Chaos and the Ergodic Theorem

PHY 313 - Statistical Mechanics

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1 Motivating the Need for Understanding Chaos

There are two main purposes of the study of science. The first is its practical application in the calculation of numbers / parameters and relationships that help man conquer his environment. The second is the more philosophical pursuit of understanding the true nature of our surroundings. Sometimes mathematical tricks and formulas allow us to calculate various parameters and since these methods work there is often little motivation to pursue the more fundamental laws that govern the systems. Sometimes theories which attempt to explain the workings of the universe are not complete and while they provide satisfactory results at some scale they fail at the macroscopic or microscopic levels.

This paper aims to delve into the validity and basis of the formative axioms of statistical mechanics because 'it is not less important to understand the foundation of such a complex issue than to calculate useful quantities' [6].

Chaotic orbits follow trajectories that flow through phase space only restricted by the conservation of total energy. Furthermore, the trajectory is so sensitive to initial conditions that the motion is in effect irriversibile. This bears uncanny similarity to the ergodic hypothisys of statistical mechanics where we say that a trajectory will pass through all points in phase space. Can the presence of chaos be used as a sufficient condition to show that a trajectory will pass through all points in phase space and hence allow us to use the ergodic hypothesis? [1].

2 The Ergodic Hyphothesis

2.1 A brief History of the Ergodic Hypothesis

Boltzmann and Gibbs founded statistical mechanics without much emphasis on the dynamics of their systems but focused on the joint behaviour of the large number of particles. The only part in which dynamics came into account was the ergodic hypothesis. Therefore in our discussion of chaos which bases itself in dynamical systems a brief foray into the history seems relevant.

Boltzmann believed that an energy surface consisted of a finite number of cells and during the time evolution of a system it would pass through each cell. Therefore, he concluded that we could replace a time average by a far simpler phase average that gave rise to the various ensembles [6]. Ehnfests then realized the impossibility of the trajectory to visit every point in phase space and so formulated the 'quasi-ergodic hypothesis' in which he said that the evolutions would cover the energy surface very densely.

Our current understanding of ergodicity has come very far from the original problem and has become very mathematically rigorous. This is in part due to the exceptions to the case introduced by the understanding of chaos that the simple intuitive statement of the ergodic hypothesis is not enough anymore. And it is these exceptions that we are very interested in. We start with a phase space Γ and evolve a single point X_o over time under the evolution law U^t as shown by Equation (1). A small measure $d\mu$ is invariant under the same evolution law.

$$X(t) = U^t X_0 \tag{1}$$

$$d\mu(X) = d\mu(U^{-t}X) \tag{2}$$

Then the dynamic system defined by $(\Gamma, U^t, d\mu(X))$ is called ergodic if for every function F(X) it follows the relation of Equation (3). That is the time average is equal to the average of phase space.

$$\bar{A} \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \int_{t_0}^{t_0+\tau} A(X(t)) = \int A(X) d\mu(X) \equiv < A > \tag{3}$$

Clearly, this is only stating it in a rigorous way and gives no result whether F is ergodic or not.

2.2 Statically Proving Ergodicity

2.2.1 Birkhoff

George D. Birkhoff Birkhoff further laid down more conditions under which ergodicity is valid. Firstly he proved that the time average as $t \to \infty$ exists for almost all initial conditions and secondly that a sufficient condition for a system to be ergodic is that the phase space Γ be metrically indecomposable (transitive) [2]. These results were more of an abstract attempt to understand ergodicity from more of a mathematical perspective.

2.2.2 Kinchin

Kinchin's approach is more relevant to the statistical mechanics domain as it operates under the assumption that the number of particles are large and hence the number of degrees of freedom is very large. He shows that initial conditions for which (3) is not valid go to zero as $N \to \infty$. Kinchin considered a seperable Hamiltonian i.e no interaction forces and showed ergodicity only for a special class of functions (sum functions) that were not sensitive to microscopic details. Examples of such functions are pressure, kinetic energy and total energy. His results were later extended to non seperable Hamiltonians aswell.

Now using the fact that the ensemble average of the time average is equal to the ensemble average and the Markov inequality he gives the relation given in Equation (4).

$$Prob(\frac{|\bar{f} - < f >|}{| < f > |} \geq \frac{K_1}{N^{1/4}}) \leq \frac{K_2}{N^{1/4}} \tag{4}$$

It is clear that in the limit $N \to \infty$ the probability that the ensemble average will be different from the time average goes to 0. Conversely, for finite N there are finite regions in phase space for which the ergodic hypothesis does not hold. Unfortunatly dynamics play no major role in Kinchin's results.

2.3 Coming a full circle

Kinchin's results can be taken and manipulated to show Equation (5). Here we replace the time average with the simple function value. We can see that the sum functions that Kinchin was interested in are in a way 'self averaging' i.e as $N \to \infty$ the value of the observable will not vary from the ensemble average. This allows us to develop the ensemble approach without using the ergodic theory (only for sum functions). Infact Boltzmann also beleived this. Hence, we have shown how the evolution of the ergodic theory did not contain much dynamic analysis and when it did this was eliminated in the limit for large N. Some theorists such as Jaynes have even formed very 'anti-dynamical' approaches where the ergodicity is unnecessary. His approach treats statistical mechanics as a form of statistical inference. His Maximum entropy principle can find the probability of given events when only partial information is available. In the case of statistical mechanics it gives rise to the various ensembles. There is no need for specific dynamics in this approach nor the previous analysis of the ergodic hypothsis.

$$Prob(\frac{|f - < f >|}{| < f > |} \geq \frac{K_1}{N^{1/4}}) \leq \frac{K_2}{N^{1/4}} \tag{5}$$

Yet again I reiterate that science is not just about doing calculations but about understanding the fundamental laws that govern these calculations. We will now look at statistical mechanics by following the trajectories of individual particles and then try to justify the ergodic hypothesis with the help of chaos in the dynamics. It is these trajectories that are physical and true as and must be understood and not ensembles that are but tools for calculation.

3 A Quantitative Analysis of Chaos

3.1 The Lyapunov exponents

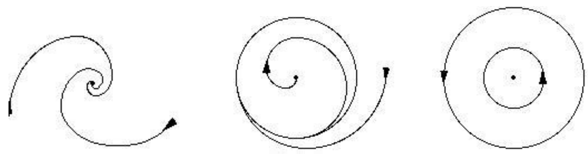
One of the critical hallmarks of chaos is the sensitivity of chaotic systems to initial conditions. That is two points very close in phase space will follow seperate trajectories over time. The rate of seperation of these trajectories is measured by the Lyapunov exponents as shown in Equation (6).

$$|\delta Z(t)| \approx e^{\lambda t}|\delta Z_o| \tag{6}$$

Here δZ_o is the initial seperation of the points in phase space and $\delta Z(t)$ the final seperation after time t. We can see that the final seperation depends on the Lyapunov λ in the exponent. In statistical mechanics we are interested with limits to infinite times and so we can define the maximum Lyapunov exponent [4] as the normal exponent in the limit as time goes to infinity and the initial seperation is infinitesmaly close so we have the MLE as given in Equation (7). The growth of a small segment of phase space is goverened bythe largest exponent.

$$\lambda = \lim_{t\to\infty} \lim_{\delta Z_o \to 0} \frac{1}{t} \ln \frac{|\delta Z(t)|}{\delta Z_o} \tag{7}$$

When $\lambda > 0$ we enter the chaotic regime. Nearby points no matter how close will seperate and the trajectory will visit all neighbourhoods in the phase space [5].



(a) $\lambda < 0$ attractive fixed point (b) $\lambda < 0$ attractor (c) $\lambda = 0$

Figure 1: Gives an intuitive feel for various values of the Lyapunov exponent

4 Chaos in Statistical Mechanics

4.1 Non-Linear Springs

The Hamiltonian of N particles with mass m connected with non-linear springs is given in Equation (8).

$$H = \sum_{i=0}^{N} [\frac{p_i^2}{2m} + \frac{K}{2}(q_{i+1} - q_i)^2 + \frac{\epsilon}{r}(q_{i+1} - q_i)^r] \tag{8}$$

If $\epsilon = 0$ then the system reduces to non-interacting harmonic oscillators with energy given by Equation (9) which clearly stays constant. This means that the time average $\bar{E_k}$ can only be equal to the ensemble average $< E_k >$ only if $\epsilon > 0$ so that the normal modes interact,transfer energy to each other and lose memory of their intitial conditions. Here we are hoping that the presence of the non-linearity that causes chaos will lead the system to travel through all points in phase space that are allowed by the total energy and our ensemble formulation based on the ergodic theorem will not be threatened. We expect that any initial condition i.e any combination energy in initial modes after some relaxation time will transfer to the other modes and each mode will fluctuate around the ensemble average.

$$E_k = 1/2(\dot{a_k} + \omega_k^2 a_k^2) \tag{9}$$

4.1.1 Simulation Parameters

I simulated this Hamiltonian with N = 32 as at this value of N the thermodynamic limit of large N is closely approximated. The code was in part adapted from [7].

4.1.2 Results and Analysis

The results are indeed highly non-intuitive but are in agreement with published simulations [3]. The initial phase is expected. The first mode starts to lose energy and the other modes slowly populate. We expect that all mode will aqcuire similar energies and remain at this equilibrium rate. Somewhat like when perfume is sprayed in a room we do not expect it to return to the bottle but spread out evenly throughout the room. The first suprising result is that first mode regains almost all of its inititial energy after losing it.After some time the system returns close to its initial state. This is shown in Figure 2. While time is between 50 - 100 the energy in the first mode has died out whereas other modes are slowly being occupied. At around time = 120 the strange result kicks in where all modes die out and only the first mode is repopulated almost entirely. One may argue that this is transitive behaviour and that in the limit as t becomes very large the modes will aqcuire the same energyies. Here is our second very suprising result. Even after long times as shown by Figure **??** the first mode still retains a significant amount of the total energy and the other modes only get small amounts of the total energy!

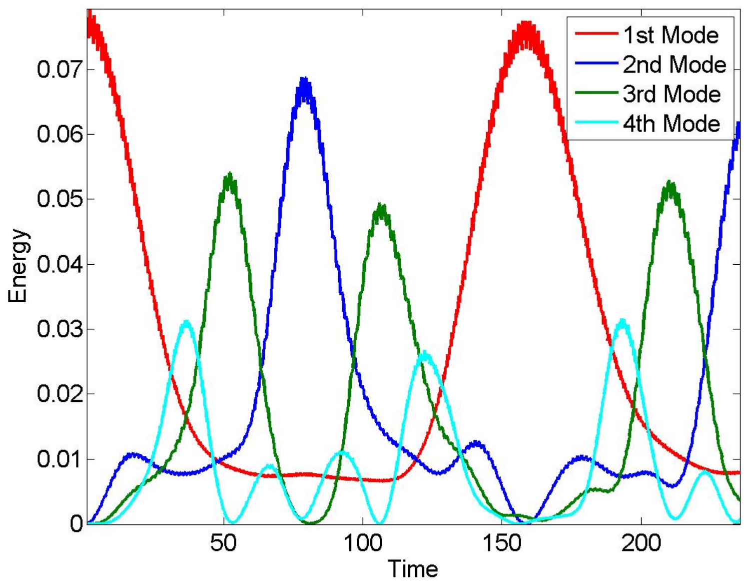


Figure 2: Energy spread of the first 4 modes over time

4.1.3 The KAM theorem and Integrable Hamiltonians

KAM gave a satisfactory solution to this problem but to truly understand it we must first look into how ergodicity is linked to conserved quantities and Poincare's contribution to this topic.

Suppose that the Hamiltonian in question, $H(q, p)$, through a change of variables from the position, momentum variables (p,q) to the action-angle variables (I,ϕ) be made to depend only on I i.e $H = H_0(I)$ then the system is known to be integrable. In this case the time evolution can be given simply by Equation (10) and (11). The subscript i denotes the coordinates for each particle so i=1,...,N.

$$I_i(t) = I_i(0) \tag{10}$$

$$\phi_i(t) = \phi_i(0) + \frac{\partial H_0}{\partial I_i}(I(0))t \tag{11}$$

This Hamiltonian has clear time evolution and the motion evolves on an N-dimensional tori. The Solar System can be shown to be integrable if planet-planet interactions are ignored and so future positions of planets can theoretically be predicted.

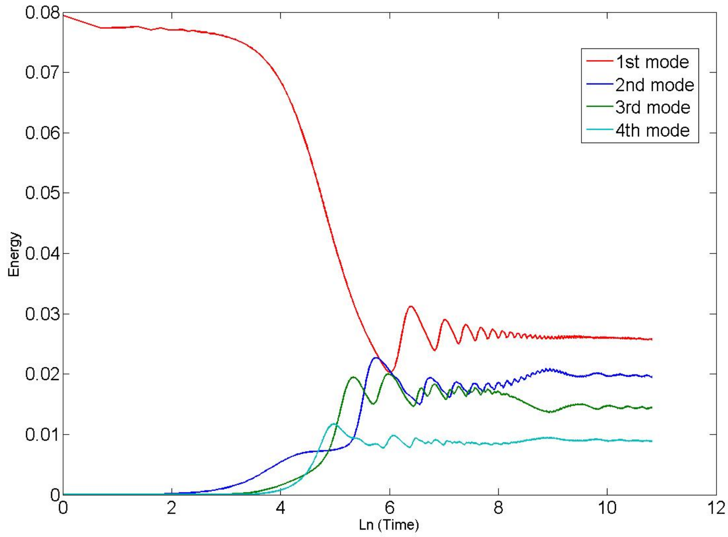


Figure 3: Energy spread of the first 4 modes over time

Now when we introduce a small pertubation as in Equation (12) is included things become slightly complicated. The question is now whether the new system is integrable. For the case of statistical mechanics we hope that it is not so that we can justify the ergodic hypothesis. Poincare showed that when $\epsilon \neq 0$ the system cannot be transformed to make it integrable. This result helped justify the ergodic theory as non-integrability was taken to mean ergodic.

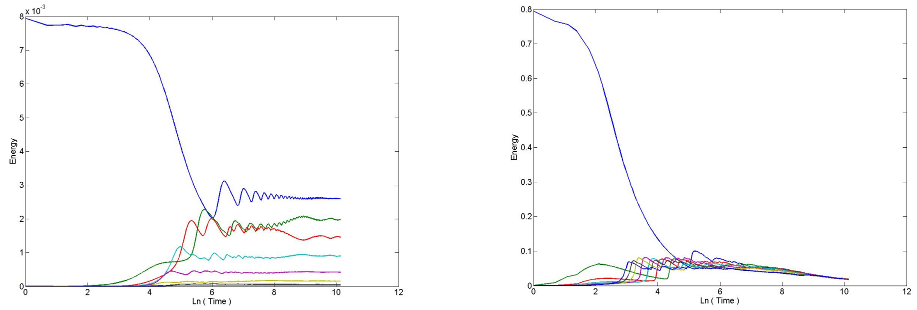
$$H(I, \phi) = H_0(I, \phi) + \epsilon H_1(I, \phi) \tag{12}$$

Now we can appreciate the KAM theorem. It states that for the perturbed Hamiltonian in (12) if ϵ is small enough then on the constant energy surface invariant tori survive. Their measure goes to 1 as $\epsilon \to 0$ as we recover our unperturbed integrable Hamiltonian. For small ϵ most of the initial tori is destroyed, i.e the movement in phase space will not be over the constant energy loop as given in Equation (9) and hence the Hamiltonian will be considered non-integrable. However, for small ϵ some tori survive and are perhaps different (deformed) from the original tori. The initial condition chosen in the FPU simulations happened to be in the region of phase space that these tori existed in and hence the evolution did not go towards equipartition of energy but was confined to oscillate on this KAM tori. As is clear this tori is perturbed, the orignal tori of the unperturbed Hamiltonian would not have let any energy escape from the first normal mode.

4.2 The Thresholds of Chaos

When similar computations are repeated with higher non-linear coefficients (ϵ) it can be seen [8] that the KAM tori are completely destroyed even for the initial conditions of the FPU experiment. And so the energy is equipartitioned. Moreover, for a given energy denisty ($\frac{E_{tot}}{N}$) there is a threshold ϵ_c which determines what effect the pertubation will have. In most physical scenarios ϵ_c is fixed based on the Hamiltonian. In these cases there is a threshold Energy density that seperates regular and irregular behaviour. For ease of simulation we increased the energy density of our simulations by putting more energy in the initial mode to see the same effect. The results are shown in Figure 4

We are finally in a position to come to a conclusion about this weird system. Chaos clearly plays a role in determining whether the system can be called ergodic or not but just the presence of chaos is clearly not a sufficient condition. If $\epsilon < \epsilon_c$ then the KAM tori are still dominant and the system will not reach equipartition as shown by Figure 4 a. However if $\epsilon > \epsilon_c$ then chaos helps us reach ergodicity and the system follows equipartition and is in agreement with normal statistcal mechanics theory. From the surface we can see that since increasing the energy density decreases ϵ_c we can conjecture



(a) E = 1/32 (b) E = 10/32

Figure 4: Energy vs Time graph for the first 8 modes for different energy density E

that in the limit as $N \to \infty$ $\epsilon_c \to 0$ as energy density depends inversely on N and we will reconfirm Kinchin's approach as discussed earlier. However, other researchers [9] have shown that other non-linearly perturbed Hamiltonians show regular behavior even as $N \to \infty$. Also, sometimes to reach equipartition the relaxation times are proportional to N and so if one takes the limit $N \to \infty$ to reduce the effect of left over KAM tori the relaxation time goes up so much that equilibrium may never be reached for some initial conditions even if $\epsilon > \epsilon_c$ [10].

5 A note on non-equilibrium dynamics

The long relaxation times do not let us reach equipartition. Perhaps chaos can help us in the understanding of system dynamics before equilibrium something that is hard to accomplish with ensembles. Dynamic properties such as thermal and electrical conductivity, viscosity etc have been known to take place while systems are chaotic. An example being shown in Figure 5 as how a chaotic system (represented in a channel configuration) helps promote heat conduction. However, a counter example Figure 6 with straight edges can also exhibit heat conduction when the traingle angles are chosen correctly. While straight edges cannot seperate two close trajectories the presence of angles can. There are numerous simulations which show a close relationship between these transport coefficients and chaos [11] along with many that provide counter examples [12] hence it is unwise to reach a conclusion of the sufficiency of chaos present simply as a positive lyapunov coefficient as the relationships are far deeper and more complicated.

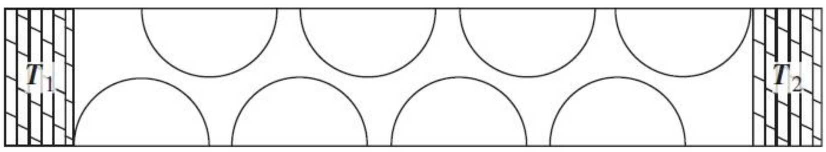


Figure 5: Channel geometry of low dimensional chaos

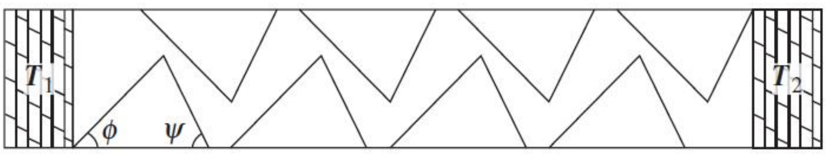


Figure 6: Non-chaotic Billiard channel

6 Summary

The presence of ϵ_c in the above arguement hints at the possibility that large positive Lyapunov exponents are a sufficient condition to procede with calculations based on the standard statistical theory. As we take the limit for large N we can see that Kichin's results are reverified but in this case we have gone though a dervivation taking into account the unique dynamics of the system, as we have agreement because $\epsilon_c \to 0$ in the same limit. Unfortunatly however, this conclusion is not general at all. Other researchers have shown [3] that other non linear systems specifically that of coupled rotators the time average disagrees sharply with the canonical value of heat capacity at high temperatures even in this limit. In my understanding while chaos looked promising to provide the answers to questions regarding molecular dynamics for infinite time it has failed to do so in several situations. There are scenarios as the FPU where even the presence of chaos does not imply ergodicity and scenarios such as Kinchin's approach where the time and ensemble averages can agree even in the absence of chaos. Even in the non equilibrium case we have chaotic and non-chaotic systems behaving in similar ways and so we must conclude again that chaos is an inexhausitive condition. Therefore, we conclude that the presence of positive lyapunov coefficients is only loosely linked to the statistical behaviour and further analysis of systems in always nessasry. Yet one does not lose hope in chaos as it is present in some form in many places. Chaos problems as they are hard to solve analytically depend heavily on computing power. Statistical mechanics problems either deal with huge particles or infinite times and so perhaps with better formed simulations we will come across a general dynamical explanation of ergodicity with the help of chaotic trajectories.

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