On Norton's No-Go Result

G. Barış Bağcı, reply by John Norton

In response to "A Hot Mess" (Vol. 4, No. 4).

To the editors:

In his essay, John Norton presents many arguments against the thermodynamics of computation. On the question of whether the field lacks a consistent foundation, I am in agreement with Norton, although occasionally for different reasons. Physicists in particular should pay close attention to the arguments Norton provides. One of these is his no-go result, which states that a single particle interacting with an infinite bath cannot undergo an isothermal reversible process due to the large fluctuations. Rolf Landauer took this process for granted in his formulation of the thermodynamics of computation.

In order to understand Norton's no-go result, we must begin with the work of Albert Einstein.¹ Already convinced about the statistical nature of entropy, Einstein inverted Boltzmann's entropy formula, $S = k_B \log (\Omega)$, where k_B is the Boltzmann constant and Ω denotes the number of accessible microstates.² The result was an expression $\Omega = \exp (S/k_B)$, where exp denotes the usual exponential function. The equilibrium state corresponds to the state with maximum number of microstates, $\Omega_{eq} = \Omega_{max}$. Due to the statistical nature of the processes, even though it is isolated, the system will exhibit spontaneous fluctuations around the equilibrium state such that Einstein considered the following expression,

$$\frac{\Omega_{neq}}{\Omega_{eq}} = \exp\left(-\frac{\Delta S_{total}}{k_{\rm B}}\right),\,$$

where Ω_{neq} denotes the microstates of the fluctuating state away from the equilibrium or so-called neighboring state. The total entropy change is $\Delta S_{total} = S_{eq} - S_{neq}$. To fully appreciate Einstein's construction, consider the

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case $\Delta S_{total} = 2.3 k_B$. The equation above yields a 1:10 ratio for $\frac{\Omega_{neq}}{\Omega_{eq}}$. This indicates that there is a much larger probability of the system being at equilibrium, whereas fluctuations away from the equilibrium state are rare. They are, nevertheless, bound to occur. The above expression indicates that the fluctuations are more likely to occur around the close neighborhood of the equilibrium state with maximum entropy.

The canonical version of the equation above was obtained by Richard Tolman, so that

$$\frac{p\left(\lambda_{neq}\right)}{p\left(\lambda_{eq}\right)} = \exp(-\beta\Delta F),$$

where *p* denotes the probability and ΔF is the Helmholtz free energy difference between equilibrium and non-equilibrium states.³ As usual, β is the inverse temperature equal to $(k_{\rm B} T)^{-1}$, where the temperature is considered to be constant. Following Norton, the states are labeled λ , which can be any extensive variable allowed to fluctuate.

Norton states that for a reversible isothermal process with zero work done, thermodynamic reversibility means that the net sum of the generalized thermodynamic forces should be zero. This condition, according to Norton,

is tantamount to $\left(\frac{\partial F}{\partial \lambda}\right)_{eq} = 0$. Norton further deduces $\frac{dF}{d\lambda} = 0$, such that $\Delta F = 0$, yielding $p(\lambda_{neq}) = p(\lambda_{eq})$ due to the equation above.⁴ The system can be found in an equilibrium state and in a state away from equilibrium with the same probability. This is Norton's no-go result.

In order to see what this result implies, it is necessary to continue following the work of Tolman. His next move was to expand the free energy around the equilibrium,

$$\Delta F = F\left(\lambda_{neq}\right) - F\left(\lambda_{eq}\right) = \left(\frac{\partial F}{\partial \lambda}\right)_{eq} \left(\lambda_{neq} - \lambda_{eq}\right) + \frac{1}{2} \left(\frac{\partial^2 F}{\partial \lambda^2}\right)_{eq} \left(\lambda_{neq} - \lambda_{eq}\right)^2 + O(\geq 3),$$

where $O(\geq 3)$ denotes terms such as $(\lambda_{neq} - \lambda_{eq})^3$ or higher. Following

common practice, he then drops the term $\left(\frac{\partial F}{\partial \lambda}\right)_{eq}$ since there is minimal free energy at equilibrium for a system with constant temperature. Norton, in his derivation of the no-go result, not only sets this term to zero by relying on thermodynamic arguments; he also adds that this term being zero implies $\frac{dF}{d\lambda} = 0$ at all equilibrium states. According to Norton, $F(\lambda_{eq}) = F(\lambda_{neq})$. An immediate obstacle now becomes apparent. The equilibrium state is defined as the state with minimum free energy. One wonders how these two states can ever have the same free energy because for any state other than equilibrium one cannot attain the minimum free energy value or any value below it.

Tolman neglects the terms of order three and higher—terms such as $O(\leq 3)$ —by invoking the law of large numbers so that the fluctuations are assumed to be sufficiently small, leaving:

$$\Delta F = F\left(\lambda_{neq}\right) - F\left(\lambda_{eq}\right) = \frac{1}{2} \left(\frac{\partial^2 F}{\partial \lambda^2}\right)_{eq} \left(\lambda_{neq} - \lambda_{eq}\right)^2.$$

Norton's no-go result relies on ΔF being zero. In the above expression, it is not zero at all, at least not in the presence of small fluctuations. The free energy difference can only be zero if the second-order term is assumed to be zero. But neglecting the second-order term would mean suppressing the fluctuations even for large systems. Norton's arguments would then seem even less plausible. Tolman uses the last expression to obtain

$$p(\lambda_{neq}) = p(\lambda_{eq}) \exp\left(-\frac{\beta}{2}\left(\frac{\partial^2 F}{\partial \lambda^2}\right)_{eq}\left(\lambda_{neq} - \lambda_{eq}\right)^2\right)$$

He was then able to correctly calculate the deviation of the mean kinetic energy per degree of freedom, $k_{\rm B}T/2$, as is the case for canonical settings in general. There is no way to get rid of these fluctuations in the usual canonical setting. This is a rigorous mathematical result known as the central limit theorem. Contrary to Norton's claim, the free energy difference can never be zero in a large enough system exactly because of the fluctuations.

I do not consider the consecutive sequences of the equilibrium states in my argument, but rather the fact that Norton chooses $\frac{dF}{d\lambda} = 0$ as a condition for

an equilibrum state. He obtains this formulation on purely thermodynamic grounds because the net sum of the thermodynamic forces should be zero at each stage of the equilibrium. This definition leaves no room for fluctuations. To define an equilibrium state, Tolman only considered

 $\left(\frac{\partial F}{\partial \lambda}\right)_{eq} = 0$, rather than $\frac{dF}{d\lambda} = 0$, as Norton does. In statistical mechanics, even the free energy at equilibrium is not constant in the usual sense of the term, but is allowed to fluctuate. The result of this small fluctuation is underwritten all over the canonical ensemble through the central limit theorem. Yet there is no room for fluctuations in thermodynamics.

Imagine a system at equilibrium. According to thermodynamics, if I measure its free energy at equal time intervals, I should always obtain the same value for the free energy. Alternatively, according to statistical mechanics, the free energy fluctuates around its mean value. Even for an equilibrium state, the value of the free energy is not constant. The first point worth noting about the no-go result is that it considers the equilibrium state as defined in thermodynamics, but then goes on to apply this strictly thermodynamic idea to another idea in statistical mechanics where even the thermodynamic limit does not suffice to converge.

Thus far we have considered the impact of small fluctuations and shown that Norton's argument can be only be correct if these fluctuations are ignored. But Norton presents his case with large fluctuations in mind. This leads to an even more drastic impasse. Assuming the fluctuations are not small, in order to maintain the free energy constant at an equilibrium state, not only the second-order term should be set to zero, but also all the other terms, i.e., $O(\leq 3) = 0$. In order to achieve this, Norton would need to suppress all terms related to the fluctuations for all orders if the fluctuations are small. In both cases, the core of his argument would be contradicted, since he defines the equilibrium state as the one with constant free energy.

Norton generally provides examples within a canonical setting. In this setting, the aforementioned second-order term must be taken into account because there will be a fluctuation on the order of $k_{\rm B}T/2$ for the deviation of the mean kinetic energy per degree of freedom. In order to illustrate his no-go result, Norton uses a canonical ensemble, which is valid only for small fluctuations. Yet his no-go result is supposed to be about large fluctuations.

Norton presents his no-go result to show that a single particle in contact with an infinite reservoir cannot be treated as Landauer had assumed. The use of canonical formalism involves a commitment to the small fluctuations regime. An equivalent question is whether a single particle can have a canonical distribution. This is possible, provided that the bath with which it interacts is large enough. Since one can talk about the canonical distribution of a single particle interacting with an infinite bath, one can also frame the issue in the regime of small fluctuations. It is the size of the thermal reservoir that determines the distribution, provided that the heat capacity of the bath is constant.⁵ If the bath is not infinite, then one might talk about large fluctuations. When this is the case, the distribution is no longer canonical, but follows the inverse power law.⁶ As a result, when the fluctuations are indeed genuinely large, almost none of the equations in this letter are valid, nor are any of the equations related to the no-go result.⁷

G. Barış Bağcı

John Norton replies:

G. Barış Bağcı and I differ only on technical issues in the derivation of the no-go result.

The no-go result applies to thermodynamically reversible processes implemented in molecular scale systems. In ordinary thermodynamics, a reversible process is one that passes through a sequence of states that come arbitrarily close to equilibrium with each other. These equilibrium states are of equal thermodynamic entropy *S*. The process can only proceed if there is a very slight entropy increase along the sequence of actual states. If the entropy were to remain constant, then the process would be frozen. There would be no entropic forces to advance the process.

Bağcı considers a special case not mentioned in the main article but treated by me elsewhere. If the system is in thermal equilibrium with a large heat bath at temperature T, with which it exchanges heat but no work, then the condition of increasing entropy of the total system is expressed by a condition of decreasing free energy F of the system, excluding the heat bath.

These are equivalent conditions. In both cases, a reversible process is characterized by the fact that each of its stages comes arbitrarily close to states with the same entropy of the total system, or with the same free energy of the system excluding the heat bath, in the general and special cases, respectively. The no-go result arises from the fact that thermal systems have molecular constitutions. A new effect, thermal fluctuations, enables the process to move among its states. This second process is active even if the stages of the process achieve the states of equal entropy or free energy. In this case, the probability W that fluctuations deliver the system to any particular stage is given by the familiar formulas. That is, either the inverted Boltzmann formula, $W = \exp(S/k)$, or the version of it that Bağcı uses, $W = \exp(-F/kT)$. Since the entropy S or free energy F at each of the stages is the same, all the stages are of equal probability. Fluctuations dominate and move the process with equal probability to each of its stages, undoing the possibility of any assured completion.

Bağcı's concern is how to arrive at the constancy of free energy F over all the stages. It is built in from the start through the definition of a reversible process. The constancy comes from ordinary thermodynamics. If the free energies of the stages of a process are equal, then the sum of thermodynamic forces acting at each stage is zero. Each stage is in static equilibrium, and the process does not advance. When that equality is implemented in statistical physics, it requires only that the mean value of the sum of these forces is zero. Fluctuations around the mean will produce momentary, non-zero driving forces that will advance or retard the process.

In place of this reasoning, Bağcı tries to derive the constancy of the free energy from a power series expansion that relates the free energy of an equilibrium state to that of the non-equilibrium states to which it fluctuates. As he recounts, the effort fails and for the reason he indicates: the fluctuation states involved are not small fluctuations amenable to power series analysis. I am not clear on the details of Bağcı's application of this power series expansion to the case at hand. His analysis considers an equilibrium state and fluctuations from it. But in statistical physics, all the stages become non-equilibrium fluctuation states. There is, however, a single equilibrium state from which they arise as fluctuations.

Since fluctuations can cause the process to migrate over all its stages, these stages can be taken together to form a single, larger thermal system at equilibrium. The individual stages are then states to which the system migrates through fluctuations. One might try to use Bağcı's power series expansion to recover the free energies and probabilities of the various stages. A more straightforward method is simply to apply directly to the fluctuation states the free energy analog of Boltzmann's $S = k \ln W$. This is the canonical expression for free energy mentioned above. It is given more fully as $F = -kT \ln Z$, where Z is the partition integral over the subvolume of phase space corresponding to the fluctuation state. It is also the probability of the fluctuation state up a constant, normalizing factor.

A simple example illustrates how the combined stages of the process form one larger system at thermal equilibrium. It is perhaps the simplest possible example: a Brownian particle in a Petri dish of water. When the dish is level, all positions of the particles are states of equal entropy or free energy. To have a process that moves the particle across the dish, one must tilt the dish, introducing a dissipative entropy gradient. If the molecular character of the thermal system is added in, the dish does not need to be tilted for the particle to move. Thermal fluctuations lead it to jiggle about in the celebrated effect of Brownian motion. Over a long period, the particle will fully explore the dish and with equal probability in all its parts. Over this long timescale, the Brownian particle behaves like a single molecule of gas. If the desired process is to move the particle assuredly from one side of the dish to the other, the dish must be tilted enough to overcome the Brownian motion that would deflect the particle away from the final position sought. This results in added entropy, creating dissipation whose magnitude can be computed from the formula in the no-go result using the probability of completion sought.

For a microscopically visible particle, the overall effect is small. It will take a long time for the Brownian particle to explore the whole dish. For smaller particles approaching molecular scales, the motion becomes more rapid and the amount of tilting needed becomes significant. In the extreme case of a molecule in air, mere tilting no longer suffices. A dissipative process that creates considerable amounts of entropy must be employed to confine the particle.⁸

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- Albert Einstein, "Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen," Annalen der Physik 17 (1905): 549–60. ↔
- 2. From this point on, I use the natural basis for the logarithmic function. \leftarrow
- 3. Richard Tolman, *The Principles of Statistical Mechanics* (London: Oxford University Press, 1938), 637–41. ↔

- 4. John Norton, "Thermodynamically Reversible Processes in Statistical Physics," American Journal of Physics 85 (2017): 135–45. ↔
- 5. Michele Campisi, Fei Zhan, and Peter Hänggi, "On the Origin of Power Laws in Equilibrium," *EPL* 99 (2012): 60004. ←
- 6. M. Michele Campisi, Fei Zhan, and Peter Hänggi, "On the Origin of Power Laws in Equilibrium," *EPL* 99 (2012): 60004. ←
- 7. G. Baris Bağcı and Thomas Oikonomou, "Tsallis Power Laws and Finite Baths with Negative Heat Capacity," *Physical Review E* 88 (2013): 042126. ↔
- 8. For a quantitative analysis of these last processes, see John Norton, Section 10
 "Simplest Illustration of the No-go Result: Bead on a Wire," in "All Shook Up: Fluctuations, Maxwell's Demon and the Thermodynamics of Computation," *Entropy* 15 (2013): 4,432–83. ↔

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