

[Temperature]

(Chapter 1.11.1 of *Elements*)

The notion of *temperature* in the subject of thermodynamics (which is where we are) needs some explanation. We present a conceptually simple argument (as we have it, a plausibility argument, although it is very general) for temperature that has deep roots in thermodynamics and the physics of many-body systems (see Osborn 1988). Consider a many-body system (“Sample”) that is in a stationary state. The probability operator D describes all there is to know about the system, and satisfies the Liouville equation $\frac{\partial D}{\partial t} = \frac{i}{h}[D, \mathcal{H}]$, where \mathcal{H} is the Hamiltonian, the total energy operator for the system, and the brackets indicate commutation of operators. The steady state $\frac{\partial D}{\partial t} = 0$ implies that $[D, \mathcal{H}] = 0$, that is, that the probability operator, representing the enormously complicated wave function of the system, is a function only of the total energy, $D = D(\mathcal{H})$.

If there are two systems, Sample and Environment, in thermodynamic equilibrium, the probability operator for the combined system is a function of the sum of energies of the two, $D^{both}(\mathcal{H}^S + \mathcal{H}^E)$. We intuitively know that the probability operators of the two systems separately depend on the particular properties of each, which are independent of each other. This independence of probabilities suggests that the joint probability operator for the combination System plus Environment is the product of probability operators

$$D^{both}(\mathcal{H}^S + \mathcal{H}^E) = D^S(\mathcal{H}^S)D^E(\mathcal{H}^E). \quad (1)$$

The solutions of this functional equation are of exponential form because that is the one function of which the function of the sum of its arguments is the product of the same functions of each of its arguments

$$\begin{aligned} D^S(\mathcal{H}^S) &= C^S \exp(-\beta \mathcal{H}^S) \\ D^E(\mathcal{H}^E) &= C^E \exp(-\beta \mathcal{H}^E). \end{aligned} \quad (2)$$

Here, C^S and C^E are constants and the two functions must share the parameter β . The parameter must be a positive real number in order to satisfy the requirement on probability operators that the sum of its diagonal elements of the operator is unity, that is,

$$\text{Tr}[D^S] = C^S \text{Tr}[\exp(-\beta \mathcal{H}^S)] = 1 \quad (3)$$

so that

$$C^S = \frac{1}{\text{Tr}[\exp(-\beta \mathcal{H}^S)]} = \frac{1}{Z^S}, \quad (4)$$

where Z^S is the *partition function* of the system, which is a function of the temperature, and the probability operator is

$$D^s = \frac{1}{Z^s} \exp(-\beta \mathcal{H}^s) \quad (5)$$

The physical dimension of $1/\beta$ is energy, a measure of the total energy of a system, which we sometimes express as a *temperature*, T , $\beta = 1/k_B T$, where k_B is *Boltzmann's constant*. So we would say that, in the state of thermodynamic equilibrium, the System has the same temperature as the Environment.