

# All States are Universal Catalysts

## In Quantum Thermodynamics

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## Outline

1. Introduction to resource theoretic approach to q. thermodynamics
2. Quantum Catalysis
3. Results:
  - (a) multicopy catalysis (analytic)
  - (b) large dimension (numerical)
4. Outlook & open questions

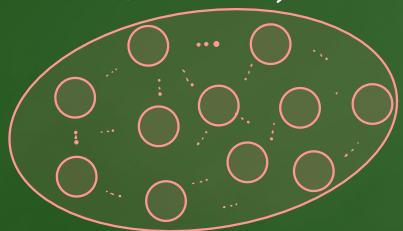
Resource-theoretic approach  
to quantum thermodynamics

# Resource-theoretic approach to q. thermodynamics I

- Framework suited to studying fundamental limits of q. thermo.<sup>1,2</sup>
  - Highly idealised, powerful framework.

## Ingredients:

- thermal bath  
(free state)



- Arbitrary Hamiltonian  $H_B$
- in thermal state at inv. temp  $\beta$

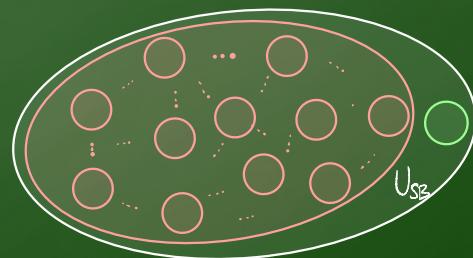
$$\tau_\beta(H_B) = e^{-\beta H_B}/Z$$

- non-equilibrium system  
(resource state)



- Arbitrary Hamiltonian  $H_S$
- state  $\rho_s \neq \tau_\beta(H_S)$

- energy-conserving  
interactions  
(allowed operations)



$$[U_{SB}, H_S + H_B] = 0$$

[1] Janzing, Wocjan, Zeier, Geiss & Beth, Int. J. Theor. Phys. (2000)

[2] Brandao, Horodecki, Oppenheim, Renes & Spekkens, PRL (2013)

## Resource-theoretic approach to q. thermodynamics II

- Usually interested in state transformations:

- thermal operations  
(TO)  $T_s[\rho_s] = \text{tr}_B [U_{SB} (\rho_s \otimes T_p(H_B)) U_{SB}^\dagger] = \sigma_s$

- write  $\rho_s \xrightarrow{\text{TO}} \sigma_s$  if  $\sigma_s = T_s[\rho_s]$  for some TO  $(T_p(H_B), U_{SB})$

Basic Question: Which state transformations  $\rho_s \xrightarrow{\text{TO}} \sigma_s$  are possible? (2nd law)

- for quasi-classical states: characterised by thermo-majorisation<sup>3</sup>  
(diagonal in energy eigenbasis)

- equivalent entropic formulation:<sup>4</sup>

$$D_H^\varepsilon(\rho_s \| T_s) \geq D_H^\varepsilon(\sigma_s \| T_s) \quad \forall 0 \leq \varepsilon \leq 1$$

- refinement of 2nd law

Hypothesis-testing relative entropy

$$D_H^\varepsilon(\rho \| \tau) = -\log \inf_M \text{tr}[M\tau]$$

s.t.  $0 \leq M \leq 1$   
 $\text{tr}[Mp] \geq 1 - \varepsilon$

[3] Horodecki & Oppenheim, Nat. Commun. (2013)

[4] Renes, J. Math. Phys. (2016)

# Quantum Catalysis

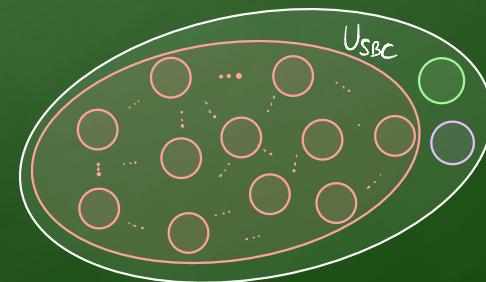
## Catalytic thermal operations I

- Thermal machines have both 'working substance' and 'rest'
  - Can view 'the rest' as a type of catalyst
    - auxilliary system that is returned to its initial state in some process.

Question: Do catalysts help in quantum thermodynamics? Ans: Yes!

New ingredient in resource-theoretic approach:

- Catalyst
  - - Arbitrary Hamiltonian  $H_c$
    - Must be returned in initial state.



## Catalytic thermal operations II

- New set of state transformations:

- Catalytic thermal operations  $T_{Sc}[\rho_s \otimes w_c] = \text{tr}_B \left[ U_{SBC} (\rho_s \otimes T_\beta(H_B) \otimes w_c) U_{SBC}^\dagger \right]$   
 $= \overline{\rho_s} \otimes w_c$

- Catalyst left unchanged
- Catalyst uncorrelated from system

- write  $\rho_s \xrightarrow{\text{CTO}} \overline{\rho_s}$  if there is a catalyst  $w_c$  s.t.

$$T_{Sc}[\rho_s \otimes w_c] = \overline{\rho_s} \otimes w_c$$

λ some TO  $(T_\beta(H_B), U_{SBC})$

## Catalytic thermal operations III

Basic question: which state transformations  $\rho_s \xrightarrow{\text{CTO}} \sigma_s$  are possible?

- Remarkably catalysis helps: exist  $\rho_s, \sigma_s$  s.t.  $\rho_s \xrightarrow{\text{TO}} \sigma_s$   
 $\rho_s \xrightarrow{\text{CTO}} \sigma_s$

- For quasi-classical states: characterised by "second laws"<sup>5</sup>

$$D_\alpha(\rho_s \parallel \tau_s) \geq D_\alpha(\sigma_s \parallel \tau_s) \quad \forall \alpha > 0$$

Rényi relative entropy (divergence)

$$D_\alpha(\rho \parallel \tau) = \frac{1}{\alpha-1} \log \text{tr} [\rho^\alpha \tau^{1-\alpha}]$$

## Catalytic thermal operations IV

- $D_\alpha(\rho_s \parallel \tau_s) \geq D_\alpha(\sigma_s \parallel \tau_s)$  guarantees existence of catalyst  $w_c$  s.t.  
 $\rho_s \otimes w_c \xrightarrow{\text{TO}} \sigma_c \otimes w_c$

but doesn't tell us anything about its properties

- e.g.
- what is the smallest dimension necessary?
  - Is the catalyst unique or highly special?
    - ↳ what properties must it have? low/high entropy? spread of energies?

Overarching goal: Understand how special quantum catalysts are

Initial intuition: catalysts should be very specialised

e.g. catalytic converters, tin openers doesn't seem to be true!

# Approximate quantum catalysis I

- Exact catalysis appears very strong or idealised.
  - Catalyst must be returned exactly.
- More reasonable to consider approximate catalysis

$\rho_s \xrightarrow[\epsilon_s, \epsilon_c]{CTO} \sigma_s$  if there is a catalyst  $w_c$  & TO s.t.

$$\sigma'_{sc} = T_{sc} [\rho_s \otimes w_c]$$

$$\| w_c - \sigma'_c \|_1 \leq \epsilon_c$$

$$\| \sigma_s - \sigma'_s \|_1 \leq \epsilon_s$$

- Consider approximation on both system & catalyst
- Recover exact catalysis when  $\sigma'_{sc} = \sigma_s \otimes w_c$ 
  - $\rightarrow$  (i)  $\epsilon_s = \epsilon_c = 0$
  - (ii) no correlation between  $S + C$

## Approximate quantum Catalysis II

- Care must be taken on the size of the error:

- if  $\epsilon_c = \text{constant}$ : All state transformations become possible<sup>5</sup>

i.e.  $\rho_s \xrightarrow[0, \epsilon_c]{\text{CTO}} \sigma_s$  possible for all quasiclassical  $(\rho_s, \sigma_s)$

- theory is unconstrained

In fact when<sup>6</sup>  $\epsilon_c \geq \frac{d_s - 1}{1 + (d_s - 1) \log d_s}$  theory unconstrained

- boundary of "embezzlement regime" of entanglement theory.

- if  $\epsilon_c = \frac{1}{\log d_s}$   $\rho_s \xrightarrow[0, \epsilon_c]{\text{CTO}} \sigma_s$  possible if  $\underbrace{\text{tr}(H_s \rho_s)}_{F(\rho_s)} - \text{TS}(\rho_s) \geq F(\sigma_s)$

[equivalent to  $D_1(\rho_s \| \sigma_s) \geq D_1(\sigma_s \| \sigma_s)$ ]

- i.e. "second laws" collapse back to "standard 2nd law"<sup>5</sup>

## Results

### (a) Multi-copy catalysts

- Consider a situation where the catalyst is a large collection of identical particles i.e. catalyst is  $w_c^{\otimes n}$  where  $w_c$  is arbitrary &  $n$  is large.

Question: Which states  $w_c$  are useful catalysts when  $n$  is large?

Intuition: • In asymptotic regime state transformations become reversible<sup>2</sup>



• transform  $w_c^{\otimes n}$  in useful catalyst  $w_c'^{\otimes m}$

• use  $w_c'^{\otimes m}$  to perform  $\rho_s \xrightarrow{\text{CTO}} \sigma_s$

• Reversibly transform  $w_c'^{\otimes m}$  back to  $w_c^{\otimes n}$  post-processing

i.e. full process appears catalytic for  $w_c^{\otimes n}$

## Embeddement regime protocol

Main idea . pre-process catalyst into target state  $\omega_c^{\otimes n} \xrightarrow{T_0} \sigma_c^{\otimes m}$

- probabilistically swap system with one of catalyst particles:

$$T_{sc}^{(mix)} [\rho_s \otimes \sigma_c^{\otimes m}] = \frac{1}{m+1} (\rho_s \otimes \sigma_c^{\otimes m} + \sigma_s \otimes \rho_{c1} \otimes \sigma_c^{\otimes (m-1)} + \dots + \sigma_s \otimes \sigma_c^{\otimes (m-1)} \otimes \rho_{cm})$$

$$\begin{array}{ccc} \otimes & \bigcirc & \dots \bigcirc \\ \rho_s & \sigma_c & \sigma_c \end{array} \longrightarrow \frac{1}{m+1} \left( \begin{array}{c} \otimes \bigcirc \dots \bigcirc + \bigcirc \otimes \dots \bigcirc \\ + \dots + \bigcirc \bigcirc \dots \otimes \end{array} \right)$$

Convex split lemma<sup>7</sup>

$$\| T_{sc}^{(mix)} [\rho \otimes \sigma^{\otimes m}] - \sigma \otimes \sigma^{\otimes m} \|_1^2 \leq \frac{2 D_\infty(\rho \parallel \sigma)}{m}$$

$$\longrightarrow \quad \epsilon_c \sim \frac{1}{\sqrt{n}} \quad \epsilon_s \sim \frac{1}{n} \quad d_c = d^n$$

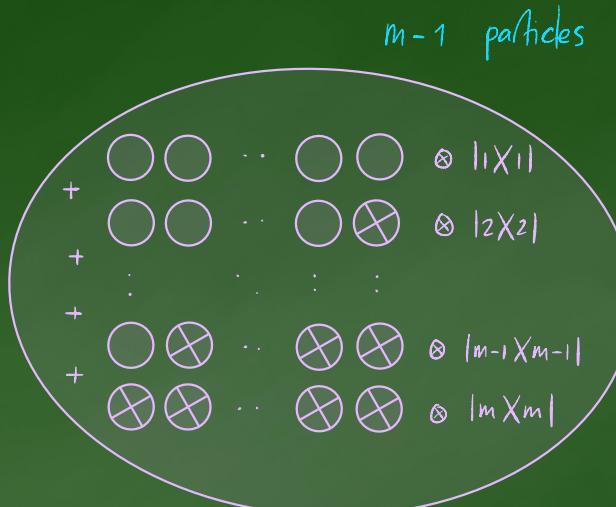
## Genuine catalysis regime protocol

- Smarter choice of target state: 'Duan state'<sup>8</sup>

$$\omega_c^D = \frac{1}{m} \sum_{i=1}^m \sigma^{\otimes(m-i)} \otimes \rho^{\otimes(i-1)} \otimes |i\rangle\langle i|$$

- Assume  $\rho_s^{\otimes m} \xrightarrow{\text{To}} \sigma_s^{\otimes m}$  for some  $m$

then  $\rho_s \otimes \omega_c^D \xrightarrow{\text{To}} \sigma_s \otimes \omega_c^D$



$$\begin{array}{c}
 + \quad \bigcirc \otimes \bigcirc \cdots \bigcirc \otimes \bigcirc \otimes |1 \times 1| \\
 + \quad \bigcirc \otimes \bigcirc \cdots \bigcirc \otimes \bigcirc \otimes |2 \times 2| \\
 + \quad \vdots \quad \ddots \quad \vdots \quad \vdots \\
 + \quad \bigcirc \otimes \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |m-1 \times m-1| \\
 + \quad \bigcirc \otimes \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |m \times m|
 \end{array}$$

$$\rho_s \otimes w_c^D$$

$\xrightarrow{\text{m-copy}}$   
 Conditional  
 on  $|m \times m|$

$$\begin{array}{c}
 + \quad \bigcirc \otimes \bigcirc \cdots \bigcirc \otimes \bigcirc \otimes |1 \times 1| \\
 + \quad \bigcirc \otimes \bigcirc \cdots \bigcirc \otimes \bigcirc \otimes |2 \times 2| \\
 + \quad \vdots \quad \ddots \quad \vdots \quad \vdots \\
 + \quad \bigcirc \otimes \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |m-1 \times m-1| \\
 + \quad \bigcirc \otimes \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |m \times m|
 \end{array}$$

↓

permute labels  $|i\rangle\langle i|$

$$\begin{array}{c}
 \bigcirc \otimes \bigcirc \cdots \bigcirc \otimes \bigcirc \otimes |1 \times 1| \\
 \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |2 \times 2| \\
 \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes \bigcirc \otimes |3 \times 3| \\
 \vdots \quad \ddots \quad \vdots \quad \vdots \\
 \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes \bigcirc \otimes |m \times m|
 \end{array}$$

$\xleftarrow[\text{systems}]{\text{permute}}$

$$\begin{array}{c}
 \bigcirc \otimes \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |1 \times 1| \\
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 \vdots \quad \ddots \quad \vdots \quad \vdots \\
 \bigcirc \otimes \bigcirc \otimes \cdots \bigcirc \otimes \bigcirc \otimes |m \times m|
 \end{array}$$

↑



$$\sigma_s \otimes w_c^D$$

## Genuine catalysis regime protocol

- Smarter choice of target state: 'Duan state':<sup>8</sup>

$$\omega_c^D = \frac{1}{m} \sum_{i=1}^m \sigma^{\otimes(m-i)} \otimes \rho^{\otimes(i-1)} \otimes |i\rangle\langle i|$$

- Assume  $\rho_s^{\otimes m} \xrightarrow{T_0} \sigma_s^{\otimes m}$  for some  $m$

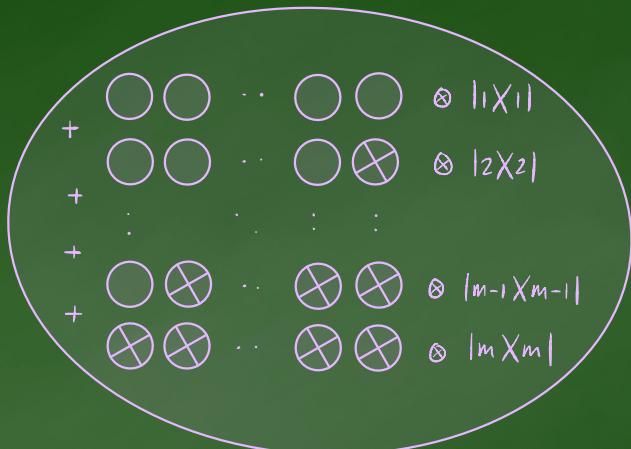
then  $\rho_s \otimes \omega_c^D \xrightarrow{T_0} \sigma_s \otimes \omega_c^D$

Lemma For quasi-classical states if  $D_\alpha(\rho_s \parallel \tau_s) > D_\alpha(\sigma_s \parallel \tau_s) \quad \forall \alpha$   
 (i.e. 2nd laws hold)

then for sufficiently large  $m$  there is a  $T_0$  such that

$$\rho_s^{\otimes m} \xrightarrow{T_0} \sigma_s^{\otimes m}$$

$$\longrightarrow \quad \epsilon_c \sim \frac{1}{n} \quad \epsilon_s \sim \frac{1}{n}$$



## (b) Large dimensional catalysts (numerical)

- Interesting to extend results beyond multi-copy catalysts
- first steps: numerical investigation of high-dimensional catalysts.  
restrict attention to 'noisy operations'  
i.e.  $H_S = H_B = H_C = 0$  (constant)

- Fix  $\rho$  and  $\sigma$  such that

$$\begin{array}{c} \rho \xrightarrow{\text{TO}} \sigma \\ \rho \xrightarrow{\text{CTO}} \sigma \end{array}$$

i.e. catalyst required.

- Choose a prob. distr.  $P_{\text{dist}}$  and pick  $d_C$  numbers + normalise  
→ simple method of sampling random catalysts
- Consider 3 possibilities:

$P_{\text{uni}}$  uniform  
 $\sim \text{const}$

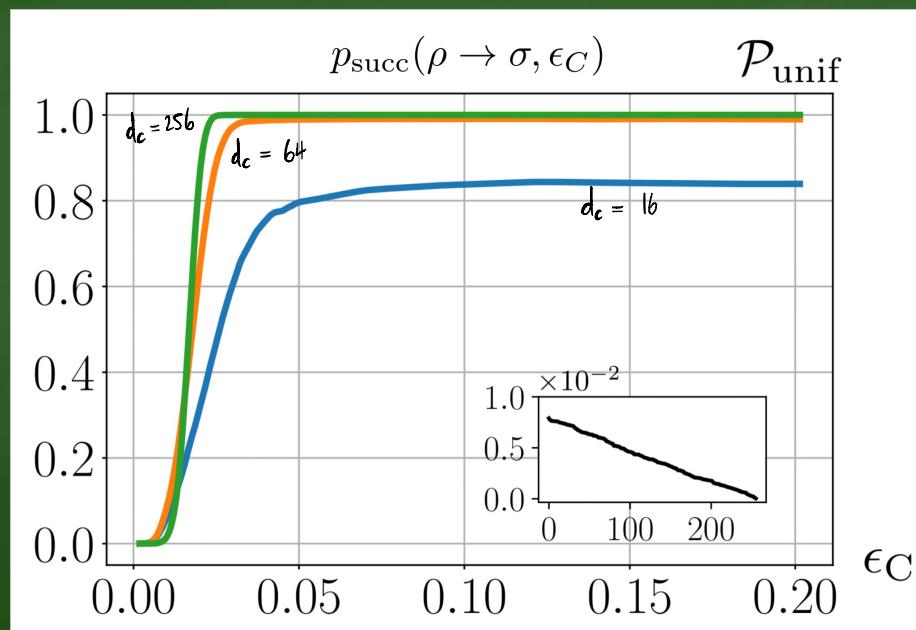
$P_{\text{exp}}$  exponential  
 $\sim e^{-x}$

$P_{\text{ray}}$  Rayleigh  
 $\sim x e^{-x^2/2}$

## (b) Large dimensional catalysts (numerical)

Question: How frequently does a randomly chosen catalyst catalyse  $\rho \rightarrow \sigma$  for a fixed error  $\epsilon_c$ ?  
→  $p_{\text{succ}}(\rho \rightarrow \sigma, \epsilon_c)$  prob. of catalysing.

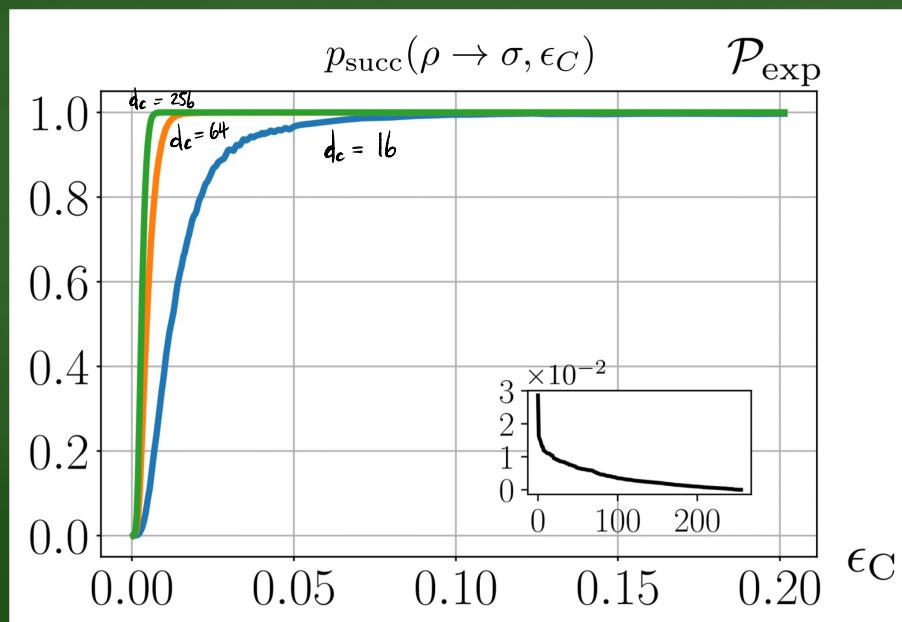
### Results



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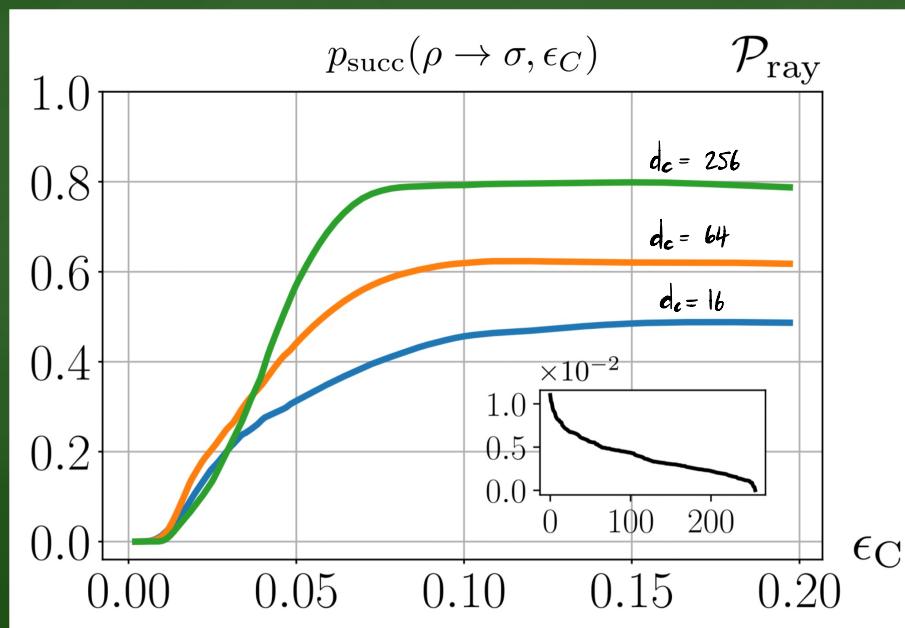
### Results



## (b) Large dimensional catalysts (numerical)

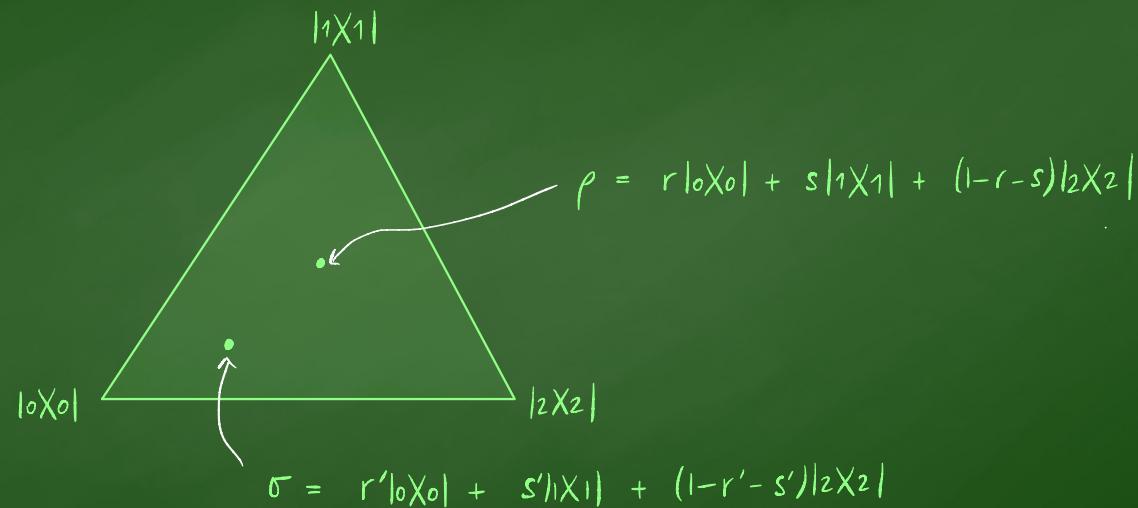
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→  $p_{\text{succ}}(\rho \rightarrow \sigma, \epsilon_c)$  prob. of catalysing.

### Results



## (b) Large dimensional catalysts (numerical)

- Above was for a single transformation. Important to understand how generic this is.  
→ Consider fixed initial state  $\rho$  and arbitrary final state  $\sigma$
- When  $d_s = 3$  all quasi-classical states can be represented as point in prob simplex.

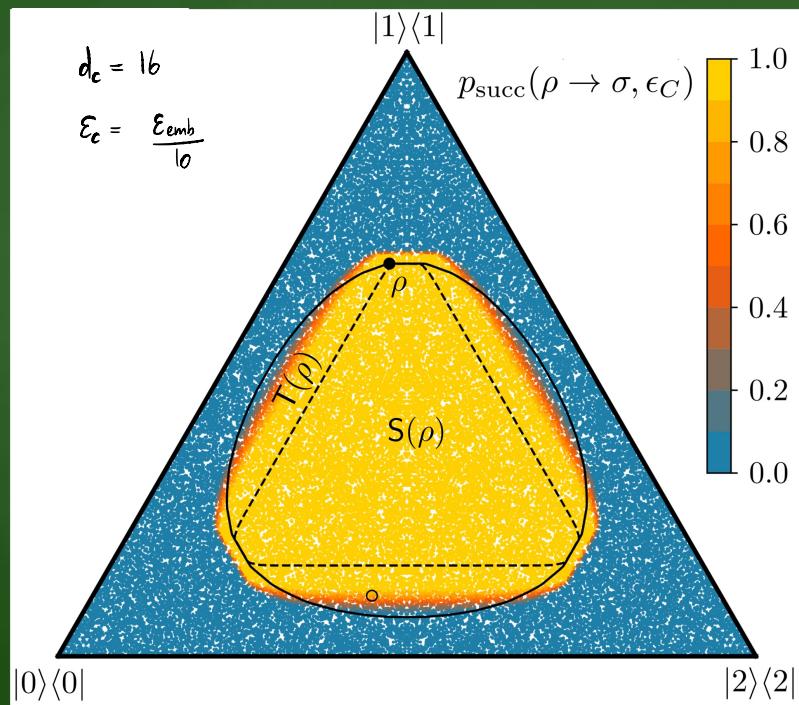


- Sets:  
 $S(\rho) = \{ \sigma \mid \rho \xrightarrow{\text{TO}} \sigma \}$  accessible set by TO  
 $T(\rho) = \{ \sigma \mid \rho \xrightarrow{\text{CTO}} \sigma \}$  accessible set by CTO

## (b) Large dimensional catalysts (numerical)

Question: How much of the catalytically accessible set  $T(\rho)$  does a random catalyst recover?

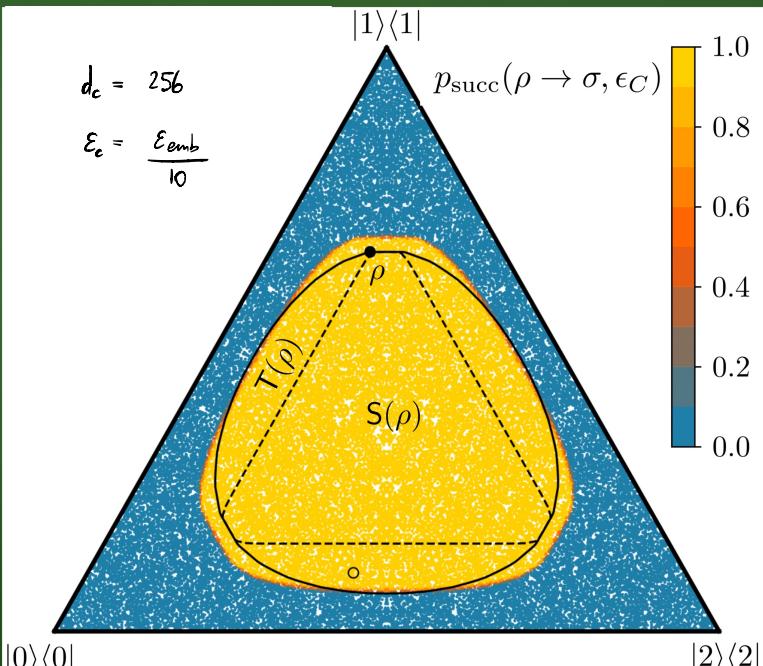
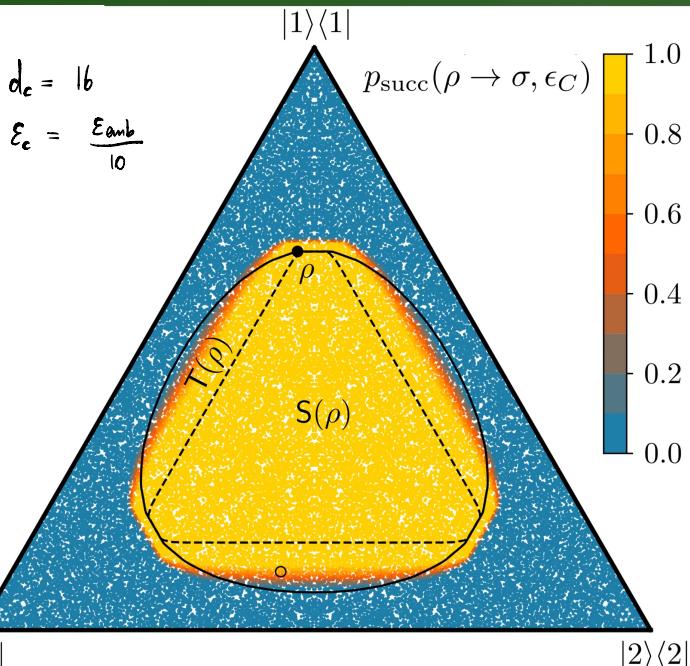
Results:



## (b) Large dimensional catalysts (numerical)

Question: How much of the catalytically accessible set  $T(\rho)$  does a random catalyst recover?

Results:



$P_{\text{exp}}$  used for sampling.

## (b) Large dimensional catalysts (numerical)

- Above was still for a fixed initial state  $\rho$ . Final step is to analyse arbitrary initial state.

- Define  $D(\rho) = T(\rho) \setminus S(\rho)$  region only accessible using catalyst  
 $= \{ \sigma \mid \rho \xrightarrow{\text{To}} \sigma, \rho \xrightarrow{\text{cto}} \sigma \}$

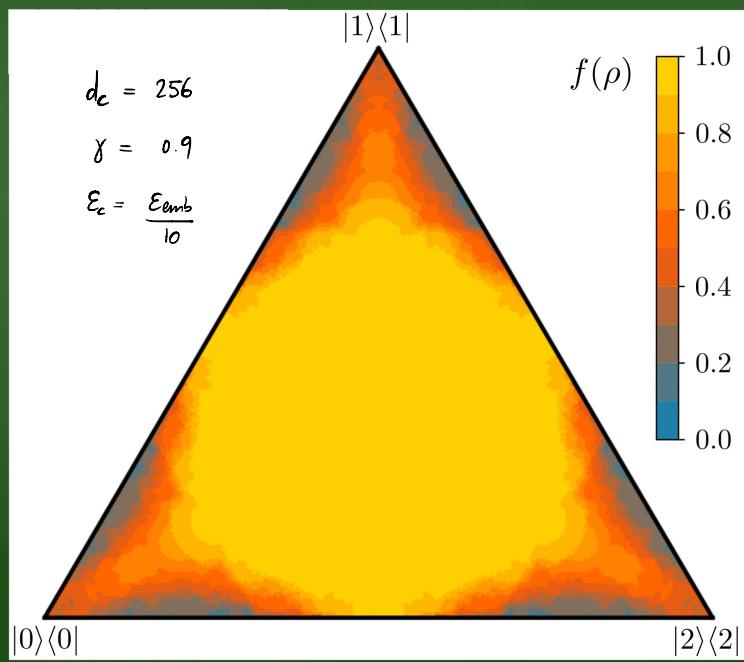
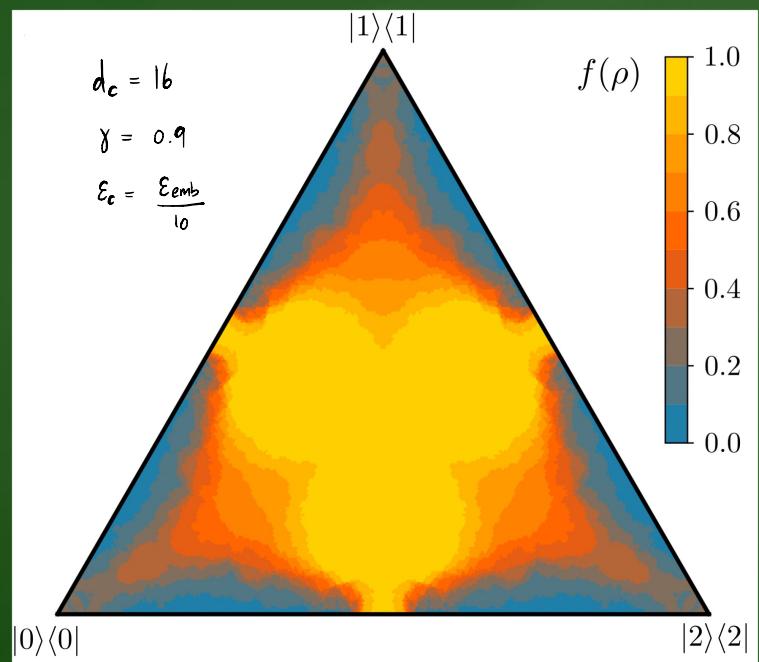
Question: what fraction of states inside  $D(\rho)$  have  $P_{\text{succ}}(\rho \rightarrow \sigma, \varepsilon_c) \geq \gamma$  ?

i.e. how likely is it that a catalytically-accessible transformation can be performed with high prob. using a catalyst of dimension  $d_c$  ?

(b) Large dimensional catalysts (numerical)

Question: What fraction of states inside  $D(\rho)$  have  $P_{\text{succ}}(\rho \rightarrow \sigma, \varepsilon_c) \geq \gamma$ ?

Results:



Outlook &

Open Questions

## Summary

- Any state can act as a quantum catalyst given sufficiently many copies
- catalytic property is universal - all possible transformations can be catalysed
- holds beyond q. thermodynamics - any majorisation-based q. resource theory
- Numerical investigations indicate that catalytic universality is generic
  - high dimensional q. systems are generally useful catalysts.

## Open Questions

- Big question: what is the mechanism underlying q. catalysis?
  - what physical properties are relevant / irrelevant? what is the resource?
- Prove analytically that all high-dimensional states are universal catalysts
  - + fix gap in proof of multi-copy states
- Understand the role that correlations & independence play in q. catalysis
- How much changes when we consider states with coherence between energy levels?
- Does universality hold in non-majorisation-based q. resource theories?