Quantum Thermalization and Localization

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These notes provide a skeleton (including hyperlinks to references) for a 3 hour workshop lecture at Busan, Korea (November 2015). The PDF file can be downloaded from my homepage (Google "Doron Cohen" and then search the page for "Korea").

[1] Outline

Quantum chaos: RMT and ETH.
Equilibration (getting a quasi steady-state).
Ergodization (isolated subsystem), fluctuations.
Thermalization (coupled subsystems), the GGE.

Weak quantum chaos; Memory of initial state?
Classical evolution: KAM, Chirikov, standard map.
Arnold-web, Arnold diffusion, stochastic pump model.

Prototype model: BHH (quantum) DNLS (classical)
Stat-Mech description: Fokker-Plank.
Thermalization of long DNLS chains.

Quantum Localization; breaktime concept; Anderson criterion.
Examples: Dynamical localization; Quantum metastability.
Disorder and MBL - quantum phase transition at finite temperature?

[2] Quantum Chaos, RMT, and ETH

RMT conjecture [Wigner, Bohigas]: Originally refers to strongly interacting many-body systems (nuclear physics context). Then same framework has been extended to chaotic systems (few degrees of freedoms, e.g. billiards).

Periodic orbits theory: The smoothed density of states can be calculated from phase-space volume. The fluctuations can be obtained from the "Gutzwiller trace formula", which is a sum over (unstable) periodic orbits.

Berry's conjecture: The Wigner function of a chaotic eigenstate can be approximated as a microcanonical distribution. It is implied that an eigenfunction of a chaotic billiard looks like a random superposition of plane waves. Related: Shnirelman's theorem.

Scar theory [Heller]: Inspired by the Gutzwiller trace formula, also the eigenstates can expanded as a sum of a microcanonical background plus periodic-orbit corrections ("scars").

Eigenstate thermalization hypothesis (ETH): Synonym for Berry's conjecture in the many body context. Speculated to hold under more flexible circumstances, where the "quantum chaos" assumptions do not hold.

The canonical Stat-Mech picture [Landau]: If the system (called "universe") is in (say) microcanonical state, then any weakly coupled subsystem is in a thermal (canonical) state. Accordingly 'reduced" probability functions are universal. For example one obtains the canonical distribution for the momentum distribution of a particle in a dilute gas.

Srednicki, Chaos and quantum thermalization [PRE 1994]
Rigo, Dunjko, Olshanii, Further discussion of ETH [Nature 2008]

- Regarding dilute hard sphere gas (formally like a Sinai billiard system).
- Energy eigenstate that satisfies ETH predicts a thermal distribution for the single particle momentum.
- For the (marginal) single-particle momentum-distribution scar corrections are not important.
- Starting from a non-stationary state, non-thermal features fade away at least as fast as $1/t$.

[3] The probability matrix

d [classical context] = number of possible outcomes (classical probability theory)
d [quantum context] = Hilbert space dimension (quantum measurement theory).

In order to specify a classical statistical state we need $d-1$ probabilities.

$$\langle A \rangle = \sum_r p_r A_r \tag{1}$$

In order to specify a quantum state we need d^2-1 probabilities. From these probabilities we can contrast the "probability matrix". For example: for spin 1/2 these might be the probabilities to be polarized in the x,y,z directions. By the basic postulate of quantum mechanics any expectation value can be deduced as follows:

$$\langle A \rangle = \sum_j \rho_{ji} A_{ij} = \mathrm{trace}[\rho A] \tag{2}$$

`Cohen`, Lecture notes in Quantum Mechanics [arXiv 2013] [PDF 2015]

Measure for purity - the number of states that participate in the mixture:

$$d[\rho] \equiv \frac{1}{\mathrm{trace}[\rho^2]} \tag{3}$$

Measure for the difference between two states:

$$D[\rho^1, \rho^2] \equiv \frac{1}{2}\mathrm{trace}\Big[\,\big|\rho^1 - \rho^2\big|\,\Big] \tag{4}$$

Meaning of this measure is that for any A

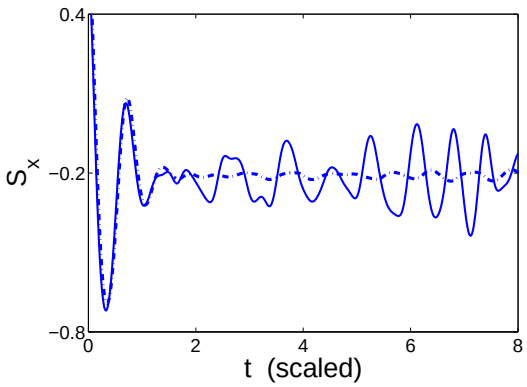
$$\Big|\,\langle A\rangle_1 - \langle A\rangle_2\,\Big| \leq \Big(\max[A] - \min[A]\Big)\; D[\rho^1, \rho^2] \tag{5}$$

Trace distance [Wikipedia]

[4] The quasi steady state

If we start with some initial state, and propagate it for a long time, then generically (for an ergodic system) we get a quasi steady-state.

Classical - no fluctuations in the expectation value $\langle A \rangle_t$
Quantum - residual fluctuations due to finite d



We denote that initial state as ρ. The evolved state is

$$\rho(t) = \sum_{n,m} \mathrm{e}^{-i(E_n - E_m)t}\; |E_n\rangle\, \rho_{n,m}\, \langle E_m| \tag{6}$$

The quasi steady-state is

$$\bar{\rho} \;=\; \sum_n |E_n\rangle\, \rho_{n,n}\, \langle E_n| \;\equiv\; \sum_n |E_n\rangle\, p_n\, \langle E_n| \tag{7}$$

The number of states that participate in the evolution is

$$d\,[\bar{\rho}] \;=\; \left[\sum_n p_n^2\right]^{-1} \tag{8}$$

Typical scenario is that we start with state $|x_0\rangle$ of basis $|x_j\rangle$ and look on the spreading.
In such scenario $p_n = P(n|x_0)$ where

$$P\,(E_n|x) \;=\; |\langle E_n|x\rangle|^2 \qquad \text{"LDOS"} \tag{9}$$

For the steady state profile we get a convolution

$$P_\infty(x|x_0) \;=\; \sum_n P\,(E_n|x)\;\; P\,(E_n|x_0) \tag{10}$$

Sometimes we want to work in the Heisenberg picture.
Accordingly we can define the time averaged observable $\bar{A}$.
Note the following trivial identities:

$$\langle A\rangle_t \;=\; \sum_{n,m} \mathrm{e}^{-i(E_n-E_m)t}\; \rho_{n,m} A_{m,n} \tag{11}$$

$$\overline{\langle A\rangle_t} \;=\; \mathrm{trace}[\bar{\rho}A] \;=\; \mathrm{trace}[\rho\bar{A}] \;=\; \mathrm{trace}[\bar{\rho}\bar{A}] \;=\; \sum_n p_n A_{n,n} \tag{12}$$

By inspection we see that non-stationary features decay as $1/t$. The argument is as follows: Consider a state that occupies an energy shell of width Δ_E that contains N_E energy levels. The time dependent phase-factors randomize all the systematic interferences except of those that originate from the strip $|E_n - E_m| < \hbar/t$. Accordingly the number of terms that contribute to the non-thermal feature is

$$N_c \;=\; \left[\frac{\hbar}{\Delta_E t}\right]\; N_E^2 \tag{13}$$

═══ [5] Fluctuations of dynamical variables

Fluctuations of the expectation value $\langle A\rangle_t$ is not the same as "fluctuations" in the sense of statistical mechanics.
The latter are the Fourier transform of the correlation function.

$$C(\tau) \;=\; \langle A(t+\tau)A(t)\rangle \tag{14}$$

$$\tilde{C}(\omega) \;=\; \mathrm{FT}\,[C(\tau)] \tag{15}$$

Quantum spectral decomposition:

$$\tilde{C}(\omega) \;=\; \sum_n p_n \sum_m |A_{nm}|^2\; 2\pi\delta(\omega - (E_n - E_m)) \tag{16}$$

From here follows the `Feinglod-Peres` relation:

$$|A_{nm}|^2 \;\approx\; \frac{1}{2\pi\varrho}\; \tilde{C}_{cl}(E_n - E_m) \tag{17}$$

Generically observables are represented by *banded* matrices.
The GOE/GUE ensembles assume zero correlation time $\rightsquigarrow$ infinite bandwidth. We deduce the following practical

estimates

$$\tau_{cl} \;=\; \text{classical correlation time that characterizes } C(\tau) \tag{18}$$

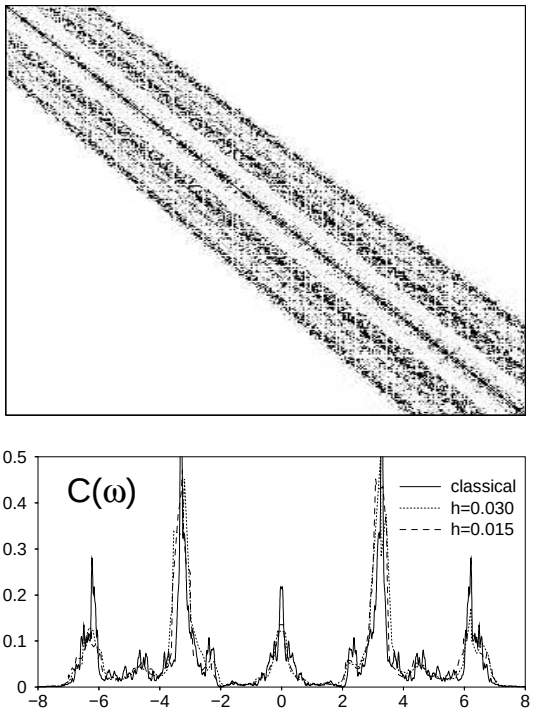
$$\Delta_b \;=\; \frac{2\pi}{\tau_{cl}} \;=\; \text{bandwidth that characterizes } \tilde{C}(\omega) \tag{19}$$

$$\Delta_0 \;=\; \frac{1}{\rho} \;=\; \text{mean level spacing} \tag{20}$$

$$\mathrm{Var}\,[A] \;=\; \left\langle A^2 \right\rangle - \langle A \rangle^2 \;=\; C(0) \tag{21}$$

$$\overline{|A_{nm}|^2} \;\approx\; \left[\frac{\Delta_0}{\Delta_b}\right] \mathrm{Var}\,[A] \;\equiv\; \frac{1}{b}\,\mathrm{Var}\,[A] \tag{22}$$

Example: motion is 2D chaotic well, Cohen, Kottos [PRE 2001]



[6] Fluctuations of expectation values

Consider a system with mean level spacing Δ_0, and bandwidth $\Delta_b = b\Delta_0$. We prepare the system in some state ψ. We now look on the temporal fluctuations of the expectation value

$$\langle A \rangle_t \;=\; \sum_{n,m} \mathrm{e}^{i(E_n - E_m)t}\; \langle n|\psi\rangle^*\, \langle m|\psi\rangle\; A_{n,m} \tag{23}$$

$$\overline{\langle A \rangle_t} \;=\; \sum_{n} p_n A_{n,n} \tag{24}$$

$$\overline{\langle A \rangle_t^2} \;=\; \sum_{n,m} p_n p_m |A_{n,m}|^2 \tag{25}$$

$$\mathrm{Var}_T[\langle A \rangle_t] \;=\; \overline{\langle A \rangle_t^2} \;-\; \left[\overline{\langle A \rangle_t}\right]^2 \qquad \text{[temporal variance]} \tag{26}$$

Using the Feinglod-Peres relation we get

$$\mathrm{Var}_T\,[\langle A \rangle_t] \;=\; \frac{1}{\max(b[A],\, d[\rho])}\,\mathrm{Var}\,[A] \tag{27}$$

where $d[\rho]$ is the number of eigenstates that participate, and $b[A]$ is the bandwidth of the matrix.
Note: The case $b > d$ is trivial because the ps sum to unity,

hence the result equals to the semiclassical estimate of the near-diagonal $|A_{nm}|^2$.
In the case $b < d$ the fraction of in-band terms is $(bd)/(d^2)$.
To provide a visualization of the double sum.
Note: As expected the temporal variance diminishes in the classical limit.

[7] Equilibration of local observables

Here we consider fluctuations of the expectation values $\langle A \rangle_t$ of local observables.

d_S = Hilbert space dimension of the subsystem
d_B = Hilbert space dimension of the environment ("bath")
$d = d_S\, d_B$

ρ = arbitrary probability matrix, dimension $d \times d$
ρ_S = reduced probability matrix, dimension $d_S \times d_S$

d_Ω = subspace dimension (e.g. all pure-states that have a given energy)
Ω = the maximally mixed state in the Ω subspace

$$d_\Omega \;<\; d_S\; d[\Omega_B] \tag{28}$$

(visualization of this inequality in "S-B" space)

Ensemble average over all states of the Ω subspace:

$$\langle A \rangle_\Omega \;=\; \mathrm{trace}\,[\Omega A] \tag{29}$$

(below subscript Ω is omitted).

Stat-Mech ensemble theorem, `Popescu, Short, Winter` [Nature Phys 2006]

$$\langle D\,[\rho_S, \Omega_S] \rangle \;\leq\; \frac{1}{2}\left(\frac{d_S}{d[\Omega_B]}\right)^{1/2} \;\leq\; \frac{1}{2}\frac{d_S}{\sqrt{d_\Omega}} \tag{30}$$

This holds irrespective of whether Ω_S is canonical.
A more tight bound depends on entanglement.

Note: The traditional reasoning concerns microcanonical-like ensembles, and assumes weak coupling.
Here these assumptions are not taken.

Dynamical equilibration theorem, `Linden, Popescu, Short, Winter` [PRE 2009]
Here the role of Ω is played by $\bar\rho$, and the role of the ensemble is played by time.

$$\overline{D\,[\rho_S(t), \bar\rho_S]} \;\leq\; \frac{1}{2}\left(\frac{d_S}{d[\bar\rho_B]}\right)^{1/2} \;\leq\; \frac{1}{2}\frac{d_S}{\sqrt{d[\bar\rho]}} \tag{31}$$

A secondary theorem is

$$\langle d[\bar\rho] \rangle \;\geq\; \frac{1}{2} d_\Omega \tag{32}$$

Hence typically

$$\overline{D\,[\rho_S(t), \bar\rho_S]} \;\leq\; \frac{d_S}{\sqrt{2 d_\Omega}} \tag{33}$$

Non-thermalization theorem, `Gogolin, Muller, Eisert` [PRL 2011]

Assume that the system is prepared in a factorized state $\rho = \rho_S \otimes \rho_B$, we get some stead state $\bar\rho_S$. The question is whether we have memory for the initial condition: whether we can resolve steady states that originate from different

preparation. For this purpose a difference measure Δ is defined:

$$\Delta = D\left[\overline{\rho}_S^1, \overline{\rho}_S^2\right] - \sum_{1,2} \overline{D\left[\rho_S(t), \bar{\rho}_S\right]} \tag{34}$$

$$> D\left[\rho_S^1, \rho_S^2\right] - \sum_{1,2} \overline{D\left[\rho_S, \bar{\rho}_S\right]} - \sum_{1,2} \overline{D\left[\rho_S(t), \bar{\rho}_S\right]} \tag{35}$$

The theorem implies that the difference Δ might be positive, because the first term might be large (preparing very different initial states), while the other terms are typically small. Thus it is implied that the respective steady states can be resolved, so there is a memory of the initial state.

Alert: One may argue that the above notion of non-thermalization is misleading. The preparations do not have the same energy distribution. In a classical context thermalization is trivially not expected in such circumstances.

Bottom line:
If the ensemble is large, the fluctuations of the expectation values are small.
The approach to the classical limit is like $1/\sqrt{d_\Omega}$.
Thanks to the "goodness" of the equilibration we might have "non-thermalization".

[8] Classical non-ergodic systems

- Implications of having a mixed phase space?
- Implications of having constants of motion?
- Do we have memory of the initial condition?

In order to visualize system with mixed-phase space or with constant of motion, consider a billiard system that is composed of several disconnected boxes. Say that the observable A of interest is the position of the particle. Clearly we have the following classical sum rule

$$\mathrm{Var}[A] \;=\; \mathrm{Var}[\bar{A}] \;+\; \mathrm{Var}_T[A_t] \tag{36}$$

Clearly in such non-ergodic system we have "memory of the initial box".
So in general we associate "memory with having "constants of motion".
One way to formalize this observation is provided by the "Mazur bound".

`Mazur`, Non-ergodicity of phase functions in certain systems [Physica 1969]

We want to find a non-zero lower bound for $\mathrm{Var}[\bar{A}]$.
Without loss of generality we assume $\langle A\rangle = 0$, hence $\mathrm{Var}[\bar{A}] = \langle \bar{A}^2\rangle$
If we have a constant of motion C, say the energy,
we can write the CauchySchwarz inequality $|\langle C\,\bar{A}\rangle|^2 < \langle C^2\rangle\ \langle \bar{A}^2\rangle$.
It is convenient to shift and noramlize the constant of motion such that $\langle C\rangle = 0$ and $\langle C^2\rangle = 1$.
We get $\langle \bar{A}^2\rangle > \left|\langle C\,\bar{A}\rangle\right|^2$. This is equivalent to $\langle \bar{A}^2\rangle > |\langle C\,A\rangle|^2$.
Note: for a mono-energetic preparation of an ergodic system Mazur bound is zero.
If we have several constants of motion we can assume without loss of generality $\langle C_i C_j\rangle = \delta_{i,j}$.
Then we get

$$\mathrm{Var}[\bar{A}] \;>\; \sum_j |\langle C_j\,A\rangle|^2 \tag{37}$$

An interesting application: `Mierzejewski, Prelovsek, Prosen`, Breakdown of the GGE for current-generating quenches [PRL 2014]

Ring with spinless fermions with control over the flux ϕ.
In the absence of flux $\rho = \mathrm{e}^{-\beta H}$, and $\langle J\rangle = 0$.
With flux after full thermalization $\rho = \mathrm{e}^{-\beta(H-\phi J)}$, and $\langle J\rangle = \beta\left\langle J^2\right\rangle \phi$.
After quench to zero flux $\rho = \mathrm{e}^{-\beta(H-\phi \bar{J})}$, and $\langle J\rangle = \beta\left\langle \bar{J}^2\right\rangle \phi \;\neq\; 0$.
The issue was to figure out the Mazur bound on $\left\langle \bar{J}^2\right\rangle$.
Main message: existence of quasi-local conserved quantities.

Relaxation and Prethermalization, experimental work with one-dimensional Bose gas, `Gring, Kuhnert, Langen, Kitagawa, Rauer, Schreitl, Mazets, Adu Smith, Demler, Schmiedmayer` [Science 2013]. Fast splitting leads to pre-thermalized state that is characterized by an effective temperature $T_{\mathrm{eff}} = (1/2)gN/L$.

Generalized Gibbs ensemble: Consider Hamiltonian H with short-range interactions that commutes with constant of motion Q. Assumed that $Q = \sum Q_{\mathrm{subsystems}}$. Then for each subsystem we expect

$$\rho_S \;\propto\; \mathrm{e}^{-\beta H_S - \lambda Q_S} \tag{38}$$

If Q is the number operator N then it is written as

$$\rho_S \;\propto\; \mathrm{e}^{-\beta(H_S - \mu N_S)} \tag{39}$$

Note: a somewhat trivial generalized quantum definition of GGE is as follows: all states ρ that lead to the same steady $\bar{\rho}$. Note that all the projectors $|E_n\rangle\langle E_n|$ are constants of motion.

[9] Weak quantum chaos

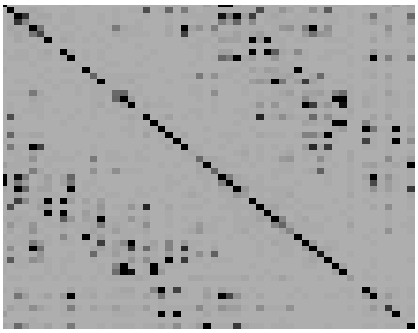
The matrix representation of quantized Hamiltonian is by a banded matrix that looks like a random matrix:

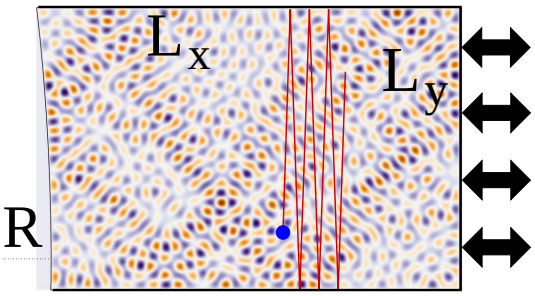
$$\mathcal{H}_{\text{total}} \;=\; \mathcal{H} \;+\; \lambda V \;=\; \text{diag}\{E_n\} + \lambda\ \text{BandedMatrix}\{V_{nm}\} \tag{40}$$

The bandprofile is given by the Feingold-Peres relation. The parametric evolution of the eigenstates as a function of λ involves generically a crossover from a perturbative to a non-perturbative regime. In the RMT work of Wigner the LDOS goes from Lorentzian to SemiCircle. For quantized hamiltonians the theory is more complicated.

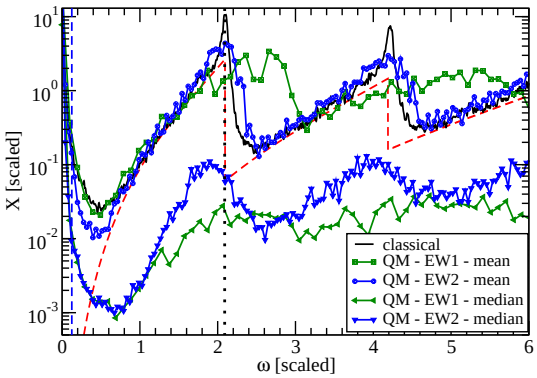
`Cohen, Heller`, Unification of perturbation theory, RMT and semiclassical considerations in the study of parametrically-dependent eigenstates [PRL 2000]. `Cohen, Kottos`, Parametric dependent Hamiltonians, wavefunctions, random-matrix-theory, and quantal-classical correspondence [PRE 2001]. See also works `with Barnett` [PRE 2001] and `with Mendez-Bermudez` [PRE 2005] [PRE 2006].

Weak quantum chaos for weakly chaotic billiards:
`Stotland, Cohen, Davidson` [EPL 2009]
`Stotland, Pecora, Cohen` [EPL 2010] [PRE 2011]
Here H is integrable, and the perturbation is small.





[not a Gaussian matrix...]

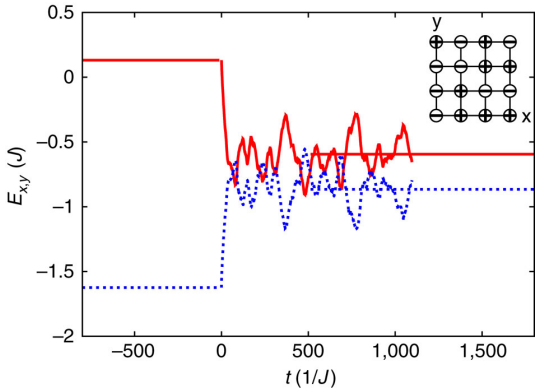


[median ≪ mean]

Major point to notice: Even in extreme quantum circumstances the alegebraic average corresponds to the classical calculation (we call it "restricted QCC"), but the median and higher moments are $\hbar$ dependent (absence of "detailed QCC" for weak quantum chaos).

Weak quantum chaos for weakly disordered lattice:
`Stotland, Budoyo, Peer, Kottos, Cohen` [EPL 2008]
`Stotland, Kottos Cohen` [PRB 2010]

Equilibration in a weakly disordered lattice:
`Olshanii, Jacobs, Rigol, Dunjko, Kennard, Yurovsky` [Nature Comm 2013] [PRL 2007]



Equipartition is not achieved - memory of the initial conditions.

Unperturbed states $|k_x, k_y\rangle$
Perturbed eigenstates $|E_n\rangle$
Initial preparation $|\boldsymbol{k}_0\rangle$, accordingly $p_n = |\langle n|\boldsymbol{k}_0\rangle|^2$
Inverse participation number of the preparation $\eta = \sum_n p_n^2$

$$\overline{\langle A\rangle_t} \;=\; \eta\,\langle A\rangle_0 \;+\; (1-\eta)\,\langle A\rangle_E \tag{41}$$

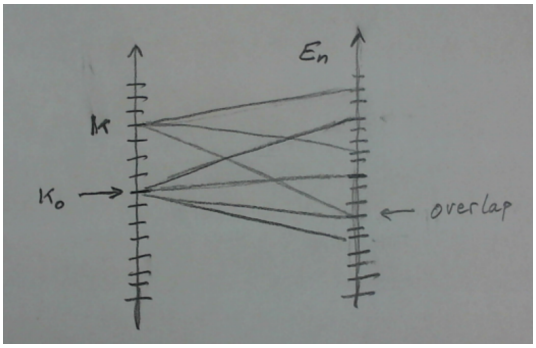
Derivation:

$$\overline{\langle A\rangle_t} \;=\; \sum_n p_n A_{n,n} \;=\; \sum_{n,k',k'} p_n\,\langle k'|n\rangle^*\,\langle k''|n\rangle\,A_{k',k''} \tag{42}$$

$$=\; \sum_k \left[\sum_n |\langle n|k_0\rangle|^2\;|\langle n|k\rangle|^2\right] A_{k,k} \;+\; \sum_n \sum_{k\neq k'} \text{neglected terms} \tag{43}$$

$$\approx\; \eta\,\langle A\rangle_{k_0,k_0} \;+\; \sum_{k(\neq k_0)} \text{overlaps}(k_0|k)\;A_{k,k} \tag{44}$$

Note: The sum of the overlaps if k_0 is excluded is $(1-\eta)$, else it would be unity. Regarding the second term: the distribution of contributing ks within the energy shell is sparse and statistically unbiased; Hence we get the microcanonical average.



[10] Classical dynamics - overview

f = number of degrees of freedom

$f = 1$
One degree of freedom is integrable (oscillator).
Action-angle canonical coordinates can be chosen (φ, J).
Motion is characterized by a frequency $\omega(E)$.
Possibility to have several regions in phase-space separated by speratrix.
The pendulum is a prototype $f = 1$ system.

$f = 2$
System with two degrees of freedom has in general mixed phase-space.
Regions of resonances for rational frequencies.
Stochastic layer are formed along the speratrix.
These regions are separated by KAM tori. Once destroyed they become cantori.
Chirikov criterion of resonance-overlap - formation of chaotic sea.
The kicked rotor (standard map) is a prototype $f = 2$ system.

$f > 2$
Energy surface is $2f - 1$ dimensional.
KAM tori are f dimensional. Note: $[(2f - 1) - (f)] > 1$.
The KAM are not able to separate the energy surface into territories.
If close to intergrable - Arnold web is formed; Arnold diffusion.
The stochastic-pump model is a prototype $f = 3$ model for Arnold diffusion.

It follows that any $f > 2$ system is ergodic, provided the energy shell is a connected domain.
But the equilibration process might be very slow.

[11] Classical dynamics - the standard map

The standard map is:

$$p_{n+1} = p_n + K \sin(\theta_n) \tag{45}$$
$$\theta_{n+1} = \theta_n + p_{n+1} \tag{46}$$

It can be generated by the Hamiltonian of a kicked rotor:

$$\mathcal{H}(p, \theta, t) = \frac{1}{2}p^2 + K \cos(\theta) \sum_{n=-\infty}^{\infty} \delta(t - n) \tag{47}$$
$$\equiv \frac{1}{2}p^2 + K \cos(x)\ f(\Omega t) \qquad [\Omega = 2\pi] \tag{48}$$

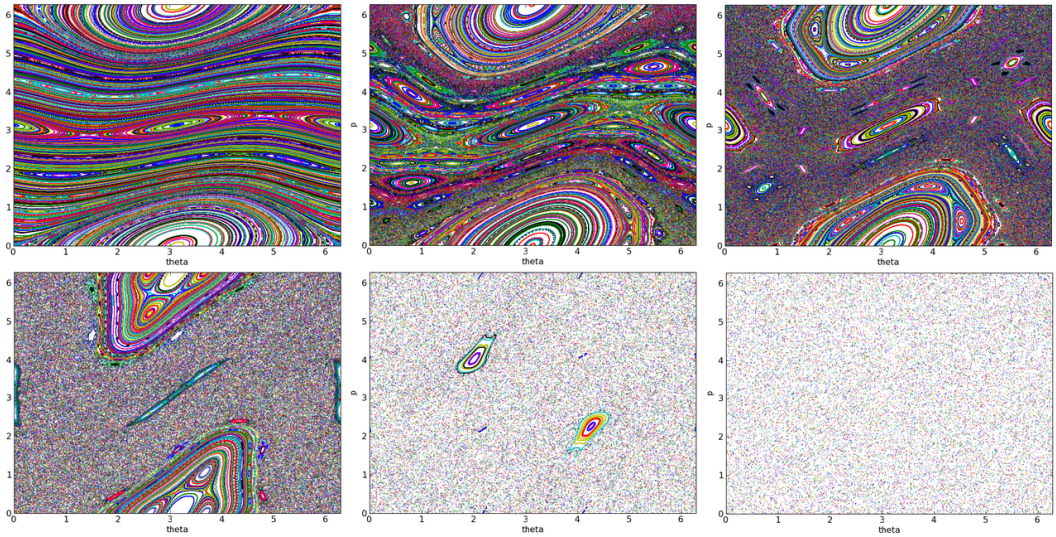
It can be regarded as a prototype $f = 2$ system:

$$\mathcal{H}(p, \theta; q, \varphi) = \frac{1}{2}p^2 + K \cos(\theta) f(\varphi) + \Omega q \tag{49}$$

The two interacting frequencies are $\Omega = 2\pi$ and $\omega(E) = \sqrt{2E}$.
The strength of the coupling is K. The critical value for getting global chaotic sea is

$$K_c \approx 0.971635... \tag{50}$$

The following figure shows how phase-space look like for different values of K.



For $K \gg 1$ we get diffusion because the following is like random walk

$$p_N - p_0 \quad = \quad K\sin(\theta_1) + K\sin(\theta_2) + \cdots + K\sin(\theta_N) \tag{51}$$

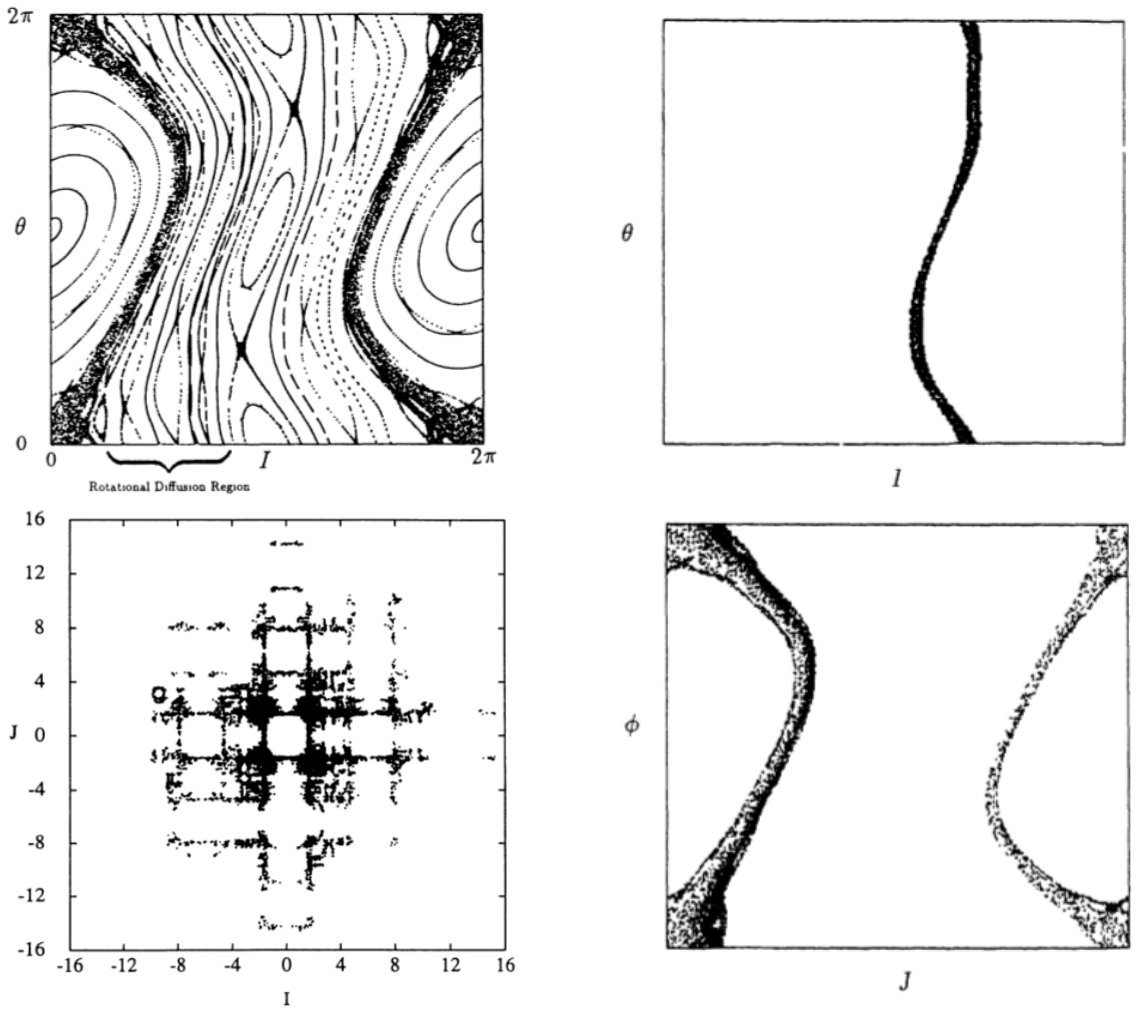
Digression: This is a prototype model for dynamical localization.

[12] Arnold diffusion - Coupled standard map

Two coupled standard maps are like $d = 3$ system.
Study of Arnold diffusion, `Wood, Lichtenberg, Lieberman` [PRA 1990]

$$I_{n+1} = I_n + K\sin(\theta_n) + \mu\sin(\theta_n + \phi_n) \tag{52}$$
$$\theta_{n+1} = \theta_n + I_{n+1} \tag{53}$$
$$J_{n+1} = J_n + K\sin(\phi_n) + \mu\sin(\theta_n + \phi_n) \tag{54}$$
$$\phi_{n+1} = \phi_n + J_{n+1} \tag{55}$$

The following figure demonstrates the idea of Arnold diffusion. Left upper: phase space of an isolated standard map. Right: Plot of a not-too-long trajectory starting at regular-stochastic region. Left bottom: Plot of $\theta = \phi = \pi$ section of a very long trajectory starting at a chaotic spot.



[13] Arnold diffusion - stochastic pump model

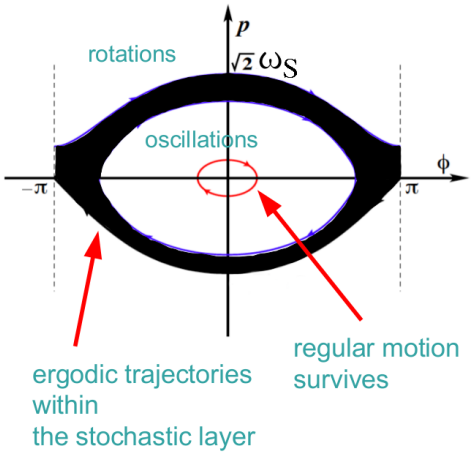
`Chirikov` [PhysRep 1979]
`Lichtenberg and Lieberman`, Regular and chaotic dynamics [book]

The minimal model for Arnold diffusion involves $f = 3$ freedoms:

- Driving source "D" that has frequency Ω.
- Pendulum ω_S that is driven into stochastic motion.
- Oscillator ω_R that is driven by the pendulum.
- The coupling between "D" and "S" is K.
- The coupling between "S" and "R" is μ.

The Hamiltonian is

$$H(\boldsymbol{\theta}, \boldsymbol{n}; \phi, p; t) \;=\; \Big[\omega_R \boldsymbol{n}\Big] \;+\; \mu\cos(\boldsymbol{\theta} - \phi) \;+\; \Big[\frac{1}{2}p^2 - \omega_S^2\cos(\phi)\Big] \;-\; K\cos(\phi - \Omega t) \tag{56}$$



The width w_S of the stochastic layer of the pendulum "S" is determined by the Melnikov-Arnold integral, involving the frequency Ω, leading to

$$w_S \;=\; 8\pi\, K \frac{\Omega}{\omega_S^2}\, \exp\left[-\frac{\pi}{2}\frac{\Omega}{\omega_S}\right] \tag{57}$$

The induced diffusion in "R" is determined by the power spectrum of $e^{i\phi}$, which is again the Melnikov-Arnold integral, but evaluated at the pertinent frequency ω_R, leading to

$$D_n \;=\; (4\pi)^2\, \frac{\mu^2}{\Omega}\, \left(\frac{\omega_R}{\omega_S}\right)^2\, \exp\left[-\frac{\pi}{2}\frac{\omega_R}{\omega_S}\right] \tag{58}$$

Note that K does not appear in the final expressions!

Quantization of the Stochastic Pump Model of Arnold Diffusion
`Leitner, Wolynes` [PRL 1997]

Manifestation of Arnold Diffusion in Quantum Systems
`Demikhovskii, Izrailev, Malyshev` [PRL 2002] [PRE 2002]

The more abstract point of view of Arnold diffusion is as follows:

- The "pendulum" is the outcome of guiding resonance involving f_S freedoms
- The "driving" is the outcome of layer resonance involving f_D freedoms
- The effective coupling is κ^{f_D} reflecting high order of perturbation theory.
- The effective pendulum frequency is proportional to κ^{f_S}
- The detuning of the layer resonance is $\Delta_D \propto e^{-f_D}$
- The effective driving frequency is Δ_D
- The detuning of the guiding resonance is $\Delta_S \propto e^{-f_S}$

Accordingly

$$w_S \;\sim\; \kappa^{f_D}\, \exp\left[-\frac{e^{-f_D}}{\kappa^{f_S}}\right] \tag{59}$$

Later we discuss the work of Basko regarding the thermalization of DNLS chain. There we have the estimate $\Delta_S \approx W e^{-f_S}$, where W is the disorder. The minimum occupation that is required to be on the guiding resonance is Δ_S/U. Accordingly the "chaotic fraction" is multiplied by a Boltzmann factor

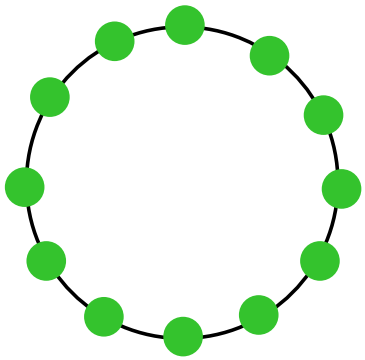
$$w \;=\; w_S\, \exp\left[-\beta\mu\, \frac{W}{U}\, e^{-f_S}\right] \;=\; \kappa^{f_D}\, \exp\left[-\frac{e^{-f_D}}{\kappa^{f_S}} - \frac{e^{-f_S}}{\rho}\right] \tag{60}$$

[14] Prototype model for thermalization

A Bose-Hubbard system with M sites and N bosons:

$$\mathcal{H} = \sum_{j=1}^{M}\left[\frac{U}{2}a_j^\dagger a_j^\dagger a_j a_j + W_j a_j^\dagger a_j - \frac{K_j}{2}\left(a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1}\right)\right] \tag{61}$$

Parameters: U (interaction), W (disorder), K (hopping), M (sites), N (particles)



In a semi-classical framework:

$$a_j = \sqrt{\boldsymbol{n}_j}\, e^{i\boldsymbol{\varphi}_j} \quad , \quad [\boldsymbol{\varphi}_j, \boldsymbol{n}_i] = i\delta_{ij} \tag{62}$$

$$z = (\boldsymbol{\varphi}_1, \cdots, \boldsymbol{\varphi}_M, \ \boldsymbol{n}_1, \cdots, \boldsymbol{n}_M) \tag{63}$$

This is like M coupled oscillators with $\mathcal{H} = H(z)$

$$H(z) = \sum_{j=1}^{M}\left[\frac{U}{2}\boldsymbol{n}_j^2 + W_j\boldsymbol{n}_j - K\sqrt{\boldsymbol{n}_{j+1}\boldsymbol{n}_j}\cos\left(\boldsymbol{\varphi}_{j+1} - \boldsymbol{\varphi}_j\right)\right] \tag{64}$$

Without hopping each "oscillator" has its own frequency:

$$\omega_j = W_j + U\boldsymbol{n}_j, \qquad W_j \in \left[-\frac{W}{2}, \frac{W}{2}\right] \tag{65}$$

The dynamics is generated by the Hamilton equation:

$$\dot{z} = \mathbb{J}\boldsymbol{\partial}H \quad , \quad \mathbb{J} = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \tag{66}$$

Discrete non-linear Schrodinger equation (DNLS)

Classically there is a single dimensionless parameter:

$$u = \frac{NU}{K} \tag{67}$$

Rescaling coordinates:

$$\tilde{\boldsymbol{n}} = \boldsymbol{n}/N \tag{68}$$

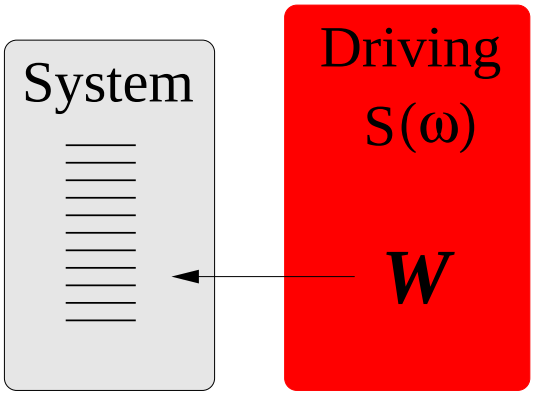
$$[\boldsymbol{\varphi}_j, \tilde{\boldsymbol{n}}_i] = i\hbar\delta_{ij} \tag{69}$$

$$\hbar = \frac{1}{N} \tag{70}$$

Thermodynamics limit: $M \to \infty$, keeping $N/M \sim$ const.
Semiclassical limit: Given M, take $N \to \infty$, such that $N/M \gg 1$.

[15] The fluctuation-diffusion-dissipation relation

`Ott` [PRL 1979] - diffusion picture for adiabatic driving
`Wilkinson` [JPA 1988] - dissipation picture based on this diffusion picture
`Jarzynski` [PRE 1995] - adding FPE perspective
`Cohen` [PRL 1999] [Annals 2000] - adding FDT perspective + addressing the quantum case
`Bunin, D'Alessio, Kafri, Polkovnikov` [Nature Phys 2011] - adding NFT based derivation



Consider a driven system $\mathcal{H} + f(t)V$. The driving source induces diffusion in energy. Fermi golden rule implies

$$D_\varepsilon \;=\; \int_0^\infty \frac{d\omega}{2\pi}\,\omega^2\,\tilde{C}_\varepsilon(\omega)\,\tilde{S}(\omega) \tag{71}$$

The Fokker-Planck description of the diffusion in energy requires to take the correct "measure", hence the appearance of the density of states $g(\varepsilon)$, namely,

$$\frac{\partial\rho}{\partial t} \;=\; \frac{\partial}{\partial\varepsilon}\left(g(\varepsilon)D(\varepsilon)\frac{\partial}{\partial\varepsilon}\left(\frac{1}{g(\varepsilon)}\rho\right)\right) \;=\; -\frac{\partial}{\partial\varepsilon}\left(A(\varepsilon)\rho - \frac{\partial}{\partial\varepsilon}\left[D(\varepsilon)\rho\right]\right) \tag{72}$$

Defining $\beta(\varepsilon)$ as the logarithmic derivative of $g(\varepsilon)$, the expression for the "drift velocity" takes the form

$$A(\varepsilon) \;=\; \partial_\varepsilon D_\varepsilon + \beta(\varepsilon)D_\varepsilon \tag{73}$$

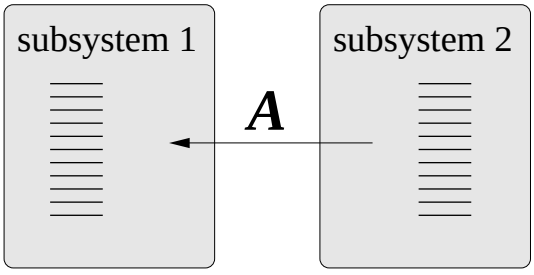
The implied expression for the rate of energy absorption is

$$J_E \;=\; \dot{W} \;=\; \frac{d}{dt}\int \varepsilon\,\varrho(\varepsilon)\,d\varepsilon \;=\; \int A(\varepsilon)\varrho(\varepsilon)\,d\varepsilon \;=\; \langle A\rangle \tag{74}$$

This can be regarded as rate of doing "work" on the system ($\dot{W}$), or as the flow of energy (J_E) from the driving source to the system.

[16] Thermalization of two subsystems

MEQ version: `Hurowitz, Cohen` [EPL 2011]
FPE version: `Tikhonenkov, Vardi, Anglin, Cohen` [PRL 2013]
NFT version: Bunin, Kafri [JPA 2013]



This is a variation on the fluctuation-diffusion-dissipation relation.
The diffusion is along constant energy lines: $\varepsilon_1 + \varepsilon_2 = \mathcal{E}$.

$$D_\varepsilon \;=\; \int_0^\infty \frac{d\omega}{2\pi}\,\omega^2\,\tilde{S}^{(1)}(\omega)\,\tilde{S}^{(2)}(\omega) \tag{75}$$

A Fokker-Planck description is implied.
The proper Liouville measure is: $g(\varepsilon) = g_1(\varepsilon)g_2(\mathcal{E}-\varepsilon)$.

Rate of energy transfer:

$$A(\varepsilon) \;=\; \partial_\varepsilon D_\varepsilon + (\beta_1 - \beta_2)D_\varepsilon \tag{76}$$

If one would assume a canonincal preparation of the two subsystems:

$$J_E \;=\; \langle A(\varepsilon)\rangle \;=\; \left(\frac{1}{T_1}-\frac{1}{T_2}\right)\langle D_\varepsilon\rangle \tag{77}$$

What we have here is a Fick-type law that related a current to the gradient of a thermodynamic potential. If the two subsystems can exchange both particles and energies the relation between (J_N, J_E) and the gradient in (μ,β) will involve a 2×2 transport matrix of transport coefficients.

═══ [17] Thermalization of long DNLS chains

`Basko`, Weak chaos in the disordered nonlinear Schrodinger chain: Destruction of Anderson localization by Arnold diffusion [Annals Phys 2011]

Assumes weakly coupled sites:

$$\kappa \;\equiv\; \frac{K}{W} \;\ll\; 1 \tag{78}$$

Recall that each site has frequency $\omega_j = W_j + U\boldsymbol{n}_j$. We assume that in the dynamical range of interest the non-linearity is small, and nothing is trapped in a local minimum.

$$\rho \;\equiv\; \frac{U\boldsymbol{n}}{W} \;\ll\; 1 \tag{79}$$

Technical remark: In the detailed derivation each segment is characterized by local $\boldsymbol{X} = (\beta\mu, -\beta)$ that can be translated via a grand-canonical ansats to local $\boldsymbol{Y} = (N(x), E(x))$. The objective is to derive macroscopic transport description that is based on a continuity equation $\partial_t \boldsymbol{Y} = -\partial_x \boldsymbol{J}$ with currents $\boldsymbol{J} = -\boldsymbol{\sigma}\partial_x \boldsymbol{X}$. Here we simplify the discussion referring only to the occupation which is described by the scaled density $\rho(x)$.

The basic idea of the calculation is as follows:
The chain is composed of segments;
Each location is characterized by a chaotic fraction w.
In the stochastic-pump-model formula for w use $\kappa := \kappa^p\rho$ with $\frac{1}{3} \le p \le 3$.

$$\text{Prob}\left[w < \mathrm{e}^{-\lambda}\right] \;\approx\; \exp\left[-S(\lambda)\right] \tag{80}$$

where

$$S(\lambda) \;=\; c\rho\lambda^p\,\exp\left[\frac{\lambda}{C\ln^2\left(\frac{1}{\kappa^p\rho}\right)}\right] \tag{81}$$

The local diffusion coefficient $D \sim wD_0$ is dominated by w.
The coarse grained diffusion coefficient is implied by a resistor network picture:

$$D \;\sim\; \left[\left\langle\frac{1}{w}\right\rangle\right]^{-1} \;=\; \left[\int_0^\infty d\lambda\;\exp\left[\lambda - S(\lambda)\right]\right]^{-1} \tag{82}$$

Leading to the estimate

$$D(\rho) \;\sim\; \exp\left[-C\ln^2\left(\frac{1}{\kappa^p\rho}\right)\ln\left(\frac{1}{\rho}\right)\right] \tag{83}$$

This estimate has been based on finding the optimal λ that characterizes the bottlenecks for diffusion. This can be translated into a characteristic length scale for distance between bottlenecks

$$L^* = \exp\left[C \ln^2\left(\frac{1}{\kappa^p \rho}\right)\right] \tag{84}$$

On scales larger than that we can write $J = -D(\rho)\partial_x \rho$. Introducing into the continuity equation $\partial_t \rho = -\partial_x J$, one obtain a non-linear diffusion equation for the occupation density.

We note that the idea of using a resistor-network calculation in the context of weak-chaos has first appeared, to the best of our knowledge, in `Cohen, Kottos, Schanz` [JPA 2006], `Bandopadhyay, Etzioni, Cohen` [EPL 2006] and has been termed *semi-linear response* by `Wilkinson, Mehlig, Cohen` [EPL 2006]. It has been connected to variable range hopping by `Cohen` [PRB 2007] with further applications by the BGU group (`Stotland et al`) in [JPA 2008] [EPL 2009] [PRB 2010] [EPL 2010] [PRE 2011]

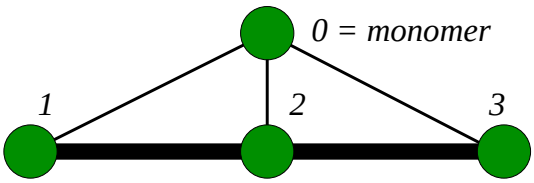
[18] Quantum Localization

Let us start with a simple example for dynamical localization in a minimal Bose-Hubbard model. The FPE description makes sense if at least one sub-system is chaotic.

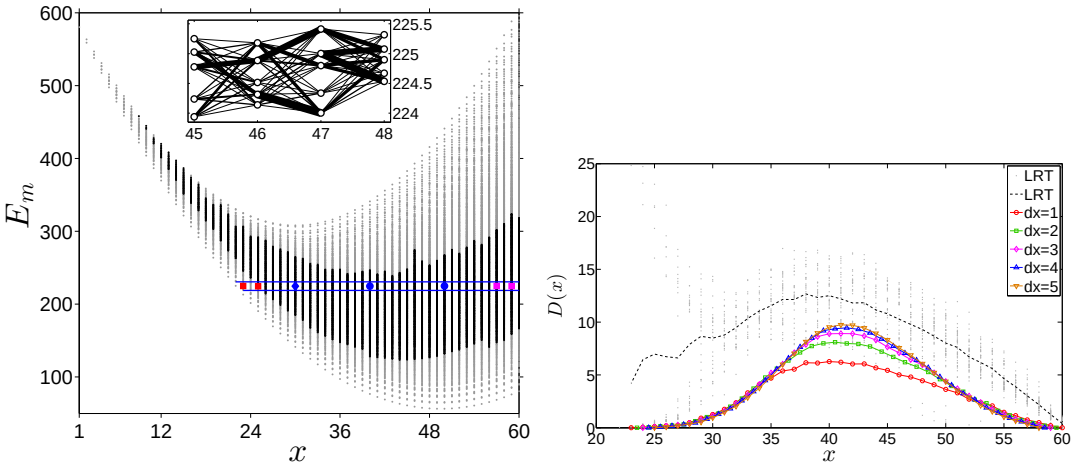
Minimal model for a chaotic sub-system: BHH trimer.

Minimal model for thermalization: BHH trimer + monomer

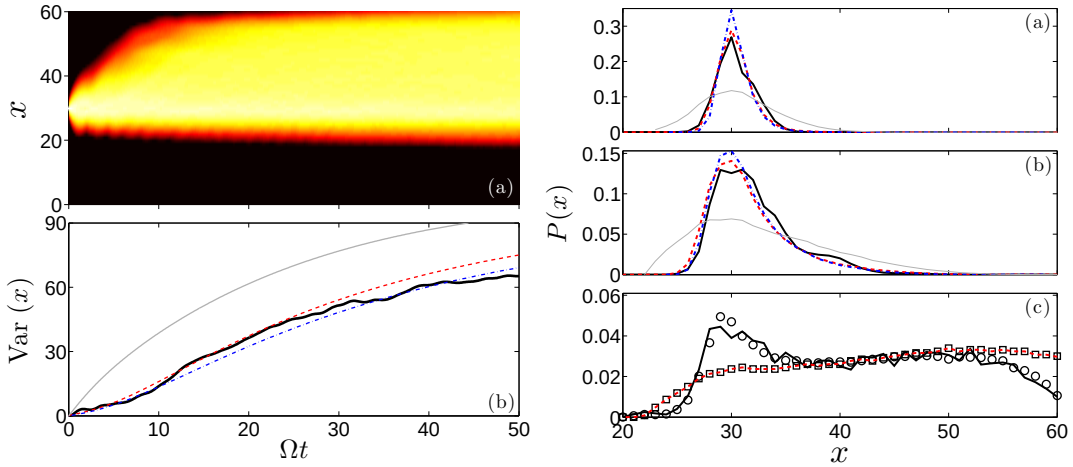
`Khripkov, Vardi, Cohen` [NJP 2015]



The trimer spectrum is characterized by the Brody parameter.
Different initial conditions are indicated.
The couplings induces FGR transitions within the energy shell.
The diffusion coefficient $D(x)$ can be calculated using a "resistor network" formalism.



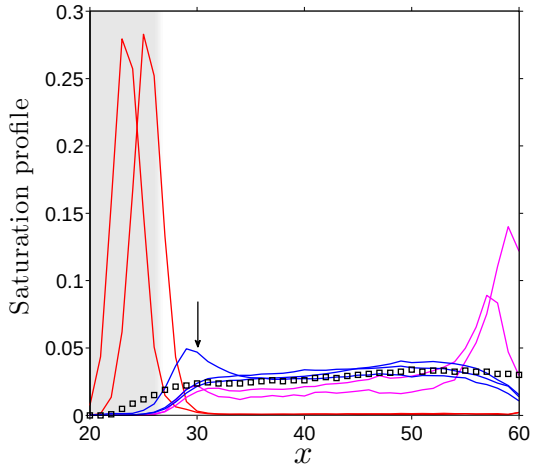
Now we follow the evolution as a function of time.



It can be described by an FPE.

$$\frac{\partial}{\partial t}\rho(x) = \frac{\partial}{\partial x}\Big[g(x)D(x)\frac{\partial}{\partial x}\Big(\frac{1}{g(x)}\rho(x)\Big)\Big] \tag{85}$$

But we see that that for some initial conditions we get localization.
For small x preparation the localization is related to phase-space structures,
while for large x it is Anderson-type localization in a chaotic sea.



Another example for manifestation of dynamical localization in the BHH context concerns a ring geometry. It is responsible for what we call quantum metastability: `Arwas, Vardi, Cohen`, Superfluidity and Chaos in low dimensional circuits [Scientific Reports (2015)]

[19] Quantum Localization - breaktime concept

The semiclassical perspective on "weak localization" is known as "scar theory". The breaktime concept has first appeared in the context of "strong" 1D dynamical localization in the kicked-rotor problem, and later generalized in various ways.

`Chirikov, Izrailev, Shepelyansky` [SovSciRevC 1981], `Shepelyansky` [PhysicaD 1987]
`Heller`, Quantum localization and the rate of exploration of phase space [PRA 1987]
`Dittrich`, Spectral statistics for 1D disordered systems [Phys Rep 1996]
`Cohen`, Periodic Orbits Breaktime and Localization [JPA 1998]

If we have a simple chaotic system (ballistic exploration of its volume) then recurrence start at the Heisenberg time

$$t_H \;=\; \frac{2\pi\hbar}{\Delta_0} \;\propto\; \frac{\Omega_\infty}{\hbar^{f-1}} \tag{86}$$

where Δ_0 is the mean level spacing, and Ω_∞ is the total volume. But if we have a more complex phase space then the exploration of the volume can be (say) as in a random walk process, described by a function $\Omega(t)$. Then we define an associated time-dependent Heisenberg time, and write the QCC condition as

$$t \;\ll\; \frac{\Omega(t)}{\Omega_\infty}\, t_H \tag{87}$$

In a diffusive systems the classical exploration grows asymptotically like $t^{1/2}$ in 1D, like $t/\ln(t)$ in 2D, and like t, with small corrections for higher dimensions. We deduce that in 1D and 2D we always have a breaktime, while in 3D there might be a mobility edge.

The well known semi-classical result for localization in 1D is easily recovered. Setting $\Omega(t) = \sqrt{Dt}$ and $t_H = 2L/v$ we get the following result

$$t^* = \frac{4D}{v^2}, \qquad \xi = \frac{2D}{v} = 2\ell \tag{88}$$

Alert: this strict 1D version s a somewhat misleading because an explicit $\hbar$ dependence is absent. The puzzle is solved by noting that in strict 1D the diffusion cannot be of classical origin. If we go to (say) an $f = 2$ quasi-1D billiard system with classical diffusion, the expression for the Heisenberg time is multiplied by an $\hbar$-dependent factor (so called "number of channels") and we deduce the $\xi \propto D_{\rm cl}/\hbar$. Hence the formula acquires an explicit $\hbar$ dependence as expected.

[20] The Anderson criterion for localization

`Anderson`, Absence of Diffusion in Certain Random Lattices [Phys Rev 1958]

Calculating the Green function for a particle in a disordered lattice. By definition the connective constant μ determines the number n^μ of self-avoiding paths that start at the origin, where $n \to \infty$ is the path length. The Green function is schematically

$$G \quad \sim \quad \sum_n \mu^n \left(\frac{K}{E-\epsilon} \right)^n \tag{89}$$

where the $\epsilon \in [-W/2, +W/2]$ are random on-site energies, and K is the hopping amplitude. The condition for convergence (implying localization) is

$$\mu \left\langle \frac{K}{E-\epsilon} \right\rangle_\epsilon \quad < \quad 1 \tag{90}$$

In the band center it leads to the Anderson criterion

$$\mu \frac{K}{W} \ln\left(\frac{W}{K} \right) \quad < \quad 1 \tag{91}$$

Or one may say roughly that there is localization if $\mu K < W$, which is the condition for not mixing the orbitals by the hopping.

[21] The MBL condition

`Basko, Aleiner, Altshuler` [Annals Phys 2006] [arXiv]
`Gornyi, Mirlin, Polyakov` [PRL 2005]

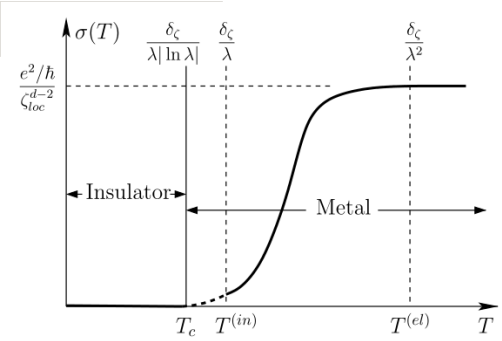
The discussion of MBL has originally appeared in the electronic context (fermions). The role of the disorder W is played by the mismatch of energies that are coupled by the two-body interaction term. Assuming that coupled orbitals reside at the same localization volume

$$\left| \epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta \right| \quad \sim \quad \Delta_\xi \tag{92}$$

It is argued that the effective connective constant is $\mu \sim T/\Delta_\xi$. The strength of the interaction (relative to Δ_ξ) is denoted λ. Hence the Anderson criterion takes the following form

$$\frac{T}{\Delta_\xi} \lambda |\ln \lambda| \quad < \quad 1 \tag{93}$$

The implications of MBL on the properties of the sample are important for both numerical and experimental studies. Clearly is does not affect the density of states, hence it is not a thermodynamic phase-transition. But we expect an abrupt change in the conductivity (see schematic plot), and it should be reflected in the sensitivity to twist boundary conditions. It also should affect the level statistic and the $\omega \sim 0$ response characteristics (see later section). Another measure is the segment-size dependence of the entanglement entropy (see later section).



The false argument against the survival of Anderson localization is as follows: Once inter-particle interaction is introduced, each particle experiences a bath that consists of all the other particles; hence decoherence destroys the Anderson localization; leading to hopping conductivity. The answer to this fallacy is that the local bath has a discrete spectrum; averaging the spectrum over disorder realization is apparently correct for the purpose of calculating dephasing rate, but wrong as far as breaktime is concerned.

[22] MBL - spectral measures

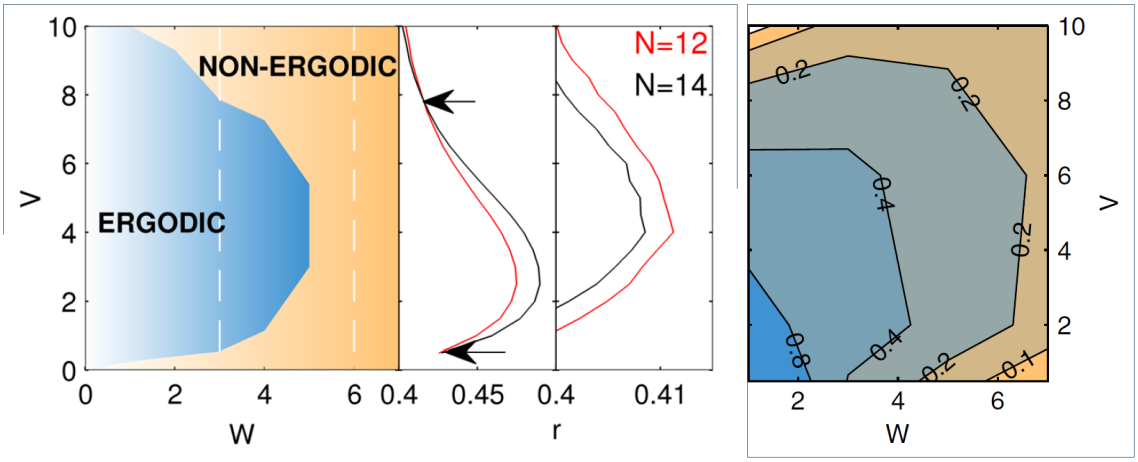
Considering spinless electrons in 1D disordered lattice, with repulsive interaction for occupation of neighboring sites.

`Bar-Lev, GuyCohen, Reichman` [PRL 2015]

Infinite temperature analysis. Calculating "Brody" vs (W, U) for increasing values of N. Identification of regions where Brody goes from Wigner to Poisson.

W_c of the ergodic-nonergodic transition becomes smaller if U is very small/large. (regions of "less chaos").

Also calculating density-density correlation function. The "spreading" exponent α can be deduced from the band profile $C(\omega)$ at the vicinity of $\omega = 0$. The system is always sub-diffusive, and the drop of α across the transition is gradual.



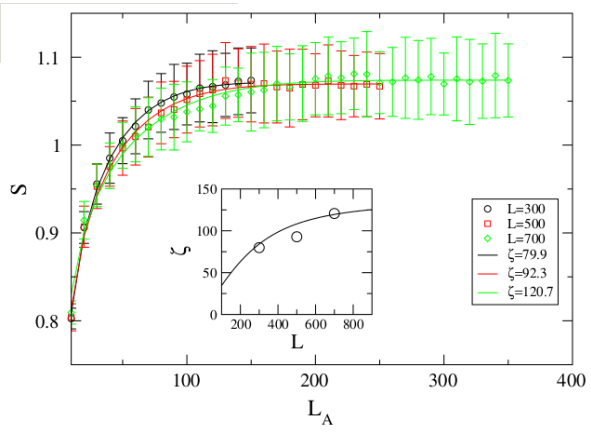
[23] MBL - entanglement measure

Considering spinless electrons in 1D disordered lattice, with repulsive interaction for occupation of neighboring sites.

`Berkovits`, Entanglement entropy in a one-dimensional disordered interacting system [PRL 2012]

Calculating entanglement entropy as a function of the segment length. Saturation reflects the finite localization length of the sample.

$$S(L_A; L, \xi) \quad = \quad \text{prefactor} \times \ln \left[\frac{L}{\pi} \text{SIN} \left(\pi \left(\frac{1}{L^2} + \frac{1}{\xi^2} \right)^{1/2} L_A \right) \right] + \text{const} \tag{94}$$



The purpose was to test the theoretical prediction for the localization length:

$$\xi(W, U) \quad = \quad [\xi(W)]^{G(U)}, \qquad G(U) < 1 \tag{95}$$

[24] Many body localization - Bose gas

`Aleiner, Altshuler, Shlyapnikov`, a finite-temperature phase transition for disordered weakly interacting bosons in one dimension [Nature Phys 2010]

The two challenging statements are:

- existence of a phase transition in one dimension;
- persistence of quantum phase-transition at finite temperature.

We consider bosons in 1D with disordered potential. It is possible to characterize the disorder by a parameter W, as if we were dealing with an Anderson lattice model. At zero temperature ($T = 0$) there is quantum phase transition form superfluid to insulator at $w = 1$, where

$$w \equiv \frac{W}{g\rho}, \qquad \rho = \text{density}, \ g = \text{GP interaction parameter} \tag{96}$$

The temperature above which the gas becomes non-degenerate is

$$T_d = \frac{\rho^2}{\mathsf{m}}, \qquad \gamma[\text{Lieb-Liniger}] = \frac{g\rho}{T_d} = \frac{\mathsf{m}g}{\rho} \tag{97}$$

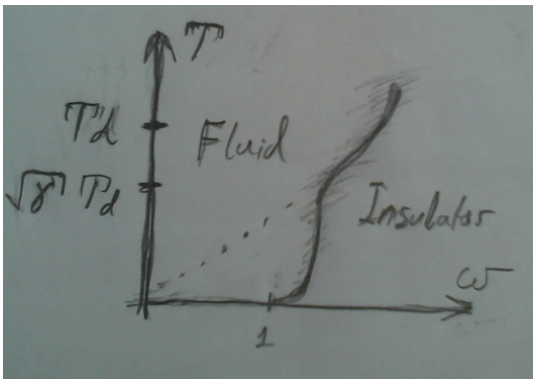
We assume weak interactions ($\gamma \ll 1$). The border of the MBL phase-transition in the (W, T) phase diagram is determined from the Anderson criterion. Namely, the insulating phase is $\mu U < \Delta_\xi$. Let us find the explicit expression for this border at the $T > T_d$ region.
The density of one-particle states at that temperature is $\nu = \sqrt{\mathsf{m}/T}$.
The localization length at that temperature is $\xi = T/(\mathsf{m}W^3)^{1/2}$.
The parameters that appear in the Anderson condition are

$$U = \frac{g}{\xi}, \qquad \Delta_\xi = \frac{1}{\nu\xi}, \qquad \mu = \rho\xi \tag{98}$$

leading to the condition

$$T \ < \ \frac{W^3}{(g\rho)^2} \tag{99}$$

Note that large density ρ implies fluid. If we start with a large density cloud of particles, the spreading will go on until ρ reach the value for which the above condition no longer satisfied.



[25] DNLS spreading problem

If we start with a very peaked preparation, then there is a remnants non-decaying piece (energetic stability?). Below we ignore this possibility and assume a wide flat region plus tails such that

$$\rho = \frac{1}{t^{\alpha/2}} \tag{100}$$

$$\langle x^2 \rangle = t^{\alpha} \tag{101}$$

It has been argued that beyond some critical value of the interaction, Anderson localization is destroyed, and there is sub-diffusion with $\alpha = 2/5$. The sub-diffusion is implied by regarding the nonlinear term as a source for white-noise, with intensity that decreases with time due to the spreading.

`Pikovsky, Shepelyansky`, Destruction of Anderson Localization by Nonlinearity [PRL 2008]

Later it has been argued by Flach et al that $\alpha = 1/3$.
`Flach, Krimer, Skokos` [PRL 2009]
`Skokos, Krimer, Komineas, Flach` [PRE 2009]

Using perturbation theory it has been argued that at least up to some stage

$$\langle x^2 \rangle \sim \ln(t) \qquad \text{for } t < u^{-\text{order}} \tag{102}$$

See `Wang,Zhang` [JStatPhys 2009] and `Fishman`, The nonlinear Schrdinger equation with a random potential [Nonlinearity 2011] (review)

The work of `Basko` provides a coarse-grained description of the transport that holds as long as the spreading width does not exceed a mesoscopic scale L^*. From this description one deduce slower than power-law spreading, namely,

$$\text{width}[x] \sim \exp\left[C\ (\ln t)^{1/3}\right] \tag{103}$$

See also discussion of weak disorder "homogeneous chaos" limit in `Basko` [PRE 2014], where $D(\rho) \propto \rho^2$ implies an intermediate stage of sub-diffusion with $\alpha = 1/2$.

If we take MBL into account, the distribution should flatten asymptotically at a density that corresponds to the fluid-insulator transition.