Quantum Thermo 1

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Based on M. Moro... & T. Oppenheim
Nat. Comm. 4, 2059, 2013

Quantum Thermodynamics: A resource theoretic perspective.

Classical / variant of 2nd Law.

Free energy $F(\rho) = E(\rho) - TS(\rho)$

System V, T

Only thermodynamical transformation that are allowed are s.t.

$$F(\rho) \geq F(\sigma) \quad \text{iff} \quad \rho \to \sigma.$$

One can calculate macroscopic work by ~~on on system by~~

$$F(\rho) - F(\sigma) \geq 0 \Rightarrow$$ Work has been extracted from the system.

e.g. for no energy exchange by work etc, this becomes entropy.

Micro-machines

(1) Three level MASERS or heat engines, PRL, 2, 262 (1959).

(2) Molecular Motors

Nature 389, 561-567 (1997)

* One can use QM to justify statistical physics.

Entanglement & foundation of stat phys.

Nature 474, 61-63 (2011)

start with a typicality argument on pure states & you'll have the bath & the sys. are entangled.

Q1: $\rho \xrightarrow[\text{operation}]{\text{Thermodynamical}} \sigma$

Observation: $F(\rho) - F(\tau) = \beta^{-1} D(\rho \| \tau)$

$$\tau = \frac{e^{-\beta H}}{Z}$$

Proof: $\text{LHS} = E(\rho) - TS(\rho) - E(\tau) - TS(\tau)$

$$S(\tau) = -\operatorname{tr}\left(\tau \ln \frac{e^{-\beta H}}{Z}\right) = -\operatorname{tr}(\tau(-\beta H)) + \ln Z$$

$$= \beta E(\tau) + \ln Z$$

$$\Rightarrow \beta(E(\tau) - TS(\tau)) = \ln Z.$$

$$\text{LHS} = E(\rho) - TS(\rho) + \beta^{-1} \ln Z$$

$$= -TS(\rho) + \beta^{-1} \ln Z + \beta^{-1} \operatorname{tr}(\rho H \beta)$$

$$= -TS(\rho) + \beta^{-1} \ln Z - \beta^{-1} \operatorname{tr}(\rho \ln(e^{-\beta H}))$$

$$= -TS(\rho) - \beta^{-1} \operatorname{tr}\left(\rho \ln\left(\frac{e^{-\beta H}}{Z}\right)\right)$$

$$= -TS(\rho) - \beta^{-1} \mathrm{tr}\left(\rho \ln \left(\frac{e^{-\beta H}}{Z}\right)\right)$$

$$= T\left[-S(\rho) - \mathrm{tr}(\rho \ln Z)\right]$$

$$= T\, D(\rho \| \tau)$$

macroscopic still; reasonable.

★ Model:

System S

$H_S \in \mathcal{H}_S$

$$H_S = \sum_{g_S E_S} E_S \, |E_S, g_S\rangle\langle E_S, g_S|$$

(Reservoir) Bath $(T = \beta^{-1})$

↳ Fixed

↳ Large

$H_R \in \mathcal{H}_R$

$$\tau_R = \frac{e^{-\beta H_R}}{Z}$$

Operations we can perform

(i) Energy conserving unitaries (V_{RS})

↳ $[V_{RS}, H_R + H_S] = 0$

(ii) We can bring additional system in thermal state at some β (zeroth law).

(iii) Partial tracing

set I

Def^n: Thermal op^n

$$\phi_{Th}(\rho_S) = \mathrm{tr}_R\left[V_{RS}(\tau_R \otimes \rho_S) V_R^{+}\right] \quad \text{set II}$$

$$[V_{RS}, H_R + H_S] = 0$$

NB. set I & set II are equivalent. | ie. set of allowed operations ⟺ thermal operations

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Question: $\rho \xrightarrow[\text{operation}]{\text{thermal}} \sigma$

Results:

Theorem 1: Consider two block diagonal states (in the energy basis) ρ_S & σ_S of system S.

Then the transition $(\rho_S, H_S) \longrightarrow (\sigma_S, H_S)$ under thermal operation is possible

iff
$$\bigoplus_{E_S} \eta_{E-E_S} \otimes P_{E_S} \rho_S P_{E_S} \succ \bigoplus_{E_S} \eta_{E-E_S} \otimes \sigma_S .$$
⟹ For system only its called Thermo-majoriz^n.

$$\eta_{E-E_S} = \frac{\mathbb{1}_{E-E_S}}{g_R(E-E_S)}$$

| E = total energy

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$\mathrm{tr}(E_S + \ldots$ [illegible]

$P_{E_S} = \sum |E_S \ldots\rangle\langle E_S \ldots|$ [illegible]

$$\eta_{E-E_S} = \frac{\mathcal{J}_{E-E_S}}{g_R(E-E_S)}$$

$$\rho_{E_S} = \sum_g |E_S, g\rangle\langle E_S, g|$$

E = total energy $= \mathrm{tr}((H_R + H_S)(\ldots))$

$\rho \succ \sigma$: ρ majorizes σ means $\sum_i \lambda_i^\downarrow(\rho) \geq \sum \lambda_i^\downarrow(\sigma)$

Block-diagonal

$$\begin{pmatrix} (\ ) & & \\ & (\ ) & \\ & & (\ ) \end{pmatrix}$$

$$\rho = \sum_i E_i |E_i\rangle\langle E_i| = \sum_{i,g} E_i |E_i, g\rangle\langle E_i, g| = \sum_i E_i \sum_g |E_i g\rangle\langle E_i, g|$$

Lemma 1: Extractable work using thermal operations from state ρ is

$$W_{ext}(\rho) = F_{min}(\rho) - F_{min}(\tau) = \beta^{-1} D_{min}(\rho\|\tau)$$

where $F_{min}(\rho) = -\beta \ln \sum_{E_1, g} h(w, E_1, g) e^{-\beta E_i}$

$h(w, E_1, g) = 1$ if local $|E_1, g\rangle$ is populated
$= 0$ else

$w = \sum_E P_E \rho P_E$; $P_E = |E\rangle\langle E|$

$D_{min}(\rho\|\tau) = -\ln \mathrm{tr}(\Pi_w \tau)$ where Π_w is proj. on the support of w.

Lemma 2

Work of formation $\tau \to \sigma$ $= \beta^{-1} D_{max}(\sigma\|\tau)$

$D_{max}(\sigma\|\tau) = \log \min_\lambda \{\lambda : \rho \leq \lambda\tau\}$

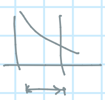
[one-shot entropy is related]

Proof of Thm 1:

(1) Assump^n on bath $0 \leq E_R \leq E_R^{max} \longrightarrow \infty$

(1a) Bath is in the Gibbs state $\tau_R = \frac{e^{-\beta H_R}}{Z}$

(1b) $\exists$ a set $\mathcal{E}_R$ s.t. $\mathrm{tr}(P_{\mathcal{E}_R} \tau) \geq 1 - \delta$



(1c) For $E \in \mathcal{E}_R$, E lie in $[\langle E\rangle - O(\sqrt{\langle E\rangle}),\ \langle E\rangle + d\sqrt{\langle E\rangle}]$

(1d) For $E \in \mathcal{E}_R$ $g_R(E) \geq e^{cE}$

(1e) For three energies E_S, E_S'; $E_R \in \mathcal{E}_R$ $\exists$ $E_R' \in \mathcal{E}_R$ s.t.
$E_R + E_S = E_R' + E_S'$

(1f) $g_R(E - E_S) \approx g_R(E) e^{-\beta E_S}$

$\epsilon_R + \epsilon_S = \epsilon_R' + \epsilon_S$

(iv) $g_R(\epsilon - \epsilon_S) \approx \underbrace{g_R(\epsilon)}_{\text{degeneracy}} e^{-\beta \epsilon_S}$

Proof:

$$H_R = \sum_{E_R} E_R \cdot \sum_{g_R(E_R)} |E_R, g_R\rangle\langle E_R, g_R|$$

$$\tau = \sum_{E_R, g_R(E)} \frac{e^{-\beta E_R}}{Z} |E_R, g_R\rangle\langle E_R, g_R|$$

$$S(E_R) = \ln g_R(E_R)$$

$$g_R(E - E_S) = e^{S(E - E_S)}$$

$$= e^{S(E) - E_S \frac{\partial S}{\partial E} + O(E_S^2)}$$

$$\approx e^{S(E)} e^{-E_S \beta} = g_R(E) e^{-\beta E_S}$$

$\beta = \frac{\partial S}{\partial E}$ (Def^n of temperature)

$\left(dE = T dS + \underbrace{P dV}_{0} \right)$ where? 0 by assump^n.

$$g_R(E - E_S) \approx g_R(E) e^{-\beta E_S}$$

Proposition: $\frac{1}{p_E} P_E^{RS} (\tau_R \otimes \rho_S) P_E^{RS} \approx \bigoplus_{E_S} \eta^R_{E - E_S} \otimes P^S_{E_S} \rho_S P^S_{E_S}$

Proof:

$$\mathcal{H}_R \otimes \mathcal{H}_S = \bigoplus_E \left(\bigoplus_{E_S} \mathcal{H}_{E - E_S} \otimes \mathcal{H}_{E_S} \right) = \bigoplus_{\underbrace{E}_{\text{energy difference}}} \left(\bigoplus_{E_S} \mathcal{H}_{E + E_S} \otimes \mathcal{H}_{E_S} \right)$$

$$E_S^{min} + E_R^{min} \leq E \leq E_S^{max} + E_R^{max}$$

$$LHS = \frac{1}{p_E} P_E^{RS} (\tau_R \otimes \rho_S) P_E^{RS}$$

$$= \frac{1}{p_E} \bigoplus_{E_S} P^R_{E - E_S} \tau_R P^R_{E - E_S} \otimes P_{E_S} \rho_S P_{E_S}$$

$$= \frac{1}{p_E} \bigoplus_{E_S} \mathbb{1}^R_{E - E_S} e^{-\beta(E - E_S)} \otimes P_{E_S} \rho_S P_{E_S}$$

$$p_E = \sum_{E_S} \underbrace{g_R(E - E_S)}_{g_R(E) \cdot e^{-\beta E_S}} \operatorname{tr}(P_{E_S} \rho_S) e^{-\beta(E - E_S)}$$

$$= g_R(E) e^{-\beta E} \sum_{E_S} \operatorname{tr}(\rho_S P_S) = g_R(E) \cdot e^{-\beta E}$$

$$LHS \approx \bigoplus_{E_S} \frac{e^{-\beta(E - E_S)}}{g_R(E) e^{-\beta E}} \mathbb{1}^R_{E - E_S} \otimes P_{E_S} \rho_S P_{E_S}$$

$$\approx \bigoplus \frac{\mathbb{1}_{E - E_S}}{g_R(E - E_S)} \otimes P_{E_S} \rho_S P_{E_S}$$

The proof: of $\overbrace{\bigoplus_E \eta_{E - E_S} \otimes P_{E_S} \rho_S P_{E_S}}^{\Omega_{RS}} > \bigoplus_{E_S} \eta_{E - E_S} \otimes \sigma_S$

$$\Updownarrow$$

$$\rho_S \xrightarrow{\text{thermal op}}$$

$\Downarrow$

$\rho_S \xrightarrow{\text{therm op}}$

if non-degen $\quad U^{\text{Energy Pres.}} |E_R, E_S\rangle = |E_R, E_S\rangle$

if degenerate $\quad U^{\text{Ener Pres}} |E_R, E_S, g_R, g_S\rangle = \underset{\text{arbitrary}}{u} |E_R, E_S, g_R, g_S\rangle$

(ii) $\rho_S^{iE} = \mathrm{tr}_R\left[U_{RS}(E)\, \Omega_{RS}\, U_{RS}(E)^\dagger\right]$

$\approx \mathrm{tr}_R \left[\sum_i p_i V_i^{RS} \Omega_{RS} V_i^{RS}\right]$

$\hookrightarrow$ random unitaries.

vis. $\quad p_i U_i \rho U_i^\dagger = \frac{\mathbb{1}}{d}$

twirling operation;

(iii) $\bigoplus_{E_S} \eta_{E-E_S} \otimes \sigma_S \approx \sum_i q_i \left(Q^{iR}_{E-E_S} \otimes \mathbb{1}^S_{E_S}\right) \sum_{E_S}\left(Q^{iR\dagger}_{E-E_S} \otimes \mathbb{1}^S_{E_S}\right)$

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(0) ρ_S

$\downarrow$ thermal op ; $\tau_R \otimes \rho_S$

(1) $\sum_i p_i U_i (\ ) U_i^\dagger$ — mixture of random unitaries

$\downarrow$

(2) $\sum_i q_i Q^i (\ ) Q^{i\dagger}$

$\downarrow$

σ_S

$\rho > \sigma \iff \sum_i p_i U_i \rho U_i^\dagger = \sigma$