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Entanglement in quantum dissipative Ising spin systems

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Abstract

We study the behavior of entanglement estimators on chains of few quantum Ising spins coupled to an environment by means of Monte Carlo simulations. We analyze the ground state value of the von Neumann entropy and the concurrence of our spins system for different couplings with the quantum bath.

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Keywords: Entanglement; Dissipation; Monte Carlo simulations

1. Introduction

Quantum spin chains have been studied very intensively during the last four decades and many results have been obtained using a variety of theoretical techniques.

A renewed interest on spin chains has arisen recently in the context of quantum phase transitions and quantum computing [1]. Spin-$\frac{1}{2}$ Ising chains coupled to different types of quantum thermal baths capture the effect of the interaction between qubits and the environment. Decoherence effects and entanglement properties can be examined in these models. The interaction with the environment turns the problem more difficult and few analytical results are available.

In this work we are interested in the behavior of quantum computing observables (like concurrence) of a small number of spins (or qubits) as a function of their coupling with an environment. This problem has been analyzed very recently in Ref. [2] for the case of one spin where an analytical treatment is possible. In this work we re-examine this problem (and correct the original claim made there, see also Ref. [3]) using numerical techniques. This technique can be used for (small) spins chains. Explicit results corresponding to two qubits are presented.

We describe the environment by a quantum thermal bath composed by independent quantum harmonic oscillators following the formulation of Feynman and Vernon for dissipation. The simulations run on an equivalent $(1+1)$-D classical spin lattice through a Trotter decomposition.

The spin chain coupled to the environment is modeled by

$$\hat{H} = \hat{H}_J + \hat{H}_B + \hat{H}_I + \hat{H}_{CT}.$$

The Hamiltonian of the quantum spin chain is described by

$$H_J = -\sum_{i=1}^{N} J\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z - \sum_{i=1}^{N} \Gamma\hat{\sigma}_i^x,$$

where J is the strength of exchange interactions. The intensity of the external transverse magnetic fields is represented by Γ. The Hamiltonian for the quantum bath reads

$$\hat{H}_B = \sum_{l=1}^{\tilde{N}} \frac{1}{2m_l}\hat{p}_l^2 + \sum_{l=1}^{\tilde{N}} \frac{m_l\omega_l^2}{2}\hat{x}_l^2,$$

and

$$\hat{H}_I = -\sum_{i=1}^{N} \hat{\sigma}_i^z \sum_{l=1}^{\tilde{N}} c_{il}\hat{x}_l,$$

and the counterterm is

$$\hat{H}_{CT} = \sum_{l=1}^{\tilde{N}} \frac{1}{2m_l\omega_l^2}\left(\sum_{i=1}^{N} c_{il}\hat{\sigma}_i^z\right)^2.$$

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We derive equilibrium properties from the partition function $Z = \mathrm{Tr}\, e^{-\beta H}$. The integration over the bath variables can be performed explicitly. We use an Ohmic bath with spectral density

$$I_i(\omega) \equiv \frac{\pi}{2}\sum_{l=1}^{\tilde{N}/N} \frac{c_{il}^2}{m_l\omega_l}\delta(\omega-\omega_l) = \begin{cases} 2\pi\alpha\omega & \text{for } \omega\Delta\tau<1, \\ 0 & \text{otherwise.}\end{cases}$$

The Trotter decomposition yields a partition in intervals of length $\Delta\tau$ of the imaginary time direction. As $\Delta\tau \to 0$ the mapping between the 1-D quantum model and the $(1+1)$-D classical model becomes exact. This equation also defines the parameter α that we use later as a measure of the strength of the bath.

2. Entanglement

The quantum state of a bipartite system, AB, can be described with the help of the density matrix, $\hat{\rho}_{AB}$. For a pure state, this system is said to be entangled if its density matrix cannot be factorized as $\hat{\rho}_{AB} = \hat{\rho}_A\hat{\rho}_B$ where $\hat{\rho}_A = \mathrm{Tr}_B(\hat{\rho}_{AB})$, and $\hat{\rho}_B = \mathrm{Tr}_A(\hat{\rho}_{AB})$ are reduced density matrices. In this case, the reduced matrices represent mixed states and the von Neumann entropy [5],

$$s = -\mathrm{Tr}(\hat{\rho}_A \log \hat{\rho}_A) = -\mathrm{Tr}(\hat{\rho}_B \log \hat{\rho}_B),$$

gives a quantitative measure of the entanglement between A and B. The von Neumann entropy has the property of being positive, and takes the zero value if the state is pure.

For our spin chain coupled to a set of harmonic oscillators, we take as subsystem A a single spin, and as subsystem B the harmonic oscillators with the rest of the chain. The reduced density matrix for a single spin can be obtained measuring spin expectation values

$$\hat{\rho}_1 = \frac{1}{2}\hat{I} + \frac{1}{2}\sum_{\mu=x,y,z}\langle\hat{\sigma}^\mu\rangle\hat{\sigma}^\mu$$
$$\langle\hat{\sigma}^\mu\rangle = \mathrm{Tr}(\hat{\sigma}^\mu\hat{\rho}_{S+B}),$$

with $\hat{\rho}_{S+B}$ the total spin-environment density matrix. Symmetry transformations show that some matrix elements must vanish. In particular, the Hamiltonian $\hat{H}$ is invariant under a global π rotation about the spin x axis yielding $\langle\hat{\sigma}^y\rangle = 0$. We can take $\langle\hat{\sigma}^z\rangle = 0$ if $\alpha<\alpha_c$. Then

$$s = -\frac{1}{2}\log_2\left(\frac{1-\langle\hat{\sigma}^x\rangle^2}{4}\right) - \frac{1}{2}\langle\hat{\sigma}^x\rangle\log_2\left(\frac{1+\langle\hat{\sigma}^x\rangle}{1-\langle\hat{\sigma}^x\rangle}\right). \quad (1)$$

When $\alpha \geqslant \alpha_c$, the spin is localized. Its reduced density matrix is $\hat{\rho}_1 = \frac{1}{2}(\hat{I} \pm \hat{\sigma}^z)$ and its von Neumann entropy vanishes, $s(\rho_1)|_{\mathrm{loc}} = 0$.

In Ref. [6] it is proved that the entanglement of formation of a general two qubits state $\hat{\rho}$ can be written in terms of the concurrence $\mathscr{C}(\rho)$

$$E(\hat{\rho}) = \mathscr{E}(\mathscr{C}(\hat{\rho})),$$

where the function $\mathscr{E}$ is given by

$$\mathscr{E}(\mathscr{C}) = h\left(\frac{1+\sqrt{1-\mathscr{C}^2}}{2}\right),$$
$$h(x) = -x\log_2 -(1-x)\log_2(1-x).$$

$\mathscr{E}(\mathscr{C})$ is monotonically increasing and ranges from 0 to 1 as $\mathscr{C}$ goes from 0 to 1, so it is usual to also take $\mathscr{C}$ as a measure of entanglement. The value of the concurrence results from

$$\mathscr{C}(\hat{\rho}) = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},$$

where λ_i are the eigenvalues, in decreasing order, of the matrix $\hat{\rho}\tilde{\hat{\rho}} \equiv \hat{\rho}\hat{\sigma}^y \otimes \hat{\sigma}^y\hat{\rho}^*\hat{\sigma}^y \otimes \hat{\sigma}^y$.

We are interested in calculating the concurrence between spin i and j of our dissipative spin chain through their reduce density matrix. Taking that $\hat{\rho}_{ij}$ is Hermitian and $\mathrm{Tr}\,\hat{\rho}_{ij} = 1$ we find that

$$\hat{\rho}_{ij} = \frac{1}{4}\sum_{\mu,\nu=x,y,z,0}\langle\hat{\sigma}_i^\mu\hat{\sigma}_j^\nu\rangle\hat{\sigma}_i^\mu\hat{\sigma}_j^\nu,$$
$$\langle\hat{\sigma}_i^\mu\hat{\sigma}_j^\nu\rangle = \mathrm{Tr}\,(\hat{\sigma}_i^\mu\hat{\sigma}_j^\nu\hat{\rho}_{S+B}),$$

where $\hat{\sigma}^0$ represents the identity operator. We use the symmetries of the Hamiltonian $\hat{H}$ to reduce the number of

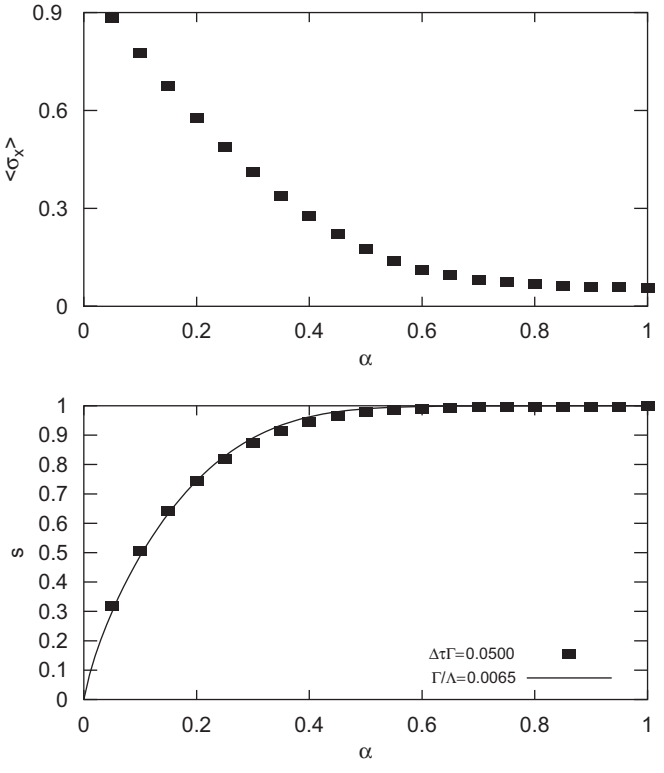

Fig. 1. $\langle\sigma_x\rangle$ (top) as function of α. The von Neumann entropy (bottom) as function of α for $N = 1$, $\Gamma = 1$. With dashed lines we show the result of fitting our data with the exact expressions given by Eq. (1). We choose the adjusting parameter Γ/Λ from Ref. [2].

expectation values needed in the calculation. After we numerically compute the four eigenvalues, we arrange them in decreasing order and make the concurrence calculation.

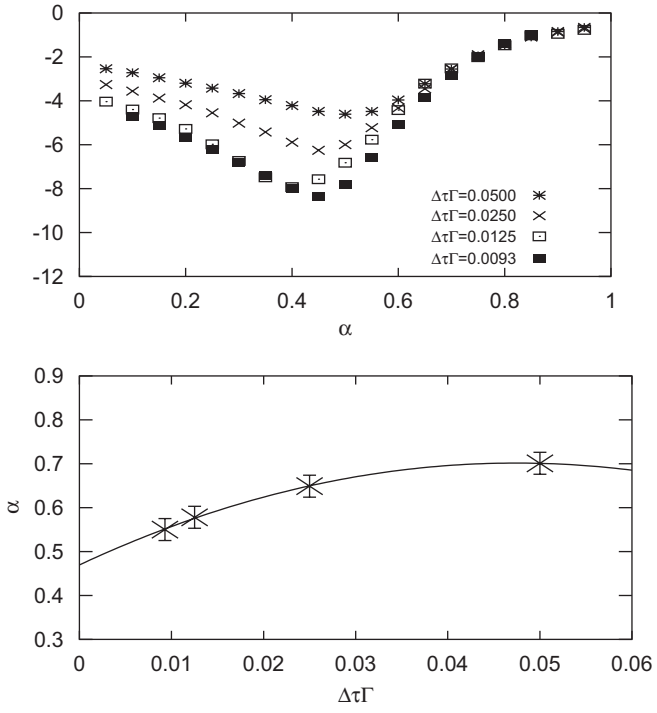

Fig. 2. Plot of $\langle \partial \log \sigma_x/\partial\alpha\rangle$ as a function of α for different products $\Delta\tau\Gamma$ (top). α for the inflection point of each curve of the left figure as function of $\Delta\tau\Gamma$ (bottom).

3. Monte Carlo simulations and results

We analyze the static properties of the system by means of Monte Carlo (MC) simulations performed on a classical equivalent partition function

$$Z_J = \sum_{s_i^t=\pm 1} \mathrm{e}^{-A},$$

$$A = -\sum_{t=0}^{N_\tau-1}\sum_{i=1}^{N} K_i s_i^t s_{i+1}^t - B\sum_{t=0}^{N_\tau-1}\sum_{i=1}^{N} s_i^t s_i^{t+1} + \frac{\alpha}{2}\sum_{t<t'}^{N_\tau-1}\sum_{i=1}^{N}\left(\frac{\pi}{N_\tau}\right)^2 \frac{s_i^t s_i^{t'}}{\sin^2(\pi|t-t'|/N_\tau)},$$

where $K_i = J_i\beta/N_\tau = J_i\Delta\tau$ and $B = \frac{1}{2}\ln(\coth(\Delta\tau\Gamma))$. The effective classical $(1+1)$-dimensional action, A, is obtained after applying the Trotter–Suzuki formula and introducing an imaginary time direction.

The classical counterpart model is defined on a rectangular lattice with size $N \times N_\tau$. The expectation values, which we denote with $\langle\cdots\rangle$, are averages over relevant sets of spin configurations in the classical equivalent $(1+1)$-dimensional system. These configurations are obtained through a modified Wolff algorithm [8] incorporating long range interactions [9].

The MC method is usually applied to the study of large chains and the thermodynamical limit ($N \to \infty$) can be achieved by using well-known scaling techniques [9]. Coupling with the bath introduces long range interactions (in the imaginary time) which increases considerably the

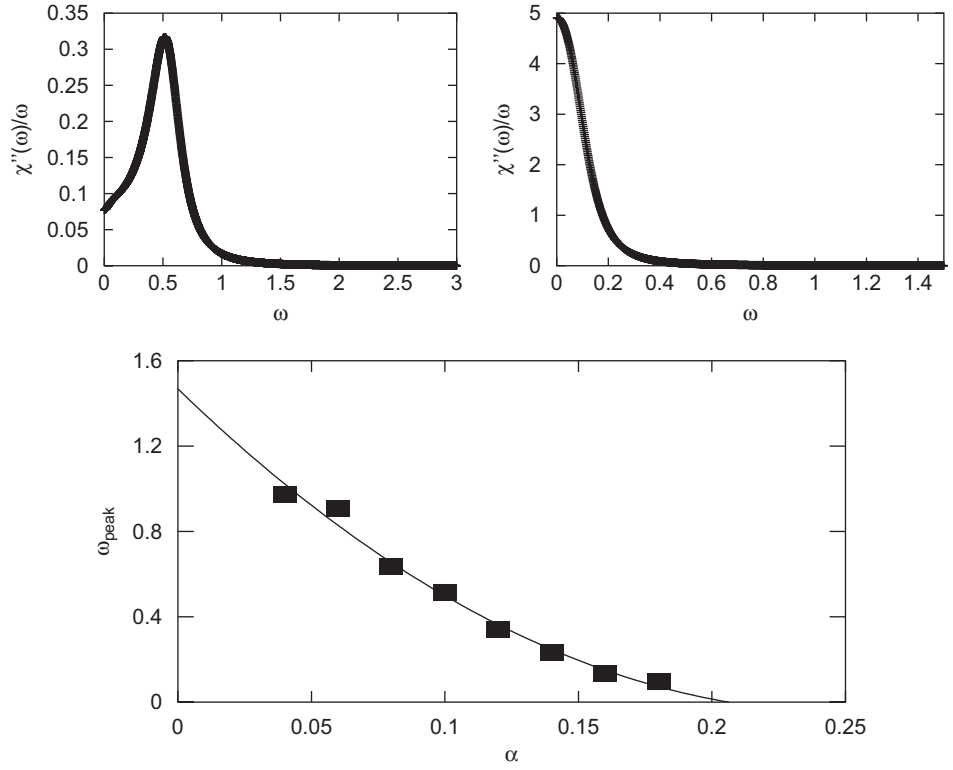

Fig. 3. $\chi''(\omega)/\omega$ plotted as a function of ω for $\alpha = 0.1$ (top left) and 0.22 (top right). ω_{peak} as a function of α (bottom).

computing time. This is not a problem in our case since we are interested in small chains.

The method can be even applied for $N = 1$ where the problem becomes the well-studied two-level Caldeira Leggett model [4]. The coherence of the system can be studied via the behavior of the correlation function $C(t) = \langle\sigma_z(t)\sigma_z(0)\rangle$. With zero coupling to the environment ($\alpha = 0$) the system will exhibit coherent oscillations. Weak coupling leads to damped oscillatory behavior and for a strong coupling the system will exhibit a completely incoherent decay of the time correlation function. The transition between underdamped and overdamped oscillations occurs at ($\alpha = \frac{1}{2}$). At $\alpha \geqslant 1$ the bath localizes the spin. With the Monte Carlo simulation we obtain the imaginary-time correlation function $C(\tau) = \langle\sigma_z(\tau)\sigma_z(0)\rangle$. Next, the Fourier transform $C(\omega_n)$ at the Matsubara frequencies is calculated. The Padé approximant method is used to continue this spectral function from de positive Matsubara frequencies onto the real axis. We obtain the imaginary part of the response function $\chi''(\omega)$. The study of this function is equivalent to the study of $C(t)$ [7]. Underdamped oscillations manifest through a peak at non-zero frequency of $C(\omega)$. Increasing the coupling of the bath shifts this frequency towards zero. For the $N = 1$ case this occurs at $\alpha = \frac{1}{2}$.

The von Neumann entropy of the $N = 1$ case was calculated by Stauber and Guinea in Ref. [2]. They calculated analytically the ground state energy as a function of the bath frequency cutoff Λ. Their result can be expressed as

$$E = \frac{C}{1-2\alpha}\left(\Gamma\left(\frac{\Gamma}{\Lambda}\right)^{\frac{\alpha}{1-\alpha}} - \frac{\Gamma^2}{\Lambda}\right), \tag{2}$$

where C is some constant. From here, $\langle\sigma_x\rangle = \partial E/\partial\Gamma$ can be calculated and the expression of the von Neumann entropy follows (see Eq. (1)). In Ref. [2], it was claimed that $f(\alpha) = \partial\log(\langle\sigma_x\rangle)/\partial\alpha$ (and consequently the von Neumann entropy) had a singular behavior at the point $\alpha = \frac{1}{2}$. As pointed originally by us (see also Ref. [3]) this is not the case, at least for finite cutoff. Nevertheless, the $f(\alpha)$ shows a qualitative change at a particular value $\alpha^*(\Lambda)$ where $f(\alpha)$ has an inflection point and it can be shown that $\alpha^*(\Lambda) \to \frac{1}{2}$ as $\Lambda \to \infty$.

We show in Fig. 1 the behavior of $\sigma(\alpha)$ and the von Neumann entropy $s(\alpha)$ as a function of the coupling to the bath α as obtained from our MC simulations for a particular value of $\Delta\tau\Gamma = 0.05$. We also show the function $s(\alpha)$ as obtained from Eq. (1) for a particular value of Λ which corresponds to our cutoff $\Delta\tau$. As evident form the figures, there is no singular behavior of this quantities.

We show in Fig. 2, the behavior of $f(\alpha)$ for different values of the cutoff. On the bottom panel the values of the inflection point are plotted. We see that this value

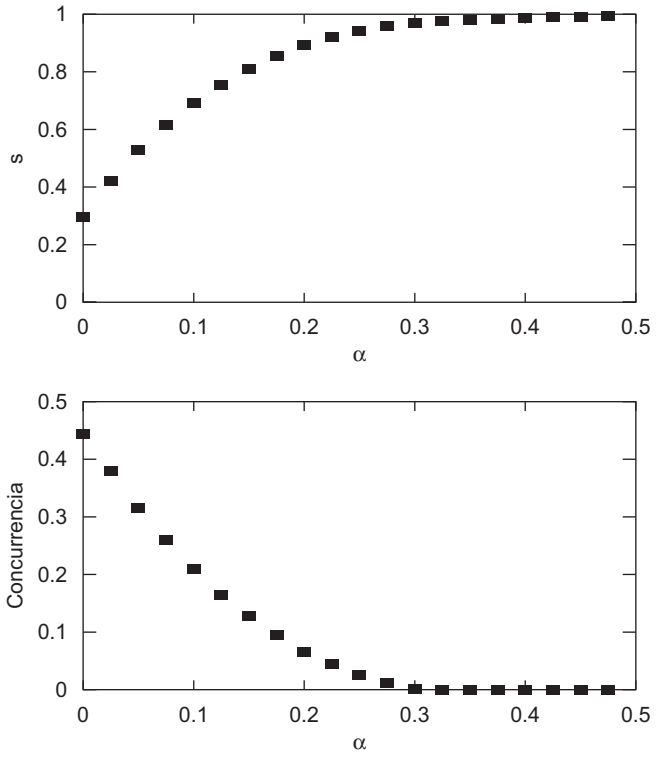

Fig. 4. The von Neumann entropy as function of α for $N = 2$, $\Gamma = 1$(top). Concurrence as function of α for $N = 2$, $\Gamma = 1$ (bottom).

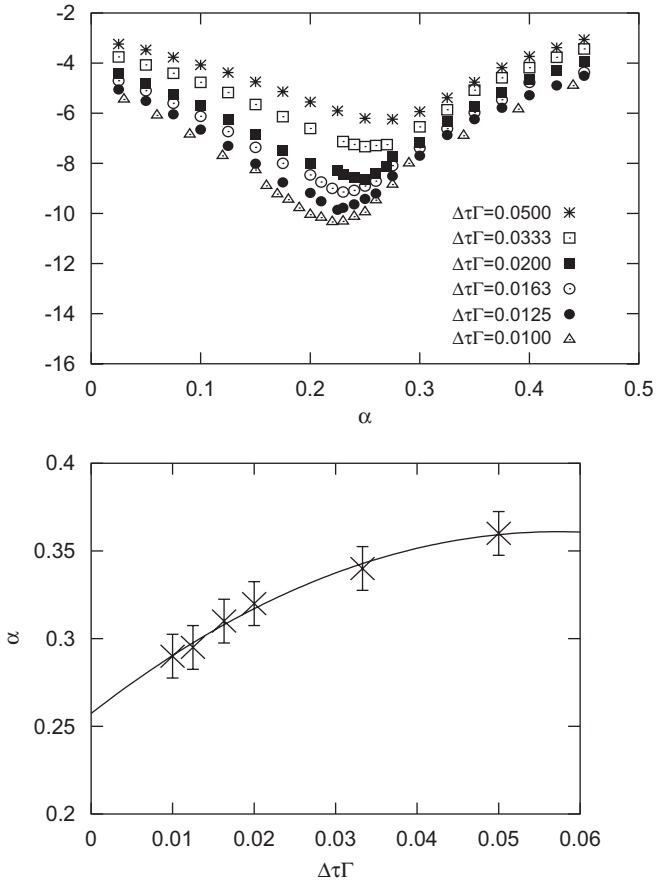

Fig. 5. Plot of $\langle\partial\log\sigma_x/\partial\alpha\rangle$ as a function of α for different products $\Delta\tau\Gamma$ (top). α for the inflection point of each curve of the left figures function of $\Delta\tau\Gamma$ (bottom).

extrapolates to a value which is compatible with the theoretical value of $\frac{1}{2}$.

We can perform numerical simulations on the system of $N = 2$ spins where there are no available analytical results. As mentioned before, we identify the transition between damped and the overdamped regime as the value of α where the peak of $\chi''(\omega)$ occurs for $\omega = 0$. We show in Fig. 3 plots of $\chi''(\omega)$ for two values of α corresponding to the underdamped and overdamped regimes. We show in the bottom panel of Fig. 3 the value of ω_{peak} as a function of α. The value of ω_{peak} becomes zero at $\alpha \approx 0.2$

We show in Fig. 4 the value of the von Neumann entropy and the concurrence as a function of α. We see that the concurrence also becomes negligible at a value of $\alpha \approx 0.2$.

Finally, in Fig. 5 we plot $f(\alpha)$ and the inflection point value for different values of the cutoff. We see here that the value of the α where the inflection occurs is slightly larger $\alpha \approx 0.25$.

We have analyzed the behavior of quantum computing observables as a function of the system–environment coupling. We have shown that for a finite cutoff the von Neumann entropy and the concurrence are not singular but there is qualitative change around the value where the overdamped-oscillatory transition occurs. A better understanding of the functional dependence of the results with the cutoff is left for future work.

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