Quantum Thermodynamics and non-Markovian physics

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Quantum Trajectories, ICTS (January 20 - February 07, 2025)

Motivation

- After motivating the need for a study of Open Quantum Systems, I introduce, briefly, some recent developments in the efforts to understand non-Markovian phenomenon.
- The discussion about non-Markovian behaviour is made in the backdrop of the Garraway model.
- This is followed by an introduction to ergotropy, entropy production, power,...in the context of quantum thermodynamics.
- Devices: Quantum Battery and Quantum Heat Engine are discussed.
- These are illustrated on open system models; (a). Garraway model, (b). central spin model, (c). Quantum Brownian Motion (QBM), (d). two-qubit decoherence.

Open Quantum Systems: A Brief Preview and Motivation

- The theory of open quantum systems addresses the problems of damping and dephasing in quantum systems by the assertion that all real systems of interest are 'open' systems, surrounded by their environments [U. Weiss: (1999); H. -P. Breuer and F. Petruccione: (2002); SB: *Open Quantum Systems: Dynamics of Nonclassical Evolution* (2019)].
- Quantum optics provided one of the first testing grounds for the application of the formalism of open quantum systems [W. H. Louisell: (1973), G. S. Agarwal: (1973), H. Carmichael: (1993)]. Application to other areas was intensified by the works of [Caldeira and Leggett: (1983)], [Grabert, Schramm and Ingold: 1988)] and [Zurek: (1993)], among others.
- The recent upsurge of interest in the problem of open quantum systems is because of the spectacular progress in manipulation of quantum states of matter, encoding, transmission and processing of quantum information, for all of which understanding and control of the environmental impact are essential [Turchette *et al.*: (2000); Myatt *et al.*: (2000); Haroche *et al.* (1996)]. This increases the relevance of open system ideas to quantum computation and quantum information.

- Hamiltonian of the total (closed system):

$$H = H_S + H_R + H_{SR}.$$

- S- system, R- reservoir (bath), $S - R$-interaction between them.
- System-reservoir complex evolves unitarily by:

$$\rho(t) = e^{-\frac{i}{\hbar}Ht}\rho(0)e^{\frac{i}{\hbar}Ht}.$$

- We are interested in the reduced dynamics of the system S, taking into account the influence of its environment. This is done by taking a trace over the reservoir degrees of freedom, making the reduced dynamics *non-unitary*:

$$\rho^s(t) = \mathrm{Tr_R}(\rho(\mathrm{t})) = \mathrm{Tr_R}\left[\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathrm{Ht}}\rho(0)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathrm{Ht}}\right].$$

- Open quantum systems can be broadly classified into two categories:

  (A). $[H_S, H_{SR}] = 0$ resulting in decoherence without any dissipation [Braginsky *et al.*: (1975), (1980); Caves *et al.*: (1980); G. Gangopadhyay, S. M. Kumar and S. Duttagupta: (2001); SB and R. Ghosh: (2007)] and

  (B). Quantum dissipative systems, where $[H_S, H_{SR}] \neq 0$ resulting in decoherence with dissipation [Caldeira and Leggett: (1983); H. Grabert, P. Schramm and G-L. Ingold: (1988); SB and R. Ghosh: (2003), (2007)].

- In the parlance of quantum information theory, an example of the noise generated by (A) would be a "phase damping channel", while that generated by (B) would be a "(generalized) amplitude damping channel".

Time scales associated with the Open System Evolution

- The open system evolution is characterized by a number of time-scales, the salient ones being:
- Scale associated with the natural frequency of the system.
- Relaxation time scale determined by the S-R coupling strength.
- Reservoir correlation time (memory time) associated with the high-frequency cutoff in the reservoir spectral density and the time scale associated with the reservoir temperature, which measures the relative importance of quantum to thermal effects.

Non-Markovian Aspects of Open Quantum Systems: Some Features

- We now make a brief excursion into non-Markovian Open Quantum Systems [Rivas, Huelga, Plenio (2014); Hall,Cresser,Li,Andersson (2014); Breuer,Laine,Piilo,Vacchini (2016); Vega,Alonso (2017); Shrikant,Srikanth,SB (2019); Shrikant,Srikanth,SB (2020)].
- This is a bigger class than the Markovian ones.
- We will illustrate our discussions using a useful model: the Garraway model
- Some promiment diagnostics of non-Markovian behavior, developed in recent years, are briefly discussed.

- A time-local master equation, providing a generalization of the usual Lindbladian type of equation would be of the form [Hall,Cresser,Li,Andersson (2014)]

$$\frac{d}{dt}\rho_S(t) = \mathcal{K}(t)\rho_S(t).$$

- The generator $\mathcal{K}(t)$ of the time-local master equation must preserve Hermiticity and trace.
- From these requirements it follows that the generator must be of the following general form

$$\begin{aligned}\mathcal{K}(t)\rho_S &= -i\left[H_S(t), \rho_S\right] \\ &\quad + \sum_i \gamma_i(t)\left[A_i(t)\rho_S A_i^\dagger(t) - \frac{1}{2}\left\{A_i^\dagger(t)A_i(t), \rho_S\right\}\right].\end{aligned}$$

  The structure of the generator provides a natural generalization of the Lindblad structure, in which the Hamiltonian $H_S(t)$, as well as the various decay rates $\gamma_i(t)$ may dependent on time.
- When $\gamma_i(t) \geq 0$, the resulting dynamics is completely positive, since the generator is then in Lindblad form for each fixed $t \geq 0$.

- A characterization of non-Markovianity was given by [Rivas, Huelga, Plenio (2010)]

$$f(t) = \lim_{\epsilon \to 0^+} \frac{|| \left[\Phi(\mathrm{t}+\epsilon, \mathrm{t}) \otimes \mathcal{I} \right] \left(|\Psi\rangle\langle\Psi| \right) ||_1 - 1}{\epsilon}$$

- Follows from Choi that $f(t) > 0$ for non-Markovian evolution.
- Measure $\mathcal{M} = \int_I dt\ f(t)$, non-Markovian behavior in $t \in I$.
- A family of dynamical maps $\Phi(t,0)$ is defined to be divisible if for all $t_2 \geq t_1 \geq 0$ there exists a CPT map $\Phi(t_2, t_1)$ such that the relation $\Phi(t_2,0) = \Phi(t_2,t_1)\Phi(t_1,0)$ holds.
- The simplest example of a divisible quantum process is given by a dynamical semigroup. For a semigroup $\Phi(t,0) = \exp[\mathcal{L}t]$ and divisibility is satisfied with the CPT map $\Phi(t_2,t_1) = \exp[\mathcal{L}(t_2 - t_1)]$.
- non-Markovian quantum processes could be described by time-local master equations whose generator involves at least one temporarily negative rate $\gamma_i(t)$ [Hall, Cresser, Li and Andersson (2014)].

- Consider two parties, Alice and Bob. Alice prepares a quantum system in one of two states ρ^1 or ρ^2 with probability $\frac{1}{2}$ each, and then sends the system to Bob. It is Bob's task to find out by a single measurement on the system whether the system state was ρ^1 or ρ^2. It turns out that Bob cannot always distinguish the states with certainty, but there is an optimal strategy which allows him to achieve the maximal possible success probability given by

$$P_{\text{max}} = \frac{1}{2}\left[1 + D(\rho^1, \rho^2)\right].$$

- The trace distance $D(\rho^1, \rho^2) = \frac{1}{2}||\rho^1 - \rho^2|| = \frac{1}{2}\text{tr}|\rho^1 - \rho^2|$ can therefore be interpreted as a measure for the distinguishability of the quantum states ρ^1 and ρ^2. Here $\text{tr}|A| = \text{tr}\sqrt{A^\dagger A}$.

- The trace distance between any pair of states satisfies $0 \leq D(\rho^1, \rho^2) \leq 1$.
- The trace distance is sub-additive with respect to tensor products of states

$$D(\rho^1 \otimes \sigma^1, \rho^2 \otimes \sigma^2) \leq D(\rho^1, \rho^2) + D(\sigma^1, \sigma^2).$$

- The trace distance is invariant under unitary transformations U,

$$D(U\rho^1 U^\dagger, U\rho^2 U^\dagger) = D(\rho^1, \rho^2).$$

More generally, all trace preserving and completely positive maps, i.e., all trace preserving quantum operations Λ are contractions of the trace distance,

$$D(\Lambda\rho^1, \Lambda\rho^2) \leq D(\rho^1, \rho^2).$$

- No quantum process describable by a family of CPT dynamical maps can ever increase the distinguishability of a pair of states over its initial value.
- When a quantum process reduces the distinguishability of states, information is flowing from the system to the environment. Correspondingly, an increase of the distinguishability signifies that information flows from the environment back to the system.
- A definition of quantum non-Markovianity, is based on the idea that for Markovian processes any two quantum states become less and less distinguishable under the dynamics, leading to a perpetual loss of information into the environment.
- Quantum memory effects thus arise if there is a temporal flow of information from the environment to the system. The information flowing back from the environment allows the earlier open system states to have an effect on the later dynamics of the system, which implies the emergence of memory effects [Breuer et al. (2009)].

- A quantum process described in terms of a family of quantum dynamical maps $\Phi(t,0)$ is non-Markovian if there is a pair of initial states $\rho_S^{1,2}(0)$ such that the trace distance between the corresponding states $\rho_S^{1,2}(t)$ increases at a certain time $t > 0$:

$$\sigma(t, \rho_S^{1,2}(0)) \equiv \frac{d}{dt} D(\rho_S^1(t), \rho_S^2(t)) > 0,$$

  where $\sigma(t, \rho_S^{1,2}(0))$ denotes the rate of change of the trace distance at time t corresponding to the initial pair of states.
- This implies that the class of quantum dynamical semigroups are Markovian.

- This suggests defining a measure $\mathcal{N}(\Phi)$ for the non-Markovianity of a quantum process through [BLP (2009)]

$$\mathcal{N}(\Phi) = \max_{\rho_S^{1,2}(0)} \int_{\sigma>0} dt\, \sigma(t, \rho_S^{1,2}(0)).$$

- The time integration is extended over all time intervals (a_i, b_i) in which σ is positive and the maximum is taken over all pairs of initial states. The measure can be written as

$$\mathcal{N}(\Phi) = \max_{\rho^{1,2}(0)} \sum_i \left[D(\rho_S^1(b_i), \rho_S^2(b_i)) - D(\rho_S^1(a_i), \rho_S^2(a_i)) \right].$$

To calculate this quantity one first determines for any pair of initial states the total growth of the trace distance over each time interval (a_i, b_i) and sums up the contribution of all intervals. $\mathcal{N}(\Phi)$ is then obtained by determining the maximum over all pairs of initial states.

[B. M. Garraway (1997)]

- The system Hamiltonian is

$$H_S = \omega_0 \sigma_+ \sigma_-,$$

describing a two-state system (qubit) with ground state $|0\rangle$, excited state $|1\rangle$ and transition frequency ω_0, where $\sigma_+ = |1\rangle\langle 0|$ and $\sigma_- = |0\rangle\langle 1|$ are the raising and lowering operators of the qubit.

- The Hamiltonian of the environment is

$$H_R = \sum_k \omega_k b_k^\dagger b_k,$$

represents a reservoir of harmonic oscillators with creation and annihilation operators $b_k^\dagger$ and b_k. The interaction Hamiltonian takes the form

$$H_{SR} = \sum_k \left(g_k \sigma_+ \otimes b_k + g_k^* \sigma_- \otimes b_k^\dagger \right).$$

- Due to the RWA, the total number of excitations in the system,

$$N = \sigma_+ \sigma_- + \sum_k b_k^\dagger b_k,$$

is a conserved quantity.

- Assuming the environment to be in the vacuum state $|0\rangle$ initially one finds:

$$\begin{aligned}
\rho_{11}(t) &= |c(t)|^2 \rho_{11}(0), \\
\rho_{00}(t) &= \rho_{00}(0) + (1 - |c(t)|^2)\rho_{11}(0), \\
\rho_{10}(t) &= c(t)\rho_{10}(0), \\
\rho_{01}(t) &= c^*(t)\rho_{01}(0),
\end{aligned}$$

  where the $\rho_{ij}(t) = \langle i|\rho_S(t)|j\rangle$ denote the matrix elements of $\rho_S(t)$.

- This is the Garraway model also called the non-Markovian Amplitude Damping (NMAD) model.
- The function $c(t)$ is the solution of the integro-differential equation

$$\frac{d}{dt}c(t) = -\int_0^t dt_1 f(t - t_1)c(t_1),$$

  corresponding to the condition of no photons in the initial state.

- where the kernel $f(t-t_1)$ represents a reservoir two-point correlation function,

$$\begin{aligned} f(t-t_1) &= \langle 0|R(t)R^\dagger(t_1)|0\rangle e^{i\omega_0(t-t_1)} \\ &= \sum_k |g_k|^2 e^{i(\omega_0-\omega_k)(t-t_1)}, \end{aligned}$$

of the environmental/reservoir operators

$$R(t) = \sum_k g_k b_k e^{-i\omega_k t}.$$

- These results hold for a generic environmental spectral density and the corresponding two-point correlation function. Taking, for example, a Lorentzian spectral density in resonance with the transition frequency of the qubit we find an exponential two-point correlation function

$$f(\tau) = \frac{1}{2}\gamma_0 \lambda e^{-\lambda|\tau|},$$

where γ_0 describes the strength of the system-environment coupling and λ the spectral width which is related to the environmental correlation time by $\tau_R = \lambda^{-1}$.

- Using this we find

$$c(t) = e^{-\lambda t/2}\left[\cosh\left(\frac{dt}{2}\right) + \frac{\lambda}{d}\sinh\left(\frac{dt}{2}\right)\right],$$

where $d = \sqrt{\lambda^2 - 2\gamma_0\lambda}$.

- For the Garraway model, the time-local generator takes the form

$$\begin{aligned}\mathcal{K}(t)\rho_S &= -\frac{i}{2}S(t)[\sigma_+\sigma_-,\rho_S] \\ &\quad +\gamma(t)\left[\sigma_-\rho_S\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho_S\}\right],\end{aligned}$$

  where $\gamma(t) = -2\Re\left(\frac{\dot{c}(t)}{c(t)}\right)$, $S(t) = -2\Im\left(\frac{\dot{c}(t)}{c(t)}\right)$.

- The quantity $S(t)$ plays the role of a time-dependent frequency shift, and $\gamma(t)$ can be interpreted as a time-dependent decay rate. Due to the time dependence of these quantities the process does not generally represent a dynamical semigroup.

- In the limit of small $\alpha = \gamma_0/\lambda$ we may approximate $c(t) \approx e^{-\gamma_0 t/2}$.
- $S(t) = 0$ and $\gamma(t) = \gamma_0$, i.e., the generator $\mathcal{K}(t)$ assumes the form of a Lindblad generator of a quantum dynamical semigroup.
- α can also be written as the ratio of the environmental correlations time $\tau_R = \lambda^{-1}$ and the relaxation time $\tau_{rel} = \gamma_0^{-1}$ of the system $\alpha = \frac{\tau_R}{\tau_{rel}}$.
- Thus we see that the standard Markov condition $\gamma_0 \ll \lambda$ indeed leads to a Markovian semigroup here.

- For the Garraway model, the necessary and sufficient condition for the complete positivity of $\Phi(t_2, t_1)$ is given by $|c(t_2)| \leq |c(t_1)|$.
- Thus the dynamical map of the model is divisible if and only if $|c(t)|$ is a monotonically decreasing function of time.
- The rate $\gamma(t)$ can be written as

$$\gamma(t) = -\frac{2}{|c(t)|}\frac{d}{dt}|c(t)|.$$

This shows that any increase of $|c(t)|$ leads to a negative decay rate in the corresponding generator, and illustrates the equivalence of the non-divisibility of the dynamical map and the occurrence of a temporarily negative rate in the time-local master equation.

- Considering the Garraway model, the time evolution of the trace distance corresponding to any pair of initial states $\rho_S^1(0)$ and $\rho_S^2(0)$ is given by

$$D(\rho_S^1(t), \rho_S^2(t)) = |c(t)|\sqrt{|c(t)|^2 a^2 + |b|^2},$$

  where $a = \rho_{11}^1(0) - \rho_{11}^2(0)$ and $b = \rho_{10}^1(0) - \rho_{10}^2(0)$.
- The time derivative of this expression yields

$$\sigma(t, \rho_S^{1,2}(0)) = \frac{2|c(t)|^2 a^2 + |b|^2}{\sqrt{|c(t)|^2 a^2 + |b|^2}} \frac{d}{dt}|c(t)|.$$

- From this we conclude that the trace distance increases at time t if and only if the function $|c(t)|$ increases at this point of time. It follows that the process is non-Markovian, $\mathcal{N}(\Phi) > 0$, if the dynamical map is non-divisible, which in turn is equivalent to a temporarily negative rate $\gamma(t)$.

Temporal Self-Similarity (S. Utagi, R. Srikanth, SB (2020))

- We identify a concept of memorylessness with *temporal self-similarity*, the property of a system dynamics whereby the propagator between two intermediate states is independent of the initial time.
- Constitutes a stronger concept of memorylessness than CP-divisibility: NCP maps are not QDS. However, there could be CP maps, for e.g., those defining the generalized OUN, PLN maps, that are *not* QDS.
- Temporal self-similarity can be identified with the quantum dynamical semigroup (QDS), generated by the GKLS (Lindbladian) evolution.
- Any deviation from QDS (whether CP-indivisible or not) makes the map dependent on initial time.

Ergotropy refers to the maximum amount of work that can be extracted from a quantum system via a unitary transformation. [Allahverdyan *et al* EPL 67 565 (2004)]

Consider a quantum state ρ with its internal Hamiltonian H having spectral decomposition

$$\rho = \sum_i r_i \left|r_i\right\rangle \left\langle r_i\right|, \text{ with eigenvalues } r_1 \geq r_2 \geq ....,$$

and

$$H = \sum_i \epsilon_i \left|\epsilon_i\right\rangle \left\langle \epsilon_i\right|, \text{ with eigenvalues } \epsilon_1 \leq \epsilon_2 \leq ....$$

Ergotropy can be obtained after minimizing the internal energy of the final state

$$\mathcal{W} = \mathrm{Tr}(\rho H) - \min\{\mathrm{Tr}(U\rho U^\dagger H)\},$$

The state $\rho_f = U\rho U^\dagger$ that achieves this minimum has the form $\rho_f = \sum_j r_j \left|\epsilon_j\right\rangle \left\langle \epsilon_j\right|$. This is known as the *passive state*.

Using the Bloch vector form, the state of a two-level system under NMAD:

$$\rho(t) = \frac{1}{2}\begin{pmatrix} 1+z(t) & x(t)-iy(t) \\ x(t)+iy(t) & 1-z(t) \end{pmatrix}. \tag{1}$$

The analytical expression for the ergotropy of the system is given by [D. Tiwari, SB (2023)]

$$\mathcal{W}(\rho(t)) = \frac{\omega_0}{2}\left(\sqrt{x(t)^2+z(t)^2}+z(t)\right). \tag{2}$$

It was recently recognized that quantum ergotropy can be separated into two different contributions, coherent ($\mathcal{W}_c$) and incoherent ($\mathcal{W}_i$) ergotropies.
(G. Francica *et.al.* Phys. Rev. Lett. (2020))

$\mathcal{W}_i = \mathrm{Tr}\{(\rho - \sigma) H\}$ is the maximal work that can be extracted from ρ without changing its coherence. Here $\mathrm{Tr}\{\sigma H\} = \min_{\mathcal{U}\in\mathcal{U}^{(i)}} \mathrm{Tr}\{\mathcal{U}\rho\mathcal{U}^\dagger H\}$, where $\mathcal{U}^{(i)}$ is the set of unitary operations without changing the coherence of ρ.

The coherent ergotropy $\mathcal{W}_c$ is the work that is exclusively stored in the coherence. The expression for the coherent ergotropy is given as

$$\beta\mathcal{W}_c(\rho) = C(\rho) + S\left(\mathcal{E}(\sigma)||\rho^{eq}\right) - D\left(\rho||\rho^{eq}\right),$$

where $S\left(\mathcal{E}(\sigma)||\rho^{eq}\right) = \mathrm{Tr}\{\sigma \ln(\sigma)\} - \mathrm{Tr}\{\mathcal{E}(\sigma)\ln(\rho^{eq})\}$ is the quantum relative entropy, $C(\rho)$ is the relative entropy of coherence and $D\left(\rho||\rho^{eq}\right) = \sum_i p_i \ln\left(\frac{p_i}{s_i}\right)$ is the classical relative entropy; p_i and s_i are the eigenvalues of the state ρ and ρ^{eq}, respectively. $\mathcal{E}(\sigma)$ is the pure dephasing operation $\left(\sum_i \langle i|\sigma|i\rangle |i\rangle\langle i|\right)$ on the coherence invariant state σ. The state ρ^{eq} is the Gibbs state $\rho^{eq} = \frac{\exp(-\beta H)}{Z}$ with $Z = \mathrm{Tr}\{\exp(-\beta H)\}$ and $\beta = 1/k_B T$.

In the case considererd here, using the Bloch vector form of a single denisty matrix at any time t, the coherent part of the ergotropy can be expressed analytically as

$$\mathcal{W}_c(\rho(t)) = \begin{cases} \frac{\omega_0}{2}\left(\sqrt{x(t)^2 + z(t)^2} - z(t)\right), & \text{for } z(t) \geq 0 \\ \frac{\omega_0}{2}\left(\sqrt{x(t)^2 + z(t)^2} + z(t)\right), & \text{for } z(t) < 0 \end{cases} \tag{3}$$

and in terms of l_1 norm of the coherence C_{l_1} as

$$\mathcal{W}_c(\rho(t)) = \begin{cases} \frac{\omega_0}{2}\left(\sqrt{\mathcal{C}_{l_1}(\rho(t))^2 + z(t)^2} - z(t)\right). & \text{for } z(t) \geq 0 \\ \frac{\omega_0}{2}\left(\sqrt{\mathcal{C}_{l_1}(\rho(t))^2 + z(t)^2} + z(t)\right). & \text{for } z(t) < 0 \end{cases} \tag{4}$$

The incoherent ergotropy of the system is

$$\mathcal{W}_i(\rho(t)) = \begin{cases} \omega_0 z(t). & \text{for } z(t) \geq 0 \\ 0. & \text{for } z(t) < 0 \end{cases} \tag{5}$$

It is interesting to note that, in this case, if $z(t) < 0$, the coherent ergotropy is equal to the ergotropy of the system.

Characterizers of quantum thermodynamics: Instantaneous and Average powers

The instantaneous charging power is defined by available work in the battery as

$$\mathcal{P}(t) = \lim_{\Delta t \to 0} \frac{\mathcal{W}(t+\Delta t) - \mathcal{W}(t)}{\Delta t} = \frac{d\mathcal{W}}{dt}.$$

It is also possible to define the average power-to-energy transfer given by

$$\mathcal{P}_{av} = \frac{\mathcal{W}(t) - \mathcal{W}(t_0)}{t - t_0},$$

where $t - t_0$ refers to the charging time of the battery.

Consider a general quantum system S interacting with a bath B. The change in the internal energy of the system at any time t is given by

$$\Delta U_S(t) = \mathrm{Tr}[H_S(\rho_S(t) - \rho_S(0))],$$

where H_S (assumed to be time-independent here) is the system's Hamiltonian and $\rho_S(t)$ is the system's state at t.

Further, the total change in the energy of the bath is given by

$$Q_B = \mathrm{Tr}[H_B(\rho_B(t) - \rho_B(0))],$$

where H_B and $\rho_B(t)$ are the Hamiltonian and the state (at time t) of the bath, respectively.

The mismatch between the total change in the internal energies of the system and bath is the work W [G.T. Landi and M. Paternostro, Rev. Mod. Phys. 93, 035008 (2021)], i.e.,

$$W = \Delta U_S(t) + Q_B,$$

where $W > 0$ means that work is performed on the system. The above can be referred to as the *first law of quantum thermodynamics.*

In a general system-bath dynamics, the irreversibility is introduced when we partially trace the bath. In the process, discarding any information stored locally in the state of the bath as well as the non-local information shared between the system and the bath is the source of irreversibility. This is accounted by the entropy production [G.T. Landi and M. Paternostro, Rev. Mod. Phys. 93, 035008 (2021), M. Esposito *et. al.*, New. J. Phys. 12, 013013 (2010)], given by

$$\Sigma = \mathcal{I}_{\rho_{SB}(t)}(S:B) + S(\rho_B(t)||\rho_B(0)),$$

where $\mathcal{I}_{\rho_{SB}(t)}(S:B) = S(\rho_S(t)) + S(\rho_B(t)) - S(\rho_{SB}(t))$ is the mutual information of any bipartite system SB with $S(\rho(t)) = -\mathrm{Tr}\rho(t)\ln\rho(t)$ being the von Neumann entropy. $S(\rho||\sigma) = \mathrm{Tr}[\rho\ln\rho - \rho\ln\sigma]$ is the quantum relative entropy.

The above equation can be further simplified to give

$$\Sigma = S[\rho_{SB}(t)||\rho_S(t)\otimes\rho_B(0)].$$

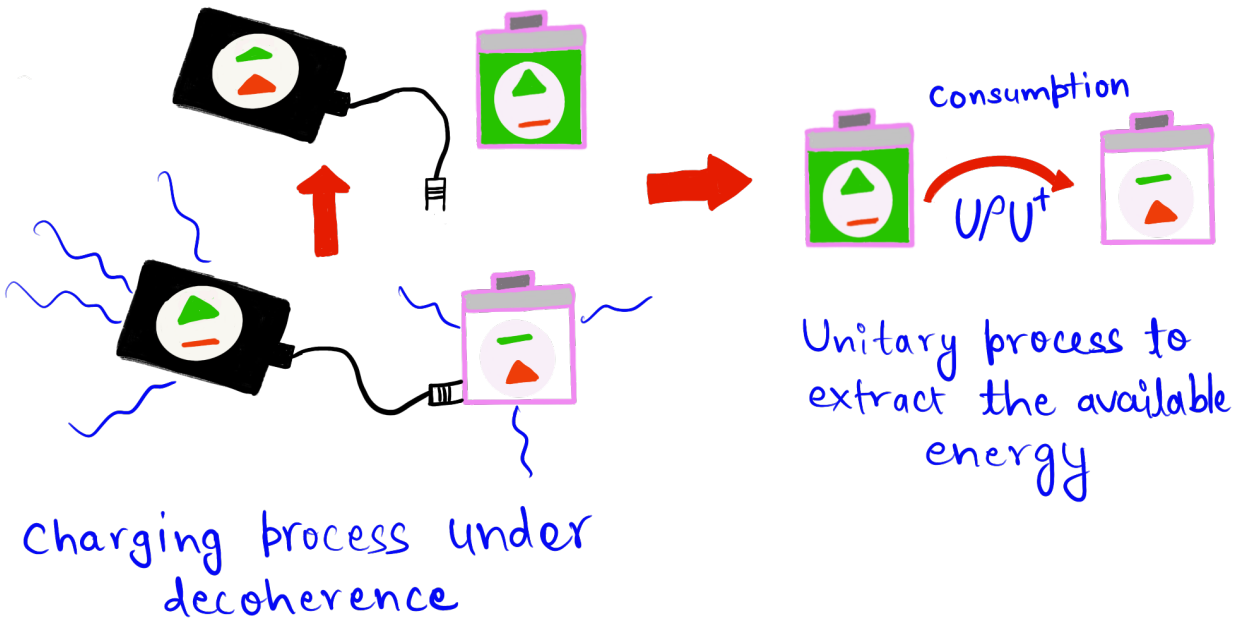
Further, if the initial state of the bath is taken to be a thermal state ($\rho_B(0) = \frac{e^{-\beta H_B}}{\mathrm{Tr}[e^{-\beta H_B}]}$ with $\beta = 1/k_B T$ being the inverse temperature), the entropy production can be given as

$$\Sigma = \Delta S_S + \beta Q_B,$$

where ΔS_S is the change in the von Neumann entropy of the system and Q_B is the total change in the bath's internal energy.

Battery:

- Quantum thermodynamics is the study of thermodynamical processes from a quantum mechanical point of view.
- Due to the constant decrement in user device sizes, several thermodynamic devices, such as quantum heat engines and quantum batteries [R. Alicki, and M. Fannes (2013], are required to be smaller as their unit cells approach the order of molecular and atomic scales.
- Various theoretical bases have been implemented to review quantum batteries, including spin chains and qubits in an optical cavity.
- The realistic implementation of quantum batteries would need to consider dissipation and decoherence effects... open systems.
- The system of interest H_S could be the battery, and its environment H_E the charger mechanism.
- We could envisage the scenario where the environment, being in a thermal equilibrium state, will not initially charge the quantum battery. To this end, we choose an initial state of the quantum battery, which has non-zero ergotropy that dissipates to the environment.
- However, due to the non-Markovian nature of the environment, the battery gets recharged. This *discharging-recharging* behavior is a uniquely non-Markovian feature and will not be observed in a Markovian scenario.

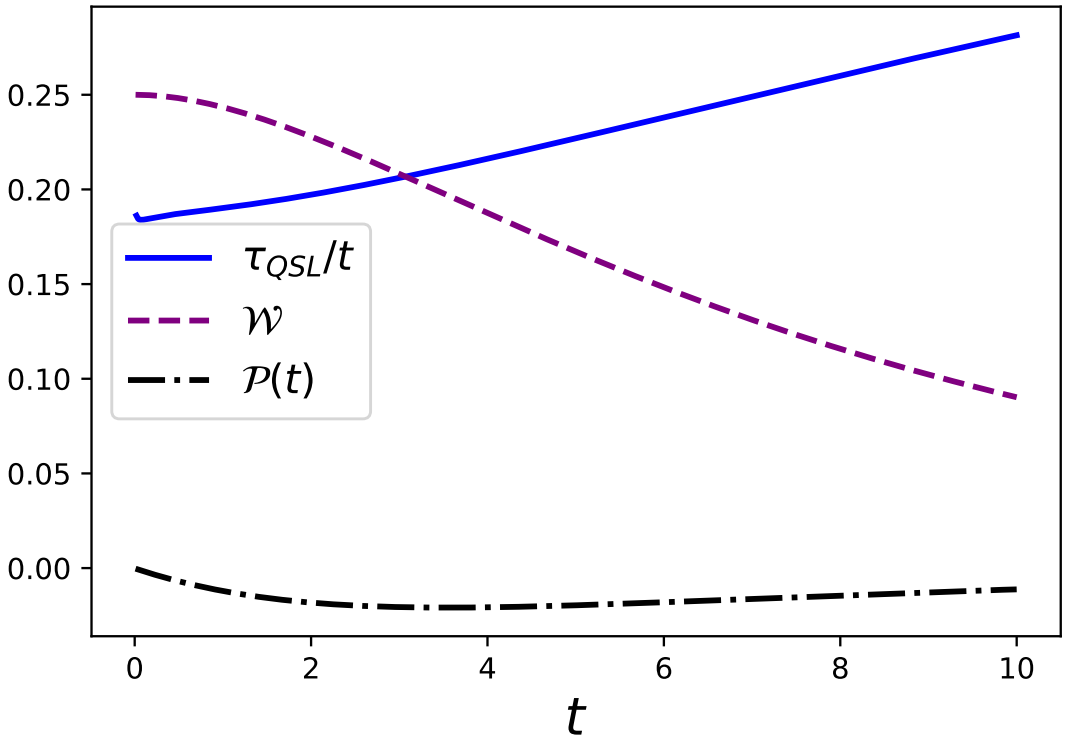


A schematic diagram of charging-discharging and work extraction processes of a quantum battery

Devices: Quantum Battery-Charger Open System Models

- NMAD model
- Central Spin model
- Quantum Brownian Motion (QBM) model

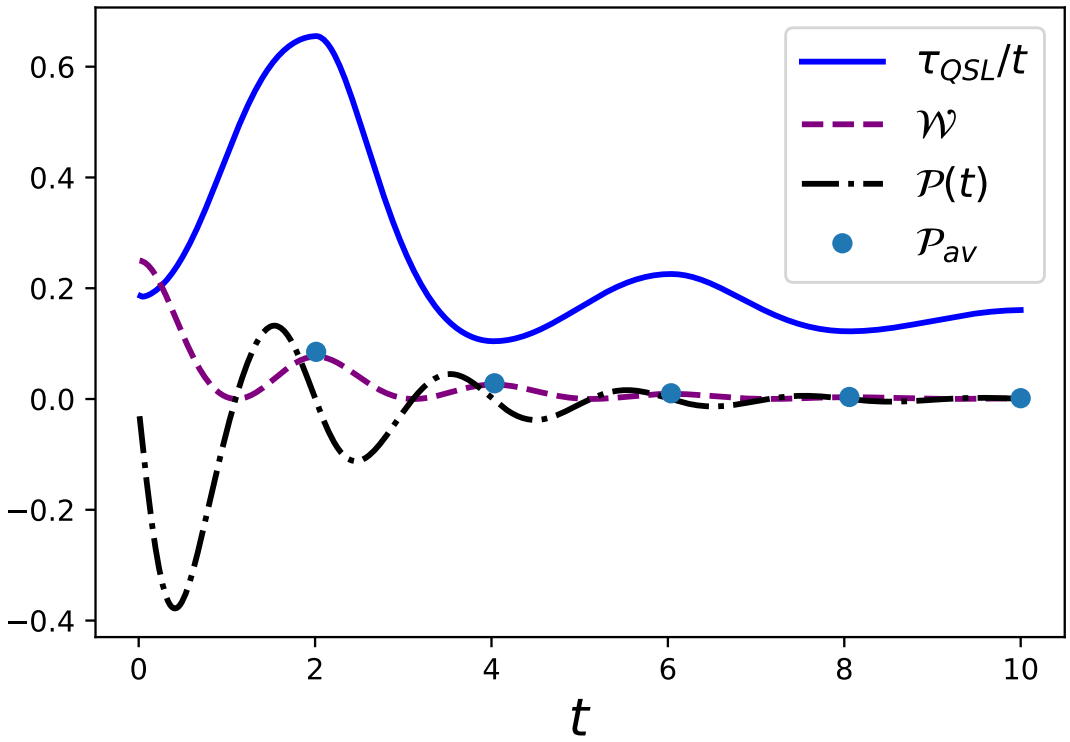
Discharging of battery under Markovian evolution:



Variation of QSL time using Fisher information metric (τ_{QSL}), ergotropy ($\mathcal{W}$), instantaneous ($\mathcal{P}(t)$) and average ($\mathcal{P}_{av}$) powers, with time. The evolution of the state is through the Markovian AD channel. The parameters are taken to be $\omega_0 = 1$, $\lambda = 0.5$, $\gamma_0 = 0.1$.

In the case of Markovian dynamics, we observe that the system does not recharge via interaction from the bath.

Discharging-charging of battery under non-Markovian evolution



Variation of QSL time using τ_{QSL}, ergotropy ($\mathcal{W}$), and instantaneous ($\mathcal{P}(t)$) and average ($\mathcal{P}_{av}$) powers, with time. The evolution of the state is through the NMAD channel. The parameters are taken to be $\omega_0 = 1$, $\lambda = 0.5$, $\gamma_0 = 10$. [D. Tiwari, SB (2023)]

Battery: Ergotropy in NMAD

- Here, we observe that the peaks and valleys of the τ_{QSL} occurs exactly at the points when a cycle of discharging and charging is completed.
- This coincides with the points where average charging power is calculated.
- The revivals in the ergotropy (recharging of the battery) are completely due to non-Markovian nature of the system, indicating the role of non-Markovian evolution in modelling the system as a quantum battery.

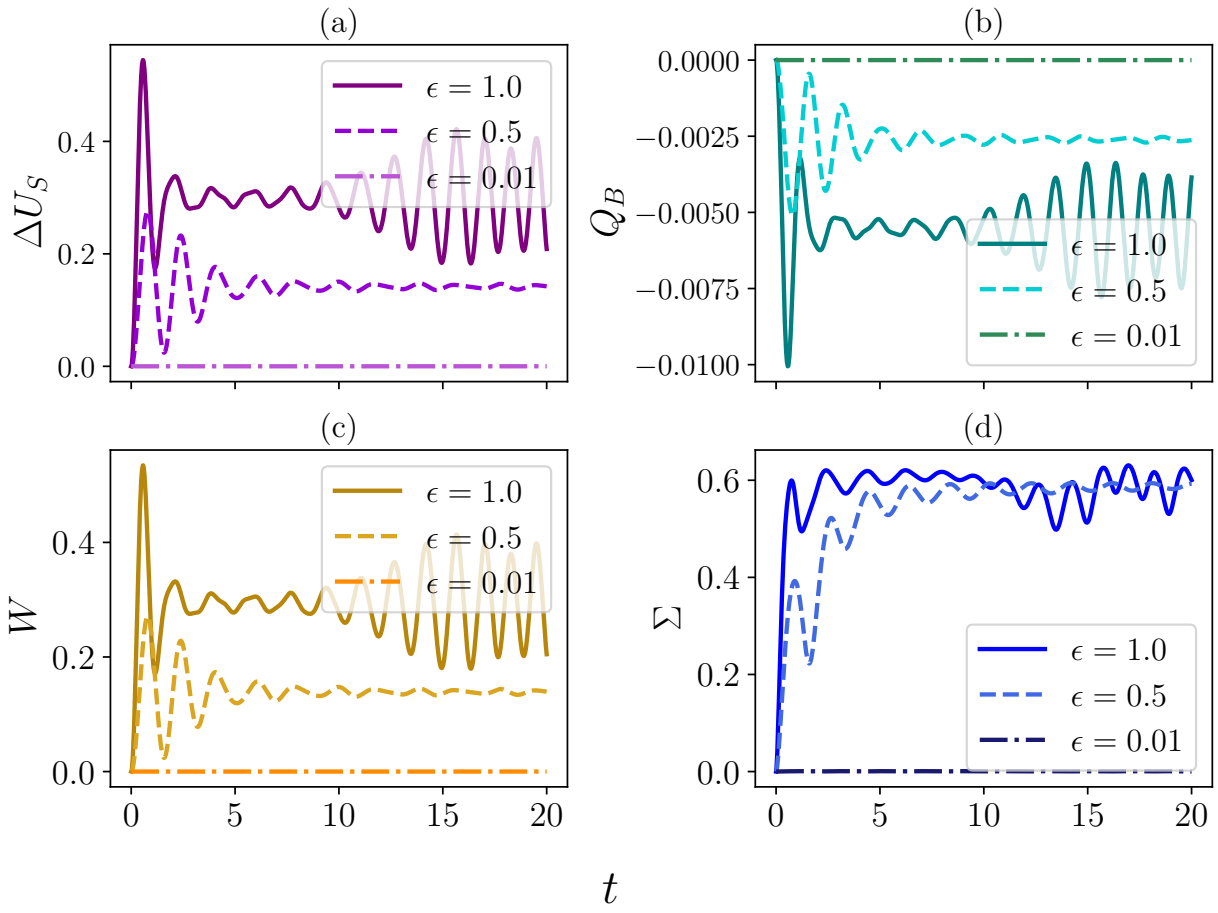
Consider, a single qubit central spin model (a single spin surrounded by a spin bath),

$$H = H_S + H_B + H_{SB} = \frac{\omega_0}{2}\sigma^z + \frac{\omega}{N}J_z + \frac{\epsilon}{\sqrt{N}}\left(\sigma^x J_x + \sigma^y J_y\right),$$

where σ^k are Pauli spin matrices and $J_k = \frac{1}{2}\sum_{i=1}^{N}\sigma_i^k$ (for $(k = x, y, z)$) are the collective angular momentum operators. N is the number of spins in the bath. ω_0 and ω are the transition frequencies for the central and the bath spins, respectively, and ϵ is the interaction strength.

We calculate the change in the internal energy of the central spin, spin bath, the corresponding work done W, and the entropy production for this model.

Internal energy, work, and entropy production in central spin model

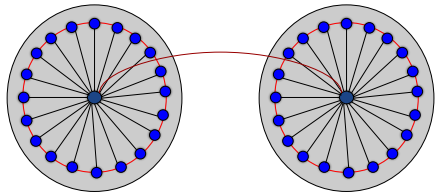


Variation of (a) change in the internal energy of the system ΔU_S, (b) change in the energy of the bath Q_B, (c) Work done by the bath W, and (d) entropy production Σ with time t. The parameters are chosen to be $N = 50$, $\omega = 3$, $\omega_0 = 3.25$, and $T = 0.25$. Further, the system's initial state is taken to be $\frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$, and the thermal state at temperature T is taken to be the bath's initial state. [D. Tiwari, B. Bose, SB (2024)]

Internal energy, work, and entropy production in central spin model

- As the internal energy of the bath decreases, system's internal energy increases and the corresponding mismatch between the system and bath internal energies is the work done by the bath on the system, consistent with the first law of thermodynamics.
- The corresponding changes in the internal energies and work done is more prominent in the strong coupling regime.
- The entropy production can be seen to be positive during the system's dynamics, consistent with the second law of thermodynamics.
- However, the rate of change in the entropy production is sometimes negative due to the non-Markovian nature of the system's dynamics.

Two-Qubit central spin model



Schematic diagram of the two-qubit central spin model.

[S. Bhattacharya and SB (2021); D. Tiwari, S. Datta, S. Bhattacharya and SB (2022)]

Here we write the two-qubit central spin model.

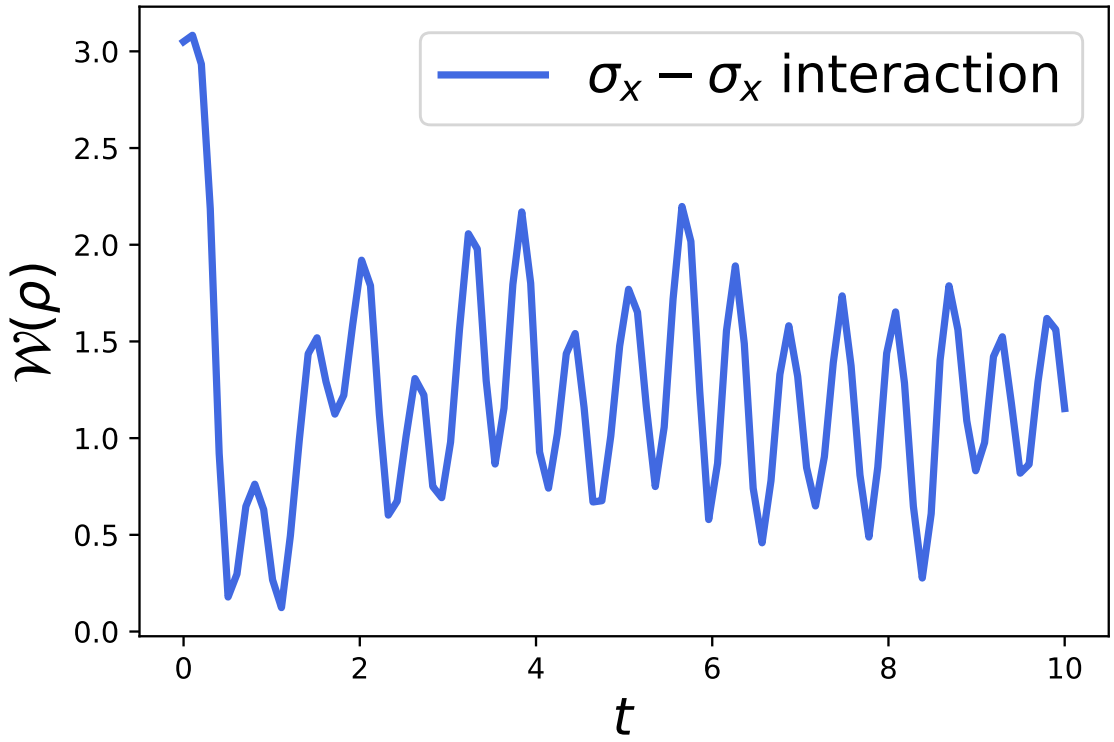
$$\mathcal{H}' = H_{S_1} + H_{S_2} + H_{S_1S_2} + H'_{E_1} + H'_{E_2} + H_{S_1E_1} + H_{S_2E_2},$$

$$= \frac{\hbar\omega_1}{2}\sigma^z_{01} + \frac{\hbar\omega_2}{2}\sigma^z_{02} + \frac{\hbar\delta}{2}V + \frac{\hbar\omega_a}{2M}\sum_{i=1}^{M}\sigma^z_{i1} + \frac{\hbar\omega_b}{2N}\sum_{i=1}^{N}\sigma^z_{i2} + \frac{\hbar\epsilon_1}{2\sqrt{M}}\sum_{i=1}^{M}(\sigma^x_{01}\sigma^x_{i1} + \sigma^y_{01}\sigma^y_{i1})$$

$$+ \frac{\hbar\epsilon_2}{2\sqrt{N}}\sum_{i=1}^{N}(\sigma^x_{02}\sigma^x_{i2} + \sigma^y_{02}\sigma^y_{i2}).$$

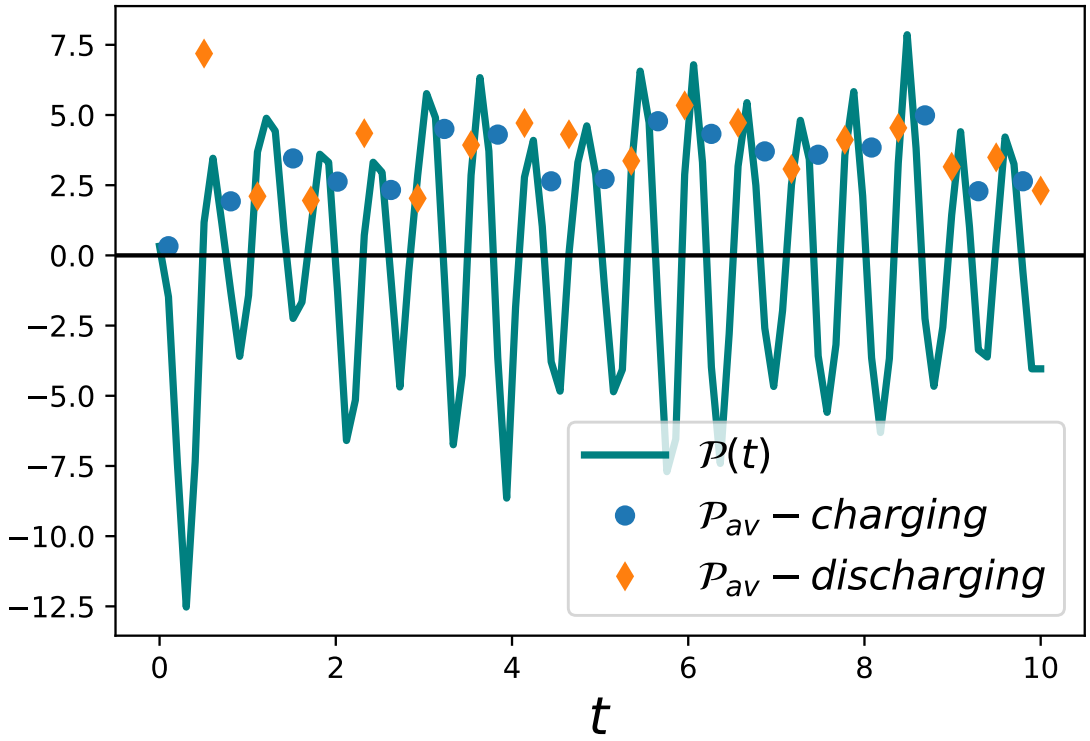
We categorise the interaction between the two central spins using two different kind of interactions. In the first case the two central spin interact using $V = \sigma^x_{01} \otimes \sigma^x_{02}$, and in the second case, there is the anisotropic Dzyaloshinskii - Moriya (DM) interaction in the z direction, $(V = \sigma^x_{01} \otimes \sigma^y_{02} - \sigma^y_{01} \otimes \sigma^x_{02})$ between the two central spins.
(G. Bhanja, D. Tiwari, and SB: work in progress)

Using $\sigma_x \otimes \sigma_x$ interaction



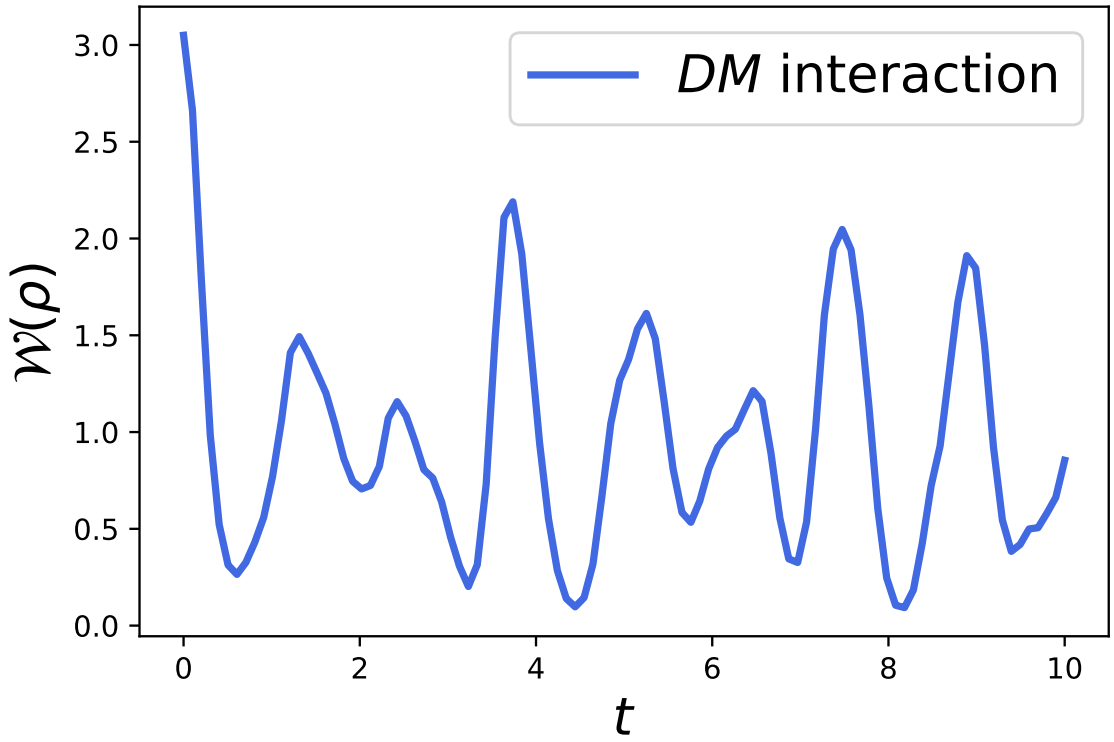
Variation of ergotropy ($\mathcal{W}$) with time in the case of the central spin model.

Using $\sigma_x \otimes \sigma_x$ interaction



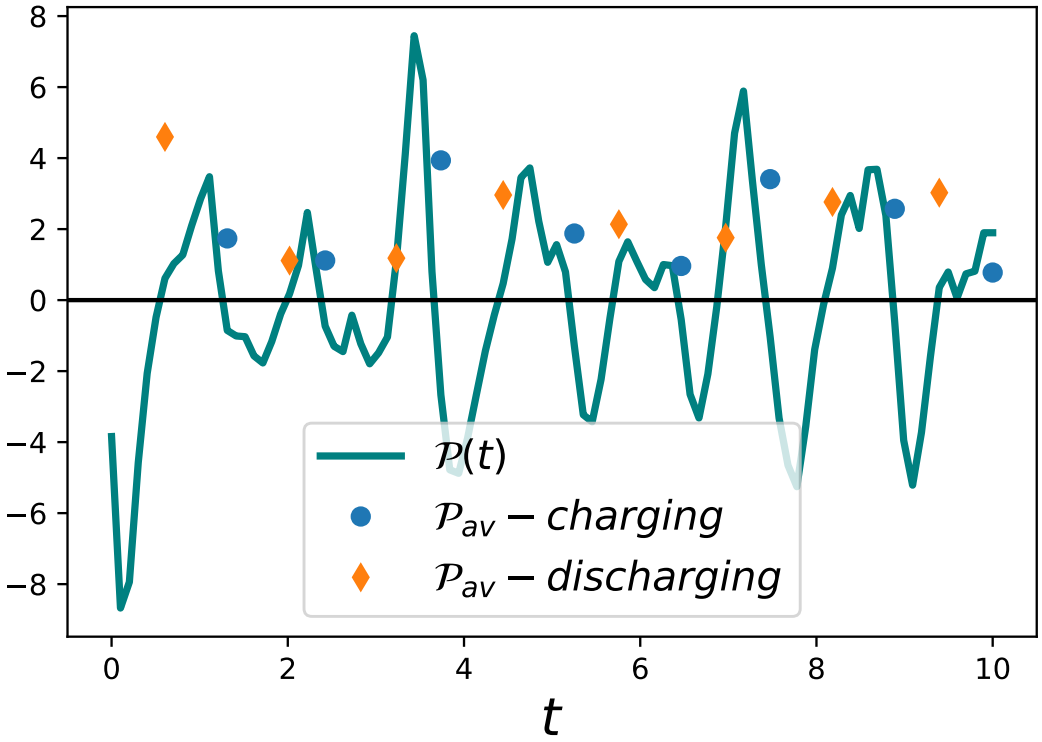
Variation of instantaneous ($\mathcal{P}(t)$) and average ($\mathcal{P}_{av}$) charging and discharging powers with time in the case of the central spin model.

Using DM interaction



Variation of ergotropy ($\mathcal{W}$) with time in the case of the central spin model.

Using DM interaction



Variation of instantaneous ($\mathcal{P}(t)$) and average ($\mathcal{P}_{av}$) charging and discharging powers with time in the case of the central spin model.

- The average discharging behavior depicts how fast or slow the battery discharges. The higher the discharging power, the quicker the battery discharges. Therefore, lower values of discharging power correspond to the slow discharging of the battery.
- In the case of the DM interaction between the two central spins, we observe that the average discharging power is lower at various points than the corresponding average charging power and the time spans of their appearance is also larger. This suggests that the DM interaction is favorable for the discharging of the collective two-spin batteries.
- Here, we have studied the collective behavior of the two-spin battery, that is, both spins are considered as a quantum battery.

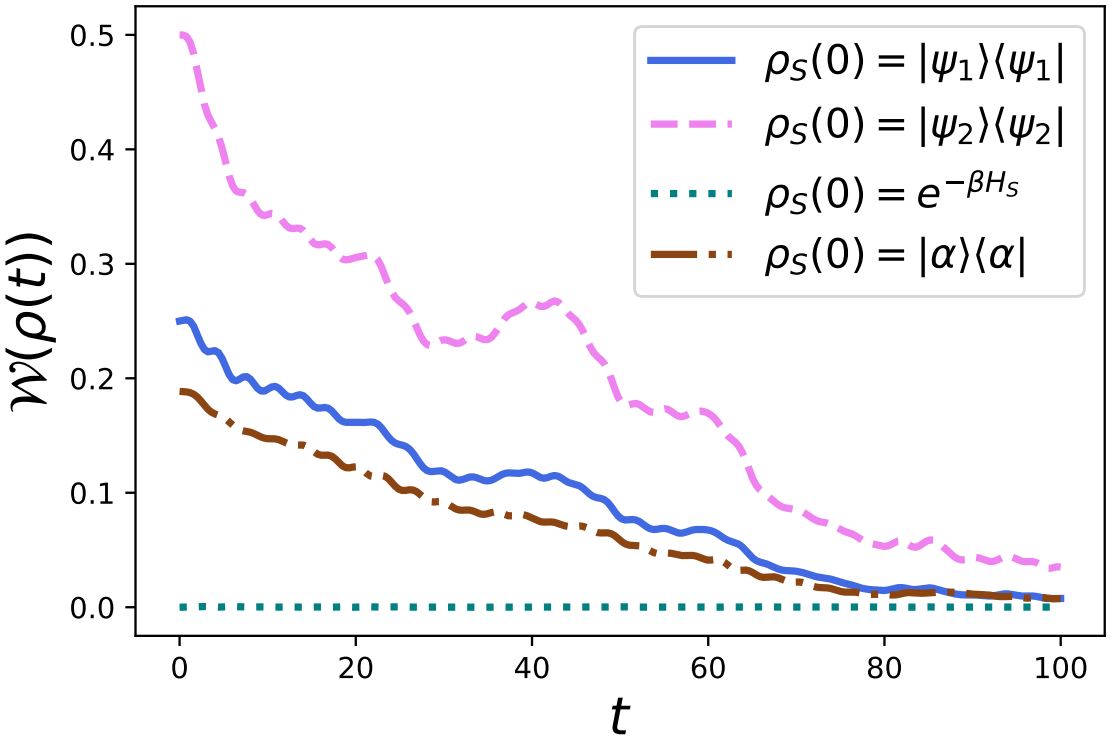
- The total Hamiltonian $\hat{H}$ of the system is [D Tiwari, SB (2024)]

$$\begin{aligned}\hat{H} &= \hat{H}_S + \hat{H}_E + \hat{H}_I, \\ &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_s^2\hat{q}^2 + \sum_n \left(\frac{\hat{p}_n^2}{2m_n} + \frac{1}{2}\omega_n^2\hat{q}_n^2\right) + (\hat{q} - \mu\hat{p})\sum_n c_n\hat{q}_n,\end{aligned}$$

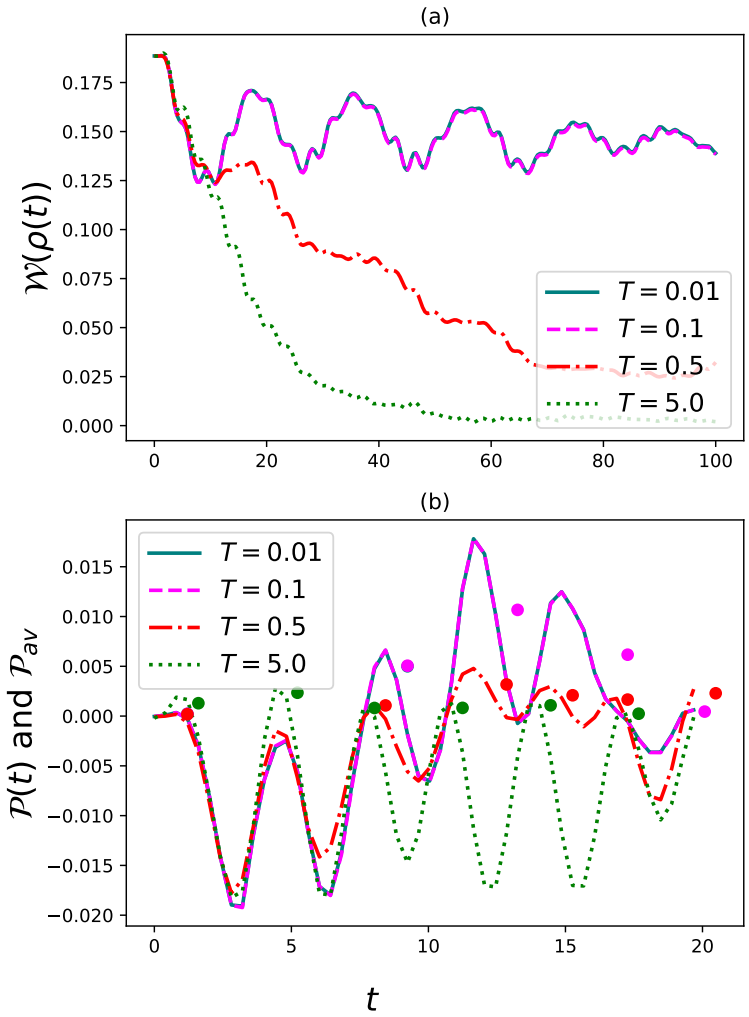
  where ω_s and m are the free frequency of the harmonic oscillator and its mass, whereas ω_n is the frequency of the n th bath mode, respectively.
- Here, $\hat{H}_S$ can be thought of as a quantum battery and the environment $\hat{H}_E$ as a charger that interacts with the quantum battery via $\hat{H}_I$.
- For $\mu = 0$, the above model reduces to the one whose master equation was obtained by Hu, Paz, and Zhang in [Hu, Paz, Zhang: 1994].
- The master equation for the system coupled via position-position coupling to an Ohmic environment and in the high-temperature limit was obtained by Caldeira-Leggett [1983].
- The reduced dynamics of the harmonic oscillator system of interest at any time t is

$$\rho_S(t) = \mathrm{Tr}_\mathrm{E}\left(e^{-i\hat{H}t}\rho(0)e^{i\hat{H}t}\right)$$

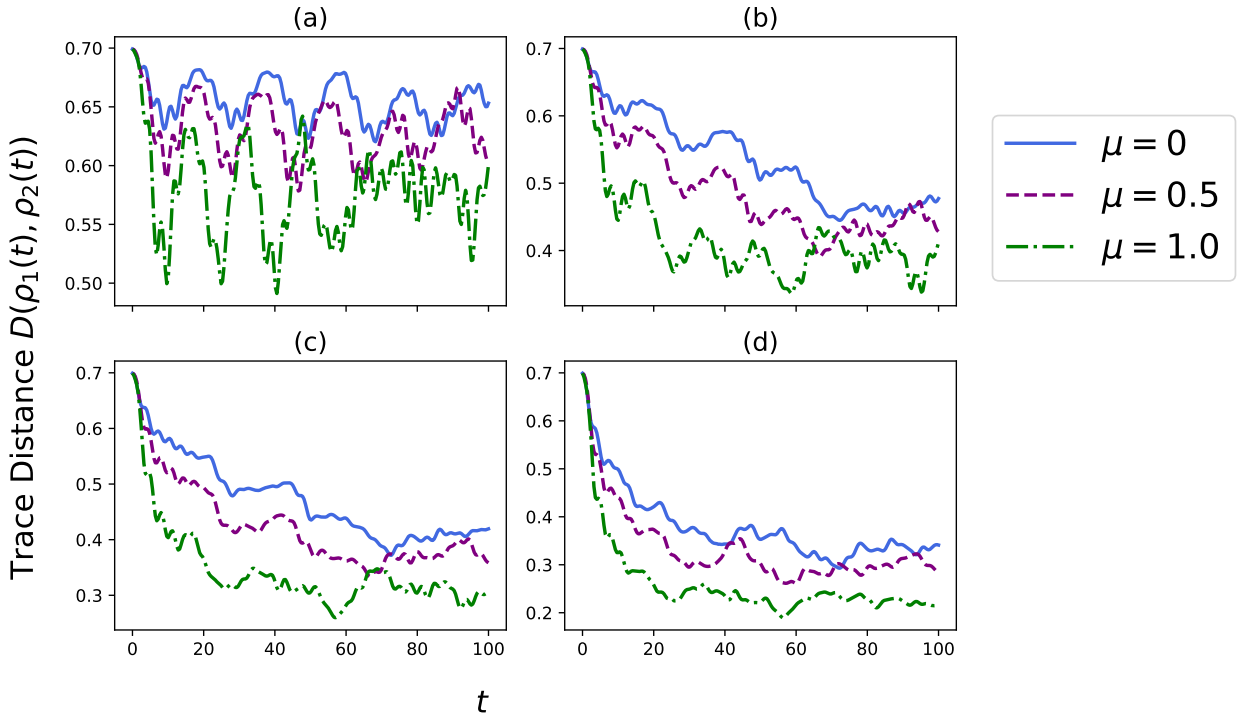
  .



Variation of ergotropy $\mathcal{W}(\rho(t))$ with time t (in natural units, where $\hbar = k_B = 1$) for different initial states $\rho_S(0)$. We have taken the following values of the parameters: $T = 1, \omega_s = 1$, and $m = 1.5$. $|\psi_1\rangle = (\sqrt{3}|0\rangle + |1\rangle)/2$, $|\psi_2\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$.



Variation of Ergotropy $\mathcal{W}(\rho(t))$ (in subplot (a)), instantaneous and average powers (in subplot (b)) with time t (in natural units, where $\hbar = k_B = 1$) for different values of temperature T. The dots of respective colors depict the average power during the charging cycle at a particular temperature. We have taken the following values of the parameters: $\mu = 0.5, \omega_s = 1$, and $m = 1.5$.



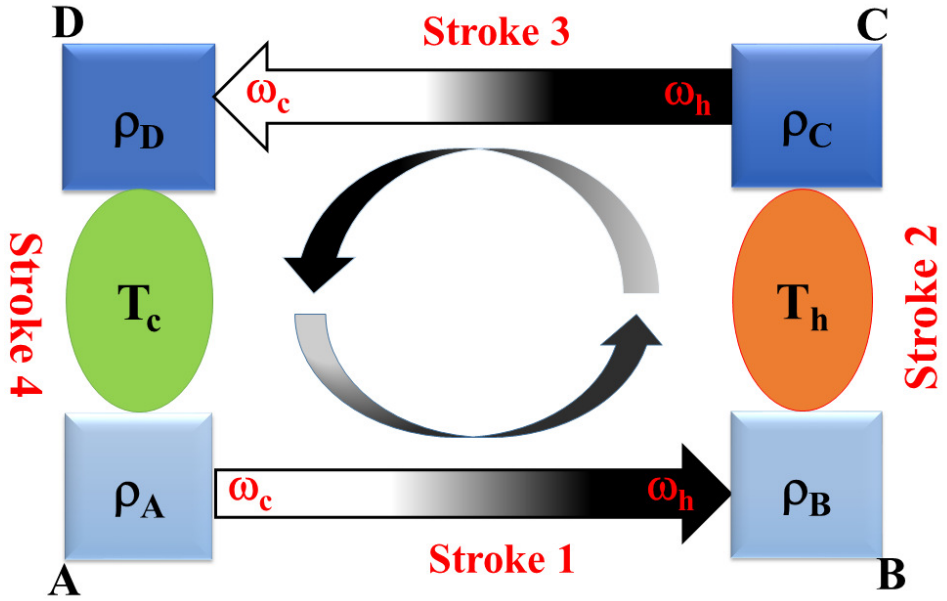
Variation of the trace distance $D(\rho_1(t), \rho_2(t))$ with time t (in natural units, where $\hbar = k_B = 1$) for states $\rho_1(t)$ and $\rho_2(t)$ using initial states $\rho_1(0) = |\alpha_1\rangle\langle\alpha_1|$ and $\rho_2(0) = |\alpha_2\rangle\langle\alpha_2|$, where $|\alpha_i\rangle = e^{\alpha_i \hat{a}^\dagger - \alpha_i^* \hat{a}} |0\rangle$ with $\alpha_1 = 3 + 4i$ and $\alpha_2 = 1$, respectively. The values of temperature T in (a), (b), (c), and (d) are $0.1, 0.5, 1.0$, and 5.0, respectively. We have chosen $\omega_s = 1$, and $m = 1.5$.

Devices: Quantum Heat Engine

- Quantum heat engines (QHEs), e.g., quantum Carnot engine (QCE), and quantum Otto engine (QOE), produce work using quantum matter as their working substance, e.g., qubit, h.o.
- QHEs offer good model systems to study the relation between thermodynamics and quantum mechanics.
- Any QHE cycle consists of several basic quantum thermodynamic processes, such as
  quantum adiabatic processes: there is no heat exchange in a quantum adiabatic process, but work can still be nonzero,
  quantum isothermal processes: working substance is kept in contact with a heat bath at a constant temperature. The particle can perform positive work, and absorb heat from the bath. Both the energy gaps and the occupation probabilities need to change simultaneously, so that the system remains in an equilibrium state with the heat bath at every instant.
  quantum isochoric processes: working substance is placed in contact with a heat bath. No work is done in this process while heat is exchanged between the working substance and the heat bath.

Quantum Heat Engine: Otto Engine

- The traditional Otto cycle has two isochoric (constant volume) and two adiabatic operations and employs an ideal gas as the working medium.
  Isochoric processes: heat exchanged with the thermal reservoirs,
  Adiabatic processes: work done
- In the quantum model of an Otto cycle, the working medium is a quantum system, such as a spin-1/2 system.
- The quantum isochoric process involving a two-level system keeps the energy-level spacing unchanged (instead of fixing the volume as in a classical system). The system being connected to a reservoir during the isochoric phase, the evolution is nonunitary in these steps, whereas it remains unitary in the adiabatic processes.



Schematic diagram of the quantum Otto cycle with squeezed thermal reservoirs.

- Working substance: two-qubit system. [A Kumar, T Bagarti, S. Lahiri, SB: (2023)].
- The evolution of working system described by the von Neumann equations in the unitary steps A→B and C→D, and by Open System Dynamics during the dissipative steps B→C and D→A.
- **Stroke 1**: Consider a quantum Otto cycle for a time-dependent Hamiltonian. The frequency of the Hamiltonian is linearly modulated with time from ω_c to $\omega_h > \omega_c$. The system Hamiltonian changes from $H(\omega_c)$ to $H(\omega_h)$;

$$\omega(t) = \omega_c(1 - t/\tau) + \omega_h t/\tau.$$

The time duration of each stroke is set to a finite time interval τ, which gives a total cycle time of 4τ: non-equilibrium process.
Stroke 2: In this stroke, the hot bath at temperature T_h is connected to the system. The energy spacing is held constant at ω_h, resulting in $H(\omega_h) = (\omega_h/2)\sigma_z$ as the final Hamiltonian at point C. Heat is transferred from the hot bath, modeled here as a squeezed thermal bath (SQTh), to the working medium during this process.
Stroke 3: The system is then decoupled from the bath. The frequency corresponding to the energy level spacing is changed linearly from ω_h to ω_c.
Stroke 4: The system is now connected to the cold bath. The energy gap is held constant at ω_c, resulting in $H(\omega_c) = (\omega_c/2)\sigma_z$ as the final Hamiltonian at the end of this stroke.

- Working substance: two-qubit system
- Interaction with SQTh modelled by [SB, V Ravishankar, R. Srikanth (2010)]

$$\begin{aligned}\frac{\partial\rho(t)}{\partial t} &= -i[\tilde{H},\rho(t)] \\ &- \frac{1}{2}\Gamma_{12}\sum_{i,j=1,2}[1+\tilde{N}](\rho S_i^+ S_j^- + S_i^+ S_j^-\rho - 2S_j^-\rho S_i^+) \\ &- \frac{1}{2}\Gamma_{12}\sum_{i,j=1,2}\tilde{N}(\rho S_i^- S_j^+ + S_i^- S_j^+\rho - 2S_j^+\rho S_i^-) \\ &+ \frac{1}{2}\Gamma_{12}\sum_{i,j=1,2}\tilde{M}(\rho S_i^+ S_j^+ + S_i^+ S_j^+\rho - 2S_j^+\rho S_i^+) \\ &+ \frac{1}{2}\Gamma_{12}\sum_{i,j=1,2}\tilde{M}^*(\rho S_i^- S_j^- + S_i^- S_j^-\rho - 2S_j^-\rho S_i^-),\end{aligned}$$

- $\tilde{H}$ consists of a total energy operator for the two qubits, and an interaction between them, which is mediated by the qubits' interaction with the bath:

$$\tilde{H} = \hbar(\omega_1 S_1^z + \omega_2 S_2^z) + \hbar\Omega_{12}(S_1^+ S_2^- + S_2^+ S_1^-),$$

where

$$\begin{aligned} S_1^z &= \frac{1}{2}(|e_1\rangle\langle e_1| - |g_1\rangle\langle g_1|) \\ S_2^z &= \frac{1}{2}(|e_2\rangle\langle e_2| - |g_2\rangle\langle g_2|) \\ S_1^+ &= |e_1\rangle\langle g_1|, \quad S_2^+ = |g_2\rangle\langle e_2| \\ S_1^- &= |e_1\rangle\langle g_1|, \quad S_2^- = |g_2\rangle\langle e_2|. \end{aligned}$$

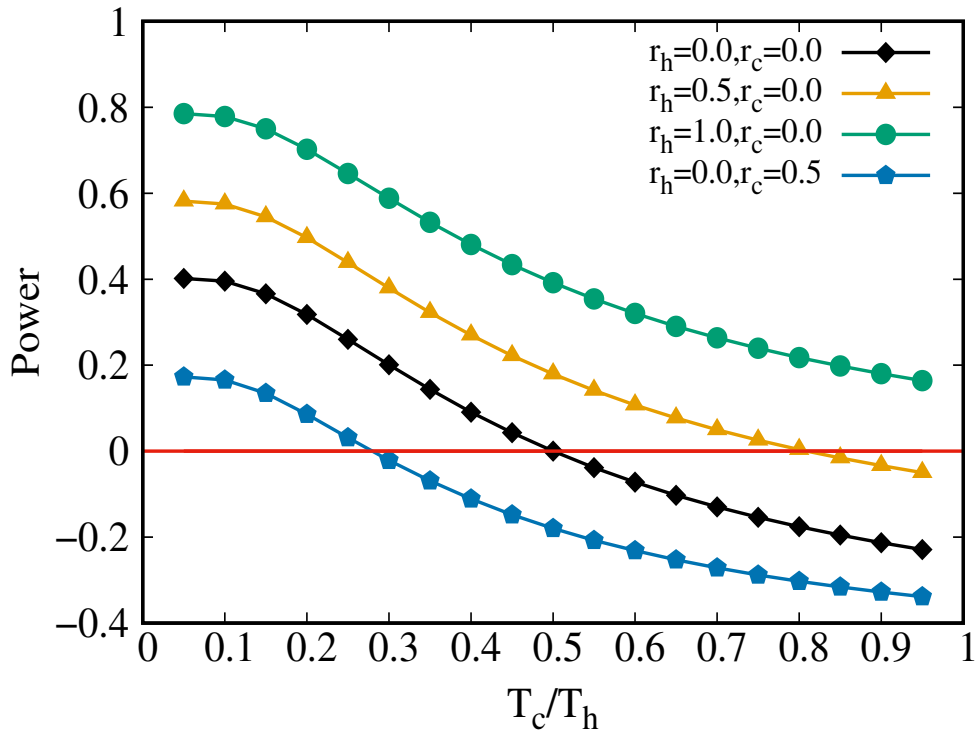
Here $S_{1,2}^{\pm}$ are the raising and lowering operators and $S_{1,2}^z$ are the energy operators of the concerned qubits.

- The strength of the interaction between the two qubits is given by

$$\Omega_{12} = \Omega_{21} = \frac{3}{4}\Gamma \left[-\{1 - (\hat{\boldsymbol{\mu}}.\hat{\boldsymbol{r}}_{12})^2\} \frac{\cos(k_0 r_{12})}{(k_0 r_{12})} + \{1 - 3(\hat{\boldsymbol{\mu}}.\hat{\boldsymbol{r}}_{12})^2\} \times \left\{ \frac{\sin(k_0 r_{12})^2}{(k_0 r_{12})} + \frac{\cos(k_0 r_{12})}{(k_0 r_{12})^3} \right\} \right].$$

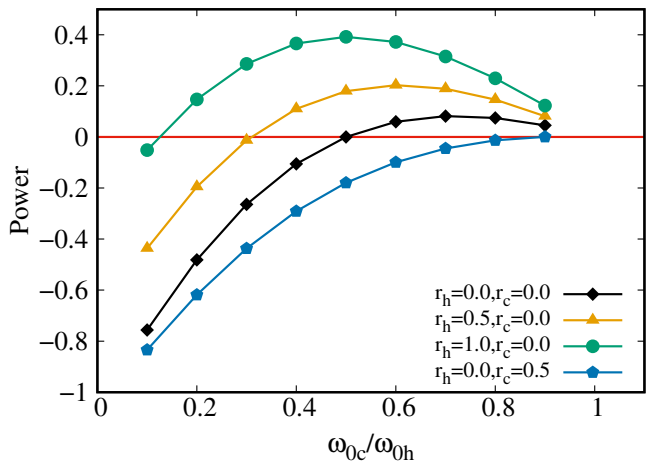
- The magnitude of the wavevector is $k_0 = 2\pi/\lambda_0 = \omega_0/c$, where λ_0 is the resonant wavelength.
- The decoherence may be broadly categorized as (a) *independent decoherence* where $\boldsymbol{k}_0.\boldsymbol{r}_{12} > 1$ and (b) *collective decoherence* where $\boldsymbol{k}_0.\boldsymbol{r}_{12} \ll 1$.
- Ω_{12} provides the shifts in atomic energy levels.

Power of Two-Qubit Engine

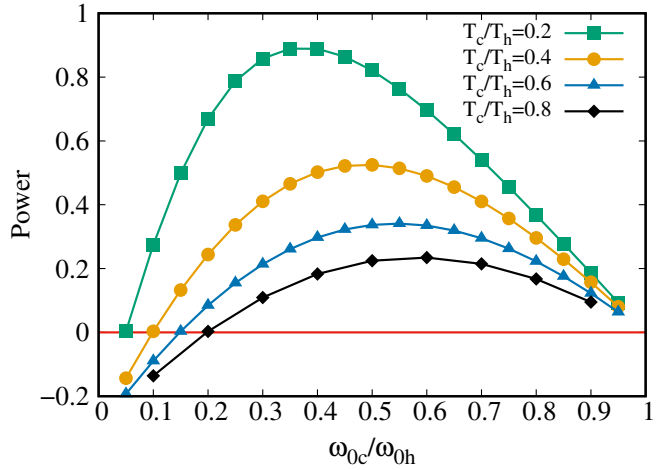


Variation of power of a TQE as a function of the temperature ratio T_c/T_h for different squeezed parameters r_h and r_c. Other parameters are: $\omega_{0h} = 20$, $\omega_{0c} = 10$, $r_{12} = 0.5$.

Power of Two-Qubit Engine

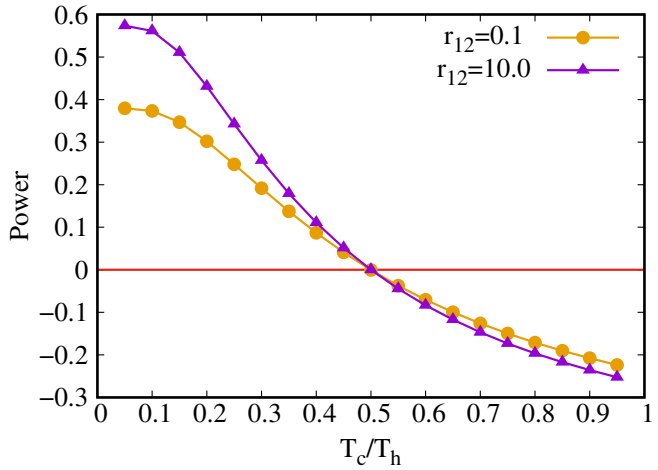


(a) Variation of power of a TQE as a function of the frequency ratio ω_{0c}/ω_{0h} for different squeezed parameters r_h and r_c. Other parameters are: $T_h = 20$, $T_c = 10$, $r_{12} = 0.5$.

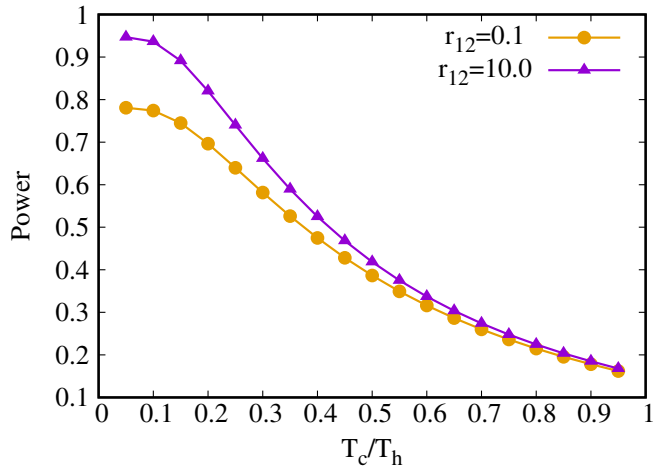


(b) Power as a function of the frequency ratio ω_{0c}/ω_{0h} for different values of bath temperature ratio T_c/T_h. The squeezing parameters are: $r_h = 1$, $r_c = 0$. Other parameters are same as in (a).

Power of Two-Qubit Engine



(a)



(b)

Variation of Engine power as the function of T_c/T_h at different r_{12}. Other parameters are $r_h = 0$, $r_c = 0$, $\omega_{0h} = 20$, $\omega_{0c} = 10$. (b) Same plots when $r_h = 1$.

Conclusions

- Some recent developments in the efforts to understand non-Markovian phenomenon were discussed.
- Quantitites like, ergotropy, entropy production, power were discussed.
- Two types of Quantum Thermodynamics Devices were discussed: Quantum Battery and Quantum Heat Engine.
- They were illustrated on open system models; (a). the Garraway type, (b). central spin model, (c). QBM, (d). two-qubit decoherence.