Compositional Thermostatics

John Baez Owen Lynch Joe Moeller

According to V.I. Arnol'd, "Every mathematician knows it is impossible to understand an elementary course in thermodynamics." (quoted in [1], chapter 1). Not content with this state of affairs, in this talk we extract some sense out of thermodynamics, in the form of a compositional theory.

One of the confusions of the subject is that there are many things called entropy, viz.

- Shannon entropy
- Thermodynamic entropy (i.e., entropy as empirically measured by temperature and heat flows)
- von Neumann entropy

In physics, there is an intuition that these are pointing towards similar concepts, and one of the aims of statistical mechanics is to derive the macroscale thermodynamic entropy from the microscale Shannon entropy [2].

However, for most mathematicians, to compare these entropies directly would be a type error; Shannon entropy is defined on probability distributions, thermodynamic entropy is defined on macroscopic variables, and von Neumann entropy is defined on mixed states in a quantum system.

In this talk, we will present an framework in which each of these entropies can be modeled in the same way. One should note that although our systems model more than just thermodynamical entropy, it is the thermodynamical context that our nomenclature derives from. We call this subject "thermostatics" because we use the maximum entropy principle to derive the *equilibria* of thermodynamical systems, just as in electrostatics one might use Maxwell's laws to derive the equilibria of an electrical system.

Definition 1. A **thermostatic system** is a convex space X along with a concave function $S\colon X \to \bar{\mathbb{R}}$ called the **entropy function**, where $\bar{\mathbb{R}} = \mathbb{R} \cup \{\pm\infty\}$ is the extended reals.

In ([3], section 2) we detail a generalized definition of convex space, originally due to Stone [4]. Convex spaces and concave functions formalize the notion that "mixing increases entropy." Concave functions also have some nice properties; for instance they are easy to maximize, and they are the setting in which Legendre transforms can be performed [5].

Example 2. An ideal gas is modeled by the convex space $\mathbb{R}^3_{>0}$ and entropy function $S(U, V, N)$. This entropy function encodes the temperature T, pressure p, and chemical potential μ by

$$\frac{1}{T} = \frac{\partial S}{\partial U}, \quad \frac{p}{T} = -\frac{\partial S}{\partial V}, \quad \frac{\mu}{T} = \frac{\partial S}{\partial N}$$

In ([3], section 3), we provide many more examples of thermostatic systems, including the oft-neglected heat bath.

Next, we form a theory of how to compose systems. The underlying idea behind this theory is the maximum entropy principle, which tells us that given several systems, their joint equilibrium maximizes total energy subject to constraints arising from conserved quantities in their interactions. This is a "thermodynamical" interpretation of the maximum entropy principle; it also has other interpretations for other types of entropy.

In order to apply category theory to composing thermostatic systems, we turn to operads and operad algebras. The use of operads and operad algebras in applied category theory to formalize composition has a rich history, dating at least back to Spivak [6], and more recently Libkind [7].

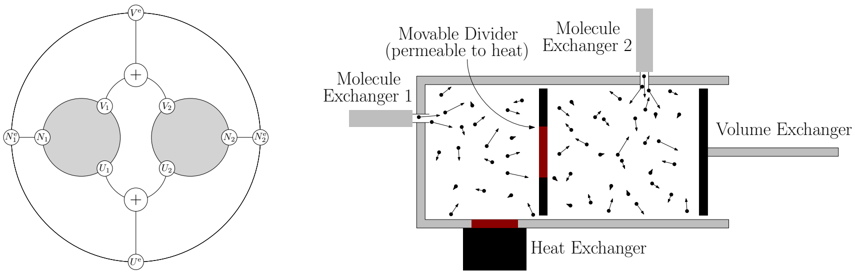

Figure 1. Symbolic and pictoral representations of thermostatic equilibriation

We then construct a operad $\mathcal{CR}$ where the types are convex sets X, and the operations are convex relations $R \subset X_1 \times \cdots \times X_n \times Y$. Such a convex relation describes how a "high-level" description of a system $y \in Y$ constrains the "low-level" possibilities for the states of several systems, $x_i \in X_i$.

Finally, we construct an operad algebra F of $\mathcal{CR}$ which assigns to a type X the set

$$F(X) = \{S\colon X \to \bar{\mathbb{R}} \mid S \text{ is concave}\},$$

and to an operation $R \subset X_1 \times \cdots \times X_n \times Y$ a map that takes entropy functions $S_i\colon X_i \to \bar{\mathbb{R}}$ and produces an entropy function

$$R^*(S_1, \ldots, S_n)(y) = \sup_{(x_1, \ldots, x_n, y) \in R} S_1(x_1) + \cdots + S_n(x_n)$$

This formalizes both the idea that entropy is additive across subsystems, and that the equilibrium is found by maximizing with respect to constraints. In ([3], sections 4 and 5) we show that these constructions are well-defined.

Theorem 3. $\mathcal{CR}$ is an operad, and F is an operad algebra.

We prove Theorem 3 using a quite general technique; we build $\mathcal{CR}$ from a symmetric monoidal category $\mathsf{ConvRel}$ and then we build F from a lax symmetric monoidal functor $\mathrm{Ent}\colon \mathsf{ConvRel} \to \mathsf{Set}$. This construction has general interest as a way of formalizing compositionality broadly within applied category theory, and so we will briefly detail it in our talk.

We finish by discussing how this framework allows us to blend statistical mechanical and thermodynamical systems. Specifically, this allows "incremental" coarse-graining, where one part of a statistical mechanical system is coarse-grained while another part remains fine-grained, something that is not expressible in standard treatments of statistical mechanics.

Bibliography

[1] W. Haddad, *A Dynamical Systems Theory of Thermodynamics*. Princeton Series in Applied Mathematics. Princeton University Press, Princeton, New Jersey, 2019.

[2] S. Friedli and Y. Velenik, *Statistical Mechanics of Lattice Systems: A Concrete Mathematical Introduction*. Cambridge University Press, first ed., Nov., 2017.

[3] J. C. Baez, O. Lynch, and J. Moeller, "Compositional Thermostatics," `arXiv:2111.10315`.

[4] M. H. Stone, "Postulates for the Barycentric Calculus," *Annali di Matematica Pura ed Applicata* **29** no. 1, (Dec., 1949) 25–30.

[5] S. Willerton, "The Legendre-Fenchel Transform from a Category Theoretic Perspective," `arXiv:1501.03791`.

[6] D. Spivak, "The Operad of Wiring Diagrams: Formalizing a Graphical Language for Databases, Recursion, and Plug-and-Play Circuits," `arXiv:1305.0297`.

[7] S. Libkind, A. Baas, E. Patterson, and J. Fairbanks, "Operadic Modeling of Dynamical Systems: Mathematics and Computation," `arXiv:2105.12282`.