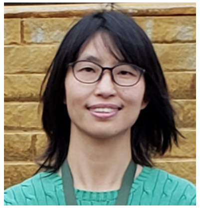
Entropy production of a small quantum system strongly interacting with an environment: A computational experiment

Ryoichi Kawai

Department of Physics
University of Alabama at Birmingham



Xian He
Nanchang University

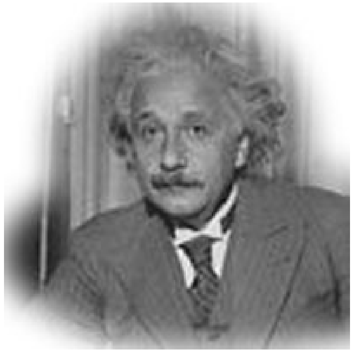
Ketan Goyal

Nordita

Sir Arthur Eddington

"The law that entropy always increases holds, I think, the supreme position among the laws of nature. If someone points out to you that your pet theory of the universe is in disagreement with Maxwell's equation – then so much the worse for Maxwell's equations … but if your theory is found to be against the second law of thermodynamics, I can give you no hope; there is nothing for it but to collapse in deepest humiliation." (1928)

"The second law of thermodynamics is the only physical theory of universal content concerning which I am convinced that, within the framework of the applicability of the basic concepts, it will never be overthrown." (1949)



Albert Einstein

When a system strongly interacts with environments,
is the second law

$$\Delta \mathcal{S} \geq \frac{Q}{T}$$

correct?

Thermal Equilibrium - Why is the Gibbs state so special?

Maximum entropy principle

$$S[\rho] = -\,\mathrm{tr}(\rho \ln \rho)$$

$$E = \mathrm{tr}(\rho H) = \mathrm{tr}(\rho_{\mathrm{G}} H)$$

$$\rho_{\mathrm{G}} = e^{-\beta H} / \,\mathrm{tr}\, e^{-\beta H}$$

$$S[\rho_{\mathrm{G}}] - S[\rho] = S[\rho \| \rho_{\mathrm{G}}] \geq 0$$

Unitary evolution

$$\partial_t S[\rho \| \rho_{\mathrm{G}}] = 0$$

Maximization

↓

Decoherence in energy basis

Decoherence Theory

- Entanglement with environment
- Why and how does the environment choose energy basis for decoherence?
- Does it have to be energy basis?
- Zurek's superselection (einselection)?

Decoherece

System + Environment

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -i[H,\rho] \qquad H = H_{\mathrm{S}} \otimes I + I \otimes H_{\mathrm{B}} + \lambda X_{\mathrm{S}} \otimes Y_{\mathrm{B}}$$

Reduced system

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}} = -i[H_{\mathrm{S}},\rho_{\mathrm{S}}] - i\lambda[X_{\mathrm{S}},\eta_{\mathrm{S}}], \qquad \eta_{\mathrm{S}} = \mathrm{tr}_{\mathrm{B}}(Y_{\mathrm{B}}\rho) \qquad \rho_{\mathrm{S}} = \mathrm{tr}_{\mathrm{B}}\,\rho$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}} = -i[H_{\mathrm{S}},\rho_{\mathrm{S}}] - {\scriptstyle i\lambda[X_{\mathrm{S}},\eta_{\mathrm{S}}]}, \qquad \lambda \ll 1$$

Diagonal in energy basis

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}} = {\scriptstyle -i[H_{\mathrm{S}},\rho_{\mathrm{S}}]} - i\lambda[X_{\mathrm{S}},\eta_{\mathrm{S}}], \qquad \lambda \gg 1$$

Diagonal in pointer basis

Measurement = Decoherence in observable basis

system state

$$|\psi_{\mathrm{s}}\rangle = \sum_i c_i |\omega_i\rangle$$

observable

$$\hat{\Omega} |\omega_i\rangle = \omega_i |\omega_i\rangle$$

before measurement

$$\rho_< = \sum_{ij} c_i c_j^* |\omega_i\rangle\langle\omega_j|$$

$$\Rightarrow$$

after measurement

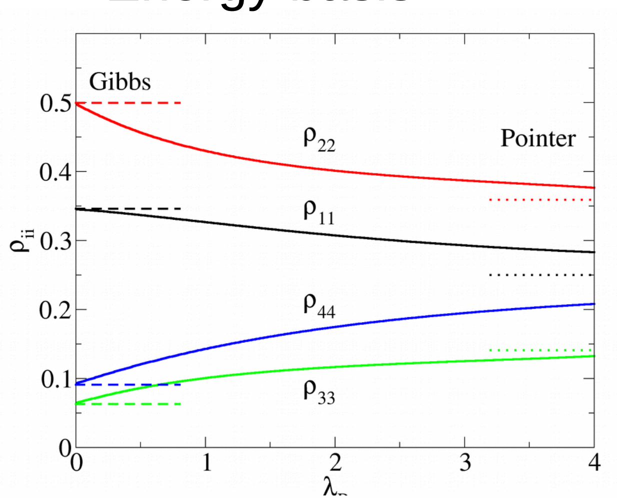
$$\rho_> = \sum_i |c_i|^2 |\omega_i\rangle\langle\omega_i| = \sum_i |\omega_i\rangle\langle\omega_i| \rho_< |\omega_i\rangle\langle\omega_i|$$

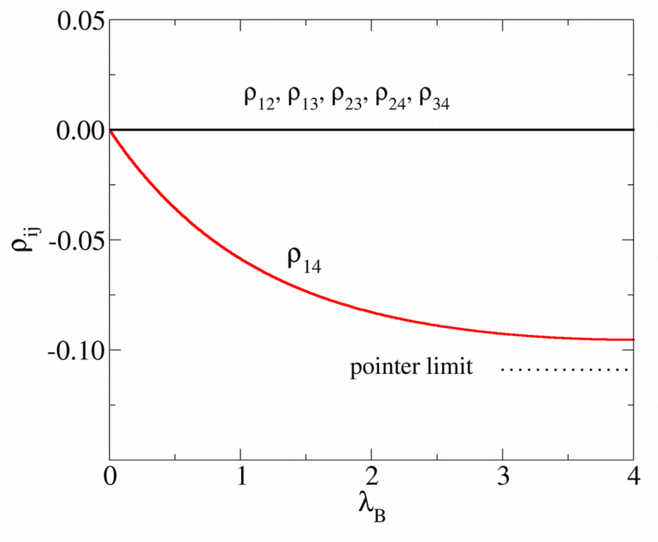
Continuous measurement by environment

$$\rho \longrightarrow \sum_j |e_j\rangle\langle e_j| \rho_{\mathrm{G}} |e_j\rangle\langle e_j| \qquad \lambda \ll 1 \qquad |e_j\rangle = \text{energy basis}$$

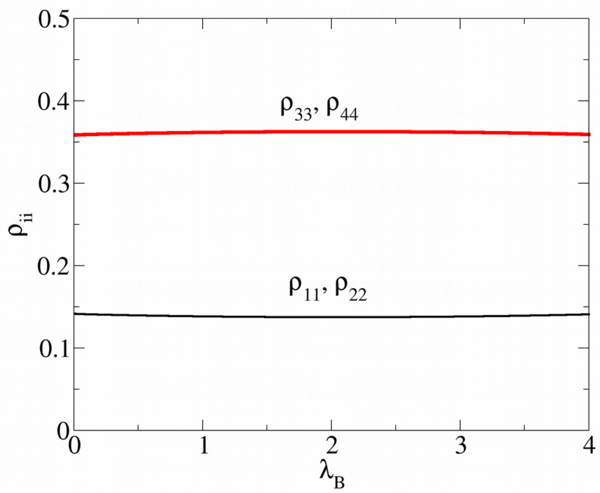
$$\rho \longrightarrow \sum_j |\pi_j\rangle\langle \pi_j| \rho_{\mathrm{G}} |\pi_j\rangle\langle \pi_j| \qquad \lambda \gg 1 \qquad |\pi_j\rangle = \text{pointer basis}$$

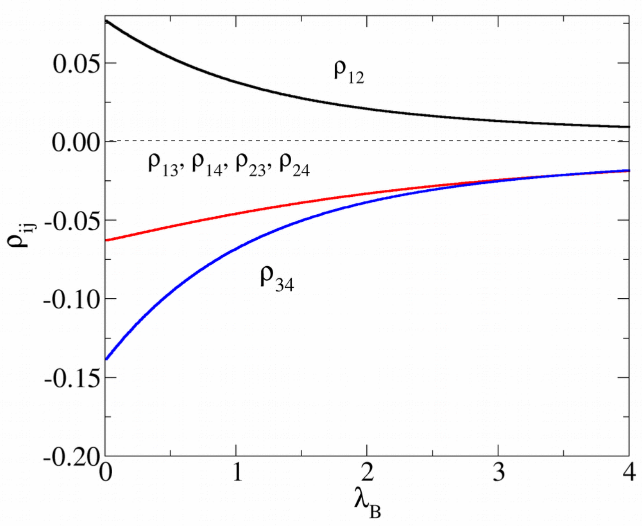
Energy basis

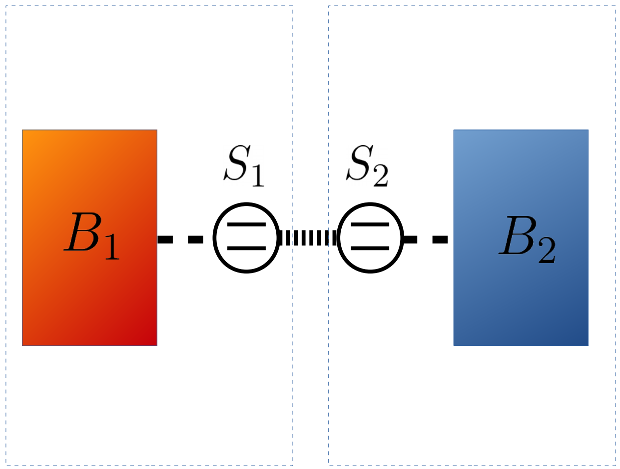




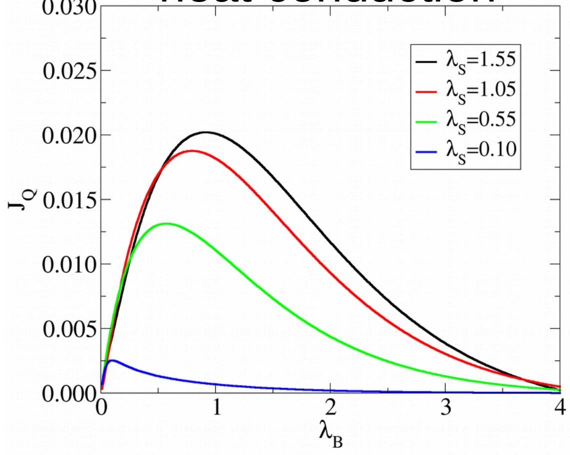
Pointer basis



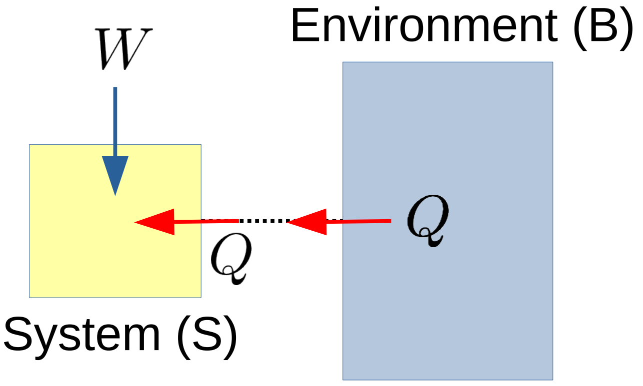




heat conduction



Weak coupling



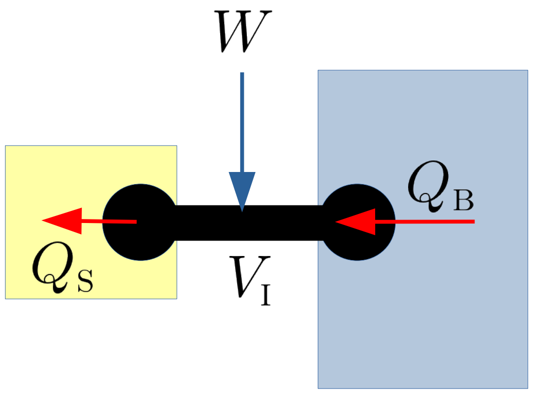
S and B are separable
(Thermodynamics concerns only S)

Equilibrium $\rho_{\rm S} = e^{-\beta H_{\rm S}}/Z_{\rm S}$

Maximum entropy principle

$(\max S(\rho_s), {\rm tr}\{\rho_{\rm S} H_{\rm S}\} = E)$

Strong coupling



S and B are not well separated.
($V_{\rm I}$ belongs to both S and B)

Maximum entropy?

Extremely strong coupling

Equilibrium: diagonal in pointer basis

Quantum Zeno effects

Question

The laws of thermodynamics determine the energy transaction between the system and its exterior *without knowing the state of the exterior.*

Is the thermodynamics of systems strongly interacting with the environment consistent with the conventional laws of thermodynamics?

Yes, but needs some modification.

↓

Hamiltonian of mean force

No, the laws of thermodynamics depend on the state of the environment.

No, we need a completely new set of laws.

Hamiltonian of Mean Force

G. Kirkwood (1935), U. Seifert (2016)

Equilibrium

$$\rho_{SB} \neq \frac{e^{-\beta H_S}}{Z_S} \otimes \frac{e^{-\beta H_B}}{Z_B}$$

$$E_{\text{total}} = \text{tr}_{SB}\left\{(H_S + H_B + H_I)e^{-\beta(H_S+H_B+H_I)}\right\}/Z_{SB}$$

$$\tilde{U} = U + \tilde{U}' + \tilde{U}''$$

$$\tilde{S}_S = S_S + \beta\tilde{U}''$$

$$\tilde{F} = F + \tilde{U}'$$

$$\tilde{W} = W$$

$$\tilde{Q} = Q - \Delta V_{SB} + \tilde{U}' + \Delta\tilde{U}''$$

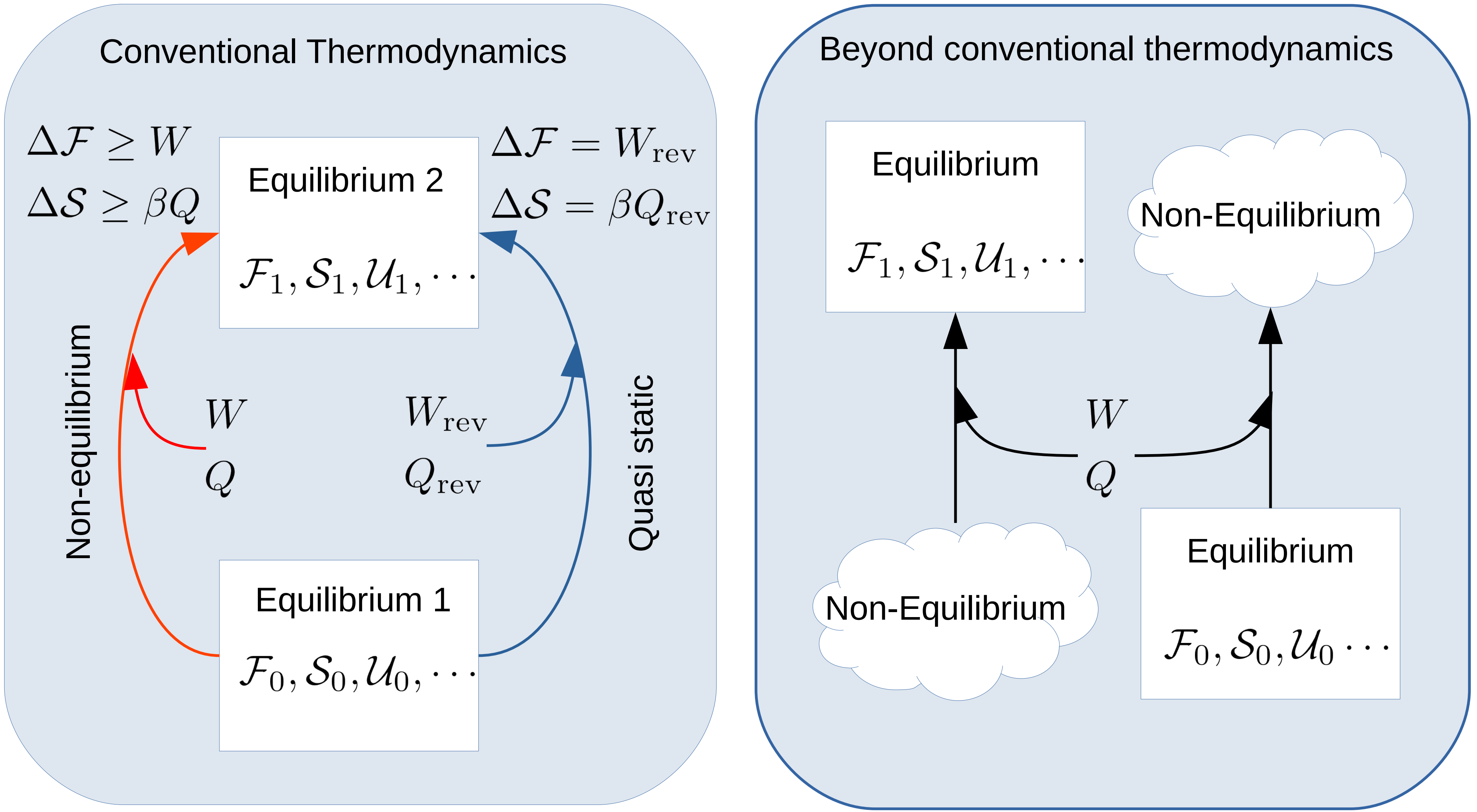
Effective System Hamiltonian

$$\tilde{H}_S = -\frac{1}{\beta}\ln\left[\text{tr}_B\left\{e^{-\beta(H_S+H_B+H_I)}\right\}/Z_B\right]$$

$$\tilde{U}' = \text{tr}_S\{\rho_S(t)(\tilde{H}_S - H_S)\}$$

$$\tilde{U}'' = \text{tr}_S\{\rho_S(t)\tilde{\beta}\partial_\beta\tilde{H}_S\}$$

P. Strasberg and M. Esposito,, Phys. Rev. E 99 (2019) 012120.



Conventional Thermodynamics
$\Delta\mathcal{F} \geq W$
$\Delta\mathcal{S} \geq \beta Q$
Equilibrium 2
$\mathcal{F}_1, \mathcal{S}_1, \mathcal{U}_1, \cdots$
$\Delta\mathcal{F} = W_{\mathrm{rev}}$
$\Delta\mathcal{S} = \beta Q_{\mathrm{rev}}$
Non-equilibrium
W
Q
W_{rev}
Q_{rev}
Quasi static
Equilibrium 1
$\mathcal{F}_0, \mathcal{S}_0, \mathcal{U}_0, \cdots$
Beyond conventional thermodynamics
Equilibrium
$\mathcal{F}_1, \mathcal{S}_1, \mathcal{U}_1, \cdots$
Non-Equilibrium
W
Q
Non-Equilibrium
Equilibrium
$\mathcal{F}_0, \mathcal{S}_0, \mathcal{U}_0 \cdots$

Measurable Quantities

Internal energy

$$U(t) = \mathrm{tr}_{\mathrm{S}}\{\rho_{\mathrm{S}}(t)H_{\mathrm{S}}\}$$

Work = energy injected into the whole system by a “classical external agent”
= change of the total energy

$$W(t) = \mathrm{tr}_{\mathrm{SB}}\{\rho_{\mathrm{SB}}(t)H_{\mathrm{SB}}\} - \mathrm{tr}_{\mathrm{SB}}\{\rho_{\mathrm{SB}}(t_0)H_{\mathrm{SB}}\}$$

Heat = energy released from the environment

$$Q(t) = \mathrm{tr}_{\mathrm{B}}\{\rho_{\mathrm{B}}(t_0)H_{\mathrm{B}}\} - \mathrm{tr}_{\mathrm{B}}\{\rho_{\mathrm{B}}(t)H_{\mathrm{B}}\}$$

Coupling energy

$$V_{\mathrm{I}}(t) = \lambda(t)\,\mathrm{tr}_{\mathrm{SB}}\{\rho_{\mathrm{SB}}(t)H_{\mathrm{I}}\}$$

Energy conservation law:

$$W(t) + Q(t) = \Delta U(t) + \Delta V_{\mathrm{I}}(t)$$

1^{st} law?

2nd law and Entropy Production

Thermodynamics

$$\Sigma_{\mathrm{Q}} = \Delta\mathcal{S} - \beta Q \geq 0$$

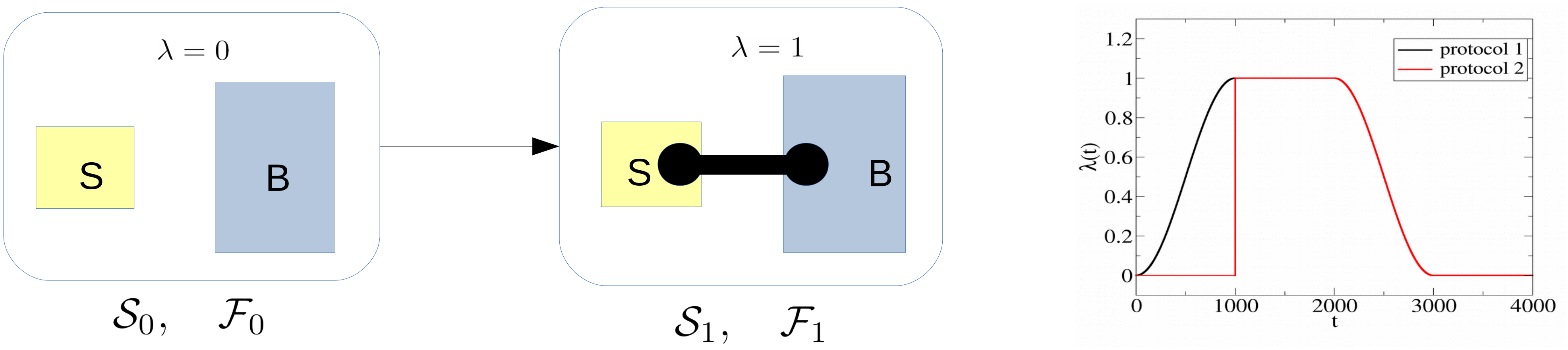
$$\Sigma_{\mathrm{W}} = \beta(W - \Delta\mathcal{F}) \geq 0$$

Non-equilibrium statistical mechanics

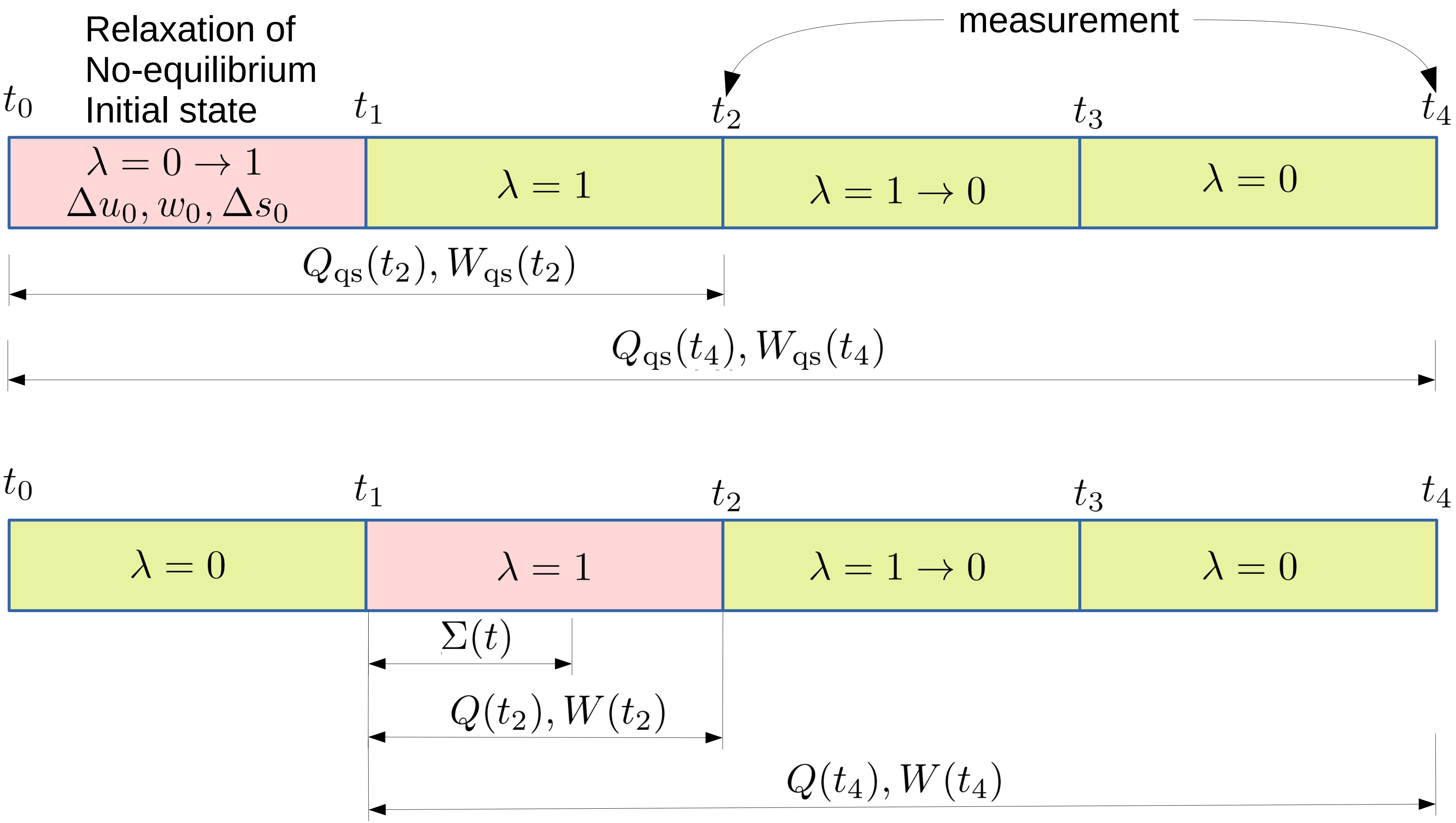
$$\Sigma_{\mathrm{S}} = \Delta S_{\mathrm{S}} - \beta Q \geq 0, \qquad S_{\mathrm{S}} = -\operatorname{tr}_{\mathrm{S}} \rho_{\mathrm{S}} \ln \rho_{\mathrm{S}}$$

$$\Sigma_{\mathrm{MF}} = \Sigma_{\mathrm{S}} + \beta\tilde{U}' \quad (\geq 0?)$$

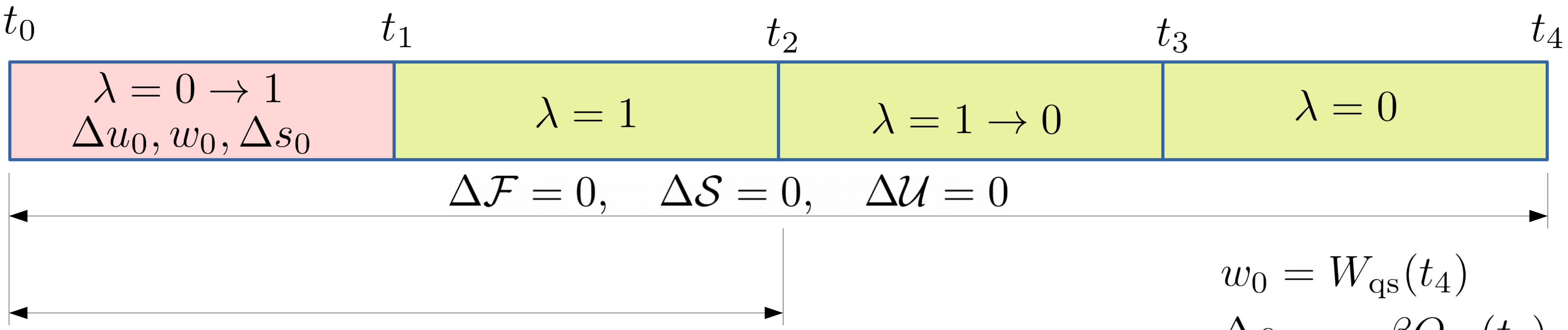
Designing experiments



$$\lambda(t) = \begin{cases} \text{slowly turn on the coupling for } \lambda_1 \text{ and } 0 \text{ for } \lambda_2 & t_1 > t > t_0 \\ \text{keep the coupling constant} & t_2 > t > t_1 \\ \text{slowly turn off the coupling} & t_3 > t > t_2 \\ \text{keep the coupling off} & t_4 > t > t_3 \end{cases}$$


measurement
Relaxation of
No-equilibrium
Initial state
t_0
t_1
t_2
t_3
t_4
$\lambda = 0 \to 1$
$\Delta u_0, w_0, \Delta s_0$
$\lambda = 1$
$\lambda = 1 \to 0$
$\lambda = 0$
$Q_{\rm qs}(t_2), W_{\rm qs}(t_2)$
$Q_{\rm qs}(t_4), W_{\rm qs}(t_4)$
t_0
t_1
t_2
t_3
t_4
$\lambda = 0$
$\lambda = 1$
$\lambda = 1 \to 0$
$\lambda = 0$
$\Sigma(t)$
$Q(t_2), W(t_2)$
$Q(t_4), W(t_4)$

Protocol 1 (quasi static)

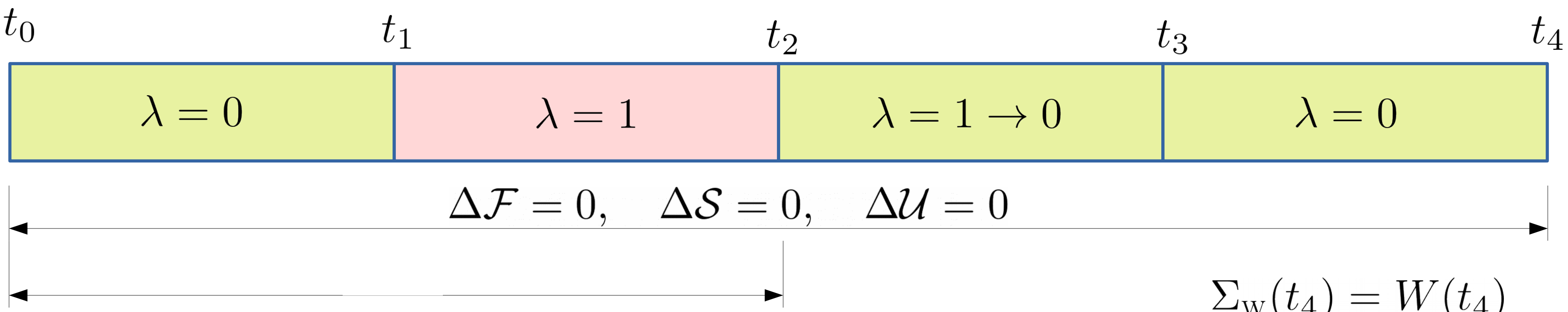


$$w_0 = W_{\mathrm{qs}}(t_4)$$
$$\Delta s_0 = -\beta Q_{\mathrm{qs}}(t_4)$$
$$\Delta u_0 = \Delta U_{\mathrm{qs}}(t_4)$$

$$\Delta\mathcal{F} = W_{\mathrm{qs}}(t_2) - w_0$$
$$\Delta\mathcal{S} = \beta Q_{\mathrm{qs}}(t_2) + \Delta s_0$$
$$\Delta\mathcal{U} = \Delta U_{\mathrm{QS}}(t_2) - \Delta u_0$$

$$\Delta\mathcal{F} = W_{\mathrm{qs}}(t_2) - W_{\mathrm{qs}}(t_4)$$
$$\Delta\mathcal{S} = \beta \left[Q_{\mathrm{qs}}(t_2) - Q_{\mathrm{qs}}(t_4)\right]$$
$$\Delta\mathcal{U} = U_{\mathrm{qs}}(t_2) - U_{\mathrm{sc}}(t_4)$$

Protocol 2 (Relaxation)



$$\Sigma_{\mathrm{W}}(t_4) = W(t_4)$$

$$\Sigma_{\mathrm{Q}}(t_4) = -\beta Q(t_4)$$

$$\begin{aligned}
\Sigma_{\mathrm{W}}(t_2) &= W(t_2) - \Delta\mathcal{F} \\
&= W(t_2) - W_{\mathrm{qs}}(t_2) + W_{\mathrm{qs}}(t_4) \\
\Sigma_{\mathrm{Q}}(t_2) &= \Delta\mathcal{S} - \beta Q(t_2) \\
&= \beta\left[Q(t_2) - Q_{\mathrm{qs}}(t_2) + Q_{\mathrm{qs}}(t_4)\right]
\end{aligned}$$

Various expression of entropy production

Experimental

$$\Sigma_{\mathrm{W}}(t) = W(t) - W_{\mathrm{qs}}(t) + W_{\mathrm{qs}}(t_4)$$

$$\Sigma_{\mathrm{Q}}(t) = \beta\left[Q(t) - Q_{\mathrm{qs}}(t) + Q_{\mathrm{qs}}(t_4)\right]$$

Theoretical

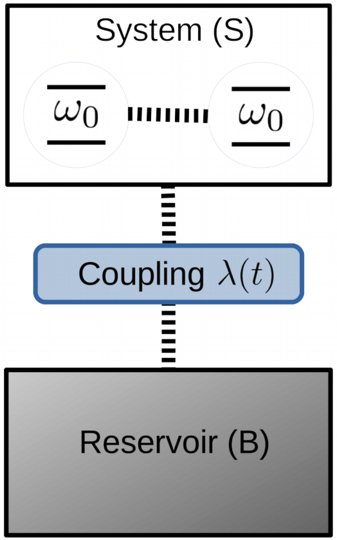
$$\Sigma_{\mathrm{S}}(t) = \Delta S_{\mathrm{S}}(t) - \beta Q(t)$$

Ad hoc correction

$$\Sigma_{\mathrm{QV}}(t) = \Sigma_{\mathrm{Q}} + \frac{\beta}{2}\left[V_{\mathrm{I}}(t) - V_{\mathrm{I}}^{\mathrm{qs}}(t)\right]]$$

$$\Sigma_{\mathrm{SV}}(t) = \Sigma_{\mathrm{S}} + \frac{\beta}{2}\Delta V_{\mathrm{I}}(t)$$

Spin-Boson Model



$$H_{\mathrm{SB}} = H_{\mathrm{S}} + H_{\mathrm{B}} + \lambda(t) H_{\mathrm{I}}, \qquad 1 \geq \lambda(t) \geq 0$$

$$H_{\mathrm{S}} = \frac{\omega_0}{2}\sigma_z \otimes I + \frac{\omega_0}{2} I \otimes \sigma_z + \Lambda(\sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+)$$

$$H_{\mathrm{B}} = \sum_{j\geq 1} \omega_j a_j^\dagger a_j$$

$$H_{\mathrm{I}}(t) = \lambda(t)\, X_{\mathrm{S}} \otimes Y_{\mathrm{B}}.$$

$$Y_{\mathrm{B}} = \sum_j \nu_j \left(a_j^\dagger + a_j \right), \qquad J(\omega) = \frac{2\kappa}{\pi} \frac{\omega\gamma}{\omega^2 + \gamma^2}$$

$$X_{\mathrm{S}} = H_{\mathrm{S}} \text{ and } \sigma_x \otimes I + I \otimes \sigma_x$$

Computation

$$\mathrm{tr}_{\mathrm{B}}\left\{\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{SB}} = -i[H_{\mathrm{SB}}, \rho_{\mathrm{SB}}]\right\} \quad \rightarrow \quad \boxed{\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}} = -i[H_{{\mathrm{S}}, \rho_{\mathrm{S}}}] - i\lambda(t)[X_{\mathrm{S}}, \eta_{\mathrm{S}}] \\ \text{where } \eta_{\mathrm{S}} = \mathrm{tr}_{\mathrm{B}}\{Y_{\mathrm{B}}\rho_{\mathrm{SB}}\}\end{aligned}}$$

$$W(t) = \int_{t_0}^{t} \dot{\lambda}(\tau)\,\mathrm{tr}_{\mathrm{S}}\{X_{\mathrm{S}}\eta_{\mathrm{S}}(\tau)\}\,\mathrm{d}\tau\,,$$

$$Q(t) = \int_{t_0}^{t} [\mathrm{tr}_{\mathrm{S}}\{H_{\mathrm{S}}\dot{\rho}_{\mathrm{S}}(\tau)\} + \lambda(\tau)\,\mathrm{tr}_{\mathrm{S}}\{X_{\mathrm{S}}\dot{\eta}_{\mathrm{S}}(\tau)\}]\,\mathrm{d}\tau$$

$$V_{\mathrm{I}}(t) = \lambda(t)\,\mathrm{tr}_{\mathrm{S}}\{X_{\mathrm{S}}\eta_{\mathrm{S}}(t)\}$$

$$\begin{aligned} C_{\mathrm{SB}}(t) &\equiv \langle X_{\mathrm{S}} \otimes Y_{\mathrm{B}}\rangle - \langle X_{\mathrm{S}}\rangle\langle Y_{\mathrm{B}}\rangle \\ &= \mathrm{tr}_{\mathrm{S}}\{X_{\mathrm{S}}\eta_{\mathrm{S}}(t)\} - \mathrm{tr}_{\mathrm{S}}\{X_{\mathrm{S}}\rho_{\mathrm{S}}(t)\}\cdot\mathrm{tr}_{\mathrm{S}}\{\eta_{\mathrm{S}}(t)\}\,. \end{aligned}$$

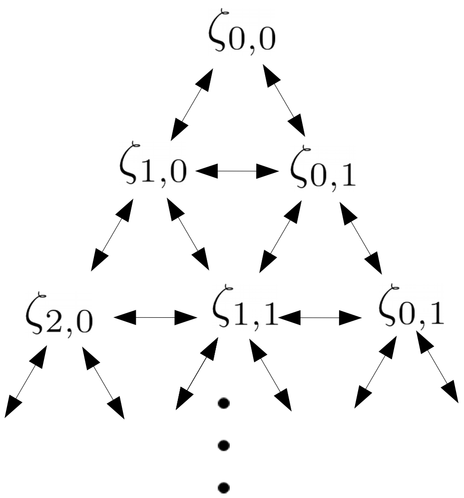
Hierarchical Equations of Motion (HEOM)

Non-equilibrium initial state $\rho_{\mathrm{SB}}(t_0) = \rho_{\mathrm{S}}(t_0) \otimes e^{-\beta H_{\mathrm{B}}}/Z_{\mathrm{B}}$

Environment correlation $\langle Y_{\mathrm{B}}(\tau) Y_{\mathrm{B}}(0)\rangle \approx \left(c_1 e^{-\gamma_1 \tau} + c_2 e^{-\gamma_2 \tau} + 2c_0 \delta(\tau)\right)$

$$\zeta_{n,m} = \text{auxiliary operators} \in \mathcal{H}_{\mathrm{S}}$$

HEOM



$$\frac{\mathrm{d}}{\mathrm{d}t}\zeta_{n_1,n_2}(t) = -i[H_{\mathrm{S}}, \zeta_{n1,n2}]_{-}$$
$$-(\gamma_1 n_1 + \gamma_2 n_2)\zeta_{n1,n2}(t) - \lambda c_0 \lambda^2(t)\mathcal{S}^{-}\mathcal{S}^{-}\,\zeta_{n1,n2}(t)$$
$$-in_1\lambda(t)\mathcal{G}_1\,\zeta_{n_1-1,n_2}(t) - in_2\lambda(t)\mathcal{G}_2\,\zeta_{n_1,n_2-1}(t)$$
$$-i\lambda(t)\mathcal{S}^{-}\left\{\zeta_{n_1+1,n_2}(t) + \zeta_{n1,n2+1}(t)\right\}$$

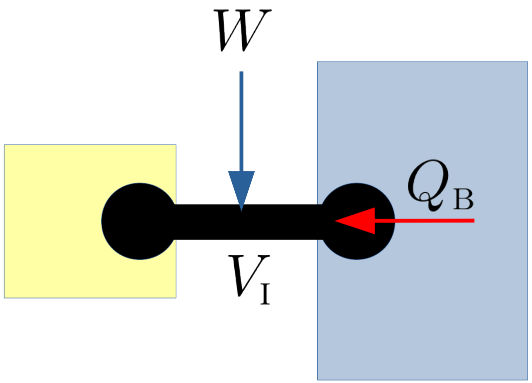
$$\text{where } \mathcal{S}^{\pm} = [X_{\mathrm{S}}, \cdot]_{\pm}, \quad \mathcal{G}_j = \mathrm{Re}\{c_j\}\mathcal{S}^{-} + i\,\mathrm{Im}\{c_j\}\mathcal{S}^{+}$$

Depth = 50
\# of ζ =1326

$$\rho_{\mathrm{S}} = \zeta_{0,0}, \qquad \eta_{\mathrm{S}} = \lambda(t)\left(\zeta_{1,0} + \zeta_{0,1}\right) + ic_0\mathcal{S}^{-}\zeta_{0,0}$$

Choice of X_S in $H_I = \lambda(t) X_S \otimes Y_B$

Extreme case: $X_S = H_S \rightarrow [H_S, H_{SB}] = 0 \rightarrow \Delta U = 0$



Diagonal elements of $\rho_S(t)$ in energy basis conserves but not off-diagonal elements

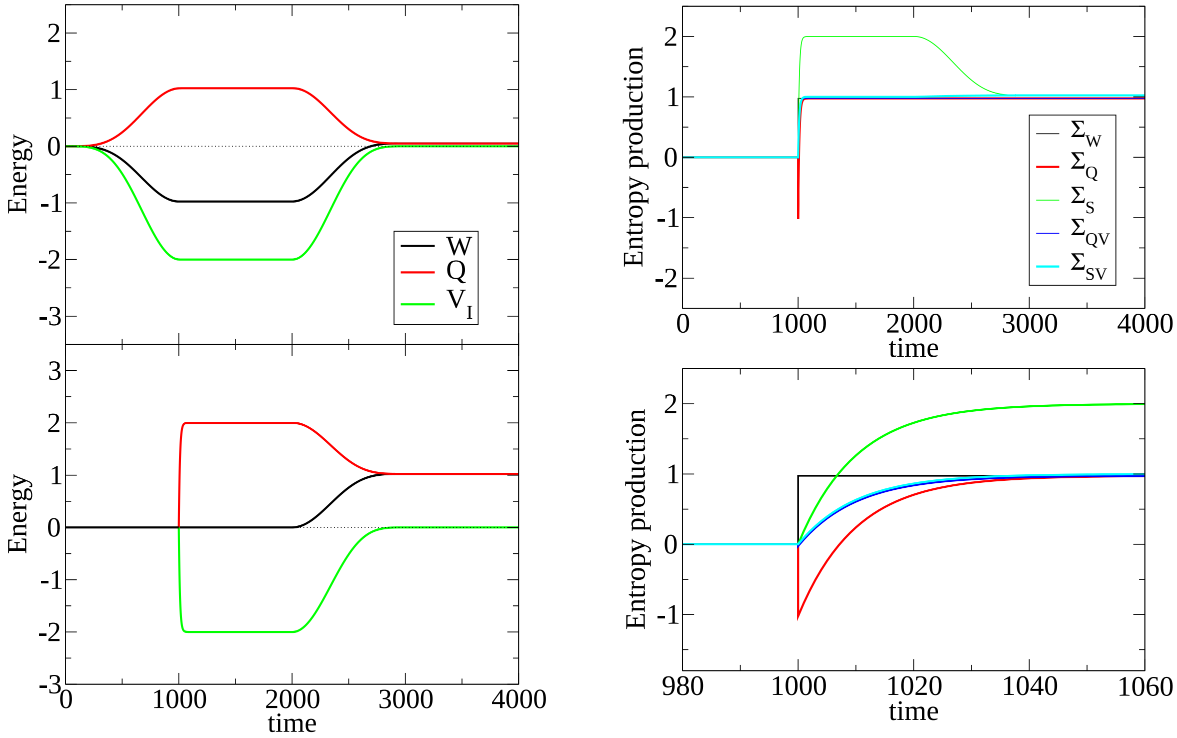
Dissipation takes place outside the system

A less extreme case: $X_S = \sigma_x \otimes I + I \otimes \sigma_x$

Decoherence free state: $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$

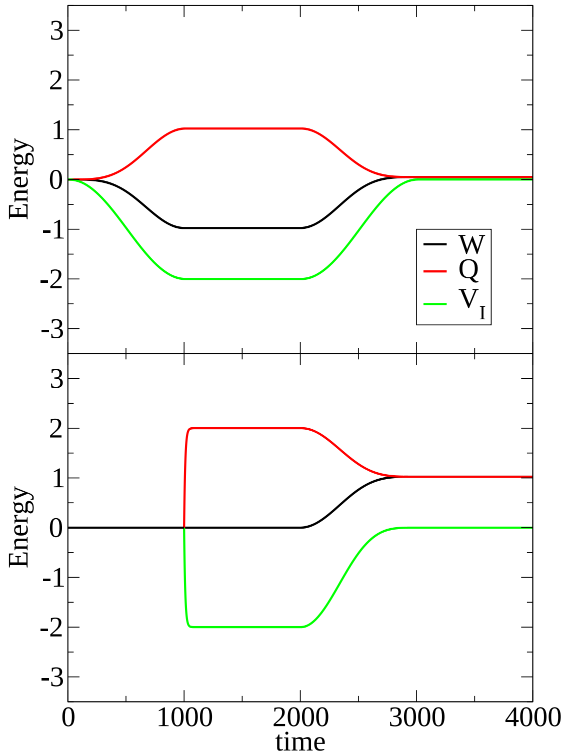
Final steady state ≠ conventional canonical equilibrium

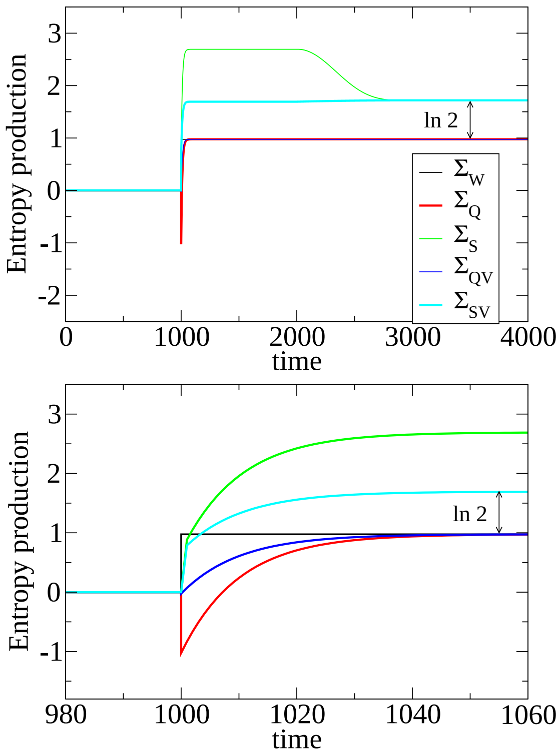
Case I: $X_{\mathrm{S}} = H_{\mathrm{S}}$ $\rho_{\mathrm{S}}(t_0) = |00\rangle\langle 00|$



- $\rho_{\mathrm{S}}(t) = \rho_{\mathrm{S}}(t_0)$
- Pure state
- Diagonal in energy basis
- No correlation with environment

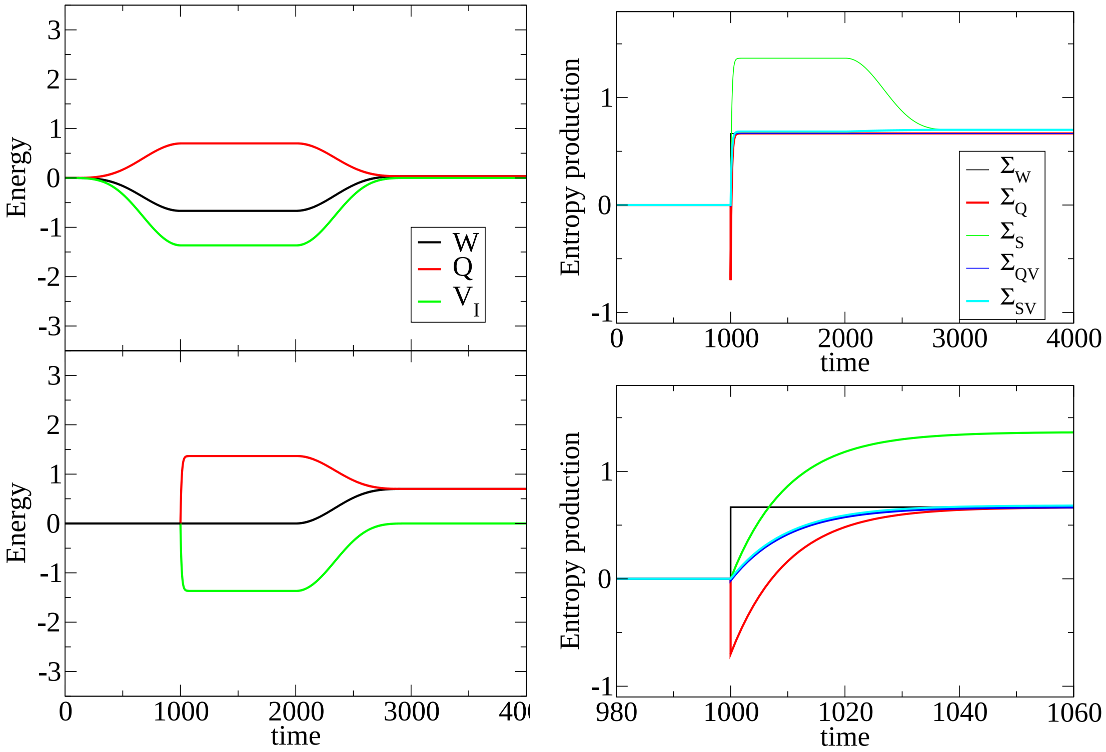
Case II: $X_S = H_S$, $|\psi(t_0)\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$





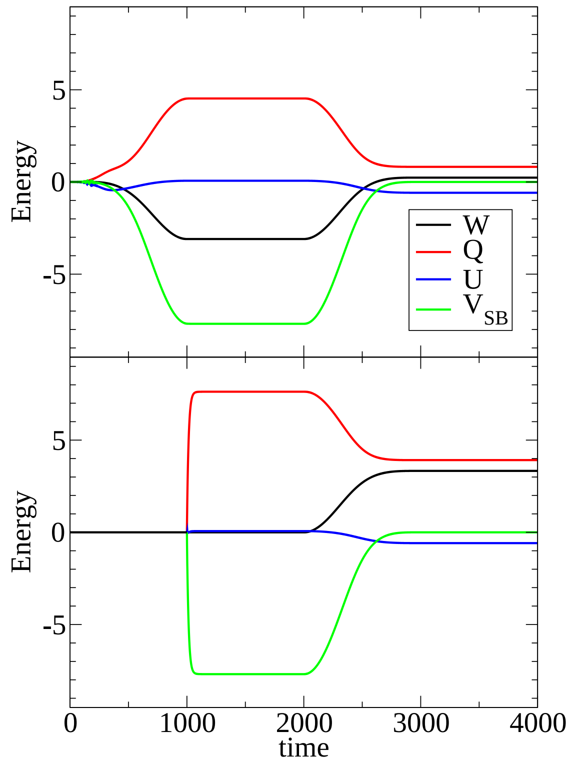
- $\rho_S(t) \neq \rho_S(t_0)$
- Pure state
- Not diagonal in energy basis
- Entanglement with environment
- Decoherence

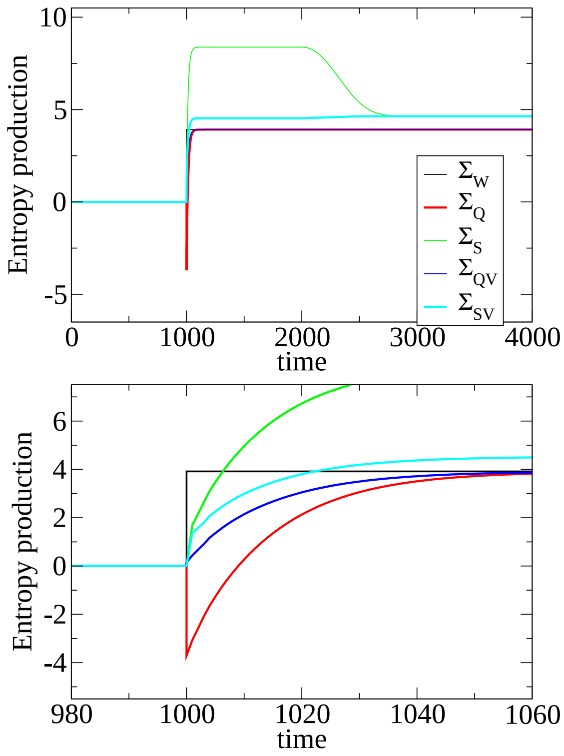
Case III: $X_{\rm S} = H_{\rm S}$, $\rho_{\rm S}(t_0) = e^{-\beta H_{\rm S}}/Z_{\rm S}$



- $\rho_{\rm S}(t) = \rho_{\rm S}(t_0)$
- Mixed state
- Diagonal in energy basis
- Classical correlation with environment
- Decoherence

Case IV: $X_S = \sigma_x \otimes I + I \otimes \sigma_x, \quad |\psi(t_0)\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$





Decoherence free state

$$|\psi(t_0)\rangle = \frac{1}{\sqrt{2}}(|01 - |10\rangle)$$

Partial thermalization

Dissipation due to decoherence

Conclusions

Empirical Thermodynamic Laws for systems with strong coupling

$$\widetilde{U} = U + V_{\mathrm{I}}$$

$$\widetilde{S} = S_{\mathrm{S}} + \frac{\beta}{2} V_{\mathrm{I}} \qquad \widetilde{F} = F + \frac{1}{2} V_{\mathrm{I}}$$

$$\widetilde{Q} = Q \qquad \widetilde{W} = W$$

1st law: $\widetilde{W} + \widetilde{Q} = \Delta \widetilde{U}$

$$(W + Q = \Delta U + \Delta V_{\mathrm{I}})$$

2nd law: $\widetilde{\Sigma} = \widetilde{S}_{\mathrm{S}} - \beta \widetilde{Q} \quad (\geq 0?)$

$$= S_{\mathrm{S}} - \beta Q + \frac{\beta}{2} V_{\mathrm{I}}$$

Mean Force Theory

$$\tilde{U}' = \tilde{U}'' = \frac{1}{2} V_{\mathrm{I}}$$

$$\tilde{U} = U + \tilde{U}' + \tilde{U}''$$

$$\tilde{S}_{\mathrm{S}} = S_{\mathrm{S}} + \beta \tilde{U}''$$

$$\tilde{F} = F + \tilde{U}'$$

$$\tilde{W} = W$$

$$\tilde{Q} = Q - \Delta V_{\mathrm{I}} + \tilde{U}' + \Delta \tilde{U}''$$

Professors Eddington and Einstein,

I hope you tell me if I collapsed in deepest humiliation.