period of the potential. The Reynolds number, $Re = L\tilde{v}/\nu \ll 1$ where L is a characteristic length, $\tilde{v}$ is the average velocity, and ν is the kinematic viscosity, is used to determine if Stokes drag force is applicable. For typical TWE, $L \approx 10\mu\text{m}$ and $\nu = 10^{-6}\text{m}^2/\text{s}$ for water. Since $Re \approx 10^{-2} \ll 1$, we see that Stokes drag force is indeed applicable here.

The ion is assumed to be spherical since a cloud of oppositely charged particle surround the ion. If the ion has a shape that cannot be considered spherical due to the affect of the cloud of oppositely charged particles, a correction factor can be introduced into the Stokes drag force $\mathbf{F}_D = -6\pi\eta r_V\lambda K/T\mathbf{v}$, where r_V is the radius of a sphere with the same volume as the ion and K is the correction factor for the shape of the ion. [17]. Since $1 < K \ll 10$ for ellipsoids, cylinders and other common

shapes the qualitative aspects of the analysis will not be affected.

Inserting the electric force and Stokes drag force into Newton's second law gives

$$\mathbf{F}_E + \mathbf{F}_D = \frac{m\lambda}{T^2} \dot{\mathbf{v}}. \quad (2.2.6)$$

For a constant applied electric field $\mathbf{E}$, this equation immediately yields

$$\mathbf{v} = R\mathbf{E}(1 - e^{-t/\tau}), \quad (2.2.7)$$

where $R = q\phi_o T / 6\pi\eta r \lambda^2$ is the dimensionless electrophoretic mobility of the ion and $\tau = mR\lambda^2 / q\phi_o T^2$ is the dimensionless time required for the ion to achieve its terminal velocity $\mathbf{v} = R\mathbf{E}$. Using values from experiments carried out previously [6] and R to the dimensional electrophoretic mobility $\mu = \lambda^2 R / \phi_o T$ results in $\tau = m\mu / qT$. From the previous experiments, $\mu \approx 10^{-4} \text{cm}^2 / \text{V} \cdot \text{s}$ resulting in $\tau \approx 10^{-12}$. Since τ is small compared with the dimensionless time scales for changes in the electric field (of order 1), it is assumed that ions respond instantaneously to changes in the electric field. This allows for the inertial effects to be ignored, and therefore resulting in $\mathbf{F}_E + \mathbf{F}_D = 0$ and $\mathbf{v} = R\mathbf{E}$. Thus our two first order equations are

$$\dot{x}(x, z, t) = \quad (2.2.8)$$

$$2R\pi \cos(2\pi t) \sin(2\pi x) \left[\delta \sin^2 \frac{\pi\Gamma z}{2} + (1 - \delta) \cos^2(2\pi t) \right] -$$

$$2R\pi \sin(2\pi t) \cos(2\pi x) \left[\delta \cos^2 \frac{\pi\Gamma z}{2} + (1 - \delta) \sin^2(2\pi t) \right]$$

$$\dot{z}(x, z, t) = -(R\delta\pi\Gamma/2) \sin(\pi\Gamma z) \cos[2\pi(x + t)]. \quad (2.2.9)$$

From now on, we will refer to R as simply the mobility.

To prevent the centers of mass of ions from contacting the walls and becoming stuck in a potential well there, we give the ions an effective radius $\xi = 0.0125$ and restrict them to the range $\xi \leq z \leq 1/\Gamma - \xi$.

2.3 Numerical Methods

In order to analyse the behavior of an ion subject to the potential, the position of an ion must be tracked over time. The new position of the ion is determined after a time of dt has elapsed with respect to the current time t . The exact position an ion at time $t + dt$ can be determined using the Taylor series method. The Taylor series method is given by

$$\mathbf{r}(t + dt) = \mathbf{r}(t) + dt\mathbf{r}'(t) + \frac{dt^2}{2}\mathbf{r}''(t) + \frac{dt^3}{6}\mathbf{r}'''(t) + \cdots = \sum_{i=0}^{\infty} \frac{dt^i}{i!}\mathbf{r}^{(i)}(t), \quad (2.3.1)$$

where

$$\mathbf{r}(t) = \begin{bmatrix} x(t) \\ z(t) \end{bmatrix}. [3] \quad (2.3.2)$$

We see that in order to determine this exact position using the Taylor series method, the position at time t and all the derivatives of the position with respect to time at time t must be known. The position of the ion at time t is known and Eqns. 2.2.8 and 2.2.9 give the first derivative of position with respect to time at time t . Since the information about the higher order derivatives are not known for time t then $\mathbf{r}(t + dt)$ must be approximated. Even if the information about the higher order derivatives is known, an approximation would still have to be used due to the infinite sum and subsequent infinite derivatives.

The simplest approximation that can be made is the truncation of the Taylor series after the second term. This method is known as Euler's method. For simplicity, let $\mathbf{r}_n$ be the position of the ion at time t_n which occurs after n iterations of Euler's method. For this system, Euler's method is given by

$$t_{n+1} = t_n + dt \quad (2.3.3)$$

$$\mathbf{r}_{n+1} = \mathbf{r}_n + dt \cdot \mathbf{f}(t_n, \mathbf{r}_n) \quad (2.3.4)$$

where

$$\mathbf{f} = \dot{\mathbf{r}} = \begin{bmatrix} \dot{x}(t, \mathbf{r}) \\ \dot{z}(t, \mathbf{r}) \end{bmatrix} \cdot [3, 7] \quad (2.3.5)$$

Due to the truncation of the Taylor series method, the local truncation error in Euler's method is of the order dt^2 for each step. Since the error is cumulative, the error after the large number of steps required in the computations can be large. The only way to mitigate this potentially large error in Euler's method is set dt sufficiently small. The result of decreasing dt is that more iterations are required to analyse the system over the same overall timespan.

To reduce the potential error without sacrificing the computing time required when the number of iterations is increased as would be necessary when using Euler's method, the fourth-order Runge-Kutta method is implemented. The fourth-order Runge-Kutta method is the result in keeping more terms from the Taylor series. The difficulty of simply keeping more terms from the Taylor series method is that it still requires derivatives of higher order than the first order. To circumvent this issue, substitutions are made along so that only the first-order derivatives are required. The form used in the approximation used in Euler's method is expanded to include five terms. The addition of three terms results in

$$\mathbf{r}_{n+1} = \mathbf{r}_n + \omega_1 dt \mathbf{K}_1 + \omega_2 dt \mathbf{K}_2 + \omega_3 dt \mathbf{K}_3 + \omega_4 dt \mathbf{K}_4 \quad (2.3.6)$$

where

$$\mathbf{K}_1 = \mathbf{f}(\mathbf{r}_n, t_n) \quad (2.3.7a)$$

$$\mathbf{K}_2 = \mathbf{f}(\mathbf{r}_n + \alpha_1 \mathbf{K}_1, t_n + \beta_1 dt) \quad (2.3.7b)$$

$$\mathbf{K}_3 = \mathbf{f}(\mathbf{r}_n + \alpha_2 \mathbf{K}_2, t_n + \beta_2 dt) \quad (2.3.7c)$$

$$\mathbf{K}_4 = \mathbf{f}(\mathbf{r}_n + \alpha_3 \mathbf{K}_3, t_n + \beta_3 dt). \quad (2.3.7d)$$

Equation 2.3.6 gives Euler's method when $\omega_1 = 1$ and $\omega_2 = \omega_3 = \omega_4 = 0$. Substitutions are made to determine values for $\omega_1, \omega_2, \omega_3, \omega_4, \alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2$, and β_3 that allow for as much of the Taylor series to be retained as possible. The result of the appropriate substitutions is

$$\mathbf{r}_{n+1} = \mathbf{r}_n + \frac{dt}{6} (\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4) \quad (2.3.8)$$

where

$$\mathbf{K}_1 = \mathbf{f}(\mathbf{r}_n, t_n) \quad (2.3.9a)$$

$$\mathbf{K}_2 = \mathbf{f}\left(\mathbf{r}_n + \frac{1}{2}dt\mathbf{K}_1, t_n + \frac{1}{2}dt, \right) \quad (2.3.9b)$$

$$\mathbf{K}_3 = \mathbf{f}\left(\mathbf{r}_n + \frac{1}{2}dt\mathbf{K}_2, t_n + \frac{1}{2}dt, \right) \quad (2.3.9c)$$

$$\mathbf{K}_4 = \mathbf{f}(\mathbf{r}_n + dt\mathbf{K}_3, t_n + dt). [3] \quad (2.3.9d)$$

The resulting truncation error for the fourth-order Runge-Kutta method is of the order dt^5 .

In comparing the two numerical methods, we see that for $dt = 10^j$, where $j = -1, -2, -3, \dots$, the local truncation error is small when using the Runge-Kutta method verses Euler's method. If $dt = 10^j$ is increased by one order of magnitude for the Runge-Kutta method verses Euler's method, then the local truncation error is still smaller for the Runge-Kutta method for $j = -2, -3, -4, \dots$

$$(10^j)^2 = 10^{2j} < (10^{j+1})^5 = 10^{5j+5} = 10^{2j}10^{3j+5}; j = -2, -3, -4, \dots \quad (2.3.10)$$

By increasing the order of magnitude for dt , this reduces the total number of steps needed to evaluate the system of differential equation by 1/10. This can be done to help compensate for the increased number of operations required in the Runge-Kutta method.

Figure 2.1: Maps of the trigonometric potential for $\delta = 0.0$ at times (a) $t = 0$, (b) $t = 1/16$, (c) $t = 1/8$, and (d) $t = 3/16$.

Figure 2.2: Maps of the trigonometric potential for $\delta = 0.5$ at times (a) $t = 0$, (b) $t = 1/16$, (c) $t = 1/8$, and (d) $t = 3/16$.

Figure 2.3: Maps of the trigonometric potential for $\delta = 1.0$ at times (a) $t = 0$, (b) $t = 1/16$, (c) $t = 1/8$, and (d) $t = 3/16$.

Chapter 3

Results

3.1 Chapter Introduction

In the analysis of the trigonometric model using the fourth-order Runge-Kutta method, the average velocity of ions with different mobilities are investigated. This determines if ions with different mobilities can travel with the same average velocity, potentially forming packet of ions containing ions with a range of mobilities. This may be useful in the analysis of a sample containing ions of different mobilities. The presence of chaotic trajectories is also important to consider. This may disrupt the separation of ions in a sample. Just because an ion exhibits a chaotic trajectory, it is may not affect the separation of ions. The affect of chaotic trajectories depends upon if the trajectories are narrowband or broadband in nature. The existence of chaos will be investigated by determining the largest Lyapunov exponent for an ion. The types of chaos, if an ion has a chaotic trajectory, is investigated using contact maps.

It is important to select an iterative time step dt in the analysis that will yield as qualitatively accurate results. This is to be done with the realization that as dt is decreased, resulting in more accurate analysis, the computing time is increased.

In order to select an appropriate dt , some initial analysis is done using varying values. An example of this process can be seen in Fig. 3.1 where time steps of $dt = 1/10, 1/100, 1/1000$, and $1/10000$ are used. It is seen that there is a noticeable difference between Figs. 3.1(a), (b), and (c). There is little difference between Figs. 3.1(c) and (d). This leads to the use of $dt = 1/1000$ in the analysis since it is the time step used in Fig. 3.1(c) and requires less computing time than $dt = 1/10000$ used in Fig. 3.1(d).

3.2 Average Velocity

Figure 3.2 shows average ion velocities $\bar{v}$ as a function of the mobility R for a variety of values of δ . The average ion velocity is determined by dividing the distance the ion travels in the x -direction by the total number of periods the ion is allowed to travel. Plateaus in $\bar{v}$ occur for all $\delta > 0$. As δ approaches 1, the plateaus become more pronounced. The minimum mobility required for trapping ($\bar{v} = 1$) increases as δ increases. This is due to increased variation of the potential in the z direction as seen in Figs. 2.1 - 2.3. We find negative average velocity values for $0.848 \leq \delta \leq 1.00$. As δ increases within this range, the maximum negative average velocity begins to increase until a value of $-1/3$ is reached. The negative average velocities develop when a portion of the wave front is weak and is allowed to move past the ion, leaving it on the backside of the wave pushing it in the negative direction. Figure 3.3(a) shows a trajectory with a negative average velocity of $\bar{v} = -1/7$.

Figure 3.4 shows a Devil's staircase for $\delta = 0.84$. The ascending Devil's staircases in the average velocity curves are well defined for $0.834 < \delta \leq 1.0$. This structure is called a Devil's staircase since there is an infinite number of steps from top to bottom.

There are also an infinite number of steps between any two steps. The average velocity values corresponding to the steps in the Devil's staircase can be calculated using Farey addition.[1] Farey addition is the addition of two fractions, but instead of adding the numerators when the denominators are the same, you simply add the numerators and add the denominators according to $(A/B) \oplus (C/D) = (A + C)/(B + D)$. [20] For example, $(1/3) \oplus (1/5) = 2/8$. It is important not to reduce any fractions or you will not get the appropriate values for the steps. We use $0/4$ for the base of the stairs and $1/1$ for the top of the stairs. The value of $0/4$ is used for the base of the stairs since there are four nodes in one wavelength of the channel. The values for the stairs are found by constructing the Farey tree in Fig. 3.5(a). Figure 3.5(b) gives the values of the stairs for the negative regions of the average velocity curves. Only the first few rows in the Farey trees are shown in Fig. 3.5, since the trees continue indefinitely.

The reciprocal of the average velocity is the orbital period for periodic orbits. An ion with an average velocity of $1/3$ has a period of 3. This means that the ion will travel one wavelength for every three periods of the electric potential. Therefore the ion falls behind the wavefront, traveling at $1/3$ its speed. Every time the ion falls behind the wavefront, we call this a retrograde cycle. Figure 3.3(b) shows a trajectory for ions with a period of 3. For the ion with period 3, one can see that the ion undergoes one retrograde cycle for every three periods of the wave. If the average velocity is a rational value that can describe the number of retrograde cycles over a certain number of periods of the electric potential, can we rule out chaos?

In order to determine whether chaos is present, we examine the rate at which nearby ions separate over time. This is accomplished by graphing the separation as a function of time on a log-plot and determining the initial average slope of the curve.

This slope is called the largest Lyapunov exponent, which we will denote as Λ , and is motivated by the assumption that the separation of nearby chaotic trajectories increases exponentially with time; i.e. $\varepsilon(t) \propto e^{\Lambda t}$.

3.3 Largest Lyapunov Exponent

For $0 < \delta < 0.834$, there are intervals of R for which the average velocity does not increase monotonically with R . The breakdown in the Devil's staircase can be seen in Fig. 3.6 for $\delta=0.6$. If I is an interval of R values for which the average velocity is non-monotonic, then there exists some ϵ -neighborhood of I in which chaos occurs. For example, the largest Lyapunov exponent is found to be positive for $\delta = 0.6$ and $R = 0.28$, which we see in Fig. 3.7, indicating the presence of chaos.

The method for computing the largest Lyapunov exponent described above is useful for illustrative purposes, but is not efficient for computing Λ for large sets of input parameters. For this reason a more efficient method was used for producing the required data in a reasonable time.[26]

The procedure involves calculating the trajectories of two initialized ions over one iteration of the 4th-order Runge-Kutta method. One of the ions is displaced a small distance, δ_0 , from the other. After the iteration is calculated the distance the ions are from each other, δ_n , is determined and their distance is reset to be δ_0 . This procedure is then repeated over many iterations and the logarithm of each δ_n/δ_0 divided by the time step t_0 (with respect to the period of field oscillation) is calculated. These values are averaged and the result is an approximation for the largest Lyapunov exponent.

That is, for N total iterations,

$$\Lambda \approx \frac{1}{N} \sum_{n=1}^N \frac{\ln(\delta_n/\delta_0)}{t_0}. \quad (3.3.1)$$

Figure 3.8 was generated using this technique and shows the average velocity $\bar{v}$ and largest Lyapunov exponent Λ verses mobility R for $\delta = 1.0$. In this case the Devil's staircase is decreasing on average and, as in the case for increasing staircases, chaos is found near regions where the curve is non-monotonic. The existence of this chaos is confirmed by the positive Λ value seen for $R > 0.1531$. Figure 3.3(a) shows a periodic ion trajectory for $R = 0.15$ corresponding to the largest plateau of this staircase. With larger mobilities of $R = 0.158$ and $R = 0.169$, the ion trajectories in Fig. 3.9 illustrate how the ion moves when $\Lambda > 0$.

Figure 3.10 shows an extended view of the graphs in Fig. 3.8. This wider view reveals the existence of peaks in Λ which correspond to each jump in $\bar{v}$ for $R > 0.892$. Each of the peaks in Figure 3.10(a) consists of an infinite number of smaller peaks which also correspond to jumps in the average velocity curve, as Figure 3.10(b) shows. Taking into account the limited mesh size of the R -axis and the truncating error associated with computing Λ , one can extrapolate that each of the peaks in the Λ -curve will converge to $\Lambda = 0$ from below as the mesh size of the R -axis tends to zero. We predict that this indicates the existence of quasi-periodic motion for each mobility value yielding these peaks. However, further investigation is needed to confirm this.

Using the above technique, we can construct a complete view of the distribution of Λ values across the (R, δ) parameter space. This is seen in Figure 3.11(a). The data in the figure was generated over 250 periods with a time step of $t_0 = 0.01$ and an initial displacement of $\delta_0 = \sqrt{2} \times 10^{-6}$. In the figure the color scale has been modified to emphasize positive Λ . Since positive Λ values in this system are typically two

orders of magnitude smaller in absolute value than most of the negative Λ values, the positive Λ coordinates have been colored white or gray; with gray signifying $\Lambda \leq 0.1$ and white signifying $\Lambda > 0.1$.

Due to the computational round-off errors and the limits of the mesh-grid, Fig. 3.11(a) does not reveal the location of all positive Λ . In particular, any $|\Lambda| < 0.015$ is considered as equal to zero and is not distinguished. This is the cause of the the sparse scattering of slightly positive Λ for $R < 0.18$.

The graph has also been augmented with three superimposed curves which separate the space into the regions labelled *I* where $\bar{v} < 0$, *II* where $\bar{v} = 0$, *III* where $0 < \bar{v} < 1$, and *IV* where $\bar{v} = 1$.

Figure 3.11(b) shows average ion velocities over the same (R, δ) space as Fig. 3.11(a). In Fig. 3.11(a), one can see a number of bands of stability scattered throughout the chaos. Figure 3.11(b) suggests that these bands correspond to mode-locked regions. Mode-locked regions are regions of the (R, δ) space where the average velocity does not change as either R or δ changes. This is confirmed by observing plots like those in Fig. 3.8 and Fig. 3.10.

3.4 Contact Maps

Figures 3.8 - 3.11 do not make any distinction between chaos that occurs in mode-locked regions and chaos that does not. For this reason we create maps displaying the set of points for which the ion collides with either the upper or lower wall. Since the number of wall contacts per orbit of an ion is affected by its average velocity, such data will help visualize the evolution of chaos as a parameter is varied through mode-locked regions. We will refer to these maps as contact maps. These maps are

similar to logistic maps.[27]

In particular, we map the spread of x coordinates relative to the nearest node to the left of a wall contact for a given value of either R or δ (see Fig. 1.1). We shall use x_ℓ to denote these coordinates relative to the leftmost node. As an example, if an ion were to contact the upper wall at $x = 0.8$, then we plot $x_\ell = 0.8 - 0.5 = 0.3$ on the contact map. Since the nodes are equally spaced $\lambda/2$ apart along a given wall, the maximum possible value of x_ℓ is $1/2$.

Figure 3.12 shows two contact maps for $\delta = 1$. In the maps, the wall contact positions, x_ℓ , are plotted vertically for each R value used to compute them. The contact maps have also been periodically wrapped such that $x_\ell = 0$ and $x_\ell = 1/2$ coincide. This enables the data to be viewed as a continuous set. Overlayed on the maps are the average velocities over the same domain of R values.

Figure 3.12(a) illustrates the ion's behavior over a range of R values also visible in Fig. 3.8. Values of R for which there is a finite and distinct collection of x_ℓ values correspond to periodic orbits. For such R values, the number of x_ℓ points will be called the contact period of the orbit. Values of R for which the collection of x_ℓ values fill an entire interval correspond to chaotic orbits. Informally, such orbits would then have an infinite contact period.

A number of important features are present in this figure. First, there exist intervals of R values where period doubling (or halving) leads to chaos. Also, there are intervals in which chaos occurs over a broader range of x_ℓ values (compared to adjacent chaotic regions) and do not develop out of a period doubling (or halving) sequence. Finally, there exists a correlation between the average velocity in an interval without chaos and the contact period in that interval.

In Fig. 3.12(a), most intervals of R in which periodicity occurs contain a period doubling (or halving) sequence of bifurcations. These sequences lead to chaos and this chaos is called narrowband chaos since the spread of x_ℓ values is confined to a narrow range with respect to the other type of chaos, i.e. broadband chaos.[5] Broadband chaos does not develop out of such sequences and instead appears abruptly at distinct values in the domain. Narrowband chaos is also found to occur only in mode-locked regions where the average velocity is constant. In this we see that chaos can occur when an average velocity is a rational value. In contrast, broadband chaos need not occur where $\bar{v}$ is rational and it is this type of chaos that occurs in regions where the average velocity does not change monotonically with R . Figure 3.9(a) shows a narrowband chaotic trajectory at $R = 0.158$ and Fig. 3.9(b) shows a broadband chaotic trajectory at $R = 0.169$.

Figure 3.12(b) shows the intricacies of the branching structure between $R = 0.12$ and $R = 0.14$. This particular range of R values effectively illustrates the period adding property of the system. To precisely define this property, let $P(R, \delta)$ be the minimum contact period of any trajectory in the mode-locked region containing mobility R and discreteness value δ . Let R'_ℓ be the greatest $R < R'$ such that $P(R'_\ell, \delta') < P(R', \delta')$ and R'_r be the least $R > R'$ such that $P(R'_r, \delta') < P(R', \delta')$. Then we say the system undergoes period adding over R if $P(R', \delta') = P(R'_\ell, \delta') + P(R'_r, \delta')$ for some fixed δ' .

It can be seen in Fig. 3.12(b) that $P(0.125, 1) = 3$ is the sum of $P(0.12, 1) = 2$ and $P(0.135, 1) = 1$. The figure also suggests that the number of retrograde cycles an ion undergoes in a mode-locked region is the same as the minimum contact period in that region. This is because the number of retrograde cycles an ion undergoes is

equal to the absolute value of numerator of the Farey fraction form of the average velocity, i.e $|p|$ for $\bar{v} = p/q$, and the figure suggests that $|p|$ is equal to the minimum contact period. For example, $P(0.125, 1) = 3$ and the Farey fraction form of the average velocity in this mode-locked region is $\bar{v} = -3/25$. This association between the number of retrograde cycles of an ion's orbit and the minimum contact period is seen over other ranges of R and δ .

The information Fig. 3.12 provides is related to taking a horizontal cross-section through Fig. 3.11(a) at $\delta = 1$. Therefore, Fig. 3.12 shows how the system's dynamics change as R is varied. Further insight can be obtained by looking at vertical cross-sections as well, i.e. with R fixed. Figure 3.13 shows a contact map at a fixed $R = 0.24$ for $0.75 \leq \delta \leq 0.85$ with the average velocity curve over-layed. Hence, the figure reveals some of the dynamics which occur across the band of stability seen to occur immediately below region *I* in Fig. 3.11(a).

Figure 3.13 shows that as δ increases the ion's orbit changes from being broadband chaotic to being stable when it "falls" into a mode-locked region corresponding to $\bar{v} = 0$ at $\delta = 0.78490 \pm 10^{-5}$. This is associated with crossing over the curve separating regions *II* and *III* in Fig. 3.11(a). Upon stabilizing, the orbit attains a contact-period of 2. This contact-period undergoes period doubling which culminates with narrow band chaos. At $\delta = 0.7950 \pm 10^{-4}$, the ion's orbit stabilizes again and repeats a sequence of period doubling bifurcations culminating in another region of narrowband chaos.

Finally, at $\delta = 0.8122 \pm 10^{-4}$ the orbit stabilizes once more with a contact period of 2, which reduces to a contact period of 1 as δ increases. This final stabilization corresponds to entering the band of stability mentioned before in Fig. 3.11(a). As δ

is increased further, the z variation in the electric potential becomes great enough that at $\delta = 0.84750 \pm 10^{-5}$ the wave front begins to overtake the ion and so gives the ion a negative average velocity. This change is associated with crossing the curve separating regions *I* and *II* in Fig. 3.11(a). This change is dramatic since the ion's orbit goes from having a contact period of 1 to effectively having an infinite contact period as it becomes broadband chaotic.

The fact that the ion has $\bar{v} = 0$ in regions *N* and *P* (identifying where narrowband chaos and periodic motion occur, respectively) is a result of the ion being localized. This localization is seen in Fig. 3.14(a) with example trajectories corresponding to a narrowband chaotic orbit at $\delta = 0.807$ and a periodic orbit at $\delta = 0.83$. The dramatic change of the orbit's dynamics when wave front overtakes the ion is exemplified by the broadband chaotic orbit in Fig. 3.14(b) at $\delta = 0.849$.

Figure 3.1: Plots used to determine the appropriate time step dt to be used in the analysis of the trigonometric model. The time steps used are (a) $dt = 1/10$, (b) $dt = 1/100$, (c) $dt = 1/1000$, and (d) $dt = 1/10000$.

Figure 3.2: Graphs of the average ion velocity $\bar{v}$ verses its mobility R for discreteness values $\delta=0.0, 0.2, 0.4, 0.6, 0.8, 0.9$, and 1.0 . The $\delta = 0$ curve is a smooth curve from $\bar{v} = 0$ up to the trapping value of $\bar{v} = 1$, while velocity plateaus are apparent for $\delta > 0$. As δ increases, increased variation in the z direction results in larger R required for trapping. Increased variation in the z direction allows for negative average velocities for $\delta = 0.9$ and $\delta = 1.0$.

Figure 3.3: Select trajectories for the discreteness value of $\delta = 1.0$. (a) A mobility of $R = 0.15$ gives an average velocity of $-1/7$, so the ion moves on average one node in the negative x direction for every $7/4$ periods. (b) A mobility of $R = 1.13$ gives an average velocity of $1/3$, so the ion moves on average one node in the positive x direction for every $3/4$ of a period. The primed numbers are included to indicate the periodic nature of the trajectory.

Figure 3.4: The graph of the average velocity $\bar{v}$ versus the electrophoretic mobility R for $\delta = 0.84$. This discreteness value displays no chaos and no negative average velocities. The result is a monotonic Devil's staircase.

Figure 3.5: Farey trees for the Devil's staircase. (a) The Farey tree for positive average velocities. The values for the start of the tree come from the bottom and the top of the Devil's staircase in Fig. 3.4. The fraction $0/4$ is used for the zero value since we have a four nodal pattern. (b) The Farey tree negative average velocities. This Farey tree starts with the values of $0/4$, like the positive Farey tree, and $-1/3$, the maximum negative velocity for an ion.

Figure 3.6: The graph of the average velocity $\bar{v}$ versus the electrophoretic mobility R for $\delta = 0.6$. This is an example of a δ value for which the average velocity does not increase monotonically.

Figure 3.7: The natural log of the separation ε with respect to time for two particles starting at almost identical positions when $\delta = 0.60$ and $R = 0.28$, where the monotonicity of the Devil's staircase breaks down. The line in the first part of the graph is the linear fit used to find the largest Lyapunov exponent, whose value is approximately 0.58. Largest Lyapunov exponents that are greater than zero show extreme sensitivity to initial conditions that characterize chaos.

Figure 3.8: The average velocity $\bar{v}$ and largest Lyapunov exponent Λ verses mobility R for $\delta = 1.00$. For this discreteness value, the largest Lyapunov exponents are positive only when $\bar{v}$ is decreasing from $\bar{v} = 0$ to $\bar{v} = -1/3$ indicating regions of chaos. As for all δ , we find chaos over intervals of R corresponding to non-monotonic regions of the average velocity curve.

Figure 3.9: Chaotic trajectories for the discreteness value of $\delta = 1.0$. (a) Narrowband chaos is exhibited for $R = 0.158$. (b) Broadband chaos is exhibited $R = 0.169$.

Figure 3.10: (a) Largest Lyapunov exponents and average velocities for $\delta = 1.0$. (b) Magnified view of the first major jump near $R = 0.89$ in the average velocity curve in (a).

Figure 3.11: (a) Largest Lyapunov exponents as a function of R and δ . Values of (R, δ) where $\Lambda > 0$ have been colored white/gray for distinction. Curves are included to separate the space into regions *I*, *II*, *III*, and *IV*. These regions identify the locations of ion trajectories with $\bar{v} < 0$, $\bar{v} = 0$, $0 < \bar{v} < 1$, and $\bar{v} = 1$, respectively. (b) Average velocities as a function of R and δ . The color-scale for $\bar{v}$ emphasizes the chaotic regions.

Figure 3.12: Contact maps for $\delta = 1$ showing the spread of x coordinates relative to the leftmost node at which the ion collides with either wall. The corresponding average velocities have been included for comparison. The maps have been periodically wrapped such that $x_\ell = 0$ and $x_\ell = 0.5$ coincide.

Figure 3.13: Bifurcation map for $R = 0.24$ showing the horizontal distance from the nearest node to the left of the ion upon contact with a wall as a function of δ . Overlaid is the average velocity (blue). The map has been divided into regions to identify where broadband chaos (B), narrowband chaos (N), and periodic motion (P) occur.

Figure 3.14: Orbit traces for $R = 0.24$. (a) At $\delta = 0.807$ the orbit (black) is narrow-band chaotic and at $\delta = 0.83$ the orbit (blue) is periodic with contact-period 1. (b) At $\delta = 0.849$ the orbit is broadband chaotic and has a negative average velocity of $\bar{v} \approx -0.01$.

Chapter 4

Conclusion

A simple two-dimensional model of traveling-wave electrophoresis is developed which allows for more efficient computation and analysis while preserving many of the characteristic features present in the logarithmic series based model previously studied.[6, 5] Like in the previous model, the presence of mode-locking and chaos is found. Unlike that model, the existence of negative average velocities is found. These negative average velocities result from including the discreteness value parameter δ unique to our model. The inclusion of this parameter (in addition to the mobility R included previously) yields a two-dimensional parameter space. In this study, maps of the largest Lyapunov exponent and average velocity over (R, δ) parameter space are generated. Together with graphs over R with fixed δ , these maps reveal that chaos can occur whether the system is mode locked or not.

Contact maps showing the locations of initial wall contacts throughout an ion's orbit help in distinguishing between chaos occurring in mode-locked regions of (R, δ) space and chaos otherwise. These contact maps are physically and structurally similar to the contact-angle maps used in the earlier model.[5] The contact maps reveal the

existence of narrowband and broadband chaos which occur when the system is mode-locked and not mode-locked, respectively. Hence, our simplified model of traveling-wave electrophoresis is able to resolve the intricate chaotic structures previously seen.

The mode-locked regions indicate the feasibility of separating ions of different packets according to ranges of mobility. The system can then be adjusted to further separate the packets into ever smaller packets. This can be done in hopes of isolating particular ions. The hope is that this can be utilized in the medical field in lab-on-a-chip devices.

This study has focused primarily on the dynamics within regions of the (R, δ) parameter space for which the average velocities are less than one. It is in these regions that chaotic motion occurs. Future work may include a detailed study of the effect of chaos on the distribution of average velocities over parameter space. Some of our current hypotheses posit that characteristic “bending and folding” of the mode-locked regions may occur when chaos is present.

Other plans for future study include a detailed analysis of the dynamics occurring in the region of the parameter space for which the average velocity is 1; this corresponds to region *IV* in Fig. 3.11(a). There remain many questions regarding the distribution of Λ in this region. For example, we do not yet understand the dynamics which result in the segmented elliptical structure of $\Lambda \approx -20$ seen for $0.7 < \delta < 0.2$. Other future work may involve incorporating diffusion or Brownian motion into the model in order to more closely simulate experimental results as well as to determine the effect of such physics on the evolution of chaos in the system.

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Appendix A

C++ Code

A.1 Average Velocity Code

```
include "stdafx.h"
include <cmath>
include <iostream>
include <fstream>
include <sstream>
using namespace std;

const double pi = 3.14159265358979;
const int a = 4;
const double delta = 0.85;
const double dt = 1.0/1000.0;

void RK4(double& x, double& y, double t, double mu);
double DeltaX(double x, double y, double t, double mu);
double DeltaY(double x, double y, double t, double mu);

int _tmain(int argc, _TCHAR* argv[])
{
    double mu = 0.0;
    double muFinal = 1.0;
    double dmu = 0.005;
    int muSteps = (muFinal - mu)/dmu;
```

```

int totalstep = 10000000;
int deltaInt = delta*100.0;
int muStartInt = mu*100.0;
int muFinalInt = muFinal*100.0;

stringstream filename;
filename << "AveVel_Delta" << deltaInt << "Mu" << muStartInt << "_"
    << muFinalInt << ".txt";

ofstream outStream;
outStream.open(filename.str().c_str());
outStream.setf(ios::showpoint);
outStream.precision(10);
cout.setf(ios::fixed);
cout.precision(10);
double ymin, ymax, xi, yi, t;
double x, y, dx, dy, vavex, vmax = 0.0;

int percentage;
ymin = 1.0/80.0;
ymax = (1.0/a)-ymin;
xi = 0.20;
yi = 0.125;
for (int i = 0; i≤muSteps; i++)
{
    percentage = (i*100.0)/muSteps;
    system("cls");
    cout << percentage << "% complete" << endl;
    x = xi;
    y = yi;
    t = 0;
    for (int ii = 1; ii≤totalstep ; ii++)
    {
        RK4(x, y, t, mu);

        if(y ≥ ymax)
        {
            y = ymax;
        }
        if(y ≤ ymin)

```



```

        {
            y = ymin;
        }
        t = t + dt;
    }

    vavex = (x-xi)/t;

    ostream << mu << "\t" << vavex << endl;
    mu = mu + dm;
}
ostream.close();

return 0;
}

void RK4(double& x, double& y, double t, double mu)
{
    double l1, l2, l3, l4, l, k1, k2, k3, k4, k;
    k1 = dt*DeltaX(x, y, t, mu);
    l1 = dt*DeltaY(x, y, t, mu);

    k2 = dt*DeltaX(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);
    l2 = dt*DeltaY(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);

    k3 = dt*DeltaX(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);
    l3 = dt*DeltaY(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);

    k4 = dt*DeltaX(x+k3, y+l3, t+dt, mu);
    l4 = dt*DeltaY(x+k3, y+l3, t+dt, mu);

    k = (k1+2.0*k2+2.0*k3+k4)/6.0;
    l = (l1+2.0*l2+2.0*l3+l4)/6.0;

    x = x + k;
    y = y + l;
}

double DeltaX(double x, double y, double t, double mu)
{

```

```

    double p1, p2, p3, sn1, sn3, cs1, cs3, dx;
    p1 = (pi*a*y)/2.0;
    p2 = 2.0*pi*x;
    p3 = 2.0*pi*t;
    sn1 = sin(p1);
    sn3 = sin(p3);
    cs1 = cos(p1);
    cs3 = cos(p3);
    dx = 2.0*mu*pi*(cos(p3)*sin(p2)*(delta*sn1*sn1+(1.0-delta)*cs3*cs3)-
        sin(p3)*cos(p2)*(delta*cs1*cs1+(1.0-delta)*sn3*sn3));
    return dx;
}

double DeltaY(double x, double y, double t, double mu)
{
    double dy;
    dy = -0.5*mu*delta*pi*a*sin(pi*a*y)*cos(2.0*pi*(x+t));
    return dy;
}

```

A.2 Trajectory Code

```

include "stdafx.h"
include <cmath>
include <iostream>
include <fstream>
include <sstream>
using namespace std;

const double pi = 3.14159265358979;
const int a = 4;
const double delta = 0.85;
const double dt = 1.0/1000.0;

void RK4(double& x, double& y, double t, double mu);
double DeltaX(double x, double y, double t, double mu);
double DeltaY(double x, double y, double t, double mu);

int _tmain(int argc, _TCHAR* argv[])

```

```

{
    double mu = 0.6;
    int totalstep = 125000;
    int periodSteps = 1.0/dt;
    int deltaInt = delta*100.0;
    int muInt = mu*1000.0;

    stringstream filename;
    filename << "Trajectory_Delta" << deltaInt << "Mu" << muInt
        << "PeriodSteps" << periodSteps << "TotalSteps"
        << totalstep << ".txt";

    ofstream outStream;
    outStream.open(filename.str().c_str());
    outStream.setf(ios::showpoint);
    outStream.precision(10);
    cout.setf(ios::fixed);
    cout.precision(10);
    double ymin, ymax, xi, yi, t;
    double x, y, dx, dy, vavex, vmax = 0.0;
    double l1, l2, l3, l4, l, k1, k2, k3, k4, k;
    int percentage;
    ymin = 1.0/80.0;
    xi = 0.0;
    yi = 0.2375;
    x = xi;
    y = yi;
    t = 0;
    for (int i = 1; i≤totalstep ; i++)
    {
        percentage = (i*100.0)/totalstep;
        system("cls");
        cout << percentage << "% complete" << endl;

        RK4(x, y, t, mu);

        if(x ≥ 1.0)
        {
            x = x - 1.0;
        }
    }
}

```

```

        else if(x < 0.0)
        {
            x = x + 1.0;
        }

        if(y ≥ ymax)
        {
            y = ymax;
        }
        else if(y ≤ ymin)
        {
            y = ymin;
        }

        if(i ≥ 100000)
        {
            outStream << x << "\t" << y << endl;
        }

        t = t + dt;
    }

    outStream.close();

return 0;
}

void RK4(double& x, double& y, double t, double mu)
{
    double l1, l2, l3, l4, l, k1, k2, k3, k4, k;
    k1 = dt*DeltaX(x, y, t, mu);
    l1 = dt*DeltaY(x, y, t, mu);

    k2 = dt*DeltaX(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);
    l2 = dt*DeltaY(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);

    k3 = dt*DeltaX(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);
    l3 = dt*DeltaY(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);

    k4 = dt*DeltaX(x+k3, y+l3, t+dt, mu);

```

```

    l4 = dt*DeltaY(x+k3, y+l3, t+dt, mu);

    k = (k1+2.0*k2+2.0*k3+k4)/6.0;
    l = (l1+2.0*l2+2.0*l3+l4)/6.0;

    x = x + k;
    y = y + l;
}

double DeltaX(double x, double y, double t, double mu)
{
    double p1, p2, p3, sn1, sn3, cs1, cs3, dx;
    p1 = (pi*a*y)/2.0;
    p2 = 2.0*pi*x;
    p3 = 2.0*pi*t;
    sn1 = sin(p1);
    sn3 = sin(p3);
    cs1 = cos(p1);
    cs3 = cos(p3);
    dx = 2.0*mu*pi*(cos(p3)*sin(p2)*(delta*sn1*sn1+(1.0-delta)*cs3*cs3)-
        sin(p3)*cos(p2)*(delta*cs1*cs1+(1.0-delta)*sn3*sn3));
    return dx;
}

double DeltaY(double x, double y, double t, double mu)
{
    double dy;
    dy = -0.5*mu*delta*pi*a*sin(pi*a*y)*cos(2.0*pi*(x+t));
    return dy;
}

```

A.3 Largest Lyapunov Exponent Code

```

include "stdafx.h"
include <cmath>
include <iostream>
include <fstream>
include <sstream>
using namespace std;

```

```

const double pi = 3.14159265358979;
const int a = 4;
const double delta = 1.00;
const double dt = 1.0/100.0;

void RK4(double& x, double& y, double t, double mu);
double DeltaX(double x, double y, double t, double mu);
double DeltaY(double x, double y, double t, double mu);

int _tmain(int argc, _TCHAR* argv[])
{
    double mu = 0.0;
    double muFinal = 0.25;
    double dmu = 0.001;
    int muSteps = (muFinal - mu)/dmu;
    int totalstep = 50000;
    int deltaInt = delta*100.0;
    int muStartInt = mu*100.0;
    int muFinalInt = muFinal*100.0;

    stringstream filename;      filename << "LLE_Delta" << deltaInt << "Mu"
    << muStartInt << "_" << muFinalInt << ".txt";
    ofstream outStream;
    outStream.open(filename.str().c_str());
    outStream.setf(ios::showpoint);
    outStream.precision(10);
    cout.setf(ios::fixed);
    cout.precision(10);
    double xi, yi, t, lle, dx, dy;
    double d0 = sqrt(2.0)*pow(10.0,-6.0);
    double x1, y1, x2, y2, d, vavex, vmax = 0.0, lleTotal, aveLLE;
    int percentage;

    xi = 0.20;
    yi = 0.125;

    x1 = x2 = xi;
    y1 = yi;
    y2 = yi+d0;

```

```

    t = 0;

    for (int i = 0; i ≤ muSteps; i++)
    {
        lleTotal=0.0;
        percentage = (i*100.0)/muSteps;
        system("cls");
        cout << percentage << "% complete" << endl;

        for (int ii = 1; ii ≤ totalstep ; ii++)
        {
            RK4(x1, y1, t, mu);
            RK4(x2, y2, t, mu);

            dx = x2 - x1;
            dy = y2 - y1;

            d = sqrt(dx*dx + dy*dy);
            lle = log(d/d0);
            lleTotal=lleTotal+lle;

            x2 = x1 + d0*(x2-x1)/d;
            y2 = y1 + d0*(y2-y1)/d;

            t = t + dt;
        }

        aveLLE = (lleTotal/totalstep)/dt;

        ostream << mu << "t" << aveLLE << endl;
        mu = mu + dmu;
    }
    ostream.close();

    return 0;
}

void RK4(double& x, double& y, double t, double mu)
{
    double l1, l2, l3, l4, l, k1, k2, k3, k4, k;

```

```

k1 = dt*DeltaX(x, y, t, mu);
l1 = dt*DeltaY(x, y, t, mu);

k2 = dt*DeltaX(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);
l2 = dt*DeltaY(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);

k3 = dt*DeltaX(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);
l3 = dt*DeltaY(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);

k4 = dt*DeltaX(x+k3, y+l3, t+dt, mu);
l4 = dt*DeltaY(x+k3, y+l3, t+dt, mu);

k = (k1+2.0*k2+2.0*k3+k4)/6.0;
l = (l1+2.0*l2+2.0*l3+l4)/6.0;

x = x + k;
y = y + l;

if(y ≥ ymax)
{
    y = ymax;
}
else if(y ≤ ymin)
{
    y = ymin;
}

}

double DeltaX(double x, double y, double t, double mu)
{
    double p1, p2, p3, sn1, sn3, cs1, cs3, dx;
    p1 = (pi*a*y)/2.0;
    p2 = 2.0*pi*x;
    p3 = 2.0*pi*t;
    sn1 = sin(p1);
    sn3 = sin(p3);
    cs1 = cos(p1);
    cs3 = cos(p3);
    dx = 2.0*mu*pi*(cos(p3)*sin(p2)*(delta*sn1*sn1+(1.0-delta)*cs3*cs3)-

```



```

        sin(p3)*cos(p2)*(delta*cs1*cs1+(1.0-delta)*sn3*sn3));
    return dx;
}

double DeltaY(double x, double y, double t, double mu)
{
    double dy;
    dy = -0.5*mu*delta*pi*a*sin(pi*a*y)*cos(2.0*pi*(x+t));
    return dy;
}

```

A.4 Contact Map Code

```

include "stdafx.h"
include <cmath>
include <iostream>
include <fstream>
include <sstream>
using namespace std;

const double pi = 3.14159265358979;
const int a = 4;
const double delta = 0.85;
const double dt = 1.0/1000.0;

void RK4(double& x, double& y, double t, double mu);
double DeltaX(double x, double y, double t, double mu);
double DeltaY(double x, double y, double t, double mu);

int _tmain(int argc, _TCHAR* argv[])
{
    double mu = 0.0;
    double muFinal = 1.0;
    double dmu = 0.005;
    int muSteps = (muFinal - mu)/dmu;
    int totalstep = 10000000;
    int deltaInt = delta*100.0;
    int muStartInt = mu*100.0;
    int muFinalInt = muFinal*100.0;
}

```

```

stringstream filename;
filename << "ContactMap_Delta" << deltaInt << "Mu" << muStartInt <<
" "
-
    << muFinalInt << ".txt";

ofstream outStream;
outStream.open(filename.str().c_str());
outStream.setf(ios::showpoint);
outStream.precision(10);
cout.setf(ios::fixed);
cout.precision(10);
double ymin, ymax, xi, yi, t;
double x, y, dx, dy, yPrev, xContact;
int percentage;

ymin = 1.0/80.0;
ymax = (1.0/a)-ymin;
xi = 0.20;
yi = 0.125;

x = xi;
y = yi;
t = 0;

for (int i = 0; i≤muSteps; i++)
{
    percentage = (i*100.0)/muSteps;
    system("cls");
    cout << percentage << "% complete" << endl;

    for (int j = 1; j≤transients; j++)
    {
        RK4(x, y, t, mu);
        t = t + dt;
    }

    for (int k = 1; k≤totalstep ; k++)
    {
        yPrev = y;

```

```

    RK4(x, y, t, mu);
    t = t + dt;

    if (y==ymin  yPrev<ymin)
    {
        if (x<0.25)
            xContact = x + 0.25;
        else if (x<0.75)
            xContact = x - 0.25;
        else if (x<1.00)
            xContact = x - 0.75;
        outStream << mu << "\t" << xContact << endl;
    }
    else if (y==ymax  yPrev>ymax)
    {
        if (x<0.5)
            xContact = x;
        else if (x<1.00)
            xContact = x - 0.5;
        outStream << mu << "\t" << xContact << endl;
    }
}

    mu = mu + dmU;
}
outStream.close();

return 0;
}

void RK4(double& x, double& y, double t, double mu)
{
    double l1, l2, l3, l4, l, k1, k2, k3, k4, k;
    double ymin, ymax;
    ymin = 1.0/80.0;
    ymax = (1.0/a)-ymin;

    k1 = dt*DeltaX(x, y, t, mu);
    l1 = dt*DeltaY(x, y, t, mu);

```

```

k2 = dt*DeltaX(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);
l2 = dt*DeltaY(x+0.5*k1, y+0.5*l1, t+0.5*dt, mu);

k3 = dt*DeltaX(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);
l3 = dt*DeltaY(x+0.5*k2, y+0.5*l2, t+0.5*dt, mu);

k4 = dt*DeltaX(x+k3, y+l3, t+dt, mu);
l4 = dt*DeltaY(x+k3, y+l3, t+dt, mu);

k = (k1+2.0*k2+2.0*k3+k4)/6.0;
l = (l1+2.0*l2+2.0*l3+l4)/6.0;

x = x + k;
y = y + l;

if(x ≥ 1.0)
{
    x = x - 1.0;
}
else if(x < 0.0)
{
    x = x + 1.0;
}

if(y ≥ ymax)
{
    y = ymax;
}
else if(y ≤ ymin)
{
    y = ymin;
}

}

double DeltaX(double x, double y, double t, double mu)
{
    double p1, p2, p3, sn1, sn3, cs1, cs3, dx;
    p1 = (pi*a*y)/2.0;
    p2 = 2.0*pi*x;

```

```

    p3 = 2.0*pi*t;
    sn1 = sin(p1);
    sn3 = sin(p3);
    cs1 = cos(p1);
    cs3 = cos(p3);
    dx = 2.0*mu*pi*(cos(p3)*sin(p2)*(delta*sn1*sn1+(1.0-delta)*cs3*cs3)-
        sin(p3)*cos(p2)*(delta*cs1*cs1+(1.0-delta)*sn3*sn3));
    return dx;
}

double DeltaY(double x, double y, double t, double mu)
{
    double dy;
    dy = -0.5*mu*delta*pi*a*sin(pi*a*y)*cos(2.0*pi*(x+t));
    return dy;
}

```