Thermalization in the XYZ Spin Chain immersed in a Weak Magnetic Field

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ABSTRACT

We study, using exact diagonalisation methods, the thermalisation of a 2-site subsystem in a non-integrable 12-site XYZ spin chain immersed in a weak magnetic field. In particular, we investigate the existence of a steady state, decoherence, the existence of a canonical thermal state, and the relaxation dynamics of this 2-site subsystem.

MODEL AND THEORETICAL FRAMEWORK

We use as a model system the XYZ spin-1/2 chain coupled to a weak magnetic field, with a Hamiltonian $H = H_S + H_B + \lambda V$.

$$H_S = J_S \sum_{\alpha=x,y,z} J_\alpha S_1^\alpha S_2^\alpha - h \sum_{i=1}^{2} S_i^z \,, \quad (1)$$

$$H_B = J_B \sum_{i=3}^{N-1} \sum_{\alpha=x,y,z} J_\alpha S_i^\alpha S_{i+1}^\alpha - h \sum_{i=3}^{N} S_i^z \,, \quad (2)$$

$$\lambda V = \lambda \sum_{\alpha=x,y,z} J_\alpha \left(S_N^\alpha S_1^\alpha + S_2^\alpha S_3^\alpha\right) \,, \quad (3)$$

Notation - H_S and H_B describe the decoupled subsystem and bath respectively. λV couples the subsystem and bath with a coupling strength λ. Eigenvalues and eigenstates of H_S, H_B, and H are denoted E_s and $|s\rangle_S$, E_b and $|b\rangle_B$, E_A and $|A\rangle$ respectively. $h = 0.4J$, $J_S = J$, $J_B = 1.1J$, $J_x = 1.0$, $J_y = 2.0$, $J_z = 3.0$, unless stated otherwise.

- For times $t < 0$, $\lambda = 0$ (bath and subsystem decoupled). Eigenstates of system are $|sb\rangle = |s\rangle_S \otimes |b\rangle_B$. System prepared in a separable initial state - subsystem (bath) state constructed from $|s\rangle_S$ ($|b\rangle_B$). Choose this initial state $|\Psi(t=0)\rangle$ within a narrow energy window centred at an E_0 away from edges of spectrum. High density of states needed.
- Local quench at $t = 0$ by coupling subsystem and bath with λV. Evolve system under full H now: $|\Psi(t)\rangle = e^{-iHt} |\Psi(0)\rangle$.
- Reduced density matrix (RDM) of subsystem by tracing out bath states from full density matrix:

$$\begin{aligned}\rho(t) &= \mathrm{Tr}_B \,|\Psi(t)\rangle \langle \Psi(t)| \\ &= \sum_{A,B,b} \exp(-i(E_A - E_B)t) \langle A| |\Psi(0)\rangle \langle \Psi(0)| |B\rangle \langle b| |A\rangle \langle B| |b\rangle \end{aligned} \quad (4)$$

Link to Eigenstate Thermalization Hypothesis - $\langle A| |\Psi(0)\rangle$ non-zero only within chosen energy window. High density of states within this window suppresses regularity/periodicity in time evolution, yielding a steady state in the strong sense (no time averaging). Assume projections onto subsystem energy basis $\sum_b \langle A| |sb\rangle \langle sb| |A\rangle$ weakly dependent on $|A\rangle$ within window.

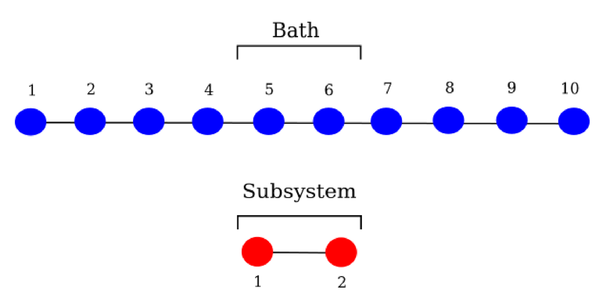

Figure 1: For times $t < 0$

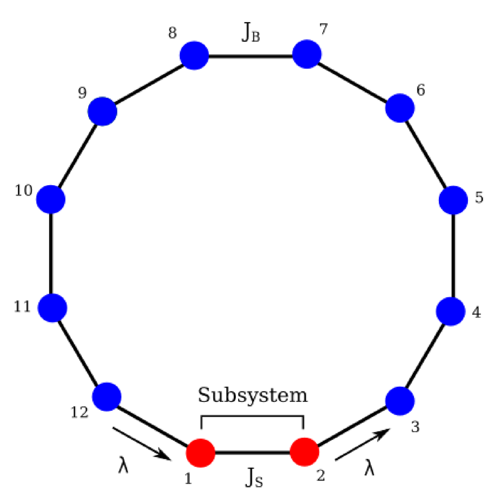

Figure 2: For times $t > 0$

DECOHERENCE AND EQUILIBRATION

Diagonal subsystem steady states in eigenbasis of H_S for subsystem-bath couplings $0.05J \leq \lambda \leq 3.5J$. Split peaks in density of states for larger λ - strongly interacting spins at chain links are effectively decoupled with energy scale proportional to λ.

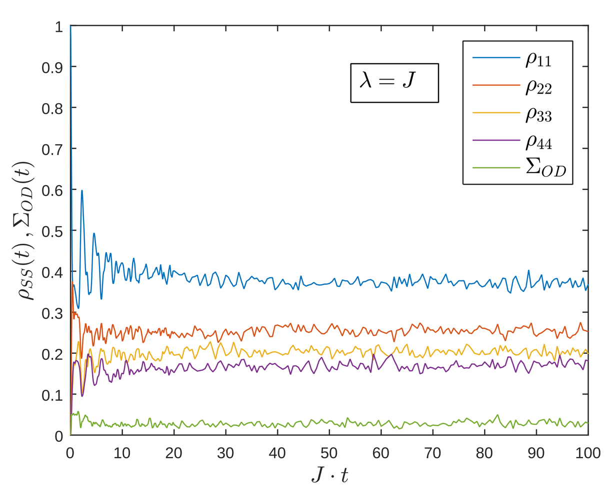

Figure 3: Steady state with decoherence for $\lambda = J$, initial subsystem state $\rho(0)_{11} = 1$

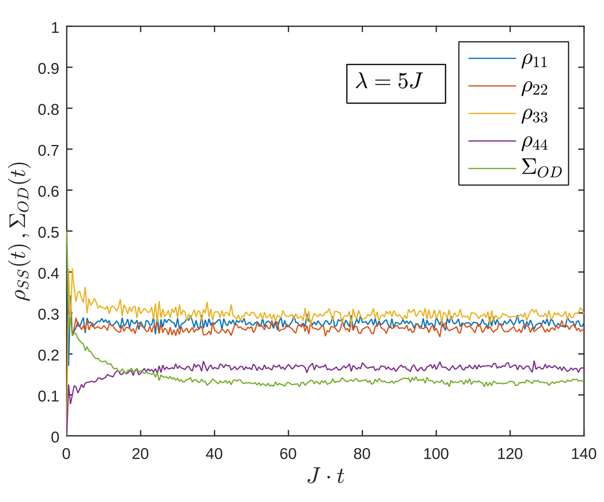

Figure 4: Steady state without decoherence for $\lambda = 5J$, initial subsystem state $\rho(0)_{11} = \rho(0)_{22} = \rho(0)_{12} = 0.5$

In results above, initial bath state is an equal-weights superposition of bath eigenstates ($|b\rangle$) in energy window centred at $E_b = -0.75J$ with a full width $\delta_b = 3J$. We quantify coherence (off-diagonal elements) using the measure:

$$\Sigma_{OD}(t) = \sqrt{\sum_{s<s'} |\rho_{ss'}(t)|^2} \quad (5)$$

FUTURE WORK

- Introduce disorder (randomise spin-spin couplings or site-dependent coupling to external magnetic field) to realise a many-body localised (MBL) phase. Study statistics of level spacings to see difference from corresponding Wigner-Dyson statistics in thermalising systems. Also check for logarithmic growth in time of entanglement entropy in the MBL case.

RELAXATION DYNAMICS

The initial state of the subsystem is prepared in an eigenstate of H_S - in this section, the ground state $\rho_{11} = 1$. We see 3 regimes of relaxation - **(A)** Exponential decay of initial state occupation probability ρ_{11} for perturbative $\lambda \leq 0.2J$ **(B)** Gaussian decay for large, non-perturbative $\lambda \geq 1.2J$ **(C)** A crossover regime for intermediate values of λ where decay is Gaussian for short times and exponential for long times.

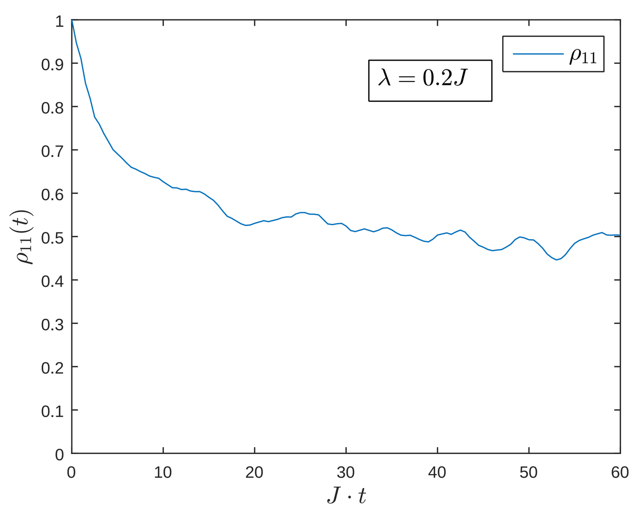

Figure 5: Exponential decay of $\rho_{11}(t)$ for $\lambda = 0.2J$.

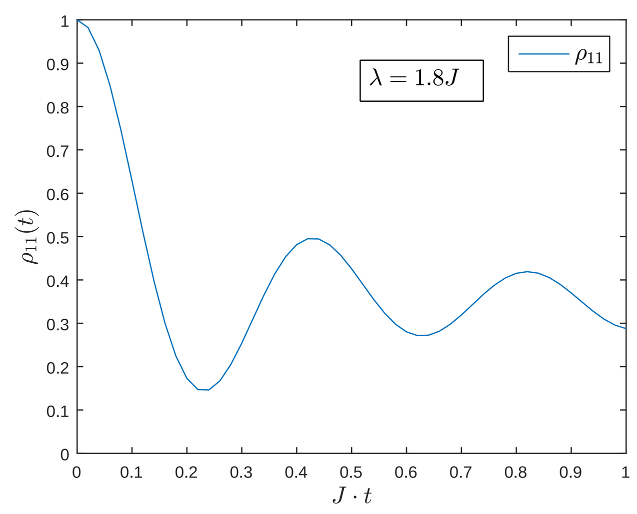

Figure 6: Gaussian decay of $\rho_{11}(t)$ for $\lambda = 1.8J$.

In results above, initial bath state is an equal-weights superposition of bath eigenstates ($|b\rangle$) in energy window centred at $E_b = -0.75J$ with a full width $\delta_b = 3J$. Decay rates in the exponential regime scale exponentially with λ, contrary to results in random matrix models [3], Fermi-Hubbard ring [1], and spin chains in the absence of external magnetic field [4]. Gaussian decay rates scale linearly with λ, similar to results of [3, 1, 4].

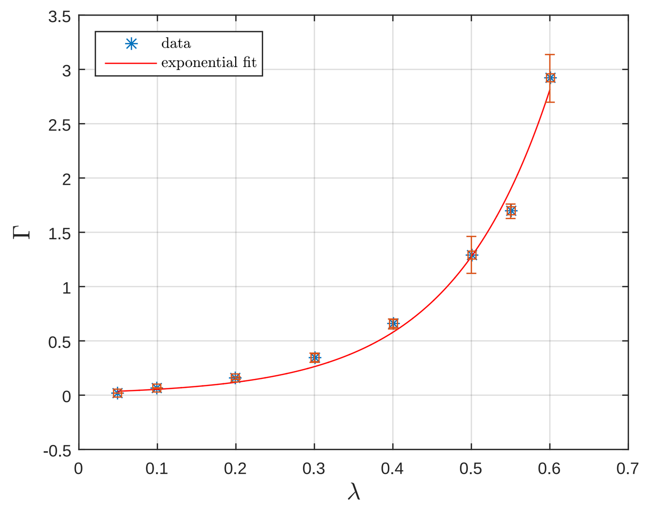

Figure 7: Decay rate Γ of $\rho_{11}(t)$ in the exponential regime as a function of λ

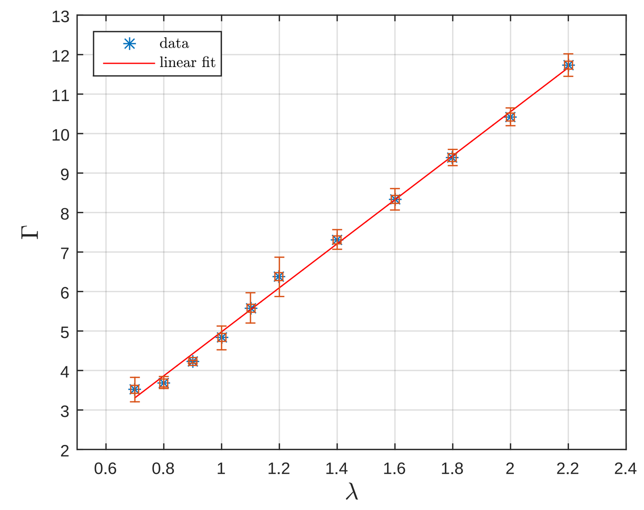

Figure 8: Decay rate Γ of $\rho_{11}(t)$ in the Gaussian regime as a function of λ

CANONICAL THERMALIZATION

System size too small to test for subsystem state independence of a thermal state. Effects of subsystem initial state is not outweighed by size of bath, and equilibrium energy of bath different to initial bath energy, implying subsystem-bath coupling changes bath temperature at equilibrium. The subsystem is prepared initially in the ground state of energy $-6J$; initial bath state is an equal-weights superposition of bath eigenstates ($|b\rangle$) in energy window centred at $E_b = -0.75J$ with a full width $\delta_b = 3J$.

- For $\lambda = 1.8J$, equilibrium bath energy is $(-13.6262J)$. At this mean energy, inverse temperature $J\beta$ of bath derived from density of states of bath is 0.0689264. Subsystem energy levels are $(-6J, 0J, 1.27J, 4.28J)$ and so the canonical thermal state (Boltzmann form) is $\omega = \mathrm{diag}(0.3648, 0.2413, 0.2143, 0.1796)$. In this case, $\rho(\infty) \approx \mathrm{diag}(0.3378, 0.2486, 0.2192, 0.1943)$ (see Figure 9). Trace distance $D = 0.5\,\mathrm{Tr}\sqrt{(\rho(\infty) - \omega)^2} = 0.03$.
- For $\lambda = J$, equilibrium bath energy is $(-12.8971J)$, with an inverse temperature $J\beta = 0.0652596$. In this case, $\omega = \mathrm{diag}(0.3582, 0.2422, 0.2165, 0.1831)$ and $\rho(\infty) = \mathrm{diag}(0.3702, 0.2535, 0.2030, 0.1734)$ (see Figure 10). Trace distance $D = 0.02$.

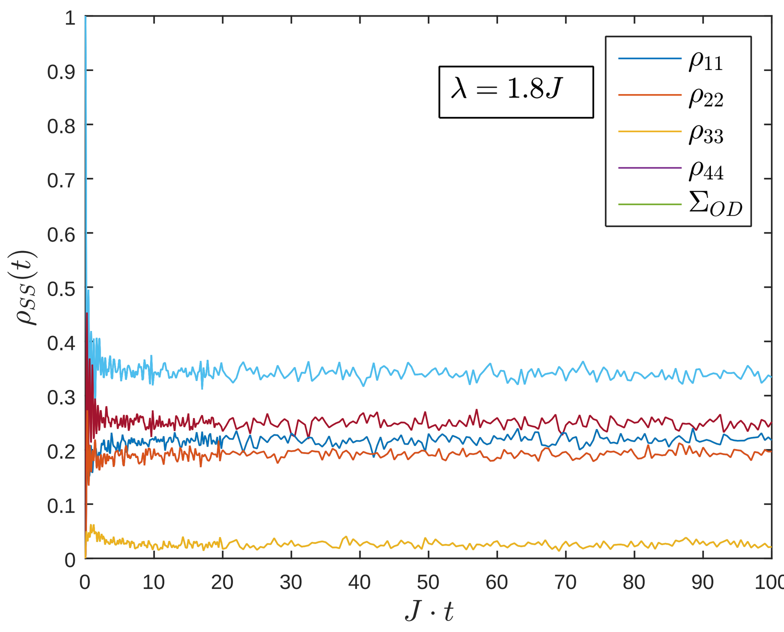

Figure 9: Relaxation of $\rho(t)$ for $\lambda = 1.8J$, initial subsystem state $\rho_{11}(0) = 1$

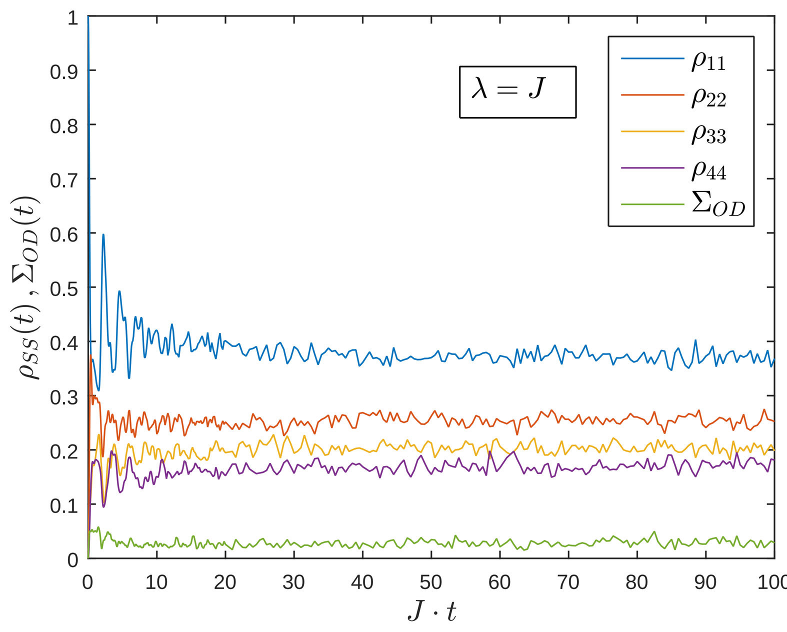

Figure 10: Relaxation of $\rho(t)$ for $\lambda = J$, initial subsystem state $\rho_{11}(0) = 1$

Trace distances $D \leq 0.03$ for $0.6 \leq \lambda \leq 2.0$. Range of subsystem-bath couplings in which we see canonical thermalisation is remarkably similar to that observed in the Fermi-Hubbard ring of [2], which seems to indicate that the steady state results we derive are only dependent on the energy scales involved and not on the specifics of the model system considered.

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