Reaching Thermal States in Quantum Systems

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Outline

• Introduction: thermalisation

• Thermalisation protocol: sudden turn on of system (S) - bath (B) coupling

• Canonical Typicality and Eigenstate Thermalisation Hypothesis

• exact diagonalization: small (2+7 sites) Hubbard ring
  • (A) Long time: thermalisation as function of S-B coupling
  • (B) Dynamics of thermalisation
Thermalisation

- subsystem reaches equilibrium with bath through energy/particle exchange
- independent of the initial subsystem state
- independent of microscopic details of the bath: only macroscopic quantities matter, eg. $T, \mu$
- loss of coherence/entanglement with bath
- states of the subsystem are occupied with probability given by Gibbs distribution
Thermalisation: main results here

- Thermalisation in a small closed quantum system?
  - yes, for surprisingly small systems
  - dynamics of approach to thermalisation: exponential and Gaussian regimes

**Thermalisation**

- prepare system in product state of decoupled system and bath:
  \[ |\Psi(0)\rangle = |s_0b\rangle \equiv |s_0\rangle \otimes |b\rangle \]
  \[ \leftarrow \frac{1}{N_{\text{shell}}^{1/2}} \sum_{\epsilon_b \in [E_0, E_0 + \delta_b]} |\epsilon_b\rangle \]

- switch on coupling \( \lambda V \) suddenly: Dynamics of the Hubbard Model

- unitary evolution:
  \[ |\Psi(t)\rangle = e^{-i\hat{H}t} |\Psi(0)\rangle \]

- Subsystem described by reduced density matrix
  \[ \rho(t) \equiv \text{Tr}_{\text{bath}} |\Psi(t)\rangle \langle \Psi(t)| \]

- diagonal elements \( \langle s|\rho|s\rangle \) = occupation probabilities of subsystem states: becomes Gibbs distribution/canonical ensemble?

- off-diagonal elements = quantum coherence / entanglement: shrinks to zero?
Canonical Ensemble

- Gibbs-Boltzmann distribution
  - subsystem state $|s\rangle$ with energy $\varepsilon_s$
    $$\rho \propto \sum_s N_{\text{bath}}(E_0 - \varepsilon_s)|s\rangle\langle s|$$
    $$\sim \sum_s e^{-\beta \varepsilon_s} |s\rangle\langle s| \quad \text{for large bath} \ (E_0 \gg \varepsilon_s)$$
  - temperature defined from:
    $$\beta \equiv \frac{1}{k_B T} = \left. \frac{d \ln N_{\text{bath}}}{dE} \right|_{E_0}$$
Canonical Typicality

Goldstein et al. PRL 96, 050403 (2006)

- Pick a random state
  - $|\Psi\rangle = \sum_{A} C_{A} |E_{A}\rangle$
    - $|E_{A}\rangle$: eigenstate of whole system
  - $C_{A} \neq 0$ only in energy shell: $[E_{0}, E_{0} + \delta]$
- Reduced density matrix $\rho$ is approximately thermal for almost all choices of $|\Psi\rangle$
Eigenstate Thermalisation Hypothesis


- Project eigenstate \(|E_A\rangle\) to subsystem state \(|s\rangle\) (energy \(\varepsilon_s\)):

  \[ P_s \equiv \sum_b |sb\rangle\langle sb| \text{ for product states } |sb\rangle \]

  Hypothesis: \( \langle E_A|P_s|E_A \rangle \simeq e^{-\beta\varepsilon_s} \)

- Subsystem thermal behaviour encoded into \(|E_A\rangle\)

\[
\begin{aligned}
|E_{352}\rangle &= |\varepsilon_1\rangle|\varepsilon_{172}\rangle \\
|E_{351}\rangle &= |\varepsilon_2\rangle|\varepsilon_{98}\rangle \\
|E_{350}\rangle &= |\varepsilon_1\rangle|\varepsilon_{171}\rangle \\
\vdots &= \vdots \\
\end{aligned}
\]

\(\lambda^V e^{-\beta\varepsilon_1}|\varepsilon_1\rangle|B_1\rangle + e^{-\beta\varepsilon_2}|\varepsilon_2\rangle|B_2\rangle + \ldots \)

- For any state \(|\Psi\rangle = \sum_A C_A|E_A\rangle\), time average \(\rho_{ss} = \sum_A |C_A|^2\langle E_A|P_s|E_A \rangle\) is the thermal state independent of \(C_A\)
Eigenstate Thermalisation Hypothesis

Hamiltonian

\[ H_S = - \sum_{\sigma = \uparrow, \downarrow} J_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.}) + U (n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) \]

\[ H_B = - \sum_{i=3}^{L-1} \sum_{\sigma = \uparrow, \downarrow} J_{\sigma} (c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) + U \sum_{i=3}^{L} n_{i\uparrow}n_{i\downarrow} \]

\[ \lambda V = -\lambda \sum_{\sigma = \uparrow, \downarrow} J_{\sigma} \left[ (c_{2\sigma}^\dagger c_{3\sigma} + c_{1\sigma}^\dagger c_{L\sigma}) + \text{h.c.} \right] \]

- 8 fermions: 4\uparrow, 4\downarrow
- \( J_{\sigma} = J (1 + \xi \text{sgn}\sigma), \quad \xi = 0.05 \)
- \( U = J = 1 \)
- 15876 energy levels
- 16 subsystem energy levels
- \( \lambda = 1 \rightarrow \) homogeneous ring
Initial State

• Product states

\[ |\Psi(t = 0)\rangle = |s\rangle \frac{1}{N_{\text{shell}}^{1/2}} \sum_{b \in \text{shell}} |\epsilon_b\rangle \]

overlaps many exact eigenstates \( |E_A\rangle \) in energy shell
Initial State

- Product states
  \[ |\Psi(t = 0)\rangle = |s\rangle \frac{1}{N_{\text{shell}}^{1/2}} \sum_{b \in \text{shell}} |\epsilon_b\rangle \]

  overlaps many exact eigenstates \[ |E_A\rangle \] in energy shell

- Switch on \( \lambda V \) for \( t > 0 \)

- Evolve \[ \rho(t) = \text{Tr}_{\text{bath}}(|\Psi(t)\rangle\langle\Psi(t)|) \]
  with \[ |\Psi(t)\rangle = e^{-iHt}|\Psi\rangle \]
Subsystem evolution

Diagonal elements of $\rho$ ($U/J = \lambda = 1$)
Subsystem evolution

Off-diagonal elements of $\rho$ ($U/J = \lambda = 1$)

$|a\rangle = \frac{1}{\sqrt{2}}(|\uparrow,0\rangle + |0,\uparrow\rangle)$, $|b\rangle = \frac{1}{\sqrt{2}}(|\uparrow,0\rangle - |0,\uparrow\rangle)$
(A) Long-time averages show thermalisation

Initial states
| ↑↓, ↑⟩ (solid)
| ↑, ↑⟩ (dashed)
| ↑, ↓⟩ (dotted)
thermal (black)
δ = 0.5

|ε₁,2,3,4⟩: subsystem eigenstates with 2 fermions and S_z = 0
Effective Temperature

$T_{\text{eff}}$ down to quantum degeneracy for $\lambda \lesssim 1$
Memory of Initial State

Loss of memory for wide range $0.1 \leq \lambda \leq 4$

\[
\Delta r = \frac{1}{2} \sum_s \left[ \langle \rho_{ss}^2 \rangle - \langle \rho_{ss} \rangle^2 \right]^{1/2}
\]


Closeness to the Thermal State

Subsystem thermalises for $\lambda \gtrsim 0.1$

$$\sigma_\omega = \frac{1}{2} \sum_s \langle |\rho_{ss} - \omega_{ss}| \rangle$$
Eigenstate Thermalisation

Projections on to subsystem ground state:

\[ \langle E_A | P_s | E_A \rangle \]

\[ P_s = \sum_b |s_b\rangle\langle s_b| \]
How does the subsystem reach thermalisation?
Initial state $|\varepsilon_s\rangle = |\uparrow, \uparrow\rangle$ with composite energy $E_0 = -2$

Exponential, $A e^{-\gamma t} + \text{const} \quad \longleftrightarrow \quad$ Gaussian $A' e^{-\Gamma^2 t^2} + \text{const}$
Short Time Dynamics: perturbation theory

- Initial state \( |\Psi(t = 0)\rangle = |s_0\rangle \frac{1}{N^{1/2}_{\text{shell}}} \sum_{b \in \text{shell}} |\epsilon_b\rangle \)

- Times greater than \( t_1 = 1/4J = 1/\text{single-particle bandwidth} \)
  - Perturbation theory for small \( \lambda \)

\[
\rho_{ss}(t) = \frac{4\lambda^2}{N_{\text{shell}}} \sum_b \left| \sum_{b_i = b} \frac{\sin[(E_{sb} - E_{s0b_i})t/2]}{E_{sb} - E_{s0b_i}} \right|^2 \langle s \ b \ |V|s_0 \ b \rangle^2
\]

- Fermi Golden Rule: \( \frac{d\rho_{ss}}{dt} = -\gamma_{\text{FGR}} \propto \lambda^2 \)

  .....start of an exponential decay for small \( \lambda \)

- "Very short" times: \( t \ll t_1 \)
  - just one hop: \( |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle \sim (1 - iHt)|\Psi(0)\rangle \)

\[
\rho_{ss}(t) \sim 1 - \Gamma^2_{\text{short}}t^2 \text{ with } \Gamma_{\text{short}} = \lambda \left[ \sum_{sb} |\langle sb|V|\Psi(0)\rangle|^2 \right]^{1/2}
\]

  ..... start of Gaussian for \( \lambda > 1 \)
Relaxation Rates

Points:
Fits to Gaussian/exponential curves

Lines:
\( \gamma_{FGR} \propto \lambda^2 \)
\( \Gamma_{short} \propto \lambda \)
Is Gaussian Behaviour Generic?

- Gaussian rate $\Gamma \sim \Gamma_{\text{short}}$ short-time rate?
  - exponential behaviour excluded if FGR rate becomes comparable to $\Gamma_{\text{short}}$ (single particle hopping rate)
  - $\Gamma_{\text{short}} \sim \lambda J \sim \lambda$ independent of system size: Gaussian regime persists to larger systems?
  - fast decoherence after hopping into bath: short inelastic scattering length $\sim$ lattice spacing ($l_{\text{inel}} \sim J^2/U^2$ for small $U/J$ and states far from Fermi level)

- Test numerically by considering
  - Random couplings between system and bath: $\langle sb|V|s'b' \rangle$ replaced with random numbers, preserving $\text{Tr}(V^2)$
  - Bose-Hubbard model
Random Couplings

Shift in crossover. Here $t_{1}^{-1} = \text{full bandwidth} \sim 20$

\begin{align*}
\lambda & \text{ Exp} \\
\lambda & \text{ Gauss}
\end{align*}

\begin{align*}
\Gamma &= \lambda^E \\
E &= 1.77, -2
\end{align*}
Bose-Hubbard Model

\[ \gamma_{\text{FGR}}, \Gamma_{\text{short}} \quad \text{(lines)} \]

Fits to Gaussian/ exponential curves
(points)

7 bosons on 9+2 sites, \( U = J = 1 \)
initial state: no boson in subsystem
Conclusions

- Understanding thermalisation of systems from a purely quantum-mechanical perspective is possible
- Surprisingly small Hubbard-model systems in pure states demonstrate subsystem thermalisation for a range of coupling strengths: short inelastic length
- Dynamics is strongly dependent on coupling strength, with Gaussian behaviour seen at moderate/strong coupling strength
- Believe that the Gaussian behaviour is generic and that it holds in the limit of large bath