

Thermalization Hypothesis - Classical and Quantum

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In this article we try to make a comprehensive introduction to the Eigenstate Thermalization Hypothesis. We will first review thermalization mechanism in classical systems, then introduce eigenstate thermalization as a possible explanation for thermal behavior in quantum systems.

INTRODUCTION

It is widely known that the **fundamental postulate of equilibrium statistical mechanics** is sufficient to derive all of equilibrium in statistical mechanics. The postulate may be stated as follows:

In a state of thermal equilibrium, all the accessible micro-states of the system are equally likely.

Now our objective is to break down the postulate and understand each of the terms.

Thermal equilibrium: In a system which is in thermal equilibrium, the long-time averages of the macroscopic quantities are time-independent (e.g. temperature, pressure, chemical potential). The probability distribution from which the average is taken is also time-independent.

Micro-states: If the generalized coordinate and momenta of each particle maybe determined, then that would be called a micro-state. On the other hand total momenta would be a macro-state of the system.

Accessible Micro-states: If the total energy of the system is E , no individual particle can have a kinetic energy greater than that. Therefore some micro-states are not accessible to the system. If we increase E , then more micro-states will be accessible to the particle. Now, how *all microscopic states become equally likely* is an area of active current research. There is no general proof, because although this assumption is an extremely successful one in statistical mechanics, it doesn't always happen. A lot of modern research tests its limits: like, *if you begin with an isolated system in a highly non-equilibrium state, will it actually evolve such that a description in terms of something remarkable like a micro-canonical ensemble eventually becomes appropriate?*

In the micro-canonical ensemble, we usually assume, that all microscopic configurations, that are consistent with global energy and particle number conservation, become equally likely. If the system requires it, we can also extend the treatment to additional global conservation laws like, restricting the set of possible microscopic

configurations further, but keep the assumption of equal likelihood of the remaining configurations. Taking this to the extreme though, there are some models that have as many conservation laws as they have degrees of freedom. These are called **integrable systems**, and their highly-constrained evolution prevents them from approaching anything close to resembling a microcanonical ensemble.

One curious thing about closed quantum systems in particular is that, in a sense, they always have as many conserved quantities as the size of the state space. In the eigen-basis $|\phi_j\rangle$ of the time-independent (since the system is closed) Hamiltonian:

$$|\psi(t)\rangle = \sum_j c_j \exp\left(\frac{-iEt}{\hbar}\right) |\phi_j\rangle$$

and the amplitudes $|c_j|^2$ are invariant in time. This is a different notion than the more familiar conservation laws that are mentioned above, but it still demonstrates that $|\psi(t)\rangle$ can't fully explore the state space. To reconcile this with the ergodicity that's needed for thermalization (essentially, the ability to eventually sample the whole configuration space), researchers in the 90s proposed the **Eigenstate thermalization hypothesis (ETH)**. In systems that satisfy the **ETH**, thermal distributions are actually encoded in each eigenstate of the Hamiltonian. The quantum dynamics mentioned above then play an auxiliary role of revealing the thermal distribution by destroying the special phase relations that characterize the initial non-equilibrium state.

The **ETH** has been verified theoretically in specific model systems.

THERMALIZATION IN CLASSICAL SYSTEMS

We take an **isolated system**¹. An isolated system obeys the conservation law that its total energy mass stays constant. consisting of N particles with total energy E confined within volume V . It's state is a point in phase space Γ :

$$(p, q) = (p_1, \dots, p_{3N}, q_1, \dots, q_{3N}) \in \Gamma$$

Dynamics are specified by the Hamiltonian $\mathcal{H} = \mathcal{H}(p, q)$ via

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} \quad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}$$

This system is a part of **microcanonical ensemble** as suggested by the conservation of triple $\mathbf{N}, \mathbf{V}, \mathbf{E}$. Classical thermodynamics is usually presented as postulating the existence of isolated systems. It is also usually presented as the fruit of experience. Obviously, no experiment has reported an ideally isolated system. Classical thermodynamics is usually also presented as postulating that an isolated system can, and indeed it eventually always does, reach its own state of internal thermodynamic equilibrium.

Now that we have introduced the desired isolated system, let us have a look at the the **fundamental postulate of statistical mechanics** more formally :

Let all states of the isolated system satisfying the macroscopic boundary conditions be on the hypersurface $\Gamma_{N, V, E}$. In equilibrium all have an equal a-priori probability, i.e. they are uniformly distributed with a (stationary) density:

$$\rho_{\mathbf{mc}}(p, q) = \begin{cases} \text{const.} & \text{if } (p, q) \in \Gamma(N, V, E) \\ 0 & \text{otherwise} \end{cases}$$

where $\rho_{\mathbf{mc}}$ is the density function of the microcanonical ensemble.

We denote by $\Gamma(N, V, E)$ the volume of the phase space

occupied by the microcanonical ensemble as:

$$\begin{aligned} \Gamma(N, V, E) &= \int_{\Gamma} d^{3N}q \, d^{3N}p \, \rho_{\mathbf{mc}}(p, q) [\Theta(\mathcal{H}(p, q) - E \\ &\quad + \Delta E) - \Theta(\mathcal{H}(p, q) - E - \Delta E)] \\ &= \int \int_{E - \Delta E \leq \mathcal{H}(p, q) \leq E + \Delta E} d^{3N}q \, d^{3N}p \, \rho_{\mathbf{mc}}(p, q) \end{aligned}$$

This is the volume enclosed by the two energy surfaces with energy $E - \Delta E$ and $E + \Delta E$.

If $\Phi(E)$ denotes the volume of the phase space enclosed by the energy surface E , then

$$\Gamma(E) = \Phi(E + \Delta E) - \Phi(E)$$

and for $\Delta E \ll E$,

$$\Gamma(E) = \frac{\partial \Phi(E)}{\partial E} \Delta E \equiv \Omega(E) \Delta(E)$$

The quantity $\Omega(E)$ is the density of states at energy E . Now in terms of the density of states, $\rho_{\mathbf{mc}}$ is given by:

$$\rho_{\mathbf{mc}}(p, q) = \begin{cases} \frac{1}{\Omega(E)\Delta E} & \text{if } \mathcal{H}(p, q) \in [E - \Delta E, E + \Delta E] \\ 0 & \text{otherwise} \end{cases}$$

Chaos theory concerns deterministic systems whose behavior can in principle be predicted. Chaotic systems are predictable for a while and then *appear* to become random. A chaotic system must be **sensitive to initial conditions**. Sensitivity to initial conditions means that each point in a chaotic system is arbitrarily closely approximated by other points with significantly different future paths, or trajectories. Thus, an arbitrarily small change, or perturbation, of the current trajectory may lead to significantly different future behavior. For chaotic systems it is useful to:

1. Address the issue of possible relaxation of certain measurable quantities to stationary values (thermalization)
2. Attempt at a statistical description of a system in such thermal equilibrium

Equilibrium is now conceived as most probable macro-state instead of stationary macro-state (in time). It is highly probable for a system initially in a non-equilibrium state to move towards equilibrium state (real space density distribution in accordance with external conditions or potentials and Maxwellian velocity distribution) as the phase space volume of the equilibrium macro-state is fantastically large as compared to non-equilibrium state. Thus the equilibrium is most probable state but arbitrary deviations from it are also probable, but it turns out that the probability is fantastically small. This gives birth to the notions of typicality.

¹ An isolated system is either: (1) a thermodynamic system which is completely enclosed by walls through which can pass neither matter nor energy, though they can move around inside it; or (2) a physical system so far removed from others that it does not interact with them.

The walls of an isolated thermodynamic system are adiabatic, rigid, and impermeable to matter.

Now we come to the famous **Ergodic Hypothesis**, which simply states that to take the mean value of one micro state with respect to time or take the mean of the whole ensemble are equivalent operations.

Definition : Let $A(p, q)$ be an integrable function, and γ be a trajectory on the hypersurface $\Gamma_{N,V,E}$. Let the long-time and microcanonical averages of A be defined respectively as:

$$\bar{A} = \lim_{T \rightarrow \infty} \int_0^T dt A(p(t), q(t))$$

$$\langle A \rangle_{mc} = \frac{1}{\Gamma_E} \int_{\Gamma} d^{3N}q d^{3N}p A(p, q) \rho_{mc}(p, q)$$

By ergodic hypothesis $\bar{A} = \langle A \rangle_{mc}$. The basic notions of **ergodic theory**, in particular ergodicity and mixing, are believed to play a crucial role in the foundations of statistical mechanics. Ergodicity, roughly speaking the absence of constants of the motion other than functions of the energy \mathcal{H} , implies the equality of time-averages and phase-space averages, i.e., of the long-time average of a quantity as it changes under the dynamics and the uniform average of that quantity. This is supposed to justify the use, to define the equilibrium values of thermodynamic quantities, of such phase-space averages with respect to the microcanonical ensemble, the uniform distribution over the energy surface, the idea being that the observed values of these quantities are time-averages, since measurement takes time. There are objections to this use of ergodicity. Boltzmann figured out that once we specify the energy of a system, the maximum number of phase points corresponding to that energy are equilibrium phase points, all of which look the same macroscopically. This means that the value of any thermodynamic quantity, a physical observable, is constant on that energy surface, and averaging over the energy surface will thus reproduce that constant value, regardless of whether or not the system is ergodic. There is another problem associated with this use of ergodicity, which regards a mismatch of time-scales. The time scale appropriate for the ergodicity of a gas in a box is, roughly speaking, the time necessary for a trajectory for the motion in phase space to traverse all across it, hence of order $10^{10^{20}}$ in any unit of time, a time far far larger than that believed to be the age of the universe. Thus ergodicity could not possibly be very relevant to an account of phenomena, such as those with which thermodynamics is concerned, taking place on reasonable time scales.

The concept of **mixing** is supposed to explain why systems evolve to a state of equilibrium. The idea here is that, since such a state is in a sense, characterized by a special probability distribution, the microcanonical ensemble, evolution of the system to its equilibrium

amounts to the convergence of a generic (nonequilibrium) distribution to the special one, under the dynamics on probabilities arising from the phase space motion. Since the energy surface corresponding to an energy E consists almost entirely of a single macrostate, the equilibrium macrostate Γ_{eq} , the mixing property of the evolution on the energy surface pretty much amounts to the condition that even small subregions of Γ_{eq} become uniformly spread over Γ_{eq} after a sufficiently long time. But this could not possibly be relevant to the problem of approach to equilibrium, since it concerns only phase points that describe a system that is already in equilibrium. Approach to equilibrium concerns the passage of a nonequilibrium phase point, lying outside of Γ_{eq} , into Γ_{eq} , and this tends to happen, in fact typically rather quickly, merely because Γ_{eq} is so extremely large.

THE EIGENSTATE THERMALIZATION HYPOTHESIS

The **Eigenstate Thermalization Hypothesis** (or **ETH**) is a set of ideas which purports to explain when and why an isolated quantum mechanical system can be accurately described using equilibrium statistical mechanics. In particular, it is devoted to understanding how systems which are initially prepared in far-from-equilibrium states can evolve in time to a state which appears to be in thermal equilibrium. However the mechanism of dynamical chaos is absent in Quantum Mechanics due to the linear time evolution of the quantum systems, due to the strictly linear time-evolution of the Schrodinger equation,

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{\mathcal{H}} |\psi(t)\rangle$$

where $\hat{\mathcal{H}}$ is the Hamiltonian of the system and $|\psi(t)\rangle$ is the state-vector at any time t . Thus it becomes an open question as to whether an isolated quantum system prepared in an arbitrary initial state which resembles thermal equilibrium. While one may naively expect, on the basis of the linear evolution of the Schrödinger equation, that such a situation is not possible, a variety of experiments in cold atomic gases have indeed observed thermal relaxation in systems which are, to a very good approximation, completely isolated from their environment, and for a wide class of initial states.

THE SETTING

Quantum System: We shall consider isolated, bounded quantum systems with Hamiltonian \mathcal{H} and prepared in an initial state: $|\psi(t=0)\rangle \equiv |\psi(0)\rangle$ Here

bounded-ness implies a discrete energy spectrum. Let

$$\hat{\mathcal{H}}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$$

where $\{|\psi_\alpha\rangle\}_\alpha$ is a complete orthonormal state. Then:

$$|\psi(0)\rangle = \sum_\alpha C_\alpha|\psi_\alpha\rangle, \quad C_\alpha = \langle\psi_\alpha|\psi(0)\rangle, \quad \sum_\alpha |C_\alpha|^2 = 1$$

For total energy of the system we obtain :

$$\langle E \rangle = \langle\psi(0)|\hat{\mathcal{H}}|\psi(0)\rangle = \sum_\alpha |C_\alpha|^2 E_\alpha$$

Generic Initial State: We restrict our attentions to initial states $|\psi(0)\rangle$ sufficiently narrow in energy i.e. the distribution of $|C_\alpha|^2$ will be narrow. More precisely

$$\begin{aligned} \Delta E &= \left(\sum_\alpha |C_\alpha|^2 E_\alpha^2 - \langle E \rangle^2 \right)^{\frac{1}{2}} \\ &= \left(\sum_\alpha |C_\alpha|^2 (E_\alpha - \langle E \rangle)^2 \right)^{\frac{1}{2}} \ll \langle E \rangle \end{aligned}$$

For our purposes such a initial state shall be called generic.

Time Evolution : The temporal evolution of the state vector is given by :

$$|\psi(t)\rangle = \sum_\alpha C_\alpha e^{-\frac{iE_\alpha t}{\hbar}} |\psi_\alpha\rangle$$

We want to understand how thermal behavior is encoded into this equation. The time-dependence of the expectation value of any observable A is given by :

$$\langle A(t) \rangle = \langle\psi(t)|A|\psi(t)\rangle = \sum_{\alpha,\beta} C_\alpha^* C_\beta A_{\alpha\beta} e^{-i\frac{(E_\beta - E_\alpha)t}{\hbar}}$$

where we define $\langle\psi_\alpha|A|\psi_\beta\rangle \equiv A_{\alpha\beta}$.

Equivalence of the Diagonal and Microcanonical Ensembles : We can define a long time average of the expectation value the operator A according to the expression:

$$\bar{A} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle\psi(t)|A|\psi(t)\rangle dt$$

Explicitly we can write :

$$\bar{A} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left[\sum_{\alpha,\beta} C_\alpha^* C_\beta A_{\alpha\beta} e^{-i\frac{(E_\beta - E_\alpha)t}{\hbar}} \right] dt$$

When the integration is explicitly performed it gives the following result :

$$\begin{aligned} \bar{A} &= \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha} + \\ & i\hbar \lim_{T \rightarrow \infty} \left[\sum_{\alpha \neq \beta} \frac{C_\alpha C_\beta A_{\alpha\beta}}{E_\beta - E_\alpha} \left(\frac{e^{-i\frac{(E_\beta - E_\alpha)T}{\hbar}} - 1}{T} \right) \right] \end{aligned}$$

When we take the limit to infinity, the terms in the second sum will vanish, provided that the phase coherence between the different exponential terms in the second sum does not ever become large enough.²

Thus the long-time average expectation value is given by

$$\bar{A} = \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha}$$

This result is explicitly dependent on how the system is prepared now that the C_α 's are retained.

Quantum Ergodicity : Now, because the system is truly isolated the quantum statistical average is the microcanonical ensemble:

$$\langle A \rangle_{mc}(\langle E \rangle) = \frac{1}{N_{\langle E \rangle, \Delta E}} \sum_\alpha A_{\alpha\alpha},$$

where α belongs to an energy window equivalent to $[\langle E \rangle - \Delta E, \langle E \rangle + \Delta E]$ and $N_{\langle E \rangle, \Delta E}$ is the number of microstates contributing to the microcanonical average. If A behaves thermally then, it should settle down to the prediction of the microcanonical ensemble, i.e.:

$$\begin{aligned} \bar{A} &= \langle A \rangle_{mc}(E) \\ &\implies \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha} = \frac{1}{N_{\langle E \rangle, \Delta E}} \sum_\alpha A_{\alpha\alpha} \end{aligned}$$

Now our concern is to explain the **thermodynamic universality** in this equation. The L.H.S. of the above equation depends on the initial conditions via $\langle\psi_\alpha|\psi(0)\rangle$ while R.H.S. depends only on $\langle E \rangle$.

ETH is based on the intuition that $A_{\alpha\alpha}$ are effectively constant over the relevant energy-window and there is negligible fluctuations between the eigenstates. If this is true let $A_{\alpha\alpha}$ be equal to a constant A . Then

$$\bar{A} = \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha} \approx A \sum_\alpha |C_\alpha|^2 = A$$

² An alternate, although naive, justification for the vanishing term may be found by considering that $|e^{-i\frac{(E_\beta - E_\alpha)T}{\hbar}} - 1|$ always fluctuates between two finite quantities. Thus as $T \rightarrow \infty$, $\frac{(e^{-i\frac{(E_\beta - E_\alpha)T}{\hbar}} - 1)}{T} \rightarrow 0$.

where we have assumed that the initial state is normalized appropriately. Also the prediction of the microcanonical ensemble becomes

$$\langle A \rangle_{mc} = \frac{1}{N} \sum_{\alpha} A_{\alpha\alpha} \approx \frac{1}{N} \sum_{\alpha} A = A$$

The two ensembles are therefore in agreement. Now let's formally state the **Eigenstate Thermalization Hypothesis** :

The Eigenstate Thermalization Hypothesis says that for an arbitrary initial state, the expectation value of \hat{A} will ultimately evolve in time to its value predicted by a microcanonical ensemble, i.e. $A_{\alpha\alpha} = \langle A \rangle_{mc}(E)$ for all α 's and thereafter will exhibit only small fluctuations around that value, provided that the following two conditions are met:

1. The diagonal elements of the matrix, $A_{\alpha\alpha}$ vary smoothly as a function of energy, with the difference between neighboring values, $A_{\alpha+1\alpha+1} - A_{\alpha\alpha}$, becoming exponentially small with respect to the system size.
2. The off-diagonal matrix elements $A_{\alpha\beta}$, with $\alpha \neq \beta$, are much smaller than the diagonal matrix elements, and in particular are themselves exponentially small in the system size.

The Auxiliary Role of time evolution: There is no time variable in the equation. Due to time evolution, the coherence between $A_{\alpha\beta}$ is destroyed and \bar{A} is reached. Time evolution does not construct the thermal state, it only reveals it. The thermal state exists at $t=0$, but the coherence hides it.

Alternatives to Eigenstate Thermalization Hypothesis :

(i) Even for eigenstates close in energy, there are large eigenstate-to-eigenstate fluctuations of both the eigenstate expectation values $A_{\alpha\alpha}$ and of the eigenstate occupation numbers $|C_{\alpha}|^2$. However, for physically interesting initial conditions, the fluctuations in the two quantities are uncorrelated. A given initial state then performs an unbiased sampling of the distribution of the eigenstate expectation values $A_{\alpha\alpha}$, resulting in the

equivalence.

(ii) For physically interesting initial conditions, the eigenstate occupation numbers $|C_{\alpha}|^2$ practically do not fluctuate at all between eigenstates that are close in energy. Again, the equivalence immediately follows.

However in some specific cases, calculations have shown that (ii) is not possible because the fluctuations in the eigenstate probabilities $|C_{\alpha}|^2$ are large. Thermal behavior also requires that both the diagonal and the chosen thermal ensemble have sufficiently narrow energy distributions ruling out the possibility of (i) that there could be large eigenstate to eigenstate fluctuations of the eigenstate values. ETH is in fact the accepted mechanism responsible for the thermal behaviour in specific quantum systems. So although at present there are no general theoretical arguments supporting the ETH, some results do exist for restricted classes of systems supporting it.

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