Quantum Ergodicity

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Thermalization: From Glasses To Black Holes., ICTS, Bangalore, June 2013







United States-Israel Binational Science Foundation Simons Foundation

Outline.

Part I. Quantum ergodicity and the eigenstate theramization hypothesis (ETH).

Part II. Applications of ETH to equilibrium and nonequilibrium thermodynamics.

Three different approaches describing isolated systems of particles (systems with stationary Hamiltonian).

Microscopic based on studying long time limit of Hamiltonian dynamics

$$\frac{dq_i}{dt} = \{q_i, \mathcal{H}\} = \frac{\partial \mathcal{H}}{\partial p_i}, \ \frac{dp_i}{dt} = \{p_i, \mathcal{H}\} = -\frac{\partial \mathcal{H}}{\partial q_i}$$

Works for small few-particle systems. Can be prohibitively (exponentially) expensive in chaotic systems.





Chaotic



II. Statistical. Start from equilibrium statistical description (system is in the most random state satisfying constraints). Use Hamiltonian (Lindblad) dynamics perturbatively: linear response (Kubo)

$$Z = \int dX dP \exp[-\beta (H_0(X, P) + H_{int}(X, P))] = Z_0 \langle \exp[-\beta H_{int}(X, P)] \rangle_0$$

III. Mixed: kinetic equations, Master equation, Fokker Planck equation,...: use statistical information and Hamiltonian dynamics to construct rate equations for the probability distribution:

$$\frac{d\rho_n}{dt} = \sum_m (p_{m \to n}\rho_n - p_{n \to m}\rho_n), \ \rho_n = \exp[-\beta E_n] = \operatorname{const}(t), \ \sum_m p_{n \to m} = 1.$$

What is the fundamental problem with the first microscopic approach? Imagine Universe consisting of three particles (classical or quantum)



Can this universe describe itself? – No. There is no place to store information.

Increase number of particles: can simulate three particle dynamics. Complexity of the total system grows exponentially, much faster than its ability to simulate itself.

It is fundamentally impossible to get a complete microsopic description of large interacting systems.

How do we connect these three approaches?

Classical ergodicity: over long periods of time, the time spent by an ensemble of particles in some region of the phase space the same energy (and other conserved integrals) is proportional to the volume of this region.

In simple words classical ergodicity is delocalization in phase space





Chaotic (ergodic)

$$\overline{\delta(X - X(t))} \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \, \delta(X - X(t)) = \rho_{\rm mc}(E),$$

Intergrable (non-ergodic). Number of conserved quantities = number of degrees of freedom

Most interacting many-particle systems are chaotic even with regular interactions (no disorder)

Famous counter example: Fermi-Pasta Ulam problem. First numerical study of ergodicity (thermalization) in an interacting many-body system.



Onset of chaos and thermalization in classical systems

Integrable system of N degrees of freedom has N integrals of motion

 I_j for $j = 1, \cdots, N$

 $[I_i, I_j] = 0$ for all i, j N constraints in 2N dimensional phase space:

each I_i corresponds to the hyper-surface in phase space

Trajectories are confined to intersection of all these surfaces forming



N-dimensional invariant tori.

KAM theorem: weak perturbation preserves `almost all' tori under the condition:

$$\det \left| \frac{\partial \omega_i}{\partial I_j} \right| = \det \left| \frac{\partial^2 H_0}{\partial I_i \partial I_j} \right| \neq 0$$

Thermalization (chaos) occurs though destruction of KAM tori

Similar scenario for the FPU problem

F. M. Izrailev and B. V. Chirikov, Soviet Physics Doklady 11,1 (1966)

Parametric resonance width matches resonance in 1st order perturbation theory:

Spectral Entropy: (Livi et. al, PRA 31, 2, 1985)



Strong stochasticity threshold: $R \simeq 0.03$

Setup: isolated quantum systems. Arbitrary initial state. Hamiltonian dynamics.

Easiest interpretation of density matrix: start from some ensemble of pure states

$$|\psi_0\rangle = \sum_n c_n |n\rangle \Rightarrow |\psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$$

Look into expectation value of some observable O at time t. $\langle O(t) \rangle = \langle \psi(t) | O | \psi(t) \rangle = \sum_{nm} c_n^* c_m e^{i(E_n - E_m)t} O_{nm}$

In order to measure the expectation value need to perform many measurements unless $\psi(t)$ is an eigenstate of *O*.

Each measurement corresponds to a new wave function due to statistical fluctuations. So unless we can prepare identical states we can only measure

$$\overline{\langle O(t)\rangle} = \overline{\langle \psi(t)|O|\psi(t)\rangle} = \sum_{nm} \overline{c_n^* c_m} e^{i(E_n - E_m)t} O_{nm} = \sum_{nm} \rho_{mn}(t) O_{nm}$$

$$\rho_{mn}(t) = \rho_{mn}(0)e^{-i(E_m - E_n)t} = \overline{c_n^* c_m}e^{-i(E_m - E_n)t}$$

If Hamiltonian is fluctuating need to average over the Hamiltonians -> non-unitary evolution.

Ergodicity in Quantum Systems

Classical system: time average of the probability distribution becomes equivalent to the microcanonical ensemble. Implies thermalization of all observables.

$$\overline{\delta(X - X(t))} \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \,\delta(X - X(t)) = \rho_{\rm mc}(E),$$

Quantum systems (quantum language?) – no relaxation of the density matrix to the microcanonical ensemble (von Neumann, 1929).

$$|\Psi(t)\rangle\langle\Psi(t)| = \sum |c_{\alpha}|^{2}|\Psi_{\alpha}\rangle\langle\Psi_{\alpha}| = \hat{\rho}_{\text{diag}}$$

Thermalization must be built in to the structure of Eigenstates and revealed through observables (von Neuman, 1929; Mazur, 1968; Sredniki, 1994; Rigol et. al. 2008, Riemann 2008, ...)

$$\langle \Psi(t) \mid M_{\beta}(t) \mid \Psi(t) \rangle \rightarrow_{t \to +\infty} \text{Tr}[M_{\beta}\hat{\rho}_{\text{mc}}] \equiv \langle M_{\beta} \rangle_{\text{mc}}$$

The limit is understood as at long times at almost all times. In a way in quantum language thermalization is prebuilt in the system. Time evolution is just dephasing.

Berry conjecture, semiclassical limit (M.V. Berry, 1977)

$$\psi^*\left(\mathbf{x} - \frac{\mathbf{s}}{2}\right)\psi\left(\mathbf{x} + \frac{\mathbf{s}}{2}\right) = \frac{1}{\Sigma}\int d\mathbf{p}\,e^{i\mathbf{p}\cdot\mathbf{s}/\hbar}\delta[E - H(\mathbf{x},\mathbf{p})]$$

Average is taken over the energy shall vanishing in the limit $\hbar \rightarrow 0$ but containing many states. Equivalently

$$W_E(\mathbf{x}, \mathbf{p}) \equiv (2\pi\hbar)^{-D} \int d\mathbf{s} \,\psi_E^* \left(\mathbf{x} - \frac{\mathbf{s}}{2}\right) \psi_E\left(\mathbf{x} + \frac{\mathbf{s}}{2}\right) e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}$$
$$W_E^{\rm sm}(\mathbf{x}, \mathbf{p}) \approx \frac{1}{\Sigma} \,\delta[E - H(\mathbf{x}, \mathbf{p})]$$

For non-relativistic particles Berry $\langle f(\mathbf{p}) \rangle = \int d\mathbf{p}_2 d\mathbf{p}_3 \dots \langle | \Psi_{\alpha}(\mathbf{p}, \mathbf{p}_2, \dots) |^2 \rangle$ conjecture implies Maxwell-Bolzmann distribution $= \frac{e^{-\frac{\mathbf{p}^2}{2mkT}}}{(2\pi mkT)^{3/2}} = f_{MB}(p),$

This follows from $\langle p_1^n \rangle = \int \prod_j dp_j dq_j \ p_1^n W(\mathbf{x}, \mathbf{p})$

Thermalization through eigenstates (J. Deutsch, 1991, M. Srednicki 1994, M. Rigol et. al. 2008)

Main idea: thermalization is encoded in eigenstates of the Hamiltonian. Dynamics is just dephasing between the eigenstates.

Prepare a quantum system in some state, characterized by the density matrix ρ_0 and let it evolve with the Hamiltonian *H*.

$$\rho(t) = \sum_{n,m} \rho_{nm}^0 |n(t)\rangle \langle m(t)| = \rho_{nm}^0 \exp[-i(E_n - E_m)t]$$

Look into the long time limit of the expectation value static observable, O

$$\langle O(t) \rangle = \sum_{nm} O_{mn} \rho_{nm} \exp[-i(E_n - E_m)t] \rightarrow_{t \to \infty} \sum_n \rho_{nn} O_{nn}$$

In typical situations (both equilibrium and not) energy is extensive and energy fluctuations are sub-extensive (consequence of locality of the Hamiltonian). If all eigenstates within a subextensive energy shell are similar then

$$\langle O(t) \rangle \to_{t \to \infty} O_{nn} \sum_{n} \rho_{nn} = O_{nn}$$

The long time limit of an observable does not depend on the details of the initial state.



M. Rigol, V. Dunjko & M. Olshanii, Nature **452**, 854 (2008)

a, Two-dimensional lattice on which five hard-core bosons propagate in time.

b, The corresponding relaxation dynamics of the central component *n* $(k_x = 0)$ of the marginal momentum distribution, compared with the predictions of the three ensembles

Diagonal/relaxation **c**, Full momentum distribution function dynamics Microcanonical in the initial state, after relaxation, and Canonical in the different ensembles.

Fluctuations of the observables. Off-diagonal matrix elements (M. Srednicki, 1999)

Consider ultimate microcanonical ensemble, a single energy eigenstate

$$\delta O_n^2 = \langle n | O^2 | n \rangle - \langle n | O | n \rangle^2 = \sum_{m \neq n} \langle n | O | m \rangle \langle m | O | n \rangle$$

There are exponentially many terms in this sum ~ exp[S], recall that the entropy is the measure of the density of states (number of states within microscopic energy window)

Make an ansatz (M. Srednicki, 1996)

$$\langle n|O|m\rangle = \overline{O}(E)\delta_{nm} + f_O(E,\omega)\exp[-S/2]\sigma_{nm}, \quad E = \frac{E_n + E_m}{2}, \omega = E_n - E_m$$

Expect that f_o is a slow function of E (changing on extensive scales) but fast function of ω , on inverse relaxation time scale, σ is a random variable with a unit variance.

$$\delta O_n^2 = \sum_{m \neq n} O_{nm}^2 = \int d\omega \Omega(E + \omega/2) |f_O(E, \omega)|^2 \exp[-S(E)] = \int d\omega |f_O(E, \omega)|^2 \exp[\beta \omega/2]$$

The function $f_o(\omega)$ should decay faster than exponentially on intensive energy scales.

Let us look into non-equal time correlation function

$$\langle O(t)O(0)\rangle_{n,c} = \sum_{m\neq n} O_{nm}^2 \exp[i(E_n - E_m)t] = \frac{1}{2} \int d\omega |f_O(E,\omega)|^2 \exp[\beta\omega/2 - i\omega t]$$

Long (Markovian) times (small frequencies): expect exponential decay.

$$|f_0(E,\omega)|^2 \sim \exp[-\beta\omega/2] \frac{\Gamma}{\Gamma^2 + \omega^2}$$

Lorentz or Breit-Wigner distribution

Short (non-Markovian) times (large frequencies): expect Gaussian decay. Also follows from short time perturbation theory (Zeno effect).

$$|f_0(E,\omega)|^2 \sim \exp[-\tau^2 \omega^2]$$

Can recover fluctuation-dissipation relations under the same conditions (V. Zelevinsky 1995, M. Srednicki 1999, E. Khatami et al 2013)

How representative is time average? (M. Srednicki, 1999)

$$\overline{(\langle O_t \rangle - \overline{O})^2} = \frac{1}{t} \int_0^t d\tau \left(\sum_{nm} \rho_{nm} O_{mn} \exp[i(E_m - E_n)\tau] \right)^2 - \left(\sum_n \rho_{nn} O_{nn} \right)^2 \to_{t \to \infty} \sum_{n \neq m} \rho_{nm} \rho_{mn} O_{mn} O_{nm}$$

Using that

$$O_{mn} \sim \exp[-S/2], \ Tr[\rho^2] < 1 \Rightarrow (\langle O_t \rangle - \overline{O})^2 < C \exp[-S]$$

If ETH applies we see that deviations of the expectation value from the time average are exponentially small.

So the system remains exponetially close to the equilibrium state at almost all times.

Quantum chaos and Wigner-Dyson distribution

Consider a fully chaotic random NxN matrix with the Gaussian probability distribution

 $H = \{H_{ij}\}, \ P(H) \sim \exp[-N/4 \operatorname{Tr}[H^2]]$

One can show that there is a level repulsion so that the probability of the level spacing is:

Wigner-Dyson distribution for orthogonal ensembles.



Level spacing distribution in heavy nuclei

K.H. Böchhoff (Ed.), Nuclear Data for Science and Technology, Reidel, Dordrecht (1983)



Level spacing distribution in Sinai billiard

O. Bohigas, M.J. Giannoni, C. Schmit Phys. Rev. Lett., 52 (1984)



Hydrogen in a strong magnetic field D. Wintgen, H. Friedrich Phys. Rev. A, 35 (1987),



A histogram of spacings between bus arrival times in Cuernavaca (Mexico), in crosses; the solid line is the prediction from random matrix theory. (Source: Krbalek-Seba, J. Phys. A., 2000)



Spacing distribution for a billion zeroes of the Riemann zeta function, and the corresponding prediction from random matrix theory. (Source: Andrew Odlyzko, Contemp. Math. 2001)

Many-body quantum systems

Integrable (in a compliated way) bosonic(L. Santos and M. Rigol, 2010)

$$\begin{split} H_B &= \\ \sum_{i=1}^{L} \left[-t \left(b_i^{\dagger} b_{i+1} + h.c. \right) + V \left(n_i^b - \frac{1}{2} \right) \left(n_{i+1}^b - \frac{1}{2} \right) \\ - t' \left(b_i^{\dagger} b_{i+2} + h.c. \right) + V' \left(n_i^b - \frac{1}{2} \right) \left(n_{i+2}^b - \frac{1}{2} \right) \right] \end{split}$$

The onset of chaos coincides with the onset of thermalization defined through the observables.



FIG. 1: (Color online) Level spacing distribution for the Hamiltonian in Eqs. (1) with L = 15, 5 spins up, $\omega = 0$, $\epsilon_d = 0.5$, $J_{xy} = 1$, and $J_z = 0.5$ (arbitrary units); bin size = 0.1. (a) Defect on site d = 1; (b) defect on site d = 7. The dashed lines are the theoretical curves.



Interacting spin-chain with a single impurity

(A. Gubin and L. Santos, 2012)

$$H_{z} = \sum_{i=1}^{L} \omega_{i} S_{i}^{z} = \left(\sum_{i=1}^{L} \omega S_{i}^{z}\right) + \epsilon_{d} S_{d}^{z}$$
$$H_{NN} = \sum_{i=1}^{L-1} \left[J_{xy} \left(S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y}\right) + J_{z} S_{i}^{z} S_{i+1}^{z}\right]$$

Quantum ergodicity and localization in the Hilbert space

Why does ETH work? Why does the single state describe equilibrium?

Imagine the most integrable many-body system: collection of non-interacting Ising spins. The dynamics is very simple: each spin is conserved.

A typical state with a fixed magnetization is thermal. This is how we derive Gibbs distribution in statistical mechanics. We do not need non-integrability.

More sophisticated language: quantum typicality. If we take a typical many-body state of a big system (Universe) and look into a small subsystem then it will look like the Gibbs state (von Neumann 1929, Popescu et. al. 2006, Goldstein et. al. 2009)

Can we create typical states in the lab doing local perturbations? Let us flip 10 spins in the middle doing the Rabi pulse

By performing a local quench we create a very atypical state, which is not thermal, whether the system is integrable or not. In an integrable system this state will never thermalize.

More sophisticated example

Weak interaction quench in the Hubbard model (M. Moeckel and S. Kehrein, 2008)

$$\begin{split} H(B) &= \sum_{k\sigma=\uparrow,\downarrow} \epsilon_k : c_{k\sigma}^{\dagger} c_{k\sigma} : \\ &+ \sum_{p'pq'q} U_{p'pq'q}(B) : c_{p'\uparrow}^{\dagger} c_{p\uparrow} c_{q'\downarrow}^{\dagger} c_{q\downarrow} : \end{split}$$

Start from U=0. Short time dynamics is approximated by non-interacting dressed quasi-particles.



System relaxes to the atypical state with wrong quasi-particle residue.

Simpler example: take noninteracting fermions and hit with a local Hammer.

Can not possibly create new Fermi-Dirac distribution, too much fine tuning.



We do not need ergodicity, ETH, chaos to understand statistical mechanics.

We need them to understand dynamics.

There are always atypical states. These are the states, which we usually excite in experiments. ETH says that there are no atypical stationary states (eigenstates of the Hamiltonian)

Fluctuations of observable between eigenstates (M. Rigol et. al. 2008)



Nonintegrable

Integrable

All eigenstates in a non-integrable system are indeed typical.

Physical reason: each eigenstate consists of (exponentially) many eigenstates of other local Hamiltonians, e.g. of a noninteracting Hamiltonian.

Corollary: each energy eigenstate contains (exponentially) many noninteracting states. Each non-interacting state is projected to many eigenstates (by a local perturbation)

C. Neuenhahn, F. Marquardt , 2010; G. Biroli, C. Kollath, A. Laeuchli, 2009



Nearly integrable (non-ergodic) Noninterable (ergodic)

Quantum ergodicity is a delocalization of the initial state in the Hilbert space The picture is thus similar to classical. Phase space \rightarrow Hilbert space.

While each eigenstate is enough to thermalize we always populate many!

Measures of (de)localization in the Hilbert space

(L. Santos and M. Rigol, 2010)



FIG. 13: (Color online.) Inverse participation ratio in the mean field basis vs energy for bosons, L = 24, k = 2, and t' = V'. The GOE result IPR_{GOE} ~ D/3 is beyond the chosen scale.



FIG. 6: (Color online.) Shannon entropy in the mean field basis vs effective temperature for bosons, L = 24, k = 2, and t' = V'. The dashed line gives the GOE averaged value $S_{GOE} \sim \ln(0.48D)$.

Nonintegrable systems are more delocalized

More direct measure of delocalization – diagonal entropy (von Neumann's entropy of the diagonal ensemble)

$$S_d = -\sum_n \rho_{nn} \log(\rho_{nn})$$

Hard core bosons



FIG. 2: (Color online) Normalized distribution function of energy. Bosonic system, L = 24, T = 3.0 and the values of t' = V' are indicated. Top panels: quench from $t_{\text{ini}} = 0.5$, $V_{\text{ini}} = 2.0$; bottom panels: quench from $t_{\text{ini}} = 2.0$, $V_{\text{ini}} = 0.5$. Solid smooth line: best Gaussian fit $(\sqrt{2\pi}a)^{-1}e^{-(E-b)^2/(2a^2)}$ for parameters a and b; dashed line: $(\sqrt{2\pi}\delta E)^{-1}e^{-(E-E_{\text{ini}})^2/(2\delta E^2)}$.

L. Santos, A. P. and M. Rigol (2012)



Nonintegrable systems: delocalization in the energy space after the quench.

Each eigenstate is thermal

Always densely occupy eigenstates

Either condition is sufficient for thermalization.

How robust are the eigenstates against small perturbation?

В

Consider two setups preparing the system in the energy eigenstate

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Setup I: trace out few spins (do not touch them but no access to them)

A

Setup II: suddenly cutoff the link

A

In both cases deal with the same reduced density matrix (right after the quench in case II)

$$\langle n|O_A|n\rangle = \sum_{n_A, n_B, m_A, m_B} \langle n|n_A, n_B \rangle \langle n_A, n_B|O_A|m_A, m_B \rangle \langle m_A, m_B|n\rangle$$

$$= \sum_{n_A, m_A, n_B} \langle n|n_A, n_B \rangle \langle n_A|O|m_A \rangle \langle m_A, n_B|n\rangle = \operatorname{Tr}[\rho_A, O_A]$$

$$\rho_A = \operatorname{Tr}_B \rho$$

$$= \sum_{n_B, n_A, m_A} |n_A \rangle \langle n_A, n_B|n \rangle \langle m_A, n_B \rangle \langle m_A, n_B|n\rangle$$

$$Quench: the reduced density matrix evolves with the Hamiltonian H_A.$$

Define two relevant entropies (both are conserved in time after quench):

$$S_{A,vn} = -\text{Tr}[\rho_A \log(\rho_A)] \qquad \qquad S_{A,d} = -\sum \rho_{A,nn} \log(\rho_{A,nn})$$

Entanglement (von Neumann's entropy)

Diagonal (measure of delocalization), entropy of time averaged density matrix after quench

n





B>>A, trace out most of the system. Eigenstate is a typical state so expect that $\rho_A \sim \exp[-\beta H_A] \Rightarrow S_{A,vn} \approx S_{A,d} \approx S_{eq}$

B<<A, trace out few spins, perhaps only one (say out of 10²²). What happens? $S_{A,vn}=S_{B,vn}\sim N_B$

Remove one spin. Barely excite the system. Density matrix is almost diagonal (stationary)?

 $S_{A,d} \gg A, vn$? Wrong (in nonintegrable case)

Use ETH: Perform quench, deposit non extensive energy δE . Occupy all states in this energy shell.

$$S_{A,d} \approx \log(\Omega(E_A)\delta E) \approx S_{A,eq}$$

ETH tells us that even cutting one degree of freedom is enough to recreate equilibrium (microcanonical) density matrix.



Check: hard-core bosons in 1D

(with L. Santos and M. Rigol, 2012)



Corollary: entropy – energy uncertainty. There is no temperature in a single eigenstate. In order to measure temperature – need to couple to thermometer, e.g. a calibrated two level system. This always mixes exponentially many states by ETH.

Otherwise would have contradictions with fundamental relation: dE = TdS - FdX

Quantum ergodicity and localization in real space

Non-interacting electrons in a disordered potential. Anderson localization

g – number of conducting channels (number of energy levels within the Thouless energy shell, which behave according to the Wigner-Dyson statistics $E_D = \hbar/\tau$, $\tau = L^2/D$, $\delta N \sim L^d E^d$



dg



Gang of four scaling theory (P.W. Anderson et. al., 1959)

Figure 4. According to scaling theory, Anderson localization is a critical phenomenon, at least in three dimensions. The scaling function $\beta(g)$ describes how—or more precisely, with what exponent—the average conductance g grows with system size L. For a normal ohmic conductor in D dimensions, the conductance varies as L^{D-2} ; consequently, $\beta(g) \sim D - 2$ for large g. Thus the beta function is positive for three-dimensional conductors, zero for two-dimensional conductors, and negative in one dimension. In the localized regime, g decays exponentially with sample size so that $\beta(g)$ is negative. In three dimensions, that leads to a critical point at which β vanishes for some special value for g associated with the mobility edge. Lower-dimension systems do not undergo a genuine phase transition because the conductance always decreases with system size. A small 2D conductor, for instance, will look like a metal in the quasi-extended regime, but all its states are eventually localized if the medium is large enough.

A. Lagendijk, B. van Tiggelen, and D. S. Wiersma (2009)

In 3D and above there is a transition between localized and delocalized states. Hi energy states are typically localized. Localization means no ergodicity.

At finite temperature the system is always delocalized (ergodic).

Interacting were thought to be always ergodic Insulator coupled to phonons. All states are localized



At finite T can always hop and get the missing energy from the phonons. In our language many-body levels are ergodic (satisfy ETH).

Pure two-body short range interactions between electrons. Altshuller et. al. (1997), Basko, Aleiner, Altshuller (2005)



Anderson localization in Ndimensional hypercube at small interactions.

Many-body localization with the activation barrier scaling as the system size.

1D disordered spin chains at infinite temperature

(A. Pal, V. Oganesyan, D. Huse, 2007+)



Strong numerical indications of many-body localization as a localization in the Hilbert space. No analytic theory yet near the transition. Ergodicity -> ETH.

What happens when the systems are not ergodic.





Chaotic system: rapid (exponential) relaxation to microcanonical ensemble Integrable system: relax to constraint equilibrium: $P(x,p) \rightarrow \delta(p-p_0)\delta(\theta-\theta_0)$

Quantum language: in both cases relax to the diagonal ensemble

$$\rho_{mn} \to \rho_{nn} \delta_{mn}$$
 $\rho_{nn} = \frac{1}{Z} \exp\left[-\sum_{n} \beta_n I_n\right]$

Integrable systems: generalized Gibbs ensemble (Jaynes 1957, Rigol 2007, J. Cardy, F. Essler, P. Calabrese, J.-S. Caux, E. Yuzbashyan ...)

F. Essler, talk at KITP, 2012

Let Im be local (in space) integrals of motion [Im, In]=[Im, H(h)]=0

Define GGE density matrix by:

$$\rho_{gG}=exp(-\Sigma \lambda_m I_m)/Z_{gG}$$

 $\lambda_m \, \mbox{fixed}$ by

 $\text{tr}[\rho_{gG} I_m] = \left< \psi(0) \right| I_m \left| \psi(0) \right>$

Reduced density matrix of B:

 $\rho_{gG,B}$ =tr_A ρ_{gG}

Prove for a particular (transverse field Ising) model

ρ_B(∞)= ρ_{gG,B}

Works both for equal and non-equal time correlation functions. Need only integrals of motion, which "fit" to the subsystem

$$I_n = \sum_j I_n(j, j+1, \dots, j+\ell_n)$$

If we can not measure $I_n - have too many fitting parameters. <math>\bullet$ \bullet \bullet \bullet

What if integrability is slightly broken?

More familiar example of GGE: Kolmogorov turbulence



A. N. Kolmogorov



Images from Wikipedia

Pump energy at long wavelength. Dissipate at short wavelength. Non-equilibrium steady state Scaling solution of the Navier Stokes equations $\partial v + (v \nabla) v = - \nabla p + v \Delta v \quad E_k \propto C \nu^{2/3} k^{-5/3}$

 $\nabla \mathbf{v} = \mathbf{0}$ $E(k) \simeq P^{2/3} k^{-5/3} \rho^{1/3}$

This energy can be thought of as the mode dependent temperature. A particular type of GGE.

Zakharov, L'vov, Fal'kovich: derived this solution from the kinetic equations

Victor Gurarie (1994): Scaling solution from as the GGE

Weakly interacting (weakly nonintegrable) Bose gas

$$H = \sum_{p} \omega_{p} a_{p}^{\dagger} a_{p} + \sum_{p_{1}p_{2}p_{3}p_{4}} \lambda_{p_{1}p_{2}p_{3}p_{4}} a_{p_{1}}^{\dagger} a_{p_{2}}^{\dagger} a_{p_{3}} a_{p_{4}}$$

Look for a stationary probability distribution

$$\rho = \exp[-F], \ F = \sum_{p} f_{p} a_{p}^{\dagger} a_{p} + \lambda F^{(1)} + \lambda^{2} F^{(2)} + \dots, \ F^{(1)} = \sum_{p_{1}, p_{2}, p_{3}, p_{4}} \Lambda_{p_{1}, p_{2}, p_{3}, p_{4}} a_{p_{1}}^{\dagger} a_{p_{2}}^{\dagger} a_{p_{3}} a_{p_{4}} a_{p$$

Find F⁽¹⁾, F⁽²⁾ perturbatively. Problem: perturbation theory is very singular because of small denominators

$$\Lambda_{p_1p_2p_3p_4} = \frac{f_{p_1} + f_{p_2} - f_{p_3} - f_{p_4}}{\omega_{p_1} + \omega_{p_2} - \omega_{p_3} - \omega_{p_4} - i\epsilon} \lambda_{p_1p_2p_3p_4}$$

Possible nonsingular solutions:

$$f_p = A\omega_p + B \Rightarrow \langle E_p \rangle = \frac{\omega_p}{A\omega_p + B}$$

Thermal equilibrium with chemical potentials.

With additional power-law constraint – additional Kolmogorov solution $\omega_p = p^{\alpha}, \quad \lambda_{\vec{p}_1 \vec{p}_2 \vec{p}_3 \vec{p}_4} = \lambda_0 (p_1 p_2 p_3 p_4)^{\frac{\beta}{4}} U(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4)$

Weak interactions select possible GGE!

Summary of part I

- Ergodic quantum systems satisfy ETH: each eigenstate of the Hamiltonian (each stationary state) is equivalent to the micro-canonical ensemble.
- Ergodicity can be understood as a process of delocalization in the eigenstate basis. Delocalized states are always ergodic (irrespective of integrability).
- Direct analogy between (many-body) Anderson localization and ergodicity.
- Many-body states are very fragile: tiny perturbation mixes exponentially many eigenstates. Ensembles are stable.
- Integrable systems relax to asymptotic states which can be described by the GGE (generalized Gibbs ensembles) composed of local integrals of motion.
- Weak interaction can select possible classes of stable GGE state, which ultimately thermalize (prethermalization scenario). But still many open problems remain.

Part II. Applications of ETH to thermodynamics



FIGURE 1–3 Heat flows in the direction of decreasing temperature.



Thermodynamics (unlike statistical physics) typically deals with non-equilibrium processes, which at each stage can be approximated as approximate local equilibrium

Setups considered



1. Prepare system A in a stationary state (diagonal ensemble)

 $\rho_{nm}(0) = \rho_n^0 \delta_{nm}$

- 2. Apply some time-dependent perturbation (quench)
- Let the system relax to a new steady state

1. Prepare systems A and B in stationary states

- 2. Connect them by a weak coupling (quench) for a period of time .
- 3. Disconnect and let the systems relax to the steady states. (Markov process).

Fundamental thermodynamic relation for open and closed systems

Start from a stationary state. Consider some dynamical process

$$E = \sum_{n} E_{n} \rho_{nn} \Rightarrow \Delta E = \sum_{n} E_{n} \Delta \rho_{nn} + \Delta E_{n} \rho_{nn}$$

$$S_{d} = -\sum_{n} \rho_{nn} \log(\rho_{nn}) \Rightarrow \Delta S_{d} = -\sum_{n} \Delta \rho_{nn} \log(\rho_{nn}) + \Delta \rho_{nn}$$
Assume initial Gibbs Distribution

$$\rho_{nn} = \frac{1}{Z} \exp[-\beta E_n] \Rightarrow \log(\rho_{nn}) = -\beta E_n - \log(Z)$$

Combine together

$$\Delta E = \frac{\partial E}{\partial \lambda} \Big|_{S_d} \Delta \lambda + \frac{1}{T} \Delta S_d \iff \Delta E = T \Delta S - \mathcal{F}_\lambda \Delta \lambda, \ \mathcal{F}_\lambda = -\frac{\partial E}{\partial \lambda} \Big|_S$$

Recover fundamental relation with the only assumption of Gibbs distribution

What if we do not have the Gibbs distribution?



Imagine we are umping some energy into an isolated system. Does fundamental relation still apply?

$$S_d = -\sum_n \rho_{nn} \log(\rho_{nn}) = -\int dE \,\Omega(E)\rho(E) \log(\rho(E))$$

$$\rho(E)\Omega(E) = W(E) - \text{Energy distribution}$$

 $\log(\Omega(E)) = S_m - \text{microcanonical entropy}$

$$S_d(\epsilon) = \int d\epsilon W(\epsilon) S_{micro}(\epsilon) - \int d\epsilon W(\epsilon) \ln(W(\epsilon))$$

Entropy is a unique function of energy (in the thermodynamic limit) if the Hamiltonian is local and density matrix is not (exponentially) sparse. I.e. if the system is not localized in the Hilbert space

Gaussian approximation for W(E), applies even for small systems:

$$S(E) \approx \ln(\sqrt{2\pi}\delta E\Omega(E)) + \frac{1}{2}\left(1 - \frac{\delta E^2}{\delta E_c^2}\right) \delta E_c^2 = T^2 C_v = -\partial_\beta E_c(T)$$

In delocalized regime, which is always the case if ETH applies

$$S_d(E) \approx -\int dE \ W(E) S_m(E) \approx S_m(\overline{E})$$

Recover fundamental relation + sub-extensive corrections from ETH Integrable systems: sparse distributions

 $dE \, W(E) \log(W(E))$ Gives extensive contribution comparable to S_m

Can we use GGE density of states?

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Integrable Hamiltonian (with L. Santos and M. Rigol) Filling 1/5, period P=5, quench A

Solid line S_d

Dashed lines S_m, S_{GGE}

GGE is not constraining enough

Isolated systems. Unitary dynamics. Initial stationary state.

$$\rho_{nm}(0) = \rho_n^0 \delta_{nm}$$

Unitarity of the evolution:

$$\rho_{mm} = \sum_{n} U_{mn} \rho_{n}^{0} U_{nm}^{-1} = \rho_{m}^{0} + \sum_{n} p_{n \to m} (\rho_{n}^{0} - \rho_{m}^{0})$$
$$U_{nm}^{-1} = U_{mn}^{*}; \quad p_{n \to m} = |U_{mn}|^{2} - \text{doubly stochastic matrix}$$

Transition rates $p_{m \rightarrow n}$ are non-negative numbers satisfying sum rule

$$\sum_{n} p_{n \to m}(t) = \sum_{n} p_{m \to n}(t) = 1$$

In general there is no detailed balance even for cyclic processes (but within the Fremi-Golden rule or for symmetric protocols there is).

The only stable distribution under these transformations is the infinite temperature maximum entropy state $\rho_n^0 = \mathrm{const}(n)$

Second law of thermodynamics



Start from a stationary state with monotonically decreasing probability (e.g. Gibbs distribution). Energy can only increase or stay constant, see picture Thirring, Quantum Mathematical Physics, 1999, A. E. Allahverdyan, Th. M. Nieuwenhuizen, (2002).

Likewise (diagonal) entropy satisfies the second law:

$$S_d = -\sum_n p_n \log(p_n)$$

For any initial stationary state

$$S_d(t) \ge S_n(t) = S_n(0) = S_d(0),$$

$$S_{d1}(t) + S_{d2}(t) \ge S_{d1}(0) + S_{d2}(0)$$

Also immediately follows from the sum rule.

Follows from Araki-Lieb subbaditivity (thanks to C. Gogolin)

Fluctuation theorems (Bochkov, Kuzovlev, Jarzynski, Crooks)



Initial stationary state + time reversability:

 $p_{mn} = p_{nm}$ Microscopic probabilities are the same Eigenstate thermalization hypothesis: microscopic probabilities are smooth (independent on m,n)

$$P_E(w) = \sum_m p_{mn} \delta(E_m - E_n - w) = p_{mn} \Omega(E + w)$$
$$\tilde{P}_{E+w}(-w) = p_{nm} \Omega(E)$$

$$P_E(w)\Omega(E) = \tilde{P}_{E+w}(-w)\Omega(E+w)$$

Bochkov, Kuzivlev, 1979, Crooks 1998

robability to do work
$$w$$
 $P(w) = \int dE \Omega(E) \rho(E) P_E(w)$

If we assume the Gibbs distribution

P

$$P(w) = \frac{1}{Z_i} \int dE \Omega(E) \exp[-\beta E] P_E(w) =$$
Crooks equality, C. Crooks, 1998,
$$\frac{1}{Z_i} \int dE \Omega(E+w) \exp[-\beta(E+w-w)\tilde{P}_{E+w}(-w)] = \frac{Z_f}{Z_i} \exp[\beta w]\tilde{P}(-w)$$

 $Z = \exp[-\beta F] \Rightarrow \langle \exp[-\beta w] \rangle = \exp[-\beta \Delta F]$

Jarzynski equality, 1997

Jarzynski equality heavily relies on having Gibbs distribution, no equivalence of ensembles. Probe large deviations

However, if interested in cumulants can use arbitrary ensembles. Assume for simplicity a cyclic process $Z_f = Z_i$.

 $P_E(w)\Omega(E) = \tilde{P}_{E+w}(-w)\Omega(E+w) \approx \tilde{P}_{E+w}(-w)\Omega(E)\exp[\beta w]$

Now can integrate with an arbitrary distribution $\rho(E)$.

 $\langle \exp[-eta w]
angle = 1$ Require that high cumulants are small, narrow distribution

$$-\beta \langle w \rangle + \frac{\beta^2}{2} \delta w^2 = 0 \implies \langle w \rangle = \frac{\beta}{2} \delta w^2 \ge 0$$
 Second law of thermodynamics. Einstein-like drift diffusion relations.

Fokker-Planck (diffusion) equation:

$$W(E, t + \delta t) = W(E, t) + \int dw [W(E - w)P_{E-w}(w) - W(E)P_{E}(-w)]$$

Exercise: expand to the second order in w. Beat subtleties $\partial_t W(E,t) = -\partial_E(AW) + \frac{1}{2}\partial_{EE}^2(BW)$ $\langle w \rangle = A(E)$ - heating rate (drift), $B(E) = \delta w^2$ - diffusion Hint, at small dt $\langle w \rangle$, $\delta w^2 \propto dt$, $\langle w^2 \rangle = \delta w^2 + \langle w \rangle^2 \approx \delta w^2$ It is sufficient to know only the heating rate to find the energy distribution! Simple way to derive the drift diffusion relation

$$\partial_t W(E,t) = -\partial_E(AW) + \frac{1}{2}\partial_{EE}^2(BW)$$

For unitary dynamics with arbitrary time dependent Hamiltonian the attractor is $\rho_{nn} \equiv \rho(E) = \text{const} \Rightarrow W(E) = \Omega(E)\rho(E) = C\Omega(E) = C\exp[S(E)]$

Plug back to the FP equation

$$-A(E) \exp[S(E)] + \frac{1}{2} \partial_E(B(E) \exp[S(E)]) = 0$$

The last term is usually suppressed in large systems. It Solution $2A(E) = \beta B + \partial_E B$ can be also recovered from the Crooks relatiom

 $A(T_{1})$

Example (particle in a deforming cavity C. Jarzynski, 1992)





Exercise: compute $r_1/2$

 $W(E) \propto \exp[-f]$

$$A(E) = c E^{3/2}$$
$$B(E) = \frac{4c}{(d+1)} E^{3/2}$$
$$\beta(E) = (d-2)/(2E)$$

Equivalent to the Lorenz gas solvable by kinetic equations: L. D'Alessio and P. Krapivsky.

Example: universal energy fluctuations for driven thermally isolated systems (microvawe heating) (G. Bunin, L. D'Alessio, Y. Kafri, A. P., 2011)

Conventional heating



Gibbs distribution

fluctuation-dissipation relations

universal width: $\delta E^2 = T^2 C_v$

Nonadiabatic (microwave) heating



Universal non-Gibbs distribution

Dynamical phase transitions as a function of the heating protocol (to the superheated regime).

Can prepare arbitrarily narrow distributions.

Open systems (A can be a single spin or macroscopic)



Time reversal symmetry implies Crooks equality: $p_A(n \to m)p_B(m' \to n') = p_A(m \to n)p_B(n' \to m')$

Sum over eigenstates of B. Use ETH for the system B.

$$\frac{p_A(n \to m)}{p_A(m \to n)} = \frac{\Omega_B(E_B - \Delta E)}{\Omega_B(E_B)} \approx \exp[-\beta_B \Delta E]$$

Detailed balance follows from the Crooks equality for the two systems and ETH for the system B.

Open systems (G. Bunin and Y. Kafri, 2011)



Time reversal symmetry implies Crooks equality:

$$p_A(n \to m)p_B(m' \to n') = p_A(m \to n)p_B(n' \to m')$$

Hence

 $P_{E_A,E_B}(-w,w)\Omega_A(E_A)\Omega_B(E_B) = P_{E_A-w,E_B+w}(w,-w)\Omega_A(E_A-w)\Omega_B(E_B+w)$

Jarzynski type relation for an open system (require narrow distributions)

$$\langle \exp[(\beta_A - \beta_B)w] \rangle = 1 \Rightarrow \langle w \rangle \approx \frac{\Delta\beta}{2} \delta w^2, \ \Delta\beta = \beta_B - \beta_A$$

Heat flows from hot to cold because of ETH

Example: two coupled black bodies at different temperatures (with G. Bunin, Y. Kafri, V. Leconte, D. Podolsky)



$$\begin{split} H &= \sum_{\mathbf{k},\alpha} \hbar c k a_{\mathbf{k},\alpha}^{\dagger} a_{\mathbf{k},\alpha} + \sum_{\mathbf{k},\alpha} \hbar c k b_{\mathbf{k},\alpha}^{\dagger} b_{\mathbf{k},\alpha} + H_{\text{int}} \\ H_{\text{int}} &= \lambda \hbar c \sum_{\alpha=1}^{2} \int dx \, dy \, a_{(x,y,0),\alpha}^{\dagger} b_{(x,y,0),\alpha} + h.c. \\ \text{Recoloring operator,} \end{split}$$

 λ – transmission amplitude

$$H_{int} = \frac{\lambda \hbar c}{i} \sum_{\alpha=1}^{2} \int dx \, dy \, a^{\dagger}_{(x,y,0),\alpha} \partial_{z} b_{(x,y,z),\alpha} \Big|_{z=0} + h.c.$$

Different gauge b->b $e^{i\pi/2}$ – flux operator

Use Fermi golden rule (exercise)

 $W_{a\to b} = \frac{|\lambda|^2 \hbar c^2 L^2}{4\pi^2} \int_0^\infty dk \, k^3 n_k^{(a)} (1 + n_k^{(b)}) \qquad A_{ab} = W_{a\to b} - W_{b\to a} = |\lambda|^2 \sigma (T_a^4 - T_b^4)$ $B_{ab} = \frac{|\lambda|^2 \hbar^2 c^3 L^2}{(2\pi)^2} \int dk \, k^4 \left[n_k^{(a)} (1 + n_k^{(b)}) + n_k^{(b)} (1 + n_k^{(a)}) \right] \qquad B_{ab} = 8|\lambda|^2 \sigma \left[(T_a T_b)^{5/2} + \frac{45}{\pi^4} \left(T_a^{5/2} - T_b^{5/2} \right)^2 \right]$ (approximate expression)

A-B relation is satisfied when $\beta_A \approx \beta_B$ otherwise high third order cumulant

(Non-equilibrium) Onsager relations. Two or more conserved quantities.

in progress with L. D'Alessio, G. Bunin, Y. Kafri, also P. Gaspard and D. Andrieux (2011)

$$\begin{array}{c} \beta_A, \mu_A \\ \hline A & \blacksquare \\ w, \delta n \end{array} \begin{array}{c} \beta_B, \mu_B \\ \hline B \\ \hline B \end{array} \end{array}$$

Time reversibility and ETH imply the Crooks relation

 $P(w,\delta n)\exp[-\beta_B w - \lambda_B \delta n] = P(-w,-\delta n)\exp[-\beta_A w - \lambda_A \delta n], \ \lambda = \partial S/\partial N = -\beta\mu$

Two independent Jarzynski relations: $\langle \exp[-\Delta\beta w] \rangle = \langle \exp[-\Delta\lambda\delta n] \rangle,$ $\Delta\beta = \beta_B - \beta_A, \ \Delta\lambda = \lambda_B - \lambda_A \ \langle \exp[-\Delta\beta w - \Delta\lambda\delta n \rangle = 1$

Onsager relations (cumulant expansion)

$$\left(\begin{array}{c} w\\\delta n\end{array}\right) = \left(\begin{array}{cc} \delta w^2 & \langle w\delta n\rangle_c\\ \langle w\delta n\rangle_c & \delta n^2\end{array}\right) \left(\begin{array}{c} \Delta\beta\\ \Delta\lambda\end{array}\right)$$

This is not a gradient expansion. E.g. temperatures can but need not be close! Two currents and one current fluctuation set the other fluctuation and the crosscorrelation. Possible applications from spintronics to black hole radiation.

Energy localization transition in periodically driven systems (with L. D'Alessio)

Instead of a single quench consider a periodic sequence of pulses:



Fermi-Ulam problem (prototype or the Fermi acceleration problem).



oscillating wall (G. M. Zaslavskii and B. V. Chirikov, 1964 M. A. Liberman and J. Lichenberg 1972)



Fig. 7.14. Poincaré phase space section for a harmonic wall oscillation with M = 20. Iterations of several selected trajectories.

Small energies: chaos and diffusion. Large energies – periodic motion. Energy stays localized within the chaotic region.

Stochastic motion – infinite acceleration.

Kicked rotor (realization of standard Chirikov map)

$$H(p, x, t) = \frac{p^2}{2} + K\cos(x)\sum \delta(t - n)$$

Transition from regular (localized) to chaotic (delocalized) motion as K increases. Chirikov, 1971



Delocalization transition at $K_c \cong 1.2$ (B. Chirikov (1979)).

Quantum systems: (dynamical) localization due to interference even in the chaotic regime (F. Izrailev, B. Chirikov, ... 1979).

What about periodically driven ergodic systems in thermodynamic limit?

New non-equilibrium phases and phase transitions

Example: Kapitza pendulum (emerged from particle accelerators, 1951)



Stable inverted equilibrium for $\frac{a}{l} \frac{\gamma}{\omega_0} > \sqrt{2}$ Stability: experimentally proven by Kapitsa using Singer sewing machine and by Arnold using razor.

Theoretically proven by Arnold using KAM theorem



Further experimental progress

Light induced Superconductivity in a Stripe-ordered Cuprate

D. Fausti, et all, Science 331, 189 (2011)



Image taken from A. Cavalleri web page

Exciton-Polariton condensates in drivendissipiative system



J. Kasprzak et. al, Nature, 443, 409 (2006)

Interesting unpublished results from R. Averitt group in VO_2 driven by THz pump.

Periodic drive: wave function (density matrix) after n-periods $|\psi(nT)\rangle = [U(T)]^n |\psi_0\rangle, \quad U(T) = \exp[-iH_2T_2] \exp[-iH_1T_1] = \exp[-iH_FT]$ $|\psi(nT)\rangle = \exp[-iH_F nT]|\psi_0\rangle$ a) H(t) H_1 b) H(t) T_1 T_1 T_1 H_{eff} T_0 T_0 H_0 H_0 Time evolution is like a single quench to the Floquet Hamiltonian Ho $H_F = H_0 + V, V = H_F - H_0.$ If V is small and local expect that the energy $\langle H_0 \rangle$ is localized.

Magnus expansion:

$$H_F = \frac{i}{T} \log[\exp[-iH_1T_1] \exp[-iH_2T_2]] = \frac{1}{T} \int_0^T dt H(t) - \frac{i}{2T} \int_0^T dt_1 \int_0^T dt_2 \left[H(t_1), H(t_2)\right] + \dots$$

- Each term in the expansion is extensive and local (like in high temperature expansion)
- Higher order terms are suppressed by the period T but become more and more non-local.
- Competition between suppression of higher order term and their non-locality similar to many-body localization.
- The expansion is well defined classically if we change commutators to the Poisson brackets.

Theory progress: no general framework yet but a good progress Magnus (short-period) expansion for the Kapitza pendulum L. D'Alessio and A.P. 2013 (original explanation, Kapitza 1951)

 $\hat{H}(t) = \frac{1}{2m}\hat{p}_{\theta}^{2} + f(t)\cos\hat{\theta} \qquad f(t) = -m\left(\omega_{0}^{2} + \frac{a}{l}\gamma^{2}\cos\left(\gamma t\right)\right)$ $H_{eff} = \frac{i}{T}\log[\exp[-iH_{1}T_{1}]\exp[-iH_{2}T_{2}]] = \frac{1}{T}\int_{0}^{T}dtH(t) - \frac{i}{2T}\int_{0}^{T}dt_{1}\int_{0}^{T}dt_{2}\left[H(t_{1}), H(t_{2})\right] + \dots$

$$\begin{aligned} \hat{H}_{eff}^{(1)} &= \frac{1}{T} \int_{0}^{T} dt \hat{H}(t), \quad \hat{H}_{eff}^{(2)} &= \frac{1}{2T(i\hbar)} \int \int_{0 < t_{2} < t_{1} < T} dt_{1} dt_{2} [\hat{H}(t_{1}), \hat{H}(t_{2})] \\ \hat{H}_{eff}^{(3)} &= \frac{1}{6T(i\hbar)^{2}} \int \int \int \left(\left[\hat{H}(t_{1}); \left[\hat{H}(t_{2}); \hat{H}(t_{3}) \right] \right] + \left[\hat{H}(t_{3}); \left[\hat{H}(t_{2}); \hat{H}(t_{1}) \right] \right] \right) \\ \hat{H}_{eff}^{(1)} &= \frac{1}{2m} \hat{p}_{\theta}^{2} - m\omega_{0}^{2} \cos \hat{\theta} \quad H_{eff}^{(2)} &= 0 \quad H_{eff}^{(3)} \approx m \left(\frac{a\gamma}{2l} \right)^{2} \sin^{2}(\hat{\theta}) \end{aligned}$$

Other terms are down by powers of γ at fixed $a\gamma/l$. Stable upper equilibrium for $a\gamma/l > \sqrt{2}\omega_0$.

Emergent steady state is an equilibrium for effective and nontrivial Hamiltonian.

Thermalization with an undriven bath? Generality?

Specific model: classical or quantum spin chain

$$H = -h\sum_{j} s_{j}^{z} - J\left[g\sum_{j} s_{j}^{z} s_{j+1}^{z} + \sum_{j} (s_{j}^{+} s_{j+1}^{-} + s_{j}^{-} s_{j+1}^{+})\right]$$



Singularity (phase transition?) at $hT_0 = \pi$

Quantum spin chain: energy in the infinite time limit



Two different regimes. Is it a crossover or a transition?

Quantum spin chain (comparison with Magnus expansion)

Energy

Entropy



Clear evidence for the phase transition as a function of the driving period.

Exact-Heff(3)

Very similar behavior in a classical chain.

Temporal simulations of a quantum spin chain.

Exact Time Evolution, NS=16



tion for a harmonic wall oscillation with M = 20. Iterations of several selected trajectories.

Entropy (log of number if occupied states)

Exact Time Evolution, NS=16



Potential implications for driven dissipative systems

Diagonal Entropy divided Smax=Log(N)



More common heat engines: only one reservoir like atmosphere.

Ergodic and non-ergodic single reservoir engines



Ergodic engine

Non-ergodic engine

What does second law tell us about maximum efficiency?

Application to heat engines (with P. Mehta). Consider cyclic process. Small perturbation: dE = TdS

Large perturbations. Can write inequalities



The second inequality implies that the free energy can only decrease during the relaxation; the first inequality is less known.

Extension of the fundamental relation to arbitrary processes. Relative entropy (Kullback-Leibler Divergence).



Main results (also Deffner, Lutz, 2010). Proofs are straightforward calculus. $\Delta Q^{I} = T\Delta S^{I} + TS_{r}(q||p^{(2)}) - TS_{r}(p^{(1)}||p^{(2)}), \quad S_{r}(q||p) = \sum_{n} q_{n} \log(q_{n}/p_{n})$ $\Delta Q^{II} = T\Delta S^{II} - TS_{r}(q||p^{(2)}), \quad \Delta Q^{II} = -T\Delta S_{B} \Rightarrow S_{r}(q||p^{(2)}) = \Delta S_{A} + \Delta S_{B}$

All inequalities follow from non-negativity of the relative entropy.

Ergodic engines.

Assume that the energy is first deposited without change of external couplings. $\lambda^{(1)}=\lambda^{(2)},\ p_n^{(1)}=p_n^{(2)}$



Magnetic gas engine.



$\Delta Q = 2BRN(p_{\uparrow} - p_{\downarrow}) = 2BRN \tanh[\beta B]$

Ergodic engine: allow to thermalize with kinetic degrees of freedom and then push the piston.

Non-ergodic engine: for inverted spin population (R>1/2) first perform the work on B by rotating around x-axis $q_{\uparrow} \leftrightarrow q_{\downarrow}$ and then use the residual energy to push the piston.



0.2

0.0

Ergodic engine: allow to thermalize with kinetic degrees of freedom and then push the piston.

Non-ergodic engine: for inverted spin population (R>1/2) use macroscopic magnetic energy to extract work

$$\eta_{mne} = \frac{TN \left(q_{\uparrow} \log(q_{\uparrow}/p_{\uparrow}) + q_{\downarrow} \log(q_{\downarrow}/p_{\downarrow})\right)}{\Delta Q},$$

0.4

0.6

0.8

1.0

Can beat maximum equilibrium efficiency by using non-ergodic setup.

 $\eta_{mne} = 1$ if $R = 1 (q_{\uparrow} = p_{\downarrow})$

Possible applications in small systems?