Strong localization and the exploration of phase space for quantum thermalization

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Short version of talk prepared for Celebrating 70th birthday of Rick Heller (Cuernavaca 2017)
The Bose Hubbard Hamiltonian

The system consists of $N$ bosons in $M$ sites. Later we add a gauge-field $\Phi$. 

$$H_{BHH} = \frac{U}{2} \sum_{j=1}^{M} a_j^\dagger a_j^\dagger a_j a_j - \frac{K}{2} \sum_{j=1}^{M} \left( a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1} a_j + 1 \right)$$

$$u \equiv \frac{NU}{K} \quad \text{[classical, stability, superfluidity, self-trapping]}$$

$$\gamma \equiv \frac{Mu}{N^2} \quad \text{[quantum, Mott-regime]}$$

Dimer ($M=2$): Minimal BHH; Bosonic Josephson junction; Pendulum physics [1,5].

Driven dimer: Landau-Zener dynamics [2], Kapitza effect [3], Zeno effect [4], Standard-map physics [5].

Trimer ($M=3$): Minimal model for low-dimensional chaos; Coupled pendula physics.

Triangular trimer ($M=3$): Minimal model with topology, Superfluidity [6], Stirring [7].

Larger rings ($M>3$) High-dimensional chaos; web of non-linear resonances [7].

Coupled subsystems ($M>3$): Minimal model for Thermalization [8,9].

The minimal model for thermalization

The FPE description makes sense if the sub-systems are chaotic.

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

Minimal model for thermalization: BHH trimer + monomer

\[ N = 60 \text{ = number of particles} \]

\[ x = \text{occupation of the trimer} \]

\[ N - x = \text{occupation of the monomer} \]

\[ f(x) = \text{probability distribution} \]

\[ \frac{\partial f(x)}{\partial t} = \frac{\partial}{\partial x} \left[ g(x) D(x) \frac{\partial}{\partial x} \left( \frac{f(x)}{g(x)} \right) \right] \]
Dynamical localization

Here we start the simulation with $x_0 = 60$, meaning that initially all the particles are in the trimer. We plot the saturation profile $P_\infty(x,\varepsilon)$. 

Classical  Quantum
The LDOS of the initial preparation

We observed dynamical localization if we start with $x_0 < 30$ or with $x_0 > 55$.

Let us look on the LDOS of representative preparations:

Localization does not always manifests as sparsity. It depends on the geometry of the $r = (x, \epsilon)$ space.
Localization of the eigenstates

Upper panel:
The unperturbed states $|r\rangle = |x, \varepsilon\rangle$, color-coded according to $F_{qm}$, arranged by $(x, \varepsilon)$.

Lower panel:
The perturbed states $|E_{\alpha}\rangle$, color-coded according to $\text{var}(x)_{\alpha}$, sorted by $(\langle x \rangle_{\alpha}, \langle \varepsilon \rangle_{\alpha})$. 
Participation, Exploration, and Breaktime

We display $\Omega_{cl}(t)$, and $\Omega_{sc}(t)$, and $\Omega_{qm}(t)$, and $\mathcal{N}(t)$.

The breaktime is determined by the intersection of the scaled $\mathcal{N}_{sc}(t)$ with the scaled $\Omega_{cl}(t)$.

Prediction:

$$\mathcal{F}_{s} \equiv \frac{\Omega_{qm}}{\Omega_{sc}}$$

$$\Omega_{\infty} \approx \mathcal{F}_{erg} \Omega_{t^*}$$
Localization measures

\[ \mathcal{F}^{cl} = \frac{\Omega^{cl}}{\Omega_E} \]
\[ \mathcal{F}^{qm} = \frac{\Omega^{qm}}{N_E} \]
\[ \mathcal{F}^{s} = \frac{\Omega^{sqm}}{\Omega^{sc}} \]
\[ \mathcal{F}_{predicted} \]

For ergodic system

\[ \Omega^{cl} \sim \Omega_E \]
\[ \Omega^{sc} \sim \sqrt{[N_E(r_0)]^2 + \Omega_E^2} \]
The "classical exploration" notion of random walk

Spreading (semiclassical or quantum):
\[ \Omega_{sc/qm}^t = \left\{ \sum_r [P_t(r|r_0)]^2 \right\}^{-1} \equiv \text{PN} \{ [r_0], t \} \]

Classical exploration:
\[ \Omega_{cl}^t = \text{PN} \{ r_0, [0, t] \} \]

Which can be written as
\[ \Omega_{cl}^t \equiv \left\{ \text{trace} \left[ \rho_{cl}(t)^2 \right] \right\}^{-1} \]

Classical exploration for random walk on a lattice [Montroll and Weiss 1965]:
\[ \Omega_t \sim \sqrt{D_0 t} \quad \text{for } d = 1 \]
\[ \Omega_t \sim \frac{v_0 t}{\log(t)} \quad \text{for } d = 2 \]
\[ \Omega_t \sim v_0 t \quad \text{for } d > 2 \]

Example:
Random walk in 3D
\( t = 100 \) steps
explored volume \( \sim 99 \)
spreading radius \( \sim 10 \)
spreading volume \( \sim 1000 \)
The breaktime concept

- Stationary view of strong localization: interference of trajectories.
- Scaling theory of localization: the importance of dimensionality.
- Dynamical view of strong localization: breakdown of quantum-classical correspondence.

\[
t_H[\Omega] = \frac{2\pi}{\Delta_0} \propto \Omega
\]

\[t \ll t_H[\Omega_t] \sim t^*
\]

\[\Omega_t = \sqrt{D_0 t} \quad \text{for } d = 1 \quad \sim \quad \text{always localization}
\]

\[\Omega_t = c_0 + v_0 t \quad \text{for } d > 2 \quad \sim \quad \text{mobility edge}
\]

For diffusion in 1D we get \(\xi = gD\), where \(g\) is the local DOS.

Manifestation of localization in thermalization?

\[
\frac{\partial f(\varepsilon)}{\partial t} = \frac{\partial}{\partial \varepsilon} \left( g(\varepsilon) D(\varepsilon) \frac{\partial}{\partial \varepsilon} \left( \frac{1}{g(\varepsilon)} f(\varepsilon) \right) \right)
\]

\(g(\varepsilon)\) - local density of states

Rate of energy transfer [FPE version]:

\[ A(\varepsilon) = \partial_\varepsilon D + (\beta_1 - \beta_2) D \]

For canonical preparation:

\[ \langle A(\varepsilon) \rangle = \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \langle D(\varepsilon) \rangle \]

Here we considered a Bose-Hubbard system where the diffusion is in \(x\)

\(x = \) the occupation of subsystem 1

\(N-x = \) the occupation of subsystem 2

Hurowitz, DC (EPL 2011) - MEQ version
Tikhonenkov, Vardi, Anglin, DC (PRL 2013)] - FPE version
Bunin, Kafri (JPA 2013) - NFT version
Khripkov, Vardi, DC (NJP 2015) - Resistor network calculation of \(D(\varepsilon)\)

**Question:** Do we have \(\xi = g(\varepsilon) D(\varepsilon)\)?
Phase space formulation of the QCC condition

We propose a generalized QCC condition for the purpose of breaktime determination:

Rough version: \[ t < \left[ \frac{\Omega_{t}^{cl}}{\Omega_{E}} \right] t_H \]

Refined version: \[ N_{sc}^{t} < \mathcal{F}_{erg}^{qm} \left[ \frac{N_{E}}{\Omega_{E}} \right] \Omega_{t}^{cl} \]

- \( N_{E} \) = total number of states within the energy shell (\( r_0 \) dependent)
- \( \mathcal{F}_{erg}^{qm} \) = filling fraction for a quantum ergodic state, say = 1/3
- \( \Omega_{E} \) = number of cells that intersect an energy-surface
- \( \Omega_{t}^{cl} \) = explored phase-space volume during time \( t \) (starting at \( r_0 \))
- \( N_{sc}^{t} \approx t/t_{E} \) = semiclassical number of participating-states during time \( t \)

\[ |\langle r_{j} | E_{\alpha} \rangle |^2 \]

It is unavoidable to use in the semiclassical analysis improper Planck cells. Namely, a chaotic eigenstate is represented by a microcanonical energy-shell of thickness \( \propto \hbar^{d} \) and radius \( \propto \hbar^{0} \). For some preparations it is implied that \( N_{E} \ll \Omega_{E} \) rather than \( N_{E} \sim \Omega_{E} \).

Cartoon: \( \Omega_{E} = 8 \), while \( N_{E} = 5 \).

Proper Planck cell: \( \Delta Q \Delta P > \hbar/2 \) for each coordinate.
The "quantum exploration" notion of Heller

The LDOS:  \( \varrho(E) = \sum p_\alpha \delta(E - E_\alpha) \)

- \( \Delta_0 = \) The mean level spacing
- \( \Delta_E = \) The width of the energy shell
- \( N_E = \) States within the energy shell
- \( N_\infty = \) Participating states
- \( \mathcal{F}^{qm} = \) Localization measure

\[
\begin{align*}
    t_H &= \frac{2\pi}{\Delta_0}, \\
    t_E &= \frac{2\pi}{\Delta_E}, \\
    N_E &= \frac{\Delta E}{\Delta_0}, \\
    N_\infty &= \left[ \sum p_\alpha^2 \right]^{-1}, \\
    \mathcal{F}^{qm} &\equiv \frac{N_\infty}{N_E}
\end{align*}
\]

The number of states that participate in the dynamics up to time \( t \) is:

\[
N_t \equiv \left\{ \operatorname{trace} [\bar{\rho}(t)^2] \right\}^{-1} = \left[ \frac{2}{t} \int_0^t \left( 1 - \frac{\tau}{t} \right) \mathcal{P}(\tau) d\tau \right]^{-1} \quad \bar{\rho}(t) \equiv \frac{1}{t} \int_0^t \rho(t') dt'
\]

Short times: \( N_t^{qm} \approx N_t^{sc} \approx t/t_E \) (based on the classical envelope)

Long times: \( N_t^{cl} \to N_\infty \) (due to the discreteness of the spectrum)
Quantum Chaos perspective on Metastability and Ergodicity

Stability of flow-states (I):
- Landau stability of flow-states ("Landau criterion")
- Bogoliubov perspective of dynamical stability
- KAM perspective of dynamical stability

Stability of flow-states (II):
- Considering high dimensional chaos ($M > 3$).
- Web of non-linear resonances.
- Irrelevance of the familiar Beliaev and Landau damping terms.
- Analysis of the quench scenario.

Coherent Rabi oscillations:
- The hallmark of coherence is Rabi oscillation between flow-states.
- Ohmic-bath perspective $\sim \eta = (\pi/\sqrt{\gamma})$
- Feasibility of Rabi oscillation for $M < 6$ devices.
- Feasibility of chaos-assisted Rabi oscillation.

Thermalization:
- Spreading in phase space is similar to Percolation.
- Resistor-Network calculation of the diffusion coefficient.
- Observing regions with Semiclassical Localization.
- Observing regions with Dynamical Localization.
The Model (non-rotating ring)

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

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

In a semi-classical framework:

$$a_j = \sqrt{n_j} e^{i\varphi_j}, \quad [\varphi_j, n_i] = i\delta_{ij}$$

$$z = (\varphi_1, \cdots, \varphi_M, \ n_1, \cdots, n_M)$$

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

$$H(z) = \sum_{j=1}^{M} \left[ \frac{U}{2} n_j^2 - K \sqrt{n_{j+1}n_j} \cos(\varphi_{j+1} - \varphi_j) \right]$$

The dynamics is generated by the Hamilton equation:

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

(DNLS)

Classically there is a single dimensionless parameter:

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

Rescaling coordinates:

$$\tilde{n} = n/N$$

$$[\varphi_j, \tilde{n}_i] = i\frac{1}{N} \delta_{ij}$$

$$\gamma \equiv \frac{m^* g}{\rho} = \frac{Mu}{N^2}$$
The model (rotating ring)

In the rotating reference frame we have a Coriolis force, which is like magnetic field $B = 2m\Omega$. Hence is is like having flux 

$$\Phi = 2\pi R^2 m \Omega$$

Note: there are optional experimental realizations.

$$\mathcal{H} = \sum_{j=1}^{M} \left[ \frac{U}{2} a_j^\dagger a_j^\dagger a_j a_j - \frac{K}{2} \left( e^{i(\Phi/M)} a_{j+1}^\dagger a_j + e^{-i(\Phi/M)} a_j^\dagger a_{j+1} \right) \right]$$

Summary of model parameters:

The ”classical” dimensionless parameters of the DNLS are $u$ and $\Phi$.

The number of particles $N$ is the ”quantum” parameter (optionally $\gamma$).

The system has effectively $d = M - 1$ degrees of freedom.

- $M = 2$  Bosonic Josephson junction (Integrable)
- $M = 3$  Minimal circuit (mixed chaotic phase-space)
- $M > 3$  High dimensional chaos (Arnold diffusion)
- $M \to \infty$ Continuous ring (Integrable)
Flow-state stability regime diagram

The $I$ of the maximum current state is imaged as a function of $(\Phi, u)$

- solid lines = energetic stability borders (Landau)
- dashed lines = dynamical stability borders (Bogoliubov)

The traditional paradigm associates flow-states with stationary fixed-points in phase space. Consequently the Landau criterion, and more generally the Bogoliubov linear-stability-analysis, are used to determine the viability of superfluidity.
Energetic vs Dynamical stability

Poincare section $n_2 = n_3$ at the flow-state energy.

1. Energetic stability;
2. Dynamical stability.

Red trajectories = large positive current
Blue trajectories = large negative current

The flow-state fixed-points are located along the symmetry axis:

$n_1 = n_2 = \cdots = N/M, \quad \varphi_i - \varphi_{i-1} = \left(\frac{2\pi}{M}\right) m$

Forced region

\begin{align*}
\varphi_1 - \varphi_3 & \quad n_1 - n_3
\end{align*}
KAM stability - elliptic islands and chaotic ponds

\( u = 2.5, \Phi = 0.95\pi \)

\( u = 2.5, \Phi = 0.6\pi \)

\( u = 2.5, \Phi = 0.44\pi \)

Forbidden region

\( \phi_1 - \phi_3 \)

\( n_1 - n_3 \)
Swap transition

In (4) and (5) dynamical stability is lost \( \sim \) chaotic motion. But the chaotic trajectory is confined within a chaotic pond; uni-directional chaotic motion; superfluidity persists! At the separatrix swap-transition superfluidity diminishes.

Swap transition (dotted line):

\[
u = 18 \sin \left( \frac{\pi}{6} - \frac{\Phi}{3} \right)\]
Manifestation of phase space topology for $M > 3$ circuits

Number of freedoms: $d = (M-1)$

$d = 2$ Mixed phase space: islands, ponds, and chaotic sea

$d > 2$ High dimensional chaos: Arnold web and chaotic sea

- The energy surface is $2d - 1$ dimensional
- KAM tori are $d$ dimensional
- The KAM tori are not effective in blocking the transport on the energy shell if $d > 2$.
- Resonances form an “Arnold Web” $\leadsto$ “Arnold diffusion”
- As $u$ becomes larger this non-linear leakage effect is enhanced, stability of the motion is deteriorated, and the current is diminished.

For $M = 3$ the 3 dimensional energy surface is divided into territories by the 2 dimensional KAM tori.

For $M = 4$ the 5 dimensional energy surface cannot be divided into territories by the 3 dimensional KAM tori.
Non-linear resonances

Regime diagram for flow-state metastability:
- Via quantum eigenstates
- Via quantum quench simulation
- Via semiclassical simulation

Observation:
The linear-stability analysis of Bogoliubov is not a sufficient condition for strict dynamical stability. A non-linear resonance between the frequencies can destroy the dynamical stability.

The “1:2” resonance for the $m = 1$ flow-state of $M = 4$ ring:

$$u = 4 \cot \left( \frac{\Phi}{4} \right) \left[ 3 \cos \left( \frac{\Phi}{4} \right) - \sqrt{6 + 2 \cos \left( \frac{\Phi}{2} \right)} \right]$$

Addressing all flow-states in one diagram:

$$\phi = \Phi - 2\pi m = \text{unfolded phase} \in [-M\pi, M\pi]$$
The non-linear terms

\[ H = \sum_k \epsilon_k b_k^\dagger b_k + \frac{U}{2M} \sum_{k_1 \ldots k_4} b_{k_4}^\dagger b_{k_3}^\dagger b_{k_2} b_{k_1} \]

Assuming condensation at the \( k=0 \) orbital the Hamiltonian can be expressed in terms of Bogoliubov quasi-particles creation operators:

\[ b_q^\dagger = u_q c_q^\dagger + v_q c_{-q} \]

\( q = \frac{2\pi}{M} m \)

\( m = \text{integer} \neq 0 \)

\[ \frac{M}{2} < m \leq \frac{M}{2} \]

Approximated Hamiltonian at the vicinity of the condensate:

\[ H = \sum_q \omega_q c_q^\dagger c_q + \frac{\sqrt{N}U}{M} \sum_{\langle q_1, q_2 \rangle} \left[ A_{q_1, q_2} (c_{-q_1 - q_2} c_{q_2} c_{q_1} + \text{h.c.}) + B_{q_1, q_2} \left( c_{q_1 + q_2} c_{q_2} c_{q_1} + \text{h.c.} \right) \right] \]

- The ”B” terms are the Beliaev and Landau damping terms. [gray lines]
- The ”A” terms are usually ignored. [red lines]
Mapping the non-linear resonances

\[
\begin{align*}
\omega_{q_1} + \omega_{q_2} - \omega_{q_1+q_2} &= 0 \\
\omega_{q_1} + \omega_{q_2} + \omega_{-q_1-q_2} &= 0
\end{align*}
\]

[gray lines]

[red lines]

Considering the “1:2” resonance for the \( m = 1 \) flow-state of the \( M = 4 \) ring, setting \( q_1 = q_2 = q = 2\pi/4 \), we get from \( 2\omega_q + \omega_{-2q} = 0 \) the resonance condition

\[
u = 4 \cot \left( \frac{\Phi}{4} \right) \left[ 3 \cos \left( \frac{\Phi}{4} \right) - \sqrt{6 + 2 \cos \left( \frac{\Phi}{2} \right)} \right]
\]
**Metastability - The Big Picture**

- **(traditional)** Energetic metastability, aka Landau criterion.
- **(traditional)** Dynamical metastability via linear stability analysis, aka BdG.
- Strict dynamical metastability (KAM, applies if $d = 2$)
- Quasi dynamical metastability (might be the case for $d > 2$)

In the absence of constants of motion, a generic system with $d > 2$ degrees-of-freedom tends to be ergodic. But the equilibration might be an extremely slow process.

**Quasi stability** might become **Quantum stability** due to **dynamical localization**. The breaktime is determined from the breakdown of the QCC condition.