Reaching Thermal States in Quantum Systems

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S. Genway, A.F. Ho and D.K.K. Lee, PRL 105, 260402 (2010)
S. Genway, A.F. Ho and D.K.K. Lee, PRA 86, 023609 (2012)
S. Genway, A.F. Ho and D.K.K. Lee, PRL 111, 130408 (2013)

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Outline

- Thermalisation protocol: sudden turn on of system (S) - bath (B) coupling
- key to thermalisation in quantum systems: 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
- Random matrix dynamics - analytical theory
- Conclusions

Introduction + background

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. chemical potential
- loss of coherence/entanglement within subsystem
- 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, to canonical distribution
  - dynamics of approach to thermalisation: exponential and Gaussian relaxation regimes
  - both numerics for a range of systems, and analytical result (last part)

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Canonical Ensemble

- Gibbs-Boltzmann distribution
  - subsystem state $|s\rangle$ with energy ε_s , S+B total energy E_0

$$\rho \propto \sum_s N_{\text{bath}}(E_0 - \varepsilon_s)|s\rangle\langle s|$$

$$\sim \sum_s e^{-\beta\varepsilon_s}|s\rangle\langle s| \qquad \text{for large bath } (E_0 \gg \varepsilon_s)$$

assumed: weak S-B coupling

  - temperature defined from:

$$\beta \equiv \frac{1}{k_{\text{B}}T} = \left.\frac{d\ln N_{\text{bath}}}{dE}\right|_{E_0}$$

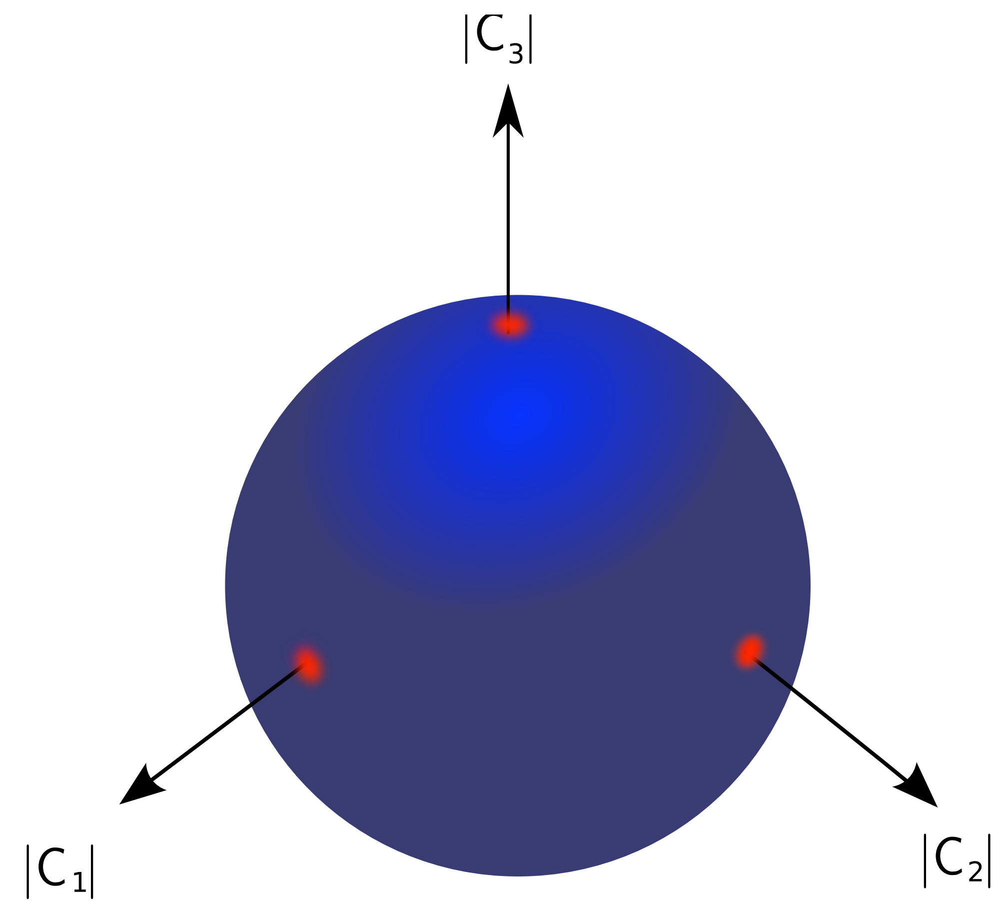
standard textbook derivation: assumed weak system-bath coupling

- Canonical ensemble in a closed quantum system? Two concepts: Canonical Typicality & Eigenstate Thermalisation

Canonical Typicality

Goldstein et al. PRL 96, 050403 (2006)
Popescu et al. Nature Phys. 2, 754 (2006), ...

- Pick a pure 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 ρ is approximately thermal for almost all choices of $|\Psi\rangle$



Eigenstate Thermalisation Hypothesis

Deutsch PRA 43, 206 (1991), Srednicki PRE 50, 888 (1994), Rigol et al., Nature 452, 854 (2008), ...
cf. quantum ergodicity theorem:
von Neumann (1929), Snirelman (1974), de Verdiere (1985), Zelditch (1987), ...

- Measurement of *local / few-body* observable for an energy eigenstate $|A\rangle$ gives thermal result
- Project eigenstate $|A\rangle$ to subsystem state $|s\rangle$ (energy ε_s):

  $P_s \equiv \sum_b |sb\rangle\langle sb|$ for product states $|sb\rangle$

  Hypothesis: $\langle A|P_s|A\rangle \simeq e^{-\beta\varepsilon_s}$

  - For any state $|\Psi\rangle = \sum_A C_A|A\rangle$, time average of the reduced density matrix is the thermal state independent of C_A

$$\rho_{ss} = \sum_A |C_A|^2 \langle A|P_s|A\rangle \sim \overline{\langle A|P_s|A\rangle}$$

Thermalisation

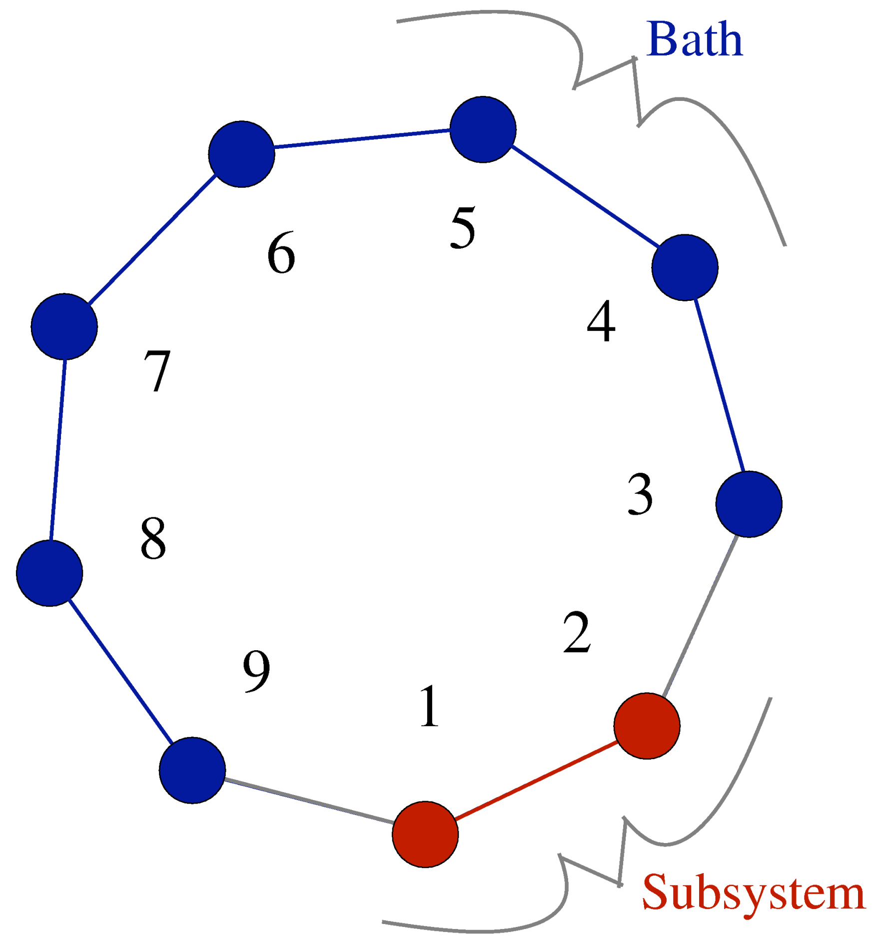
Hamiltonian

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

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

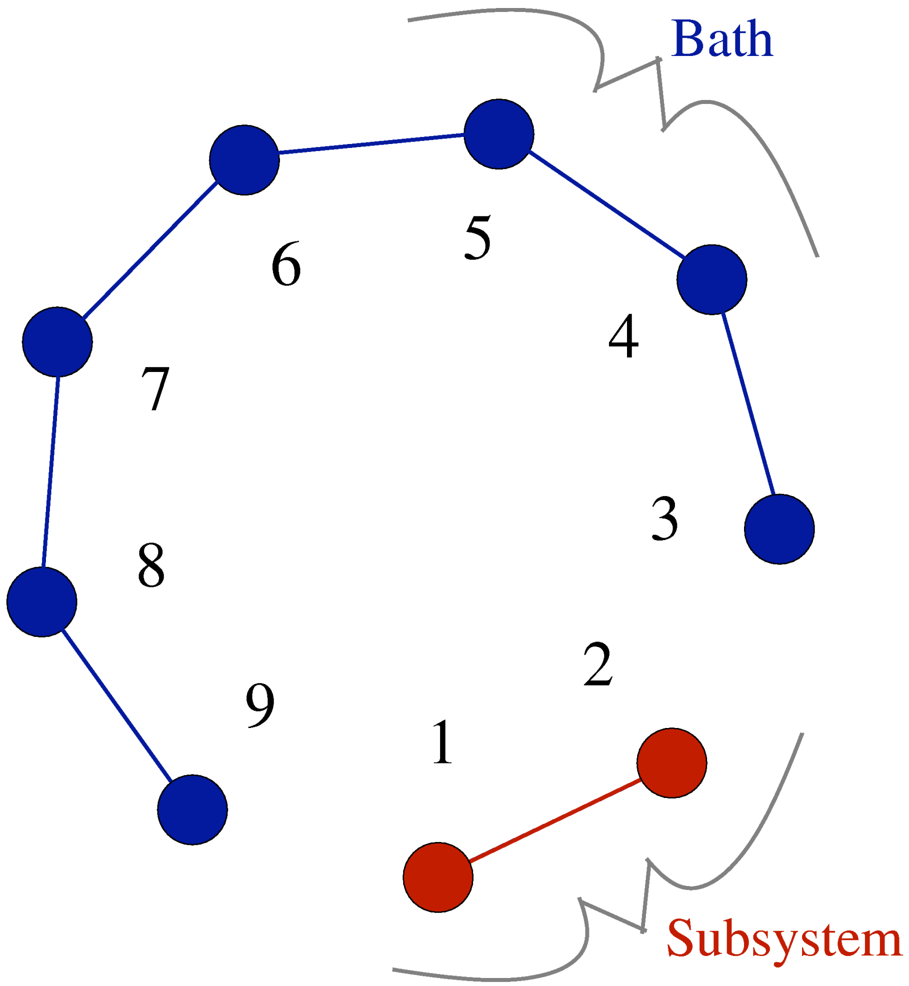
$$\lambda V = -\lambda \sum_{\sigma=\uparrow,\downarrow} J_\sigma \left[(c^\dagger_{2\sigma}c_{3\sigma} + c^\dagger_{1\sigma}c_{L\sigma}) + \text{h.c.}\right]$$

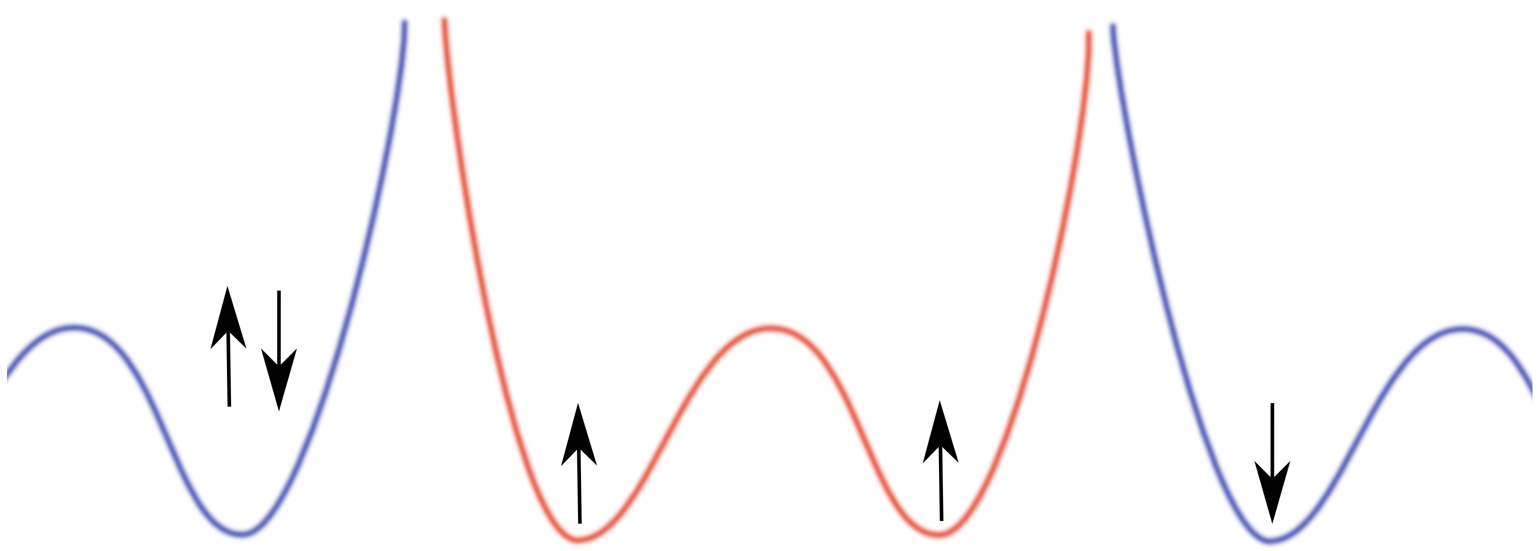
- 8 fermions: 4↑, 4↓
- $J_\sigma = J(1 + \xi \text{sgn}\sigma)$, $\xi = 0.05$
- $U = J = 1$
- 15876 energy levels
- 16 subsystem energy levels
- $\lambda = 1 \rightarrow$ homogeneous ring



Initial State

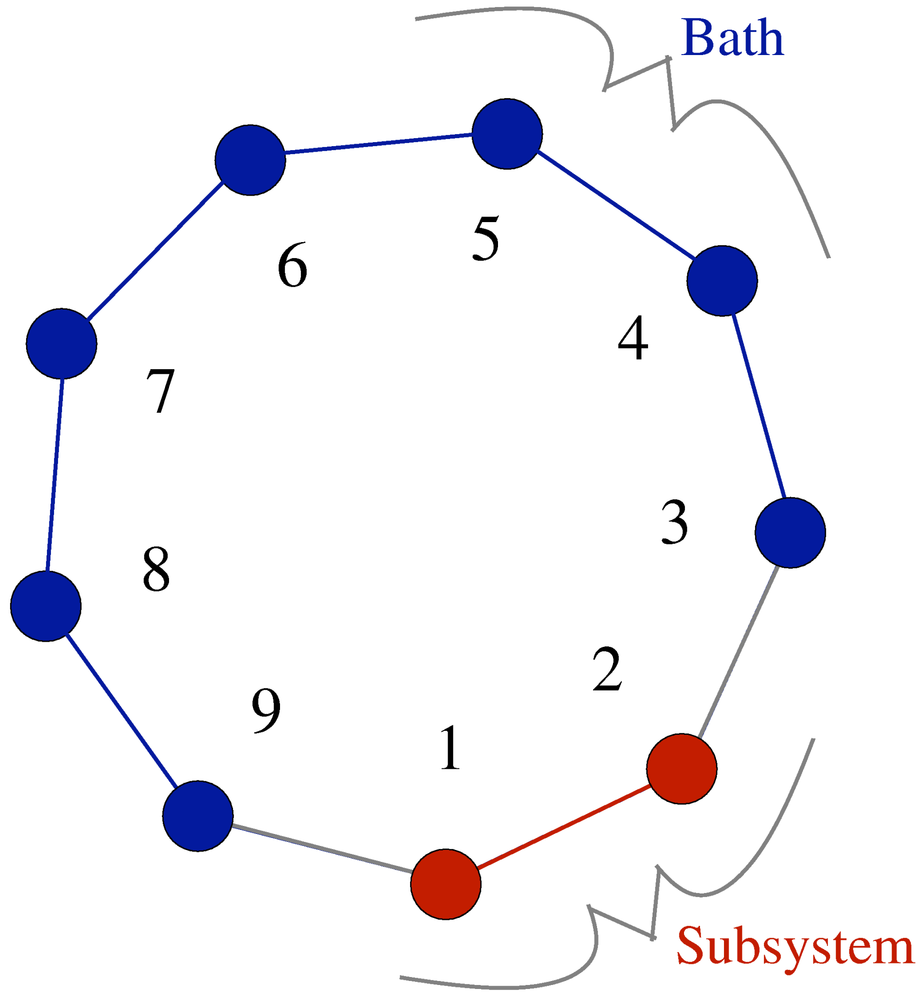
- Product states
  $$|\Psi(t=0)\rangle = |s\rangle \frac{1}{N_{\text{shell}}^{1/2}} \sum_{b \in \text{shell}} |\epsilon_b\rangle$$
  overlaps many exact eigenstates $|E_A\rangle$ in energy shell

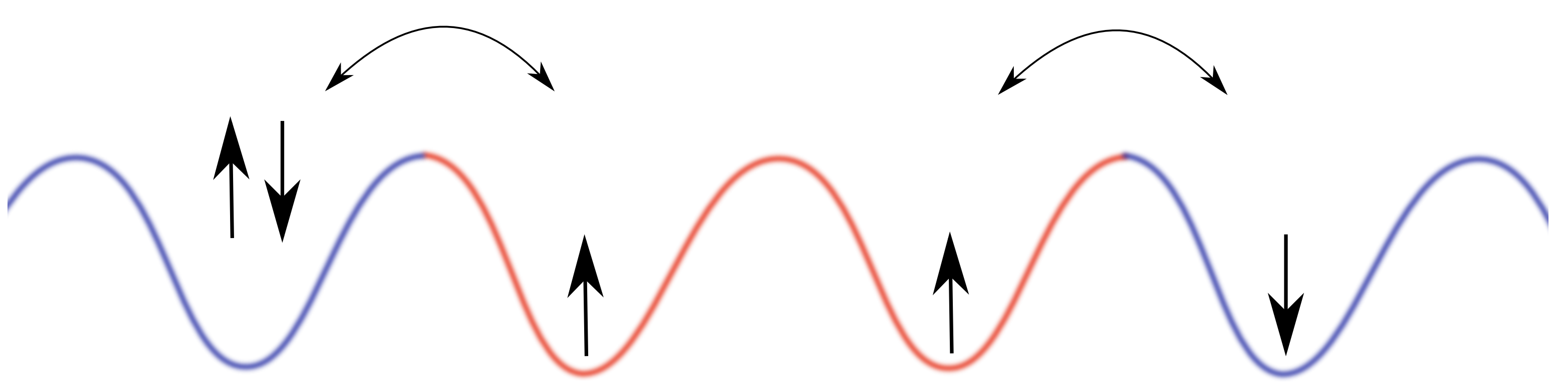




Initial State

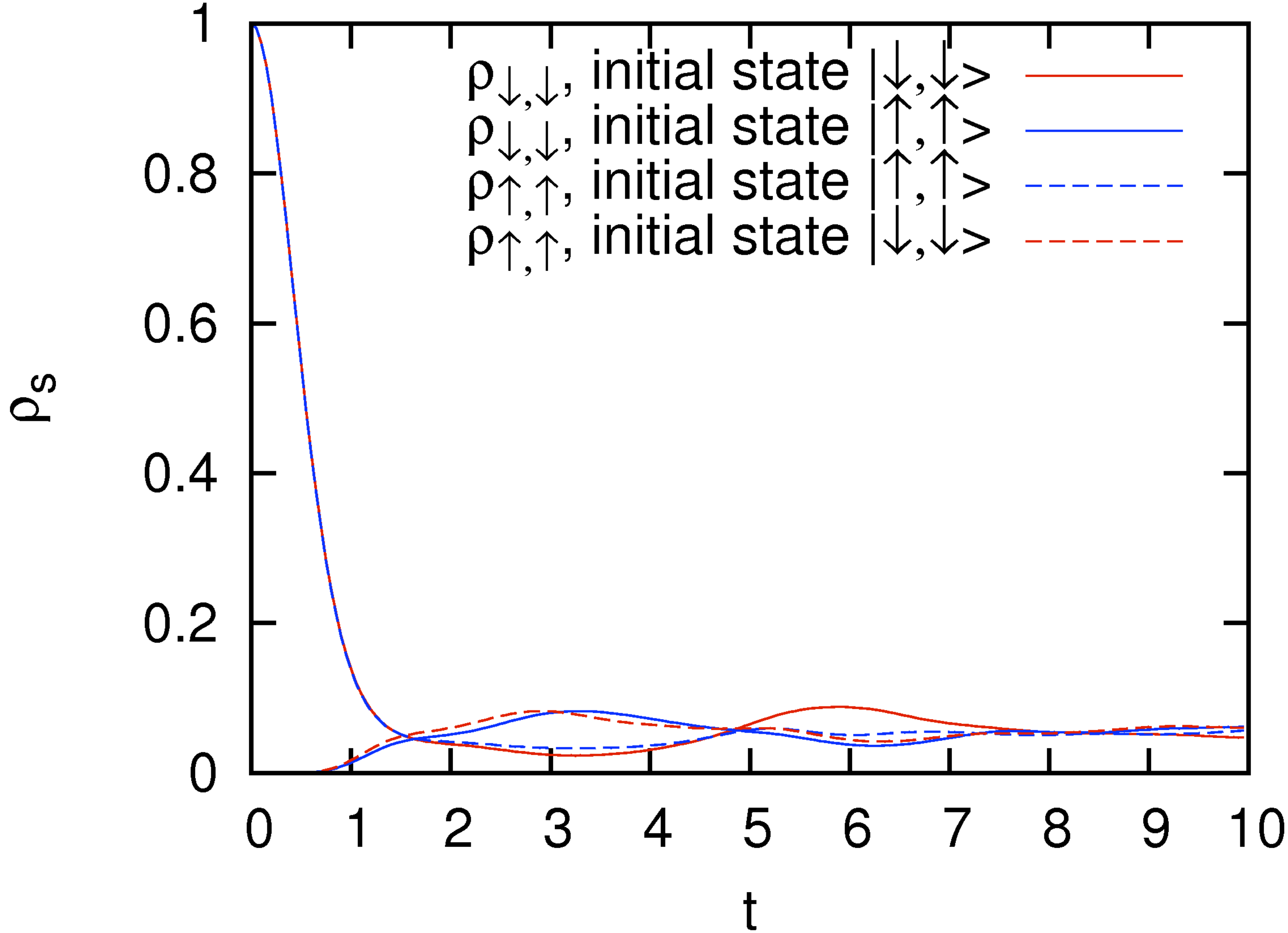
- Product states
  $$|\Psi(t=0)\rangle = |s\rangle \frac{1}{N_{\text{shell}}^{1/2}} \sum_{b\in\text{shell}} |\epsilon_b\rangle$$
  overlaps many exact eigenstates $|E_A\rangle$ in energy shell
- Switch on λV for $t > 0$
- Evolve $\rho(t) = \text{Tr}_{\text{bath}}\left(|\Psi(t)\rangle\langle\Psi(t)|\right)$ with $|\Psi(t)\rangle = e^{-iHt}|\Psi\rangle$





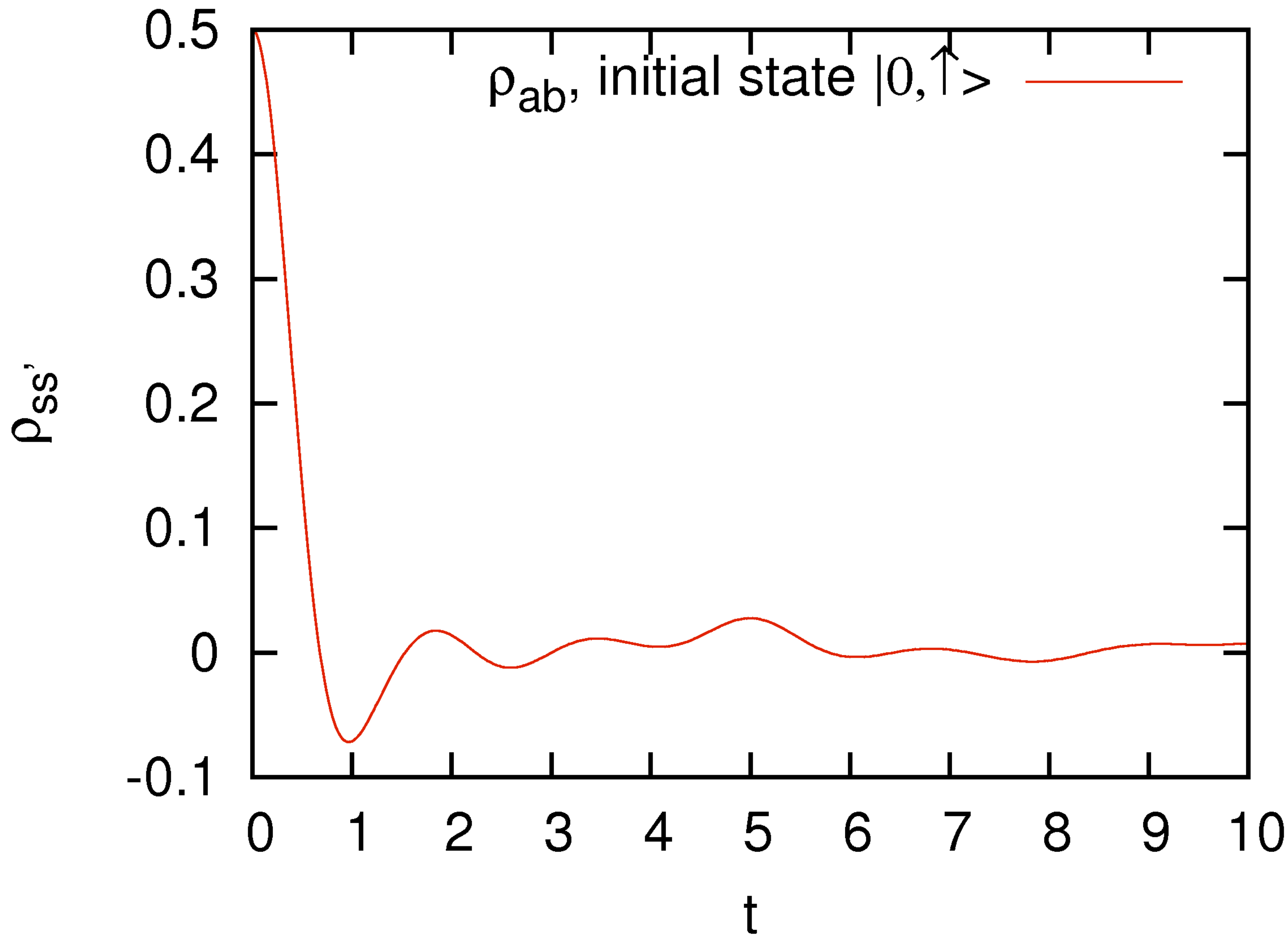
Subsystem evolution

Diagonal elements of ρ $(U/J = \lambda = 1)$



Subsystem evolution

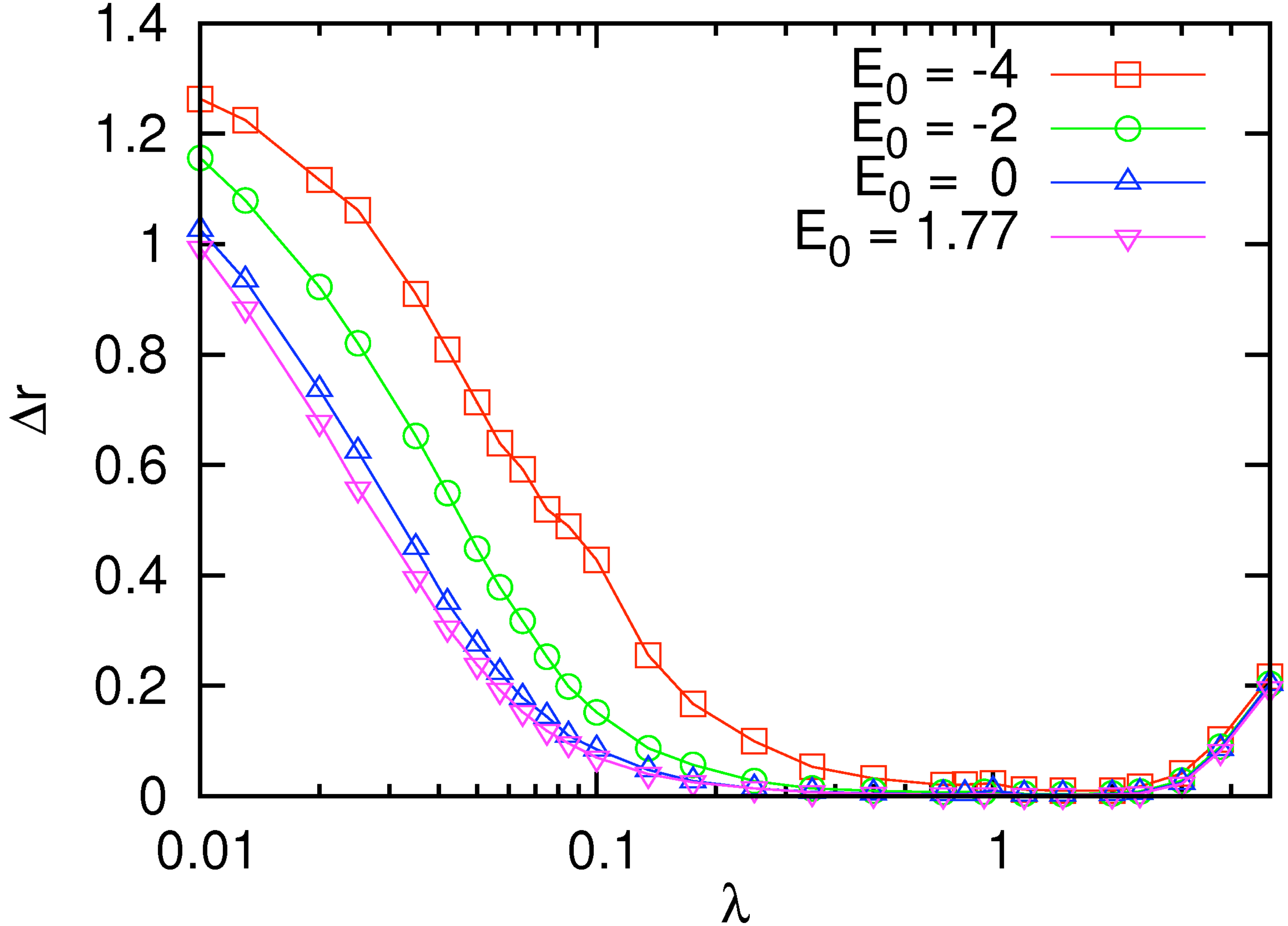
Off-diagonal elements of ρ $(U/J = \lambda = 1)$



$$|a\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow, 0\rangle + |0, \uparrow\rangle\big), \quad |b\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow, 0\rangle - |0, \uparrow\rangle\big)$$

Memory of Initial State

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

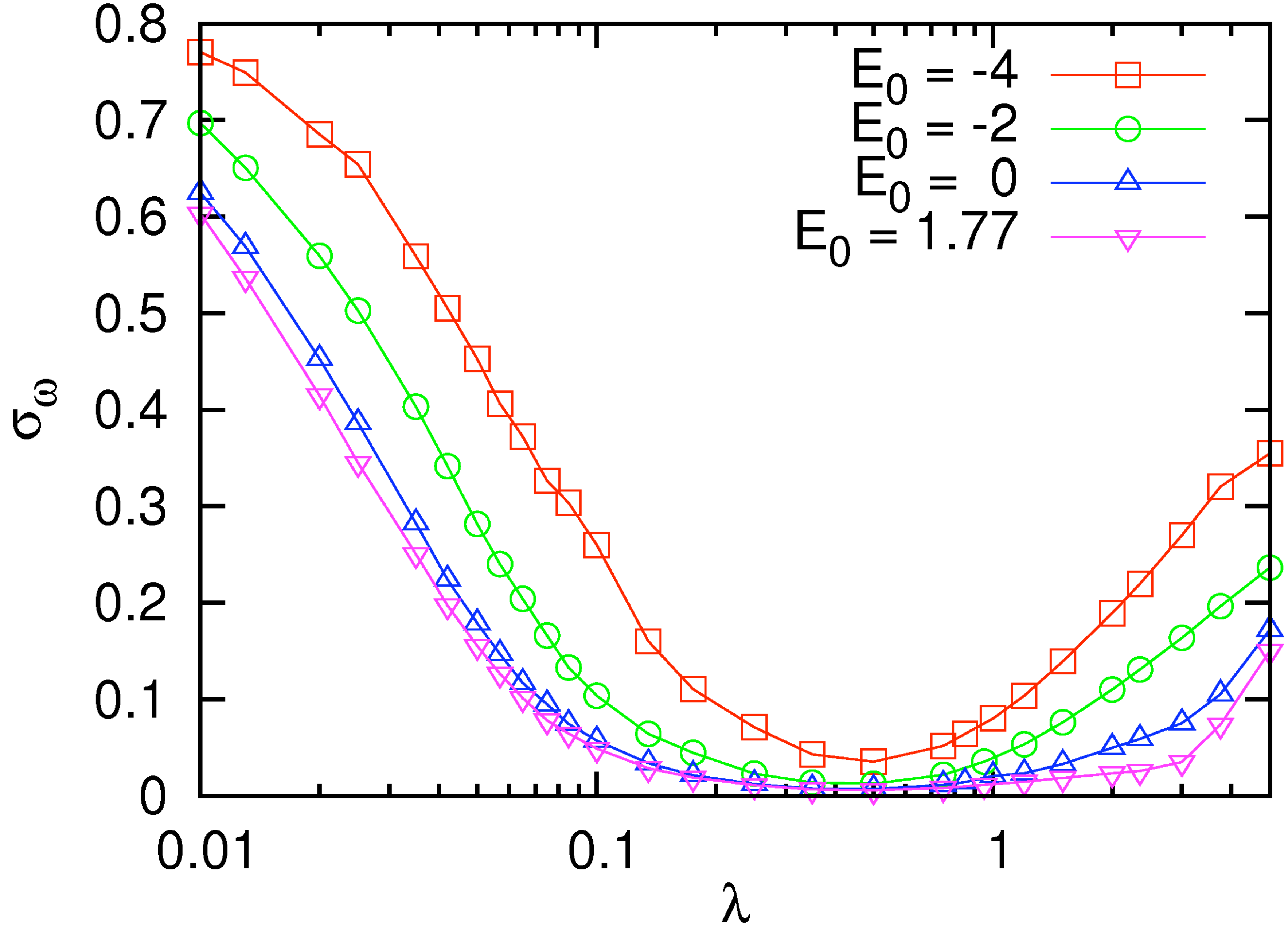


$$\Delta r = \frac{1}{2} \sum_s \left[\langle \rho_{ss}^2 \rangle - \langle \rho_{ss} \rangle^2 \right]^{1/2}$$

angular bracket: average over all (16) initial subsystem states

Closeness to the Thermal State

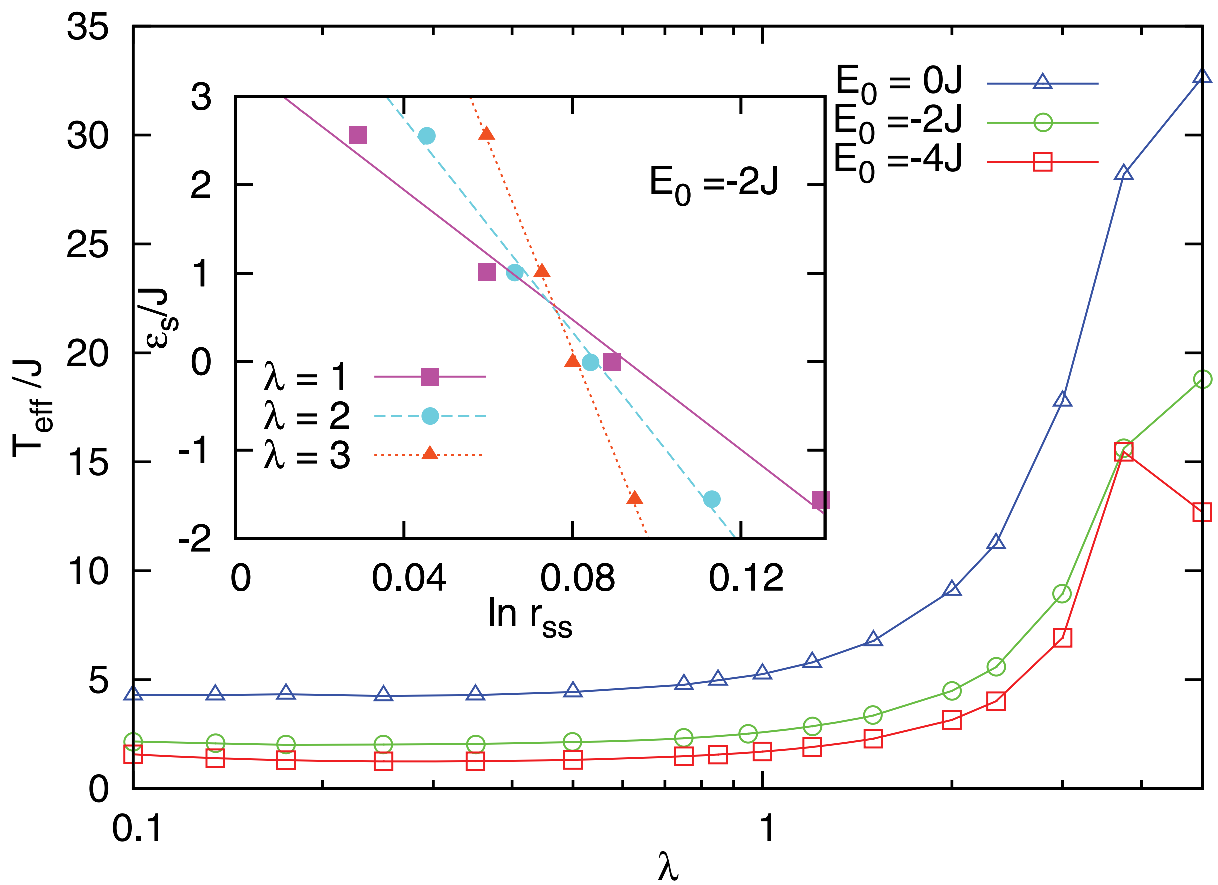
Subsystem thermalises for $\lambda \gtrsim 0.1$

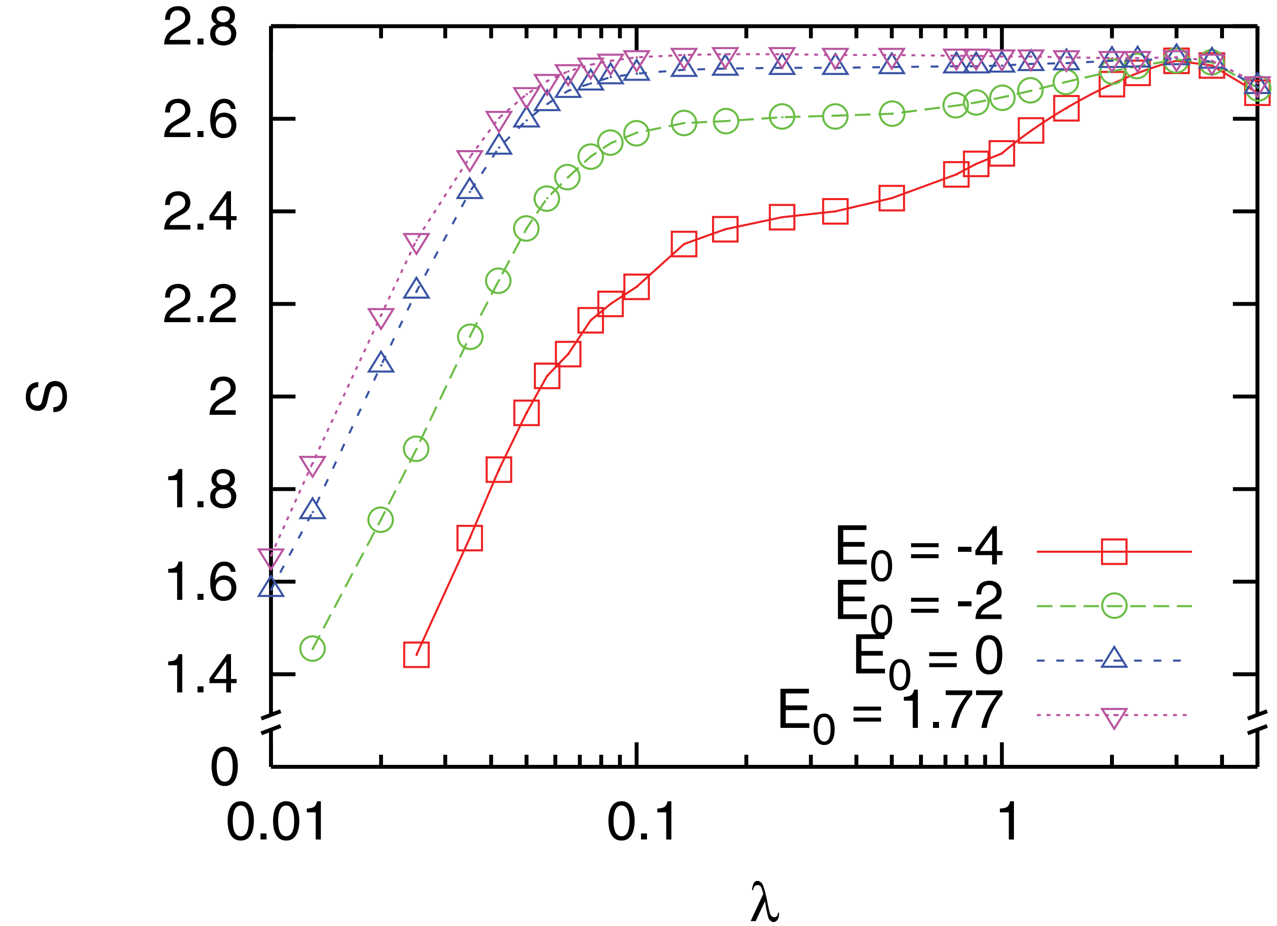


$$\sigma_\omega = \frac{1}{2}\sum_s \langle|\rho_{ss} - \omega_{ss}|\rangle$$

angular bracket: average over all (16) initial subsystem states

Thermal state





$$\log \rho_{ss} = -\frac{\epsilon_s}{T_{\text{eff}}} + \text{const}$$

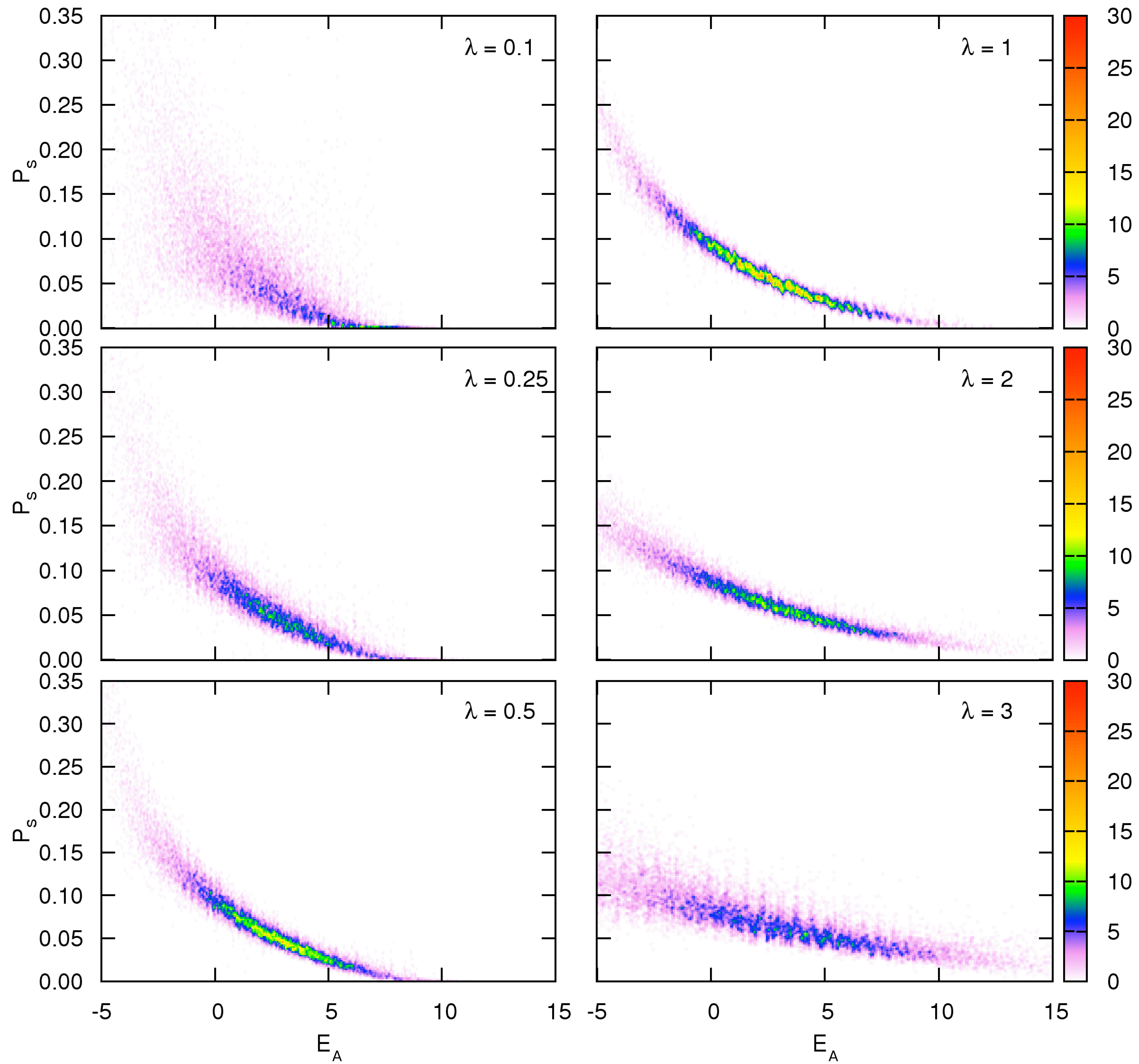
$$S = -\sum_s \langle \rho_{ss} \ln \rho_{ss} \rangle$$

angular bracket: average over all (16) initial subsystem states

Effective temperature T_{eff} down to quantum degeneracy for $\lambda \lesssim 1$

von Neumann entropy: plateau in thermalised regime

Eigenstate Thermalisation



Projections on to subsystem ground state : for $N_s = 2, S_z = 0$

$$\langle E_A | P_s | E_A \rangle$$

$$P_s = \sum_b |sb\rangle\langle sb|$$

scattered values at weak S-B coupling, well defined at intermediate coupling

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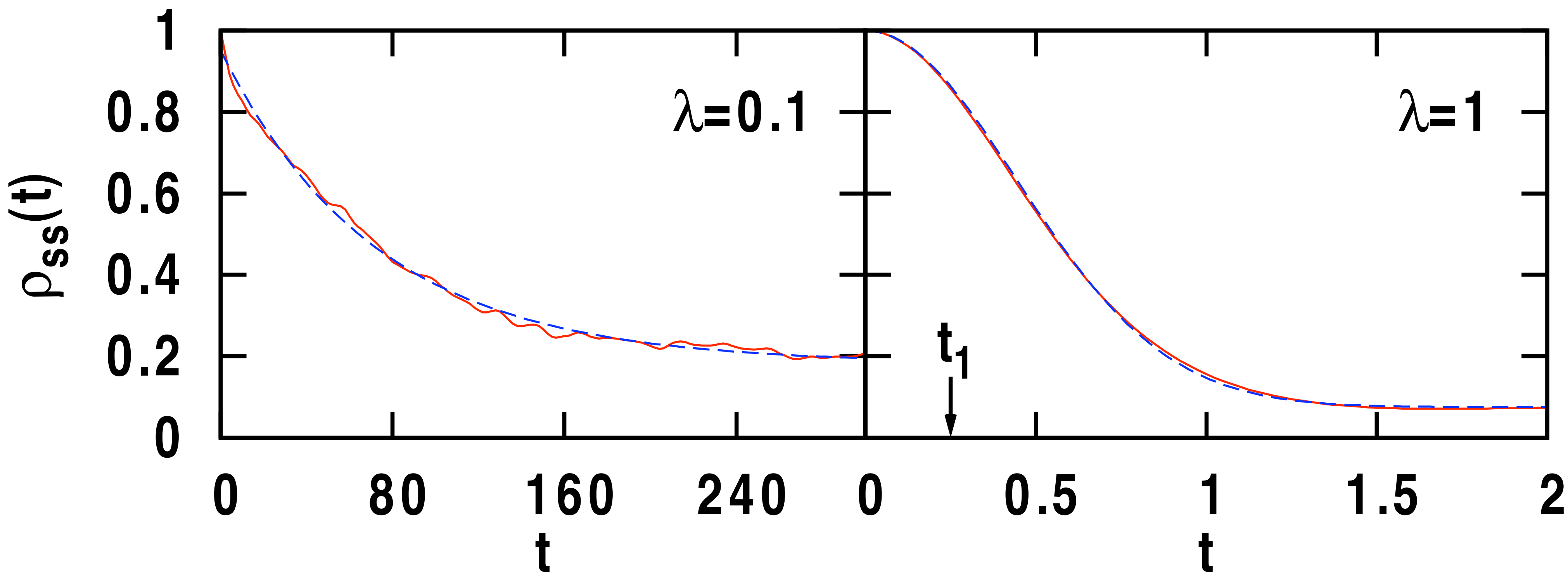
Dynamics

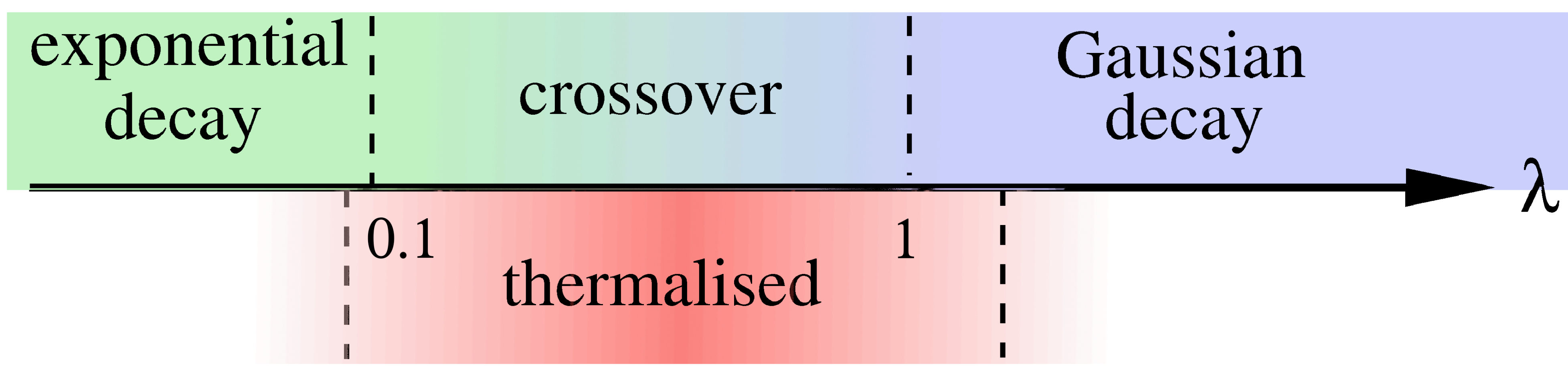
(B) Dynamics of Thermalisation

How does the subsystem reach thermalisation?

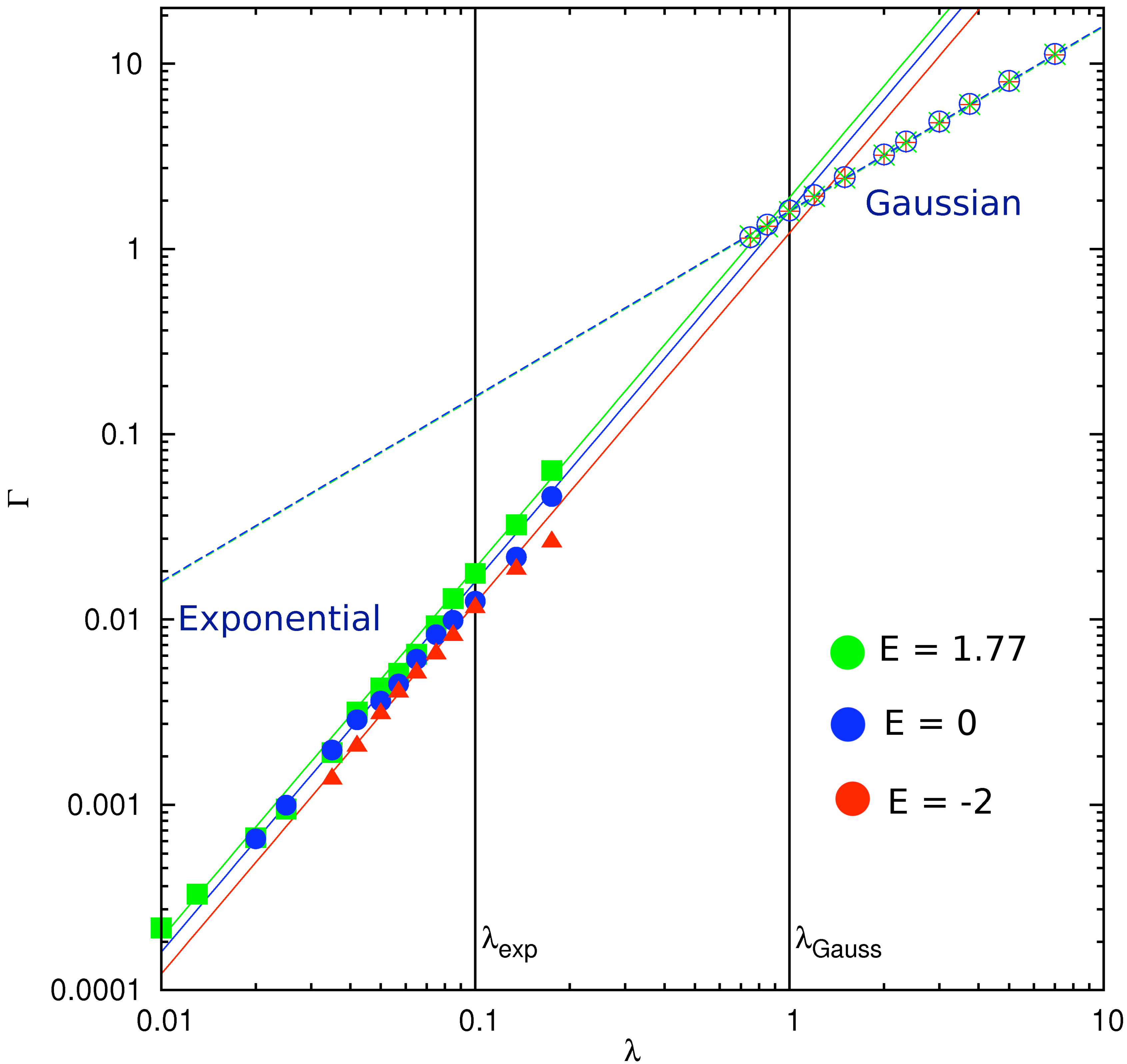
Initial state $|\varepsilon_s\rangle = |\uparrow,\uparrow\rangle$ with composite energy $E_0 = -2$



Exponential, $Ae^{-\gamma t}$ + const $\longleftrightarrow$ Gaussian $A'e^{-\Gamma^2 t^2}$ + const



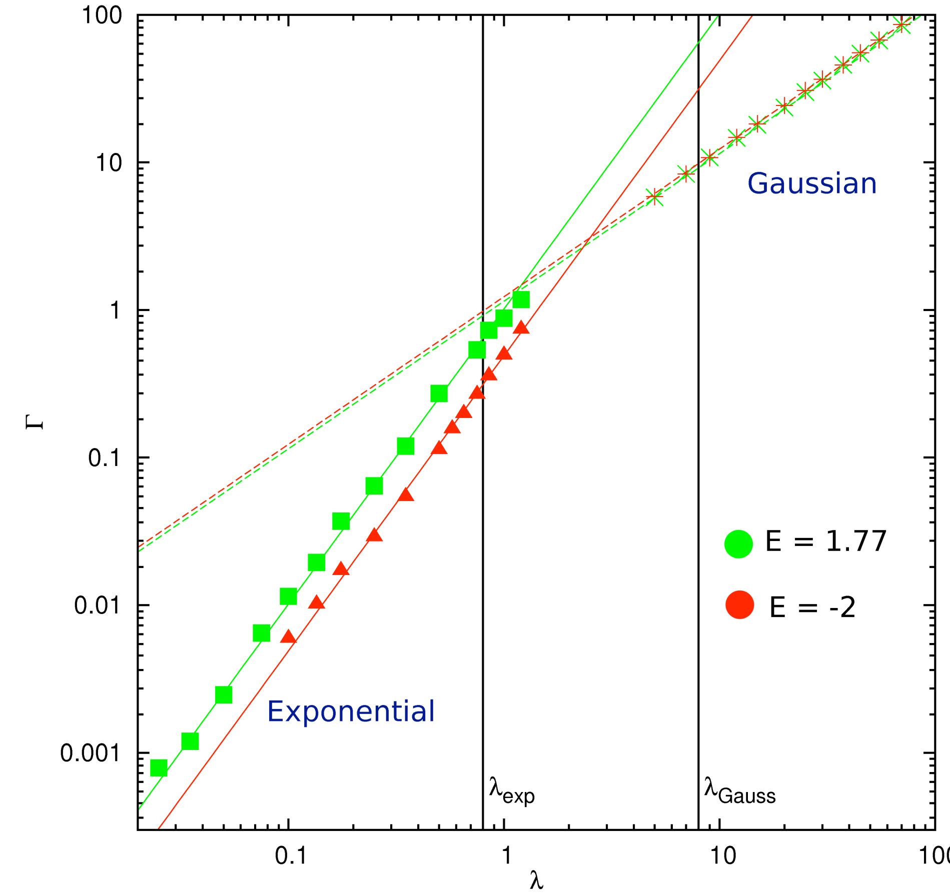
Relaxation Rates



Points:
Fits to Gaussian/
exponential curves

Lines:
$\gamma_{\mathrm{FGR}} \propto \lambda^2$
$\Gamma_{\text{short}} \propto \lambda$

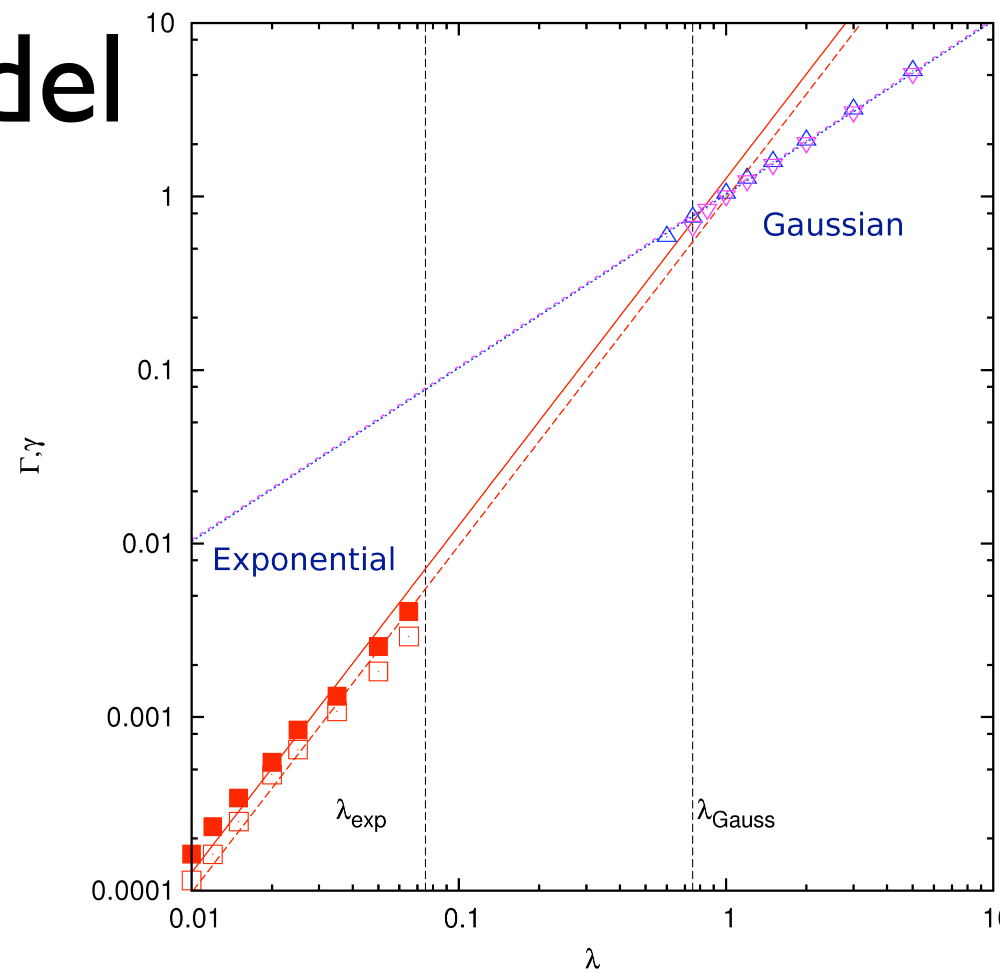
Random Couplings



Shift in crossover.
Here t_1^{-1} = full bandwidth ~ 20

Bose-Hubbard Model

Gaussian regime universal



γ_{FGR}, Γ_{short} (lines)
Fits to Gaussian/ exponential curves (points)

7 bosons on 9+2 sites, $U = J = 1$
initial state: no boson in subsystem

Short Time Dynamics: perturbation theory

- Initial state $|\Psi(t=0)\rangle = |s_0\rangle \frac{1}{N_{\text{shell}}^{1/2}} \sum_{b \in \text{shell}} |\epsilon_b\rangle$
- Times greater than $t_1 = 1/4J =$ 1/single-particle bandwidth
  - Perturbation theory for small λ

$$\rho_{\substack{ss \\ s \neq s_0}}(t) = \frac{4\lambda^2}{N_{\text{shell}}} \sum_b \left| \sum_{b_i=b_l}^{b_u} \frac{\sin[(E_{sb} - E_{s_0 b_i})\frac{t}{2}]}{E_{sb} - E_{s_0 b_i}} \langle s \;\; b\, |V| s_0\, b_i \rangle \right|^2$$

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

.....start of an exponential decay for small λ

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

$$\rho_{\substack{ss \\ s = s_0}}(t) \simeq 1 - \Gamma_{\text{short}}^2 t^2 \text{ with } \Gamma_{\text{short}} = \lambda \left[\sum_{sb} |\langle sb|V|\Psi(0)\rangle|^2 \right]^{1/2}$$

.... start of Gaussian for $\lambda > 1$

Random matrix dynamics

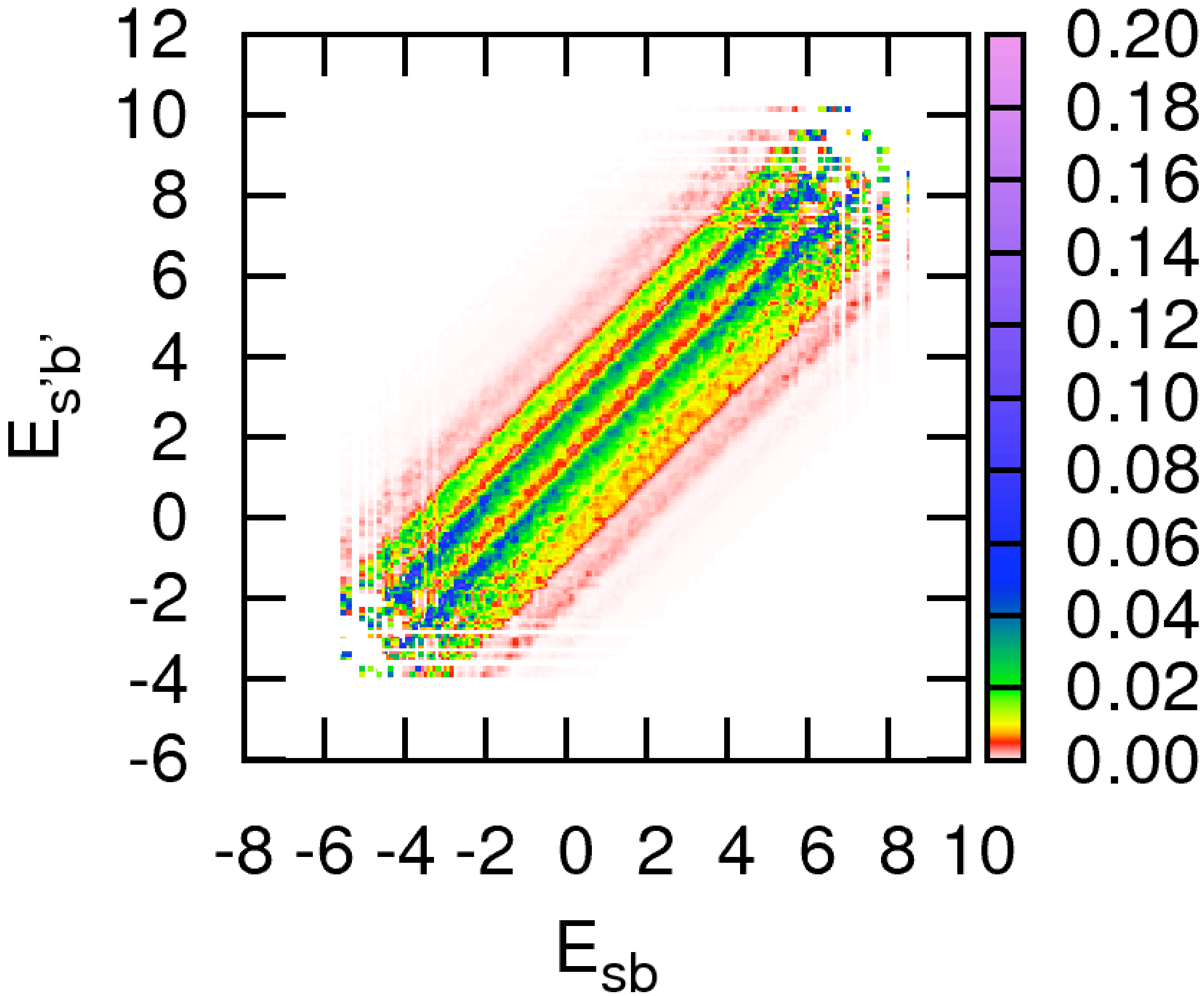
A random matrix model

- Banded random coupling

$$H = \sum_{sb} (\varepsilon_s + \epsilon_b)|sb\rangle\langle sb| + \sum_{ss'bb'} |sb\rangle\langle sb|V|s'b'\rangle\langle s'b'|$$

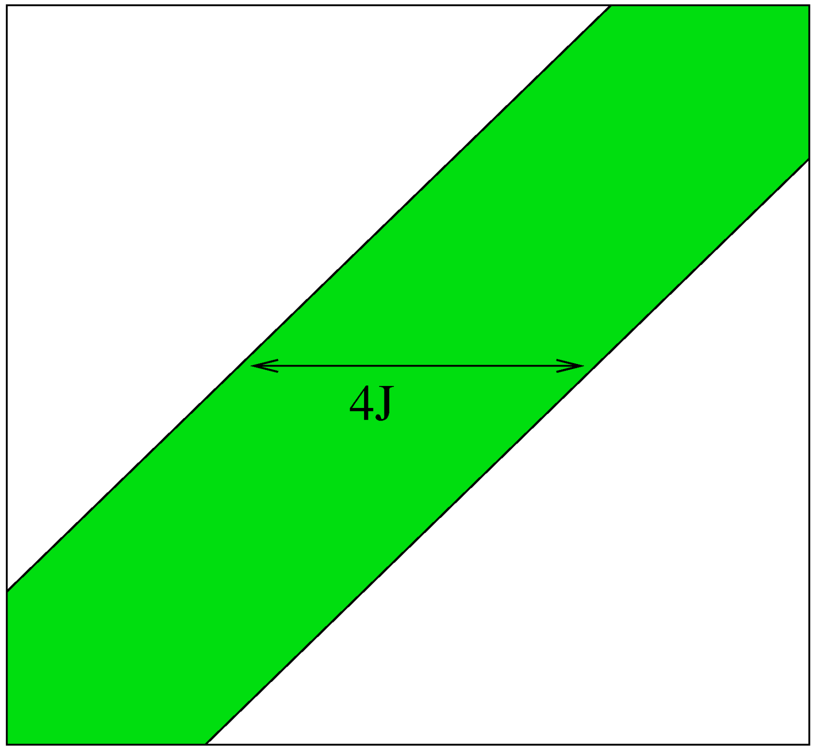
  - bath levels ϵ_b obeys Wigner-Dyson statistics
  - coupling matrix elements $\langle sb|V|s'b'\rangle$ zero for $|E_{sb} - E_{s'b'}| > W$
  - each non-zero element has variance $c\Delta$
  - $\Delta =$ level spacing
- Two energy scales: c and W
- For Hubbard ring with local quench
  - strength of coupling: $c \sim \lambda^2 J$
  - coupling width: $W = 4J$, single-particle bandwidth

coupling matrix structure



Hubbard Model coupling matrix

in $|sb\rangle$ basis looks like...



Origin of dynamics: overlaps

- Dynamics given by overlap of exact eigenstates $|A\rangle$ with product states $\langle A|sb\rangle$
  - initial state $|s_0 b_0\rangle$
  - reduced density matrix

$$\rho_{ss'}(t) = \sum_{ABb} \langle B|s_0 b_0\rangle\langle s_0 b_0|A\rangle\langle A|sb\rangle\langle s'b|B\rangle\, e^{-iE_{AB}t}$$

  - diagonal elements for subsystem state $s = s_0$

$$\rho_{ss}(t) = \sum_{ABb} \langle B|sb_0\rangle\langle sb_0|A\rangle\langle A|sb\rangle\langle sb|B\rangle\, e^{-iE_{AB}t}$$

NB: this is like Fourier transform in t if the overlap combo depends only on E_{AB} .

- Need to understand statistics of overlaps...

Origin of dynamics: overlaps

- Variance $\sigma^2 = \overline{|\langle A|sb\rangle|^2}$
  - a function only of $\Delta E_A \equiv E_A - E_{sb}$ after averaging over small windows of $|E_A\rangle$ and $|sb\rangle$ **(ETH ! see later)**
- Reduced density matrix has Fourier components:

$$\tilde{\rho}_{ss}(\omega) \sim \sum_A \sigma^2(\Delta E_A - \hbar\omega)\sigma^2(\Delta E_A)$$

$$\rho_{ss}(t) \sim |\tilde{\sigma}^2(t)|^2$$

dropping terms of random signs

- Relaxation of $\rho_{ss}(t)$
  - exponential decay $\leftrightarrow$ Lorentzian profile for $\sigma^2(\Delta E)$
  - Gaussian decay $\leftrightarrow$ Gaussian profile for $\sigma^2(\Delta E)$

Method: Dyson Brownian motion model

Build up S-B coupling V as a sequence in fictitious time τ of random kicks:

Dyson, 1962, 1972

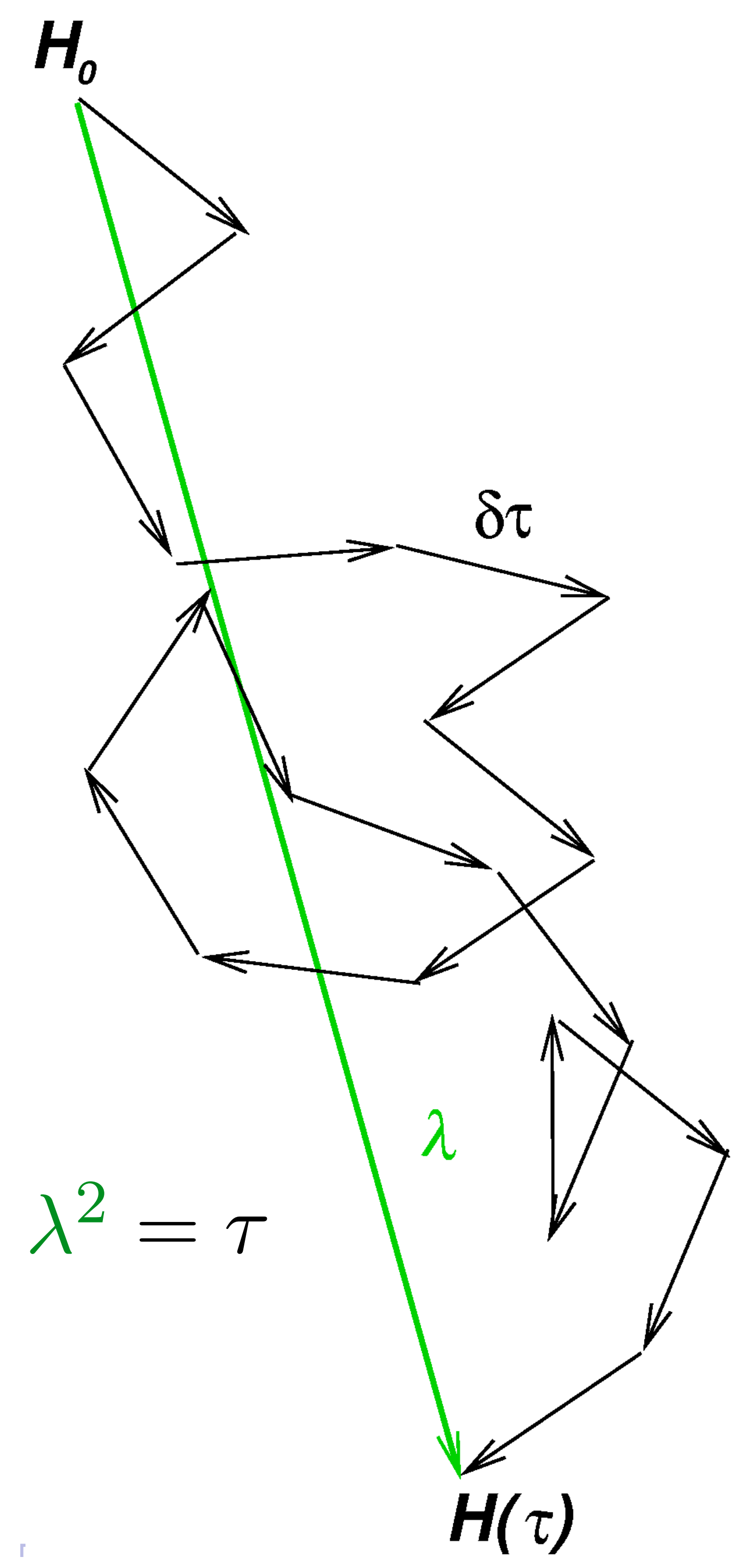
$$H(\tau) = \underbrace{H_S + H_B}_{H_0} + \int_0^\tau d\tau' \xi(\tau')$$

$$\langle A(\tau)|\xi\delta\tau|B(\tau)\rangle = \xi_{AB}$$ Gaussian random variables

$$\overline{\xi_{AB}(\tau)\xi_{BA}(\tau')} = c_{AB}\,\delta(\tau-\tau')$$

perturbation theory at each fictitious time step $\delta\tau$:

$$\delta|A\rangle = \underbrace{\sum_{B\neq A}\frac{\xi_{AB}\,\delta\tau}{E_A-E_B}|B\rangle}_{\text{diffusion}} - \underbrace{\frac{1}{2}\sum_{B\neq A}\frac{c_{AB}\,\delta\tau}{(E_A-E_B)^2}|A\rangle}_{\text{drift}}$$



Wilkison & Walker, J. Phys A 26, 6143 (1995)
Chalker, Lerner & Smith, PRL (1996)

Mean-square overlaps: results

S. Genway, A.F. Ho and D.K.K. Lee, PRL 111, 130408 (2013)

- Brownian motion (imaginary time $\tau = \lambda^2$)
  - Equation of motion for $\sigma^2_{Asb}(\Delta E = E_A - E_{sb}) = \overline{\langle A|sb\rangle^2}$:

$$\frac{\partial\sigma_A^2}{\partial\tau} = -\int dE_B \frac{c(E_A - E_B)}{(E_A - E_B)^2}(\sigma_A^2 - \sigma_B^2)$$

coupling matrix: $c(E) = J/4 \quad (|E| \leq 4J),$ (zero otherwise)

  - Fourier transform of $\sigma_A^2(\Delta E)$: $\tilde{\sigma}^2(t) = e^{-c\tau\Lambda(t)}$

$$\Lambda(t) = 2\int_\Delta^{4J} \frac{1-\cos Et}{E^2}\, dE \sim \begin{cases} \pi|t| & J^{-1} \ll t \ll \Delta^{-1} \\ 4Jt^2 & t \ll J^{-1} \end{cases}$$

  - $\lambda \ll 1$: $\tilde{\sigma}^2(t)$ exponential decay $\Rightarrow$ σ_A^2 Lorentzian
  - $\lambda \gtrsim 1$: $\tilde{\sigma}^2(t)$ Gaussian (small exponential tail) $\Rightarrow$ σ_A^2 Gaussian

$$\begin{aligned} \rho_{ss}(\lambda^2, t) &= \rho_{ss}(\tau,\infty) + [1 - \rho_{ss}(\tau,\infty)]\, e^{-2c\lambda^2\Lambda(t)} \\ \rho_{ss}(\lambda^2,\infty) &= N_{\text{bath}}(E_0 - \varepsilon_s)\Delta \sim e^{-\beta\varepsilon_s} \end{aligned}$$

Mean-square overlaps and ETH

- analytical demonstration of ETH via result for $\overline{\sigma^2_{Asb}}$ in Dyson Brownian motion model

$$\langle A|P_s|A\rangle = \sum_b |\langle A|sb\rangle|^2 \longrightarrow \sum_b \overline{|\langle A|sb\rangle|^2} \simeq \nu_b(E_A - \epsilon_s)\Delta$$

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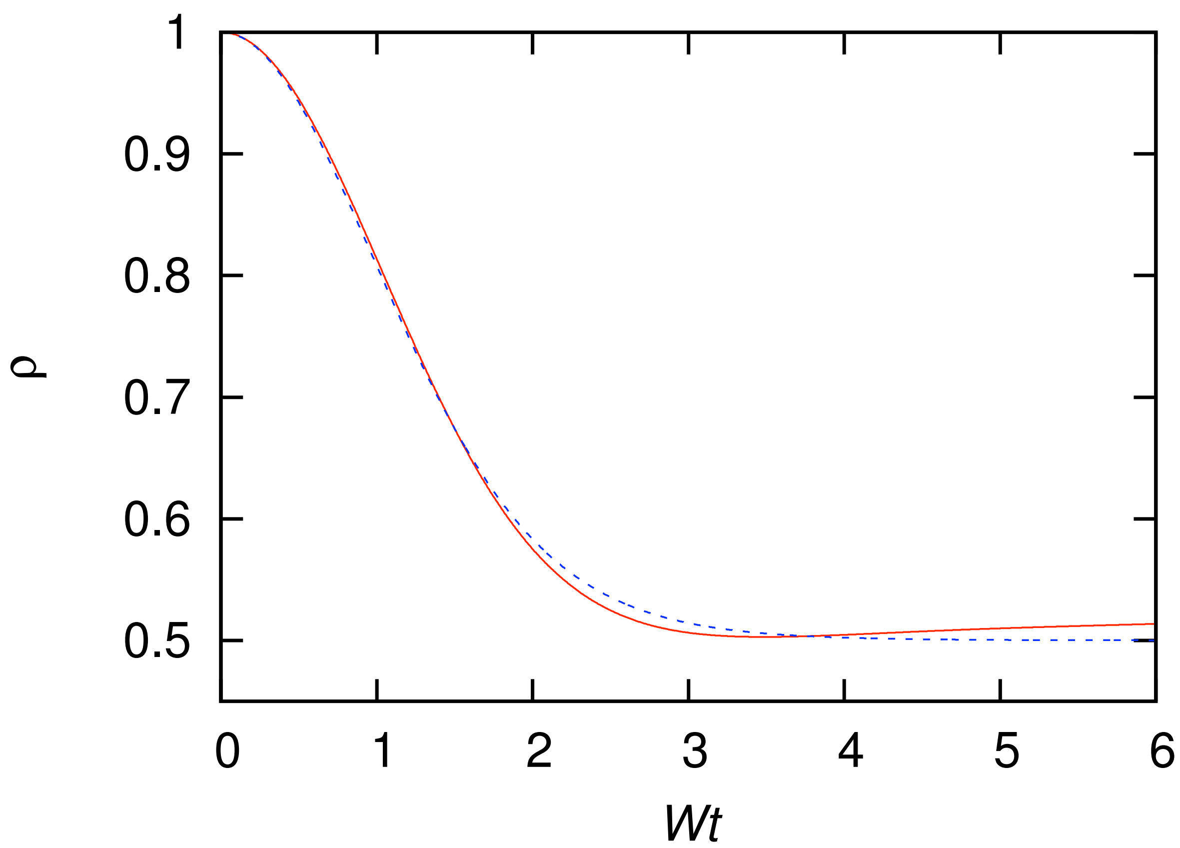
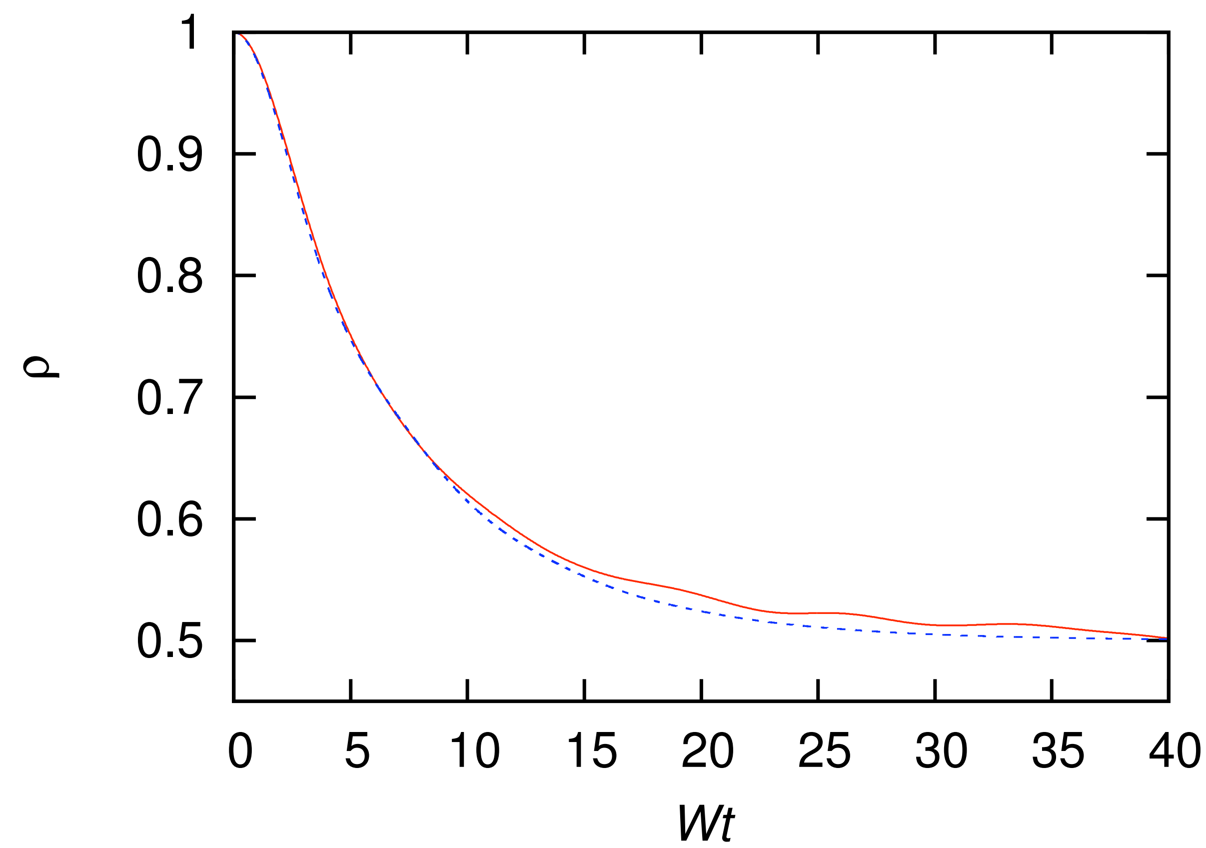
Reduced density matrix

- Diagonal element $\rho_{ss}(t)$ with $s = s_0$ (initial prepared state s_0)
  - two-level system at high effective temperature



strong coupling $\lambda \sim 1$:
Gaussian with exponential tail



weak coupling $\lambda \sim 0.1$:
exponential decay

red line: random matrix numerics
blue dashed line: approximate theory

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
- Gaussian behaviour is generic and holds in the limit of large bath in ring geometry
- Random matrix theory gives full time dependence: Gaussian decay with exponential tail
- Cold atom experiment: single-site addressability, local measurements and initial state preparation