Quantum Thermodynamics: An Open System Approach

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Motivation

- Motivate the need for Open Quantum Systems.
- Focus on Quantum Thermodynamics
- Discuss well known characterizers of quantum thermodynamics and the Hamiltonian of Mean Force
- Focus on devices, such as Quantum Battery and Heat Engine, whose underpinnings are provided by Quantum Thermodynamics
- Devices discussed from the perspective of some Open System Models
- Finally, I discuss a panoramic schematic of quantum thermal analogs of electric circuits in the steady state regime.

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.

$$\rho^{s}(t) = \operatorname{Tr}_{R}(\rho(t)) = \operatorname{Tr}_{R}\left[e^{-\frac{i}{\hbar}\operatorname{Ht}}\rho(0)e^{\frac{i}{\hbar}\operatorname{Ht}}\right].$$

- 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 $[H_5, H_{SR}] \neq 0$ 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

- 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.

Non-Markovian Master Equation: Time-Local Master Equations

 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)]

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

- ullet 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

$$\mathcal{K}(t)\rho_{S} = -i\left[H_{S}(t), \rho_{S}\right] + \sum_{i} \gamma_{i}(t) \left[A_{i}(t)\rho_{S}A_{i}^{\dagger}(t) - \frac{1}{2}\left\{A_{i}^{\dagger}(t)A_{i}(t), \rho_{S}\right\}\right].$$

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 $t \geq 0$.



Quantum Thermodynamics

- The fundamental laws of thermodynamic equilibrium and non-equilibrium in the quantum regime are the subject of quantum thermodynamics [Gemmer, Michel, and Mahler, Lecture notes in physics (2004); Binder, et al: Thermodynamics in the quantum regime: Fundamental aspects and new directions, fundamental theories of physics, Springer (2019)].
- This is facilitated by the rapid experimental control of quantum systems and the engineering of small environments.

Characterizers of quantum thermodynamics: Ergotropy

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 ${\cal H}$ having spectral decomposition

$$ho = \sum_{i} r_{i} \ket{r_{i}} ra{r_{i}}$$
, with eigenvalues $r_{1} \geq r_{2} \geq$,

and

$$H = \sum_{i} \epsilon_{i} \ket{\epsilon_{i}} \bra{\epsilon_{i}}$$
, with eigenvalues $\epsilon_{1} \leq \epsilon_{2} \leq ...$

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

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

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



Characterizers of quantum thermodynamics: Ergotropy

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: Front. Qu. Sci. Technol. **2**, 1207552 (2023)]

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

Coherent and Incoherent Ergotropy

It was recently recognized that quantum ergotropy can be separated into two different contributions, coherent (W_c) and incoherent (W_i) ergotropies. (G. Francica *et.al.* Phys. Rev. Lett. (2020))

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

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

where $S\left(\mathcal{E}(\sigma)||\rho^{eq}\right)=\operatorname{Tr}\left\{\sigma\ln(\sigma)\right\}-\operatorname{Tr}\left\{\mathcal{E}(\sigma)\ln(\rho^{eq})\right\}$ 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 $\left(\sum_{i}\langle i|\sigma|i\rangle\langle i|\right)$ on the coherence invariant state σ . The state ρ^{eq} is the Gibbs state $\rho^{eq}=\frac{\exp(-\beta H)}{Z}$ with $Z=\operatorname{Tr}\left\{\exp(-\beta H)\right\}$ and $\beta=1/k_{B}T$.

Coherent and Incoherent Ergotropy (Contd.)

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

$$W_{c}(\rho(t)) = \begin{cases} \frac{\omega_{0}}{2} \left(\sqrt{x(t)^{2} + z(t)^{2}} - z(t) \right), & \text{for } z(t) \geq 0 \\ \frac{\omega_{0}}{2} \left(\sqrt{x(t)^{2} + z(t)^{2}} + z(t) \right), & \text{for } z(t) < 0 \end{cases}$$
(3)

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

$$\mathcal{W}_{c}(\rho(t)) = \begin{cases} \frac{\omega_{0}}{2} \left(\sqrt{\mathcal{C}_{h_{1}}(\rho(t))^{2} + z(t)^{2}} - z(t) \right), & \text{for } z(t) \geq 0 \\ \frac{\omega_{0}}{2} \left(\sqrt{\mathcal{C}_{h_{1}}(\rho(t))^{2} + z(t)^{2}} + z(t) \right), & \text{for } z(t) < 0 \end{cases}$$
(4)

The incoherent ergotropy of the system is

$$W_i(\rho(t)) = \begin{cases} \omega_0 z(t). & \text{for } z(t) \ge 0\\ 0. & \text{for } z(t) < 0 \end{cases}$$
 (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.

Characterizers of quantum thermodynamics: internal energy, heat, and work

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

$$\Delta U_{S}(t) = \text{Tr}[H_{S}(\rho_{S}(t) - \rho_{S}(0))],$$

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

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

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*.



Characterizers of quantum thermodynamics: Heat Current

• Consider a system H_S coupled to a heat bath H_B via an interaction Hamiltonian H_I . The system heat current $Q_S(t)$, in this case, is given by $\dot{Q}_S(t) = \frac{d}{dt} \langle H_S(t) \rangle - \dot{W}(t)$, where $\dot{W}(t) = \left\langle \frac{\partial H_S(t)}{\partial t} \right\rangle$. The average $\langle \cdot \rangle = \text{Tr} \left[\rho_{SB}(t) \cdot \right]$. Using the relation between the expectation value of a quantum mechanical operator and the expectation value of the commutator between the operator and the Hamiltonian of the system, the system heat current can be rewritten as

$$\dot{Q}_{S}(t) = i \langle [H_{I}(t), H_{S}(t)] \rangle.$$

For a constant H_S , this becomes the rate of change in the system's internal energy.

• Considering the rate of change in the bath energy $\dot{Q}_B(t) = \frac{d}{dt} \langle H_B(t) \rangle$ for a constant H_B , we get the following relation between the $\dot{Q}_B(t)$ and the $\dot{Q}_S(t)$

$$\dot{Q}_B(t) = -\dot{Q}_S(t) - \frac{d}{dt} \langle H_I(t) \rangle.$$

From this

$$Q_B = -\int_0^t d\tau \left\{ i \left\langle \left[H_I(\tau), H_S(\tau) \right] \right\rangle \right\} + \left\langle H_I(0) \right\rangle - \left\langle H_I(t) \right\rangle.$$

Notice that the first term on the right side of the above equation denotes the negative of the change in the internal energy of the system for a constant H_S and the second term is the work done by the bath on the system

Characterizers of quantum thermodynamics: entropy production

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 $(\rho_B(0) = \frac{e^{-\beta H_B}}{{\rm Tr}[e^{-\beta H_B}]} \text{ with } \beta = 1/k_BT \text{ being the inverse temperature), the entropy production can be given as}$

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

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.

Hamiltonian of Mean Force

- Consider a quantum system S interacting with a thermal bath B, which is described by the Hamiltonian H.
- The global equilibrium state of the system and the reservoir at temperature $\mathcal T$ is denoted by ζ_{SB} , which is of Gibbs form,

$$\zeta_{SB} := \frac{\exp(-\beta H)}{Z_{SB}},$$

where, $Z_{SB} = \text{Tr} \left[\exp(-\beta H) \right]$ is the partition function for SB, and $\beta = (k_B T)^{-1}$.

- The interaction term causes the reduced equilibrium state of the system S, $\zeta_S^*(T) = \operatorname{Tr}_B\left[\zeta_{SB}(T)\right]$, to deviate from the thermal state $\zeta_S(T) = \exp{-\beta H_S}/\operatorname{Tr}\left[\exp{-\beta H_S}\right]$ unless the system-bath coupling is very weak.
- The reduced equilibrium state of the system S as an effective Gibbs state is then given by $\zeta_S^*(T) = \frac{\exp[-\beta \mathcal{H}_S^*(T)]}{Z_S^*}$, where the partition function for the system S can be expressed as the ratio

$$Z_S^* = Z_{SB}/Z_B$$

where $Z_{SB}=\mathrm{Tr}[e^{-\beta H]}$ and $Z_B=\mathrm{Tr}_B[e^{-\beta H_B}]$ and,

$$\mathcal{H}_{S}^{*}(T) := -\frac{1}{\beta} \log \left(\frac{\operatorname{Tr}_{B} \left[\exp(-\beta H) \right]}{\operatorname{Tr}_{B} \left[\exp(-\beta H_{B}) \right]} \right),$$

is the Hamiltonian of mean force [Binder, et al (2019)].



Hamiltonian of Mean Force: Continued...

- This operator acts as an effective Hamiltonian for the system S, incorporating both temperature T and interaction V. In the weak coupling regime, it simplifies to the bare Hamiltonian H_S . The Hamiltonian of mean force (HMF) approach is crucial for understanding key thermodynamic properties like free energy, entropy, and heat capacities in systems with significant environmental interactions. It aids in formulating generalized thermodynamic potentials and investigating equilibrium and non-equilibrium processes, shedding light on quantum dissipation and decoherence.
- In the strong coupling regime, for the thermal equilibrium state $\zeta_S(T)$, the system's thermodynamic entropy becomes [Talkner and Hanggi: RMP (2020)]

$$\mathcal{S}_S = -\mathrm{Tr}\left[\zeta_S^*(T)\log\zeta_S^*(T)\right] + \beta^2\mathrm{Tr}\left[\partial_\beta\mathcal{H}_S^*(T)\zeta_S^*(T)\right].$$

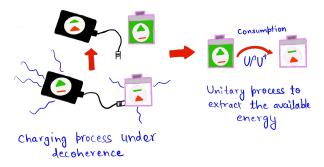
The first term is the von Neumann entropy of the system, while the second term comes from the temperature dependence of HMF. This suggests that thermodynamic entropy is not universally equivalent to the information content of the equilibrium state in systems with interactions.

Devices: Quantum Battery and Heat Engine

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.

Devices: Quantum Battery



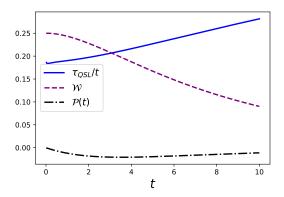
A schematic diagram of charging-discharging and work extraction processes of a quantum battery

Devices: Quantum Battery-Charger Open System Models

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

Battery: Ergotropy in NMAD

Discharging of battery under Markovian evolution:



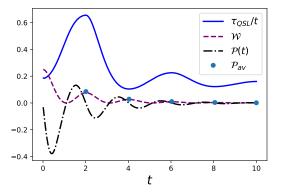
Variation of QSL time using Fisher information metric (au_{QSL}), ergotropy (au), instantaneous (au(t)) and average (au_{av}) powers, with time. The evolution of the state is through the Markovian AD channel. The parameters are taken to be $\omega_0=1$, $\lambda=0.5$, $\gamma_0=0.1$.

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



Battery: Ergotropy in NMAD

Discharging-charging of battery under non-Markovian evolution



Variation of QSL time using au_{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: Front. Qu. Sci. Technol. 2, 1207552 (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.

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

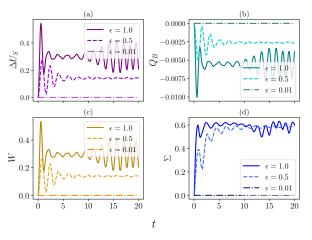
Consider, a single qubit central spin model (a single spin surrounded by a spin bath),

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

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

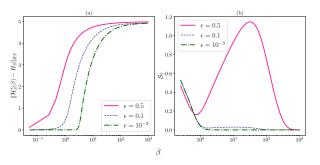


Variation of (a) change in the internal energy of the system ΔU_{S} , (b) change in the energy of the bath Q_{B} , (c) Work done by the bath W, and (d) entropy production Σ with time t. The parameters are chosen to be N=50, $\omega=3$, $\omega_{0}=3.25$, and T=0.25. Further, the system's initial state 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: J. Chem. Phys. 162, 114104 (2025)]

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.

HMF in central spin model



Variation of (a) the Hilbert-Schmidt norm of the matrix $\mathcal{H}_{S}^{*}(\beta)-H_{S}$, where H_{S} is the central spin system Hamiltonian and $\mathcal{H}_{S}^{*}(\beta)$ is the HMF, and (b) thermodynamic entropy \mathcal{S}_{S} as a function of inverse temperature β . The parameters are: $N=80, \omega=\omega_{0}=5$. [D. Tiwari, B. Bose, SB: J. Chem. Phys. **162**, 114104 (2025)]

QBM model

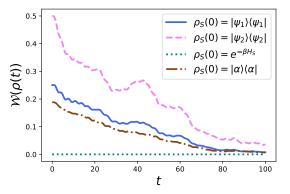
$$\begin{split} \hat{H} &= \hat{H}_{S} + \hat{H}_{E} + \hat{H}_{I}, \\ &= \frac{\hat{p}^{2}}{2m} + \frac{1}{2}m\omega_{s}^{2}\hat{q}^{2} + \sum_{n} \left(\frac{\hat{p}_{n}^{2}}{2m_{n}} + \frac{1}{2}\omega_{n}^{2}\hat{q}_{n}^{2}\right) + (\hat{q} - \mu\hat{p})\sum_{n} c_{n}\hat{q}_{n}, \end{split}$$

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.

- ullet 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

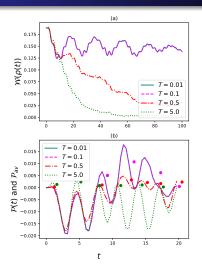
$$ho_{S}(t) = \mathrm{Tr_{E}}\left(e^{-i\hat{H}t}\rho(0)e^{i\hat{H}t}\right)$$





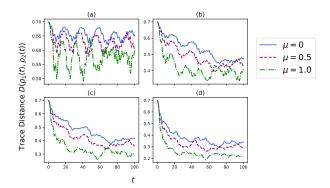
Variation of ergotropy $\mathcal{W}(\rho(t))$ with time t (in natural units, where $\hbar=k_B=1$) for different initial states $\rho_S(0)$. We have taken the following values of the parameters: $T=1, \omega_s=1$, and m=1.5. $|\psi_1\rangle=(\sqrt{3}|0\rangle+|1\rangle)/2,$ $|\psi_2\rangle=(|0\rangle+|1\rangle)/\sqrt{2}.$

QBM model



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.

QBM model



Variation of the trace distance $D\left(\rho_1(t),\rho_2(t)\right)$ 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 $|\alpha_i\rangle=e^{\alpha_i\hat{s}^{\dagger}-\alpha_i^{*}\hat{s}}|0\rangle$ 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.

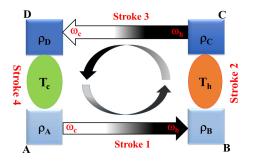
Devices: Quantum Heat Engine

- 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.

Otto Cycle



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

Otto Engine

- Working substance: two-qubit system. [A Kumar, T Bagarti, S. Lahiri, SB: Physica A 623, 128832 (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.



Otto Engine

- Working substance: two-qubit system
- Interaction with SQTh modelled by [SB, V Ravishankar, R. Srikanth: Ann. Phys. (N.Y.) 56, 277 (2010)]

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

Working Substance

 $ightharpoonup ilde{H}$ 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

$$\begin{split} S_{1}^{\mathrm{z}} &= \frac{1}{2} (\ket{e_{1}}\bra{e_{1}} - \ket{g_{1}}\bra{g_{1}}) \\ S_{2}^{\mathrm{z}} &= \frac{1}{2} (\ket{e_{2}}\bra{e_{2}} - \ket{g_{2}}\bra{g_{2}}) \\ S_{1}^{+} &= \ket{e_{1}}\bra{g_{1}}, \quad S_{2}^{+} &= \ket{g_{2}}\bra{e_{2}} \\ S_{1}^{-} &= \ket{e_{1}}\bra{g_{1}}, \quad S_{2}^{-} &= \ket{g_{2}}\bra{e_{2}}. \end{split}$$

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

Working Substance

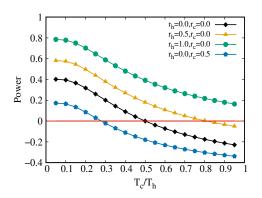
• The strength of the interaction between the two qubits is given by

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

- 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 k₀.r₁₂ > 1 and (b) collective decoherence where k₀.r₁₂ ≪ 1.
- ullet Ω_{12} provides the shifts in atomic energy levels.

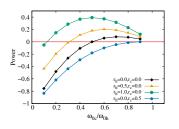


Power of Two-Qubit Engine



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

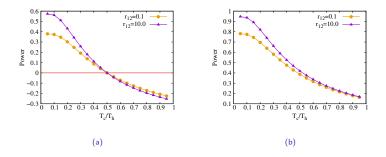


1 T/T₁-02 T/T₁-02 T/T₁-03 T/T₁-03 T/T₁-03 T/T₁-04 T/T₁-04 T/T₁-05 T/T

(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: $T_h=20,\ T_c=10,\ T_{12}=0.5.$

(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

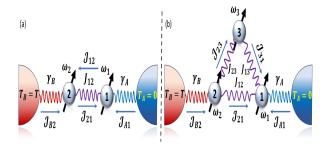


Variation of Engine power as the function of T_c/T_h at different r_{12} . Other parameters are $r_h=0$, $r_c=0$, $\omega_{0h}=20$, $\omega_{0c}=10$. (b) Same plots when $r_h=1$.

Devices: Quantum Thermal Analogs of Electric Circuits

- [D. Tiwari, S. Bhattacharya, SB: Phys. Rev. Lett. 135, 020404 (2025)]
 - We develop a panoramic schematic of quantum thermal analogs of electric circuits in the steady state regime. We establish the foundations of the said premise by defining the analogs of Kirchhoff's laws for heat currents and temperature gradients, as well as a quantum thermal step transformer.
 - The approach encompasses various circuits like thermal diode, transistor, and Wheatstone bridge.
 - Two new quantum thermal circuits are developed.
 - This sheds light on the present architecture of quantum device engineering.

- We begin by constructing a model for a quantum thermal circuit of two qubits connected to two thermal baths at different temperatures and interacting with each other via a Hamiltonian.
- By analyzing the flow of heat current through this, we seek to establish a
 relationship akin to Kirchhoff's laws. Our goal is to understand if, and under
 what conditions, temperature gradients and heat currents in quantum thermal
 devices can relate in a manner analogous to these fundamental circuit principles.



Schematic diagrams of the (a) 2-qubit and (b) 3-qubit quantum thermal circuits. Quantum thermal current from source j to qubit k, taking qubit k as a node, is \mathcal{J}_{jk} .

- The Hamiltonian of this system, Fig. a, is $H_S = \sum_{j=1}^2 \frac{\omega_j}{2} \sigma_j^z + J_{12} \left(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y \right)$, where σ^i (i=x,y,z) are the Pauli matrices. J_{12} is the interaction strength between the two qubits and models the quantum thermal resistor.
- The dynamics of the system is governed by

$$\frac{d\rho}{dt} = -i[H_{S}, \rho] + \mathcal{D}_{A1}(\rho) + \mathcal{D}_{B2}(\rho) = \mathcal{L}(\rho),$$

where $\mathcal{D}_{jk}(\rho)=$ $\gamma_j(\tilde{N}_{jk}+1)\left(\sigma_k^-\rho\sigma_k^+-\frac{1}{2}\left\{\sigma_k^+\sigma_k^-,\rho\right\}\right)+\gamma_j\tilde{N}_{jk}\left(\sigma_k^+\rho\sigma_k^--\frac{1}{2}\left\{\sigma_k^-\sigma_k^+,\rho\right\}\right),$ with $\sigma_k^\pm=\frac{1}{2}\left(\sigma_k^\times\pm i\sigma_k^\vee\right),$ and $\tilde{N}_{jk}=\frac{1}{e^{\beta_j\omega_k}-1},$ with $\beta_j=T_j^{-1}$ (here, j=A,B and k=1,2). γ_A and γ_B are the dissipative factors. $\mathcal L$ denotes the right-hand side of the master equation.

• The steady state of the system is given by the condition $\frac{d\rho^{SS}}{dt}=0$.

• Quantum heat currents: In the steady state condition, from the bath j to the qubit k (\mathcal{J}_{jk}) and from qubit l to qubit k (\mathcal{J}_{lk}) are given by

$$\mathcal{J}_{jk} = \operatorname{Tr}\left[H_k \mathcal{D}_{jk}\left(
ho^{SS}
ight)
ight] \ \ \text{and} \ \ \mathcal{J}_{lk} = i \operatorname{Tr}\left\{
ho^{SS}[H_{lk}, H_k]
ight\},$$

respectively.

We find

$$\mathcal{J}_{A1}+\mathcal{J}_{21}=0.$$

This is crucial as it allows qubit 1 to be considered as a junction node, leading to the visualization of the above equation as the quantum thermal version of *Kirchhoff's current law*.

• In fact, considering heat currents \mathcal{J}_{jk} 's from n different sources to a qubit k, it can be proved that in the steady state condition, the sum of all the heat currents is zero, i.e.,

$$\sum_{j=1}^n \mathcal{J}_{jk} = 0.$$

• It can be easily verified that $\mathcal{J}_{B2}+\mathcal{J}_{12}=0$, which shows the characteristics of the quantum thermal version of Kirchhoff's current law.

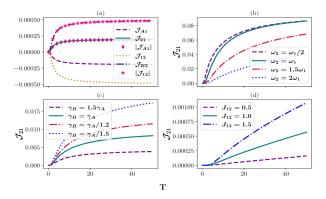


- Quantum thermal transformer: Heat currents \mathcal{J}_{21} and \mathcal{J}_{12} are interconnected by the relation $\frac{\mathcal{J}_{21}}{\omega_1} = -\frac{\mathcal{J}_{12}}{\omega_2}$, or $\left|\frac{\mathcal{J}_{21}}{\mathcal{J}_{12}}\right| = \frac{\omega_1}{\omega_2} = \left|\frac{\mathcal{J}_{A1}}{\mathcal{J}_{B2}}\right|$.
- In general, for an interaction $H_{jk} = J_{jk} \left(\sigma_j^x \sigma_k^x + \sigma_j^y \sigma_k^y \right)$ between two qubits j and k, the current between them can be shown to be

$$\frac{\mathcal{J}_{jk}}{\omega_k} = -\frac{\mathcal{J}_{kj}}{\omega_j}.$$

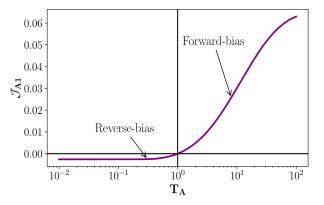
The above relation mimics the quantum thermal version of a step transformer,

- Quantum thermal voltage: Develop quantum analog of the thermal voltage driving the thermal current. To this end, we determine the effective temperature of qubits 1 and 2 in the steady state.
- The effective temperature T_1 of the qubit 1 is found by comparing the state ρ_1^{SS} with the state $e^{-H_1/T_1}/\mathrm{Tr} \left(e^{-H_1/T_1}\right)$, where $H_1 = \frac{\omega_1}{2} \sigma_1^z$.
- T_1 can be envisaged as the thermal potential difference between qubit 1 and bath A, that is, $V_{1A} = T_1 0 = T_1$. This potential difference drives the thermal current \mathcal{J}_{A1} .
- We get V₂₁ + V₃₂ + V₁₃ = 0 inside the loop of the three qubits, resembling Kirchhoff's second law of an electric circuit, stating that the sum of potential differences around a closed loop (a closed sequence of interactions connecting qubits, returning to the initial qubit) in an electric circuit is zero.
- The heat current can be seen to increase linearly in certain parameter regimes, satisfying the condition for Ohm's law.
- In general, the heat current exhibits nonlinear behavior.
- Kirchhoff's current law is satisfied universally.



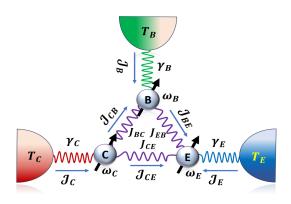
Variation of heat currents \mathcal{J}_{jk} in (a), and heat current \mathcal{J}_{21} from qubit 2 to 1 in (b), (c), and (d) with temperature T of bath B for the two-qubit quantum thermal resistor model.

Quantum Thermal Analogs of Electric Circuits: Quantum Thermal Diode



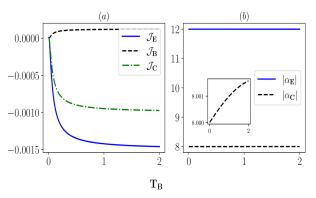
Variation of heat current \mathcal{J}_{A1} from bath A to qubit 1 as a function of temperature T_A of bath A for a quantum thermal diode. Based on the temperature difference between bath A and bath B, we call the thermal diode to be in the reverse and in the forward bias. In the forward bias region, the heat current flows from bath A to the qubit 1, whereas in the reverse bias region, the heat current flows from the qubit 1 to the bath A. Further, the heat current is zero when the temperatures T_A and T_B of the baths A and B, respectively, are equal.

Quantum Thermal Analogs of Electric Circuits: Quantum Thermal Transistor



A schematic diagram to show the arrangement of qubits and the respective baths to function as a quantum thermal transistor. The labels B, C, and E correspond to base, collector, and emitter, respectively.

Quantum Thermal Analogs of Electric Circuits: Quantum Thermal Transistor



Variation of the (a) collector (\mathcal{J}_C) , base (\mathcal{J}_B) , and emitter (\mathcal{J}_E) thermal currents and (b) the corresponding amplification factor α_C and α_E as a function of the base temperature T_B .

Quantum Thermal Transistor: Continued...

The Hamiltonian of the system is given by

$$\begin{split} H_{trans} &= \frac{\omega_{C}}{2} \sigma_{C}^{z} + \frac{\omega_{B}}{2} \sigma_{B}^{z} + \frac{\omega_{E}}{2} \sigma_{E}^{z} + J_{BC} \left(\sigma_{B}^{x} \sigma_{C}^{x} + \sigma_{B}^{y} \sigma_{C}^{y} \right) \\ &+ J_{EB} \left(\sigma_{E}^{x} \sigma_{B}^{x} + \sigma_{E}^{y} \sigma_{B}^{y} \right) + J_{CE} \left(\sigma_{C}^{x} \sigma_{E}^{x} + \sigma_{C}^{y} \sigma_{E}^{y} \right). \end{split}$$

The above Hamiltonian is along similar lines to our adaptation of thermal resistors, diodes, and other thermal circuits discussed here.

The master equation dictating the dynamics of the system is given by

$$\begin{split} \frac{d\rho}{dt} &= -i[H_{trans},\rho] + \sum_{k=B,C,E} \left(\gamma_k \left(N_{th,k} + 1 \right) \left[\sigma_k^- \rho \sigma_k^+ - \frac{1}{2} \left\{ \sigma_k^+ \sigma_k^- \right\} \right] \right. \\ &+ \left. \gamma_k N_{th,k} \left[\sigma_k^+ \rho \sigma_k^- - \frac{1}{2} \left\{ \sigma_k^- \sigma_k^+ \right\} \right] \right), \end{split}$$

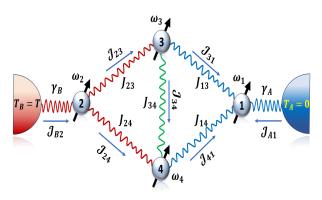
where $N_{th,k} = \frac{1}{e^{\omega_k/T_k}-1}$ for k = B, C, E.

- The base, emitter, and collector currents \mathcal{J}_B , \mathcal{J}_E , and \mathcal{J}_C , respectively, for the quantum thermal transistor are found using the steady-state ρ_{trans}^{SS} and are plotted as a function of the base temperature T_B .
- It can be observed that the base current only changes slightly, whereas, for the same change in temperature, the collector and emitter currents change rapidly.
- To quantify the amplifications in the collector and emitter currents, the factor

$$\alpha_P = \frac{\mathcal{J}_P}{\mathcal{J}_B},$$

for P = C, E is plotted. It can be observed that the collector and emitter currents get amplified by 8 and 12 times, respectively, for the given set of parameters.

Quantum Thermal Wheatstone Bridge

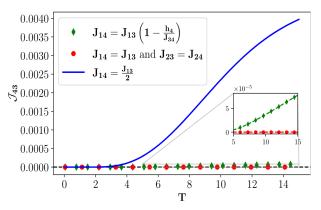


A schematic diagram of the standard quantum thermal Wheatstone bridge.

Quantum Thermal Wheatstone Bridge: Continued...

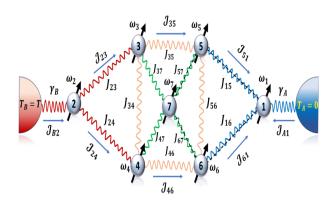
- Classical setup of a Wheatstone bridge of an electrical circuit, where an unknown resistance can be determined using a specific balance condition when the current between nodes 3 and 4 is zero.
- The Hamiltonian for the quantum Wheatstone bridge is given by $H_S^W = \frac{1}{2} \sum_{i=1}^4 \omega_i \sigma_i^z + \sum_{l,k=1,l < k}^4 J_{lk} \left(\sigma_l^x \sigma_k^x + \sigma_l^y \sigma_k^y \right)$, where $J_{12} = 0$ as the qubits 1 and 2 are non-interacting.
- The balance condition for the Wheatstone bridge is that the quantum heat current \mathcal{J}_{34} between qubits 3 and 4 should be zero. This happens when couplings follow the relation: $J_{13}=J_{14}$ and $J_{23}=J_{24}$. Note that J_{13} need not be equal to J_{23} .
- Unknown Hamiltonian strengths can be determined by the profiling of heat currents.

Quantum Thermal Wheatstone Bridge



Variation of quantum heat current \mathcal{J}_{43} between qubits 3 and 4 in the case of the quantum Wheatstone bridge model in the steady state.

Quantum Thermal super Wheatstone Bridge



A schematic diagram of the quantum thermal super Wheatstone Bridge.

Conclusions

- I tried to motivate the need for Open Quantum Systems and focused on Quantum Thermodynamics.
- A brief discussion of well known characterizers of quantum thermodynamics was followed by their implementation on devices, such as Quantum Battery and Heat Engine.
- A number of Open System Models were made use of for this purpose.
- Finally, I discussed a panoramic schematic of quantum thermal analogs of electric circuits in the steady state regime.