(LA-UR-21-21980) **March, 2021**

Geometry of Thermal States – thermodynamics of quantum and classical coherence

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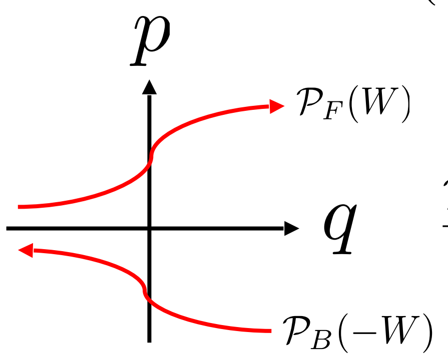
Open questions

Classical Stochastic thermodynamics

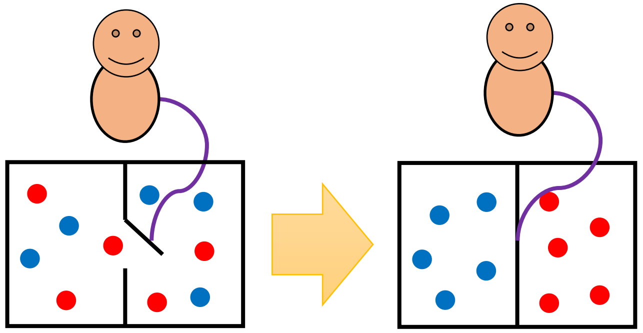
Fluctuation theorems (1990s)



$$\frac{\mathcal{P}_B(-W)}{\mathcal{P}_F(W)} = e^{-\beta(W-\Delta F)}$$

C. Jarzynski, Phys. Rev. Lett.**78**, 2690 (1997)
G. E. Crooks, Phys. Rev. E **60**, 2721 (1999)

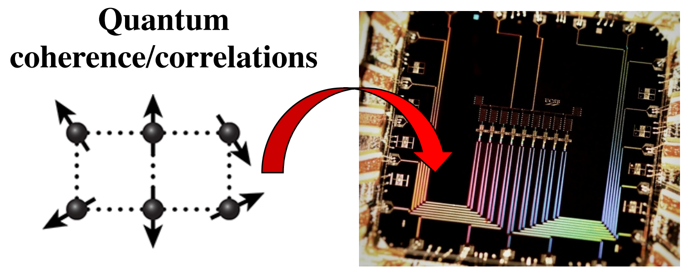
Informational thermodynamics



T. Sagawa and M. Ueda, Phys. Rev. Lett. **104**, 090602 (2010)
J. M. R. Parrondo *et al*, Nat. Phys. **11**, 131 (2015)

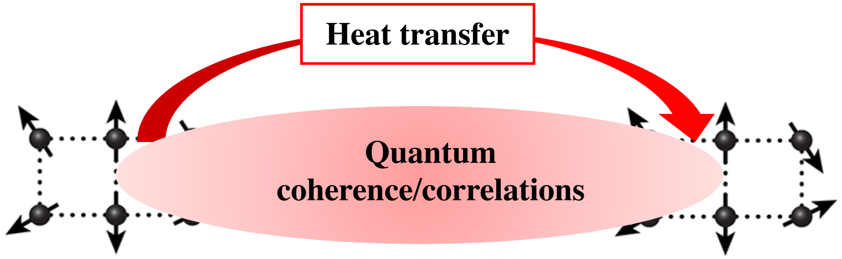
Quantum physics

Quantum Information Processing



Nielsen and Chuang (2011)

Work and Heat



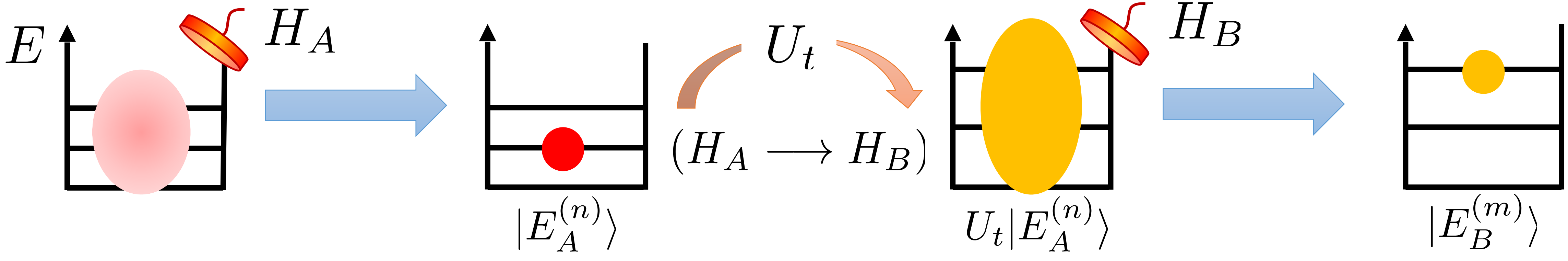
S. Lloyd et al, arXiv:1510.05035

Consistent theory
to *bridge* the classical and quantum approach?

We focus on
Second Law of Thermodynamics

Second law of thermodynamics: Quantum approach

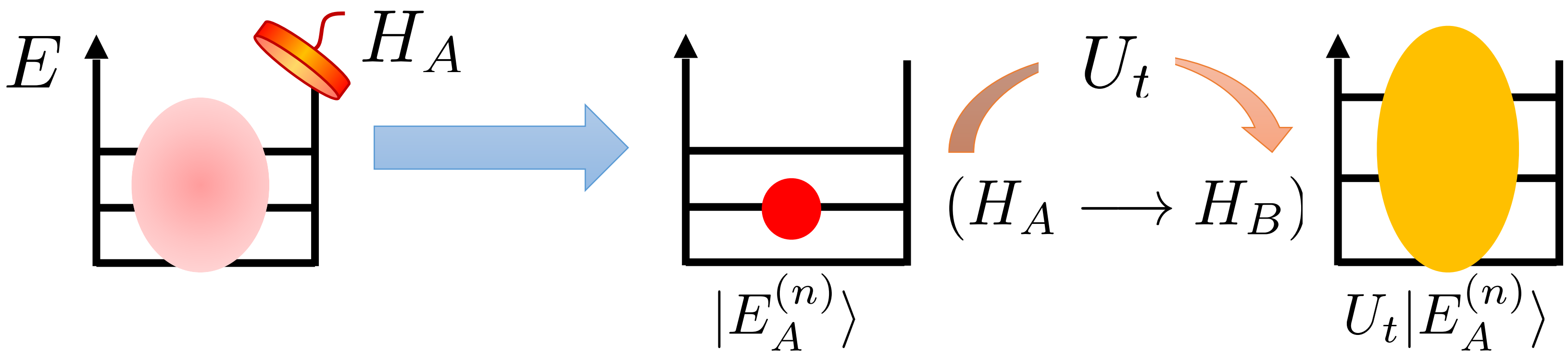
1. (Review) Two-time measurement scheme



$$\beta\langle W_{\mathrm{irr}}\rangle \geq 0$$

H. Tasaki, arXiv:cond-mat/0009244 (2000)
J. Kurchan, arXiv:cond-mat/0007360 (2001)
S. Mukamel, Phys. Rev. Lett. 90, 170604 (2003)

2. One-time measurement scheme



Benefit

(1) Quantum coherence is protected

(2) Informational contribution

(3) Classical correspondence

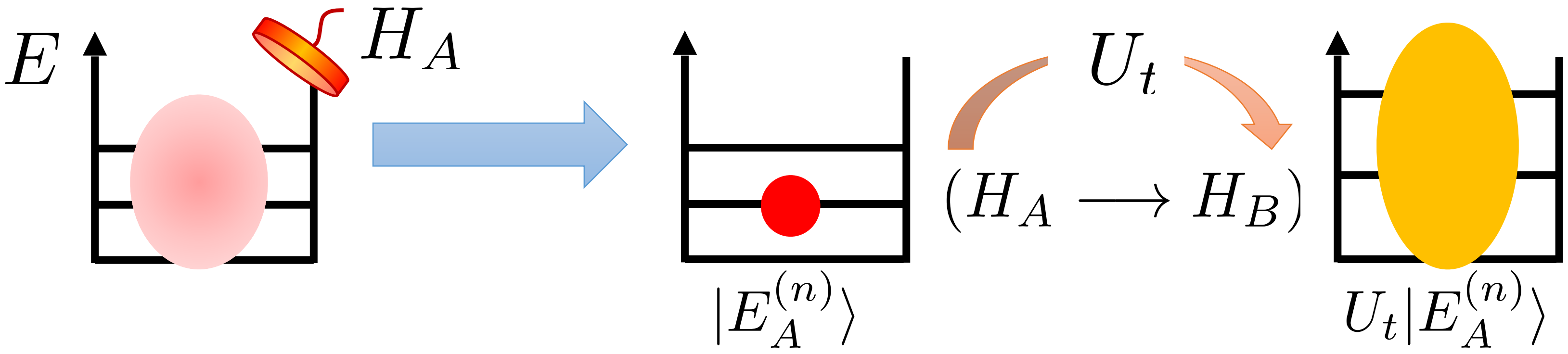
Sharper bound with quantum relative entropy

$$\beta\langle W_{\mathrm{irr}}\rangle \geq D_Q[\widetilde{\rho}_B||\rho_B^{\mathrm{eq}}]$$

S. Deffner et al, Phys. Rev. E **94**, 010103(R) (2016)

Second law of thermodynamics: Quantum approach

One-time measurement scheme



$$\beta\langle W_{\mathrm{irr}}\rangle \geq D_Q[\widetilde{\rho}_B||\rho_B^{\mathrm{eq}}]$$

Conditional Thermal State (guessed state)

$$\widetilde{\rho}_B = \sum_n \frac{e^{-\beta\left\langle E_A^{(n)}\right|U_\tau^\dagger H_B U_\tau\left|E_A^{(n)}\right\rangle}}{\mathcal{Z}(B|A)} U_\tau\left|E_A^{(n)}\right\rangle\left\langle E_A^{(n)}\right|U_\tau^\dagger$$

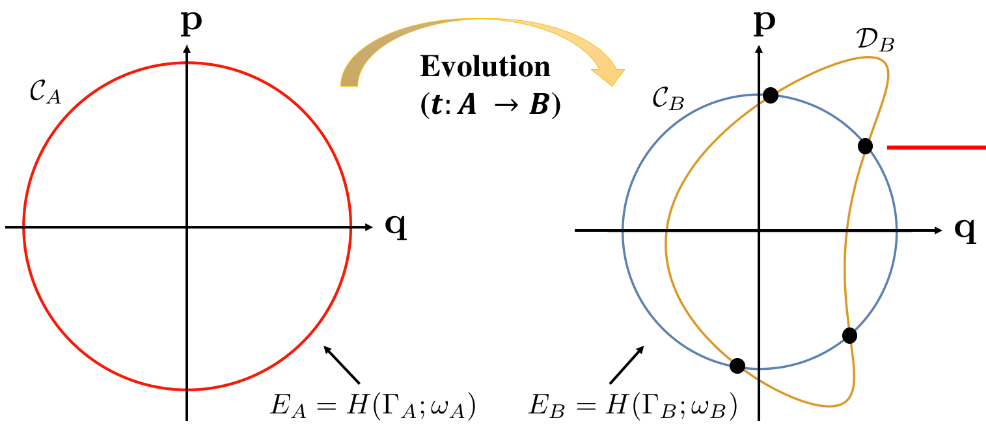
Thermal state characterized by the conditional final energy expectation conditioned on a initial energy measurement

Gibbs state with H_B

$$\rho_B^{\mathrm{eq}} = \frac{1}{Z_B} e^{-\beta H_B}$$

S. Deffner et al, Phys. Rev. E **94**, 010103(R) (2016)

Second law of thermodynamics: Classical approach



Transition probability distribution

$$p(E_B|E_A) = \frac{\int d\Gamma_A \delta(E_A - H(\Gamma_A;\omega_A))\delta(E_B - H(\Gamma_B(\Gamma_A);\omega_B))}{\int d\Gamma_A \delta(E_A - H(\Gamma_A;\omega_A))}$$

The transition probability distribution counts the intersection points of $\mathscr{D}_B$ and $\boldsymbol{C_B}$

Sharper bound with classical relative entropy

$$\beta\langle W_{\mathrm{irr}}\rangle \geq D_C[p_{B|A}||p_B^{\mathrm{eq}}]$$

Conditional Thermal Distribution

$$p_{B|A}(E_A, E_B) = p(E_B|E_A)\frac{e^{-\beta\varepsilon_B(E_A)}}{\mathcal{Z}(B|A)}$$

where

$$\varepsilon_B(E_A) = \int dE_B E_B p(E_B|E_A)$$

Thermal distribution with $\boldsymbol{H_B}$

$$p_B^{\mathrm{eq}}(E_B) = \frac{1}{Z_B}e^{-\beta E_B}$$

AS and S. Deffner, arXiv:2010.05835 (2020)

Geometric Quantum Mechanics (GQM)

Ambiguity of density matrix formalism

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_k p_k |\psi_k\rangle\langle\psi_k|$$

Different decompositions

Probabilistic interpretation based on ensemble theory is **not unique**

Manifold of quantum states

Complex projective space $\mathscr{V}_d$

$\mathbf{z} = (z_0, z_1, \cdots, z_{d-1})$

Complex homogeneous coordinate

pure state

$$|\psi(\mathbf{z})\rangle = \sum_{\alpha=0}^{d-1} z_\alpha |e_\alpha\rangle$$

coordinate-invariant volume element

$$dV = \sqrt{\det(g)} d\mathbf{z} d\bar{\mathbf{z}}$$

where

$$g_{\alpha\bar{\gamma}} = \frac{1}{2} \partial_{z_\alpha} \partial_{\bar{z}_\gamma} \ln(\mathbf{z} \cdot \bar{\mathbf{z}})$$

Ashtekar and Schilling (1999)
Bengtsson and K. Zyczkowski (2017)

Geometric quantum state (solution)

Given an observable O, the state in GQM is described as

Functional: $f_p(O) = \int_{\mathcal{V}_d} d\mathbf{z} d\bar{\mathbf{z}}\, p(\mathbf{z}, \bar{\mathbf{z}})\, O(\mathbf{z}, \bar{\mathbf{z}})$

where $O(\mathbf{z}, \bar{\mathbf{z}}) = \langle\psi(\mathbf{z})|O|\psi(\mathbf{z})\rangle$

and ***geometric quantum state*** is

$p(\mathbf{z}, \bar{\mathbf{z}})$**:** probability distribution of $(\boldsymbol{z}, \bar{\boldsymbol{z}})$

Geometric entropy (generalized entropy):

$$S_G(p) = -\int_{\mathcal{V}_d} d\mathbf{z} d\bar{\mathbf{z}}\, p(\mathbf{z}, \bar{\mathbf{z}}) \ln p(\mathbf{z}, \bar{\mathbf{z}})$$

(*it is not usually equivalent to von-Neumann entropy)

Relation to von-Neumann entropy:

$$\rho = \int_{\mathcal{V}_d} d\mathbf{z} d\bar{\mathbf{z}}\, p(\mathbf{z}, \bar{\mathbf{z}}) |\psi(\mathbf{z})\rangle\langle\psi(\mathbf{z})|$$

diagonal decomposition in eigensystems

then, the von-Neumann entropy

$$S_Q(\rho) = -\mathrm{Tr}[\rho \ln \rho]$$

becomes

$$S_Q(\rho) = S_G(p)$$

F. Anza and J. P. Crutchfield, arXiv:2008.08679 (2020)
F. Anza and J. P. Crutchfield, arXiv:2008.08682 (2020)
F. Anza and J. P. Crutchfield, arXiv:2008.08683 (2020)

Geometric Relative Entropy

Definition of Geometric Relative Entropy and its relation to Quantum Relative Entropy

Given two geometric quantum states $p_1(z, \bar{z})$ and $p_2(z, \bar{z})$, the geometric relative entropy is defined as

$$\mathcal{D}[p_1||p_2] = \int_{\mathcal{V}_d} d\mathbf{z}d\overline{\mathbf{z}}\; p_1(\mathbf{z},\overline{\mathbf{z}}) \ln \frac{p_1(\mathbf{z},\overline{\mathbf{z}})}{p_2(\mathbf{z},\overline{\mathbf{z}})}$$

Given two density matrices with diagonal decompositions in eigensystems ($p_j(\mathbf{z}, \bar{\mathbf{z}})$ is in **decreasing order**)

$$\rho_j = \int_{\mathcal{V}_d} d\mathbf{z}d\overline{\mathbf{z}}\; p_j(\mathbf{z},\overline{\mathbf{z}})|\psi_j(\mathbf{z})\rangle\langle\psi_j(\mathbf{z})|\,, \quad (j=1,2)$$

then given an unitary $K \in \mathscr{U}$, the geometric relative entropy is the minimum of the quantum relative entropy

$$\mathcal{D}[p_1||p_2] = \min_{K\in\mathcal{U}} D_Q[K\rho_1 K^\dagger||\rho_2]$$

namely

$$|\langle\psi_2(\mathbf{z}',\overline{\mathbf{z}}')|K|\psi_1(\mathbf{z},\overline{\mathbf{z}})\rangle|^2 = \delta(\mathbf{z}'-\mathbf{z},\overline{\mathbf{z}}'-\overline{\mathbf{z}})$$

→ **any relation to quantum ergotropy?**

Geometric Relative Entropy

Result 1: Quantum Ergotropy and Geometric Relative Entropy

Given a quantum state $\rho = \sum_j r_j |r_j\rangle\langle r_j| \; (r_1 \geq r_2 \geq \cdots)$ and an Hamiltonian $H = \sum_i E_i |E_i\rangle\langle E_i| \; (E_1 \leq E_2 \leq \cdots)$

the maximum work extracted by a unitary $K \in \mathscr{U}$ is given by

$$\mathcal{W}_Q(\rho) = \mathrm{Tr}[\rho H] - \min_{K \in \mathcal{U}} \mathrm{Tr}[K\rho K^\dagger H] = \sum_{ij} r_j E_i \left(|\langle r_j | E_i \rangle|^2 - \delta_{ij} \right)$$

namely

$$|\langle E_j | K | r_i \rangle|^2 = \delta_{ij}$$

A. E. Allahverdyan *et al*, Europhys. Lett. **67**, 565 (2004).

In our case, when we set ($E(\mathbf{z}, \bar{\mathbf{z}})$ is in **increasing order**)

$$\rho_2 = \rho^{\mathrm{eq}} = \int_{\mathcal{V}_d} d\mathbf{z} d\bar{\mathbf{z}} \underbrace{\frac{e^{-\beta E(\mathbf{z},\bar{\mathbf{z}})}}{Z}}_{= p^{\mathrm{eq}}(\mathbf{z},\bar{\mathbf{z}})} |E(\mathbf{z},\bar{\mathbf{z}})\rangle\langle E(\mathbf{z},\bar{\mathbf{z}})|$$

then we have

$$\beta \mathcal{W}_Q(\rho) = D_Q[\rho || \rho^{\mathrm{eq}}] - \mathcal{D}[p || p^{\mathrm{eq}}]$$

AS and S. Deffner, in preparation (2021)

Geometric Relative Entropy and Coherence Measure

Result 2: Coherent Quantum Ergotropy and Geometric Relative Entropy

Quantum Ergotropy:

$$\mathcal{W}_Q(\rho) = \mathcal{W}_Q^{(c)}(\rho) + \mathcal{W}_Q^{(i)}(\rho)$$

Coherent: $\mathcal{W}_Q^{(c)}(\rho) = C(\rho) + D_Q[\Lambda(\sigma)||\rho^{\mathrm{eq}}] - \min_{K\in\mathcal{U}} D_Q[K\rho K^\dagger||\rho^{\mathrm{eq}}]$

Incoherent: $\mathcal{W}_Q^{(i)}(\rho) = \mathrm{Tr}[(\rho-\sigma)H]$

- Coherence-invariant state: $\sigma = R\rho R^\dagger$ such that $\mathcal{W}_Q^{(i)}(\rho) = \mathrm{Tr}[\rho H] - \min_{R\in\mathcal{U}^{(i)}} \mathrm{Tr}[R\rho R^\dagger H]$

  Unitaries **without** changing coherence

- Dephasing in the energy bases: $\Lambda(\sigma) = \sum_j \langle E_j|\sigma|E_j\rangle |E_j\rangle\langle E_j|$

- Relative entropy of coherence (distillable quantum coherence): $C(\rho) = S_Q(\Lambda(\rho)) - S_Q(\rho)$

G. Francica *et al*, Phys. Rev. Lett. **125**, 180603 (2020).

$$\mathcal{D}[p||p^{\mathrm{eq}}] = \min_{K\in\mathcal{U}} D_Q[K\rho K^\dagger||\rho^{\mathrm{eq}}]$$

$$\mathcal{W}_Q^{(c)}(\rho) = C(\rho) + D_Q[\Lambda(\sigma)||\rho^{\mathrm{eq}}] - \mathcal{D}[p||p^{\mathrm{eq}}]$$

AS and S. Deffner, in preparation (2021)

Revisit Second Law of Thermodynamics

Result 3: Conditional Thermal State is Geometric Canonical Ensemble

Geometric Canonical Ensemble:

$$\widetilde{p}(\mathbf{z},\overline{\mathbf{z}}) = \frac{e^{-\beta h(\mathbf{z},\overline{\mathbf{z}})}}{\mathcal{Z}}, \quad h(\mathbf{z},\overline{\mathbf{z}}) = \langle\psi(\mathbf{z})|H|\psi(\mathbf{z})\rangle$$

Derived from the principle of maximum entropy of geometric quantum state

F. Anza and J. P. Crutchfield, arXiv:2008.08679 (2020)
F. Anza and J. P. Crutchfield, arXiv:2008.08682 (2020)
F. Anza and J. P. Crutchfield, arXiv:2008.08683 (2020)

Conditional Thermal State:

$$\widetilde{\rho}_B = \sum_n \frac{e^{-\beta\left\langle E_A^{(n)}\middle|U_\tau^\dagger H_B U_\tau\middle|E_A^{(n)}\right\rangle}}{\mathcal{Z}(B|A)} U_\tau \left|E_A^{(n)}\right\rangle\left\langle E_A^{(n)}\right| U_\tau^\dagger$$

$$\mathbf{z}_n = \mathbf{z}\left(U_\tau\left|E_A^{(n)}\right\rangle\right) \Longleftrightarrow |\psi_B(\mathbf{z}_n)\rangle = U_\tau\left|E_A^{(n)}\right\rangle$$

$$\widetilde{p}_B(\mathbf{z},\overline{\mathbf{z}}) = \sum_n \frac{e^{-\beta h_B(\mathbf{z},\overline{\mathbf{z}})}}{\mathcal{Z}(B|A)}\delta(\mathbf{z}-\mathbf{z}_n,\overline{\mathbf{z}}-\overline{\mathbf{z}}_n)$$

Density of State
(continuous-variable representation)

$$\widetilde{p}_B(\mathbf{z},\overline{\mathbf{z}}) = \int_{\mathcal{V}_d'} d\mathbf{z}'d\overline{\mathbf{z}}' \frac{e^{-\beta h_B(\mathbf{z}',\overline{\mathbf{z}}')}}{\mathcal{Z}(B|A)}\delta(\mathbf{z}-\mathbf{z}',\overline{\mathbf{z}}-\overline{\mathbf{z}}')$$

$$= \frac{e^{-\beta h_B(\mathbf{z},\overline{\mathbf{z}})}}{\mathcal{Z}(B|A)}$$: Geometric Canonical Ensemble

$$\widetilde{\rho}_B = \int_{\mathcal{V}_d} d\mathbf{z}d\overline{\mathbf{z}}\ \widetilde{p}_B(\mathbf{z},\overline{\mathbf{z}})\,|\psi_B(\mathbf{z})\rangle\langle\psi_B(\mathbf{z})|$$

AS and S. Deffner, in preparation (2021)

Revisit Second Law of Thermodynamics

Result 4: Second Law of Thermodynamics and Quantum Coherence

Sharper bound (Quantum): $\beta\langle W_{\mathrm{irr}}\rangle \geq D_Q[\widetilde{\rho}_B||\rho_B^{\mathrm{eq}}]$

Quantum Ergotropy: $\beta\mathcal{W}_Q(\widetilde{\rho}_B) = D_Q[\widetilde{\rho}_B||\rho_B^{\mathrm{eq}}] - \mathcal{D}[\widetilde{p}_B||p_B^{\mathrm{eq}}]$

- **Incoherent:** $\mathcal{W}_Q^{(i)}(\widetilde{\rho}_B) = \mathrm{Tr}[(\widetilde{\rho}_B - \widetilde{\sigma}_B)H_B]$
- **Coherent:** $\mathcal{W}_Q^{(c)}(\widetilde{\rho}_B) = C(\widetilde{\rho}_B) + D_Q[\Lambda(\widetilde{\sigma}_B)||\rho_B^{\mathrm{eq}}] - \mathcal{D}[\widetilde{p}_B||p_B^{\mathrm{eq}}]$

Second Law of Thermodynamics with quantum coherence:

$$\beta\langle W_{\mathrm{irr}}\rangle \geq \beta\mathcal{W}_Q^{(i)}(\widetilde{\rho}_B) + C(\widetilde{\rho}_B) + D_Q[\Lambda(\widetilde{\sigma}_B)||\rho_B^{\mathrm{eq}}]$$

- Incoherent quantum ergotropy of geometric canonical ensembles
- Distillable quantum coherence from geometric canonical ensembles
- Population mismatch between the geometric canonical ensembles and Gibbs state

Geometric canonical ensembles

Coherence source providing the informational contribution to second law of thermodynamics

AS and S. Deffner, in preparation (2021)

Bridging Quantum and Classical Approach

Result 5: Classical Ergotropy

Sharper bound (Classical): $\beta\langle W_{\rm irr}\rangle \geq D_C[p_{B|A}||p_B^{\rm eq}]$

Conditional Thermal State: $\widetilde{p}_{B|A}(\mathbf{z},\overline{\mathbf{z}};\mathbf{z}',\overline{\mathbf{z}}') = \underline{p(\mathbf{z}',\overline{\mathbf{z}}'|\mathbf{z},\overline{\mathbf{z}})}\,\widetilde{p}_B(\mathbf{z},\overline{\mathbf{z}})$

transition probability distribution ($A \to B$)

Definition of Classical Ergotropy:

$$\mathcal{W}_C(p) = \iint_{\mathcal{V}_d\cup\mathcal{V}_d'} d\mathbf{z}d\overline{\mathbf{z}}d\mathbf{z}'d\overline{\mathbf{z}}'p(\mathbf{z},\overline{\mathbf{z}};\mathbf{z}',\overline{\mathbf{z}}')E(\mathbf{z}',\overline{\mathbf{z}}') - \min_{\underline{q\in\mathcal{Q}}}\iint_{\mathcal{V}_d\cup\mathcal{V}_d'} d\mathbf{z}d\overline{\mathbf{z}}d\mathbf{z}'d\overline{\mathbf{z}}'q(\mathbf{z}',\overline{\mathbf{z}}'|\mathbf{z},\overline{\mathbf{z}})p(\mathbf{z},\overline{\mathbf{z}})E(\mathbf{z}',\overline{\mathbf{z}}')$$

sets of transition probabilities distributions

Solution can be $q(\mathbf{z}',\overline{\mathbf{z}}'|\mathbf{z},\overline{\mathbf{z}}) = \delta(\mathbf{z}-\mathbf{z}',\overline{\mathbf{z}}-\overline{\mathbf{z}}')$

which yields

$$\mathcal{W}_C(\widetilde{p}_B) = \int_{\mathcal{V}_d'} d\mathbf{z}'d\overline{\mathbf{z}}'\xi_B(\mathbf{z}')E_B(\mathbf{z}')$$

where

$$\underline{\xi_B(\mathbf{z}')} = \int_{\mathcal{V}_d} d\mathbf{z}d\overline{\mathbf{z}}\;\widetilde{p}_{B|A}(\mathbf{z},\overline{\mathbf{z}};\mathbf{z}',\overline{\mathbf{z}}') - \widetilde{p}_B(\mathbf{z}',\overline{\mathbf{z}}')$$

Not an explicit function of the Hamiltonian
(**classical inhomogeneities** = classical analogue of quantum coherence)

A. M. Smith, Ph.D. thesis, University of Maryland, College Park (2019).

Classical and Geometric Relative Entropy:

$$D_C[\widetilde{p}_{B|A}||p_B^{\rm eq}] = \mathcal{D}[\widetilde{p}_B||p_B^{\rm eq}] + \beta\mathcal{W}_C(\widetilde{p}_B)$$

AS and S. Deffner, in preparation (2021)

Conclusion

(1) We have introduced geometric relative entropy defined in a unified manner in both quantum and classical approach

(2) We have demonstrated the relation of geometric relative entropy to quantum ergotropy and quantum coherence.

(3) We have verified that conditional thermal state is characterized by a geometric canonical ensemble.

(4) We have explicitly clarified that this state is a source of coherence for the informational contribution to second law.

(5) We have derived the classical ergotropy, and showed that the geometric canonical ensemble in the classical is a source of classical inhomogeneities, which demonstrated the consistency to the quantum approach.