COMPOSITIONAL THERMODYNAMICS

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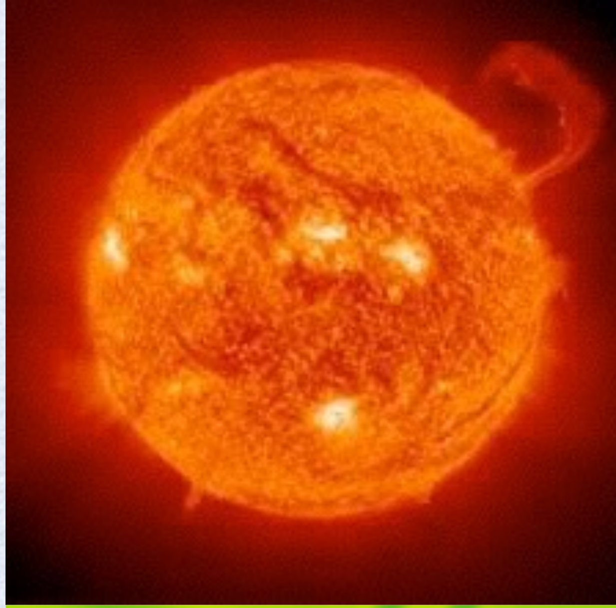
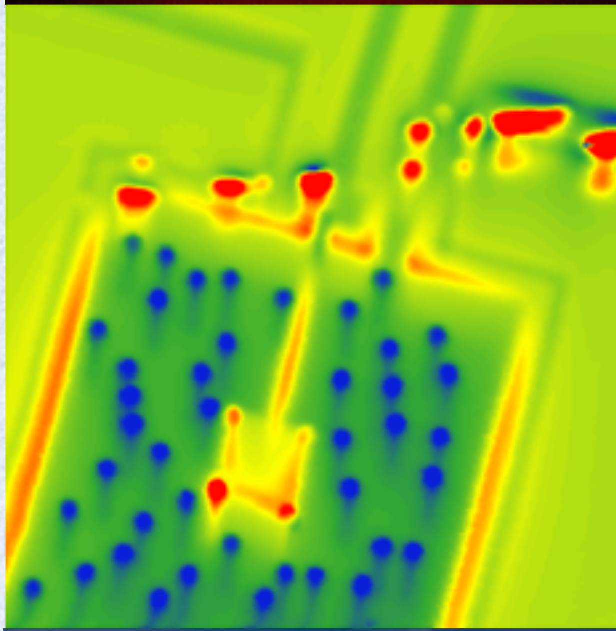
THERMODYNAMICS

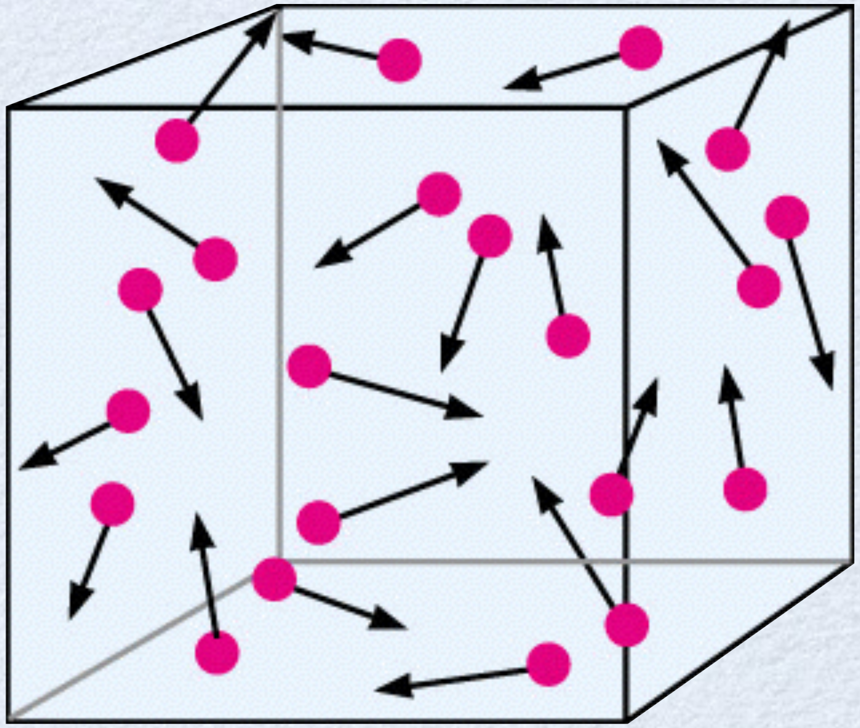
Thermodynamics provides a general paradigm that can be applied to different physical theories
(e.g. classical mechanics,
relativistic mechanics,
quantum mechanics).

Is this paradigm *universal*?
Which conditions must a physical theory satisfy in order to allow for a sensible thermodynamics?





FROM DYNAMICS TO THERMODYNAMICS



Statistical mechanics reduces thermodynamical to dynamical + probabilistic notions

- the initial state of the system is chosen at random according to a probability distribution
  e.g.
  $$p(\mathbf{r},\mathbf{p}) = \frac{1}{V}\left(\frac{\beta}{2m}\right)^{3/2} e^{-\beta\frac{|\mathbf{p}|^2}{2m}} \quad \text{or} \quad \rho = \frac{e^{-\beta H}}{\mathrm{Tr}[e^{-\beta H}]}$$

- thermodynamical quantities are expectation values

IN THE CLASSICAL WORLD: TENSION AT THE FOUNDATIONS

In the classical world of Newton and Laplace,
there is no place for probability at the fundamental level.

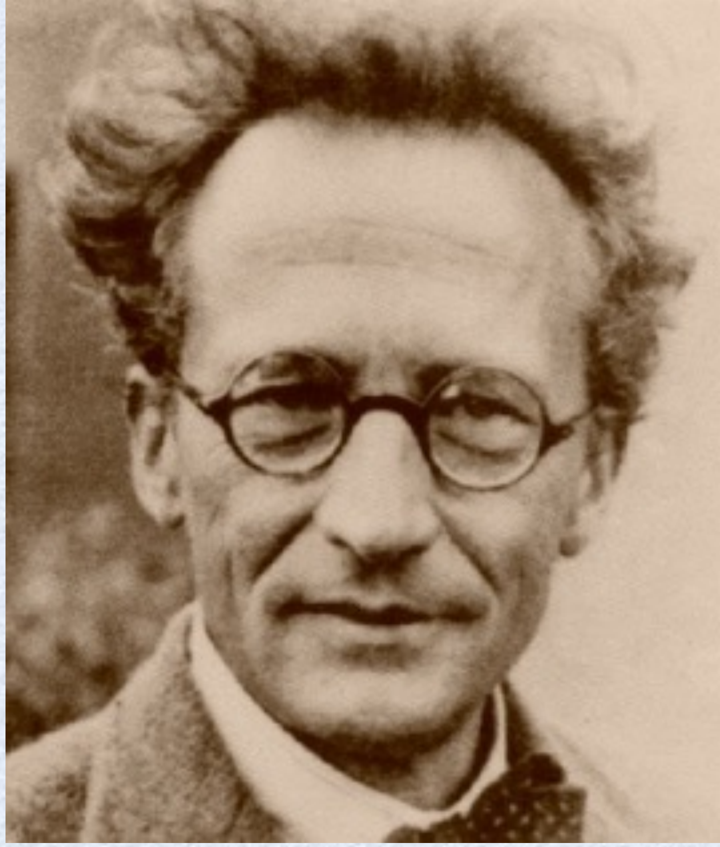
Why should measured quantities depend on the expectations of an agent?

Attempted explanations:

-ergodic theory,
-symmetries
-max ent principle
-...

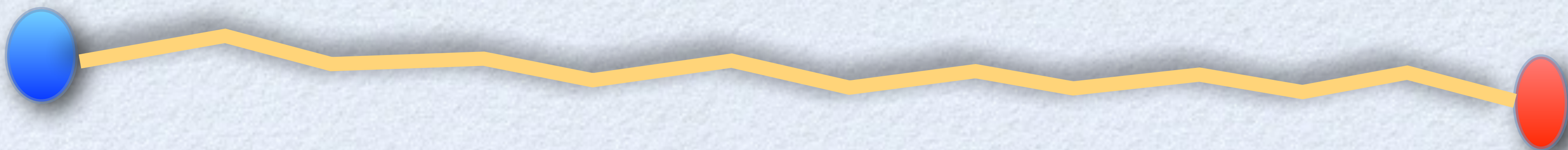
} single-system, non-compositional approaches

ENTERS COMPOSITIONALITY: THE QUANTUM CASE



In quantum theory,
probability has a different status:
mixed states can be modelled as
marginals of pure states

$$|\Psi\rangle_{AB}$$



ρ_A ρ_B

$$\rho_A = \mathrm{Tr}_B \left[|\Psi\rangle\langle\Psi| \right]$$

This property is called "purification"

PURIFICATION AS A FOUNDATION

Statistical ensembles from
pure states of the system + its environment

Popescu-Short-Winter 2006,
Gemmer-Michel-Mahler 2006,
...

Idea of this work: Abstract from quantum mechanics,
build an axiomatic foundation for
statistical mechanics in
general theories.

WHAT IS COMPOSITIONAL HERE?

1) The framework:

"general physical theories"
built on symmetric monoidal categories,
inspired by Abramsky and Coecke's
Categorical Quantum Mechanics.

2) The axioms:

specify properties of composition,
how physical systems are combined
together

PLAN OF THE TALK

1) The framework

2) The axioms

3) The results

THE FRAMEWORK:

OPERATIONAL-PROBABILISTIC THEORIES

Chiribella, D'Ariano, Perinotti,
Probabilistic Theories with Purification, Phys. Rev. A 81, 062348 (2010)

FRAMEWORKS FOR GENERAL PHYSICAL THEORIES

Single-system (non-compositional)

- Mackey
- Ludwig
- Gudder
- Piron
- Holevo

…

Composite systems

- Hardy 2001
- Abramsky-Coecke 2004
- D'Ariano 2006
- Barrett 2006
- Wilce-Barnum 2007
- CDP 2009, Hardy 2009

OPERATIONAL STRUCTURE

In a nutshell:

Strict symmetric monoidal category.

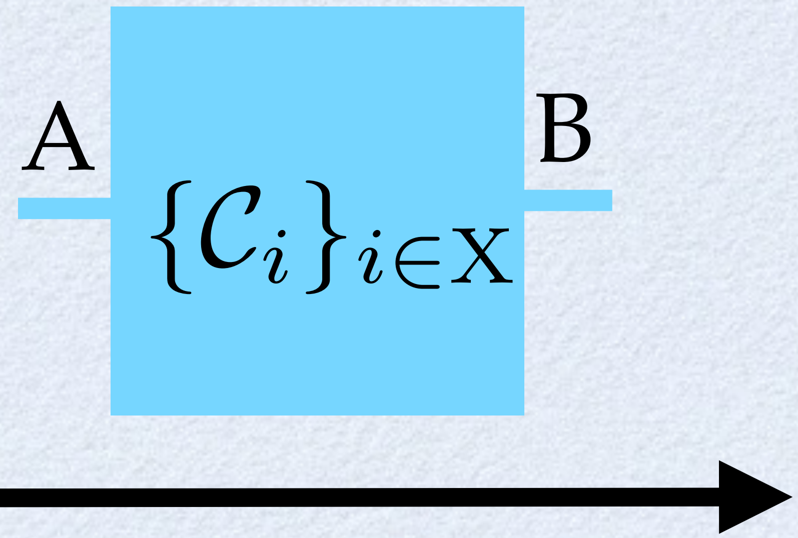
Objects = physical systems

Morphisms = (non-deterministic) physical processes

SYSTEMS AND TESTS

-Systems: A, B, C, ... , I = trivial system (nothing)

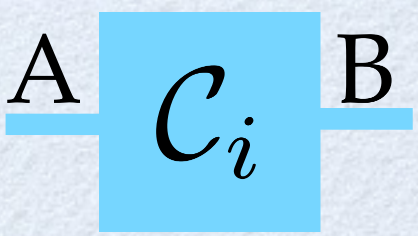
-Tests: a test represents a (non-deterministic) physical process



input-output arrow

A : input system
B : output system

i: outcome, in some outcome set X
$\mathcal{C}_i$: possible transformation,
graphically represented as

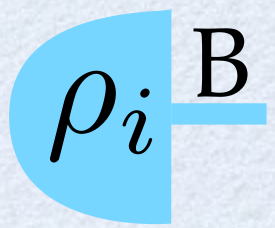


PREPARATIONS AND MEASUREMENTS

Special cases of tests:

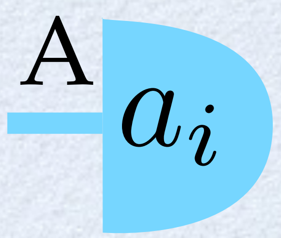
- trivial input: preparation

ρ_i : "state"



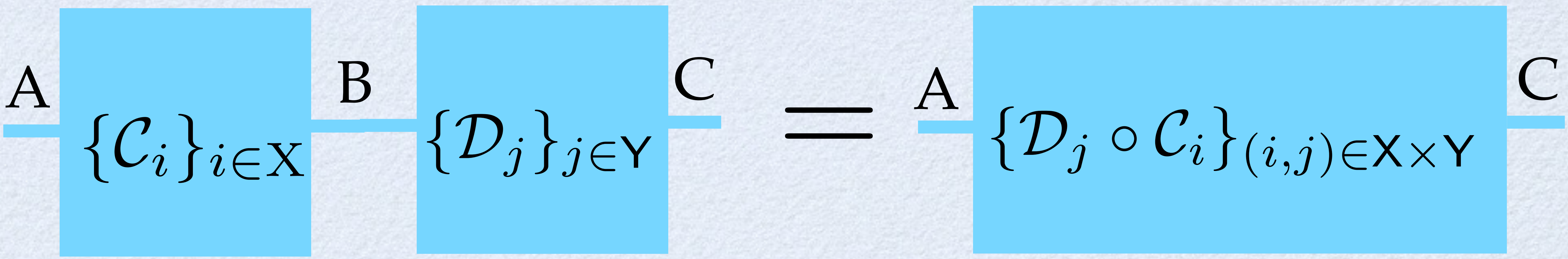
- trivial output: (demolition) measurement

a_i : "effect"

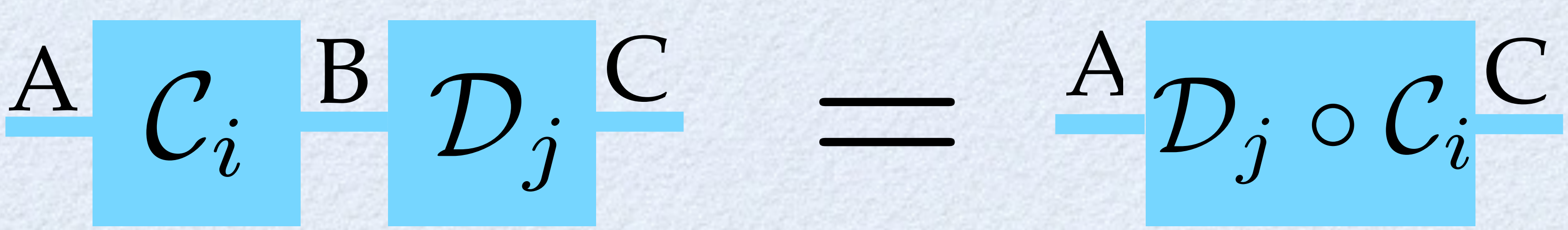


SEQUENTIAL COMPOSITION

-Sequential composition of tests:



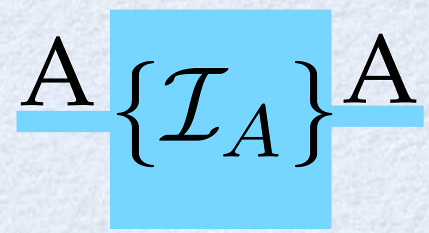
...induces sequential composition of processes:



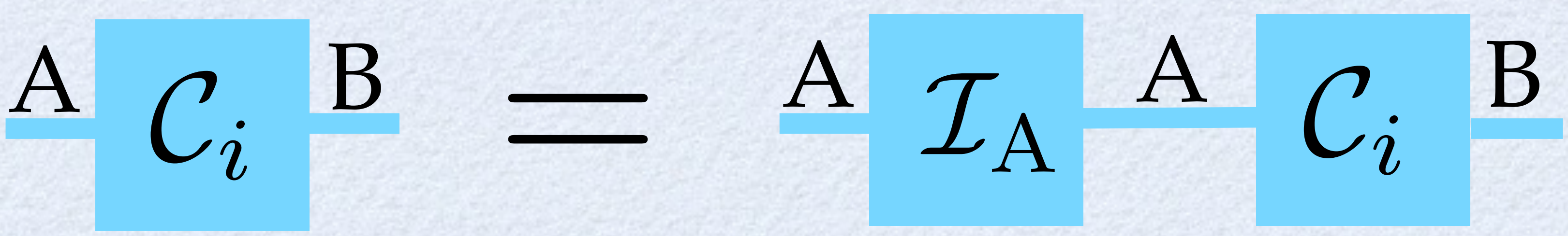
IDENTITY

Identity test on system A = doing nothing on system A

It is a test with a single outcome



where $\mathcal{I}_A$ is the identity process, defined by the relations



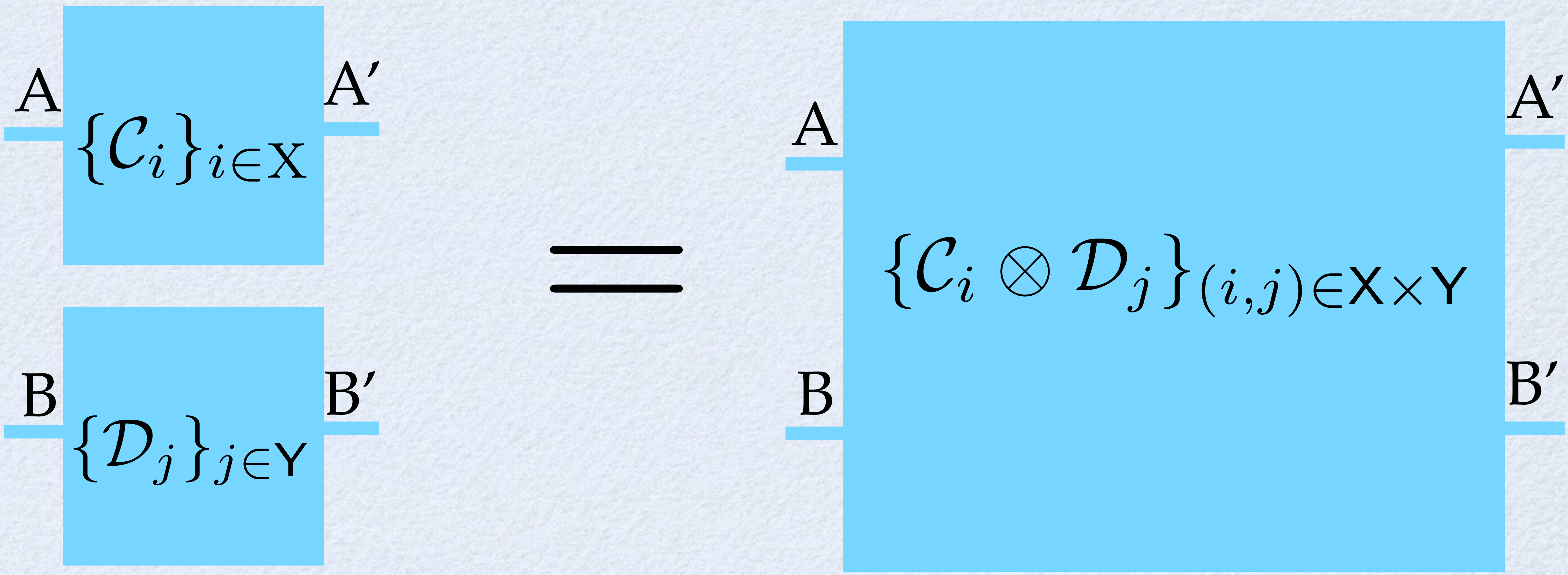
$\forall B, \forall \mathcal{C}_i$

$\forall C, \forall \mathcal{D}_j$

PARALLEL COMPOSITION

-Composite systems: $A \otimes B$ $\quad (A \otimes I = I \otimes A = A)$

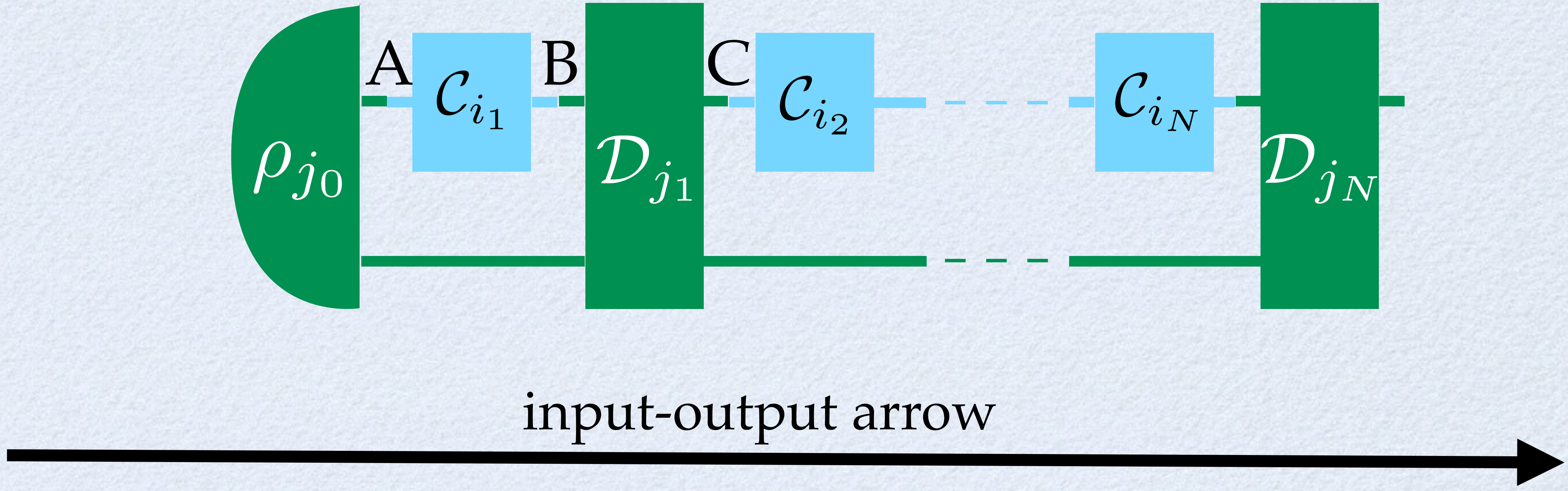
-Parallel composition of tests:



...induces parallel composition of processes
(same diagram, without brackets)

CIRCUITS

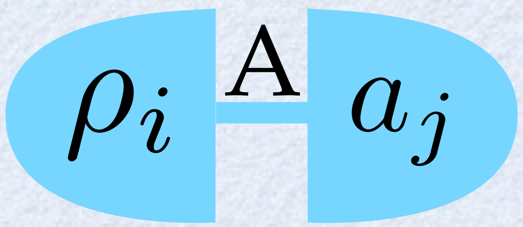
OPERATIONAL THEORY: a theory of devices that can be mounted to form circuits.



PROBABILISTIC STRUCTURE

PROBABILITY ASSIGNMENT

- Preparation + measurement = probability distribution

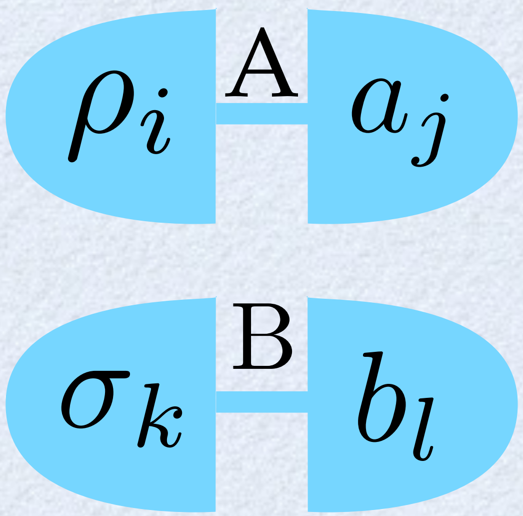


$$= \; p(a_j, \rho_i)$$

$$\begin{cases} p(a_j, \rho_i) \geq 0 \\ \sum_{i \in X} \sum_{j \in Y} p(a_j, \rho_i) = 1 \end{cases}$$

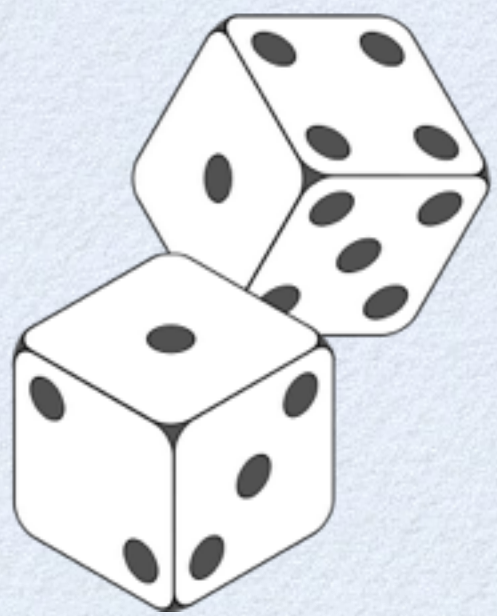
INDEPENDENT EXPERIMENTS

- Experiments performed in parallel are **statistically independent:**



$$= \quad p(a_j, \rho_i)\, p(b_l, \sigma_k)$$

e.g. the roll of two dice



OPERATIONAL-PROBABILISTIC THEORIES

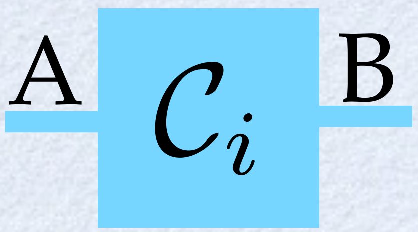
OPERATIONAL-PROBABILISTIC THEORIES (OPTS)

Operational-probabilistic theory
=
operational structure
+
probabilistic structure

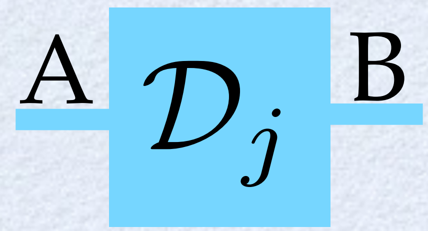
Examples:

-classical theory
-quantum theory
-quantum theory on real Hilbert spaces
-...

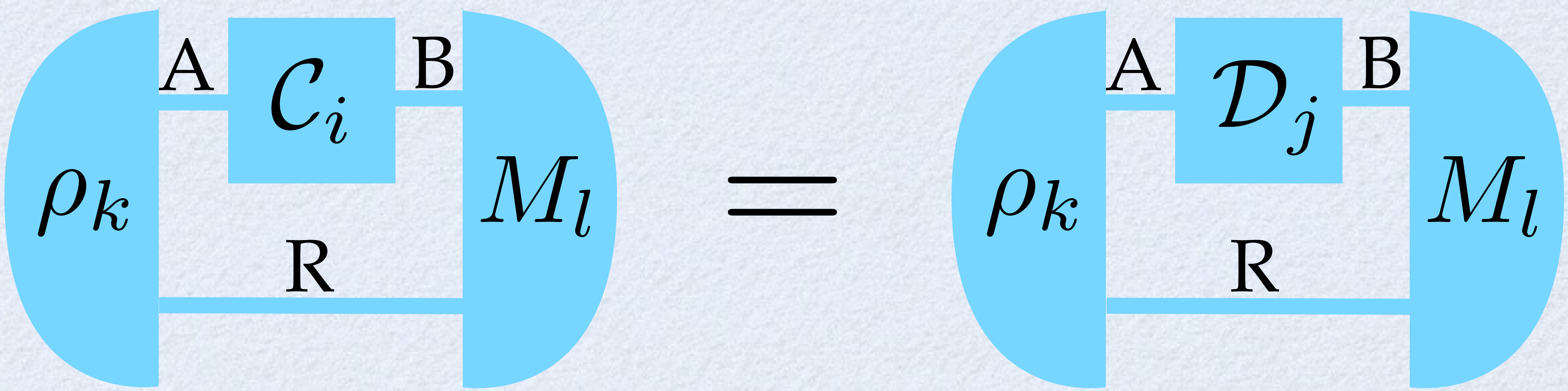
QUOTIENT THEORIES



and



are statistically equivalent iff



$$\forall R,\ \forall \rho_k,\ \forall M_l$$

The quotient yields a new OPT: the quotient theory

ORDERED VECTOR SPACE STRUCTURE

Theorem:

In the quotient theory

- the processes of type $A \to B$ span a real ordered vector space

$$\mathsf{Transf}_{\mathbb{R}}(A \to B)$$

- the sequential composition of two processes is linear in both arguments

$$\left(\sum_i x_i \, \mathcal{C}_i \right) \circ \left(\sum_j y_j \, \mathcal{D}_j \right) = \sum_{i,j} x_i y_j \, \left(\mathcal{C}_i \circ \mathcal{D}_j \right)$$

FINITARY ASSUMPTION

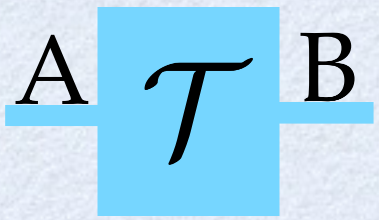
In this talk:

restrict our attention to finite systems, i.e. systems for which

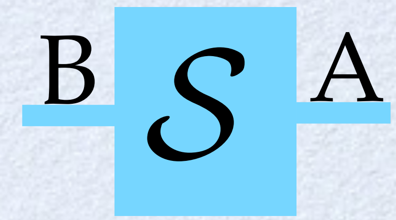
$$\dim \mathsf{St}_{\mathbb{R}}(A) < \infty$$

KEY NOTIONS

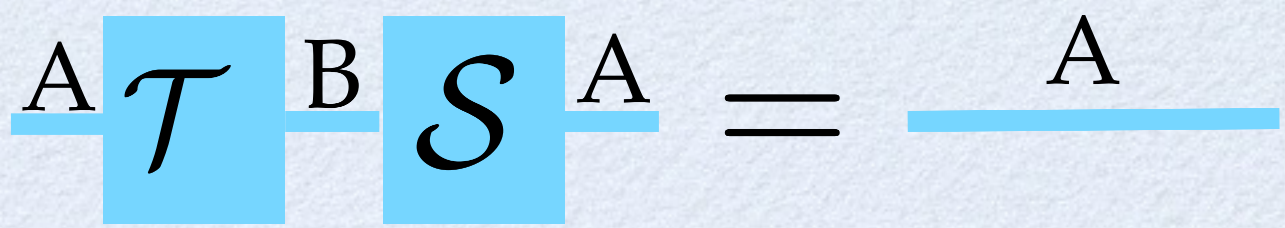
REVERSIBLE PROCESSES

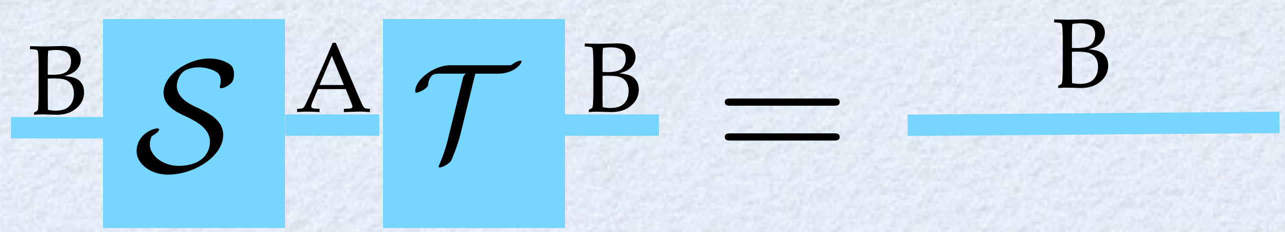


is reversible iff exists



such that





PURE PROCESSES

$\text{A}\!-\!\boxed{\mathcal{T}}\!-\!\text{B}$ is pure iff $\text{A}\!-\!\boxed{\mathcal{T}}\!-\!\text{B} = \sum_x \text{A}\!-\!\boxed{\mathcal{T}_x}\!-\!\text{B}$

implies $\text{A}\!-\!\boxed{\mathcal{T}_x}\!-\!\text{B} \propto \text{A}\!-\!\boxed{\mathcal{T}}\!-\!\text{B} \quad \forall x$

special case: pure states

$\psi\!-\!\text{A}$ is pure iff $\psi\!-\!\text{A} = \sum_x \psi_x\!-\!\text{A}$

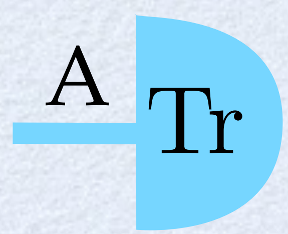
implies $\psi_x\!-\!\text{A} \propto \psi\!-\!\text{A} \quad \forall x$

AXIOMS

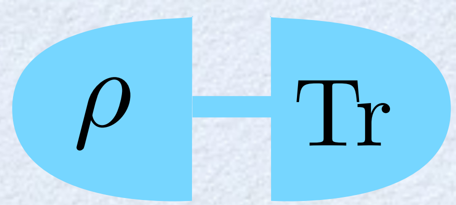
AXIOM 1: CAUSALITY

Operations performed in the future cannot affect the probability of outcomes of experiments done in the present

Equivalently: there is only one way to discard a system



e.g. in QT:

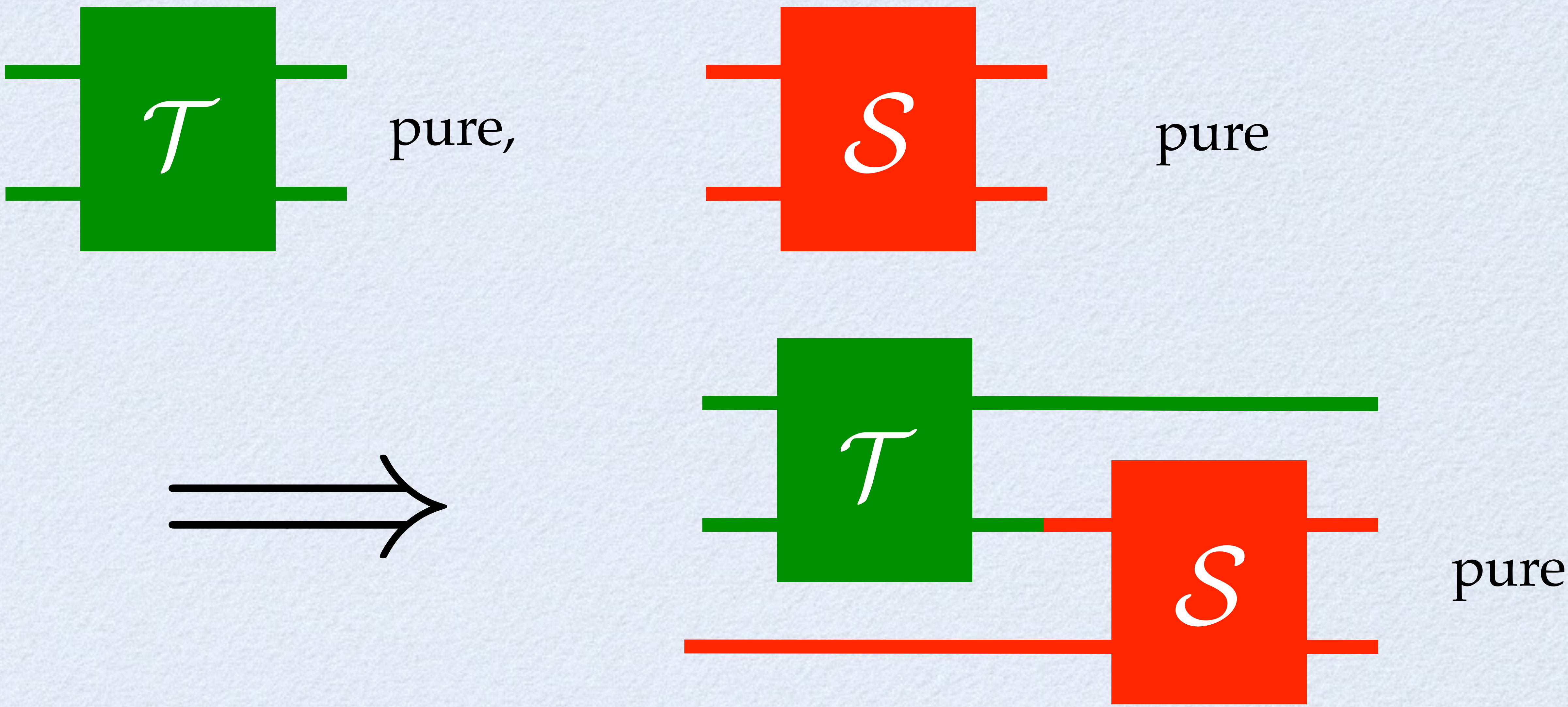


$= \mathrm{Tr}[\rho]$

$$\rho_A := \mathrm{Tr}_A[\rho_{AB}]$$

AXIOM 2: PURITY PRESERVATION

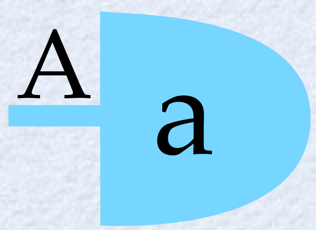
Purity Preservation: the composition of pure transformations is pure



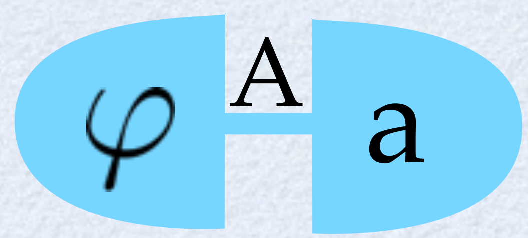
Special case: the product of two pure states is a pure state.

AXIOM3: PURE SHARPNESS

Pure Sharpness: for every system,
there exist at least one pure effect that
happens with probability 1 on some state.

$\forall A \quad \exists$ 

such that

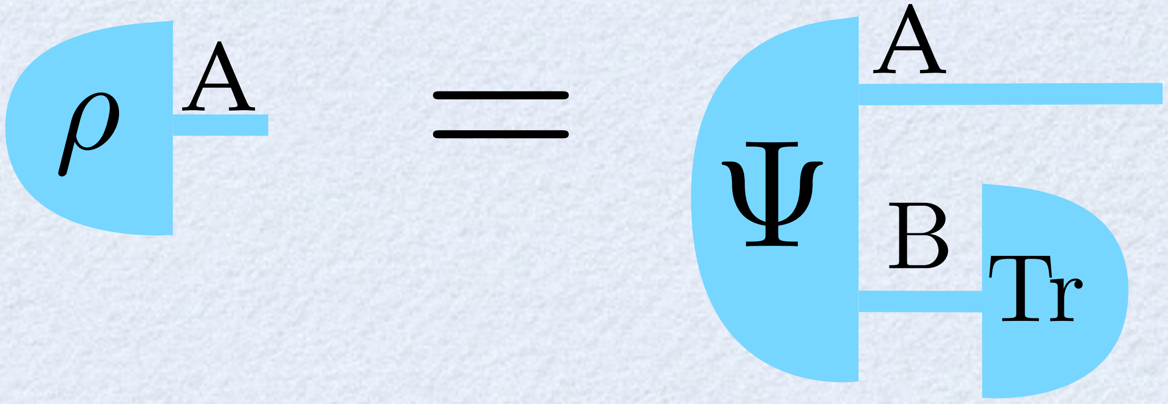
- a is pure
- 

$= 1$

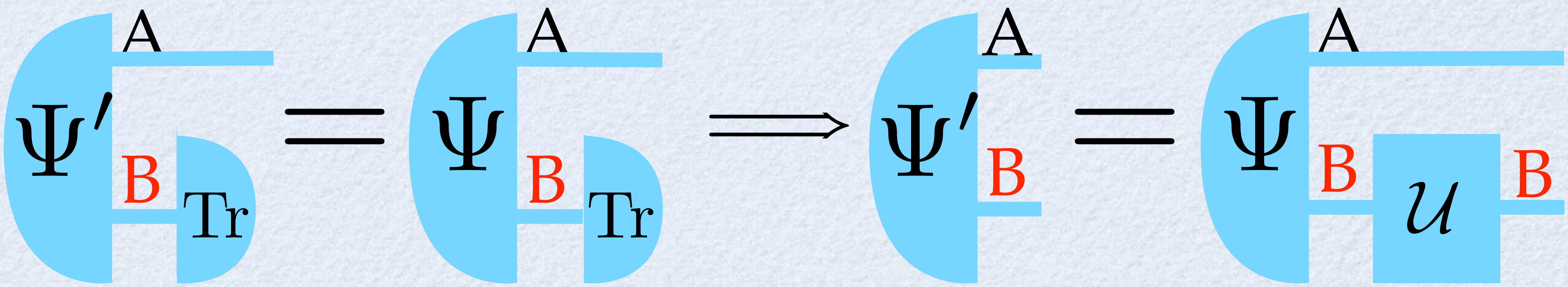
for some state φ

AXIOM 4: PURIFICATION

- **Existence:** For every state ρ of A
  there is a system B and a pure state Ψ of $A \otimes B$
  such that

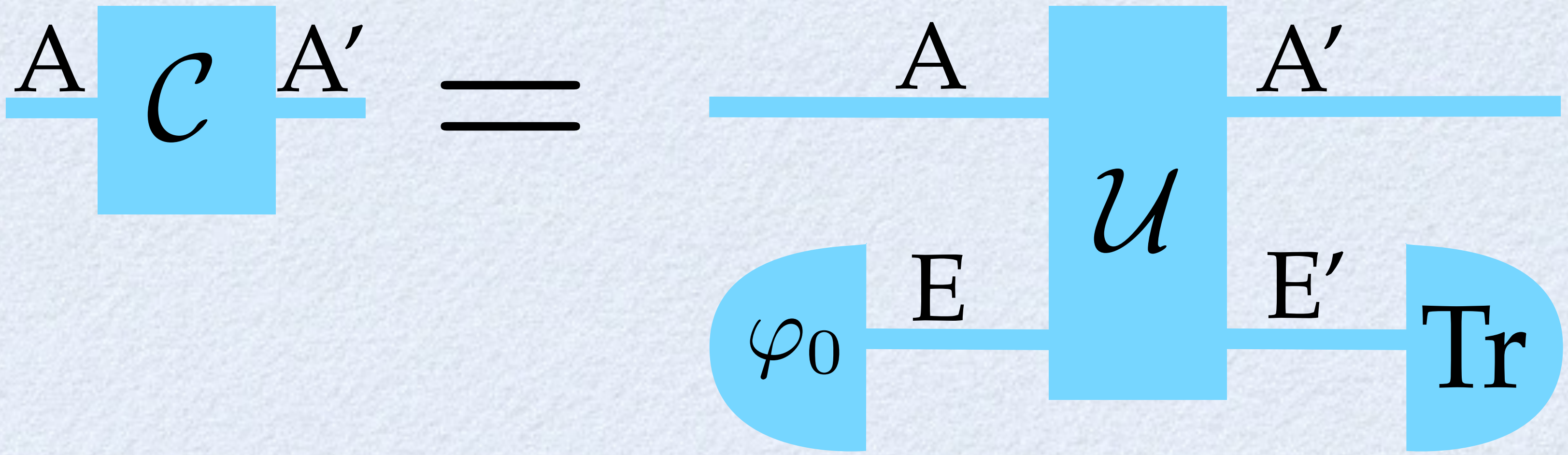


- **Uniqueness:** two purifications of the same state are equivalent
  up to a reversible transformation



PURIFICATION: EQUIVALENT FORMULATION

Theorem: For every process
there exist environments E and E′
a pure state of E ,
and a reversible process from AE to A′E′ such that



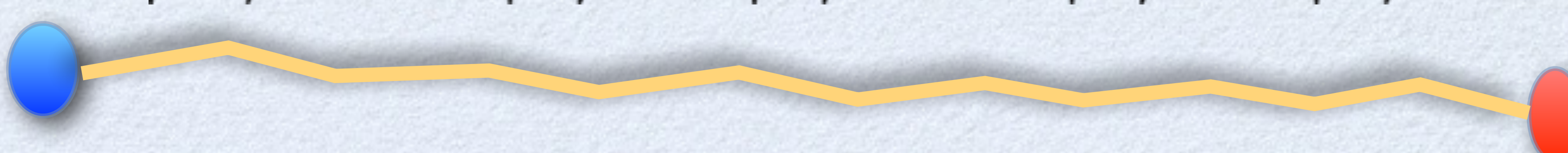
This simulation is unique up to reversible processes
on the environment.

EXAMPLES OF THEORIES SATISFYING THE AXIOMS

- quantum theory
- real vector space quantum theory
- other variants of quantum theory
- classical theory (!)

  suitably extended with non-classical systems

$$|\Psi\rangle = \alpha\,|0\rangle \otimes |0\rangle + \beta\,|1\rangle \otimes |1\rangle$$



classical bit

non-classical bit

RESULTS

Chiribella and Scandolo,
Entanglement as an axiomatic foundation for statistical mechanics
arXiv:1608.04459

THE DIAGONALIZATION THEOREM

Thm: In a theory satisfying the 4 axioms,
every state can be *diagonalized*, i.e. decomposed as

$$\rho = \sum_i p_i \psi_i$$

$\{\psi_i\}$ pure states $\{p_i\}$ probabilities (the "spectrum")

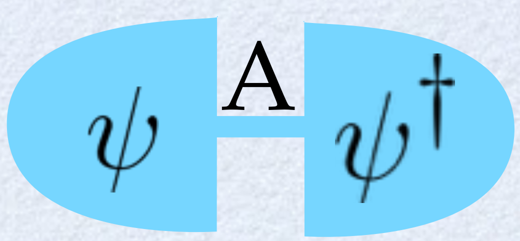
The spectrum is uniquely defined,
the diagonalization is canonical.

Corollary: There exist distinguishable states.

THE STATE-EFFECT DUALITY

Thm: For every system A,
there exists a linear, order-preserving isomorphism $\dagger$
between $\mathsf{St}_{\mathbb{R}}(\mathrm{A})$ and $\mathsf{Eff}_{\mathbb{R}}(\mathrm{A})$

For every pure normalized state ψ ,
one has



$= 1$ (cf. Hardy's Sharpness Axiom)

OBSERVABLES

Observables := elements of $\mathsf{Eff}_{\mathbb{R}}(\mathrm{A})$

Thm. Every observable H, can be diagonalized as

$$H = \sum_i E_i \, \psi_i^\dagger$$

$$\{E_i\} = \text{real numbers (the ``values'')}$$

$$\left\{\psi_i^\dagger\right\} = \text{``measurement''}$$

FUNCTIONAL CALCULUS

Given an observable $H = \sum_i E_i \, \psi_i^\dagger$

and a function $f : \mathbb{R} \to \mathbb{R}$

one can define a new observable $f(H) := \sum_i f(E_i) \; \psi_i^\dagger$

Formally, we have all the tools required to define the Gibbs state:

$$\rho_{\text{Gibbs}} = \frac{e^{-\beta H^\dagger}}{\text{Tr}\left[e^{-\beta H^\dagger}\right]}$$

But what is the interpretation of this state?

PURITY

THE RARE PARADIGM

An agent has partial control on the parameters of a reversible dynamics:

$$p_x$$

As a result, she implements a
Random Reversible (RaRe) transformation

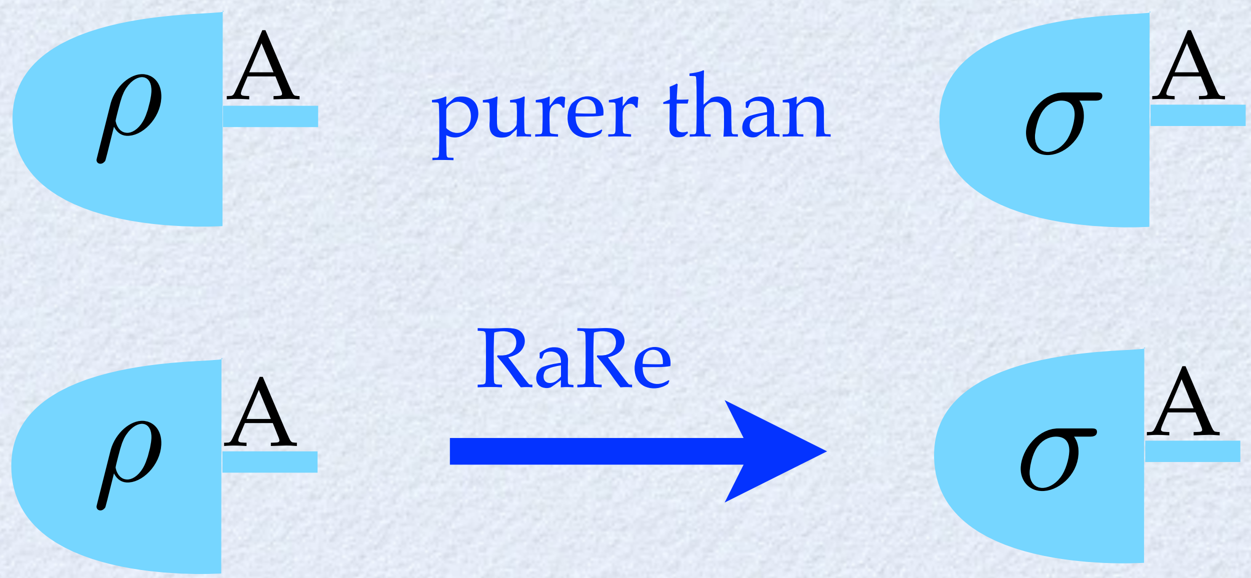
$$\mathcal{R} = \sum_x p_x \, \mathcal{U}_x$$

RaRe transformations = monoidal subcategory of the category of transformations

THE PURITY PREORDER

Definition:

iff

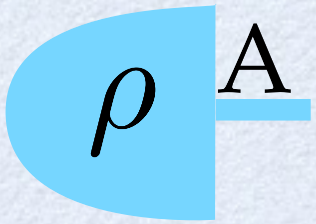


cf. group majorization by Masanes & Müller

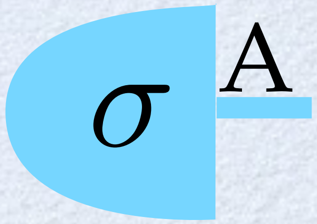
> Proposition. The pure states are maxima,
> the invariant state is the minimum.

PURITY MONOTONES AND ENTROPIES

Definition: $f : \mathsf{St}(\mathrm{A}) \to \mathbb{R}$ is a purity monotone if



purer than



implies $f(\rho) \geq f(\sigma)$

Definition: A family of functions $f_{\mathrm{A}} : \mathsf{St}(\mathrm{A}) \to \mathbb{R}$

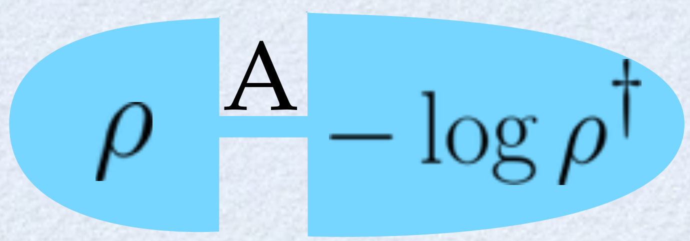
is an entropy if

- $-f_A$ is a purity monotone
- $f_{\mathrm{A}\otimes\mathrm{B}}(\rho \otimes \sigma) = f_{\mathrm{A}}(\rho) + f_{\mathrm{B}}(\sigma)$

EXAMPLE

Shannon / von Neumann entropy:

$$S(\rho) = \left\langle -\log \rho^{\dagger} \right\rangle$$

$=$ 

$$= \sum_i -p_i \log p_i \qquad \rho = \sum_i p_i \psi$$

ENTROPY / ENERGY TRADEOFF

CHARACTERIZATION OF THE GIBBS STATE

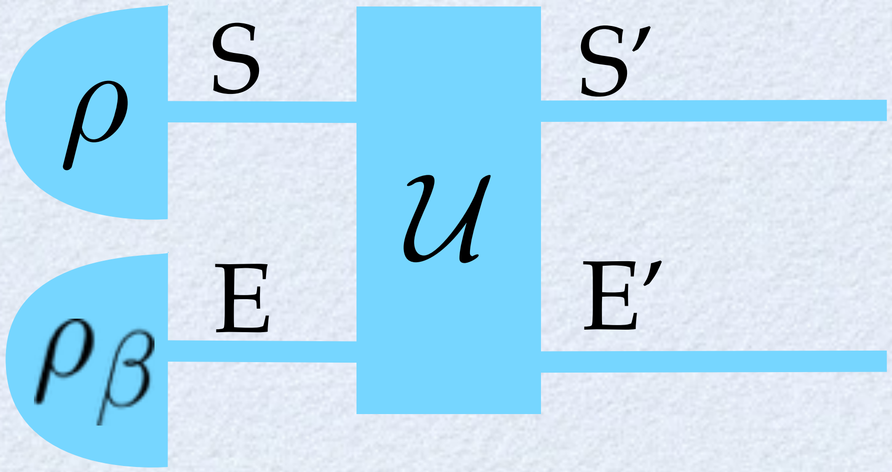
Proposition: In every theory satisfying the 4 axioms, the Gibbs state

$$\rho_{\text{Gibbs}} = \frac{e^{-\beta H^\dagger}}{\text{Tr}\left[e^{-\beta H^\dagger}\right]}$$

is the state with maximum S/vN entropy among the states with given expectation value of H.

LANDAUER'S PRINCIPLE

Suppose that the system interacts reversibly with an environment in the Gibbs state



In every theory satisfying the 4 axioms, one has

$$\langle H'_{\mathrm{E}} \rangle - \langle H_{\mathrm{E}} \rangle \geq \frac{S(\rho) - S(\rho')}{\beta}$$

CONCLUSIONS

4 axioms for thermodynamics

- Causality
- Purity Preservation
- Pure Sharpness
- Purification

Obtain diagonalization, entropies, Gibbs states, and Landauer's principle.

Conjecture: every physical theory admitting a thermodynamical description can be extended to a theory that satisfies the 4 axioms.

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