Thermalization in Quantum Systems

Jonas Larson

Stockholm University and Universität zu Köln

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Motivation

- Long time evolution of closed quantum systems not fully understood.
- Cold atom system → Not only of academic interest.
- Open questions in closed system quantum dynamics:

  i. Criteria for equilibration/thermalization.
  ii. Mechanism behind thermalization.
  iii. Properties of equilibrated states.
  iv. Definition for "quantum integrability".
  v. Many-body localization…

  vi. Open systems…

Outline

1. Quantum Thermalization.
2. Integrability. Problems.
3. Chaos. Problems.
4. Localization and absence of *ETH*.

Quantum Thermalization

Quantum Thermalization

- Characteristics of $\hat{\rho}$ for long times.

1) Weak coupling.
2) Infinite degrees of freedom (bath).
3) Delta correlated in time (bath): Markov approximation (no memory).
4) Factorizable system-bath state (Born approximation).

Thermalization of system.

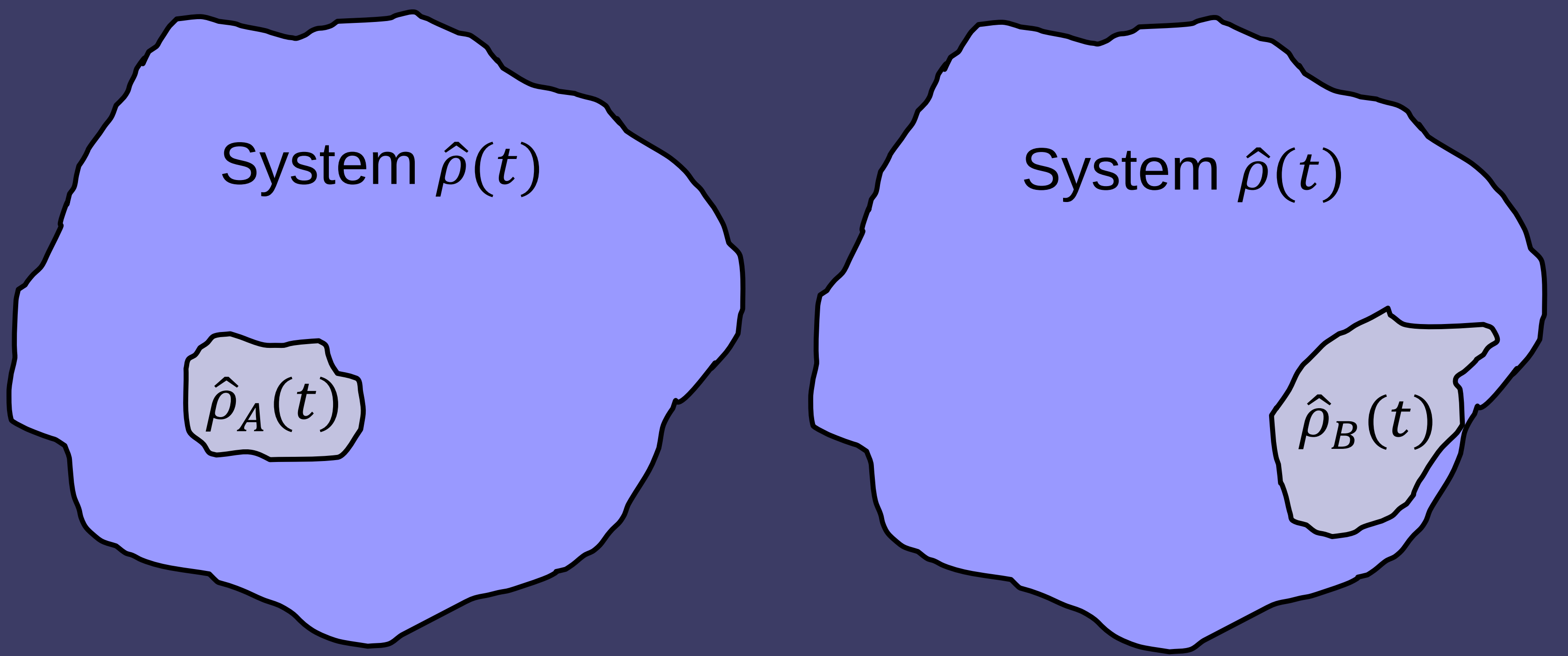
$$\partial_t \hat{\rho} = i\left[\hat{\rho}, \hat{H}_{sys}\right] + \hat{L}[\hat{\rho}]$$

Quantum Thermalization

Equilibration

Closed system

- Characteristics of $\hat{\rho}_s(t)$ for long times.
- No clear separation "system/bath", no Born-Markov nor rotating-wave approximations.



Srednicki, *Phys. Rev. E* (1994).

Quantum Thermalization

Equilibration

Closed system

- Characteristics of $\hat{\rho}(t)$ for long times.
- Equilibration:

$$\langle \hat{A} \rangle = Tr\left[\hat{A}\hat{\rho}(t)\right], \qquad \begin{cases} t - \text{independent as } t \to \infty \\ \hat{A} \quad \text{local observable.} \end{cases}$$

- Thermalization:

$$\langle \hat{A} \rangle = \langle \hat{A} \rangle_{Th} \qquad \text{at long times}$$

$$\langle \hat{A} \rangle_{Th} = \mathrm{Tr}\left[\hat{A}\hat{\rho}_{Th}\right],$$

where $\hat{\rho}_{Th}$ = thermal state. "Temperature" determined from $\langle \widehat{H} \rangle$.
No memory of initial state.

Srednicki, *Phys. Rev. E* (1994).

Quantum Thermalization

ETH – *Eigenstate Thermalization Hypotesis*

- $|\Psi(t)\rangle = \sum_\gamma C_\gamma e^{-iE_\gamma t/\hbar}|\psi_\gamma\rangle \;\rightarrow$

$$\langle \hat{A}(t) \rangle = \sum_{\gamma,\delta} C_\delta{}^* C_\gamma e^{i(E_\delta - E_\gamma)t/\hbar} A_{\delta\gamma}, \qquad A_{\delta\gamma} = \langle \psi_\delta | \hat{A} | \psi_\gamma \rangle$$

- If thermalization (long-time limit)

$$\langle \hat{A} \rangle^{LT} = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \langle \hat{A}(t) \rangle = \sum_\gamma |C_\gamma|^2 A_{\gamma\gamma}.$$

- *ETH*: $A_{\gamma\gamma}$ is approximately constant in the ”energy window” of the state Ψ .

- *ETH*: For all γ, $\hat{\rho}_A = \mathrm{Tr}_B\left[|\psi_\gamma\rangle\langle\psi_\gamma|\right]$ is thermal.

Rigol, Nature 2008.

Quantum Thermalization

Thermalization

- Which systems thermalize?

  Possible candidates:

  1) Quantum non-integrable systems.
  2) Chaotic systems.

Integrability

Integrability

101 Quantum Integrability

- Classical systems:

  Definition: A system is integrable if the number of degrees of freedom *N* is smaller than or equal to the number *K* of *independent* constants of motion.

$$\{Q_n, H\} = 0, \qquad n = 1, 2, \dots, K, \qquad \{Q_n, Q_m\} = 0 \quad \forall n, m$$

Arnold, *Mathematical Methods in Classical Mechanics*

Integrability

101 Quantum Integrability

- Quantum systems:

  Definition 1: Replace $\{\ ,\ \} \rightarrow i[\ ,\ ]/\hbar$. Fails, take $\hat{P}_\gamma = |\psi_\gamma\rangle\langle\psi_\gamma|$.

  Definition 2: Use definition 1, but consider *relevant* constants of motion - that is operators with classical counterparts. Fails, not all operators have any classical corresponding observable.

  Definition 3: Poissonian level statistics ($P(S) = e^{-S}$) implies integrability.

  Definition 4: Level crossings implies integrability.

  $\vdots$

  Definition 64: A quantum system is integrable if it is exactly solvable.

Caux, J. Stat. Mech. 2011

Integrability vs thermalization

Spin-orbit coupled particle

Rabi Model

- *Rabi Hamiltonian* of quantum optics

$$\hat{H}_R = \omega \hat{a}^+ \hat{a} + \frac{\Omega}{2}\hat{\sigma}_z + v(\hat{a}^+ + \hat{a})\hat{\sigma}_x.$$

- Z_2-parity symmetry

$$[\hat{U}_p, \hat{H}_R] = 0, \qquad \hat{U}_p = e^{i\pi\left(\hat{a}^+\hat{a} + \frac{\hat{\sigma}_z}{2}\right)}.$$

- Drive term breaks Z_2 (total energy only preserved quantity)

$$\hat{H}_{dR} = \omega \hat{a}^+ \hat{a} + \frac{\Omega}{2}\hat{\sigma}_z + v(\hat{a}^+ + \hat{a})\hat{\sigma}_x + \gamma\hat{\sigma}_x.$$

Scully & Zubary, *Quantum Optics* (CUP)

Integrability vs thermalization

Spin-orbit coupled particle

Rabi Model

- Is the driven Rabi model integrable?
- **Definition 1-2**: "Two" degrees of freedom, only one (relevant) constant of motion (energy) → Non-integrable.

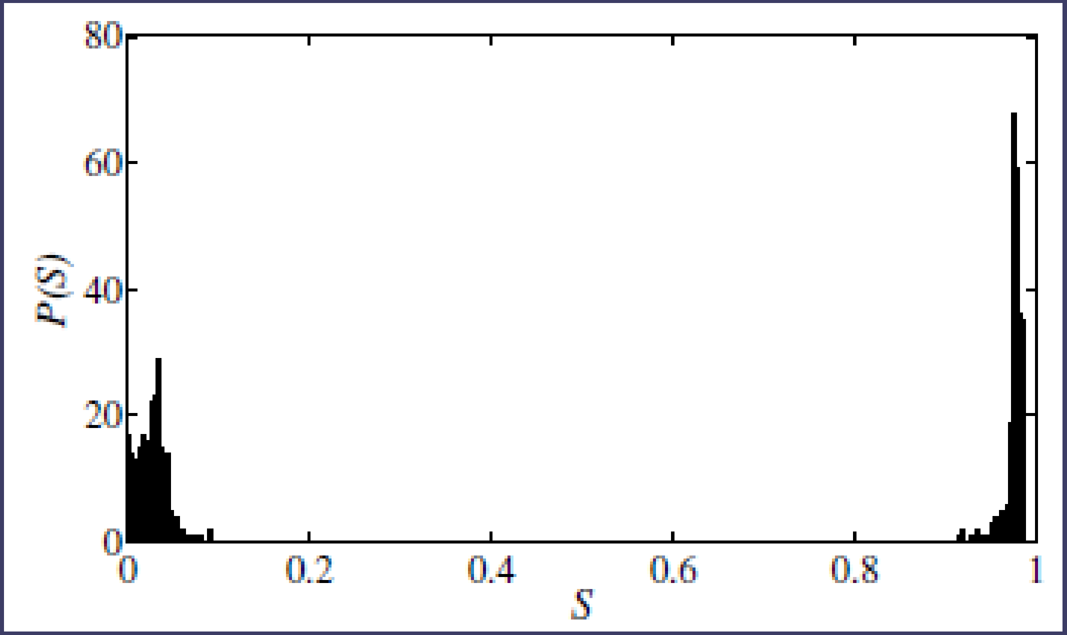
Larson, *J. Phys. B* (2013) (JC issue)

Integrability vs thermalization

Spin-orbit coupled particle

Rabi Model

- Is the driven Rabi model integrable?
- **Definition 3**: Level-statistics. Two branches, neither Poissonian → Non-integrable.



Level statistics of the Rabi model.

Larson, *J. Phys. B* (2013) (JC issue)

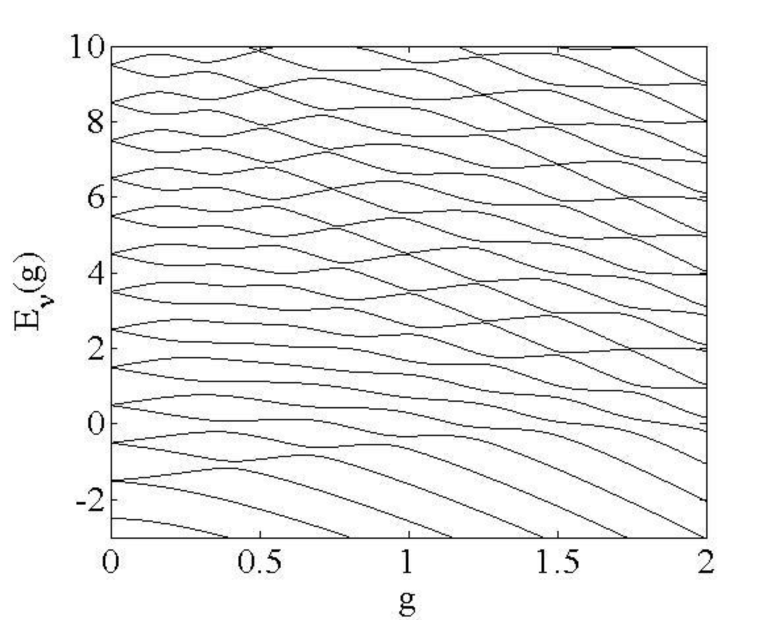
Integrability vs thermalization

Spin-orbit coupled particle

Rabi Model

- Is the driven Rabi model integrable?

- **Definition 4**: Avoided crossings. No vissible crossings → Non-integrable.



Energies of the Rabi model.

Larson, *J. Phys. B* (2013) (JC issue)

Integrability vs thermalization

Spin-orbit coupled particle

Rabi Model

- Is the driven Rabi model integrable?

- **Definition 64**: Solvable. Braak (PRL 2011) says it might be solvable but not integrable, others say it is *quasi solvable* → integrable?

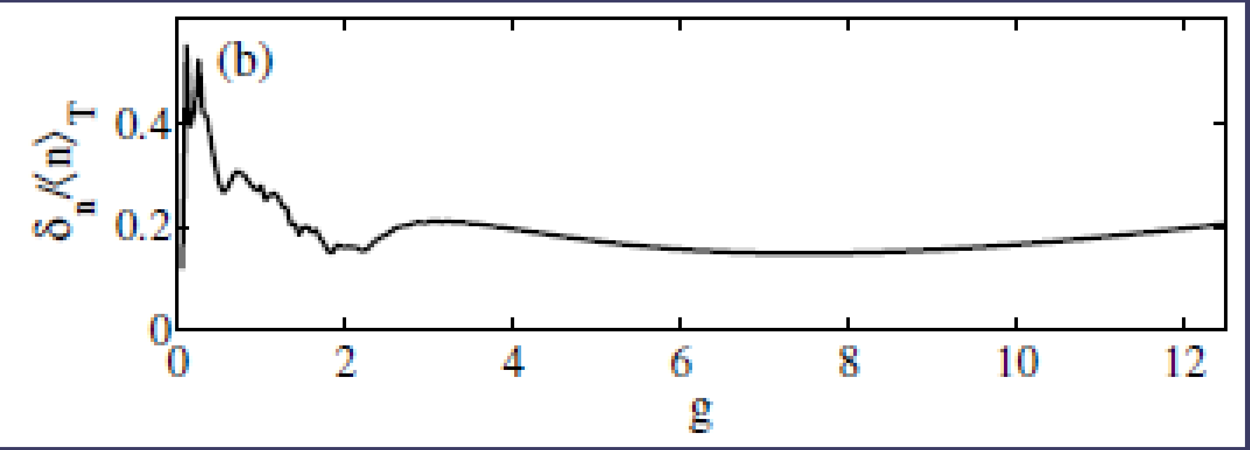
Larson, J. *Phys. B* (2013) (JC issue)

Integrability vs thermalization

Spin-orbit coupled particle

Rabi Model

- Does the driven Rabi model thermalize?
- If quantum non-integrability implies thermalization a qualified guess would be yes.



Scaled variance of $\langle \hat{n}(t) \rangle$. Thermalization $\rightarrow \delta_n = 0$. No thermalization!

Chaos

Classical chaos

Butterfly effect

Hamilton equations:

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j}, \quad \frac{dq_j}{dt} = \frac{\partial H}{\partial p_j}, \qquad j = 1,2,\dots,n.$$

- A solution $R^1(t) = \left(q_1{}^{(1)}(t), \dots, q_n{}^{(1)}(t), p_1{}^{(1)}(t), \dots, p_n{}^{(1)}(t)\right)$ lives on a surface in $2n$-dimensional phase space.
- Chaotic system – exponential spreading:

$$|R^1(t) - R^2(t)| \propto e^{\lambda t}, \qquad \lambda > 0.$$

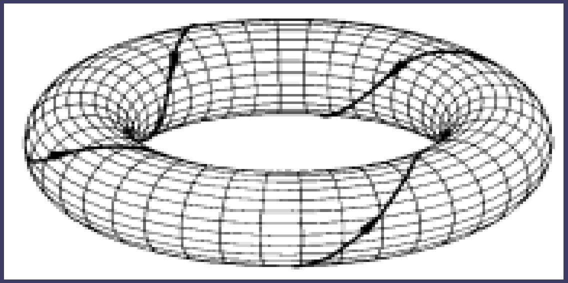
Lyapunov exponent λ

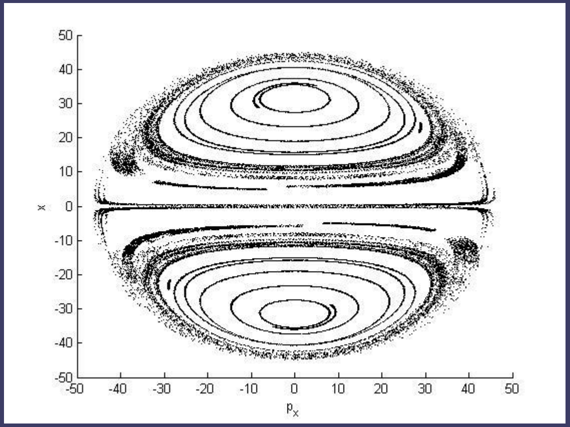
Gutzwiller, *Chaos in Classical and Quantum mechanics (Springer)*

Classical chaos

KAM Theory

- Regular motion: Any solution $R^1(t) = \left(q_1{}^{(1)}(t), \ldots, q_n{}^{(1)}(t), p_1{}^{(1)}(t), \ldots, p_n{}^{(1)}(t)\right)$ lives on a tori in the $2n$-dimensional phase space.
- Add a perturbation V that beaks integrability. KAM describes how the tori is gradually deformed.
- Cranking up V: Going from regular to full blown chaos.





Poincaré section

Quantum chaos

Butterfly effect

Schrödinger equation:

$$\frac{d\hat{\rho}}{dt} = i\left[\hat{\rho}, \hat{H}\right].$$

Unitary linear evolution

- Trace distance

$$T(\hat{\rho}_1(t), \hat{\rho}_2(t)) \equiv \frac{1}{2}\mathrm{Tr}\left[\sqrt{(\hat{\rho}_1(t) - \hat{\rho}_2(t))^2}\right] = \frac{1}{2}\sum_i |\mu_i| = \mathrm{const.}$$

μ_i eigenvalues of $(\hat{\rho}_1(t) - \hat{\rho}_2(t))$

- Quantum mechanics – linear theory.
- No Butterfly effect! Or…

Peres, *Quantum Theory, Concepts and Methods* (Kluwer)

Quantum chaos

Butterfly effect

- Perturbation $\hat{\Gamma}$: $\hat{H}_1 = \hat{H}$ and $\hat{H}_2 = \hat{H} + \hat{\Gamma}$.
- Evolution, $\frac{d\hat{\rho}_1}{dt} = i[\hat{\rho}_1, \hat{H}_1]$ and $\frac{d\hat{\rho}_2}{dt} = i[\hat{\rho}_2, \hat{H}_2]$.
- Trace distance

$$T(\hat{\rho}_1(t), \hat{\rho}_2(t)) \propto e^{\lambda t}$$

- Quantum butterfly effect!
- Non-unitary evolution → butterfly effect,

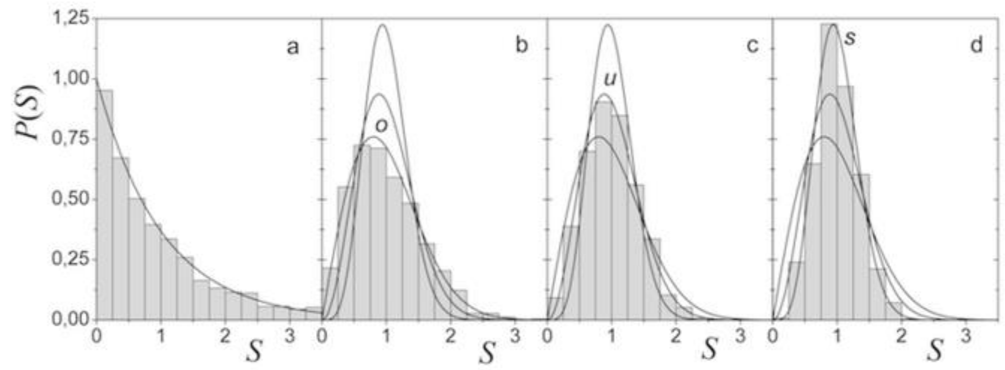
$$\frac{d\hat{\rho}}{dt} = i[\hat{\rho}, \hat{H}] + \hat{L}[\hat{\rho}].$$

Zurek, *Rev. Mod. Phys.* (2003).

Quantum chaos

Characteristics of quantum chaotic systems

- Spectrum E_n.
- Energy separation $s_n = E_{n+1} - E_n$.
- Normalized distribution $P(S)$.
- Regular motion: $P(S) = e^{-S}$ (Poisson distribution).
- Chaotic motion: $P(S) = \frac{\pi}{2} S^{\beta} e^{-\pi S^2/4}$ (Wigner distribution).



Kicked top

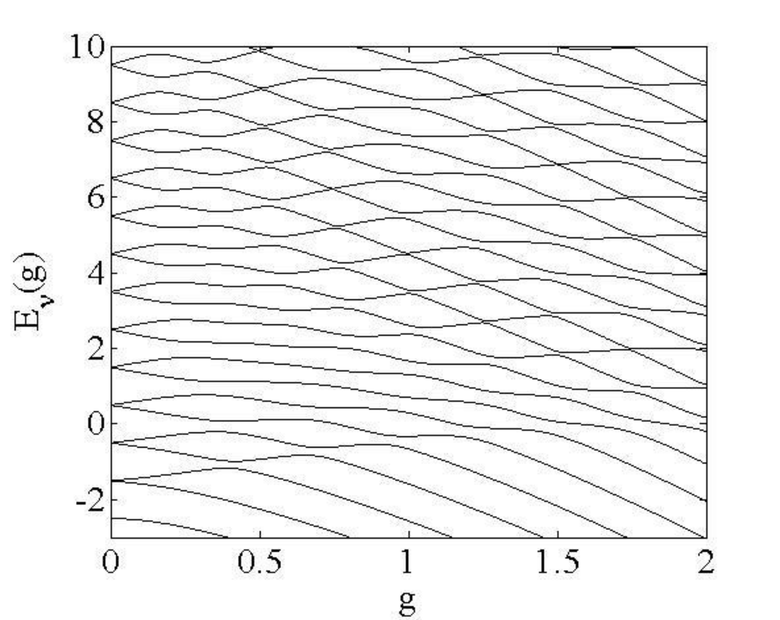
Level repulsion

Haake, *Quantum Signatures of Chaos* (Springer).

Quantum chaos

Characteristics of quantum chaotic systems

- Level repulsion → varying time-scales.
- Level repulsion → ergodicity.
- Level repuslion → avoided crossings.



Driven Rabi model

Haake, *Quantum Signatures of Chaos* (Springer).

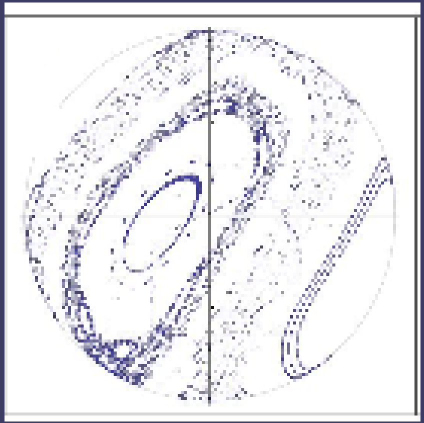
Chaos vs thermalization

Rabi Model

Spin-orbit coupled particle

- Mean-field for the bosons, parametrize the atom by

$$|\theta\rangle = \begin{bmatrix} \sqrt{(1+Z)/2} \\ \sqrt{(1-Z)/2}\, e^{i\delta} \end{bmatrix},$$



Poincaré section.

- Semi-classical Hamiltonian

$$H_{cl} = \frac{p^2}{2} + \frac{x^2}{2} + \frac{\omega}{2} Z + \left(gx\sqrt{2} + \gamma\right)\sqrt{1 - Z^2} \cos\delta.$$

- This Hamiltonian is chaotic in a classical sense → thermalization.

Larson, J. Phys. B (2013) (JC issue)

Chaos vs thermalization

Jahn-Teller Model

Spin-orbit coupled particle

- 2D SO coupling.

$$\hat{H}_{SO} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{r}^2 + v_x \hat{p}_x \hat{\sigma}_x + v_y \hat{p}_y \hat{\sigma}_y.$$

- $\omega = 0 \rightarrow$ dispersions

$$E_{\pm}(p_x, p_y) = \frac{1}{2m}\left({p_x}^2 + {p_y}^2\right) \pm \sqrt{(v_x p_x)^2 + \left(v_y p_y\right)^2}.$$

Larson, *Phys. Rev. A* (2009)

Chaos vs thermalization

Jahn-Teller Model

Spin-orbit coupled particle

- $v_x = v_y \rightarrow U(1)$ symmetry
  $\left[\hat{J}, \hat{H}_{SO}\right] = 0.$

Larson, *Phys. Rev. A* (2009).

Chaos vs thermalization

Jahn-Teller Model

Spin-orbit coupled particle

- $v_x = v_y \rightarrow U(1)$ symmetry
  $\left[\hat{J}, \widehat{H}_{SO}\right] = 0.$
- $v_x = v_y$ and $\omega \neq 0 \rightarrow \widehat{H}_{SO}$ equals dual $E \times \varepsilon$ −Jahn-Teller model.

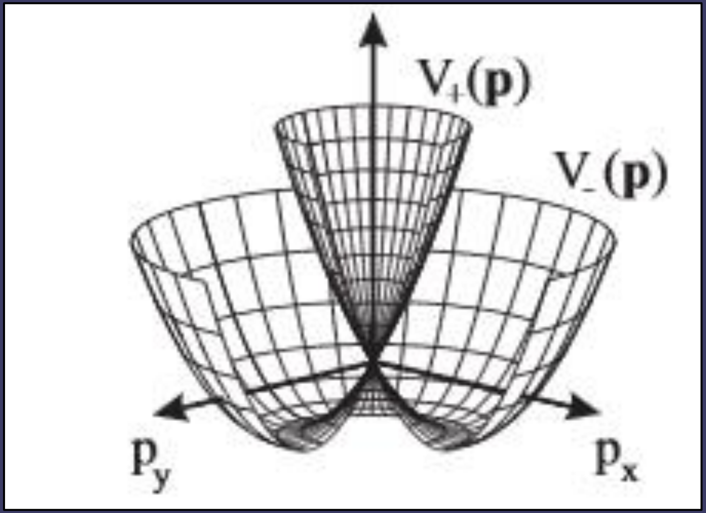
Larson, *Phys. Rev. A* (2009).

Chaos vs thermalization

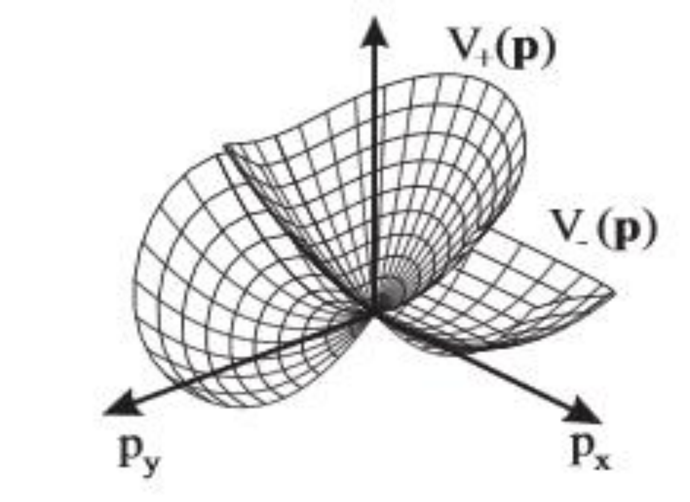
Jahn-Teller Model

Spin-orbit coupled particle

- $v_x = v_y \rightarrow U(1)$ symmetry $[\hat{J}, \widehat{H}_{SO}] = 0$.
- $v_x = v_y$ and $\omega \neq 0 \rightarrow \widehat{H}_{SO}$ equals dual $E \times \varepsilon$ –Jahn-Teller model.



- $v_x \neq v_y \rightarrow Z_2$ symmetry $[\hat{J}, \widehat{H}_{SO}] \neq 0.$
- $\widehat{H}_{SO}$ equals dual $E \times (\beta_1 + \beta_2)$ –Jahn-Teller model.



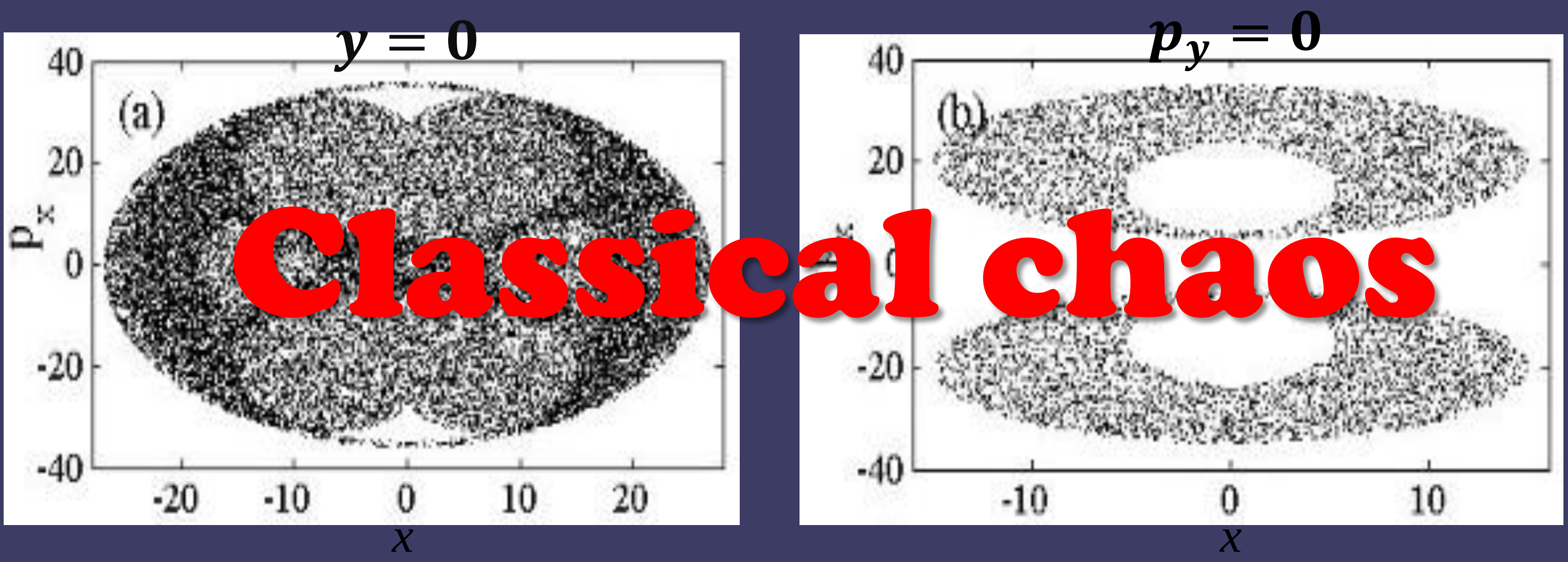
Larson, *Phys. Rev. A* (2009).

Chaos vs thermalization

Jahn-Teller Model

Classical dynamics

- Poincaré sections ($v_x \neq v_y$).



Larson, *Phys. Rev. A* (2013).

Chaos vs thermalization

Jahn-Teller Model

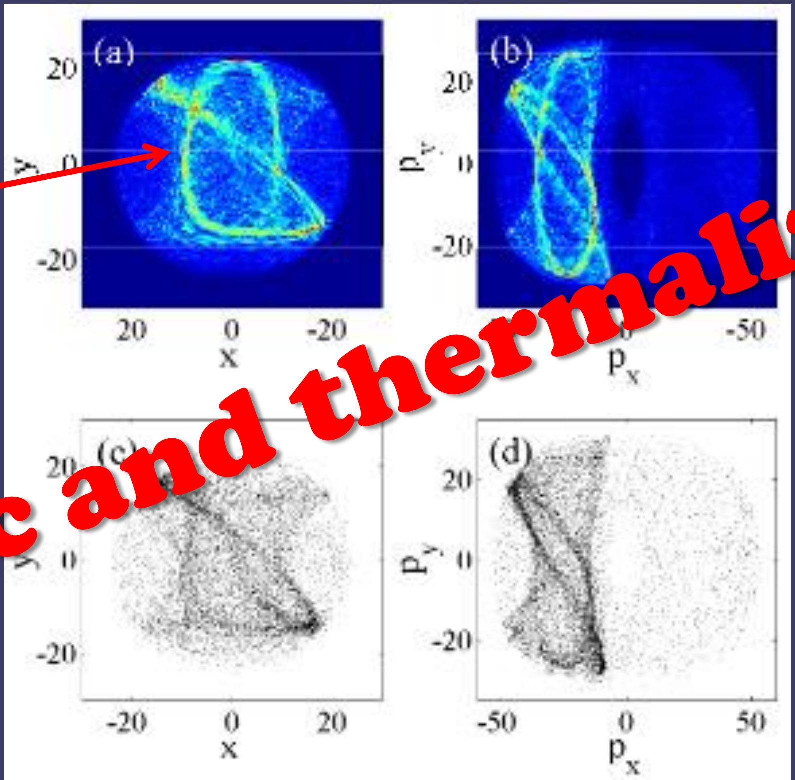
Breaking $U(1)$

Quantum dynamics

- Distributions ($v_x \neq v_y$).

Quantum Scars
Remnants of periodic classical solutions.

Heller, Phys. Rev. Lett. (1984).



Full Quantum

Truncated Wigner (Semi-classical)

Ergodic and thermalization

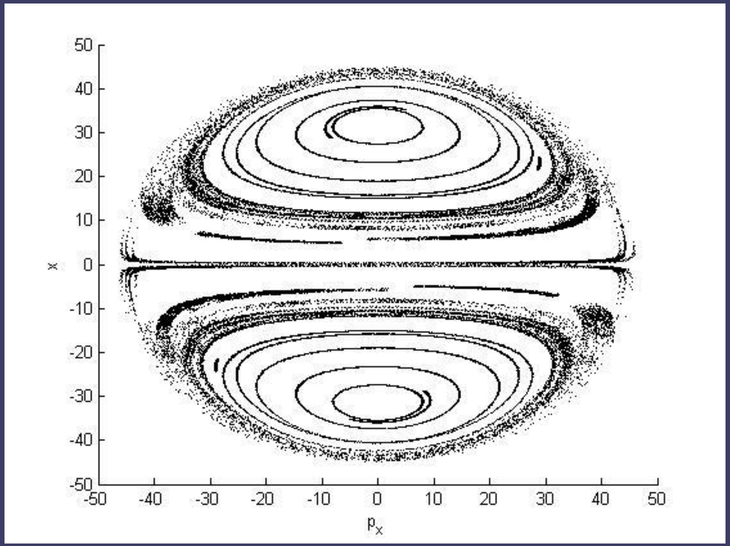
Larson, *Phys. Rev. A* (2013).

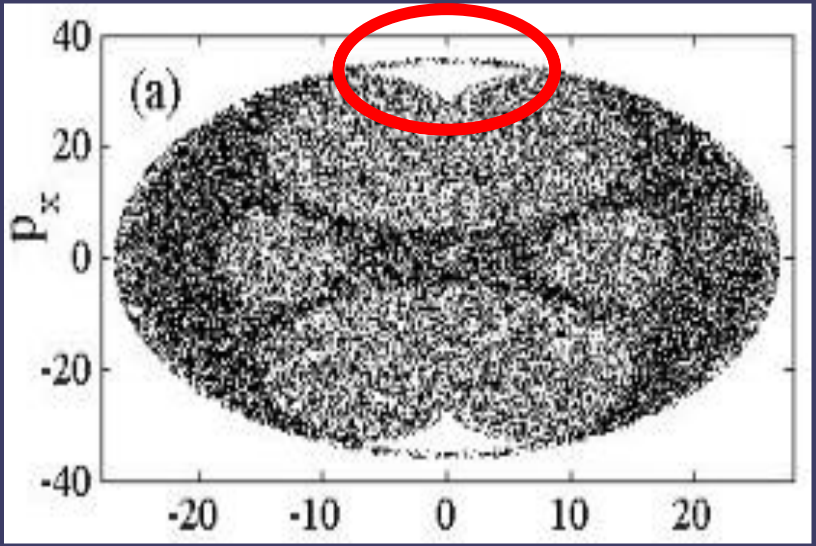
Chaos vs thermalization

Jahn-Teller Model

KAM theory

- ”Islands” may survive large integrability breaking perturbations.





Poincaré sections

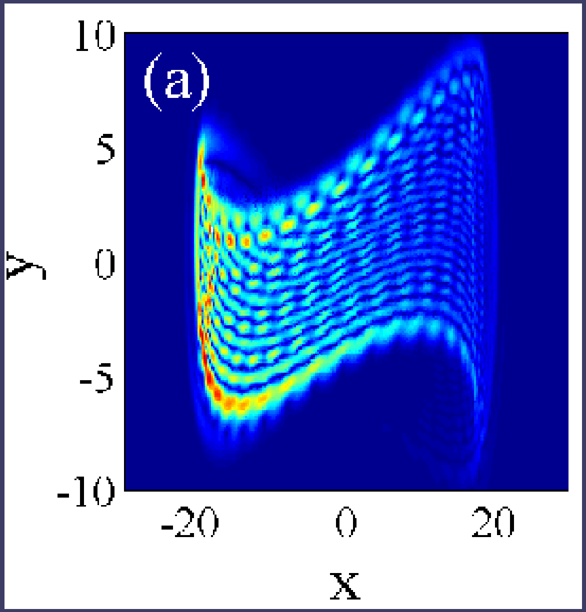
Larson, *Phys. Rev. A* (2013).

Chaos vs thermalization

Jahn-Teller Model

KAM theory

- Initiate a state in one island.



Distribution after long time when initial state in a regular island.

- No thermalization: Not all eigenstates obey *ETH*.

Larson, *Phys. Rev. A* (2013).

Localization

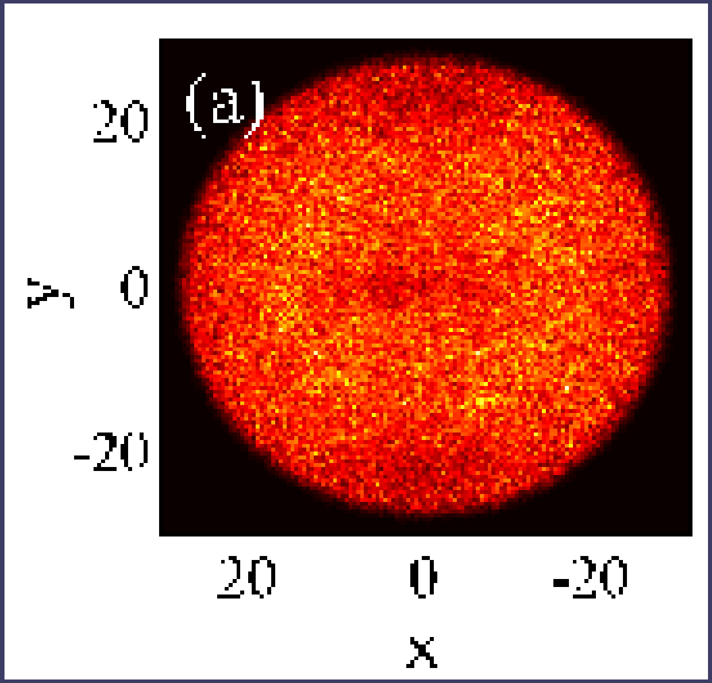
ETH revisited

Ergodicity

- Thermalization → ergodicity.
- Quantum information spreads over the whole accessible phase space.
- The information about a subsystem *A* is shared in the whole system *S*:

  $\hat{\rho}_A(t)$ diagonal/mixed.

- $\hat{\rho}_A(t)$ obeys a ”volume law”.
- Can ergodicity be lost in quantum non-integrable/chaotic systems?



Anderson localization

Quantum interference

- Add disorder to your system.
- Time inversion symmetry.
- Enhance probability to scatter into the same state (factor 2) than an arbitrary state.
- Quantum interference effect.
- No counterpart in classical systems (particles).

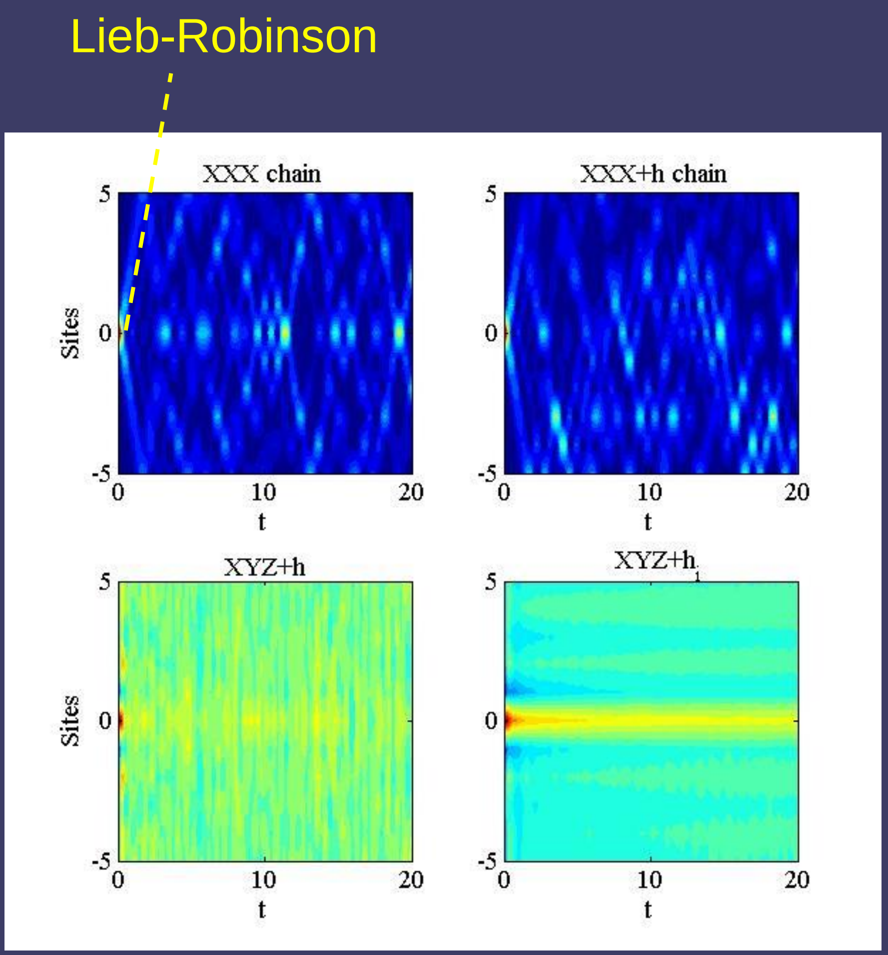
Anderson, *Phys. Rev. (1058)*.

Localization vs thermalization

- Spin models good for studying many-body localization

$$\hat{H} = \sum_i (J_x \hat{\sigma}^x{}_i \hat{\sigma}^x{}_{i+1} + J_y \hat{\sigma}^y{}_i \hat{\sigma}^y{}_{i+1} + J_z \hat{\sigma}^z{}_i \hat{\sigma}^z{}_{i+1} + h_i \hat{\sigma}^z{}_i)$$

- Clean XXX and XXY solvable, $XYZ + h$ non-integrable.
- Localization with strong enough disorder $h_i \in [-W, +W]$.
- Localized eigenstates are not thermal, no thermalization!



Larson, In progress.


Thanks!