Dynamics of a spin in a spin bath : Thermodynamics of non-Markovianity

Samyadeb Bhattacharya
Harish-Chandra Research Institute

Collaborators

Avijit Misra

Chiranjib Mukhopadhyay

Prof. Arun Kumar Pati

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Motivation

1. Derivation of exact canonical master equation of Lindblad form for a qubit immerged in a sea of completely un-polarized spins without considering the weak coupling and Born-Markov approximations.

2. Study the essential non-Markovian feature of the reduced dynamics.

3. Study the process of equilibration of the reduced system and the role of non-Markovianity in it.

Content

- Introduction
- Derivation of the master equation
- Non-Markovianity : RHP and BLP measures
- Irreversibly entropy production
- Purity and witnessing non-Markovianity
- Conclusion

Introduction

1. In many body problems the dynamics of microscopic (e.g. spin systems) or mesoscopic (e.g. SQUIDs) systems always gets complicated owing to its interaction with a background environment.
2. Two different universal classes of quantum environment are usually considered :

A. Bath as a system of uncoupled harmonic oscillators : The environment is described as a set of uncoupled harmonic oscillators. Paradigmatic examples of this kind of baths are spin-boson and Caldeira-Leggett model originating from a scheme proposed by Feynman and Vernon .

B. Bath as a system of spin half particles : *Relatively* less explored as an environment model.

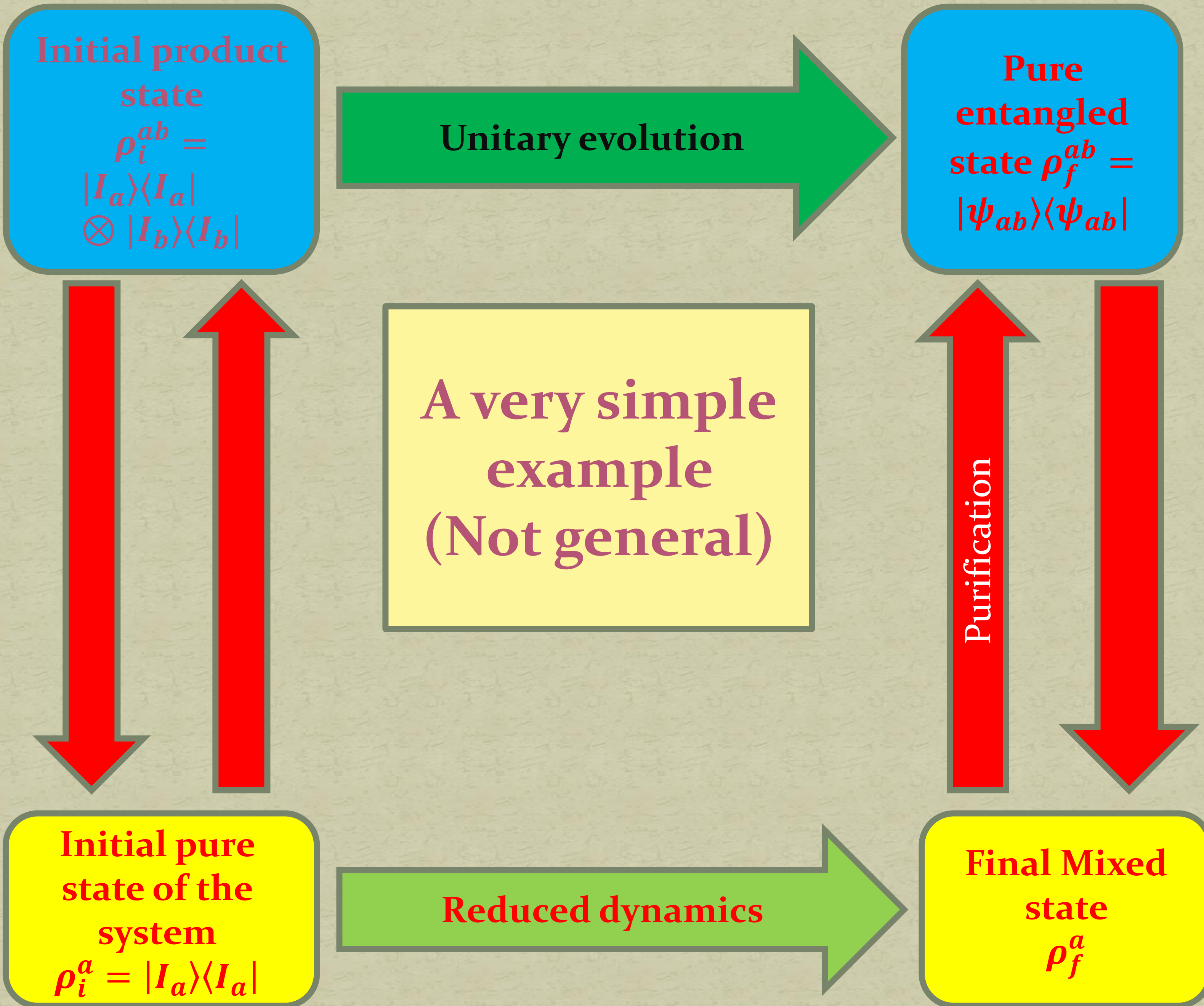
We are interested to dig deeper

Why spin bath ?

The spin bath models play a pivotal role in the quantum theory of magnetism, quantum spin glasses, theory of conductors and superconductors. To get the exact dynamics of a quantum systems under these spin bath models is of paramount importance yet a difficult task.

Why this study ?

In most of the cases the dynamics cannot be described exactly and several approximation techniques, both local and nonlocal in time, have been employed. **Whereas we derive an exact time local canonical master equation of the Lindblad form.** One of the characteristics of the spin bath models is to exhibit the non-Markovian features. The non-Markovianity has been identified as a key resource in information theoretic, thermodynamic and precision measurement protocols. We study the non-Markovian features of the reduced dynamics and its few possible thermodynamic implications.



Initial product state $\rho_i^{ab} = |I_a\rangle\langle I_a| \otimes |I_b\rangle\langle I_b|$
Unitary evolution
Pure entangled state $\rho_f^{ab} = |\psi_{ab}\rangle\langle\psi_{ab}|$
A very simple example (Not general)
Purification
Initial pure state of the system $\rho_i^a = |I_a\rangle\langle I_a|$
Reduced dynamics
Final Mixed state ρ_f^a

The master equation.

- **The model :** We consider a spin-half particle that interacts uniformly with N other spin-half particles constituting the bath. The spins of the bath do not interact with each other.
- **The Hamiltonian :** $\boldsymbol{H_T = H_s + H_{SB}}$

$$\boldsymbol{H_s = \frac{\hbar}{2}\omega_0\sigma_z \; ; \; H_{SB} = \frac{\hbar}{2}\sum_i \alpha(\sigma_x\sigma_x^i + \sigma_y\sigma_y^i + \sigma_z\sigma_z^i)}$$

The initial total state: $\boldsymbol{\rho_T(0) = \rho(0) \otimes \frac{I_B}{2^N}}$

Note that as we are only concerned with the reduced dynamics of the central spin and the bath is completely un-polarized initially, there is no loss of generality to drop the bath Hamiltonian.

The reduced map : $\mathrm{Tr_B}[\boldsymbol{U(t)(\rho(0)} \otimes \frac{\boldsymbol{I_B}}{\boldsymbol{2^N}})\boldsymbol{U^+(t)}]$

$\boldsymbol{U(t)}$ is the unitary evolution corresponding to the Schrodinger evolution.

The total angular momentum of the bath : $\boldsymbol{J} = \sum_i \boldsymbol{\sigma}^i$

The basis $|j, m\rangle$ is defined as the simultaneous eigen-basis of both $\boldsymbol{J}^2$ and J_z.

The system density matrix :

$$\boldsymbol{\rho_{11}(t) = A(t)\rho_{11}(0) + B(t)\rho_{22}(0)}$$

$$\boldsymbol{\rho_{12}(t) = C(t)\rho_{12}(0)}$$

Where

$$A(t) = \sum_{j,m} \frac{N_j}{2^N} \left[cos^2(\mu_+ t) + \frac{\Omega_+^2}{4\mu_+^2} sin^2(\mu_+ t)\right] \quad ;$$

$$B(t) = \sum_{j,m} \frac{N_j}{2^N} \frac{\alpha^2 b_+^2}{4\mu_+^2} sin^2(\mu_+ t)$$

$$C(t) = \sum_{j,m} \frac{N_j}{2^N} \left[cos(\mu_+ t) - \frac{i\Omega_+}{2\mu_+} sin\,(\mu_+ t)\right] \left[\cos(\mu_- t) + \frac{\mathrm{i}\Omega_-}{2\mu_-}\; sin(\mu_- t)\right]$$

The coefficients :

- $\Omega_\pm = \pm\omega_0 + \alpha(\pm m + \frac{1}{2})$
- $\mu_\pm = \frac{1}{2}\left(\Omega_\pm^2 + \alpha^2 b_\pm^2\right)^{\frac{1}{2}}$
- $b_\pm = (j(j+1) - m(m \pm 1))^{\frac{1}{2}}$

- Derivation of the master equation is basically finding the generator of the evolution, which is one of the fundamental problems in the theory of open quantum systems.
- The dynamical map : $\boldsymbol{\rho(t) = \phi[\rho(0)] = [F(t)r(0)]^T G}$

where $\boldsymbol{F_{kl} = Tr[G_k \phi(G_l)]}$ and $\boldsymbol{r_l = Tr[G_l \rho(0)]}$

with $\boldsymbol{G_l = \{\frac{I}{\sqrt{2}}, \frac{\sigma_x}{\sqrt{2}}, \frac{\sigma_y}{\sqrt{2}}, \frac{\sigma_z}{\sqrt{2}}\}}$;

Then the equation of motion can be derived as:

$$\boldsymbol{\frac{d}{dt}\rho(t) = \Lambda[\rho(t)] = [\mathrm{L(t)r(t)}]^{\mathrm{T}}\mathrm{G}}$$

with $$\boldsymbol{L(t) = \frac{dF(t)}{dt} F^{-1}(t)}$$

Condition : a) $\boldsymbol{F^{-1}(t)}$ **must exist and** $\boldsymbol{F(0) = I}$

- Master equation for the central spin :

$$\frac{d}{dt}\rho(t) = \frac{i}{\hbar}\,U(t)[\rho(t),\sigma_z] + \Gamma_{deph}(t)[\sigma_z\rho(t)\sigma_z - \rho(t)] + \Gamma_{dis}(t)\left[\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho(t)\}\right] + \Gamma_{abs}(t)\left[\sigma_+\rho(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+,\rho(t)\}\right]$$

where

$$\Gamma_{dis}(t) = \Gamma_{abs}(t) = \frac{1}{2}\frac{d}{dt}\,ln\left(\frac{1}{A(t)-B(t)}\right)$$ **(Unital)**

$$\Gamma_{deph}(t) = \frac{1}{4}\frac{d}{dt}\,ln\left(\frac{A(t)-B(t)}{|C(t)|^2}\right)$$

$$U(t) = -\frac{1}{2}\frac{d}{dt}\,ln\left(1+\left(\frac{C_R(t)}{C_I(t)}\right)^2\right)$$

- The master equation can be alternatively written as :

$$\frac{d}{dt}\boldsymbol{\rho}(\boldsymbol{t}) = \frac{i}{\hbar}\,\boldsymbol{U}(\boldsymbol{t})[\boldsymbol{\rho}(\boldsymbol{t}), \boldsymbol{\sigma}_z] + \boldsymbol{\Gamma}_{deph}(\boldsymbol{t})[\boldsymbol{\sigma}_z\boldsymbol{\rho}(\boldsymbol{t})\boldsymbol{\sigma}_z - \boldsymbol{\rho}(\boldsymbol{t})] + \boldsymbol{\Gamma}_x(\boldsymbol{t})[\boldsymbol{\sigma}_x\boldsymbol{\rho}(\boldsymbol{t})\boldsymbol{\sigma}_x - \boldsymbol{\rho}(\boldsymbol{t})] + \boldsymbol{\Gamma}_y(\boldsymbol{t})\left[\boldsymbol{\sigma}_y\boldsymbol{\rho}(\boldsymbol{t})\boldsymbol{\sigma}_y - \boldsymbol{\rho}(\boldsymbol{t})\right]$$

Lindblad operators are Hermitian

Where $\Gamma_x(t) = \Gamma_y(t) = \frac{\Gamma_{dis}(t)}{2}$

The dynamics is unital and hence doubly stochastic

- Kraus operators :

$$\sum_i K_i^+ K_i = 1$$
$$\sum_i K_i K_i^+ = 1$$

$$K_1 = \sqrt{B(t)}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$K_2 = \sqrt{B(t)}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$K_3 = \sqrt{\frac{A(t)-|C(t)|}{2}}\begin{pmatrix} -e^{i\theta(t)} & 0 \\ 0 & 1 \end{pmatrix}$$

$$K_4 = \sqrt{\frac{A(t)+|C(t)|}{2}}\begin{pmatrix} e^{i\theta(t)} & 0 \\ 0 & 1 \end{pmatrix}$$

With $\theta(t) = arctan\left[\frac{C_I(t)}{C_R(t)}\right]$

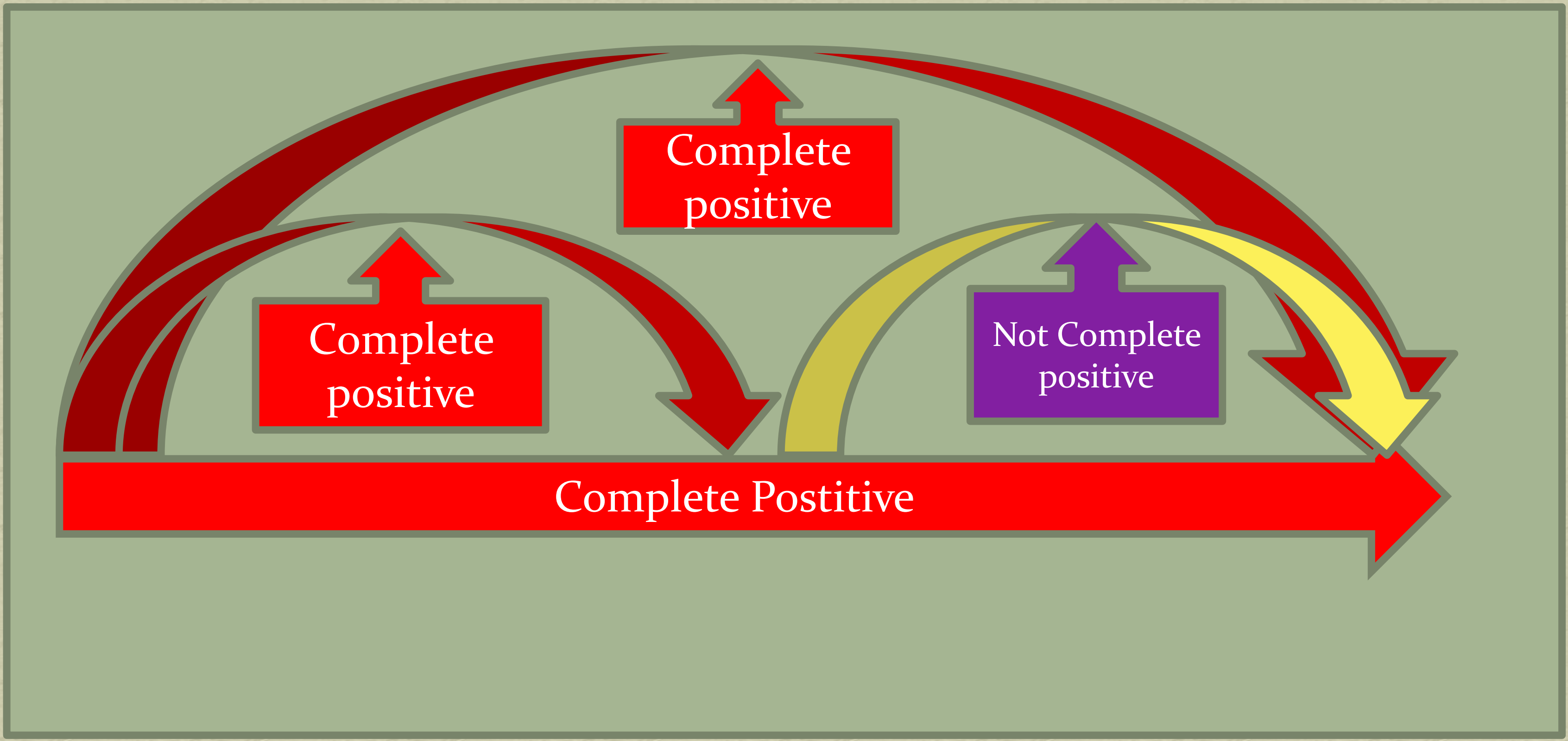
Non-Markovianity

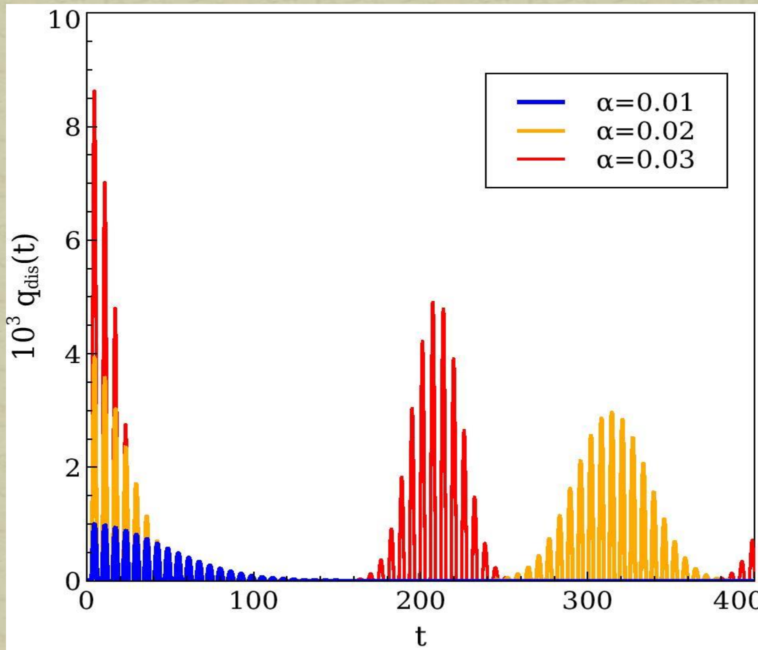
- The charecterization and quantification of the non-Markovianity is a fundamental aspect of open quantum dynamics.
- **RHP measure :** In this approach, the non-Markovian behaviour is attributed to the deviation from divisibility and the quantification of non-Markovianity is done based on the amount of the deviation.

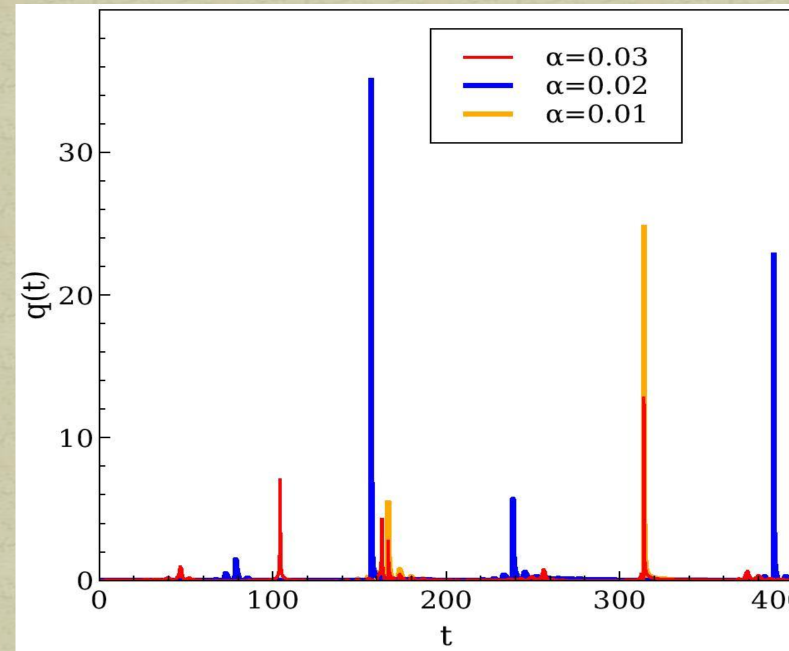
$$q(t) = \lim_{\epsilon \to 0^+} \frac{\left|\left| I_d \otimes \phi(t+\epsilon, t) |\Phi^+\rangle\langle\Phi^+| \right|\right|_1 - 1}{\epsilon}$$

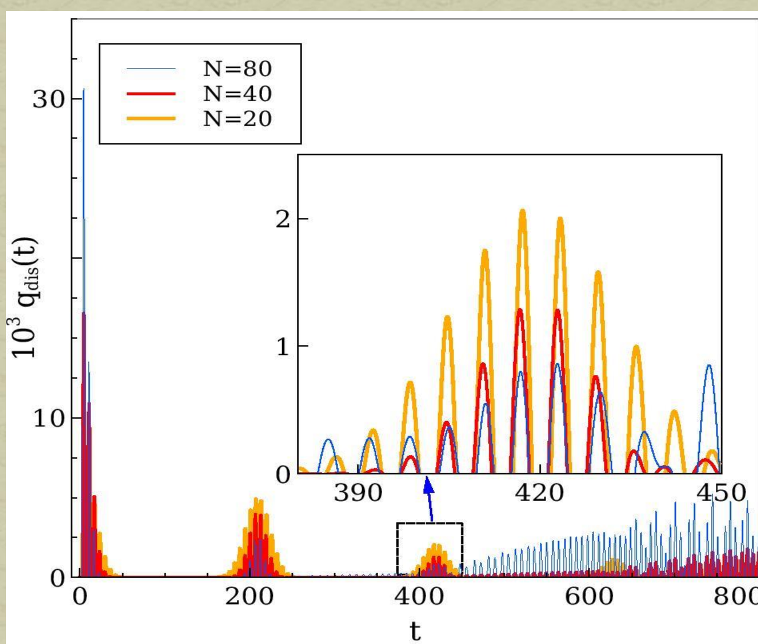
$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

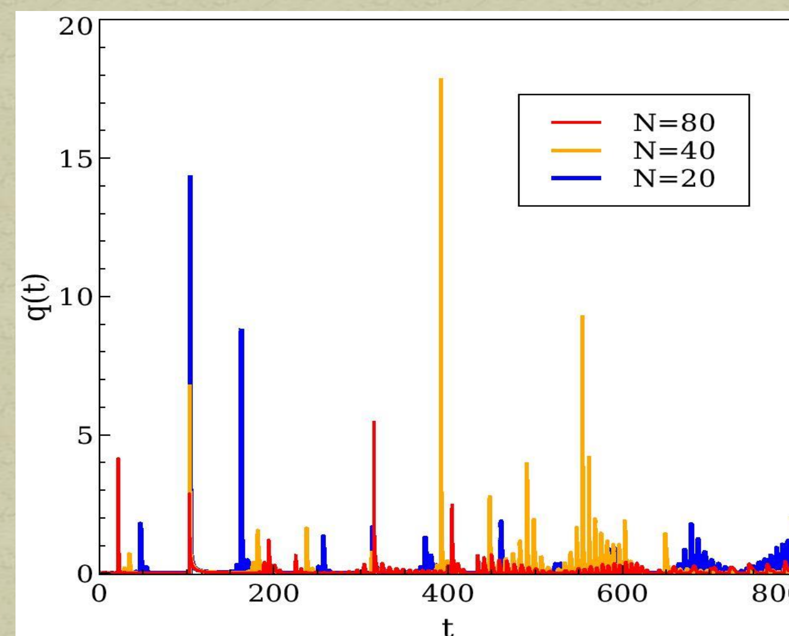
Non-Markovianity in terms of divisibility breaking




α=0.01
α=0.02
α=0.03
$10^3\, q_{dis}(t)$
t


α=0.03
α=0.02
α=0.01
q(t)
t


N=80
N=40
N=20
$10^3\, q_{dis}(t)$
t


N=80
N=40
N=20
q(t)
t

Irreversible Entropy Production

The irreversible or non-equilibrium entropy production and its rate are two fundamental concepts in the analysis of the non-equilibrium processes.

$$\boldsymbol{\sigma(t) = \frac{dS(t)}{dt} + J(t)}$$

S(t) is the von-Neumann entropy and J(t) is the entropy flux .

$$J = \frac{1}{KT}\frac{dQ}{dt}$$
$$= \frac{1}{KT}\, Tr[H(t)\Lambda(\rho(t))]$$

$$\boldsymbol{\sigma(t) = -\frac{d}{dt} S(\rho(t)||\rho_{eq})}$$

$\boldsymbol{\sigma(t) \geq 0}$ is the local version of 2nd Law

$\sigma(t) < 0$ essentially means that the system is driven away from equilibrium

For the central spin :

$$\boldsymbol{J(t) = 0}$$

Since the absorption and the dissipation rates are equal due to the infinite temperature of the bath, the net heat flow is always zero.

Therefore :

$$\boldsymbol{\sigma(t) = \frac{dS(t)}{dt}}$$

S(t) is monotonically increasing under unital operation.

In fact for hermitian Lindblad operators (V_j) :

$$\frac{dS(t)}{dt} = \sum_{jkl} \Gamma_j(t)\left(\lambda_k(t) - \lambda_l(t)\right)\left(ln\lambda_k(t) - ln\lambda_l(t)\right)\left|\langle\lambda_k(t)|V_j|\lambda_l(t)\rangle\right|^2 \text{ with}$$

$$\rho(t) = \sum_l \lambda_l |\lambda_l\rangle$$

So in the non-Markovian region ($\Gamma_j(t) < 0$), the system is driven away from equilibrium ($\sigma(t) < 0$)

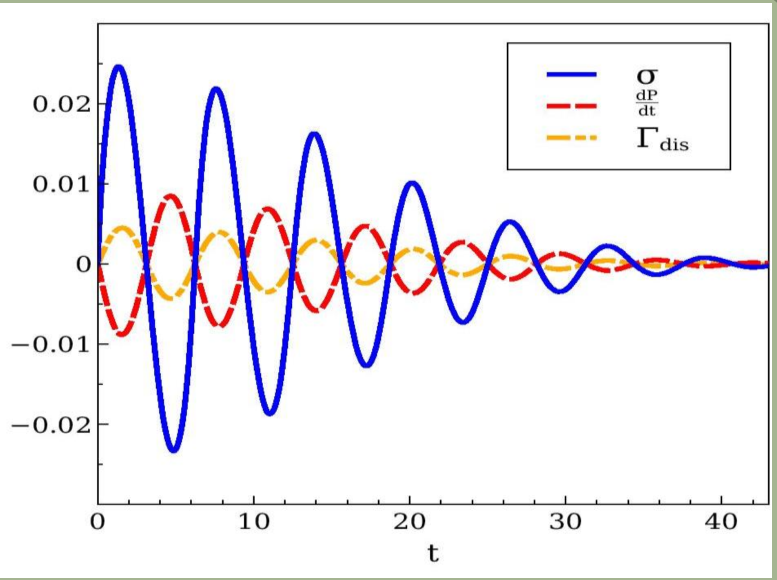
Purity and detection of non-Markovianity

Unitality of the dynamics demands that all the entropy functions are monotonically increasing under the evolution. Hence non-Markovianity can be addressed by the increase of purity P(t) of the state, which is complimentary to the linear entropy.

Under the specific evolution :

$$\frac{dP(t)}{dt} = 2Tr\left[\rho(t)\Lambda\left(\rho(t)\right)\right] = \sum_i \Gamma_i(t) Q_i(t)$$

Where $Q_i(t) = \|[V_j, \rho(t)]\|_{HS}^2$ is the "quantumness" of the system



Take home message

We derive exact canonical master equation for a central spin interacting with a completely un-polarized spin bath without weak coupling and Born Markov approximation. We also compute the Kraus operators for the mentioned unital evolution.

The non-Markovianity in terms of divisibility breaking of the channel has been studied with respect to parameters such as interaction strength and number of bath spins.

We show that non-Markovianity necessarily drives the system away from equilibrium.

As the purity is a measurable quantity, the exact canonical Lindblad type master equation of the central spin, derived in this article, could be of paramount importance to investigate the non-Markovian features and negative entropy production rate in the laboratory.

Is this it or anything else ?

The scheme used here to derive the canonical master equation has been proven to be fruitful to explore the strong coupling regime where the system-bath separability breaks down, which gives the present study a practical importance to unravel the far reaching impacts of the non-Markovian dynamics in the strong coupling regime

It allows us the possibilities of studying various quantum devices in much more realistic and practically implementable models.

There are possibilities to address fundamental issues like Thermalization or Ergoidicity and many others in the hitherto unexplored strong coupling region.

You cannot let go of the past, it does matter…