

# Five axioms are required for a proof of the second law of thermodynamics that uses the Kullback-Leibler divergence.

Brendan Lucas

Consider a physical universe with random, discrete, generalized<sup>1</sup> energy  $E$ . The second law follows from these five axioms:

**Axiom 1.** Energy is a discrete random variable  $E$  in a sample space  $\mathcal{E} \ni E_i \forall i$  with marginal probability  $p(E)$ .<sup>2</sup>

**Axiom 2.** The expected energy  $\langle E \rangle = \sum_i p_i E_i$  of the universe is a constant.

**Axiom 3:** If the universe is not in an equilibrium, it will be in equilibrium.

**Axiom 4:** The set of all energies  $\mathcal{E}$  does not change, even as the distribution  $p(E)$  may change. In other words,  $\mathcal{E}$  is invariant.

**Axiom 5:** The temperature of the universe is a constant.

You may not be inclined to accept these axioms as a physical reality. Certainly, they are dubious. But they are also intuitive; Axiom 1 mirrors the insights of quantum mechanics, Axiom 2 mirrors what we call the first law of thermodynamics (which we need not assume its traditional form), Axiom 3 almost constitutes the very definition of equilibrium, and Axiom 4 establishes energy as something objective, while the (apparently Bayesian) probabilities can be subjective. Axiom 5, I will not deny, is almost certainly false.

“Proof” of these axioms is out of scope; they may all be false. But we show they are sufficient to prove the second law of thermodynamics, so that is special about them. “Fluctuation theorems” only come so close; they only show an *expectation value* of a change in entropy to be non-negative, not the change in entropy itself.<sup>3</sup>

“Statistical mechanics,” as it is commonly understood, we call “the equilibrium theory.” This is because “The generalized Boltzmann distribution  $p_{\text{eq}}(E_i) = \frac{e^{-E_i/k_B T}}{\sum_j e^{-E_j/k_B T}}$  is the only distribution for which the Gibbs-Shannon entropy  $H = -\sum_i p_i \ln p_i$  is equal to the thermodynamic entropy  $S = k_B H$ . (Gao 2019 [https://arxiv.org/abs/1903.02121])” The generalized Boltzmann distribution is the maximum entropy distribution, the equilibrium distribution, so we call it  $p_{\text{eq}}$ . Away from equilibrium (that is to say, *in real life*), thermodynamic

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<sup>1</sup>You may prefer one related to enthalpy,  $E_i = \varepsilon_i + pV_i$ , or involve a chemical potential like  $E_i = \varepsilon_i \pm \mu N_i$ , where  $\varepsilon_i$  is defined so that  $\sum_i p_i \varepsilon_i = U$  is the internal energy, or something else. The math works out the same, but the exact expression of the (generalized) free energy will be different. Henceforth “generalized energy” is just “energy.”

<sup>2</sup> $p(E)$  describes the frequency at which different values of  $E$  can be observed, or assigns a degree of subjective belief to each possible energy level.

<sup>3</sup>“Whither Time’s Arrow?” by Gavin E. Crooks

entropy<sup>4</sup> has not been demonstrated to have statistical definition<sup>5</sup>. They won't tell you that in school! But for this derivation, we concern ourselves solely with the Gibbs-Shannon entropy, and do not worry about different thermodynamic entropies or generalized entropies such as those of Tsallis or Renyi.

$p_{\text{now}}$  is our model of the universe's energy now, and  $p_{\text{eq}}$  is the unique marginal of  $\mathcal{E}$ 's equilibrium;  $p_{\text{eq}}$  is “the heat death of the universe.”  $\beta = 1/k_B T$  is inverse temperature, or coldness of the universe.  $p_{\text{now}}$  is compared against  $p_{\text{eq}}$  with the Kullback-Leibler divergence (KLD).  $p_{\text{now}}$  can be any marginal over  $\mathcal{E}$ , including the equilibrium distribution (but hopefully not, if one likes to live). *The fourth axiom is required to define the KLD.*

1. Define KLD:

$$D[p_{\text{now}}||p_{\text{eq}}] = \sum_{i=1}^N p_{\text{now}}(E_i) \ln \left( \frac{p_{\text{now}}(E_i)}{p_{\text{eq}}(E_i)} \right) = \sum_{i=1}^N p_{\text{now}}(E_i) \ln p_{\text{now}}(E_i) - \sum_{i=1}^N p_{\text{now}}(E_i) \ln p_{\text{eq}}(E_i)$$

2. Expand and add a special zero

$$\begin{aligned} D[p_{\text{now}}||p_{\text{eq}}] &= \sum_{i=1}^N p_{\text{now}}(E_i) \ln p_{\text{now}}(E_i) - \sum_{i=1}^N p_{\text{now}}(E_i) \ln p_{\text{eq}}(E_i) \\ &\quad + \left( \sum_{i=1}^N p_{\text{eq}}(E_i) \ln p_{\text{eq}}(E_i) - \sum_{i=1}^N p_{\text{eq}}(E_i) \ln p_{\text{eq}}(E_i) \right) \end{aligned}$$

3. Convert to macroscopic variables with  $\frac{1}{k_B} S = - \sum_{i=1}^N p_i \ln p_i$

$$\begin{aligned} D[p_{\text{now}}||p_{\text{eq}}] &= \frac{1}{k_B} \Delta S - \sum_{i=1}^N p_{\text{now}}(E_i) \ln p_{\text{eq}}(E_i) \\ &\quad + \sum_{i=1}^N p_{\text{eq}}(E_i) \ln p_{\text{eq}}(E_i) \\ &= \frac{1}{k_B} \Delta S + \sum_{i=1}^N [p_{\text{eq}}(E_i) - p_{\text{now}}(E_i)] \ln p_{\text{eq}}(E_i) \end{aligned}$$

4. Plug in the “heat death” partition function:  $p_{\text{eq}}(E_i) = \frac{e^{-\beta E_i}}{\sum_{j=1}^N e^{-\beta E_j}} = \frac{e^{-\beta E_i}}{Z}$ ,

$$\begin{aligned} D[p_{\text{now}}||p_{\text{eq}}] &= \frac{1}{k_B} \Delta S + \sum_{i=1}^N [p_{\text{eq}}(E_i) - p_{\text{now}}(E_i)] \ln \left( \frac{e^{-\beta E_i}}{\sum_{j=1}^N e^{-\beta E_j}} \right) \\ &= \frac{1}{k_B} \Delta S + \sum_{i=1}^N [p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \cdot [\beta E_i] + \sum_{i=1}^N [p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \ln Z \end{aligned}$$

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<sup>4</sup>“Thermodynamic entropy” is entropy as it was understood by Clausius and Kelvin, or now by chemists and some (e.g. mechanical) engineers.

<sup>5</sup>“Gibbs-Shannon entropy” is the definition preferred by many theorists and other (e.g. electrical) engineers.

5. Notice that

$$\sum_{i=1}^N [p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \ln Z = \ln Z \left[ \sum_{i=1}^N p_{\text{now}}(E_i) - \sum_{i=1}^N p_{\text{eq}}(E_i) \right] = \ln Z - \ln Z = 0$$

So,

$$D[p_{\text{now}} \| p_{\text{eq}}] = \frac{1}{k_B} \Delta S + \sum_{i=1}^N [p_{\text{now}}(E_i) - p_{\text{eq}}(E_i)] \cdot [\beta E_i]$$

6. The following step gives a difference in the expectation values of energy if and only if every  $E_i$  is the same in  $p_{\text{eq}}$  and  $p_{\text{now}}$ ; axiomatically, the energy levels did not change, but only their probabilities changed.

$$\begin{aligned} D[p_{\text{now}} \| p_{\text{eq}}] &= \frac{1}{k_B} \Delta S + \sum_{i=1}^N p_{\text{now}}(E_i) \beta E_i - \sum_{i=1}^N p_{\text{eq}}(E_i) \beta E_i \\ &= \frac{1}{k_B} \Delta S - \beta \Delta \langle E \rangle \end{aligned}$$

7. Invoke the second axiom,

$$k_B D[p_{\text{now}} \| p_{\text{eq}}] = \Delta S,$$

8. KLD is non-negative, so

$$\Delta S \geq 0$$

QED, that is the second law of thermodynamics, in all the glory of its shaky foundation. **The entropy of a universe with these five axioms can only increase or stay the same, but never decrease!**