Theoretical Tools for Quantum Batteries:

Basic Concepts and Their Applications

Lecture 2

Gentaro Watanabe

(Zhejiang University)

Lecture 2: Ergotropy & coherence

I. Introduction & motivation

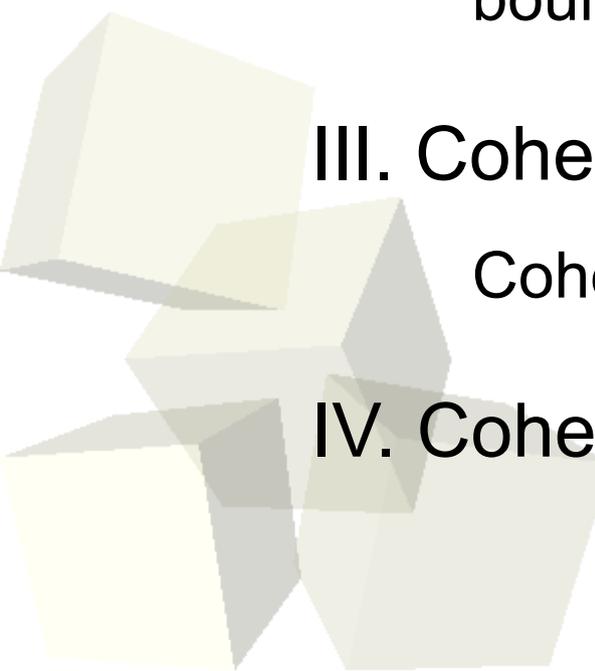Quality of the stored energy & work extraction

II. Passivity & ergotropy

Passivity, ergotropy, "asymptotic freedom" of QBs, bound ergotropy
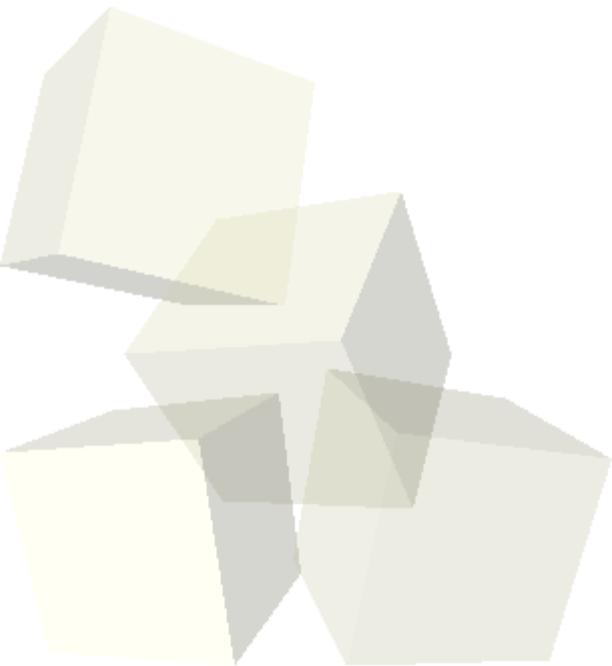
III. Coherence measure

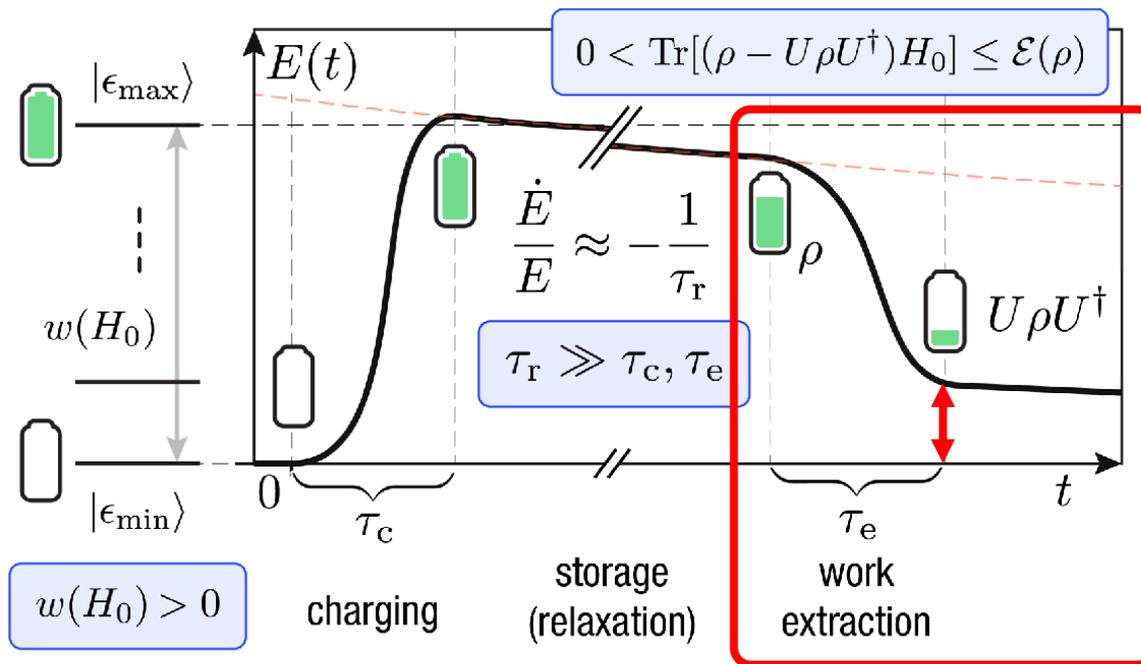Coherence monotone, relative entropy of coherence

IV. Coherent & incoherent ergotropy

I. Introduction & motivation

"Quality" of the charged energy matters.

Even if the charged energy is high, the entire amount may not be extractable.

$$0 < \mathrm{Tr}[(\rho - U\rho U^{\dagger})H_0] \leq \mathcal{E}(\rho)$$

$|\epsilon_{\max}\rangle$

$w(H_0)$

$|\epsilon_{\min}\rangle$

$\dfrac{\dot{E}}{E} \approx -\dfrac{1}{\tau_{\mathrm{r}}}$

$\tau_{\mathrm{r}} \gg \tau_{\mathrm{c}}, \tau_{\mathrm{e}}$

ρ

$U\rho U^{\dagger}$

$w(H_0) > 0$

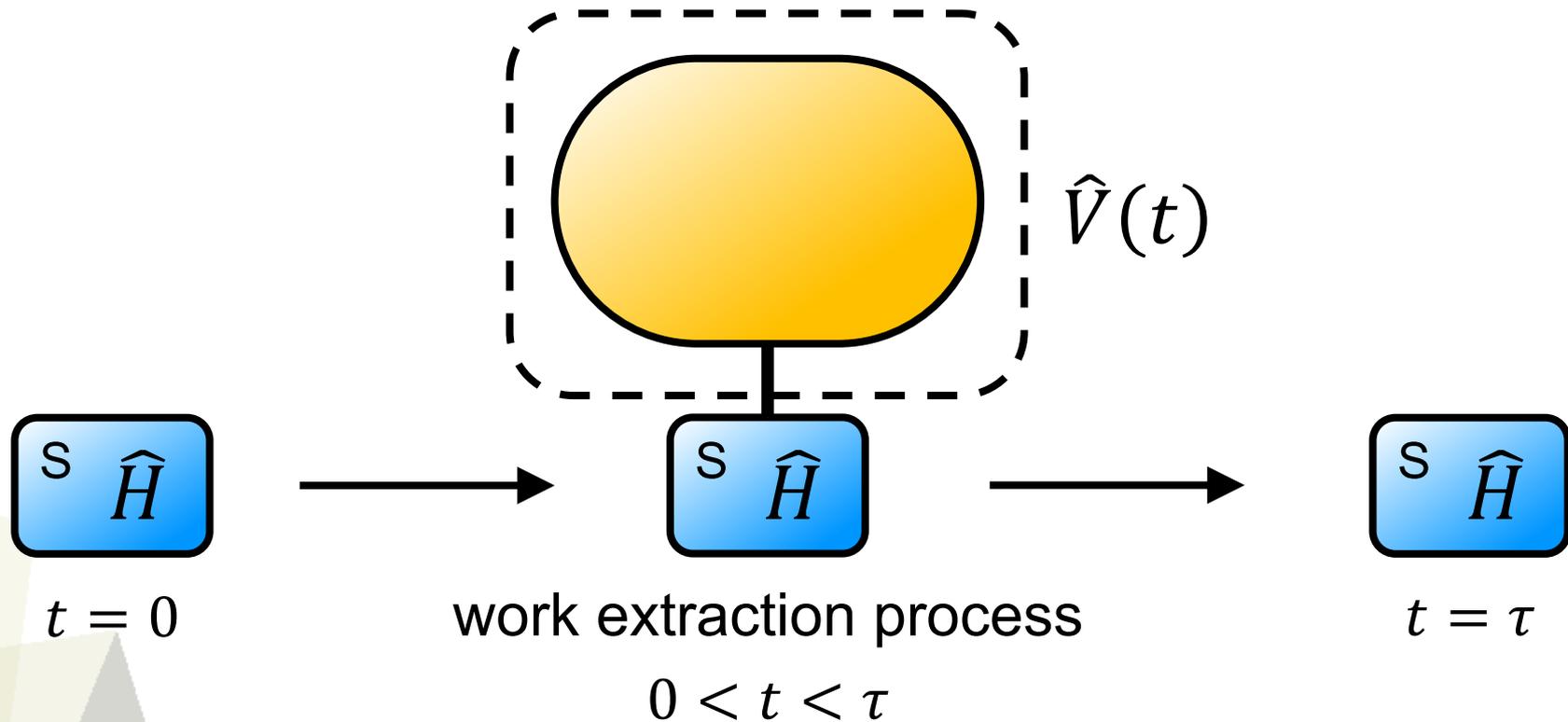| τ_{c}	storage	τ_{e}
charging	(relaxation)	work extraction

Campaioli *et al.*, ROMP **96**, 031001 (2024)

Example: For isothermal processes in macro. equilibrium sys.

max. extractable work: $W_{\max} = F = E - TS \leq E$
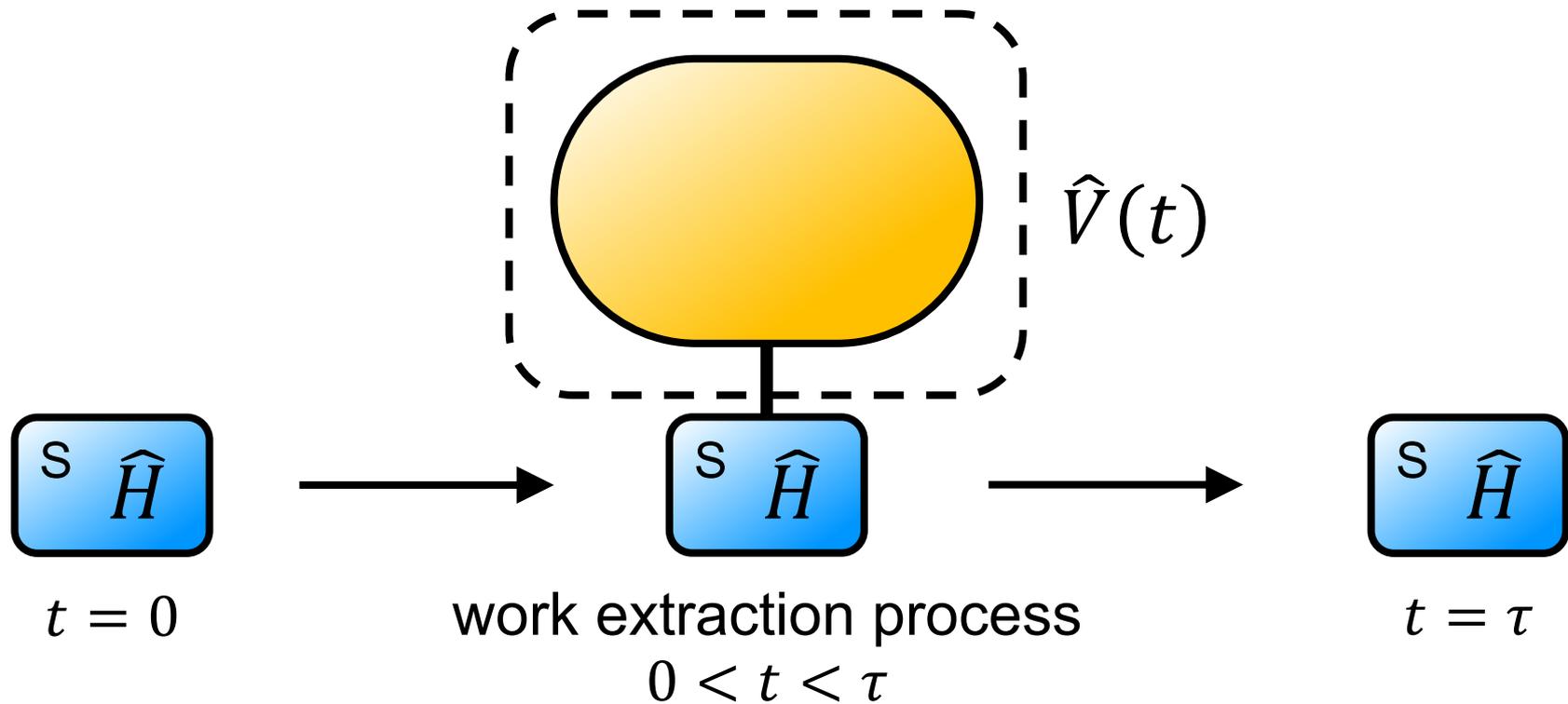
$W_{\max}$ is smaller when T, S are larger.

Work extraction: Usually, highly isolated; through coupling to an external sys. via control params.

$\hat{V}(t)$

S $\hat{H}$

$t = 0$

S $\hat{H}$

work extraction process

$0 < t < \tau$

S $\hat{H}$

$t = \tau$

$$\hat{H}_{\text{tot}}(t) = \hat{H} + \hat{V}(t) \quad \text{with} \quad \hat{V} = 0 \quad \text{at} \quad t = 0 \ \& \ \tau$$

$$\hat{V}(t)$$

$t = 0$ work extraction process $t = \tau$

$$0 < t < \tau$$

$$\hat{H}_{\text{tot}}(t) = \hat{H} + \hat{V}(t) \quad \text{with} \quad \hat{V} = 0 \quad \text{at} \quad t = 0 \ \& \ \tau$$
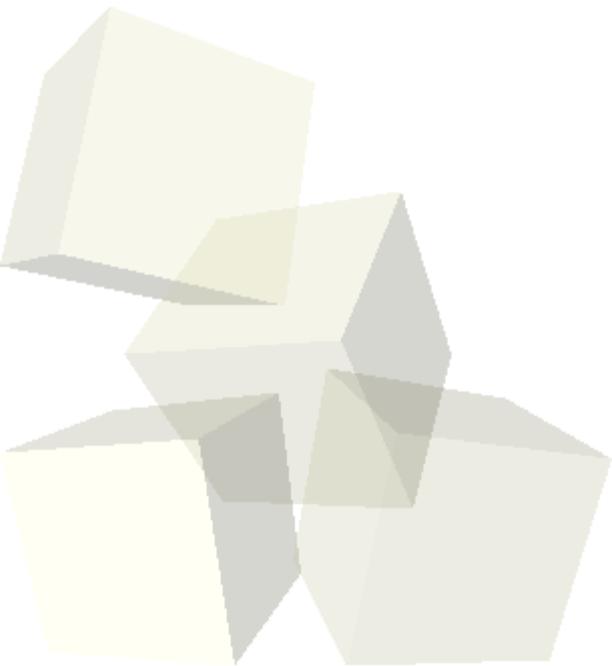
Reasonable scenario

Work extraction by "cyclic unitary" $\hat{U}$

with $\hat{H}_{\text{tot}}(0) = \hat{H}_{\text{tot}}(\tau) \equiv \hat{H}$

(mean) extracted work: $W_{\text{ext}} = \text{Tr}[\hat{H} \, \hat{\rho}_0] - \text{Tr}[\hat{H} \, \hat{U}\hat{\rho}_0\hat{U}^{\dagger}]$

II. Passivity & ergotropy

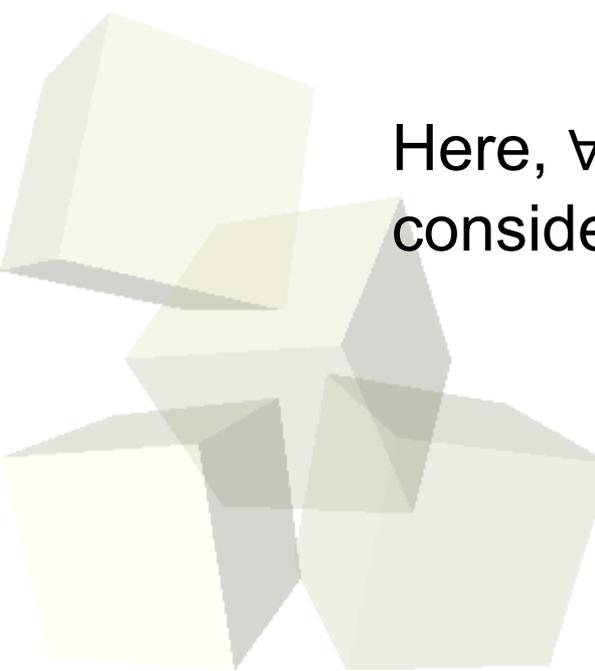· Passivity

$\hat{\rho}$ is passive w.r.t. $\hat{H}$

⟺ No work can be extracted from $\hat{\rho}$ by any unitary map defined in the Hilbert space.

i.e., $\mathrm{Tr}[\hat{H}\hat{\rho}] \leq \mathrm{Tr}[\hat{H}\,\hat{U}\hat{\rho}\hat{U}^{\dagger}]$ for $\forall \hat{U}$

Here, $\forall$ unitaries defined in the given Hilbert space are considered. Not limited to unitaries generated by $\hat{H}$.

local unitaries

global unitaries

Niedenzu, Huber, Boukobza, Quantum **3**, 195 (2019)

$\widehat{U}$: local unitary $\widehat{U}_N$: global unitary for N copies

$$\left\{\widehat{U} \otimes \widehat{U} \otimes \cdots\right\} \subset \left\{\widehat{U}_N\right\}$$

· Passivity

$\hat{\rho}$ is passive w.r.t. $\hat{H}$

$\Longleftrightarrow$ No work can be extracted from $\hat{\rho}$ by any unitary map defined in the Hilbert space.

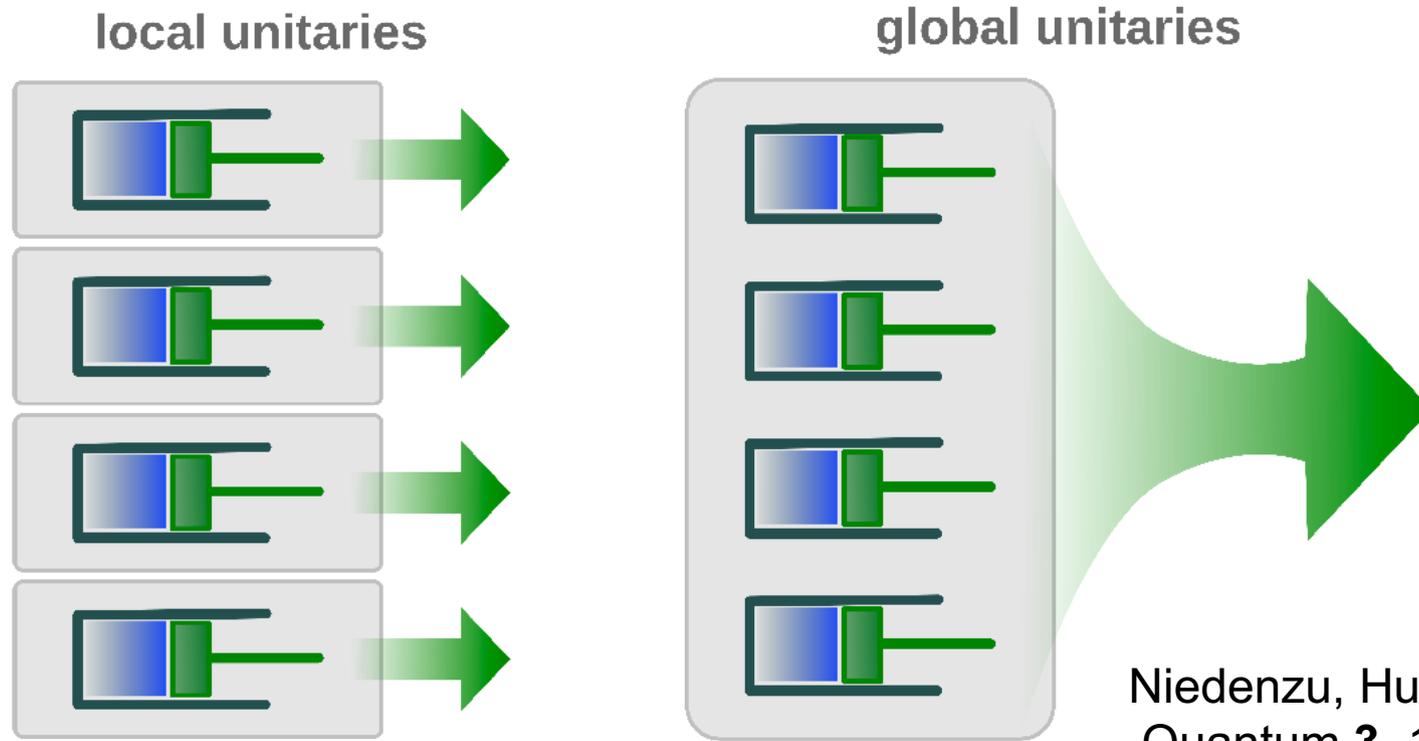$$\text{i.e.,} \quad \text{Tr}[\hat{H}\hat{\rho}] \leq \text{Tr}[\hat{H}\ \hat{U}\hat{\rho}\hat{U}^{\dagger}] \ \text{ for } \ \forall\hat{U}$$

· Complete passivity

$\hat{\rho}$ is completely passive w.r.t. $\hat{H}$

$\Longleftrightarrow$ $\hat{\rho}^{\otimes N}$ is passive for any N.
(passivity for $\forall N$ copies of the system)

$$\text{i.e.,} \quad \text{Tr}[\hat{H}^{(N)}\hat{\rho}^{\otimes N}] \leq \text{Tr}[\hat{H}^{(N)}\ \hat{U}_N\hat{\rho}^{\otimes N}\hat{U}_N^{\dagger}] \ \text{ for } \ \forall\hat{U}_N, N.$$

$$\hat{H}^{(N)} \equiv \sum_{i=1}^{N}\hat{H}_i \quad \text{with } \hat{H}_1 = \hat{H}\otimes\hat{I}\otimes\cdots,$$
$$\hat{H}_2 = \hat{I}\otimes\hat{H}\otimes\hat{I}\otimes\cdots, \ \ldots$$

Passive even by collective operations in $\mathcal{H}^{\otimes N}$.

· "active state" = non-passive state

· For a given $\widehat{H}$, there are many passive states.

· Each active state $\widehat{\rho}$ has its own "passive counterpart" $\widehat{\rho}^{\downarrow}$, accessible via some unitary map from $\widehat{\rho}$.

To discuss passive st. for a given $\widehat{H}$, need to specify $\widehat{\rho}$.

"passive state $\widehat{\rho}^{\downarrow}$ corresponding to $\widehat{\rho}$"

($\widehat{\rho}^{\downarrow}$, $\widehat{P}_{\rho}$, $\widehat{\rho}_{\text{passive}}$, etc. : passive counterpart of $\widehat{\rho}$)

· Gibbs st. (canonical st.) $\widehat{\rho} = e^{-\beta\widehat{H}}/Z$ is the unique completely passive state.

・ Gibbs st. $\hat{\rho}_{\text{th}} = e^{-\beta\hat{H}}/Z$ is the unique completely passive state.

Canonical st. (with $\beta > 0$) is obtained as a max. entropy st. for a given internal energy $E = \langle\hat{H}\rangle$.

$\because$ $S(E)$ is monotonic

$$\frac{dS}{dE} = \beta > 0$$

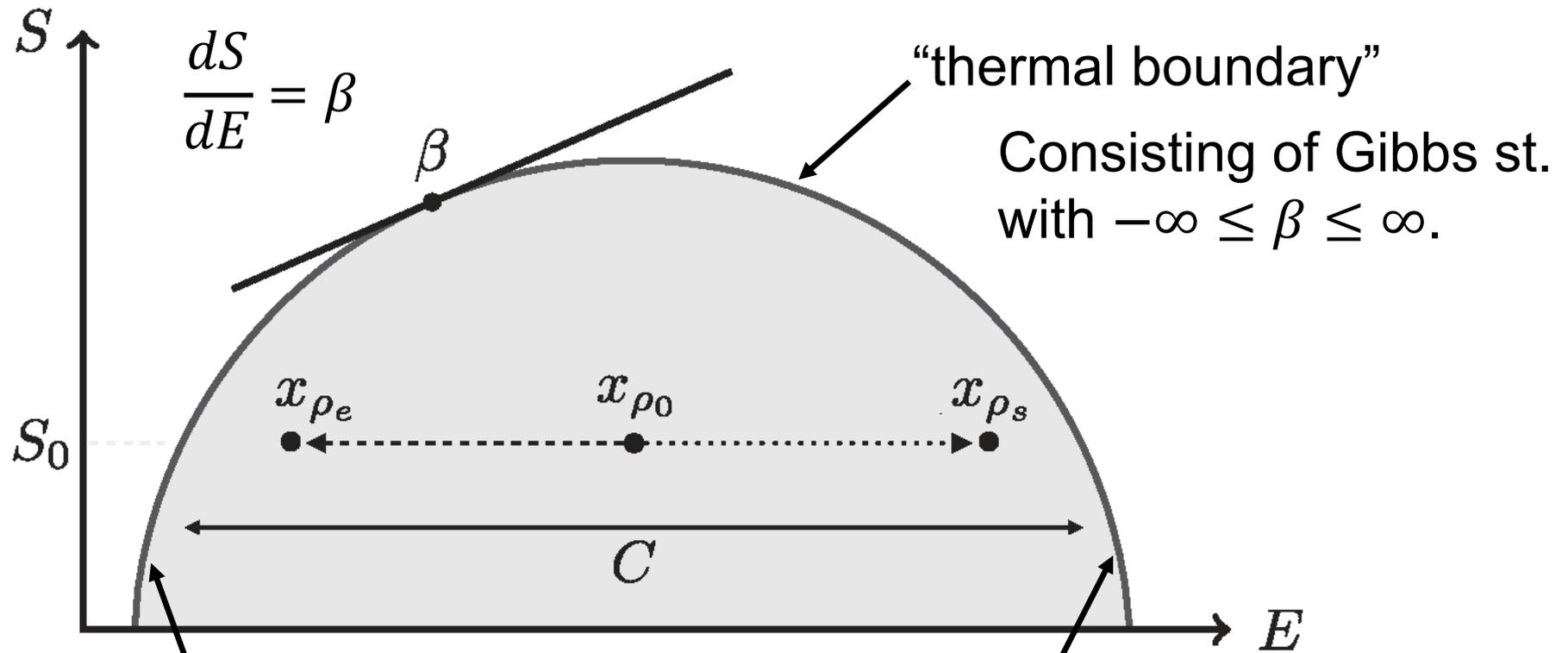Canonical st. (with $\beta > 0$) is a min. energy st. for a given entropy $S \equiv -k_B\text{Tr}[\hat{\rho}\ln\hat{\rho}]$.

Unitary map: von Neumann entropy S unchanged.

For a given $\hat{\rho}$, Gibbs st. $\hat{\rho}_{\text{th}}$ with $S(\hat{\rho}_{\text{th}}) = S(\hat{\rho})$ is the lowest-energy state associated with $\hat{\rho}$, attainable when all possible collective unitary operations are allowed.

$\dfrac{dS}{dE} = \beta$

β

"thermal boundary"

Consisting of Gibbs st. with $-\infty \leq \beta \leq \infty$.

S

S_0

x_{ρ_e} x_{ρ_0} x_{ρ_s}

C

E

completely passive
$\hat{\rho}_{\text{th}}$ with $\beta > 0$

completely active
$\hat{\rho}_{\text{th}}$ with $\beta < 0$

Any state $\hat{\rho}$ is inside the thermal boundary (shaded region).

Allahverdyan, Balian, Nieuwenhuizen, EPL **67**, 565 (2004)

Ergotropy $\mathcal{E}(\hat{\rho})$: Maximum energy extractable from $\hat{\rho}$ via a unitary map under a given $\hat{H}$ (cyclic unitary).

$$\mathcal{E}(\hat{\rho}) \equiv \mathrm{Tr}[\hat{H}\hat{\rho}] - \min_{\hat{U}} \mathrm{Tr}[\hat{H}\,\hat{U}\hat{\rho}\hat{U}^{\dagger}]$$

$$= E(\hat{\rho}) - E_{\mathrm{pas}}(\hat{\rho})$$

passive energy $E_{\mathrm{pas}}(\hat{\rho}) \equiv \min_{\hat{U}} \mathrm{Tr}[\hat{H}\,\hat{U}\hat{\rho}\hat{U}^{\dagger}] = E(\hat{\rho}^{\downarrow})$

・Minimization is performed over all the unitaries defined in $\mathcal{H}$.

・A measure to characterize the "quality" of the charged energy.

・ergotropy = ergo ("work") + tropy ("transformation").

・In literatures, ergotropy is denoted by $\mathcal{E}$, $\mathcal{W}$, etc.

$\hat{H}$ & $\hat{\rho}$ are diagonalizable. ($\because$ Hermitian)

Spectral decomposition:

$$\hat{H} = \sum_{k=1}^{d} \varepsilon_k^{\uparrow} \left|\varepsilon_k^{\uparrow}\right\rangle\left\langle\varepsilon_k^{\uparrow}\right| \quad \text{with } \varepsilon_1^{\uparrow} \leq \varepsilon_2^{\uparrow} \leq \cdots \quad \text{(ascending order)}$$

$$\hat{\rho} = \sum_{k=1}^{d} r_k^{\downarrow} \left|r_k^{\downarrow}\right\rangle\left\langle r_k^{\downarrow}\right| \quad \text{with } r_1^{\downarrow} \geq r_2^{\downarrow} \geq \cdots \quad \text{(descending order)}$$

Key point: Eigenvalues are unchanged under unitary transf.

$\left\{r_k^{\downarrow}\right\}$ is common for $\forall \, \hat{U}\hat{\rho}\hat{U}^{\dagger}$.

Min. energy st. achievable via unitaries (i.e., $\hat{\rho}^{\downarrow}$) should be the state with larger population $r_k^{\downarrow}$ in lower-energy eigenst. $\left|\varepsilon_k^{\uparrow}\right\rangle$:

$$\hat{\rho}^{\downarrow} = \sum_{k=1}^{d} r_k^{\downarrow} \left|\varepsilon_k^{\uparrow}\right\rangle\left\langle\varepsilon_k^{\uparrow}\right|$$

passive st. corresponding to $\hat{\rho}$:
$$\hat{\rho}^{\downarrow} = \sum_{k=1}^{d} r_k^{\downarrow} |\varepsilon_k^{\uparrow}\rangle\langle\varepsilon_k^{\uparrow}|$$

unitary $\hat{U}$: $\hat{\rho} \longrightarrow \hat{\rho}^{\downarrow}$ is
$$\hat{U} = \sum_{k=1}^{d} |\varepsilon_k^{\uparrow}\rangle\langle r_k^{\downarrow}|$$

$$(\because \ \hat{U}\hat{\rho}\hat{U}^{\dagger} = \sum_{i,j,k}(|\varepsilon_i^{\uparrow}\rangle\langle r_i^{\downarrow}|)(r_k^{\downarrow} |r_k^{\downarrow}\rangle\langle r_k^{\downarrow}|)(|r_j^{\downarrow}\rangle\langle\varepsilon_j^{\uparrow}|) = \sum_k r_k^{\downarrow} |\varepsilon_k^{\uparrow}\rangle\langle\varepsilon_k^{\uparrow}|\ )$$
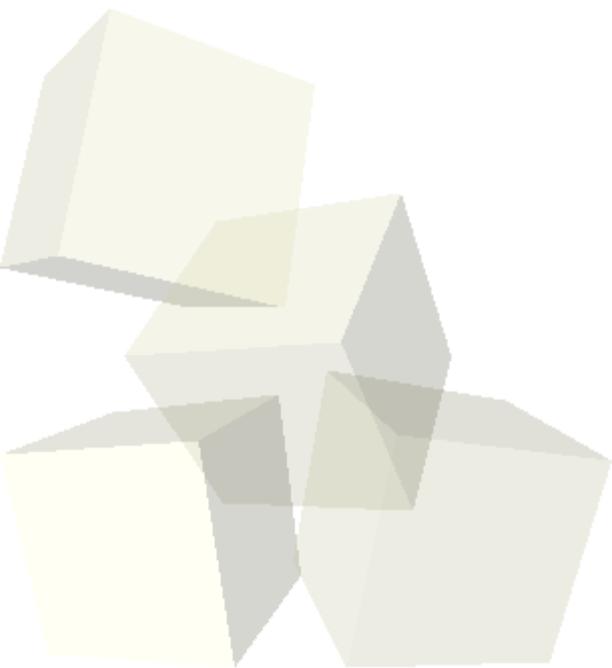
$$\mathcal{E}(\hat{\rho}) \equiv \mathrm{Tr}\big[\hat{H}\hat{\rho}\big] - \mathrm{Tr}\big[\hat{H}\,\hat{\rho}^{\downarrow}\big]$$

$$= \sum_k \varepsilon_k^{\uparrow}\left[\left(\sum_j r_j^{\downarrow} |\langle r_j^{\downarrow}|\varepsilon_k^{\uparrow}\rangle|^2\right) - r_k^{\downarrow}\right] = \sum_k \varepsilon_k^{\uparrow}(\rho_{kk} - r_k^{\downarrow})$$

with pop. in $|\varepsilon_k^{\uparrow}\rangle$: $\rho_{kk} \equiv \sum_j r_j^{\downarrow} |\langle r_j^{\downarrow}|\varepsilon_k^{\uparrow}\rangle|^2$
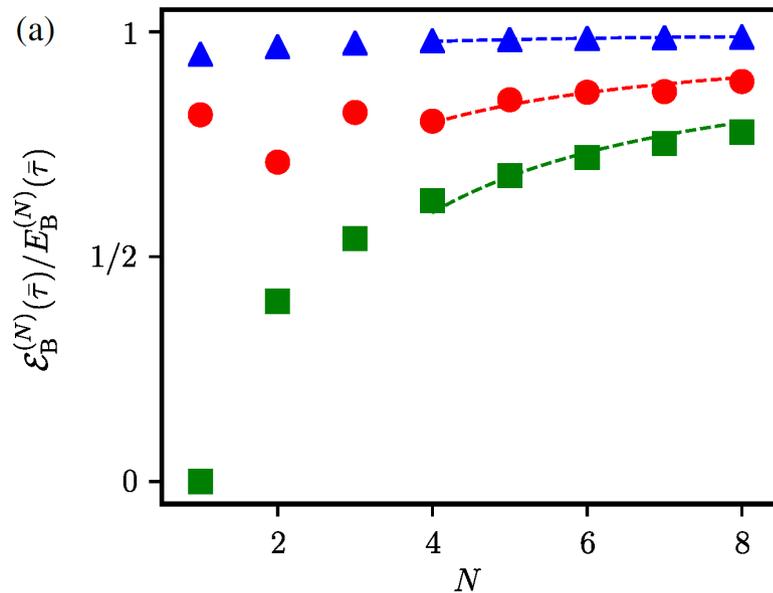
· When $\hat{\rho}$ is pure, $\hat{\rho}^{\downarrow}$ is the ground st.: $\hat{\rho}^{\downarrow} = \left|\varepsilon_1^{\uparrow}\right\rangle\left\langle\varepsilon_1^{\uparrow}\right|$

· $\mathcal{E}(\hat{\rho}) = E(\hat{\rho})$ if and only if $\hat{\rho}$ is pure.

(Assuming a non-degenerate ground state and $\varepsilon_1^{\uparrow} = 0$.)

(a)

$\mathcal{E}_{\mathrm{B}}^{(N)}(\bar{\tau}) / E_{\mathrm{B}}^{(N)}(\bar{\tau})$

1

1/2

0

2 4 6 8

N

Andolina *et al*., PRL **122**, 047702 (2019)

passive energy: $E_{\mathrm{pas}} = E - \mathcal{E}$

E_{pass} can be interpreted as "locked energy" which cannot be extracted.

Asymptotic freedom: $E_{\mathrm{pas}}/E \to 0$ (i.e., $\mathcal{E}/E \to 1$) as $N \to \infty$ in certain collective charging schemes.

Entire energy becomes "free" in the asymptotic limit of $N \to \infty$.

Bound ergotropy: Difference in passive energies (per copy) for $N = 1$ & ∞ copies.

$N = 1$: $E = \mathcal{E} + E_{\text{pas}}$ (E_{pas}: passive energy for $N = 1$)

$N > 1$: $E_N = NE$,   but $\mathcal{E}_N \geq N\mathcal{E}$

Equality: For Gibbs st. $\hat{\rho}_{\text{th}}$ with $S(\hat{\rho}_{\text{th}}) = S(\hat{\rho})$ when $N = \infty$.

($\because$ $\hat{\rho}_{\text{th}}$ is the unique completely passive st.)

For $N = \infty$, passive energy per copy is $E_{\text{th}} \equiv E(\hat{\rho}_{\text{th}}) \leq E_{\text{pas}}$.

Some portion of E_{pas} becomes extractable.

Define $\mathcal{E}_{\text{bound}} \equiv E_{\text{pas}} - E_{\text{th}} \geq 0$ (bound ergotropy)

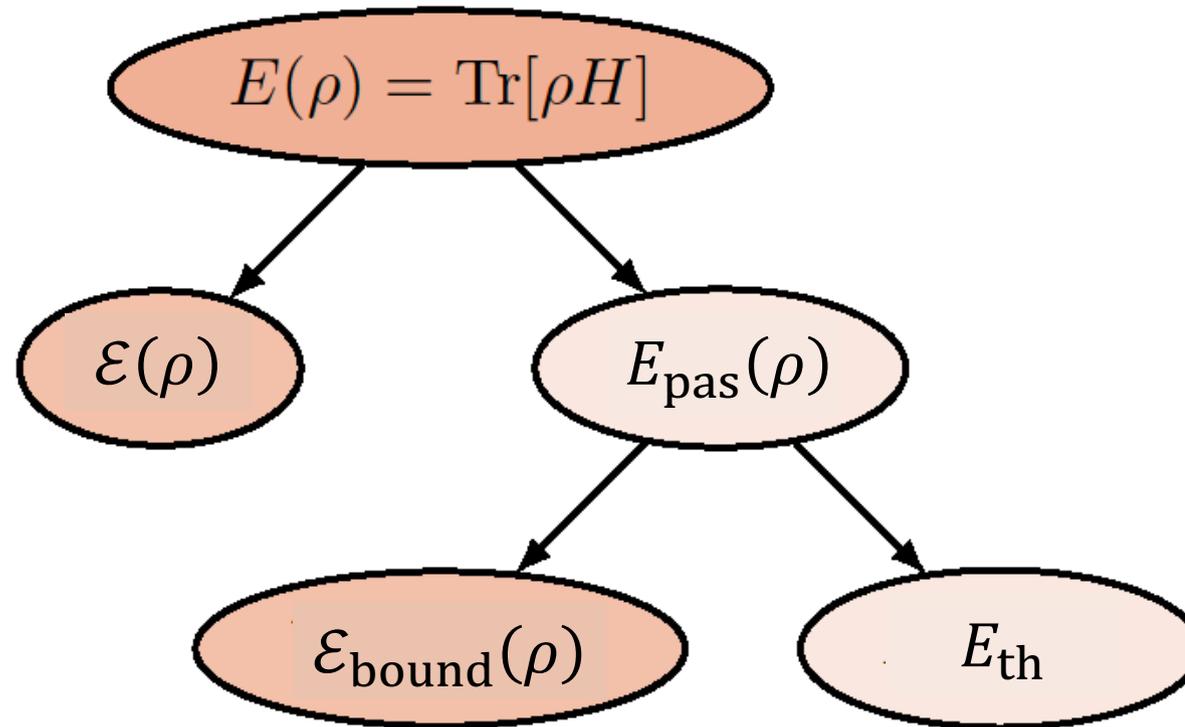Bound ergotropy: $\mathcal{E}_{\text{bound}} \equiv E_{\text{pas}} - E_{\text{th}} \geq 0$

$$E_N = NE = N\mathcal{E} + NE_{\text{pas}} \xrightarrow{N \to \infty} N\mathcal{E} + N(\mathcal{E}_{\text{bound}} + E_{\text{th}})$$

Thus, energy per copy reads: $\lim_{N \to \infty} E_N/N = \mathcal{E} + \mathcal{E}_{\text{bound}} + E_{\text{th}}$

"Total" ergotropy (per copy) for $N = \infty$: $\mathcal{E}_{\text{tot}} \equiv \mathcal{E} + \mathcal{E}_{\text{bound}}$

$$E(\rho) = \mathrm{Tr}[\rho H]$$

$$\mathcal{E}(\rho) \qquad E_{\mathrm{pas}}(\rho)$$

$$\mathcal{E}_{\mathrm{bound}}(\rho) \qquad E_{\mathrm{th}}$$

$$\lim_{N \to \infty} E_N / N = \underbrace{\mathcal{E} + \mathcal{E}_{\mathrm{bound}}}_{\mathcal{E}_{\mathrm{tot}}} + E_{\mathrm{th}}$$

$$\mathcal{E}_{\mathrm{bound}} \equiv E_{\mathrm{pas}} - E_{\mathrm{th}} \geq 0$$

Noneq. free energy: $F(\hat{\rho}) \equiv E(\hat{\rho}) - TS(\hat{\rho})$

$$= \mathcal{E}(\hat{\rho}) + E_{\text{pas}}(\hat{\rho}) - TS(\hat{\rho})$$

with T for the Gibbs st. $\hat{\rho}_{\text{th}}$ such that $S(\hat{\rho}_{\text{th}}) = S(\hat{\rho})$

Consider free energy F_N for N copies.

$$\lim_{N \to \infty} F_N/N = F(\hat{\rho}) = E(\hat{\rho}) - TS(\hat{\rho})$$

$$= \mathcal{E} + \mathcal{E}_{\text{bound}} + E_{\text{th}} - TS(\hat{\rho})$$

$$= \mathcal{E} + \mathcal{E}_{\text{bound}} + \underbrace{E_{\text{th}} - TS(\hat{\rho}_{\text{th}})}_{F(\hat{\rho}_{\text{th}})} \quad (\because S(\hat{\rho}_{\text{th}}) = S(\hat{\rho}))$$
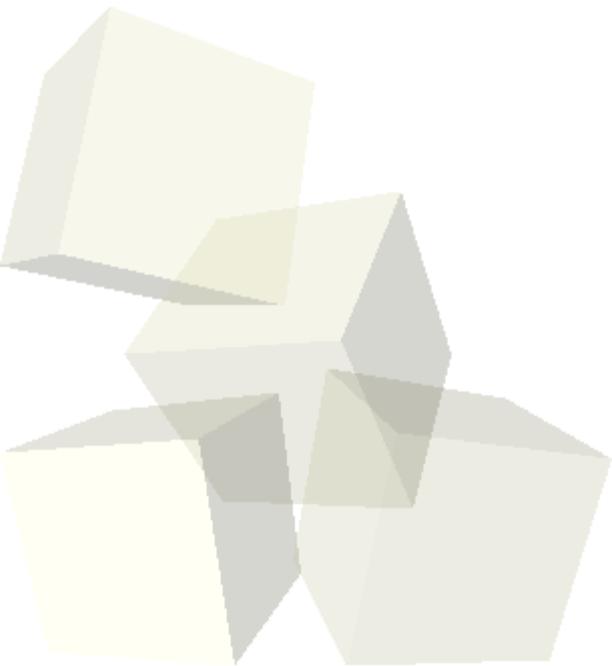
$$\boxed{\mathcal{E}_{\text{tot}} \equiv \mathcal{E} + \mathcal{E}_{\text{bound}} = F(\hat{\rho}) - F(\hat{\rho}_{\text{th}})}$$

with $\hat{\rho}_{\text{th}}$ such that $S(\hat{\rho}_{\text{th}}) = S(\hat{\rho})$

For $N = \infty$, total ergotropy is equal to free energy difference. 22

III. Coherence measure

Quantum coherence: Nonzero off-diag. elements of $\hat{\rho}$ (typically in $\hat{H}$-basis).

Originates from superposition of energy eigenst.

Such superposition is easily destroyed by the interaction with environment.

Decoherence
$\begin{cases} \text{Dissipation: Involving energy exchange with environment.} \\ \\ \text{Dephasing: Without energy exchange with environment.} \end{cases}$

Dephasing: Decay of off-diagonal elements (typically in $\widehat{H}$-basis).

(Coherence: Nonzero off-diag. elements in $\widehat{H}$-basis.)

Example: For a TLS

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|e\rangle + e^{i\theta}|g\rangle\right) \qquad \{|e\rangle, |g\rangle\} : \text{ basis of } \widehat{H}$$

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix} 1 & \boxed{e^{-i\theta}} \\ \boxed{e^{i\theta}} & 1 \end{pmatrix} \quad : \text{ pure st.}$$

Dephasing $\xrightarrow{\hspace{2cm}}$ $\dfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$: statistical mix. $\begin{cases} |e\rangle \ 50\% \\ |g\rangle \ 50\% \end{cases}$

$$\langle\widehat{H}^n\rangle \equiv \text{Tr}\left[\hat{\rho}\,\widehat{H}^n\right] \text{ unchanged.}$$

Quantum coherence is well quantified using relative entropy

quantum relative entropy: $S(\hat{\rho}\|\hat{\sigma}) \equiv \text{Tr}[\hat{\rho}\ln\hat{\rho}] - \text{Tr}[\hat{\rho}\ln\hat{\sigma}]$

Relative entropy of coherence

Coherence measure: $C(\hat{\rho}) \equiv S(\hat{\rho}\|\hat{\delta}_\rho) = S(\hat{\delta}_\rho) - S(\hat{\rho})$

$\hat{\delta}_\rho \equiv \Delta(\hat{\rho})$: diagonal part of $\hat{\rho}$ (or, dephased st.).

Δ : dephasing map

Gives a density op. obtained by keeping only the diagonal elements of a given $\hat{\rho}$.

Example

$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \longrightarrow \Delta(\hat{\rho}) = \begin{pmatrix} \rho_{11} & 0 \\ 0 & \rho_{22} \end{pmatrix}$$

$\mathcal{I}$: Set of all diagonal $\hat{\rho}$ in some chosen basis.

$\forall$density op. $\hat{\delta} \in \mathcal{I}$ are in the form of $\quad \hat{\delta} = \sum_{i=1}^{d} \delta_i |i\rangle\langle i|$

$\{|i\rangle\}$: a set of basis func.

Incoherent operation/map : An operation/map that keeps every diagonal state $\hat{\rho}$ diagonal.

Incoherent CPTP map : $\Phi_{\mathrm{ICPTP}}(\hat{\rho}) = \sum_n \widehat{M}_n \hat{\rho} \widehat{M}_n^{\dagger}$

with Kraus op. $\widehat{M}_n \mathcal{I} \widehat{M}_n^{\dagger} \subset \mathcal{I}$ for $\forall n$.

In short, an incoherent operation/map is the one that does not generate coherence.

Coherence measure: No increase under incoherent operations.

"coherence monotone"

Conditions for coherence measure $C(\hat{\rho})$; $C(\hat{\rho}) \geq 0$ & real

(C1) $C(\hat{\delta}) = 0$ iff $\hat{\delta} \in \mathcal{I}$. ($C = 0 \Longleftrightarrow$ no coherence)

(C2) Monotonicity under Φ_{ICPTP} :

$$C(\hat{\rho}) \geq C\big(\Phi_{\mathrm{ICPTP}}(\hat{\rho})\big) \quad \text{for} \quad \forall \Phi_{\mathrm{ICPTP}}.$$

(C3) Non-increasing under mixing: $\sum_n p_n\, C(\hat{\rho}_n) \geq C(\sum_n p_n\, \hat{\rho}_n)$
(convexity)

for $\forall \{\hat{\rho}_n\},\ p_n\ (\sum_n p_n = 1)$

Mixing: Loss of information about which $\hat{\rho}_n$ has been prepared.

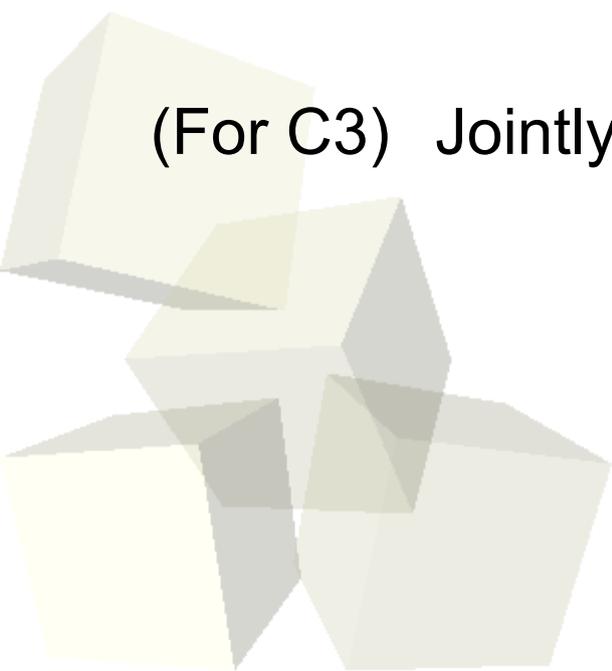$\Longrightarrow$ Coherence should not increase.

Consider $C(\hat{\rho}) \equiv \min\limits_{\hat{\delta} \in \mathcal{I}} D(\hat{\rho}, \hat{\delta})$ with some distance measure D.

Conditions (C1), (C2), and (C3) are satisfied by the above $C(\hat{\rho})$ if $D(\hat{\rho}, \hat{\delta})$ possesses the following properties.

(For C1) Iff $\hat{\rho} = \hat{\delta}$, $D(\hat{\rho}, \hat{\delta}) = 0$.

(For C2) Contracting under $\forall$CPTP Φ: $D(\hat{\rho}, \hat{\sigma}) \geq D(\Phi(\hat{\rho}), \Phi(\hat{\sigma}))$.

(For C3) Jointly convex: $\sum_n p_n D(\hat{\rho}_n, \hat{\sigma}_n) \geq D(\sum_n p_n \hat{\rho}_n, \sum_n p_n \hat{\sigma}_n)$.

Consider $\quad C(\hat{\rho}) \equiv \min_{\hat{\delta} \in \mathcal{I}} D(\hat{\rho}, \hat{\delta}) \quad$ with some distance measure D.

Conditions (C1), (C2), and (C3) are satisfied by the above $C(\hat{\rho})$ if $D(\hat{\rho}, \hat{\delta})$ possesses the following properties.

(For C1) Iff $\hat{\rho} = \hat{\delta}, \; D(\hat{\rho}, \hat{\delta}) = 0$.

$$\Longrightarrow \quad C(\hat{\rho}) \equiv \min_{\hat{\delta} \in \mathcal{I}} D(\hat{\rho}, \hat{\delta}) = 0 \quad \text{iff} \quad \hat{\rho} \in \mathcal{I}. \quad \text{(C1)}$$

(For C2) Contracting under $\forall$CPTP Φ: $\; D(\hat{\rho}, \hat{\sigma}) \geq D(\Phi(\hat{\rho}), \Phi(\hat{\sigma}))$.

$$\Longrightarrow \quad C(\hat{\rho}) = D(\hat{\rho}, \hat{\delta}^*) \geq D\left(\Phi_{\text{ICPTP}}(\hat{\rho}), \Phi_{\text{ICPTP}}(\hat{\delta}^*)\right)$$

$\hat{\delta}^*: \hat{\delta} \in \mathcal{I}$ minimizing $D(\hat{\rho}, \hat{\delta})$ $\quad \geq \min_{\hat{\delta} \in \mathcal{I}} D(\Phi_{\text{ICPTP}}(\hat{\rho}), \hat{\delta}) = C(\Phi_{\text{ICPTP}}(\hat{\rho}))$

$$\text{(C2)}$$

(For C3) Jointly convex: $\sum_n p_n D(\hat{\rho}_n, \hat{\sigma}_n) \geq D(\sum_n p_n \hat{\rho}_n, \sum_n p_n \hat{\sigma}_n)$.
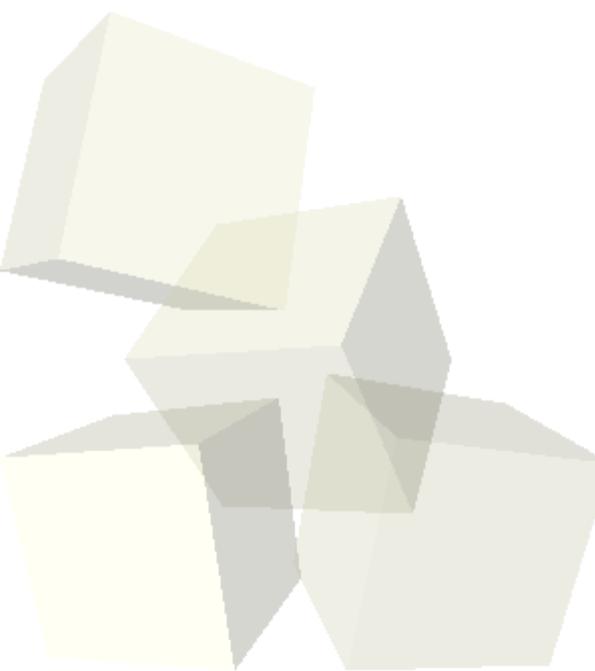
(For C3) Jointly convex: $\sum_n p_n D(\hat{\rho}_n, \hat{\sigma}_n) \geq D(\sum_n p_n \hat{\rho}_n, \sum_n p_n \hat{\sigma}_n)$.

$$C\left(\sum_n p_n \hat{\rho}_n\right) = D\left(\sum_n p_n \hat{\rho}_n, \hat{\delta}^*\right)$$

$$\hat{\delta}^*: \hat{\delta} \in \mathcal{I} \text{ minimizing } D\left(\sum_n p_n \hat{\rho}_n, \hat{\delta}\right)$$

$$= D\left(\sum_n p_n \hat{\rho}_n, \sum_n p_n \hat{\delta}^*\right)$$

Introduce $\hat{\delta}_n^*: \hat{\delta}_n \in \mathcal{I}$ minimizing $D\left(\hat{\rho}_n, \hat{\delta}_n\right)$ for each n.

Since $\hat{\delta}^*$ minimizes $D\left(\sum_n p_n \hat{\rho}_n, \sum_n p_n \hat{\delta}^*\right)$, we have

$$\leq D\left(\sum_n p_n \hat{\rho}_n, \sum_n p_n \hat{\delta}_n^*\right)$$

$$\leq \sum_n p_n \underbrace{D\left(\hat{\rho}_n, \hat{\delta}_n^*\right)}_{C(\hat{\rho}_n)} \quad (\because \text{joint convexity})$$

$$= \sum_n p_n C(\hat{\rho}_n) \quad \text{(C3)}$$

Quantum relative entropy $S(\hat{\rho}\|\hat{\sigma})$: Measure of distinguishability btwn. two density ops. $\hat{\rho}$ & $\hat{\sigma}$.

$$S(\hat{\rho}\|\hat{\sigma}) \equiv \mathrm{Tr}[\hat{\rho}\ln\hat{\rho}] - \mathrm{Tr}[\hat{\rho}\ln\hat{\sigma}]$$

(Quantum counterpart of Kullback-Leibler (KL-) divergence:

$$D(p(x)\|q(x)) \equiv \sum_x \left[p(x)\ln\left(\frac{p(x)}{q(x)}\right) \right])$$

<u>Properties</u>

(1) Klein's ineq.: $S(\hat{\rho}\|\hat{\sigma}) \geq 0$; $S(\hat{\rho}\|\hat{\sigma}) = 0$ iff $\hat{\rho} = \hat{\sigma}$. ➡ (C1)

(2) Contracting under $\forall$CPTP Φ: $S(\hat{\rho}\|\hat{\sigma}) \geq S(\Phi(\hat{\rho})\|\Phi(\hat{\sigma}))$ ➡ (C2)
Less distinguishable under information loss.

(3) Joint convexity: $\sum_n p_n S(\hat{\rho}_n\|\hat{\sigma}_n) \geq S(\sum_n p_n\hat{\rho}_n \| \sum_n p_n\hat{\sigma}_n)$ ➡ (C3)
for $\forall\{p_n\}, \{\hat{\rho}_n\}, \{\hat{\sigma}_n\}$.

Remark: (2) & (3) are equivalent.

Quantum relative entropy $S(\hat{\rho}\|\hat{\sigma})$: Measure of distinguishability btwn. two density ops. $\hat{\rho}$ & $\hat{\sigma}$.

$$S(\hat{\rho}\|\hat{\sigma}) \equiv \mathrm{Tr}[\hat{\rho}\ln\hat{\rho}] - \mathrm{Tr}[\hat{\rho}\ln\hat{\sigma}]$$

(Quantum counterpart of Kullback-Leibler (KL-) divergence:

$$D(p(x)\|q(x)) \equiv \sum_x \left[p(x)\ln\left(\frac{p(x)}{q(x)}\right) \right])$$

Coherence monotone can be constructed by using the quantum relative entropy as:

$$C(\hat{\rho}) \equiv \min_{\hat{\delta}\in\mathcal{I}} S(\hat{\rho}\|\hat{\delta})$$

"relative entropy of coherence"

$$C(\hat{\rho}) \equiv \min_{\hat{\delta} \in \mathcal{I}} S(\hat{\rho} \| \hat{\delta})$$

➡️ A closed form without minimization:

$$C(\hat{\rho}) = S(\hat{\rho} \| \hat{\delta}_\rho) = S(\hat{\delta}_\rho) - S(\hat{\rho})$$

Proof

A formula for $\forall \hat{\rho} \in \mathcal{H}$ and $\forall \hat{\delta} \in \mathcal{I}$ (shown later):

$$S(\hat{\rho} \| \hat{\delta}) = S(\Delta(\hat{\rho})) - S(\hat{\rho}) + S(\Delta(\hat{\rho}) \| \hat{\delta}). \qquad (A)$$

Substituting Eq. (A) into the definition of $C(\hat{\rho})$, we obtain:

$$C(\hat{\rho}) = \min_{\hat{\delta} \in \mathcal{I}} \left[S(\Delta(\hat{\rho})) - S(\hat{\rho}) + S(\Delta(\hat{\rho}) \| \hat{\delta}) \right]$$

$[\cdots]$ is minimized when $\hat{\delta} = \Delta(\hat{\rho})$.

$$= S(\hat{\rho} \| \Delta(\hat{\rho}))$$

$$= S(\Delta(\hat{\rho})) - S(\hat{\rho}) = S(\hat{\delta}_\rho) - S(\hat{\rho}).$$

Exercise: Show $S(\hat{\rho}\|\hat{\delta}) = S(\Delta(\hat{\rho})) - S(\hat{\rho}) + S(\Delta(\hat{\rho})\|\hat{\delta})$

for $\forall \hat{\rho} \in \mathcal{H}$ and $\forall \hat{\delta} \in \mathcal{I}$.

Proof

For $\hat{\delta} \in \mathcal{I}$: $\mathrm{Tr}[\hat{\rho} \ln \hat{\delta}] = \mathrm{Tr}[\Delta(\hat{\rho}) \ln \hat{\delta}]$.

$$\therefore S(\hat{\rho}\|\hat{\delta}) = \mathrm{Tr}[\hat{\rho}(\ln \hat{\rho} - \ln \hat{\delta})]$$

$$= -S(\hat{\rho}) - \underbrace{\mathrm{Tr}[\hat{\rho} \ln \hat{\delta}]}_{\mathrm{Tr}[\Delta(\hat{\rho}) \ln \hat{\delta}]} + \overbrace{\mathrm{Tr}[\Delta(\hat{\rho}) \ln \Delta(\hat{\rho})] - \mathrm{Tr}[\Delta(\hat{\rho}) \ln \Delta(\hat{\rho})]}^{0}$$

$$= -S(\hat{\rho}) \underbrace{- \mathrm{Tr}[\Delta(\hat{\rho}) \ln \hat{\delta}] + \mathrm{Tr}[\Delta(\hat{\rho}) \ln \Delta(\hat{\rho})]}_{S(\Delta(\hat{\rho})\|\hat{\delta})} - \mathrm{Tr}[\Delta(\hat{\rho}) \ln \Delta(\hat{\rho})]$$

$$= -S(\hat{\rho}) + S(\Delta(\hat{\rho})\|\hat{\delta}) + S(\Delta(\hat{\rho}))$$

Relative entropy of coherence: A coherence monotone.

$$C(\hat{\rho}) \equiv \min_{\hat{\delta} \in \mathcal{I}} S(\hat{\rho} \| \hat{\delta}) = S(\hat{\rho} \| \hat{\delta}_\rho) = S(\hat{\delta}_\rho) - S(\hat{\rho})$$

$C(\hat{\rho}) = S(\hat{\delta}_\rho) - S(\hat{\rho})$ can be interpreted as "entropy of coherence".

Remarks

· For any $\hat{\rho}$, we have $C(\hat{\rho}) \leq S(\hat{\delta}_\rho) \leq \ln d$.
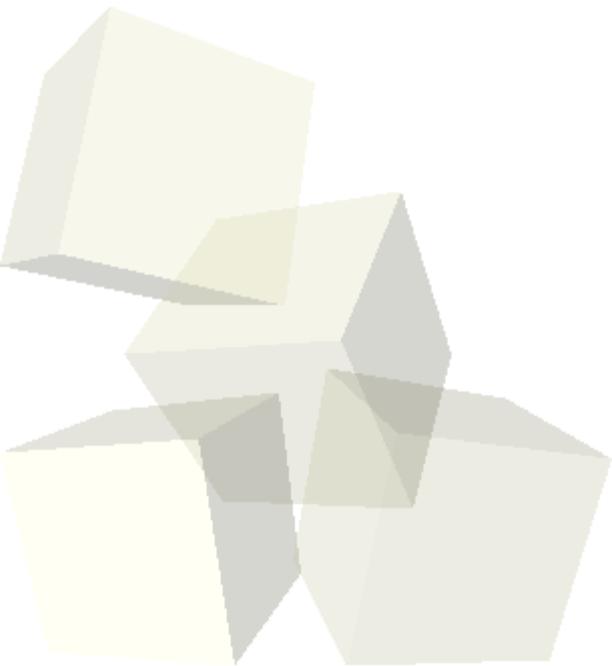
This max. value is attained by maximally coh. st.:

$$|\psi_{\max}\rangle \equiv \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle$$

· l_1-matrix norm $\|\hat{\rho} - \hat{\sigma}\|_{l_1} \equiv \sum_{i,j} |\rho_{i,j} - \sigma_{i,j}|$ can also be used to construct another coherence monotone:

$$C_{l_1}(\hat{\rho}) \equiv \min_{\hat{\delta} \in \mathcal{I}} \|\hat{\rho} - \hat{\delta}\|_{l_1} = \sum_{\substack{i,j \\ i \neq j}} |\rho_{i,j}|$$

IV. Coherent and incoherent ergotropy

✳ Hereafter, we consider the coherence in $\widehat{H}$-basis.

Incoherent ergotropy $\mathcal{E}_i(\hat{\rho})$

$\Bigg\{$

(Def. 1) Maximum extractable work from $\hat{\rho}$ by cyclic unitaries that preserve the coherence of $\hat{\rho}$.

(Def. 2) Maximum extractable work from $\Delta(\hat{\rho})$ by cyclic unitaries.

The two definitions are equivalent (shown later).

$$\mathcal{E}_i(\hat{\rho}) \equiv \mathcal{E}\big(\Delta(\hat{\rho})\big)$$
$$= E(\hat{\rho}) - E_{\mathrm{pas}}\big(\Delta(\hat{\rho})\big) = E(\hat{\rho}) - E\big(\hat{\delta}_\rho^{\downarrow}\big)$$

Coherent ergotropy $\mathcal{E}_c(\hat{\rho})$:   The rest of the ergotropy.

$$\mathcal{E}_c(\hat{\rho}) \equiv \mathcal{E}(\hat{\rho}) - \mathcal{E}_i(\hat{\rho})$$

Incoherent cyclic unitary $\hat{V}$: A cyclic unitary that leaves the coherence unchanged.

$\mathcal{U}_c^{(i)}$: A set of all incoherent cyclic unitaries.

$$\hat{V} \in \mathcal{U}_c^{(i)} \quad \Longleftrightarrow \quad \text{For } \forall\hat{\rho}, \quad C(\hat{V}\hat{\rho}\hat{V}^{\dagger}) = C(\hat{\rho}).$$

Thus, $\hat{V}$ is a reshuffling of the energy basis (up to a phase factor).

$(\because \ C(\hat{V}\hat{\rho}\hat{V}^{\dagger}) = C(\hat{\rho}) \text{ for } \forall\hat{\rho} \ \Longrightarrow \ S(\Delta(\hat{\rho})) = S\left(\Delta(\hat{V}\hat{\rho}\hat{V}^{\dagger})\right) \text{ for } \forall\hat{\rho})$

$$\hat{V} = \sum_k e^{-i\varphi_k}\left|\varepsilon_k^{\uparrow}\right\rangle\left\langle\varepsilon_{\pi_k}^{\uparrow}\right| \equiv \hat{V}_{\pi}$$

π : Permutation corresponding to a given reshuffling.

π_k: kth element of permutation π

Example: $d = 4,\ \pi(\{1,2,3,4\}) = \{3,2,4,1\} \ \Longrightarrow \ \pi_1 = 3,\ \pi_2 = 2,\ \pi_3 = 4,\ \pi_4 = 1$

$$\hat{V} = \sum_k e^{-i\varphi_k} \left| \varepsilon_k^\uparrow \right\rangle \left\langle \varepsilon_{\pi_k}^\uparrow \right| \equiv \hat{V}_\pi$$

(Def. 1)

$$\mathcal{E}_i(\hat{\rho}) \equiv \mathrm{Tr}\left[\hat{H}\hat{\rho}\right] - \min_{\hat{V} \in \mathcal{U}_c^{(i)}} \mathrm{Tr}\left[\hat{H}\,\hat{V}\hat{\rho}\hat{V}^\dagger\right] = \mathrm{Tr}\left[\hat{H}\hat{\rho}\right] - \min_\pi \mathrm{Tr}\left[\hat{H}\,\hat{V}_\pi\hat{\rho}\hat{V}_\pi^\dagger\right]$$

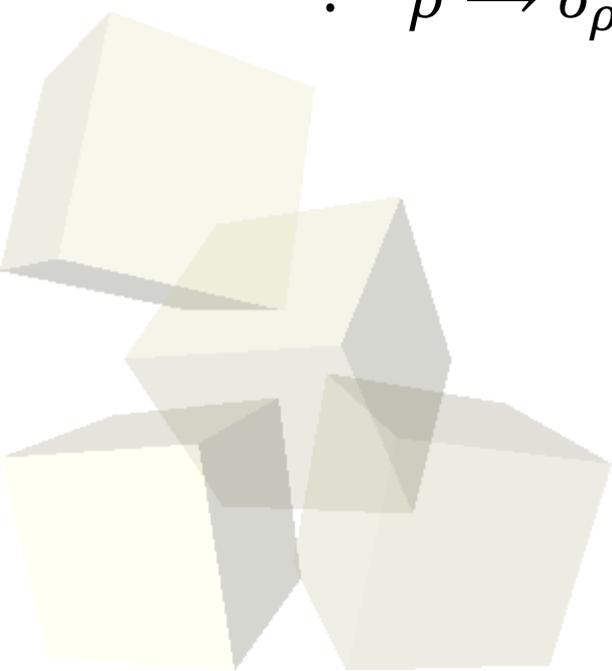Denote optimal π by $\tilde{\pi}$, and define $\hat{\sigma}_\rho$ as the state obtained by $\hat{V}_{\tilde{\pi}}$:

$$\hat{\sigma}_\rho \equiv \hat{V}_{\tilde{\pi}}\hat{\rho}\hat{V}_{\tilde{\pi}}^\dagger = \sum_{k,k'} e^{-i\varphi_k} \left| \varepsilon_k^\uparrow \right\rangle \underbrace{\left\langle \varepsilon_{\tilde{\pi}_k}^\uparrow \middle| \hat{\rho} \middle| \varepsilon_{\tilde{\pi}_{k'}}^\uparrow \right\rangle}_{\rho_{\tilde{\pi}_k,\tilde{\pi}_{k'}}} \left\langle \varepsilon_{k'}^\uparrow \middle| e^{i\varphi_{k'}} \right.$$

$$= \sum_{k,k'} \rho_{\tilde{\pi}_k,\tilde{\pi}_{k'}} \left| \varepsilon_k^\uparrow \right\rangle \left\langle \varepsilon_{k'}^\uparrow \right| e^{-i(\varphi_k - \varphi_{k'})}$$

$$\therefore \ \mathcal{E}_i(\hat{\rho}) = \mathrm{Tr}\left[\hat{H}(\hat{\rho} - \hat{\sigma}_\rho)\right] = \sum_k \varepsilon_k^\uparrow \left(\rho_{kk} - \rho_{\tilde{\pi}_k,\tilde{\pi}_k} \right)$$

$\tilde{\pi}$: Rearrange $\{\rho_{kk}\}$ in descending order, $\rho_{\tilde{\pi}_k,\tilde{\pi}_k} \geq \rho_{\tilde{\pi}_{k+1},\tilde{\pi}_{k+1}}$

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- $\hat{\rho}$ & $\hat{\sigma}_\rho$ have the same amount of coherence: $C(\hat{\rho}) = C(\hat{\sigma}_\rho)$.

- $\hat{\rho}^{\downarrow} = \hat{\sigma}_\rho^{\downarrow}$.

  $\because$ $\hat{\rho} \longrightarrow \hat{\sigma}_\rho$ is unitary. $\implies$ $\hat{\rho}$ & $\hat{\sigma}_\rho$ have the same spectrum.

(Def. 2) $\mathcal{E}_i(\hat{\rho}) \equiv \mathcal{E}(\Delta(\hat{\rho})) = \mathcal{E}(\hat{\delta}_\rho)$

$$\mathcal{E}_i(\hat{\rho}) \equiv \mathcal{E}(\hat{\delta}_\rho) = \text{Tr}[\widehat{H}(\hat{\delta}_\rho - \hat{\delta}_\rho^\downarrow)]$$ $\mathcal{E}(\hat{\rho}) = \sum_k \varepsilon_k^\uparrow(\rho_{kk} - r_k^\downarrow)$

- Both $\hat{\delta}_\rho$ & $\hat{\delta}_\rho^\downarrow$ are diagonal in $\widehat{H}$-basis.

  $\Longrightarrow$ Unitary $\hat{\delta}_\rho \longrightarrow \hat{\delta}_\rho^\downarrow$ is reshuffling of $\widehat{H}$-basis.

- $\hat{\delta}_\rho$ & $\hat{\rho}$ has the same population in $\widehat{H}$-basis: $[\delta_\rho]_{kk} = \rho_{kk}$.

$\Longrightarrow$ Optimal reshuffling unitary $\hat{\delta}_\rho \longrightarrow \hat{\delta}_\rho^\downarrow$ is equivalent to $\widehat{V}_{\widetilde{\pi}}$.

$\therefore$ $\hat{\delta}_\rho^\downarrow$ has the same population as $\hat{\sigma}_\rho$, but no coherence.

$\Longrightarrow$ $\boxed{\hat{\delta}_\rho^\downarrow = \Delta(\hat{\sigma}_\rho)}$

$$\hat{\delta}_\rho^\downarrow = \Delta(\hat{\sigma}_\rho)$$

$$\text{Tr}[\hat{H}\Delta(\hat{\sigma}_\rho)] = \sum_k \varepsilon_k^\uparrow \langle \varepsilon_k^\uparrow | \hat{\sigma}_\rho | \varepsilon_k^\uparrow \rangle$$
$$= \text{Tr}[\hat{H}\hat{\sigma}_\rho]$$

$$\Longrightarrow \quad \text{Tr}[\hat{H}\hat{\sigma}_\rho] = \text{Tr}[\hat{H}\Delta(\hat{\sigma}_\rho)] = \text{Tr}[\hat{H}\hat{\delta}_\rho^\downarrow]$$

$$\therefore \quad \text{(Def. 2)} \quad \mathcal{E}_i(\hat{\rho}) = \text{Tr}[\hat{H}(\hat{\delta}_\rho - \hat{\delta}_\rho^\downarrow)] = \text{Tr}[\hat{H}(\hat{\rho} - \hat{\sigma}_\rho)]$$

Note: (Def. 1) $\mathcal{E}_i(\hat{\rho}) = \text{Tr}[\hat{H}(\hat{\rho} - \hat{\sigma}_\rho)]$

Therefore, the tow definitions are equivalent!

$$\mathcal{E}_i(\hat{\rho}) = \text{Tr}[\hat{H}(\hat{\delta}_\rho - \hat{\delta}_\rho^\downarrow)] = \text{Tr}[\hat{H}(\hat{\rho} - \hat{\sigma}_\rho)]$$

$\mathcal{E}_c(\hat{\rho})$:   The remaining ergotropy after excluding $\mathcal{E}_i$.

$$\mathcal{E}_c \equiv \mathcal{E} - \mathcal{E}_i$$

$$= \mathrm{Tr}\big[\hat{H}(\hat{\rho} - \hat{\rho}^{\downarrow})\big] - \mathrm{Tr}\big[\hat{H}(\hat{\rho} - \hat{\sigma}_{\rho})\big] = \mathrm{Tr}\big[\hat{H}(\hat{\sigma}_{\rho} - \hat{\rho}^{\downarrow})\big] \geq 0$$

$$= \sum_k \varepsilon_k^{\uparrow}\big(\rho_{\tilde{\pi}_k,\tilde{\pi}_k} - r_k^{\downarrow}\big)$$

$(\because \hat{\sigma}_{\rho}$ is active.$)$

- $\hat{\sigma}_{\rho}^{\downarrow} = \hat{\rho}^{\downarrow}$ & $\mathcal{E}_c(\hat{\rho}) = \mathrm{Tr}\big[\hat{H}(\hat{\sigma}_{\rho} - \hat{\rho}^{\downarrow})\big]$ ➡ $\mathcal{E}_c(\hat{\rho}) = \mathcal{E}(\hat{\sigma}_{\rho})$

- If $\hat{\rho}$ has no coherence: $\hat{\rho} = \hat{\delta}_{\rho}$ ➡ $\mathcal{E}_i(\hat{\rho}) \equiv \mathcal{E}(\hat{\delta}_{\rho}) = \mathcal{E}(\hat{\rho})$

$$\therefore \quad \mathcal{E}_c(\hat{\rho}) = 0$$

$\mathcal{E}_c(\hat{\rho}) \neq 0$ is due to the presence of coherence in $\hat{\rho}$.

$\mathcal{E}_c$: A part of extractable work which cannot be obtained by incoherent op.

- $\mathcal{E}_c(\hat{\rho}) \geq 0.$ (Nonzero if $\hat{\rho}$ has coherence.)

- $\mathcal{E}_c$ is NOT a coherence monotone.

$$\because \ \exists \ \text{incoh. op. } \hat{V}; \ \mathcal{E}_c(\hat{V}\hat{\rho}\hat{V}^\dagger) > \mathcal{E}_c(\hat{\rho})$$
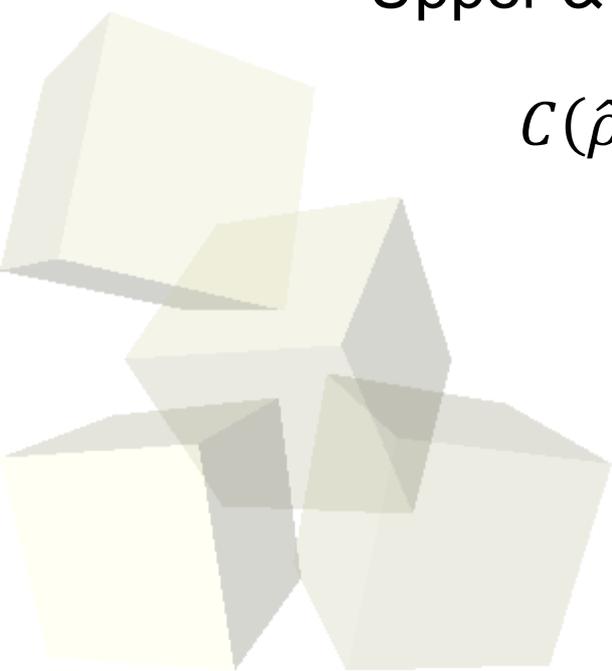
- Upper & lower bounds of $\mathcal{E}_c$ are related to C.

$$C(\hat{\rho}) - S(\hat{\rho}^\downarrow \| \hat{\rho}_\beta) \leq \beta \, \mathcal{E}_c(\hat{\rho}) \leq C(\hat{\rho}) + S(\hat{\delta}_\rho^\downarrow \| \hat{\rho}_\beta)$$

$$\text{with } \hat{\rho}_\beta \equiv e^{-\beta\hat{H}}/Z \quad \text{for } \forall\beta.$$

Upper bound when: $\hat{\rho}^\downarrow = \hat{\rho}_\beta$.

Lower bound when: $\hat{\delta}_\rho^\downarrow = \hat{\rho}_\beta$.

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(1) Derive $S(\hat{\rho}\|\hat{\rho}_\beta) = \beta \, \mathrm{Tr}[\hat{H}(\hat{\rho} - \hat{\rho}_\beta)] - S(\hat{\rho}) + S(\hat{\rho}_\beta)$

(2) Using the result of (1), derive

$$\beta \mathcal{E}_c(\hat{\rho}) = C(\hat{\rho}) + S(\hat{\delta}_\rho^{\downarrow}\|\hat{\rho}_\beta) - S(\hat{\rho}^{\downarrow}\|\hat{\rho}_\beta).$$

From this relation, confirm the upper & lower bounds and their saturation conditions.
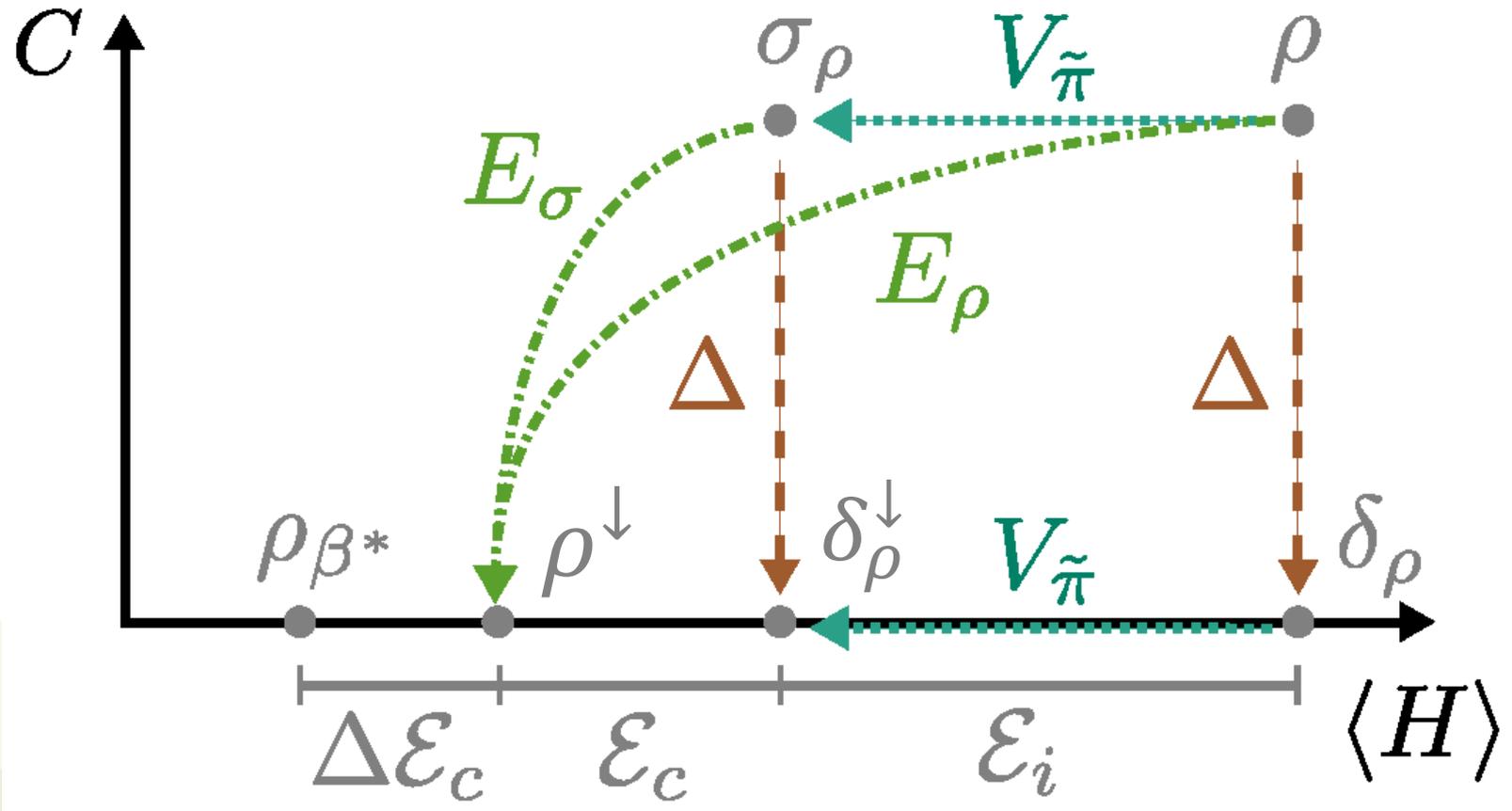
(Brief solution)

$$\beta \mathcal{E}_c = \beta(\mathcal{E} - \mathcal{E}_i) = \beta \, \mathrm{Tr}[\hat{H}(\hat{\sigma}_\rho - \hat{\rho}^{\downarrow})] = \beta \, \mathrm{Tr}[\hat{H}(\hat{\delta}_\rho^{\downarrow} - \hat{\rho}^{\downarrow})]$$

$$= \beta \, \mathrm{Tr}[\hat{H}(\hat{\delta}_\rho^{\downarrow} - \hat{\rho}_\beta)] - \beta \, \mathrm{Tr}[\hat{H}(\hat{\rho}^{\downarrow} - \hat{\rho}_\beta)]$$

Using the result of (1), we obtain:

$$= S(\hat{\delta}_\rho) - S(\hat{\rho}) + S(\hat{\delta}_\rho^{\downarrow}\|\hat{\rho}_\beta) - S(\hat{\rho}^{\downarrow}\|\hat{\rho}_\beta).$$
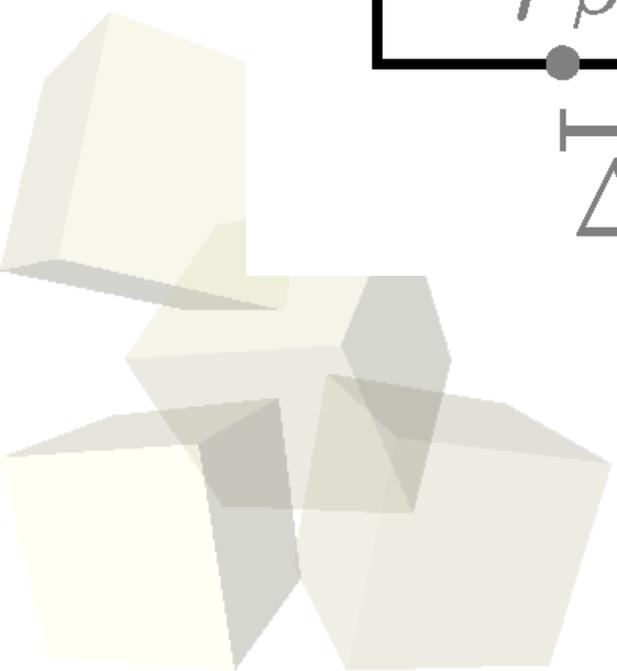
Francica *et al*., PRL **125**, 180603 (2020)

β^*: inverse temp. satisfying $S(\hat{\rho}_{\beta^*}) = S(\hat{\rho})$

Lecture 2: Ergotropy & coherence

I. Introduction & motivation

Quality of the stored energy & work extraction

II. Passivity & ergotropy

Passivity, ergotropy, "asymptotic freedom" of QBs, bound ergotropy

III. Coherence measure

Coherence monotone, relative entropy of coherence

IV. Coherent & incoherent ergotropy

A. E. Allahverdyan, R. Balian, and Th. M. Nieuwenhuizen,
EPL **67**, 565 (2004)

"Maximal work extraction from finite quantum systems"

T. Baumgratz, M. Cramer, and M. Plenio, PRL **113**, 140401 (2014)

"Quantifying Coherence"

G. Francica *et al.*, PRL **125**, 180603 (2020)

"Quantifying Coherence and Ergotropy"

W. Niedenzu, M. Huber, and E. Boukobza, Quantum **3**, 105 (2019)

"Concepts of work in autonomous quantum heat engines"

G. M. Andolina *et al.*, PRL **122**, 047702 (2019)

"Extractable Work, the Role of Correlations, and Asymptotic Freedom in Quantum Batterie"