Stochastic Simulations in Far-From-Equilibrium Thermal Systems

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ABSTRACT

The field of far-from-equilibrium thermodynamics is often quoted as work in progress despite the extensive depth in the equilibrium based theory. One of the major shortcomings of equilibrium based theory is its inability to explain the emergence of order. Some examples of far-from-equilibrium systems include, reaction diffusion systems, ordered patterns in solids such as snowflakes and alloys in a stronger molecular structure when heated. This paper looks into some of the standard far-from-equilibrium systems such as Rayleigh Bénard Cells, the Kuramoto Model, the Ising model, spatial population growth and heat flow through a simple solid. Stochastic simulations were carried out in order to explicitly compute the variations in system’s intensive properties spatially and temporally. As all of these systems evolved into a steady-state they exhibited certain similarities that were characteristically different from that of the system when at equilibrium. One of the striking differences was a non-Gaussian probability distribution of the thermodynamic parameters when driven far-from-equilibrium. This spread of thermodynamic values across systems serve as the common connection as order emerges in out-of-equilibrium systems at steady-state.
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1. INTRODUCTION

The Laws of Thermodynamics beautifully explains systems that are in thermodynamic equilibrium, the work done, the heat exchanged, and the efficiency therein to reach a point of general homogeneity in the phase-space. In the real world however, this is never the case as the systems are open to constant influxes of matter and energy. It is truly impossible to separate a system from the rest of the universe, so until the universe itself is at equilibrium all systems will also not be in equilibrium. The current problem in Statistical Thermodynamics is that there is little theory to explain these “non-equilibrium” systems and processes. Most of the existing theories extrapolate equilibrium thermodynamics to explain far-from-equilibrium behavior [7, 4, 17, 37, 18, 9, 5]. Several far-from-equilibrium physical and computational systems, such as the Rayleigh-Bénard convection, oscillatory dynamics in Bacterial colonies, the Ising model and its variants, and Kuramoto-type oscillators are explored in this work from a computational perspective. As a general theory for far-from-equilibrium thermodynamics is still ‘a work in progress’, our computational results along with experimental verifications will help to build toward a general theory in future.

1.1 Equilibrium Thermodynamics

All of the concepts discussed in this paper are grounded in the ideas of thermodynamics. General thermodynamics is used to solve for the case of equilibrium. Now thermodynamics is always used in the case of a closed system of microscopic particles interacting, in a gas they’re whizzing by each other really fast, in a liquid they’re colliding with each other and in a solid they are vibrating in place. Since, there are so many particles in this system the energy and motion of each particle cannot usually be calculated explicitly, and the statistics of the system average out on whole with fluctuations decaying as $\frac{1}{\sqrt{N}}$, as $N \to \infty$. Thermodynamics takes the general motion of these particles and solve for average values of the intensive (and extensive) variables of the system such as changes in the pressure, volume, energy, work and temperature, when processes are driven under conditions of equilibrium. It is usually expressed mathematically in the form of First Law of Thermodynamics written as so,

$$dU = \delta Q - \delta W \quad (1.1)$$

This is just the conservation of energy for a macroscopic system. Now here the case of equilibrium is when the change in energy hits zero, this is reinforced by the Second Law for closed systems at equilibrium,

$$dS = \frac{\delta Q}{T} \quad (1.2)$$

which states that the entropy of the system must not decrease, and for a closed system the entropy of the system is maximum. Empirically stated, when the system hits equilibrium it will behave ergodically, and the system will behave uniformly in both time and space [6, 31, 13]. When this is combined with the first law by redefining the heat in relation to the temperature and the entropy, $\delta Q = TdS$ it can be seen how the equilibrium condition will come about.

Now to actually calculate the thermodynamic values like entropy and energy Statistical Thermodynamics is employed. The general idea of Statistical Thermodynamics is thinking about the macroscopic system as a series of events occurring at certain probabilities on the microscopic scale and relating the two. Now from the first law of thermodynamics Boltzmann derived a way to express a probability distribution for any system heading to equilibrium, and was able to identify how to regain macroscopic thermodynamic values from the first law again. He defined the distribution through the partition function written as,

$$Z = \sum_{i=0}^{N} e^{-\beta H_i} \quad (1.3)$$
Here $N$ is the number of degrees of freedom in the system, $\beta$ is the inverse temperature $1/kT$ where $k$ is Boltzmann’s constant, $T$ is the temperature of the bath, and $H$ is the Hamiltonian of each degree of freedom. Now this is the summation of all of the probabilities of finding a particle at any energy level at the given temperature. The actual probability is found by using the partition function as a normalization constant,

$$p(E) = \frac{e^{-\beta E}}{Z} \quad (1.4)$$

Now thermodynamic values like entropy, expected energy and pressure can be re-derived in terms of this new probability distribution,

$$s = k \log(Z) \quad (1.5)$$

$$\bar{E} = -\frac{\partial}{\partial \beta} \ln(Z) \quad (1.6)$$

$$\bar{p} = \frac{1}{\beta} \frac{\partial \ln(Z)}{\partial V} \quad (1.7)$$

This new probability distribution is commonly referred to as the Grand-Canonical ensemble, the distribution is Gaussian by definition and used widely today as a statistical way to look at these macroscopic systems. In order to be able to derive similar statistical values for an ensemble under conditions that are far-from-equilibrium one needs to redefine the First Law by identifying the intensive variables of the system as functionals and not merely phase-space coordinates.

### 1.2 Thermodynamics when far-from-equilibrium

As discussed before, to be able to apply thermodynamics to a system driven far-from-equilibrium, we need to first establish the definitions of the thermodynamic variables. A key aspect of general relativity is the idea that free-fall and inertial motion are physically indistinguishable, also known as the Principle of Equivalence as long as the observer is completely clueless. If this were to be stated for large macroscopic systems, then thermodynamic values of a system when far-from-equilibrium steady-state should be indistinguishable from when it is at equilibrium. Thermal fluctuations in a system at equilibrium are centered around a small value $|X_i - \langle X_i \rangle| \sim 1/\sqrt{N}$. As the system is large it can be assumed that the measured thermal values around the system would appear constant as the mean $\langle X_i \rangle$ as $N \to \infty$. For a system out-of-equilibrium but at a steady-state the same sort of behavior should follow, the measured value should correlate to the expected value of the system $|X_i - \langle X_i \rangle| \sim \epsilon$, as fluctuations are not dominant.

But the difference between equilibrium state and far-from-equilibrium steady state, is that there is a driving flux of energy or flow through the system, which leads to the emergence of spatial and temporal scales that are larger and slower than equilibrium fluctuations. As a result of which, these equilibrium points will space out resulting into regular spatial structures. The emergent order or ‘complexity’ is the gap in our current understanding of these systems from a thermodynamic point of view. Flow equations can show how these systems move but they do not show why these systems form ordered structures. As this feature of symmetry breaking is not described within the current flow equations to describe these macroscopic systems in motion, a new thermodynamic framework needs to be implemented to describe this emergence of order within these complex systems.

This emergent order has always been hard to quantify in the thermodynamic realm where it plays a significant role in the case of entropy. We quantify it using a theoretical approach through the simple application of the Euler-Lagrange method [26, 11, 22]. The Lagrangian in classical sense is usually defined as the kinetic energy ($K$) minus the potential energy ($U$), $L = K - U$. To solve for the motion of the system the Euler-Lagrange equation can used,

$$\frac{\partial L}{\partial q} = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) \quad (1.8)$$

In a thermodynamic case a Lagrangian density can be written as, $\mathcal{L} = Ts - \phi$, where the specific work being done, $\phi$, is substituted for the potential energy and the kinetic energy is the heat which is just temperature, $T$ times specific entropy, $s$. By this combination of the First Law of Thermodynamics and
1. Introduction

Lagrangian mechanics the motion of the system can be defined. It is possible to rewrite Equation (1.8) in terms of the temperature functional, just transform \( q \rightarrow T \) and \( \dot{q} \rightarrow \dot{T} \). The equation now looks like,

\[
\frac{\partial \mathcal{L}}{\partial T} = \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{T}} \right)
\]

(1.9)

This is not the motion of a non-equilibrium system this is just the motion of a thermal system based on its thermal Lagrangian on the energy manifold defined by a temperature functional. If the system was not at equilibrium it would be assumed that \( \frac{\partial \mathcal{L}}{\partial T} \) is not at zero. Solving the equation above for that case and making some simplifications it can be said that the general First Law of Thermodynamics for a non equilibrium system can be expressed as,

\[
d(Ts - \phi) + l_x d(T\partial_x s - \partial_x \phi) + \tau d(T\partial_t s - \partial_t \phi) = 0
\]

(1.10)

Essentially the equation above is the First Law of Thermodynamics for a steady state non-equilibrium system. The impact that the equation really has is the use of \( l_x \) and \( \tau \) on the control of entropy and work balance. The characteristic length and time-scales emerge from the dynamics of the out-of-equilibrium system. The values of these constants control the motion of the system and how the system evolves. It can be attempted to try to find these scales to account for the new distribution of thermal values in this system. Equation (1.10) however is still based on the fact that the system will try to reach equilibrium and evolve as so. That also means that the system has to reach its steady-state and cannot be turbulent or still evolving from initial conditions.

1.3 Outline

This paper is split into separate sections based upon a certain simulation or experiment carried out. In section two analysis of Rayleigh-Bénard cells is looked into. Rayleigh-Bénard cells are convection patterns that form when a fluid is heated from the bottom and allowed to cool from the top. The usual pattern that appears is a circular hexagonal grid formation on the surface of the liquid. The pattern is determinant on the type of liquid as well as for certain temperatures and pressures. The connection between this and non-equilibrium thermodynamics can be seen in the sense that there is a constant heat flux through the system and the system exhibits order. These characteristics allow the analysis of the system through the thermodynamic properties, the one used specifically was temperature. The connection of the distribution of temperature through the system to length scales in the theory discussed in section two can be assessed through a tool known as as the two-point spatial autocorrelation function.

Moving away from actual physical experiments, the simulation of systems on a computer was the main case of study. The first simulation discussed is the Kuramoto model, a model of synchrony through coupled oscillators. The general mean field model regulates the angular frequency of every single oscillator in the system based on the others. This model has been applied to physical system as different as Josephson junctions in semiconductors to the correlation of fireflies shining their lights at night. The model is built around it’s own synchrony which can be tied to the order of a system. The system was simulated in multiple dimensions and thermodynamic properties were assigned to it to try to see any correlation between the ideas of section two.

Another system looked at was a spatial population growth model. The model took into account a Malthusian based growth model combined with diffusive and convective elements to guide the evolution of the system. The systems behavior although not thermodynamic in principle is a macroscopic stochastic system and it should exhibit similar properties to the other systems being looked at.

The last simulation looked at was a lattice of quantum oscillators similar in nature to the Einstein solid used to define the Einstein temperature in solids and eventually led to the Debye model which is the current
model of solids. The difference in this new approach taken is that the temperature is not just calculated for the system as a whole but for smaller subsystems within the solid. The solid was "placed" in contact with two thermal reservoirs of two different temperatures to bring about a non-equilibrium system and fluctuations were measured. The system was also analyzed and looked at with respect to the other systems as well.
2. RAYLEIGH-BÉNARD CONVECTION

One of the first experiments conducted to validate this new theory was conducted on the Rayleigh-Bénard cells. Rayleigh-Bénard cells are convection patterns that appear in fluids, when heated from the bottom at certain pressures [7, 32, 27]. The system is usually used to study convection in a fluids, but a vast majority of the system is not yet fully explored. As the system orders itself by just a driving influx of heat into the system. It is not yet known why or how it exhibits this order when other systems do not. This emergence of order as the system is heated is an easy connection between the characteristic length and time scales of the theory and a real physical system.

To compute these characteristic constants the use of a certain tool in Statistical Physics was employed, the autocorrelation function. This function is defined in a form of a convolution. The convolution operator measures how two functions affect one another. Autocorrelation in particular is a function's convolution with itself, so it quantifies how a region in space or time is similar to itself. To find these thermal characteristic constants the autocorrelation function can be used to determine different length and time scales. In an equilibrium system the autocorrelation will look like an exponential decay, \( e^{-\lambda/x} \). In the non-equilibrium case there should be a small separation in ordered systems, this will look like another exponential for the steady-state system sitting on top of the first one, like a bump. This will have a different \( \lambda \) value than the equilibrium decay in the autocorrelation.

The experiment was carried out by taking thermal video of a convection pattern created, then through that video the length scale and time scale of the system could be found. Originally an autocorrelation function program for use with AFMs was used on the data to extract the characteristic length from the videos. The final product was acceptable but the specified format for AFMs made the calculations take longer and abstract because the data was not AFM data. The AFM program only looked along one axis at a time and produced a lot of noise as can be seen in Figure 2.1. To have more reliant data for this experiment there needed to be an autocorrelation function made specifically for this experiment. Although originally the autocorrelation function was only intended to be used on the Rayleigh-Bénard cells, but it turned out to be a useful function to employ later in the project.

2.1 Autocorrelation

An Autocorrelation function is a measure of how similar values of a function are with the area around them. The range of an autocorrelation function is from 0 to 1, 1 being the same value, perfect correlation, and 0 being absolutely no correlation. The domain of an autocorrelation is from 0 to however large the domain is. This is just used to express the frequency of these values. Sometimes for some autocorrelation functions only half the domain was used. This is because the periodicity would cause the ACF to rise up at larger frequencies because of assumption of periodic boundaries from the Fourier transform in some of the libraries used.

The traditional way to calculate an autocorrelation function is to sum up the value of a function multiplied by the complex conjugate of that function a length \( m \) away. Therefore the autocorrelation function, \( \mathcal{G}(m) \), is written as the real part of this function,

\[
\mathcal{G}(m) = \sum_{i=0}^{N} f(i) \bar{f}(i + m)
\]  \hspace{1cm} (2.1)

Here the domain is discrete for \( f \) and is from 0 to \( N \) but can be any discrete or continuous range of coordinates. In the continuous case you would just replace the summation with an integral. \( \bar{f} \) is the complex conjugate of \( f \) which converts the function into some periodic form based on the fact that we are including
complex numbers (from Euler’s Identity, $e^{i\theta} = \cos(\theta) + i\sin(\theta)$). This is the most general statement of the autocorrelation function but to fully implement it on the computer would be slow and hard, because of its use of summation for every term of the function and its use of complex numbers.

There are other ways to calculate the autocorrelation function, one of the simplest and most straightforward approaches is the Weiner-Khinchin theorem [39, 19] which allows for the calculation of the autocorrelation function through a relation of the functions’ power spectral density or Fourier transform, and the complex conjugate of the spectral density/ Fourier transform. This relation can be written out as,

$$G_m = \int_{-\infty}^{\infty} \hat{f}(m) \bar{\hat{f}}(m)e^{i2\pi xm} dm$$

(2.2)

Here $\hat{f}$ is the Fourier transform of $f$ and $\bar{\hat{f}}$ is the complex conjugate of the Fourier transform of $f$. This is easy to implement because the Fourier transform is not only fast but also simpler to use on the computer. It is the main component of the JPEG compression algorithm for images. Likewise on the computer the inverse Fourier transform is very similar and the main component (the integral and exponent) of the autocorrelation function relation.

## 2.2 Spatial autocorrelation for two dimensional domains

As stated before, the two-point autocorrelation function was used to analyze the thermal camera images gathered of the Rayleigh-Bénard convection patterns. These images are essentially a discrete function of the temperature based on $x$ and $y$ position, where the tuple, $(x, y)$ denotes a pixel location. The task was to then implement the Weiner-Khinchin relation on the image to get the desired autocorrelation function. This required three main components of the program. The first was to take the image from JPEG format and convert it into a 2D matrix, and then crop the part of the image that contained the pattern. The second step was to implement this relation on the 2D matrix and normalize it with the proper autocorrelation function. The last part was to do this on every single image of every single trial of the videos and export them to CSV for analysis in OriginLab, a plotting and fitting program.

Extraction of the image into matrix form is easy in Python, the cropping of the image had to be user selected, so some user interface was designed. The goal for the window was to select the proper region of the image where the pattern is being observed. After the user selected the region the program could now start processing the images according to Equation (2.2).

Some special alterations were made beside the direct implementation of Equation(2.2) on the image however. The Fourier transform function in numpy (FFT) assumes periodic boundary conditions, so the Fourier transform has to be altered, there is a function in numpy that does this because this is a common
Fig. 2.2: The progression of the 95 W convection pattern used for determining characteristic lengths within the system.

need. The function essentially inverts the graphs so that the corners touch the center, and the new 0 frequency of maximum value is at the center of the matrix (This is what was meant earlier when splitting the domain in half was said). The Fourier transform then was multiplied by its complex conjugate and the inverse Fourier transform was taken.

Now essentially an autocorrelation function was established, but it was a 2D autocorrelation function. A one dimensional output was needed to get the characteristic length $l_x$ for the theory that was being tested. In order to implement this, a function was defined that radially averaged the autocorrelation function while returning a general one dimensional output.

This new autocorrelation function was smoother and more defined than the previous one from the AFM program. This was probably because it took the $x$ and $y$ components both into effect, the AFM program only averaged along $x$. This output was then exported to a ‘.csv’ file for each video.

This process was automated to allow the user to select the desired region from one frame of the movie and then the program would retrieve the autocorrelation function for each frame in the movie. This allowed what could not be done in the AFM software, it was slow and could only be fed one input at a time. Now an autocorrelation for every frame of all of the data could be calculated in minutes.

The AFM program also could not perform time evolution calculations, so no value of $\tau$ was found originally for the system. Now that $l_x$ was determined, a similar way was used to extract the time based characteristic constant, $\tau$. The same user interface was kept, but the radial averaging of a 2-D matrix would not work for time. Instead the value of each pixel in the video was taken for every frame in the video and created an $M \times N$ number of functions representing $T(t)$ for each pixel, $M$ is width, and $N$ is height of the user selected region. Then a one dimensional autocorrelation function for all of the $T(t)$ functions was taken using Equation (2.2) and averaged together to get $G(t)$. This was easier because the coordinate system did not have to be transformed as was done for the spatial autocorrelation function.

2.3 Results

The autocorrelation function took a lot of research and a lot of thinking on how to produce the proper result for the circumstance, in the end it reproduced the AFM software’s result and did so with less noise. This $\xi$ value estimates the observed dimensions of the cells in the pattern.

The main data looked at was the 4.74 mm oil thickness heated at 95 W power from the bottom, and the 4.74 mm oil thickness heated at 23.8 W power. The 95 W trial was the trial that produced the most defined results. The 23.8 W trial was used as a reference case because it did not produce any convection patterns at all. In the 95 W autocorrelation there is a clearly defined hump about 10 units away from the origin as can be seen in Figure 2.3. This can also be seen as the average diameter of the convection cells in the video. The 23.8 W autocorrelation looks like a regular singular exponential decay.

Both of the autocorrelation functions as expected behave as decaying exponentials, $e^{-\xi t}$, which is typical for most macroscopic systems whether in equilibrium or driven out. The higher power autocorrelation function does exhibit a hump, which can be interpreted as a second defining length because the system is driven out of equilibrium. The autocorrelation functions were fit with decaying exponentials, one for the 23.8 W case and two separate ones for the 95 W case, and all the $\xi$’s were found. The fits can be seen laid
Fig. 2.3: Shown in (a) is the autocorrelation functions for the 95 W Rayleigh-Bénard convection pattern, and the 23.8 W one. There are three fits, one for the 23.8 W pattern, and two for the two exponentials of the 95 W pattern. Seen in (b) is the values of the $\xi$ for the exponential decay fits progressing with time, the green is the 23.8 W trial ($R$) that showed no pattern, and the red and blue are the two fits for the 95 W trial that did show a pattern ($P$).

Fig. 2.4: The mean temperature (blue) and the standard deviation of the temperature (red) for six trials transitioning from transient state to steady state (heating).
Fig. 2.5: Shown in a) is the autocorrelation function generated for the time domain of the 95 W trial, red is the fitted exponential decay for the trial which corresponds to a $\xi$ value of 0.03182 with an $R^2 = 0.9952$. b) is the temperature probability distribution for the 95 W trial.

Over the data in Figure 2.3.

The fitted lengths/\(\xi\)'s where found for the entire trial of the 95 W pattern and the 23.8 W pattern. The evolution of these length scales can also be seen in Figure 2.3 where the 23.8 W pattern can be seen to be longer and not really transform at all in time, while the ordered 95 W pattern hit a rapid change and decreased when it exhibited order and a second length scale could be seen. The length scales of the steady-state patterned system were $\xi = 9.34 \text{ mm (red)}$ and $\xi = 18.5 \text{ mm (blue)}$ which do represent the average length and width of the cells in the image. Meanwhile, the non-patterned fit has a length scale of $\xi = 33 \text{ mm}$ which is close to the thickness of the oil.

The time length scale was also found for the two patterns, the length scale found for the 95 W pattern was 0.03182 minutes as seen in Figure 2.5a. The time scale was a standard decay for the non-ordered case and the ordered case, although not that interesting it can be used in calculation.

It can also be noted that this system's temperature probability distribution is comprised of two humps instead of one normal distribution as seen in Figure 2.5b. This queer distribution exemplifies the non-Gaussian distribution present in many far-from-equilibrium systems and can be compared with the other systems looked at and modeled within in this work.
3. KURAMOTO MODEL

Moving away from the analysis and more to the actual simulations carried out. The first simulation was based on the Kuramoto model, a model developed by Yoshiki Kuramoto [20, 21] in the late 20th century that describes coupling of a large system of oscillators. This model was chosen because of its property where the system can hit a steady-state synchronization of the phases of all of the oscillators. This synchronization is of macroscopic order that can be assessed in a non-equilibrium thermodynamic standpoint. The synchronization could possibly be assessed in terms of entropy [12] and show some of the qualities developed in Section 2.

To generally describe a Kuramoto system there needs to be some set of oscillators. Each oscillator in the system has its own natural frequency $\omega_n$, but is affected by every other oscillator connected to it. The coupling takes form in affecting each frequency based on the angle of every other oscillator. It is explicitly written as so,

$$\omega_i = \frac{d\theta}{dt} = \omega_n + \frac{K}{N} \sum_{j \neq i}^{N-1} \sin(\theta_j - \theta_i)$$  \hspace{1cm} (3.1)

Here the use of suffix notation is being employed where the $i^{th}$ angular total frequency, $\omega_i$, is made up of it’s natural frequency, $\omega_n$, and a coupling term, $K/N$ is the normalization of the coupling. $K$ is the coupling constant, $N$ is the total number of oscillators while $\theta$ per usual represents the angle of the $i^{th}$ or $j^{th}$ oscillator.

This equation governs the general motion of the system, and is all that is needed to achieve the synchronization of the system. The synchronization of the system can generally be attributed to the coupling term present at the end of the equation. As the system progresses in time, the coupling term will adjust the oscillators’ velocities so that their phases converge to the same value. This model although not describing any system in particular has had applications in understanding situations in real world systems such as describing the locking of josephson junctions [40] and the synchronization of fireflies shining in the night [36].

This is just a single case of the model, many other modifications can be made to Equation (3.1) to simulate the system in different domains and apply it more specifically. This equation is probably the most general case and is known as the mean-field model. The model was explored in this way as well as other ways which can be done by modifying the coupling term in Equation (3.1). The mean field model has no constraints on the domain of the coupling, so the system can be simulated simply without placing oscillators distances apart and controlling more of the system except for the number and speed of each degree of freedom.

For the mean field model a time based correlation is useful to look at the system and how synchronized it is. The correlation of all of the oscillators with respect to angle can be found with a relation that Kuramoto found himself [20, 21],

$$r e^{i\theta} = \frac{1}{N} \sum_{j=0}^{N} e^{i\theta_j}$$ \hspace{1cm} (3.2)

This is essentially a rehash of Equation(2.2) where the inverse Fourier transform is on the left side as well and the integral is now a discrete summation. This is easy to calculate in code and employed in analysis of the mean-field simulation.

Another version of the Kuramoto model that was explored which can be called the adjacent field model [23, 30]. This model doesn’t couple every oscillator to each other, it couples every oscillator to each oscillator around it. That means that this model has some spatial dependence. Usually the simulation was carried out on a two-dimensional lattice. Three and higher dimensional configurations and other lattice designs are possible but were not explored in this work. The governing equation for this model is similar to Equation...
(3.1) but slightly different,

$$\omega_i = \omega_n + \frac{K}{4} \sum_{<i,j>}^4 \sin(\theta_j - \theta_i)$$  \hspace{1cm} (3.3)

This is written for a two dimensional lattice interacting with the oscillator above, below, left and right from it. Therefore the normalization constant and the summation is just with $N = 4$, but can be tweaked, the $<i,j>$ notation just signifies the oscillators $j$ adjacent to $i$.

This model can find a characteristic length through spatial means now unlike the mean field model. This can be done with same autocorrelation function as developed for the Rayleigh-Bénard cells in section 2.

Another model briefly looked at was an inverse square coupling relationship. This relationship is a realistic relationship because most objects acted on by a central force experience an inverse square relationship. The governing equation of motion for this system would be,

$$\omega_i = \omega_n + C \sum_{i \neq j}^N \frac{K}{r^2} \sin(\theta_j - \theta_i)$$  \hspace{1cm} (3.4)

This is similar to Equations (3.1),(3.3) but the normalization constant in front of the summation is an arbitrary constant $C$ that can be played with. The coupling constant was brought inside the summation and its magnitude was regulated by its distance away from the oscillator it is affecting through the inverse square relation for the distance.

This model although realistic is very taxing on the computer, and creates a similar outcome to the motion of Equation (3.3) because of the adjacent oscillators still contributing a majority of the coupling to the oscillator they are affecting.

All of these models can have specific coupling constants if wanted, this can be done by defining a set, or matrix of individual coupling constants, $k_i$, for each matrix and bringing the coupling constant inside the summation for each term. This can be done oscillator specific by defining a a matrix or individually assigned through a set of coupling constants for each oscillator.

### 3.1 One dimensional simulation

Anyways to create the mean field model a system of oscillators was created, each with their respective natural frequency $\omega_n$, actual frequency $\omega_c$, and angle $\theta$. These were represented as variables in an object in a Python script. Then one function was defined that incremented their angles based on their angular frequency and another that changed their angular frequency based on Equation (3.1). All of the angular frequencies were given a normal distribution and the angles were given uniform distribution to initialize the simulation. This along with some animation was able to show some great synchronization that can be seen in the files attached.

To analyze the system the relation in Equation (3.2) was used. This is a quick calculation thanks to the FFT function in Numpy. The standard deviation of the angular frequencies and angles of each of the oscillators was also looked at in the analysis. The time evolution of these values was particularly interesting. Some other values that were calculated were the average angular frequency, as well as the average and standard deviation which are calculated through special circular statistics.

### 3.2 Two dimensional Kuramoto model

After fully looking into the mean field model, the two spatial models elaborated on before were looked at. The adjacent field method as characterized by Equation (3.3) was looked at first. This one was created in the same way as the mean-field model, by creating a system of oscillators. This time the oscillators were stored on a two dimensional matrix that defined their spatial position relative to the other oscillators. Doing it this way allowed for an arbitrary lattice constant $a$ to be defined representing the distance in between adjacent oscillators of the lattice. The lattice constant was not used for calculations until the inverse square field relation was looked at.

The adjacent field was carried out by implementing Equation (3.3) through a function that acted on all of the oscillators. The function only had to take into account the four adjacent oscillators, so its runtime
was much faster than the other method; The adjacent field runs at $O(n)$ efficiency, but the mean field and inverse square field run at $O(n^2)$.

The same statistical functions that were implemented on the mean-field model except for the relation in Equation (3.2) were used to analyze the adjacent field model. The autocorrelation function which was used earlier to at the characteristic length for the system was used here to measure heterogeneity in the system. When the autocorrelation was implemented on the angular frequency lattice no real bump was observed to show any sign of out-of-equilibrium order. In order to better classify the system thermally some new value needed to be calculated for the system.

This system does not have discrete energy values, therefore it is virtually impossible to calculate a canonical partition function to derive the thermal values as used in Equation (1.5) in Section 1. A new ensemble could be defined from the continuous probability of some property of the system, then some pseudo-thermal values could be calculated from this probability distribution. In particular the Shannon Entropy [34, 2] which is used in information theory could be evaluated. The term is actually based on Boltzmann’s derivation of the grand canonical ensemble used in statistical physics. It can be seen as a generalization of entropy for different probability distributions. The Shannon Entropy can be calculated as follows,

$$S = -\sum_{i=0}^{N} p_i \ln(p_i)$$

For this particular system the probability, $p_i$, is being calculated by discretizing the values being analyzed, and normalizing the distribution of them. The evolution of this entropy was looked at over time and the autocorrelation function was used on the lattice of calculated individual entropy values for each degree of freedom.

### 3.3 Results

In the case of the one dimensional Mean Field Kuramoto model two main cases exhibited the most interesting behavior. The system was tested with varying size and coupling. The size really just determined how accurate the system evolved in time according to predictions. The size had no real impact except for noise in the results, so the system was usually set to 200 oscillators within the system to get consistent results.

An obvious difference in results can be observed by changing the coupling constant as seen in Figure 3.1. The minimum coupling constant, $K$, needed to reach order depends on the probability distribution of the natural frequencies $\omega_n$. For the case seen in Figure 3.1 the probability distribution is normal with a standard deviation of one half, $\sigma_{\omega_n} = 0.5$. For this case the minimum coupling constant needed for correlation is a
Fig. 3.2: The one dimensional Kuramoto system with 200 oscillators and coupling constant $K = 5$ at varying standard deviation of natural frequencies, $\sigma_{\omega_n}$, from 0 to 2. a) is the correlation vs time of the system and b) is the standard deviation vs time of the system.

Fig. 3.3: This is the Shannon Entropy with respect to a 64 by 64 two dimensional adjacent field Kuramoto lattice at $k = 5$. a) is the Entropy evolution compared to the standard deviation in the angular frequency of all the oscillators. b) is the last frame of the system showing each individual degree of freedom’s entropy where purple is 0 and yellow is about 0.2.
3. Kuramoto Model

The effect was looked at in reverse as well and the standard deviation in the natural frequencies were varied as can be seen in Figure 3.2. This produced slightly different results in the correlations for the systems than just varying $K$. As the standard deviation increased the correlation decreased, but the overall volatility and random behavior of the system caused a lot of noise within the system and oscillations were more susceptible. The maximum standard deviation of 2 although never hitting a correlated steady-state did have some high correlations in the system at some points with a maxima of 0.4.

The standard deviation of the frequencies was also looked at for these two comparisons as can also be seen in Figures 3.1b and 3.2b. A trend can be seen that for the systems that do hit a correlated steady-state, there is an increase in the standard deviation of the frequencies. The increase is proportional to how correlated the steady state is, for larger coupling there is a larger spike in the standard deviation. The Rayleigh-Bénard cells also exhibited a similar property in standard deviation of temperature on phase transition as can be seen in Figure 2.4.

For the varying coupling and constant standard deviation only the cases with $K > 1$ showed the increase and level off at a low value as seen in the case of Section 2, those were also the only ones to correlate fully. The other two standard deviations stay mostly constant. For the varying standard deviation and constant coupling only the cases with $\sigma_{\omega_n} = 2$ showed no increase and dip in the standard deviation. The $\sigma_{\omega_n} = 1.5$ case showed a very slight amount of increase and decrease, but still was semi-ordered around $R = 0.7$. As the standard deviation increased the noise in the correlation and the standard deviation increased proportionately, while the smoothness for constant standard deviation was constant throughout. However, in the correlated case of $\sigma_{\omega_n} = 1.5$ is noisier than $\sigma_{\omega_n} = 2$. This chaotic behavior seems to be more favorable in the non-equilibrium cases.

Moving onto the two dimensional case which needed to take some different approaches to gathering the data. First, the correlation from Equation (3.2) cannot be applied to this system because it is no longer a mean field model and the phases do not align together with respect to just time. In order to classify the correlation now visual analysis needed to be employed. The lattice was extracted to an MP4 file and the synchronization of the phases into a pattern could be seen. Also the same property as seen in the one dimensional case still occurred for the two dimensional one where the standard deviation in frequency would dip and level out when it reached a correlated state, no increase beforehand can be seen however. To further analyze the system the Shannon Entropy was also calculated. Both the standard deviation and the Shannon entropy can be seen in Figure 3.3, as well as an image of the lattice’s entropy for each degree of freedom in the lattice. This lattice was processed through the same autocorrelation function as used in the prior section and can be seen in Figure 3.4. The entropy and the phase autocorrelation functions

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure3_4}
\caption{Fig. 3.4: Shown in \textit{a}) is the autocorrelation functions generated from the two dimensional lattice values for entropy, frequency and phase. Shown in \textit{b}) is the probability distribution of the angular frequency at the first frame of the simulation, and at the last frame of the simulation once it was completely ordered.}
\end{figure}
show a hump starting at around 12 lattice units, meanwhile the frequency autocorrelation function shows no superpositioned exponentials.

The most clear bump is seen in the entropy which gives a connection to the theory being built upon. This can also be seen in the net entropy where the entropy increases but starts to level out once a steady-state is achieved (this shows a similarity between this system in motion and system at equilibrium). Although this two dimensional system is not based on any real hamiltonians or any real thermal system, it does correspond to the theory developed. The probability distribution of the final frequency can be seen in Figure 3.4 overlaid on top of the initial. The standard deviation of the final frame is much tighter than the initial frame, they have about the same mean however.
4. ISING MODEL

Another case of spontaneous emergence of order in a system is ferromagnetism. In a ferromagnet all of the spins of the electrons within the structure of the metal are oriented in the same way which in turn generates a net magnetic field in the solid. This case of order was tricky to explain until the 20th century when Ernst Ising as a project from his professor came up with a model based on statistical physics to explain the phenomenon [16]. The idea was centered around a new property found from quantum mechanics called the Pauli exclusion principle which says that two fermions (electrons for this case) cannot occupy the same energy level if they are close enough to interact. Ising used this exclusion principle to define a general interaction force based on the spins of neighboring electrons. This force was written in terms of the Hamiltonian for each spin site of the electrons within the metal [33],

\[ H(S_i) = -\mu_i h - J \cdot \sum_{<i,j>} S_i S_j \] (4.1)

Here \( S \) is the spin of the electron (1/2 or -1/2), the suffix represents adjacent lattice spots. \( J \) is an interaction constant between the electrons representing the Pauli exclusion principle as described before, basically a generalized force. If \( J \) is greater than zero it is ferromagnetic and all the spins will align in the same way. \( \mu \) is the magnetic moment of the electron, and \( h \) is the magnetic field that the electron is experiencing.

The entire system’s energy is the energy from Equation (4.1) for each spin site in the lattice/metal. This type of Hamiltonian is pretty out of the ordinary and makes certain assumptions about the system, and does not predict every single aspect of ferromagnetic materials. It does however show the macroscopic order that is connected to the non-equilibrium theory. This unconventional expression for energy doesn’t make any sense in regards to the actual motion of the electrons, but is used to predict the outcome of the system through the partition function to find the probability as discussed in Equations (1.5) and (1.4), in Section 1.1. Ising used these definitions to show that there is no order in one dimension for a system that acts like this. However it was discovered by Onsager [29] much later that in two dimensions the model will reach total synchronization at a high enough value of \( J \) and a cold enough temperature. Onsager calculated explicitly that the magnetization of the electrons, the average value of the spins over the magnitude of the spins \( (|S|/\bar{S}) \), which relates to the temperature as,

\[ M(T) = \left( 1 - \frac{1}{\sinh(\frac{2J}{kT})^4} \right)^{1/8} \] (4.2)

Here, one can see that magnetization \( M \) is dependent on the temperature \( T \) of the system. When the magnetization is plotted out it forms a sharp sigmoidal curve centered at the Curie temperature. The Curie temperature is the temperature that a ferromagnetic system loses its magnetization effect. Onsager’s formula is not defined for temperatures above the Curie temperature. This makes it a low temperature phenomenon. As the interaction parameter of the Hamiltonian, \( J \) is unique based on the system, ferromagnetism does appear in the real world, and at realistic earth temperatures, that temperature is uniform throughout as it is solved in the case of equilibrium. The system, however can be driven out-of-equilibrium through the field term in Equation (4.1). On certain lattice types two peaks occurred on the magnetization transition described generally in Equation (4.2), before the effect disappeared [15]. The existence of two separate states where the system exhibits more order while it has been driven out-of-equilibrium is a direct connection to the ideas presented in Section 2.
4.1 Ising Lattice simulation

The simplest way to look at the dynamics of the Ising model is usually through a Monte-Carlo simulation, which is a simulation based on probabilities and random number generation. It is easily seen through the theory that the Ising model is centralized around statistical mechanic’s through the use of the partition function which is a direct way to calculate the probability of a certain outcome. To employ this in simulation a set of spin sites were defined that act according to their Hamiltonian, Equation (4.1). They were arranged in a two dimensional square lattice with periodic boundary conditions because that is the simplest way to see correlation in this system.

In order to actually make them flip the probability was calculated for the system to flip up or flip down. This is calculated by plugging Equation (4.1) into Equations (1.5) and (1.4) and then the most probable outcome can be selected. From here the spin sites can be flipped accordingly, and as Onsager’s prediction say the system should reach a completely correlated state as long as it is at a low enough temperature.

There is more to the simulation however, the system needed to evolve with time. It may seem like an obvious option to just flip the spins according to their probabilities over and over again, but a natural system does not behave that way. This was a mistake made when creating the simulation for the first time and the result is a goofy correlated antiferromagnetic checker pattern. This sort of pattern does occur in the Ising model, but only when the spin coupling constant, $J$, is negative, and it wasn’t set as so in this simulation. It was discovered that the system needs to evolve as a Markov chain to correlate to a single spin within the system. A Markov chain is a simple idea as not every element needs to change to their most probable outcome as the system evolves in time. This is done by choosing one, or a small percentage of the system at a time and then checking their probabilities.

Finally, when the simulation was run at low temperatures the correct correlation was seen. The simulation was a general way to see the order within the system as shown in Figure 4.1. However, this system is in no sense a non-equilibrium system, it was assumed that the entire system was in contact with a heat reservoir at constant temperature $T$. The equilibrium nature being a defining characteristic of the system allows it to correlate with time. So how is this connected with non-equilibrium thermodynamics?

The lattice consists of microscopic sites within a macroscopic system. Even if the macroscopic system is at equilibrium, the microstates of the lattice sites can still have non-equilibrium features locally. In this case, it is implemented through the field interaction term in Equation (4.1). The $\mu_i h$ term is determined independently from the neighboring spins. this field was essentially used to drive the system out-of-equilibrium and compare it with the equilibrium case. If the field is changing the system is not in equilibrium and should exhibit some of the non-equilibrium properties that are expected.

As the external field can be of any functional form, a script was written to define a field that develops both spatially and temporally, $h(x, y, t)$. This way both spatial and temporal properties of the fields could be put onto the system. The first field to be tested was just a sinusoidal field, $h(t) = \sin(\omega t)$, where $\omega$ was calculated to allow every spin on average to be checked with one of the field’s periods. The other functions that were implemented were a constant field, $h(t) = c$, where $c$ is an arbitrary constant, a linear field, $h(x) = Ax + B$ and a travelling wave field, $h(x, t) = A \sin(\omega t - kx)$. The idea behind choosing these fields was to get ones that varied with respect to time or space to see if it affects the ordering. The sinusoidal wave is the one that varies with time, and the linear varies with space. The traveling wave was implemented to vary with time and space while the constant field was a control case for no variation.
4. Ising Model

4.2 Results

The specific Ising model simulation just touched the surface of ferromagnetic research, but this simple model can be connected to the non-equilibrium theory presented in Section 2. The data includes comparisons for different applied fields on the Ising model. First with respect to time the field affected ones were brought to ordered equilibrium quicker than the control case with no field most of the time. The time to reach equilibrium can be seen in Figure 4.2. The cases where the field was not beneficial were the linear and the traveling wave case. Both of these cases are the only fields that vary spatially, the net field across the lattice always came out to around zero. This failure to reach equilibrium can be seen as a locking characteristic of spatial fields with zero net impact. The ordering instead can possibly be attributed to some spatial pattern. The steady-state of the linear and travelling fields both exhibited some non-stochastic pattern. The linear field split the flipping of the spin sites into two parts where the field was more defined. The travelling wave made a diagonal stripe effect. The only field that varied solely with respect to time was sinusoidal field. This field was slightly slower than the constant valued field. The reason that these fields order more quicker may be an example of paramagnetism [38], which is when the spin sites are swayed to orient in the direction of the external magnetic field.

It can also be seen in Figure 4.2 that the standard deviation of the spins in the system were inversely proportional to the magnetism which is expected in this binary system. The standard deviation however does lag a little in the beginning; This is not a spike as seen in Sections 2 and 3 but the fact that the standard deviation plus the magnetization are above one in the first half of the simulation does show some correlation between increased standard deviation and transition to order.

The different fields were also tested with respect to temperature as can be seen in Figure 4.3. The only field that is more susceptible to magnetization at higher temperatures than the control case is the constant field. This can again possibly be attributed to paramagnetism. On the other hand, the sinusoidal field needs to be at a colder temperature to order itself. The linear field failed to show any order before \( \beta = 1 \), and it failed to do so even before \( \beta = 10 \). The traveling wave actually did pretty well at higher temperatures. It even outperformed the regular sinusoidal field. It is interesting how the combination of temporal and spatial variance is more favorable for order with respect to temperature yet less favorable for order with respect to time where instead it makes the st. The constant field still outperformed any variance at all which may be due to paramagnetic effects.
Fig. 4.3: Shown in a) is the inverse temperature evolution of all of the different fields tested, including a theoretical value predicted by Onsager in red. b) shows the steady state of all of the fields at a low temperature of $\beta = 10$. 

**a)**

**b)** Steady-State of Fields

- No Field
- Sin Field
- Linear Field
- Constant Field
- Sinusoidal Field
- Travelling Wave
- Theoretical (red line)
5. BIOPHYSICS

Another macroscopic system looked into was the spatial population growth model. This model was based on a prior simulation in the past on the same subject. The idea is to model population growth of a biological species in a fluid medium. Generally speaking populations disperse, they spread out over an area based on competition for food. The idea of hitting a maximum population is not new, the first to really look into it mathematically was Thomas Malthus [25]. He looked into many factors that impact population growth as a function of time, most importantly being the carrying capacity of the environment. A general Malthusian growth model can be expressed in a simple differential equation [35, 14],

\[
\frac{dN}{dt} = N \left( 1 - \frac{N}{N_{\text{max}}} \right) \tag{5.1}
\]

In order to look at a spatial population growth, Equation (5.1) can be combined with the dispersion-convection equation for fluids which is written as,

\[
\frac{\partial N}{\partial t} = D \nabla^2 N + \vec{v} \nabla N \tag{5.2}
\]

The reasoning for combining these two elements is based on the stochastic growth of populations. From how many offspring a parent will reproduce, to where those offspring were to spread to, everything about the system is random. Equation (5.2) is used to express motion in fluid systems which is inherently random [3, 1]. The first term on the right hand side of the equation governs the diffusive element of fluid motion, \( D \) is just a constant to control this spread. The second term is the convective element, which governs the general correlated motion of parts of a fluid element.

This equation can be applied to a population because a population and a fluid are both made up of a large number of elements and they both behave stochastically at a microscopic level, Equation (5.2) can even be derived from the Langevin equation which describes the motion of random walks. Left to themselves, populations will generally just diffuse in a normal pattern, along every direction given no obstacle, just like a fluid. When the population reaches a certain density the convective element sets in, where the parts of the system collide and start moving collectively. When combined together the general equation of motion for a population based system in time and space is,

\[
\frac{dN}{dt} = N(1 - N/N_{\text{max}}) + D \nabla^2 N + H(N - N_{\text{crit}}) \vec{v} \nabla N \tag{5.3}
\]

The \( H(N - N_{\text{crit}}) \) is a Heaviside step function, or a smooth version of it represented by a sigmoid curve, \( N_{\text{crit}} \) is the population when the system starts experiencing convective forces to guide their motion. This was implemented because the population will not experience convection forces until it is at a certain density. Once it reaches the critical density, it can be assumed that multiple collisions within members of the species take place.

Although this is not a system that has an energy or heat flowing through it, it however, is a macroscopic system that can exhibit order. This ordering behavior can be tied to other qualities of these other thermal systems simulated such as the standard deviation of a certain property. The number of degrees of freedom in a system is also an important thermodynamic property. The change in total number is interpreted as chemical potential in classical thermodynamics because it represents the change in number of molecules from chemical reactions. This natural growth of a population, and its steady state at maximum capacity with individuals dying and being born constantly could perhaps lead to some cool oscillatory behavior.
5. Biophysics

Fig. 5.1: Shown in a) is the numerically solved average population density, $\langle N_s \rangle_t$ as a function of time with varying initial population, $n = 20, 40, 60, 80, 100$ individuals and $\sigma_c = \sigma_d = 0.4$ on a semi-logarithmic scale averaged over 5 simulation runs each for 200 time steps. The arrow indicates increasing $n$. Inset plot shows a sigmoidal fit for $n = 20$. In b) is the mean convection velocity for the system versus time for the same trial.

5.1 Three dimensional spatial population growth

To make a system like this work Equation (5.3) needs to be implemented on a population system. This was not the first attempt to simulate this sort of growth. An earlier simulation was implemented on a two-dimensional lattice, and it only took the diffusive element of Equation (5.3) into account and not the convective one. It was simulated starting with an initial random seed of parents, which were made to reproduce in a Gaussian dispersion all across the lattice in each step [24]. It also calculated the mortality at each location in the lattice by solving the differential equation via convolution with a Fourier transform of the kernel and the population.

Transforming the simulation into three dimensions only altered the dispersion calculations really. The two dimensional Gaussian distribution was transformed into a three dimensional distribution to implement the spread of offspring throughout the lattice for the simulation. The solution to the mortality differential equation was obtained by reproducing the kernel in three dimensions. A three-dimensional Fourier transform was taken on the kernel and the population density. Finally the inverse Fourier transform was taken of their product.

The convection was introduced to the script by calculating the gradient of $N$ in the $z$ direction and multiplying it by the average $z$ component of the velocity of the movement of parent offspring reproduction (The distance between the parent and the offspring per unit time). This was summed with the diffusive solution for the mortality and solved for the full Equation (5.3) with respect to time and space on the lattice.

5.2 Results

The three-dimensional system had similar results to that of the prior two-dimensional model tested. The similarities included what is seen in Figure 5.1 where as the initial seeding of the population increased the rate at which the system hit its carrying capacity increased. The three-dimensional trials still kept the same sigmoid nature as seen in the two dimensional case and historically. Figure 5.2a shows the result of having differently seeded diffusion and competition $\sigma$’s. The driving parameter in these cases seems to be $\sigma_d$ which controls the diffusion spread. This explains why the case where $\sigma_d$ was larger than $\sigma_c$ the system grew quicker, but the other two trials it behaved pretty much the same despite different having different valued $\sigma$’s.

A new trait that came up in the three-dimensional simulation seen in Figure 5.2b is that the standard deviation in population density increased sharply right before the system hit a carrying capacity and then
Fig. 5.2: a) The simulated average population density, $\langle N_s \rangle_t$ with an initial population of $n = 20$ individuals for the three cases: $\sigma_d = 0.6 > \sigma_c = 0.4$ (dashed black), $\sigma_d = \sigma_c = 0.4$ (light grey), and $\sigma_d = 0.4 < \sigma_c = 0.6$ (solid black) on a semi-logarithmic scale averaged over 5 simulation runs each for 200 time steps. b) The standard deviation of the population density, $\sigma_{N_s}$ as a function of time step for the three cases. c) The average convective velocity, $\langle V \rangle_t$ as a function of time. Inset plot shows the functional dependence of the average convective velocity on time on a log-log scale. Irrespective of the model constraint, the average velocities from the three cases almost converge as, $t^{-\alpha}$, $0.9 < \alpha < 1.1$. d) The standard deviation of the velocity, $\sigma_V$ as a function of time step for the three cases. Inset plot shows the functional dependence of the standard deviation of the convective velocity on time on a log-log scale, $\sigma_V \sim t^{-\beta}$, $0.8 < \alpha < 1.2$. 
leveled out at a lower value once the population was securely at carrying capacity. The same can be seen for the convection velocity in Figure 5.2d. This is similar to the Rayleigh-Bénard cell’s temperature and the angular frequency in the Kuramoto model.
6. QUANTUM OSCILLATOR LATTICE

The last simulation looked into drew from the previous simulations carried out. The synchronization of the Kuramoto system’s coupled oscillators had many real world applications to periodic systems. There is also a possible connection between the description of solid-state physics and the Kuramoto system. Quite often to simulate a solid material physicists model the solid as a lattice of harmonic oscillators. In statistical mechanics the most relevant version of this is the Debye Model [33, 8], which considers these harmonic oscillators within the solid and quantizes their potentials with quantum mechanics, with the solution to the harmonic oscillator plugged into the Schrodinger equation. The solution looks like this,

$$E(n) = \hbar \omega \left( n + \frac{1}{2} \right), \quad n \in \mathbb{N}$$

The energy is now a function of natural numbers, so \( n \) can only be a non-negative integer. This quantization of discrete energy values allows Equations (1.5) and (1.4) to be used to calculate thermodynamic quantities. The only dependent variable that is not a constant is now \( \omega \), the angular frequency of the oscillator. This is where the simulation differs from the Debye model, solving for the ratios of \( \omega \) is the true difficulty in solving this system, as it depends on the real world qualities of the solid in discussion such as its elasticity and physical dimensions. There is an inherent difficulty in simulating such a system, as to how should the frequencies be arranged?

The simplest way to simulate it would be to just forget about the angular frequency, and set the \( \omega \) value to a constant within the system. Although less realistic, it is still a thermal system nonetheless. Albert Einstein actually came up with this system five years before Debye came around with the more accurate model. Einstein solved for the specific heat and other thermodynamic properties from this system that were close enough to the actual values of real world solids [10]. It became one of the first solid-state systems looked at from a quantum mechanics point of view. Essentially this Einstein solid was a good enough model to simulate a solid-state object from a statistical physics perspective.

To calculate thermodynamic properties Einstein did not use the partition function like Debye. The partition function is an estimation of the number of energy states. The number of states can be found explicitly because of the constant angular frequency. In this case, each adjacent energy level has the same difference between every energy-level pair for every oscillator. In order to find the number of energy states, all of the possible energy configurations need to be summed up and divided by the product of all the different outcomes. The solution for the number of states within a given domain can be written as,

$$\Omega = \frac{(q + N - 1)!}{q!(N - 1)!}$$

The small \( q \) here represents the total number of quanta \( n \) for the given domain. \( \Omega \) is all the different arrangements of the energy within the system essentially. With this property of the system, thermodynamic values can be calculated, based on some statistical physics relations,

$$\beta = \frac{1}{kT} = \frac{ds}{dE}$$

With these relations once established, this abstract solid can now be put in contact with two thermal reservoirs each with their own unique temperatures \( T_1 \) and \( T_2 \), such that heat can flow through the solid. This is a very simple definition of a thermodynamic system, so the system should show some connections with the theory of Section 2.
6.1 Monte Carlo Simulation

To implement a non-equilibrium Einstein solid the probability of each outcome in the future needs to be determined through the thermal characteristics. Because it is not in equilibrium, there should be a temperature gradient throughout the system, as it cannot be at a single temperature equilibrium state. To find different temperatures throughout the system, many small regions need to be chosen. These regions will serve as the domain for Equation (6.2). The specific domain for the calculation of $q$ for each degree of freedom will be the degree of freedom and all the adjacent positions in the lattice to it. Therefore, in one-dimension there will be three degrees of freedom for the domain of the number of states $\Omega$, in two, five, in three, seven and so on. This is to allow for a more specific yet rougher estimate for the temperature throughout the system. The calculation for $q$ can now be written out as,

$$q_i = n_i + \sum_{<i,j>} n_j$$  \hspace{1cm} (6.4)

Where $i$ is the oscillator, for which calculations are being done, and $j$ is the oscillators adjacent to $i$. This will establish an $\Omega$ term for every oscillator in the system. With an established $\Omega$ an entropy $s$ can be defined for every oscillator, and therefore a $\beta$ based on the changes of energy and entropy.

To make the system actually evolve in time, a Markov chain was used as earlier (in the Ising model simulation). A Markov chain being the most simple way to stochastically model the evolution of a system with time has been proven to always hit a steady state at some point [28] which is crucial for the simulation to hold up to the theory of section 2. The Markov chain was implemented by choosing a single coordinate in the lattice randomly, and then the probability was determined if it would lose, gain or keep its energy level, with the constraint that it could only move one energy level at a time. The probability was then determined through the use of the grand canonical partition function as before, Equations (1.5) and (1.4). First the probability that it would go up or down was determined, then the probability of which adjacent oscillator it would take or receive energy from it was determined. The end oscillators adjacent to the heat baths were at a constant temperature same as the heat baths, and would either supply or take energy into or out of the system.

Under these conditions the system would evolve in time, and perhaps would show some ordered behavior. Even if it didn’t it should still perform under the same dynamics as Equation (1.10). There is still some difficulty in completely connecting this stochastic system to Equation (1.10), and that is because it is difficult to calculate the work done in the system.

6.2 Results

The simulation was carried out in multiple sizes, some as large as 65,536 oscillators in the system. The problem encountered was that the time for the simulation to hit steady-state was proportional to the number of oscillators in the system because the computer would have to compute more probabilities for the system to hit steady-state. This is why the results shown are from a 16 $\times$ 16 lattice. The simulation was also carried out with multiple temperatures, but the higher the temperature, the longer the system would take to reach steady-state. This is why most of the results are at temperatures of 5 and 10.

Figure 6.1 shows the time evolution of the entropy and temperature of the system. They both sharply increase at the beginning of the simulation but gradually level out as the system hits a steady-state. The temperature of the system was noisier and had greater fluctuations than the entropy that the system was at. This scaling up and leveling of the thermodynamic values of the system are signs of an out-of-equilibrium “equilibrium” state where the system has a temperature gradient throughout it, but the system still acts like an equilibrium system.

The noise in the temperature temporally can also be seen spatially in the temperature probability distribution in Figure 6.1b. The temperature is not normally distributed, it is quite spread-out and has multiple local peaks. This chaotic temperature distribution shows quite a turbulent pattern within the system. The probability distribution could be identified as superpositioned exponentials on top of one another, two near the temperatures of the heat reservoirs, and others scattered around those temperatures, probably corresponding to some length scale within the system.
Fig. 6.1: a) is the time evolution of the temperature and entropy of a 16 by 16 Einstein Lattice connected to two heat reservoirs of temperature $T = 5$ and $T = 10$. b) is the temperature probability distribution for the steady state.

Fig. 6.2: a) is the graph of the spatial autocorrelation functions for a frame of the lattice’s inverse temperature ($\beta$), entropy and energy at a steady state which can all be seen in b)
This can be further looked at by observing the autocorrelation functions in Figure 6.2a, which do not show normal exponential decays as an equilibrium system displays. The autocorrelation functions shows multiple bumps, the most prominent are seen at length 3 and length 5 units. This does point to signs of small length scales emerging in the system. It isn’t as intuitive to see as the Ising, Kuramoto and Rayleigh-Bénard systems, but the pattern can be made out from the raw images in Figure 6.2b. The length 3 unit hump in the autocorrelation function can be seen as the slight checkering in all of the frames. The same can be seen for the length 5 unit hump where canals or sort of ovals can be seen in the frames expanding diagonally from top left to bottom right. They are very faint, but for sure not the usual Gaussian homogeneity for equilibrium systems.
Although non-equilibrium thermodynamics is not fully developed, the systems can still be modeled and studied on the computer. Explicit calculation of multiple thermodynamic variables were found and their spatio-temporal evolution and distributions were looked at. All of these systems showed large variance from the usual normal distribution seen in equilibrium systems. For example this can be seen in the probability density graphs seen in Figures 2.5 and 6.1 where neither of these look like normal distributions, as both exhibit two dominant humps. This thermal property is vastly under explained, yet appears so much throughout this work and nature itself.

Moving on, how are these distributions spaced throughout the system is sometimes hard to characterize for such general macroscopic systems. The autocorrelation function then becomes the primary tool to characterize the system. Developed for analysis of the Rayleigh Bénard cell experiment, it showed pattern emergence and length-scales for other systems beside just the Bénard cells. The autocorrelation function identified irregular spatial distributions of scalars in the system, and helped identify order. The Rayleigh Bénard convection system showed much stronger spatial dependence than most of the simulations but it is historically known for its patterns in its driven state. That is not to say that the two-dimensional Kuramoto Model and the Quantum Oscillator Lattice did show some semblance of pattern both visually and through the autocorrelation function. Unfortunately the autocorrelation function could not find any pattern temporally which brings to question if there are better options for quantifying the system temporally.

The main way of analyzing these systems with respect to time was through means and standard deviations of the system as a whole. In particular with the standard deviation it was observed that when the system is in a transient state heading towards equilibrium, the standard deviation in its thermodynamic variable will spike and then drop to a minimum once it hits steady state. This can be seen in Figures 2.4, 3.1, 3.2, and 5.2b for temperature in the Rayleigh Bénard cells while heating, in the angular frequency for the one-dimensional Kuramoto model on transition to synchronization and in population density for the spatial population growth model. This, although not for every case is applicable to identify phase transition in a system. It can be thought of as forces fighting within the system to reach this state of synchronization which causes this standard deviation to dip.

The mean of some values of the system with respect to time was important for characterizing the systems as well. In all of the systems these thermodynamic values came and rested at a constant once it achieved a steady-state. The entropy did not usually violate the Second Law of Thermodynamics, and behaved monotonically except for phenomena in small sample sizes (or locally). This is important, as it helps establish similarities between equilibrium and out-of-equilibrium systems at steady-state. It is hence, also crucial to note that the laws of thermodynamics are not completely changed under this transformation.

Two time based correlations looked into were the correlations calculated for the Kuramoto Model and the Ising model. For the case of the Kuramoto model, the correlation was easily calculated through Equation (3.2). The Ising model is a simple system where each degree of freedom is given a binary option so the correlation is not hard to calculate either. Over time, both the Kuramoto model and the Ising model steadily progressed towards order, and then asymptotically saturated at a value close to one (perfectly correlated). In the Ising model, how the magnetization evolved in relation to the temperature was also looked at.

In conclusion, from looking at a variety of systems it can be seen that macroscopically these systems show order while microscopically they act completely random. This can be attributed to the non-equilibrium conditions that these systems are exposed to which cause them to evolve to these ordered steady-states. Although a not fully flushed subject yet, the present work provides some intuition as to why these systems behave like the way they do.
7.1 Acknowledgments

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APPENDIX
A. AUTOCORRELATION CODE

Here is a pseudo code form of the python program written to analyze much of the data in this paper through use of an autocorrelation function. The function’s input is a two dimensional lattice storing any sort of value such as pixel values in a camera, energy in a lattice of interacting molecules etc. The output is a one dimensional autocorrelation function which proved useful to help analyze the length scales of the system.

**Algorithm 1** The autocorrelation function pseudo code.

```plaintext
function ACF(lat)
    fftim ← fft(lat) # Takes 2-D Fourier transform of image
    conjim ← fftim.conj # Gets the complex conjugate
    acfim ← fft(conjim * fftim.real) # Finds ACF through WKT
    acfim ← fftshift(acfim) # Flips the acf so (0,0) is in center
    cor ← [min(lat.xdim//2, lat.ydim//2)] # Initialize 1-d array
    for r = 0; r++; r < min(lat.xdim//2, lat.ydim//2) do
        coords ← getCircle(lat.xdim//2, lat.ydim//2, r) # Call getCircle for r
        for c = 0; c++; c < len(coords) do
            temp ← temp + lat[c]
        end for
        cor[r] = temp/len(coords) # ACF value is average of circle
    end for
    return (cor - min(cor))/(max(cor) - min(cor)) # Return normalized ACF
end function
```

The autocorrelation code also took use of the getCircle function which was also written for use in this program. The function just returns the coordinates of a circle in a grid around a chosen center point with a given radius. This was used to help transform the two dimensional autocorrelation function into a one dimensional one just based on length away from each point.
Algorithm 2 The getCircle pseudo code.

\begin{algorithm}
\textbf{function} GETCIRCLE(center, radius) \\
\hspace{1em} coords ← [ ] # Initialize the coordinate array \\
\hspace{1em} x ← radius \\
\hspace{1em} y ← 0 \\
\hspace{1em} \textbf{while} x >= y \hspace{1em} \textbf{do} # This completes one eighth of the circle by balancing x and y within r \\
\hspace{2em} coords.append((x, y)) \\
\hspace{2em} \textbf{if} \ x^2 + (y + 1)^2 > radius^2 \hspace{1em} \textbf{then} \\
\hspace{3em} x ← x - 1 \\
\hspace{2em} \textbf{end if} \\
\hspace{1em} y ← y + 1 \\
\hspace{1em} \textbf{end while} \\
\hspace{1em} fCoords ← [ ] \\
\hspace{1em} \textbf{for} c \hspace{1em} \textbf{in} \hspace{1em} coords \hspace{1em} \textbf{do} # Now copy the coordinates 7 times to the other 7 eighths of the circle \\
\hspace{2em} fCoords.append(-c[0] + center[0], -c[1] + center[1]) \\
\hspace{2em} fCoords.append(-c[0] + center[0], c[1] + center[1]) \\
\hspace{2em} fCoords.append(c[0] + center[0], -c[1] + center[1]) \\
\hspace{2em} fCoords.append(c[0] + center[0], c[1] + center[1]) \\
\hspace{2em} fCoords.append(-c[1] + center[0], -c[0] + center[1]) \\
\hspace{2em} fCoords.append(-c[1] + center[0], c[0] + center[1]) \\
\hspace{2em} fCoords.append(c[1] + center[0], -c[0] + center[1]) \\
\hspace{2em} fCoords.append(c[1] + center[0], c[0] + center[1]) \\
\hspace{1em} \textbf{end for} \\
\hspace{1em} \textbf{return} fCoords \\
\textbf{end function}
\end{algorithm}
BIBLIOGRAPHY


