# Reaching Thermal States in Quantum Systems

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INT, University of Washington, April 2011

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Thanks:
funding: EPSRC (UK)
discussions: John Chalker, Miguel Cazalilla

S. Genway, A.F. Ho and D.K.K. Lee, PRL 105, 260402 (2010)

# 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

S. Genway, A.F. Ho and D.K.K. Lee, PRL 105, 260402 (2010)

# Thermalisation


- prepare system in product state of decoupled system and bath:

$$|\Psi(0)\rangle = |s_0 b\rangle \equiv |s_0\rangle \otimes |b\rangle \qquad \longleftarrow \frac{1}{N_{\text{shell}}^{1/2}} \sum_{\substack{\text{energy shell} \\ \epsilon_b \in [E_0, E_0+\delta_b]}} |\epsilon_b\rangle$$

- 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 $\varepsilon_s$

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

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

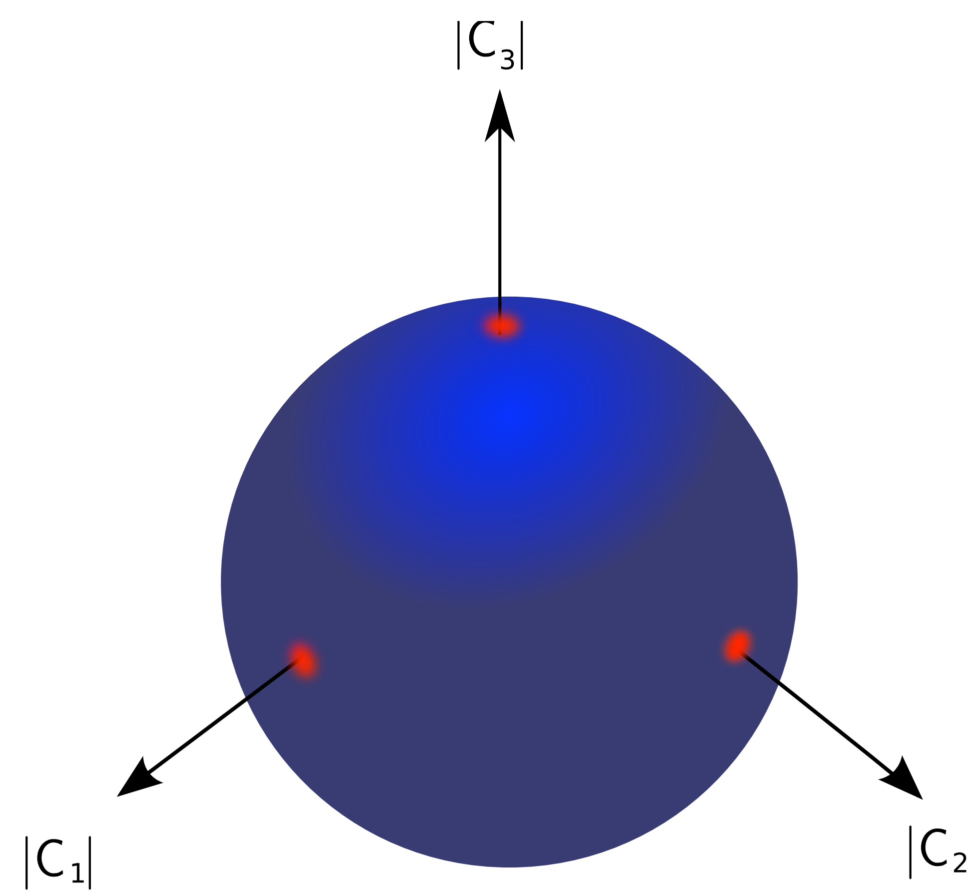
  - temperature defined from:

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

# Canonical Typicality

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

Srednicki PRE 50, 888 (1994), Rigol et al., Nature 452, 854 (2008)

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

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

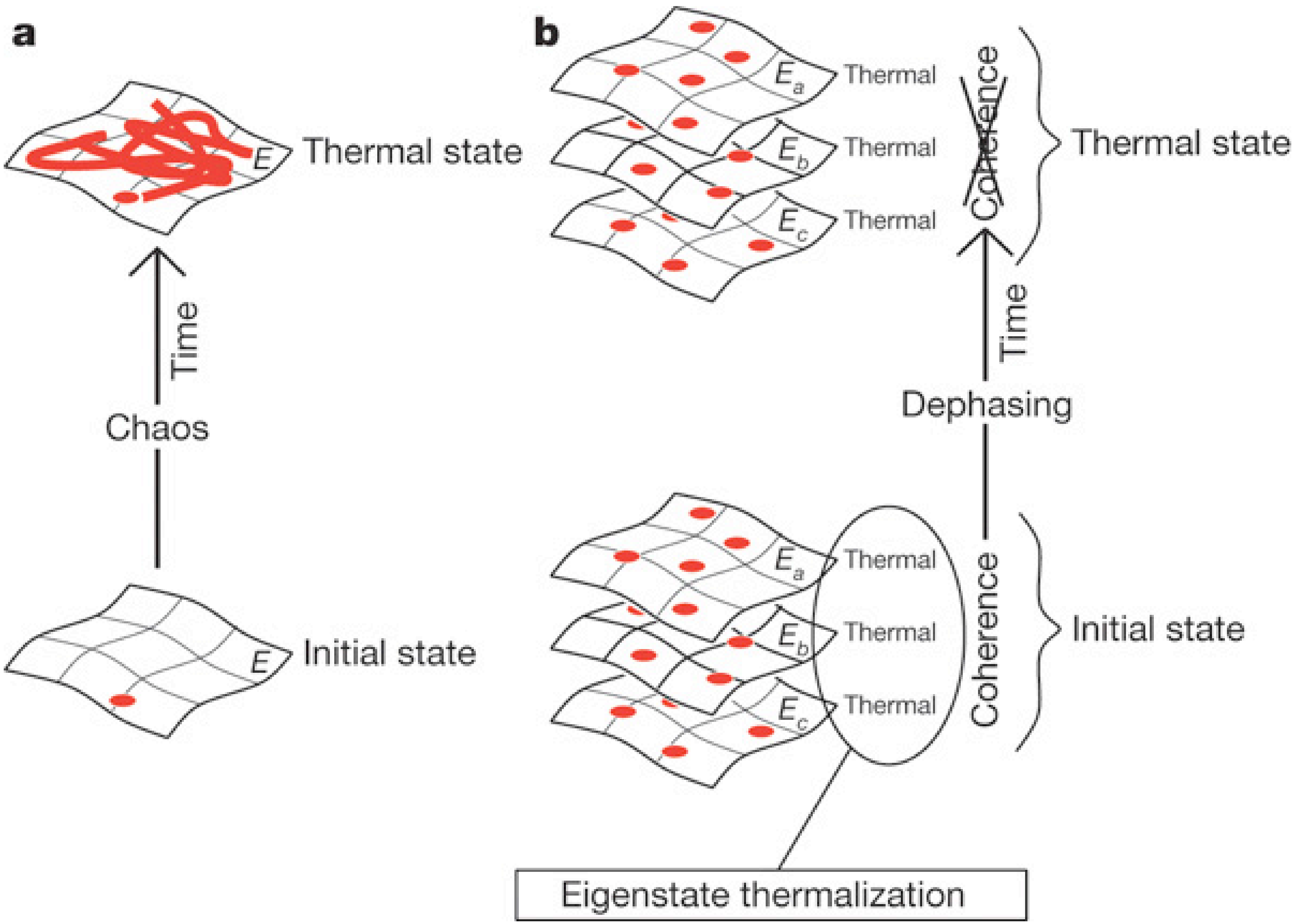
Hypothesis: $\langle E_A|P_s|E_A\rangle \simeq e^{-\beta\varepsilon_s}$

- subsystem thermal behaviour encoded into $|E_A\rangle$

$$\left.\begin{array}{ccc} \vdots & = & \vdots \quad \vdots \\ |E_{352}\rangle & = & |\varepsilon_1\rangle|\epsilon_{172}\rangle \\ |E_{351}\rangle & = & |\varepsilon_2\rangle|\epsilon_{98}\rangle \\ |E_{350}\rangle & = & |\varepsilon_1\rangle|\epsilon_{171}\rangle \\ \vdots & = & \vdots \quad \vdots \end{array}\right\} \xrightarrow{\lambda V} e^{-\beta\varepsilon_1}|\varepsilon_1\rangle|B_1\rangle + e^{-\beta\varepsilon_2}|\varepsilon_2\rangle|B_2\rangle + \ldots$$

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

# Eigenstate Thermalisation Hypothesis




Rigol et al., Nature **452**, 854 (2008)

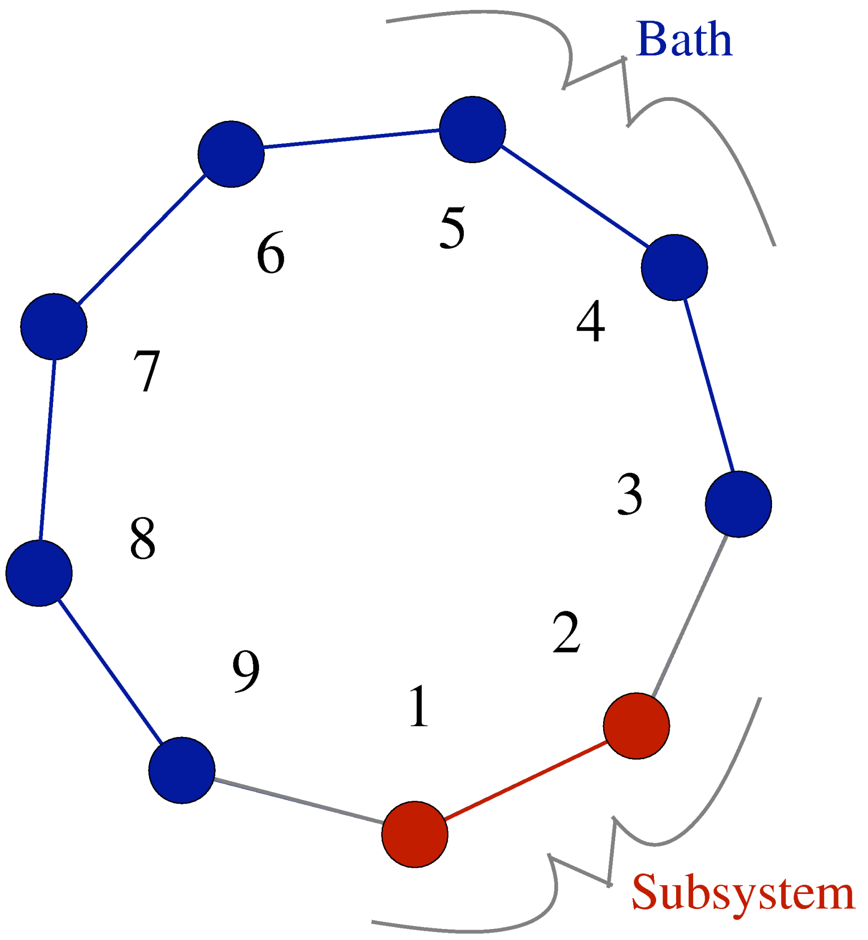
# Hamiltonian

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

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

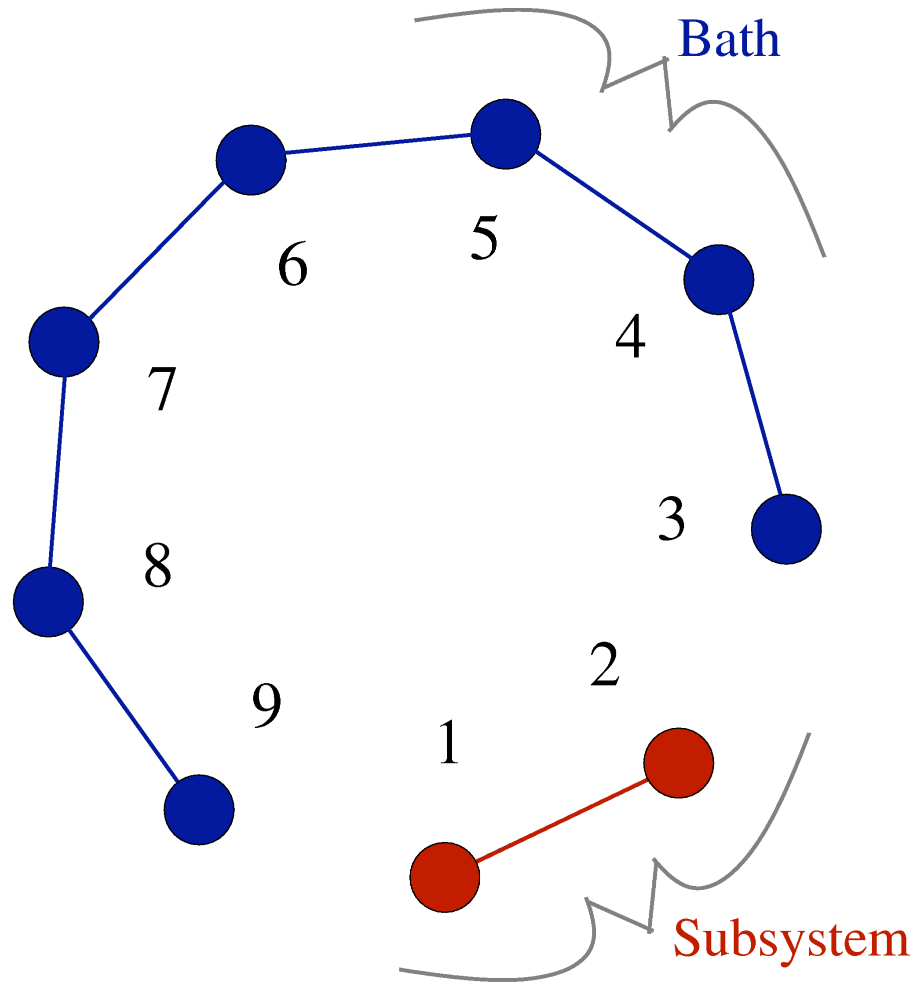
$$\lambda V = -\lambda \sum_{\sigma=\uparrow,\downarrow} J_\sigma\left[(c^\dagger_{2\sigma}c_{3\sigma} + c^\dagger_{1\sigma}c_{L\sigma}) + \text{h.c.}\right]$$

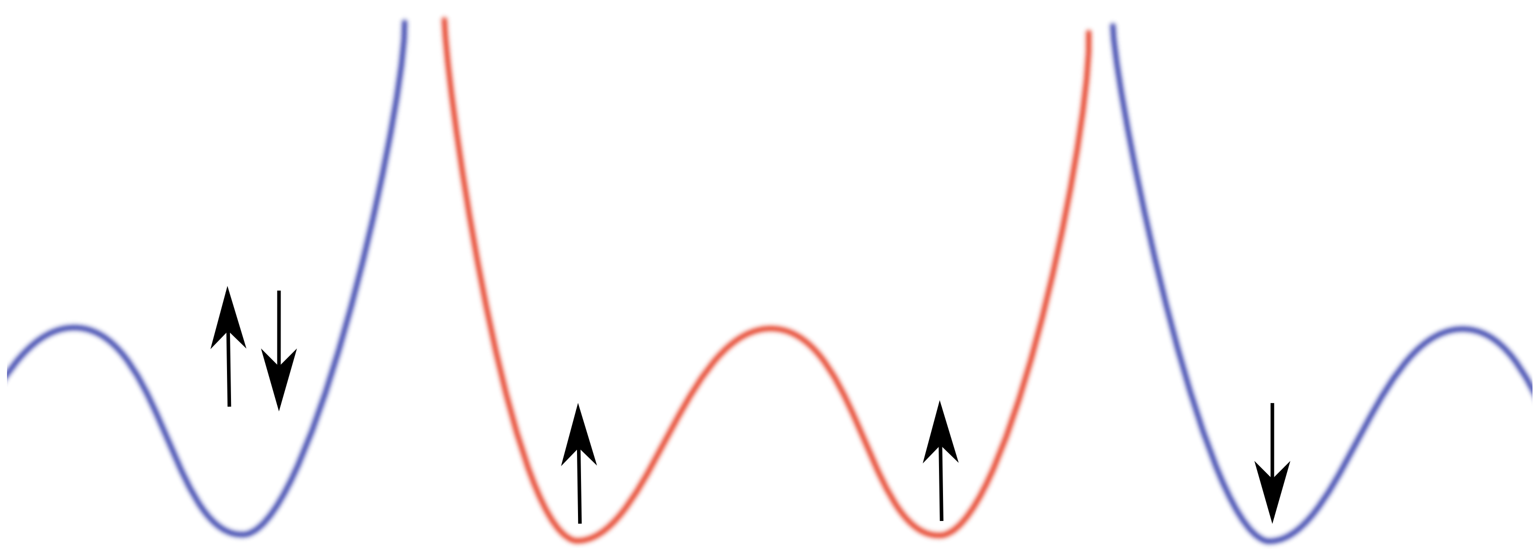
- 8 fermions: 4↑, 4↓
- $J_\sigma = J(1+\xi\,\text{sgn}\sigma)$, $\xi = 0.05$
- $U = J = 1$
- 15876 energy levels
- 16 subsystem energy levels
- $\lambda = 1 \rightarrow$ homogeneous ring



# 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



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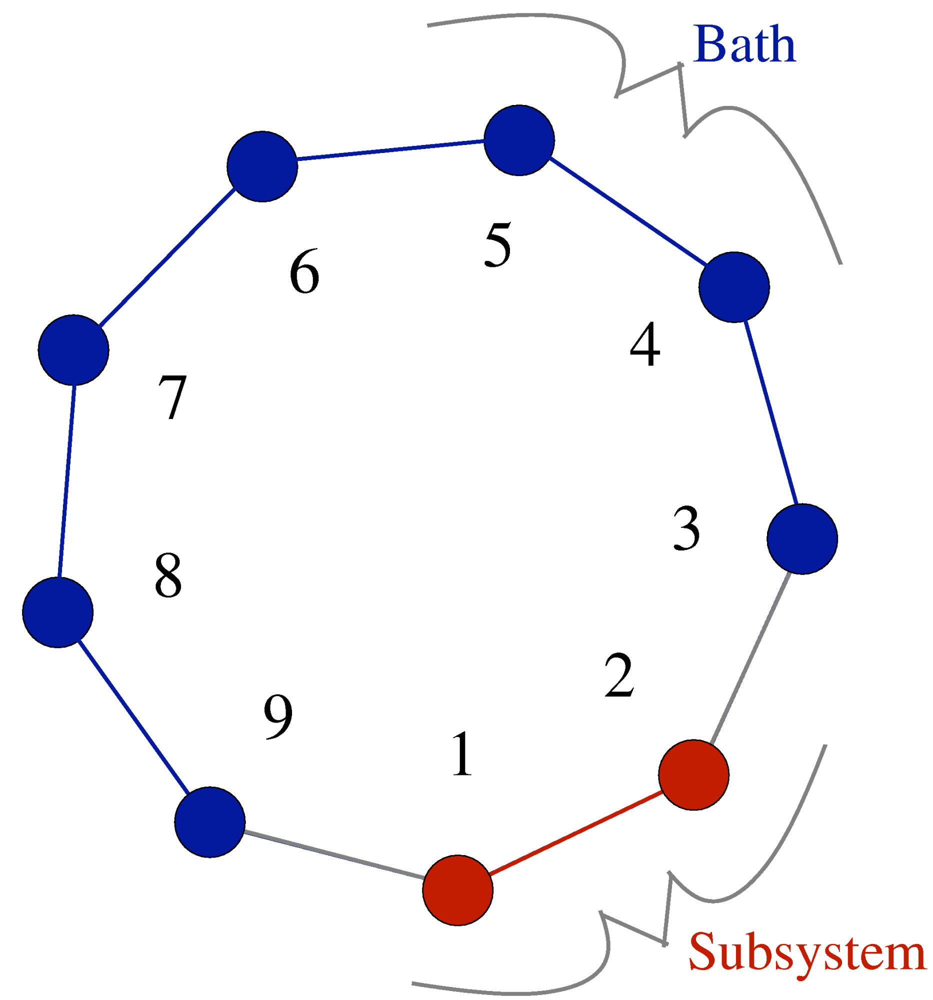
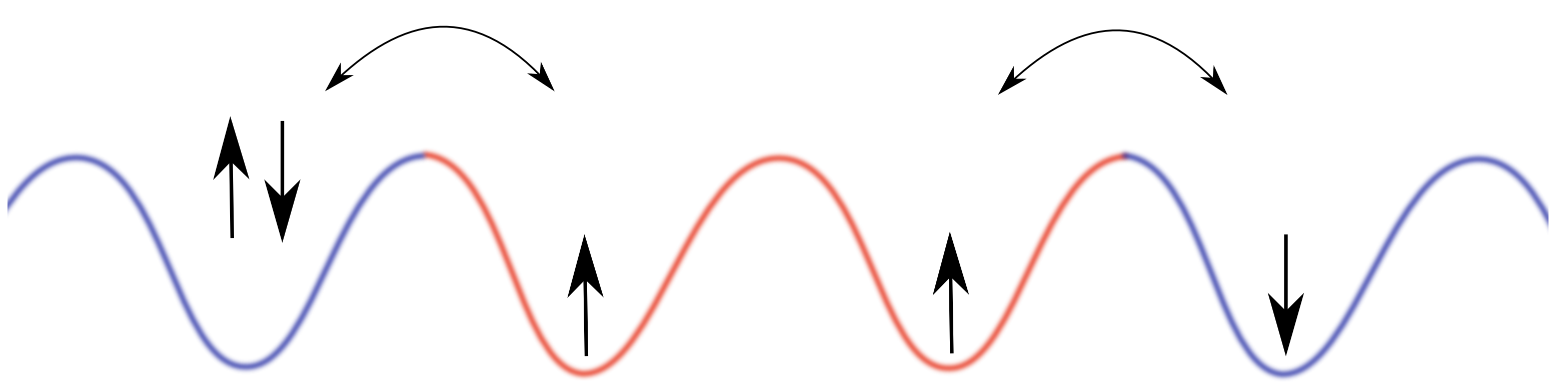
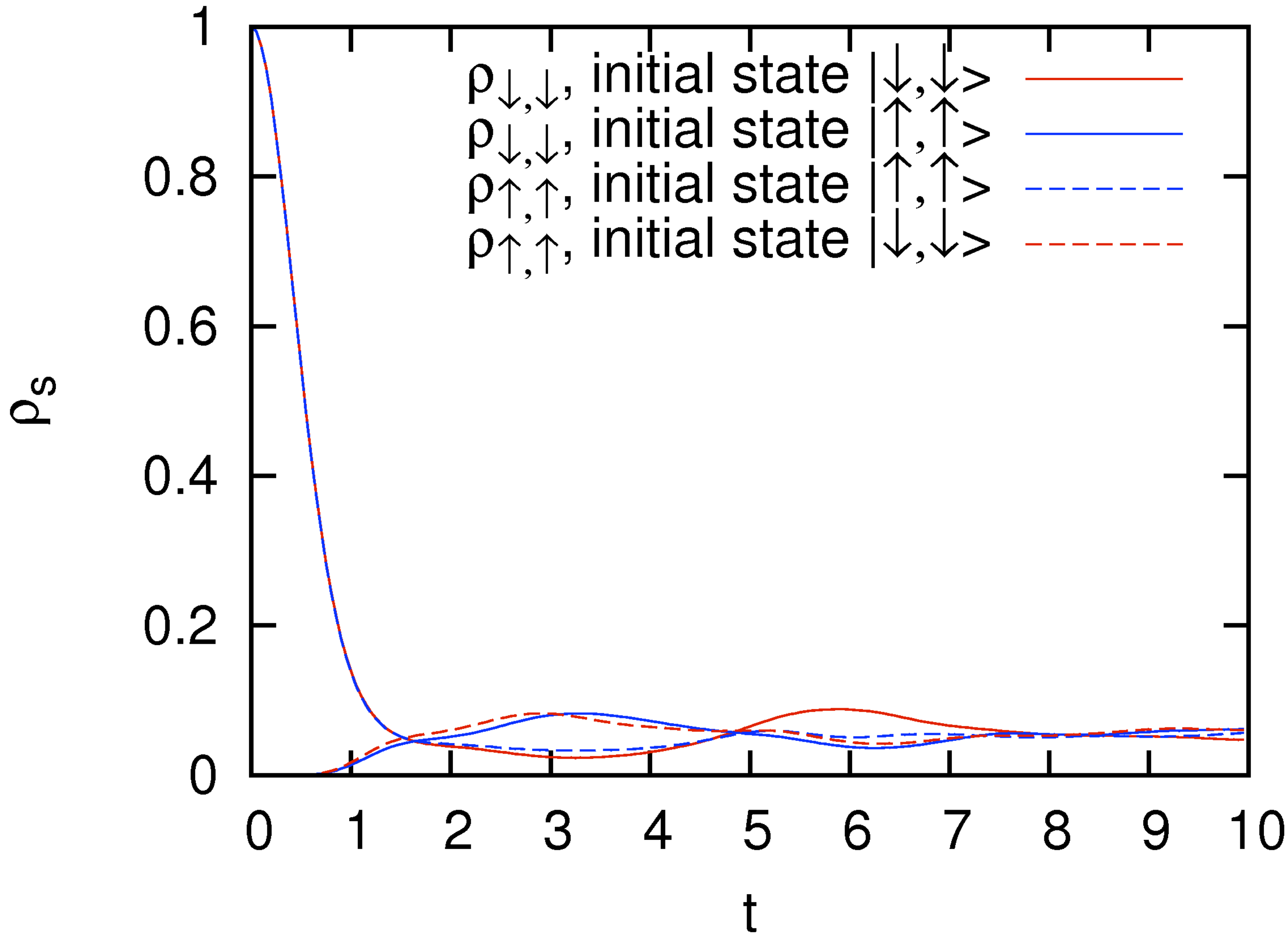
- Switch on $\lambda V$ for $t > 0$
- Evolve $\rho(t) = \text{Tr}_{\text{bath}}\left(|\Psi(t)\rangle\langle\Psi(t)|\right)$ with $|\Psi(t)\rangle = e^{-iHt}|\Psi\rangle$



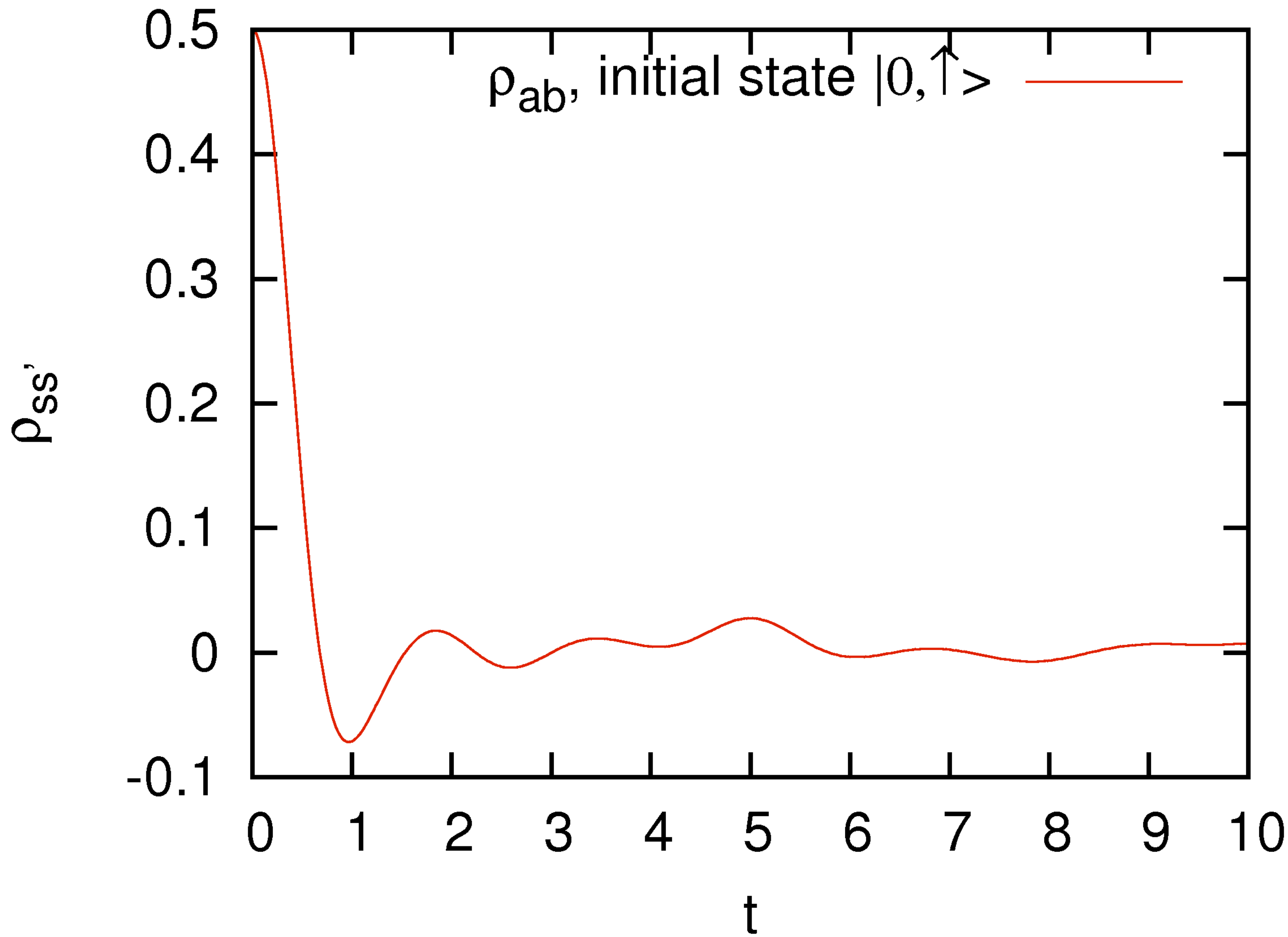
# Subsystem evolution

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



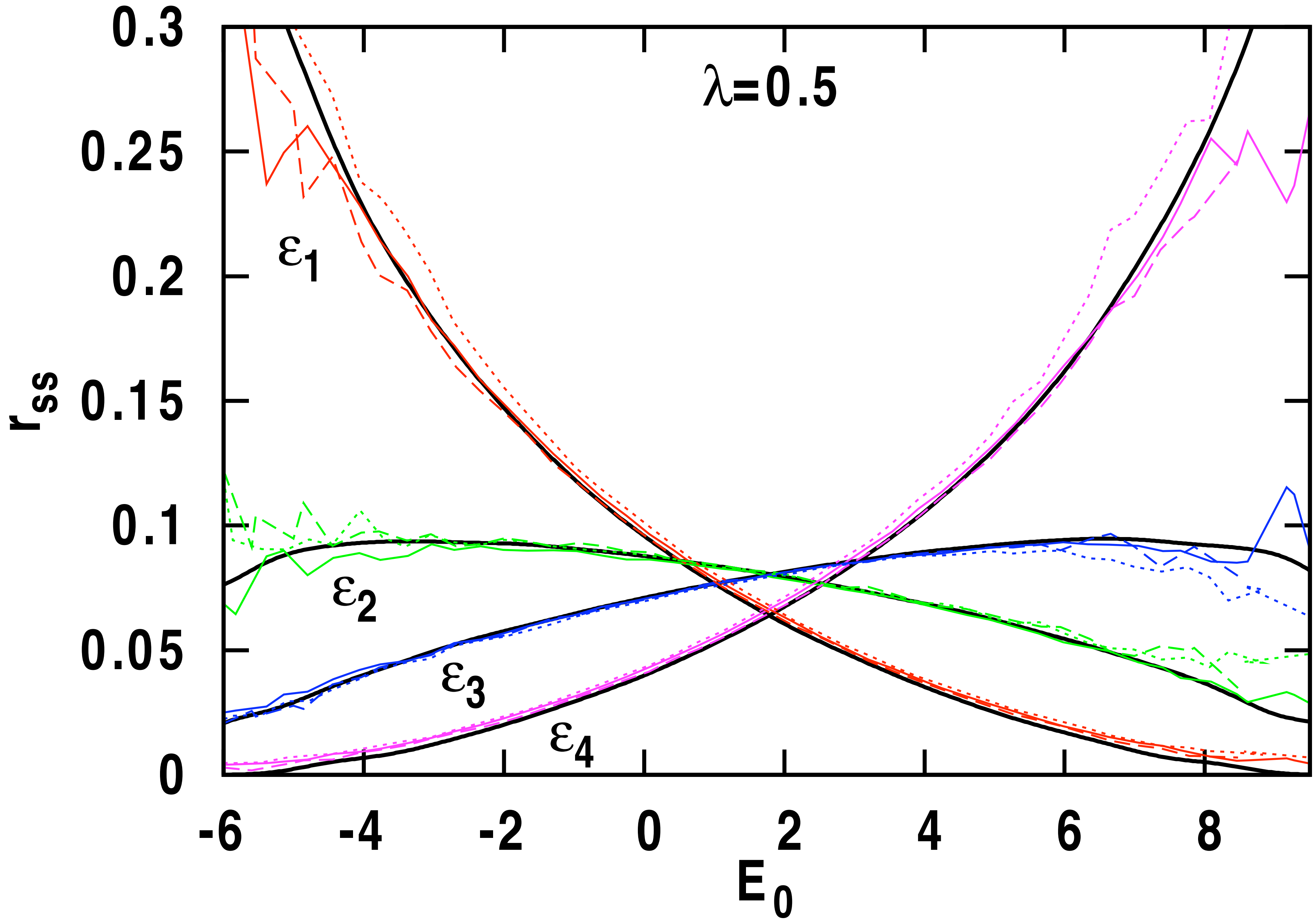
# Subsystem evolution

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




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

# (A) Long-time averages show thermalisation

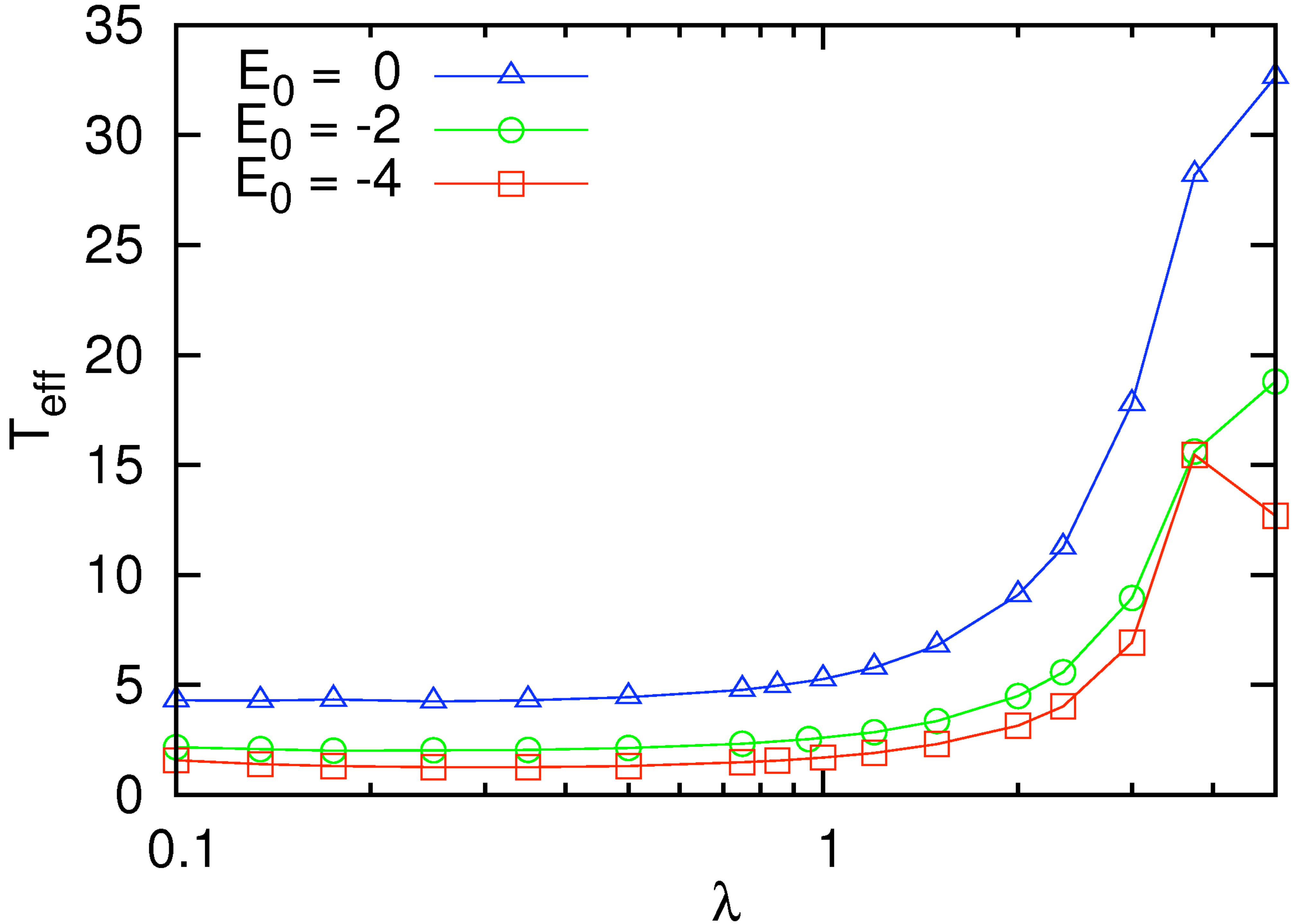



Initial states
$|\uparrow\downarrow,\uparrow\rangle$ (solid)
$|\uparrow,\uparrow\rangle$ (dashed)
$|\uparrow,\downarrow\rangle$ (dotted)
thermal (black)
$\delta = 0.5$

$|\varepsilon_{1,2,3,4}\rangle$: subsystem eigenstates with 2 fermions and $S_z = 0$

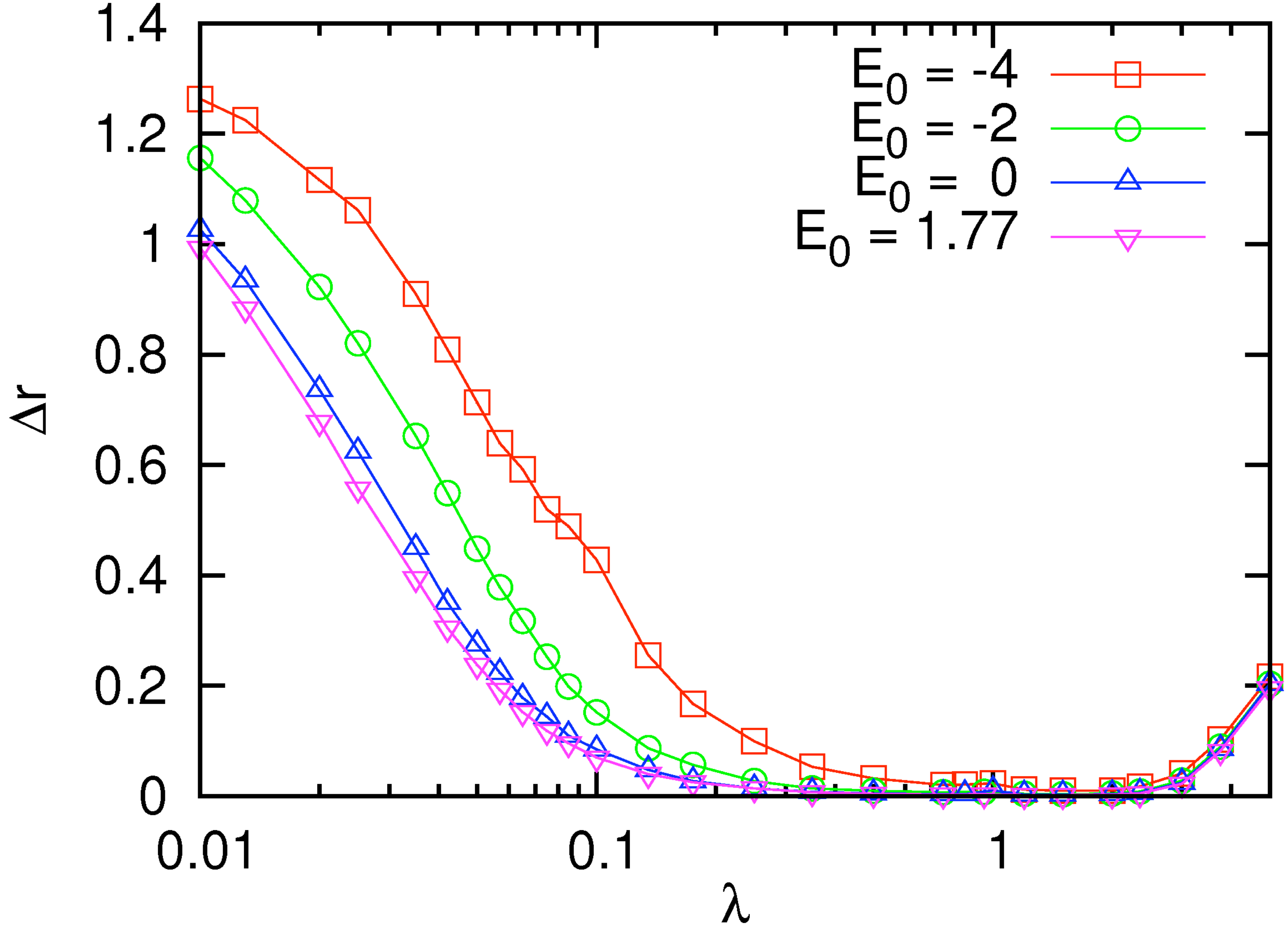
# Effective Temperature

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



# Memory of Initial State

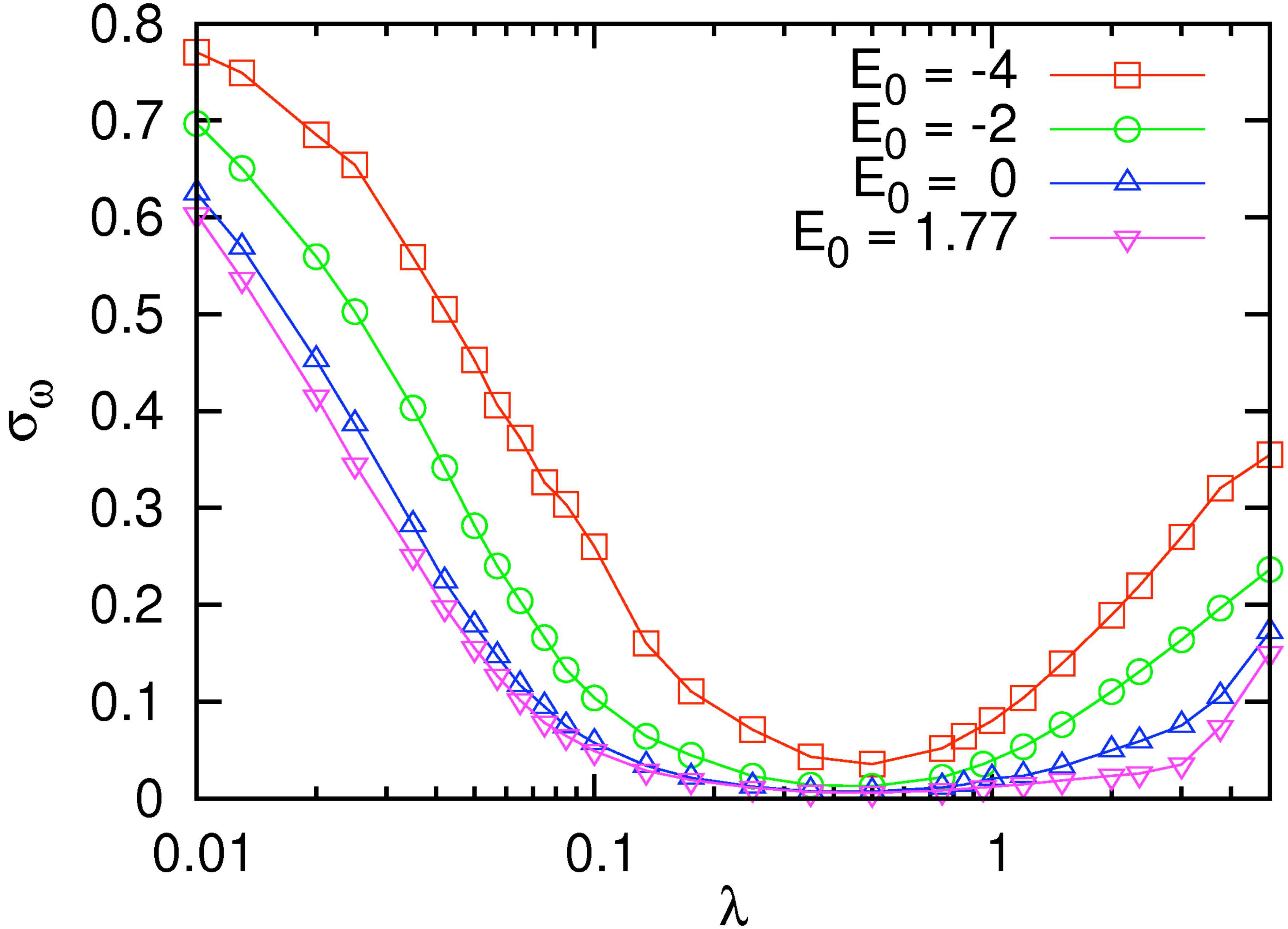
Loss of memory for wide range $0.1 \lesssim \lambda \lesssim 4$




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

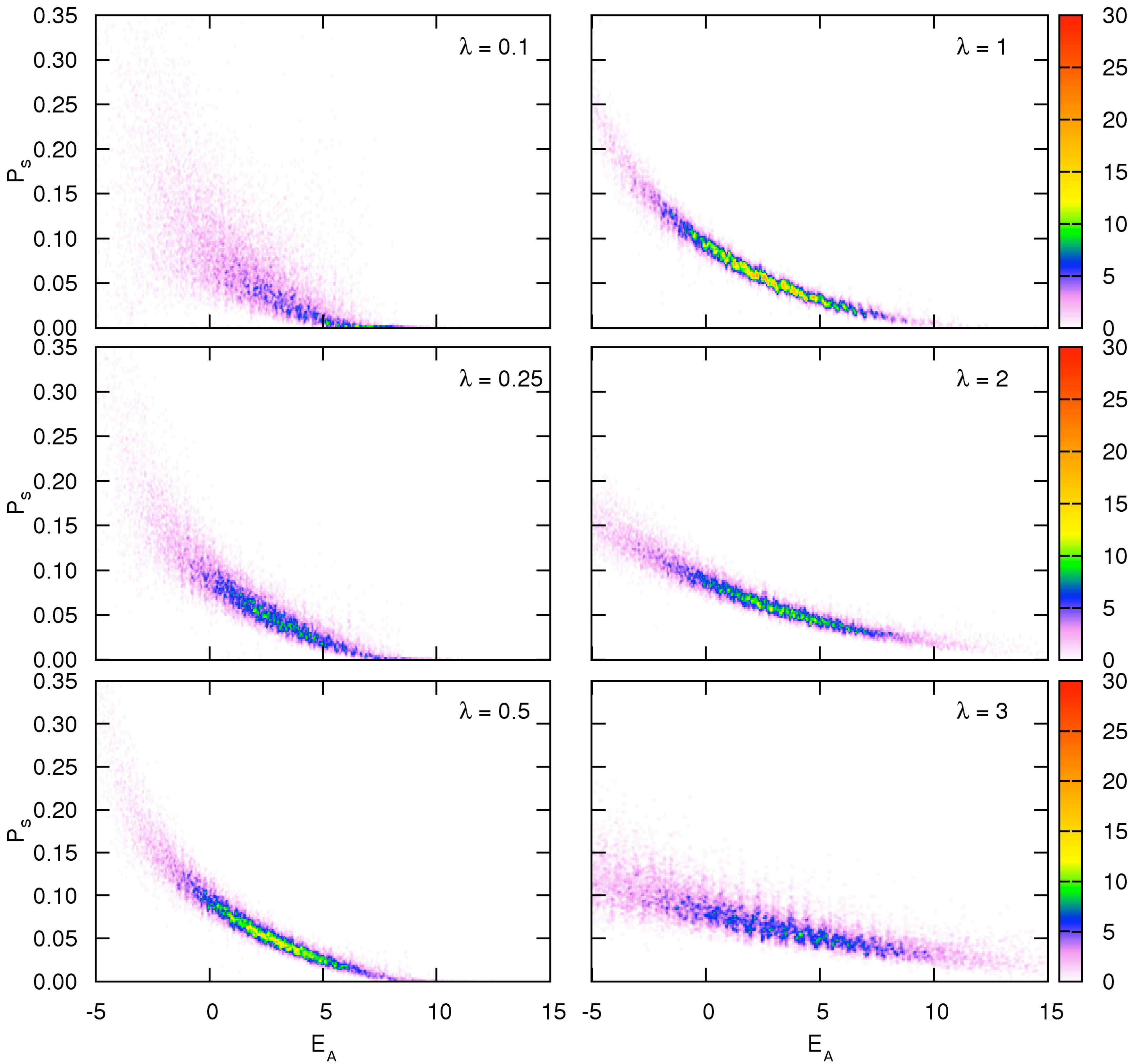
# Closeness to the Thermal State

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 :

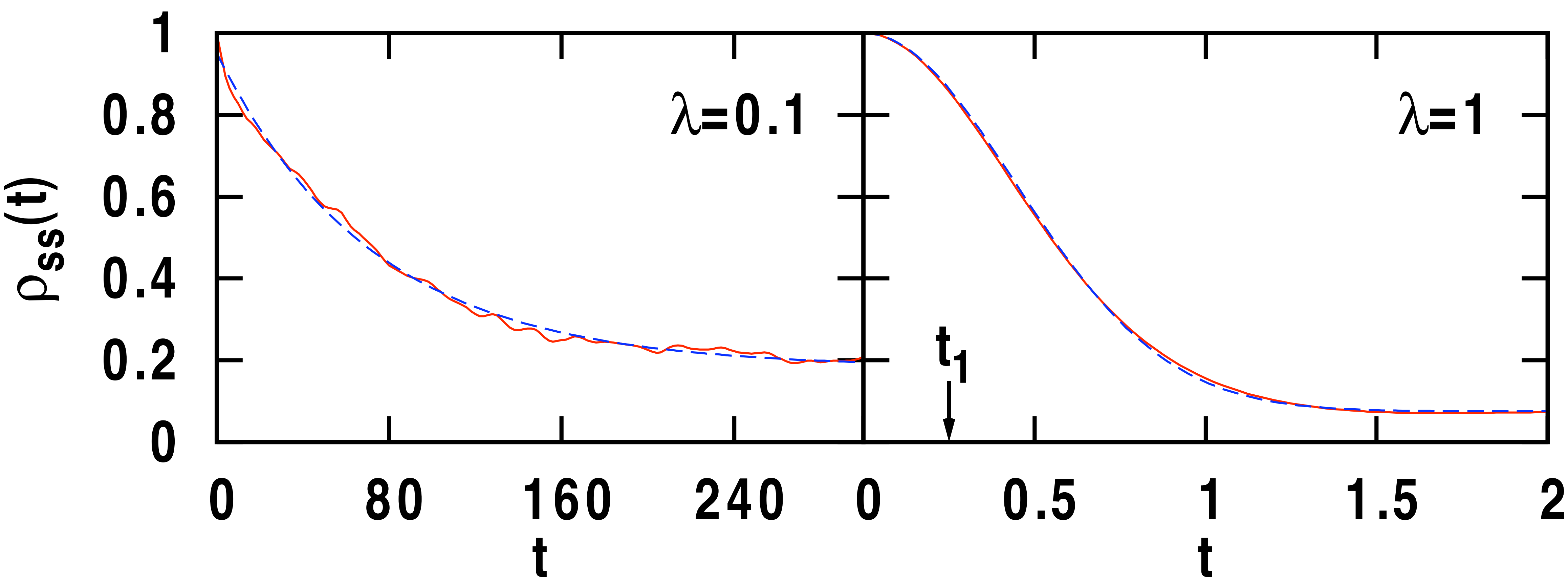
$$\langle E_A | P_s | E_A \rangle$$

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

# (B) Dynamics of Thermalisation

How does the subsystem reach thermalisation?

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




small $\lambda$ $\longleftrightarrow$ larger $\lambda$

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

# 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 $\lambda$

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

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

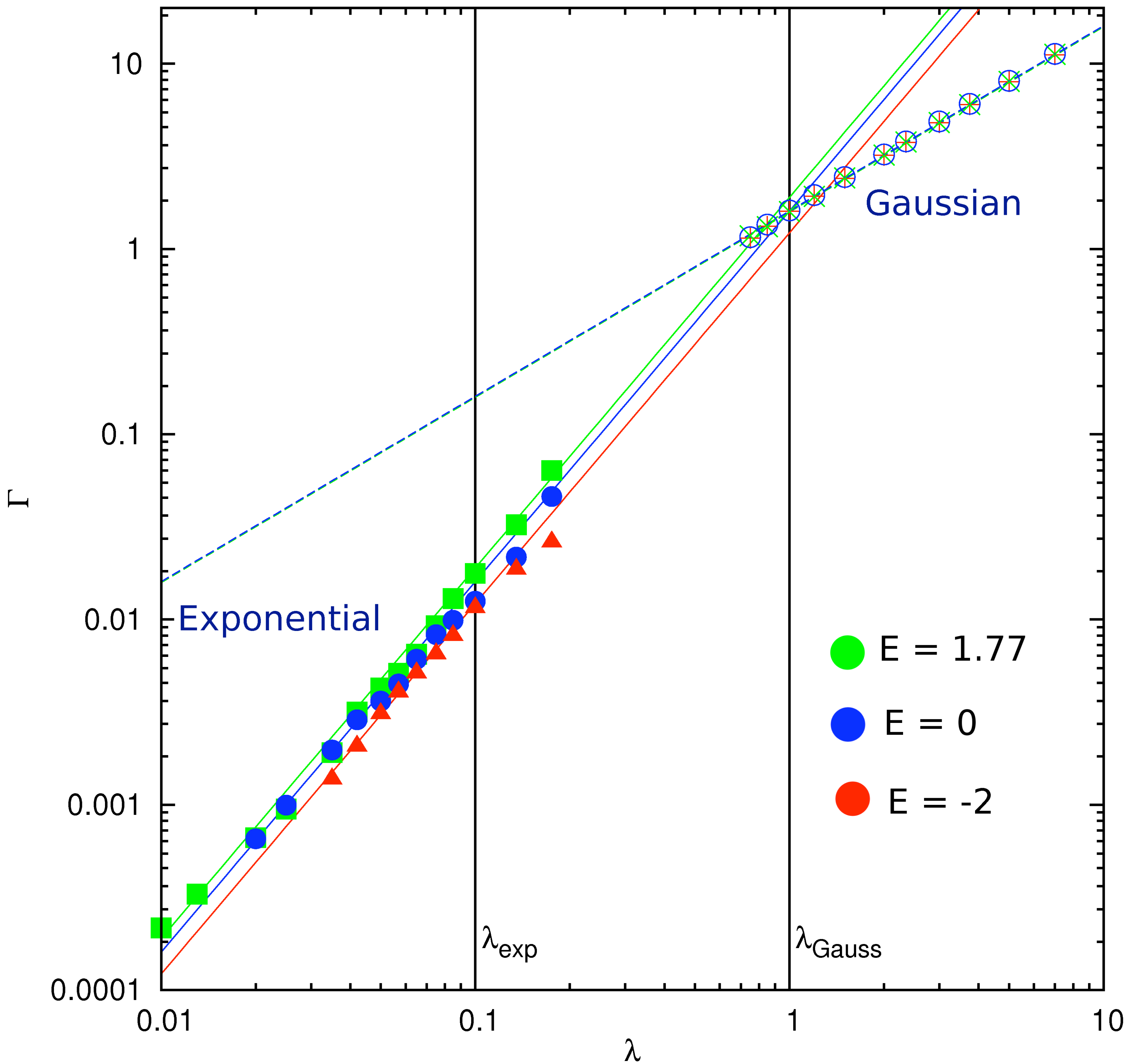
.....start of an exponential decay for small $\lambda$

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

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

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

# Relaxation Rates



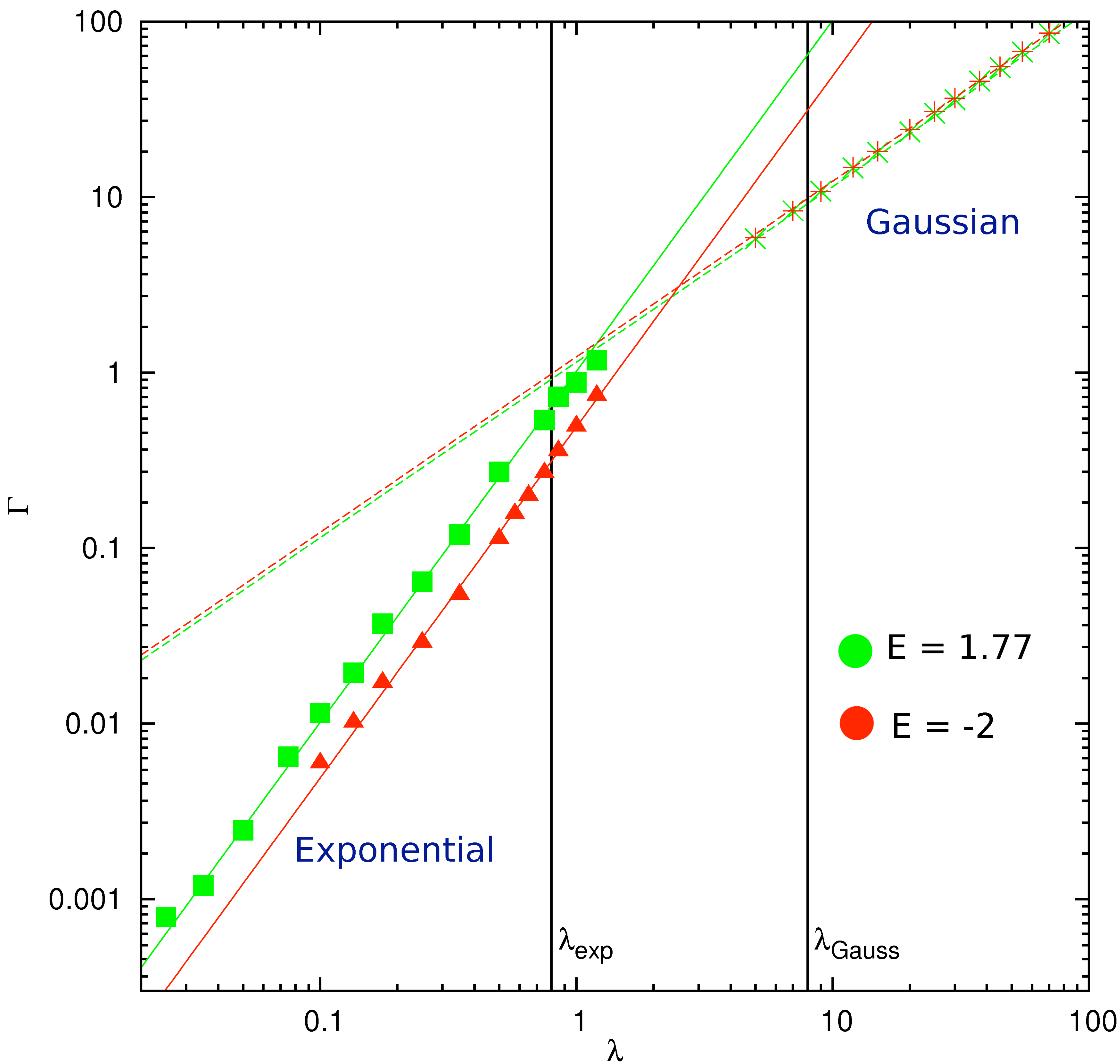

Points:
Fits to Gaussian/
exponential curves

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

# Is Gaussian Behaviour Generic?

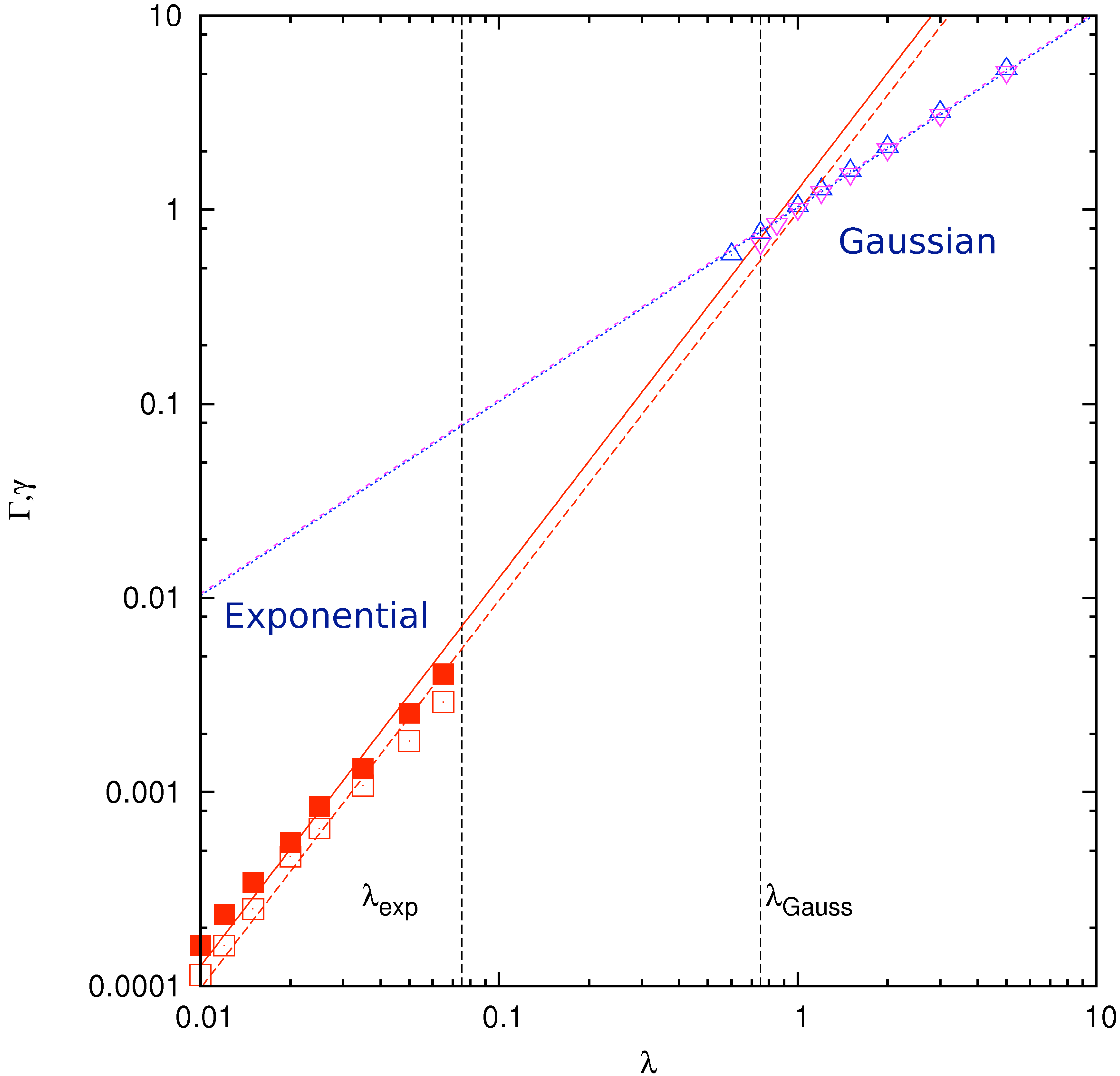
- Gaussian rate $\Gamma \sim \Gamma_{\text{short}}$ short-time rate?
  - exponential behaviour excluded if FGR rate becomes comparable to $\Gamma_{\text{short}}$ (single particle hopping rate)
  - $\Gamma_{\text{short}} \sim \lambda J \sim \lambda$ independent of system size: Gaussian regime persists 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 $t_1^{-1} =$ full bandwidth $\sim 20$

# Bose-Hubbard Model




$\gamma_{FGR}$, $\Gamma_{short}$ (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