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

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Sir Arthur Eddington

“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

“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)
When a system strongly interacts with environments, is the second law correct?

\[ \Delta S \geq \frac{Q}{T} \]

correct?
Thermal Equilibrium - Why is the Gibbs state so special?

Maximum entropy principle

\[ S[\rho] = - \text{tr}(\rho \ln \rho) \]

\[ E = \text{tr}(\rho H) = \text{tr}(\rho_G H) \]

\[ \rho_G = e^{-\beta H} / \text{tr} e^{-\beta H} \]

\[ S[\rho_G] - S[\rho] = S[\rho \| \rho_G] \geq 0 \]

Unitary evolution

\[ \partial_t S[\rho \| \rho_G] = 0 \]

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

\[ \frac{d}{dt} \rho = -i[H, \rho] \quad H = H_S \otimes I + I \otimes H_B + \lambda X_S \otimes Y_B \]

Reduced system

\[ \frac{d}{dt} \rho_S = -i[H_S, \rho_S] - i\lambda [X_S, \eta_S], \quad \eta_S = \text{tr}_B (Y_B \rho) \quad \rho_S = \text{tr}_B \rho \]

\[ \frac{d}{dt} \rho_S = -i[H_S, \rho_S] - i\lambda [X_S, \eta_S], \quad \lambda \ll 1 \quad \text{Diagonal in energy basis} \]

\[ \frac{d}{dt} \rho_S = -i[H_S, \rho_S] - i\lambda [X_S, \eta_S], \quad \lambda \gg 1 \quad \text{Diagonal in pointer basis} \]
Measurement = Decoherence in observable basis

\[ |\psi_S\rangle = \sum_i c_i |\omega_i\rangle \]

\[ \hat{\Omega} |\omega_i\rangle = \omega_i |\omega_i\rangle \]

before measurement

\[ \rho_\prec = \sum_{ij} c_i c_j^\ast |\omega_i\rangle\langle\omega_j| \quad \Rightarrow \quad \rho = \sum_i |c_i|^2 |\omega_i\rangle\langle\omega_i| = \sum_i |\omega_i\rangle\langle\omega_i| \rho_\prec |\omega_i\rangle\langle\omega_i| \]

after measurement

Continuous measurement by environment

\[ \rho \quad \rightarrow \quad \sum_j |e_j\rangle\langle e_j| \rho_G |e_j\rangle\langle e_j| \quad \lambda \ll 1 \quad |e_j\rangle = \text{energy basis} \]

\[ \rho \quad \rightarrow \quad \sum_j |\pi_j\rangle\langle\pi_j| \rho_G |\pi_j\rangle\langle\pi_j| \quad \lambda \gg 1 \quad |\pi_j\rangle = \text{pointer basis} \]
Energy basis

- $\rho_{11}$
- $\rho_{22}$
- $\rho_{33}$
- $\rho_{44}$

- $\rho_{12}$
- $\rho_{13}$
- $\rho_{23}$
- $\rho_{24}$
- $\rho_{34}$

-指针限制

heat conduction

- $\lambda_1=1.55$
- $\lambda_2=1.05$
- $\lambda_3=0.55$
- $\lambda_4=0.10$
System (S) and Environment (B)

**Weak coupling**

- System (S) and Environment (B) are separable.
- Thermodynamics concerns only S.
- Equilibrium: $\rho_S = e^{-\beta H_S}/Z_S$
- Maximum entropy principle:
  $(\max S(\rho_s), \text{tr}\{\rho_s H_S\} = E)$

**Strong coupling**

- System (S) and Environment (B) are not well separated.
  ($V_I$ belongs to both S and B)
- Maximum entropy?
- Extremely strong coupling:
  - Equilibrium: diagonal in pointer basis
  - Quantum Zeno effects
The laws of thermodynamics determine the energy transaction between the system and its exterior  \textit{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.
- 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
Hamiltonian of Mean Force


Equilibrium

\[ \rho_{SB} = \frac{e^{-\beta H_S}}{Z_S} \otimes \frac{e^{-\beta H_B}}{Z_B} \]

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

Effective System Hamiltonian

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

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

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

\[ \tilde{U} = U + \tilde{U}' + \tilde{U}'' \]

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

\[ \tilde{F} = F + \tilde{U}' \]

\[ \tilde{W} = W \]

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

Conventional Thermodynamics

\[ \Delta F \geq W \]
\[ \Delta S \geq \beta Q \]

Equilibrium 1
\[ F_0, S_0, U_0, \ldots \]

Equilibrium 2
\[ F_1, S_1, U_1, \ldots \]

\[ \Delta F = W_{\text{rev}} \]
\[ \Delta S = \beta Q_{\text{rev}} \]

Beyond conventional thermodynamics

Non-Equilibrium

Equilibrium
\[ F_1, S_1, U_1, \ldots \]

\[ W \]
\[ Q \]
\[ Q_{\text{rev}} \]

Equilibrium
\[ F_0, S_0, U_0, \ldots \]
Measurable Quantities

Internal energy
\[ U(t) = \text{tr}_S \{ \rho_s(t) H_S \} \]

Work = energy injected into the whole system by a “classical external agent”
= change of the total energy
\[ W(t) = \text{tr}_{SB} \{ \rho_{SB}(t) H_{SB} \} - \text{tr}_{SB} \{ \rho_{SB}(t_0) H_{SB} \} \]

Heat = energy released from the environment
\[ Q(t) = \text{tr}_B \{ \rho_B(t_0) H_B \} - \text{tr}_B \{ \rho_B(t) H_B \} \]

Coupling energy
\[ V_1(t) = \lambda(t) \text{tr}_{SB} \{ \rho_{SB}(t) H_I \} \]

Energy conservation law:
\[ W(t) + Q(t) = \Delta U(t) + \Delta V_1(t) \quad 1^{\text{st}} \text{law?} \]
2\textsuperscript{nd} law and Entropy Production

**Thermodynamics**

\[ \Sigma_Q = \Delta S - \beta Q \geq 0 \]
\[ \Sigma_W = \beta (W - \Delta F) \geq 0 \]

**Non-equilibrium statistical mechanics**

\[ \Sigma_S = \Delta S_s - \beta Q \geq 0, \quad S_s = - \text{tr}_s \rho_s \ln \rho_s \]
\[ \Sigma_{MF} = \Sigma_S + \beta \tilde{U}' \quad (\geq 0?) \]
Designing experiments

\[ \lambda(t) = \begin{cases} 
\text{slowly turn on the coupling for } \lambda_1 \text{ and 0 for } \lambda_2 & t_1 > t > t_0 \\
\text{keep the coupling constant} & t_2 > t > t_1 \\
\text{slowly turn off the coupling} & t_3 > t > t_2 \\
\text{keep the coupling off} & t_4 > t > t_3 
\end{cases} \]
Relaxation of No-equilibrium Initial state

\[
\begin{align*}
\lambda = 0 & \rightarrow 1 \\
\Delta u_0, w_0, \Delta s_0
\end{align*}
\]

\[
\begin{align*}
\lambda = 1 \\
\lambda = 1 \rightarrow 0 \\
\lambda = 0
\end{align*}
\]

\[
\begin{align*}
Q_{qs}(t_2), W_{qs}(t_2) \\
Q_{qs}(t_4), W_{qs}(t_4)
\end{align*}
\]
Protocol 1 (quasi static)

\[\begin{array}{|c|c|c|c|}
\hline
&t_0& t_1& t_2& t_3& t_4 \\
\hline
\lambda &= 0 \rightarrow 1 & \lambda &= 1 & \lambda &= 1 \rightarrow 0 & \lambda &= 0 \\
\Delta u_0, w_0, \Delta s_0 & & \Delta \mathcal{F} = 0, \quad \Delta \mathcal{S} = 0, \quad \Delta \mathcal{U} = 0 & & \\
\hline
\end{array} \]

\[\begin{align*}
\Delta \mathcal{F} &= W_{qs}(t_2) - w_0 \\
\Delta \mathcal{S} &= \beta Q_{qs}(t_2) + \Delta s_0 \\
\Delta \mathcal{U} &= \Delta U_{qs}(t_2) - \Delta u_0 \\
\end{align*}\]

\[\begin{align*}
\Delta \mathcal{F} &= W_{qs}(t_2) - W_{qs}(t_4) \\
\Delta \mathcal{S} &= \beta [Q_{qs}(t_2) - Q_{qs}(t_4)] \\
\Delta \mathcal{U} &= U_{qs}(t_2) - U_{sc}(t_4) \\
\end{align*}\]
Protocol 2 (Relaxation)

\[ \Delta F = 0, \quad \Delta S = 0, \quad \Delta U = 0 \]

\[ \Sigma_w(t_2) = W(t_2) - \Delta F \]
\[ = W(t_2) - W_{qs}(t_2) + W_{qs}(t_4) \]

\[ \Sigma_Q(t_2) = \Delta S - \beta Q(t_2) \]
\[ = \beta [Q(t_2) - Q_{qs}(t_2) + Q_{qs}(t_4)] \]

\[ \Sigma_w(t_4) = W(t_4) \]
\[ \Sigma_Q(t_4) = -\beta Q(t_4) \]
Various expression of entropy production

Experimental\[ \Sigma_W(t) = W(t) - W_{qs}(t) + W_{qs}(t_4) \]

\[ \Sigma_Q(t) = \beta [Q(t) - Q_{qs}(t) + Q_{qs}(t_4)] \]

Theoretical\[ \Sigma_S(t) = \Delta S_s(t) - \beta Q(t) \]

*Ad hoc* correction\[ \Sigma_{QV}(t) = \Sigma_Q + \frac{\beta}{2} [V_1(t) - V_1^{qs}(t)] \]

\[ \Sigma_{SV}(t) = \Sigma_S + \frac{\beta}{2} \Delta V_1(t) \]
Spin-Boson Model

\[ H_{SB} = H_S + H_B + \lambda(t)H_1, \quad 1 \geq \lambda(t) \geq 0 \]

\[ H_S = \frac{\omega_0}{2} \sigma_z \otimes I + \frac{\omega_0}{2} I \otimes \sigma_z + \Lambda(\sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+) \]

\[ H_B = \sum_{j \geq 1} \omega_j a_j^\dagger a_j \]

\[ H_1(t) = \lambda(t) X_S \otimes Y_B. \]

\[ Y_B = \sum_j \nu_j \left( a_j^\dagger + a_j \right), \quad J(\omega) = \frac{2\kappa}{\pi} \frac{\omega \gamma}{\omega^2 + \gamma^2} \]

\[ X_S = H_S \text{ and } \sigma_x \otimes I + I \otimes \sigma_x \]
Computation

\[
\text{tr}_B \left\{ \frac{d}{dt} \rho_{SB} = -i[H_{SB}, \rho_{SB}] \right\} \quad \Rightarrow \quad \frac{d}{dt} \rho_S = -i[H_s, \rho_S] - i\lambda(t)[X_s, \eta_s]
\]

where \( \eta_s = \text{tr}_B \{ Y_B \rho_{SB} \} \)

\[
W(t) = \int_{t_0}^{t} \lambda(\tau) \text{tr}_S \{ X_s \eta_s(\tau) \} \, d\tau
\]

\[
Q(t) = \int_{t_0}^{t} \left[ \text{tr}_S \{ H_s \rho_s(\tau) \} + \lambda(\tau) \text{tr}_S \{ X_s \eta_s(\tau) \} \right] \, d\tau
\]

\[
V_1(t) = \lambda(t) \text{tr}_S \{ X_s \eta_s(t) \}
\]

\[
C_{SB}(t) \equiv \langle X_s \otimes Y_B \rangle - \langle X_s \rangle \langle Y_B \rangle = \text{tr}_S \{ X_s \eta_s(t) \} - \text{tr}_S \{ X_s \rho_s(t) \} \cdot \text{tr}_S \{ \eta_s(t) \}.
\]
Hierarchical Equations of Motion (HEOM)

Non-equilibrium initial state

\[ \rho_{SB}(t_0) = \rho_S(t_0) \otimes e^{-\beta H_B} / Z_B \]

Environment correlation

\[ \langle Y_B(\tau) Y_B(0) \rangle \approx (c_1 e^{-\gamma_1 \tau} + c_2 e^{-\gamma_2 \tau} + 2c_0 \delta(\tau)) \]

\[ \zeta_{n,m} = \text{auxiliary operators } \in \mathcal{H}_S \]

\[ \frac{d}{dt} \zeta_{n_1,n_2}(t) = -i[H_S, \zeta_{n_1,n_2}] - \]

\[ - (\gamma_1 n_1 + \gamma_2 n_2) \zeta_{n_1,n_2}(t) - \lambda c_0 \lambda^2(t) S^- S^- \zeta_{n_1,n_2}(t) \]

\[ - i n_1 \lambda(t) g_1 \zeta_{n_1-1,n_2}(t) - i n_2 \lambda(t) g_2 \zeta_{n_1,n_2-1}(t) \]

\[ - i \lambda(t) S^- \{ \zeta_{n_1+1,n_2}(t) + \zeta_{n_1,n_2+1}(t) \} \]

where \[ S^\pm = [X_S, \cdot]_\pm, \quad g_j = \text{Re}\{c_j\} S^- + i \text{Im}\{c_j\} S^+ \]

\[ \rho_s = \zeta_{0,0}, \quad \eta_s = \lambda(t) (\zeta_{1,0} + \zeta_{0,1}) + ic_0 S^- \zeta_{0,0} \]
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: $X_S = H_S$  \[ \rho_S(t_0) = |00\rangle\langle 00| \]

- $\rho_S(t) = \rho_S(t_0)$
- 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: \( X_S = H_S \), \( \rho_S(t_0) = e^{-\beta H_S}/Z_S \)

- \( \rho_S(t) = \rho_S(t_0) \)
- Mixed state
- Diagonal in energy basis
- Classical correlation with environment
- Decoherence
Case IV: $X_S = \sigma_x \otimes I + I \otimes \sigma_x$, $|\psi(t_0)\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$

**Decoherence free state**

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

**Partial thermalization**

**Dissipation due to decoherence**
Empirical Thermodynamic Laws for systems with strong coupling

\[ \tilde{U} = U + V_1 \]

\[ \tilde{S} = S_s + \frac{\beta}{2} V_1 \quad \tilde{F} = F + \frac{1}{2} V_1 \]

\[ \tilde{Q} = Q \quad \tilde{W} = W \]

1\textsuperscript{st} law: \[ \tilde{W} + \tilde{Q} = \Delta \tilde{U} \]

\[ (W + Q = \Delta U + \Delta V_1) \]

2\textsuperscript{nd} law: \[ \tilde{\Sigma} = \tilde{S}_s - \beta \tilde{Q} \quad (\geq 0?) \]

\[ = S_s - \beta Q + \frac{\beta}{2} V_1 \]

Mean Force Theory

\[ \tilde{U}' = \tilde{U}'' = \frac{1}{2} V_1 \]

\[ \tilde{U} = U + \tilde{U}' + \tilde{U}'' \]

\[ \tilde{S}_s = S_s + \beta \tilde{U}'' \]

\[ \tilde{F} = F + \tilde{U}' \]

\[ \tilde{W} = W \]

\[ \tilde{Q} = Q - \Delta V_1 + \tilde{U}' + \Delta \tilde{U}'' \]
Professors Eddington and Einstein,

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