Operadic Composition of Thermodynamical Systems

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Overview

1. What is entropy?
2. Thermostatic systems
3. Composing thermostatic systems
   (the central dogma)
4. ... with operads!

Examples

Conclusion

References

Part 1: What is Entropy?

Can point to many things called entropy...

- Shannon Entropy
- Thermodynamic (empirically measured) entropy
- von Neumann entropy
- Rényi entropy

Why do we care about Entropy?

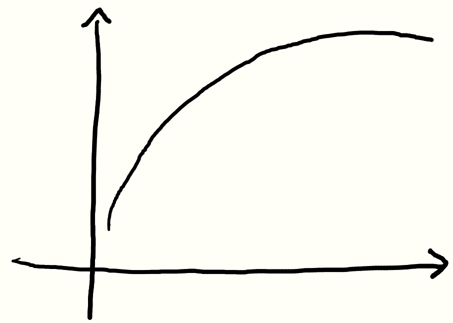
- Maximizing it subject to a constraint often gives us the answer to a question we care about.
    - What prior should we choose?
    - Where is the equilibrium?
    - What kind of large deviation is likely?

What is entropy?

Without answering completely, we can make some assumptions.

(1) Function of states
(2) "Mixing" increases it.
(3) Additive over independent subsystems
(4) Something we want to maximize subject to constraints.

This talk will formalize the above picture



Formalize (1) + (2)

Def A *thermostatic system* consists of

- A convex space X
- A concave function $S : X \to \overline{\mathbb{R}} = \mathbb{R} \cup \{\pm\infty\}$

Ex $X = \{\text{prob distributions on } \{1 \dots n\}\}$

$$S(p) = -\sum_{i=1}^{n} p_i \log p_i$$

Why / what is convexity / concavity?

Def A **convex space** is a set X along with a function $c_\lambda : X \times X \to X$ for $\lambda \in [0,1]$ called the **mixing operation**, such that

- $c_1(x,y) = x$ (identity)
- $c_\lambda(x,x) = x$ (idempotency)
- $c_\lambda(x,y) = c_{1-\lambda}(y,x)$ (symmetry)
- $c_\lambda(c_\gamma(x,y),z) = c_{\lambda\gamma}(x, c_\eta(y,z))$ if $\eta(1-\lambda\gamma) = \lambda(1-\gamma)$ (associativity)

Ex Vector spaces, with $c_\lambda(x,y) = \lambda x + (1-\lambda) y$

Note Originally "Barycentric algebras" by Stone in 1949

Def/Ex A convex subspace $U \subseteq X$ of a convex space X is a subset $U \subseteq X$ such that

$$x, y \in U \Rightarrow c_\lambda(x,y) \in U \quad \forall \lambda \in [0,1]$$

Convex subspaces are convex spaces

Ex $\Delta^n = \{ p \in \mathbb{R}^{n+1} \mid \sum_{i=0}^{n} p_i = 1,\ p_i \geq 0\ \forall i \}$

Ex If $(A, \vee)$ is a semilattice, i.e.

- $a \vee a = a$
- $a \vee b = b \vee a$
- $(a \vee b) \vee c = a \vee (b \vee c)$

Then

$$c_\lambda(a,b) = \begin{cases} a & \text{if } \lambda = 1 \\ b & \text{if } \lambda = 0 \\ a \vee b & \text{otherwise} \end{cases}$$

makes A into a convex space.

Def Let $\overline{\mathbb{R}} = \mathbb{R} \cup \{\pm\infty\}$ have convex structure

$$c_\lambda(x,y) = (1-\lambda)x + \lambda y \quad \text{for } x,y \in \mathbb{R}$$

$$c_\lambda(x,+\infty) = +\infty \quad \text{for } x \in \mathbb{R},\ \lambda \in (0,1]$$

$$c_\lambda(x,-\infty) = -\infty \quad \text{for } x \in \mathbb{R} \cup \{+\infty\},\ \lambda \in (0,1]$$

Note that $-\infty$ "beats" $+\infty$

Prop Every subset $U \subseteq \overline{\mathbb{R}}$ has a least upper bound.

Proof sup of an unbounded above set is $+\infty$

sup of an empty set is $-\infty$

Def A convex-linear function $f: X \to Y$ satisfies

$$f(c_\lambda(x,y)) = c_\lambda(f(x), f(y))$$

Def A convex relation is a convex subspace $R \subseteq X \times Y$

Ex $\{(x, f(x)) \mid x \in X\}$ is a convex relation iff f is convex-linear

Def Let **Conv** be the category of convex spaces and convex-linear functions, and let **ConvRel** be the category of convex spaces and convex relations

Def A concave function $S: X \to \bar{\mathbb{R}}$ satisfies

$$S(c_\lambda(x,y)) \geq c_\lambda(S(x), S(y))$$

Thermostatic systems revisited

Def A *thermostatic system* consists of

- Convex space X
- Concave function $S : X \to \overline{\mathbb{R}}$

energy volume number of particles

Ex Gas has $X = \mathbb{R}^3_{>0}$, with coordinates (U, V, N).

Entropy $S(U, V, N)$ encodes physical properties

$$\frac{1}{T} = \frac{\partial S}{\partial U} \qquad \frac{p}{T} = \frac{\partial S}{\partial V} \qquad \frac{\mu}{T} = \frac{\partial S}{\partial N}$$

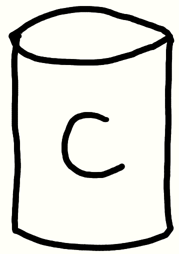
temperature pressure chemical potential

Ex $X = \Delta^n$, Shannon entropy

Ex $X = \mathrm{St}(H)$, von Neumann entropy

More Examples of Thermostatic Systems Part 2 Slide 8/8

Ex A water tank with heat capacity C has $X = \mathbb{R}_{>0}$, with coordinate U



$$S(U) = C \log U$$

$$\frac{1}{T} \overset{\text{def}}{=} \frac{\partial S}{\partial U} = \frac{C}{U} \Rightarrow U = CT$$

Note For large C, $U = CT$, small flux ΔU

Heat bath is "infinite heat capacity tank"

Ex A heat bath at temperature T has $X = \mathbb{R}$

$$S(\Delta U) = \frac{1}{T} \Delta U$$

Very simple, but not usually formalized!

Part 3: Composition of Thermostatic Systems

Recall assumptions about Entropy

(1) Function of states

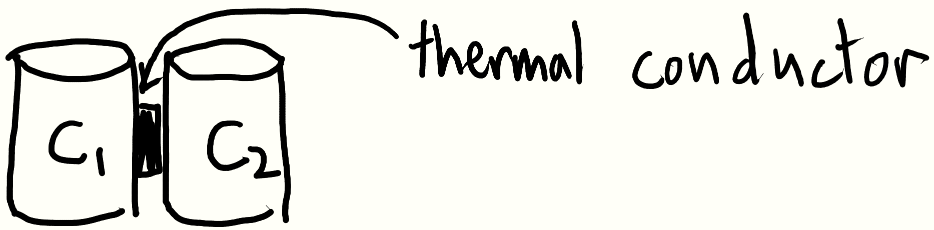
(2) Mixing increases it.

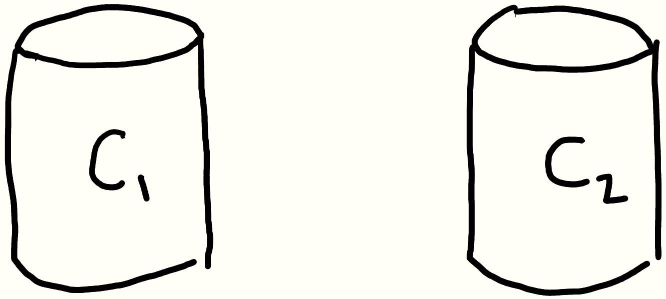
(3) Additive over independent subsystems

(4) Something we want to maximize subject to constraints.

We've formalized (1) + (2), now on to (3) + (4)

To start, we do an example: connecting two tanks





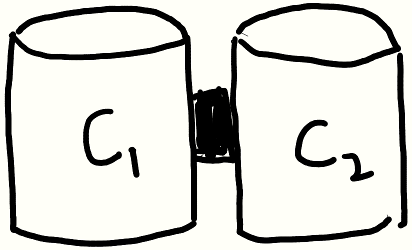
Start with $X_1 = \mathbb{R}_{>0}$, $X_2 = \mathbb{R}_{>0}$

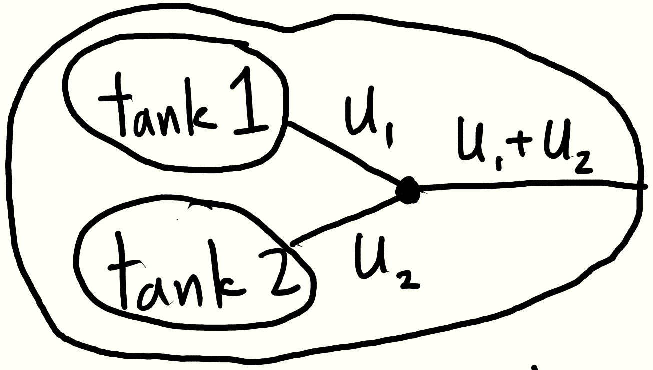
$$S_1(u_1) = C_1 \log(u_1)$$
$$S_2(u_2) = C_2 \log(u_2)$$

Make $X = X_1 \times X_2$,

$$S(u_1, u_2) = S_1(u_1) + S_2(u_2) = C_1 \log u_1 + C_2 \log u_2$$

Apply (4): Constrain with Conserved Quantities





- Total energy $U = U_1 + U_2$ is conserved.
- Relation $R \subseteq (\mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0}) \times \mathbb{R}_{\geq 0}$

$$((U_1, U_2), U) \in R \Leftrightarrow U_1 + U_2 = U$$

- Entropy of U is supremum of entropies of compatible states

$$S(U) = \sup_{U_1 + U_2 = U} S_1(U_1) + S_2(U_2)$$

- At supremum, $\dfrac{\partial S_1}{\partial U_1} = \dfrac{\partial S_2}{\partial U_2}$, i.e. $T_1 = T_2$
- New system $(\mathbb{R}_{\geq 0}, S)$, $S(U) = (C_1 + C_2)\log(U) + K$

Independent composition:

$$(X_1, S_1), \ldots, (X_n, S_n) \longmapsto (X_1 \times \ldots \times X_n,\ S_1 + \ldots + S_n)$$

Maximize over constraints

$$(X, S),\ \ R \subseteq X \times Y \longmapsto (Y,\ R_* S)$$

convex

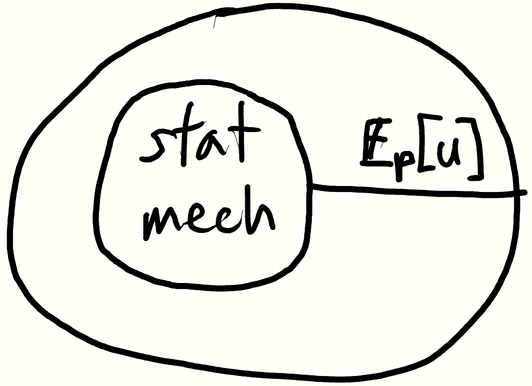
$$\underbrace{R_* S}_{\text{concave!}}(y) = \sup_{(x,y) \in R} S(x)$$

Composition = $\boxed{\text{Independent composition}}$ $\Downarrow$ $\boxed{\text{Maximize over constraints}}$

$\boxed{\text{Aside}}$ Central Dogma bridges Thermo + Stat Mech

Ω Finite, $X = \mathcal{P}(\Omega)$, $S : X \to \overline{\mathbb{R}}$ Shannon

(X, S) is "stat mech-esque"



$H : \Omega \to \mathbb{R}_{>0}$, $Y = \mathbb{R}_{>0}$

$$R \subseteq X \times Y, \quad (p, u) \in R \iff \mathbb{E}_p[H] = u$$

$$R_* S(u) = \sup_{\mathbb{E}_p[H] = u} S(p)$$

supremum is canonical distribution!

$(Y, R_* S)$ is "thermo-esque"

Raw materials:

Def ConvRel

- convex spaces as objects
- convex relations $R \subseteq X \times Y$ as morphisms

Def $\mathrm{Ent} : \mathrm{ConvRel} \to \mathrm{Set}$

$$\mathrm{Ent}(X) = \{ S : X \to \overline{\mathbb{R}},\ S \text{ concave} \}$$

$$\mathrm{Ent}(R) = S \mapsto R_* S \qquad \left(R_* S(y) = \sup_{(x,y) \in R} S(x) \right)$$

Def Natural transformation

$$\mathrm{ind}_{X_1, \dots, X_n} : \mathrm{Ent}(X_1) \times \cdots \times \mathrm{Ent}(X_n) \to \mathrm{Ent}(X_1 \times \cdots \times X_n)$$

$$(S_1, \dots, S_n) \longmapsto S_1 + \cdots + S_n$$

Note: $\mathrm{ind}_\phi : 1 \to \mathrm{Ent}(\mathbb{R}^0) \qquad * \longmapsto 0$

Def A *symmetric monoidal category* consists of

- A category C
- A functor $\otimes : C \times C \to C$
- An object $I \in C_0$

such that (assoc, unit, sym, etc.)

Ex Any category with finite (co) products

Ex $(\mathrm{Conv}, \times, \mathbb{R}^0)$

Ex $(\mathrm{ConvRel}, \times, \mathbb{R}^0)$ (because $\mathrm{Conv} \overset{\text{wide}}{\subseteq} \mathrm{ConvRel}$)

Note: $\times$ NOT product in ConvRel

Def A *lax symmetric monoidal functor* from a SMC C to a SMC D is..

- A functor $F : C \to D$
- A natural transformation

$$\varepsilon_{X_1,\ldots,X_n} : F(X_1) \otimes_D \cdots \otimes_D F(X_n) \longrightarrow F(X_1 \otimes_C \cdots \otimes_C X_n)$$

for $n \in \mathbb{N}$ (when $n=0$, $\varepsilon_\emptyset : I_D \to F(I_C)$)

...satisfying coherence conditions...

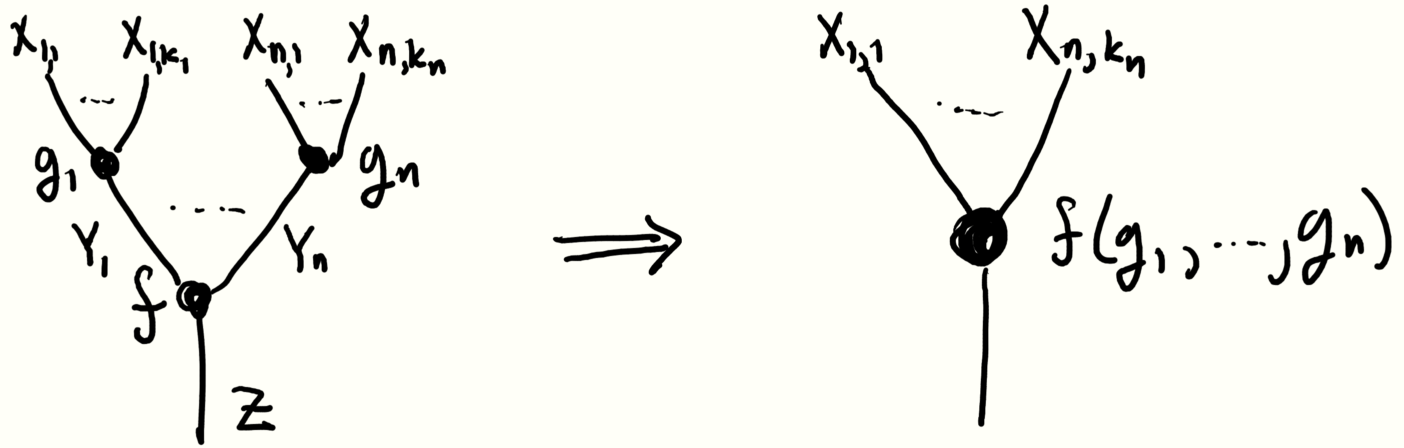
Prop (Ent, ind) is a lax symmetric monoidal functor

$$(\mathrm{ConvRel}, \times, \mathbb{R}^0) \longrightarrow (\mathrm{Set}, \times, 1)$$

Recall A (multisorted) operad $\mathcal{O}$ has

- a set of types $\mathcal{O}_0$
- for every $X_1, \dots, X_n, Y \in \mathcal{O}_0$, a set of operations $\mathcal{O}(X_1, \dots, X_n; Y)$

With (suitably well-behaved) composition



Operads from SMCs

Def Given a SMC $(\mathcal{C}, \otimes, I)$ define $\mathrm{Op}(\mathcal{C})$

$$\mathrm{Op}(\mathcal{C})_0 = \mathcal{C}_0$$

$$\mathrm{Op}(\mathcal{C})(X_1, \ldots, X_n; Y) = \mathrm{Hom}_{\mathcal{C}}(X_1 \otimes \cdots \otimes X_n, Y)$$

Ex Let $\mathcal{CR} = \mathrm{Op}(\mathrm{ConvRel})$

- types are convex sets
- operations are convex relations

$$R \subseteq (X_1 \times \cdots \times X_n) \times Y$$

Description of how to compose $(X_1, S_1) \ldots (X_n, S_n)$!

Operad Algebras

Def An operad algebra F of an operad $\mathcal{O}$ is

- A set $F(X)$ for every type $X \in \mathcal{O}_0$
- A function $F(f): F(X_1) \times \cdots \times F(X_n) \to F(Y)$ for every operation $f \in \mathcal{O}(X_1, \ldots, X_n; Y)$

respecting composition, identities, symmetries...

Prop SMC $(C, \otimes, I)$, LSM functor $F: C \to \mathrm{Set}$, then $\mathrm{Op}(F)$ is operad algebra of $\mathrm{Op}(C)$

$$\mathrm{Op}(F)(X) = F(X) \qquad X \in \mathrm{Op}(C)_0 = C_0$$

$$\mathrm{Op}(F)(f) = F(X_1) \otimes \cdots \otimes F(X_n) \xrightarrow{\varepsilon_{X_1, \ldots, X_n}} F(X_1 \otimes \cdots \otimes X_n) \xrightarrow{F(f)} F(Y)$$

$$f \in \mathrm{Op}(C)(X_1, \ldots, X_n; Y) = \mathrm{Hom}_C(X_1 \otimes \cdots \otimes X_n, Y)$$

Thm Op(Ent) is an operad algebra of Op(ConvRel).

The action of a relation $R \subseteq X_1 \times \cdots \times X_n \times Y$ on entropy functions $S_1, \ldots, S_n$ is

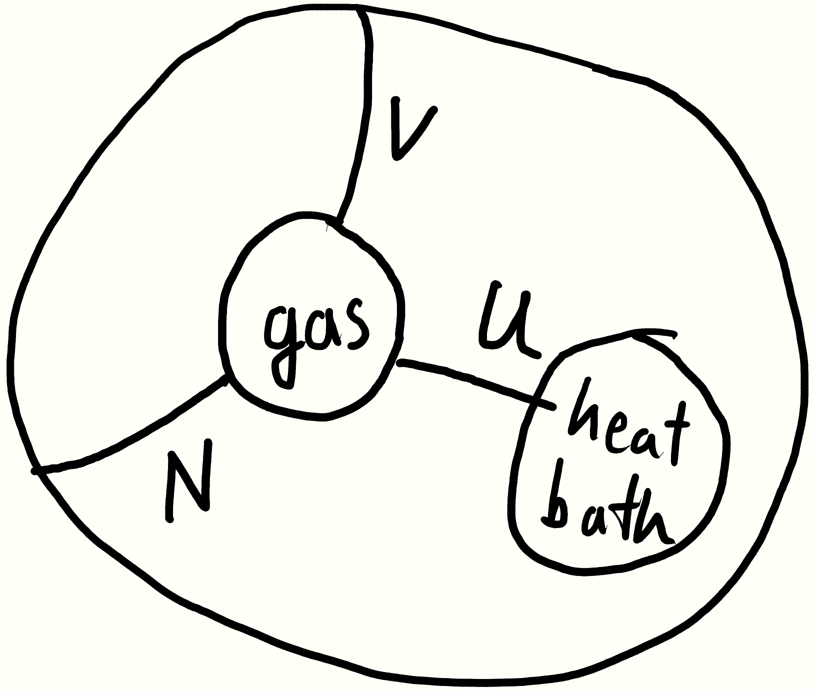
$$\mathrm{Ent}(X_1) \times \cdots \times \mathrm{Ent}(X_n) \xrightarrow{\text{ind}} \mathrm{Ent}(X_1 \times \cdots \times X_n) \xrightarrow{R_*} \mathrm{Ent}(Y)$$

$$(S_1, \ldots, S_n) \longmapsto S_1 + \cdots + S_n \longmapsto R_*(S_1 + \cdots S_n)$$

- The central dogma is precisely the rule for making an operad algebra out of a LSM functor!

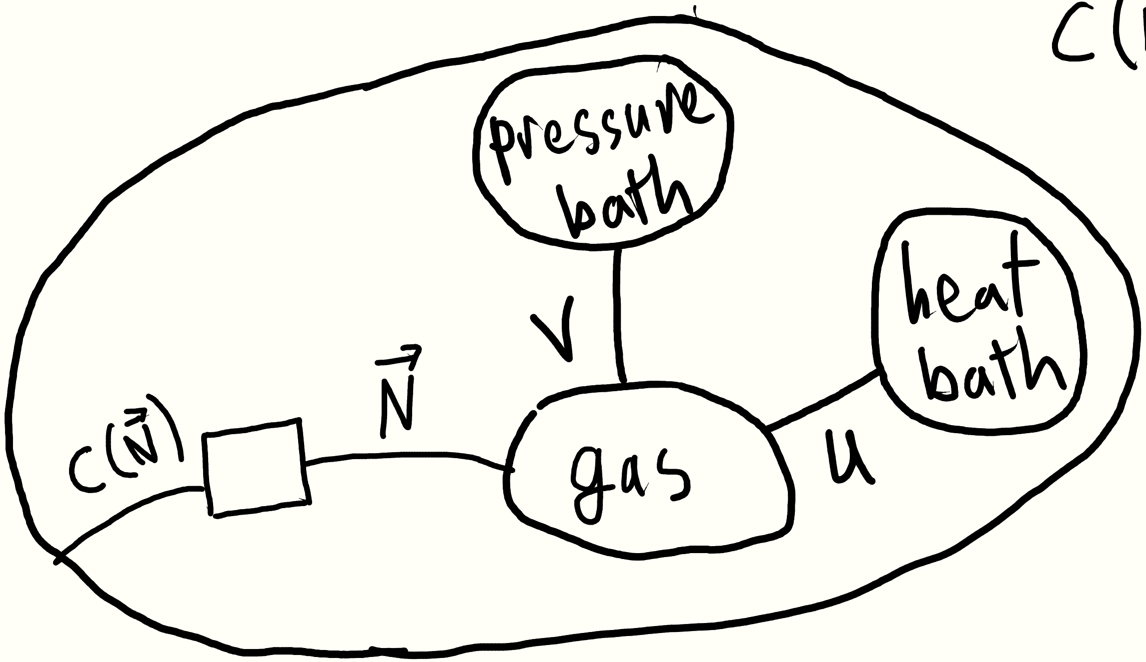
Example 1/3 : Ideal gas at constant T

$$\underset{\text{gas}}{X_1} = \mathbb{R}^3_{>0}, \quad \underset{\text{heat bath}}{X_2} = \mathbb{R}, \quad \underset{\text{gas at const. } T}{Y} = \mathbb{R}^2_{>0}$$



supremum happens at $\dfrac{\partial S}{\partial U} = \dfrac{1}{T}$

Example 2/3: Chemical Reactions



$c(\vec{N})$ = conserved quanitles

$E + S \rightleftharpoons E + P$

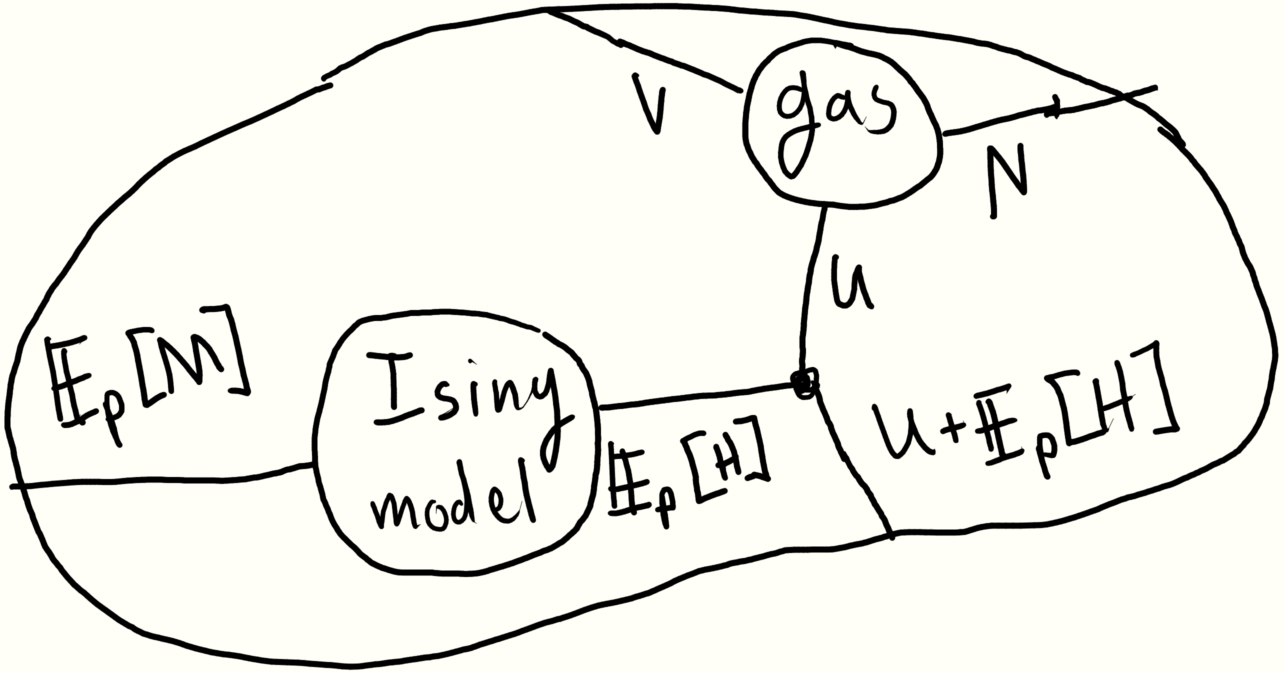
$[E]$ is conserved

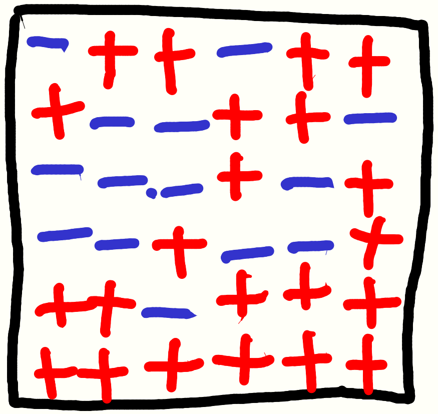
$[S] + [P]$ is conserved

Maximum entropy tells us $U, V, \vec{N}$

given $T, p, [E], [S]+[P]$

Example 3/3: Ising Model + Gas





- Traditional statistical mechanics uses a heat bath
- We can replace the heat bath with more complex system, like gas

Conclusions

- We can do a lot with our assumptions!
- Having different entropies in same framing allows composition of previously incompatible systems.
- "central dogma" = build an operad algebra from a lax symmetric monoidal functor
- Other physical systems can be composed in this way

References

Compositional Thermostatics,
John Baez, Owen Lynch, and Joe Moeller

(find it on arXiv)