Thermodynamic uncertainty relations again: A reply to Lavenda

J. Uffink and J. van Lith
Institute for History and Foundations of Science
University of Utrecht
PO Box 80.000, 3508 TA Utrecht, the Netherlands
E-mail: uffink@phys.uu.nl; j.h.vanLith@phys.uu.nl

July 5, 2001

Abstract

In a previous paper (*Found. Phys.* **29**, 655, (1999)), we have presented a review of various approaches in the literature towards the derivation of so-called thermodynamic uncertainty relations in statistical thermodynamics. This review has been critical. We have argued that some of these approaches are sound, i.e. they reach a valid conclusion, albeit under restricted conditions, whereas others were found to be incoherent and could not withstand the scrutiny of logical analysis. In the latter category we have included work of Lavenda on this topic. However, in a comment (*Found. Phys. Lett.* **13**, 487 (2000)), Lavenda claims to have uncovered "fundamental errors" in our paper . In this reply we show that these claims are mistaken.

Key words: thermodynamics, uncertainty relations, second law.

In a recent comment [1], Lavenda claims to have found "fundamental errors" in our paper [2]. In total, he raises five points, to which we reply below, following the numbering employed in his comment. We also address a sixth point which he left unnumbered.

1. The first issue concerns an elementary problem in classical thermodynamics. Consider two systems that are initially at different temperatures T_1 and T_2. They are then placed in thermal contact, while ensuring that no work is done on or by either body. An irreversible thermal equilibration process sets in, until the two systems reach a common final temperature T_f. The question is now to determine the total entropy increase $\delta S = \delta S_1 + \delta S_2$ of the two systems during this process.

   In his book [3, eqn. (4.70)], Lavenda gives the total change in entropy as:

   $$\delta S = \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \delta U_1 \geq 0, \tag{1}$$

   where δU_1 is the energy change of system 1. We have criticized this relation on the grounds that the left-hand side, i.e. the equation

   $$\delta S = \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \delta U_1 \tag{2}$$

holds for reversible processes only, and leads to the consequence $\delta S = 0$. Lavenda objects that this is "definitely wrong".

In order to see who is right on this issue, let us consider the simplest possible example, i.e. the case where the two bodies are equal masses m of some ideal gas. In that case, the entropy change can be calculated exactly, and a straightforward calculation gives

$$\delta S = mc_V \ln \frac{T_f^2}{T_1 T_2} = mc_V \ln \frac{(T_1 + T_2)^2}{4 T_1 T_2} \tag{3}$$

where we have used $T_f = (T_1 + T_2)/2$, and c_V is the specific heat of the gas.

On the other hand, since $\delta U_1 = mc_V(T_f - T_1) = mc_V(T_2 - T_1)/2$, we find

$$\left(\frac{1}{T_1} - \frac{1}{T_2} \right) \delta U_1 = mc_V \frac{(T_2 - T_1)^2}{2 T_1 T_2}. \tag{4}$$

The evaluations (3) and (4) are clearly different, and it follows immediately that equation (2) is not generally valid for this irreversible process.

Note that the discrepancy between the two sides of equation (2) remains even if the temperatures T_1 and T_2 are very close. That is to say, if we put $T_2 = T_1 + \epsilon$, with $\epsilon \ll T_1$, we get from (3):

$$\delta S \approx mc_V \frac{\epsilon^2}{4 T_1^2} \tag{5}$$

whereas (4) gives twice this amount:

$$\left(\frac{1}{T_1} - \frac{1}{T_2} \right) \delta U_1 \approx mc_V \frac{\epsilon^2}{2 T_1^2}. \tag{6}$$

Hence, Eqn. (2) cannot even be maintained as approximately true when the temperatures are only slightly different.

The reason for the failure of Lavenda's equation (2) is, of course, that it is based on the simple-minded assumptions

$$\delta S_i = \frac{\delta U_i}{T_i}, \qquad i = 1, 2 \tag{7}$$

for the entropy change of the two systems, and then using $\delta U_2 = -\delta U_1$. However, the assumptions (7) are only valid as approximations for reversible (i.e. quasi-static) processes up to first order in the energy exchange (or in ϵ, which is proportional to δU_i). In fact, however, (5) shows that the total entropy increase is a second-order effect (being proportional to ϵ^2), so that δS cannot be obtained in first-order approximation. To obtain an expression for the total entropy increase which is valid in lowest non-vanishing order, one should include the second order terms in (7).

For our example, this gives

$$\delta S_1 \approx mc_V \left(\frac{\epsilon}{2T_1} - \frac{1}{8}\left(\frac{\epsilon}{T_1}\right)^2 \right) \tag{8}$$

$$\delta S_2 \approx mc_V \left(-\frac{\epsilon}{2T_1} + \frac{3}{8}\left(\frac{\epsilon}{T_1}\right)^2 \right) \tag{9}$$

which shows that, upon addition, the first-order terms cancel, while only the quadratic terms yield the correct expression (5) for the total entropy increase.

It appears, therefore, that our paper [2] is right in claiming that the validity of (2) is limited to reversible processes. A consistent use of Lavenda's first-order approximation (7) would imply that the quadratic terms in (8) and (9) are neglected, and thus lead to the result $\delta S = 0$, as stated in this paper.

2. The second issue under dispute concerns the derivation of a thermodynamic uncertainty relation $\Delta U \Delta \beta \geq 1$ in a Bayesian version of statistical thermodynamics, as given in Lavenda's book [3, pp. 195–199]. Here, β denotes the inverse temperature $\beta = \frac{1}{kT}$, where k is the Boltzmann constant, and ΔU and $\Delta \beta$ denote standard deviations, i.e. $\Delta U = \sqrt{\langle (U - \langle U \rangle)^2 \rangle}$ etc., where the average is performed with respect to an appropriate probability distribution. This derivation rests on a lengthy argument, which we do not reproduce here, but the basic structure is that it rests on four ingredients (given in the equations (4.69), (4.73), and (4.67) in [3]), which (neglecting a second order term in the last-mentioned equation) we have summarised as :

$$\mathcal{I}_F = -\frac{\delta U}{\delta \beta} = (\Delta U)^2 = (\Delta \beta)^{-2} = c_V T_1 T_2 \tag{10}$$

Here, $\mathcal{I}_F$ is the Fisher information, and δU and $\delta \beta$ refer to changes in energy and temperature respectively. This notation is slightly different from the convention adopted in [3] where our δU and $\delta \beta$ are denoted as ΔE and $\Delta \beta$ and our $(\Delta U)^2$ and $(\Delta \beta)^2$ as $\overline{(\Delta E)^2}$ and $\overline{(\Delta \beta)^2}$ respectively.

Lavenda's book uses these ingredients to derive the uncertainty relation

$$\Delta U \Delta \beta \geq 1. \tag{11}$$

Our paper observes that, on the same basis, one actually obtains a result even stronger than (11), namely

$$\Delta U \Delta \beta = 1 \tag{12}$$

Therefore, we have concluded that there is "no indication that an uncertainty relation with an inequality sign can be derived on this basis." Lavenda counters that this conclusion displays "a lack of understanding of the statistical and thermodynamic properties of the thermodynamic uncertainty relations".

3

Let us consider the arguments he presents for this case. First, he attributes to us the relation

$$\mathcal{I}_F = -\frac{\Delta E}{\Delta \beta} = \Delta E^2 = -(\Delta \beta)^{-2} = C_V T_1 T_2 \qquad (13)$$

which differs from what we have written by an erroneous minus sign in the fourth term, and, more importantly, by obliterating the notational distinction between changes during a process (denoted by δ) and standard deviations Δ, which represent (square roots of) a statistical average. He then complains that we "do not perform any averaging". Obviously, this complaint is due to Lavenda's own failure to reproduce the distinction implied in our notation.[1]

Next, he invokes a theorem of Khinchin and other considerations, to re-establish the result (11). But all this is completely beside the point. We have not denied that the relation (11) can be derived on the basis of these assumptions; we have argued that they imply the stronger result (12). Since Lavenda's comment does not dispute that the relations (10) correctly summarize the ingredients of the argument in his book (modulo a change in notation), we see no way how anyone can deny this simple observation.

3. A next issue concerns a change of view which we have observed in the course of Lavenda's writings on the implication of the thermodynamic uncertainty relations (11) with regard to the possibility of an underlying molecular reality.

   In Lavenda's paper [4] it is stated that his approach "circumvents a more fundamental, molecular description." In his book [3, p. 6] it is stated that the thermodynamic uncertainty relation (11) "makes it all but impossible that a probabilistic interpretation of thermodynamics would ever be superseded by [a] deterministic one, rooted in the dynamics of large assemblies of molecules." The shift we have observed here is between '*circumvents*', expressing merely that a molecular-dynamical description is not needed (but still allowed), to the view that such a description is *all but impossible*, suggesting that such a description is excluded.

   In his comments, Lavenda calls our discussion "confused and circular". Again, he misrepresents our views. He claims that we have perceived a change from an early view in which the mechanical underpinning is "forbidden" to one in which such an underpinning is "excluded". He then remarks: "whether the thermodynamic uncertainty relations 'exclude' or 'forbid' a mechanical underpinning is not a change of view." This last remark is, of course, correct. But it has no bearing on our discussion.

4. In Lavenda's book, an important role is attributed to a particular new principle, which he calls "Gauss' principle". Unfortunately, we have not

---

[1]We have pointed out both errors to Lavenda in private communication. It is disappointing to see them repeated in print.

4

been able to obtain a clear and convincing formulation of this principle and, frankly speaking, we are quite skeptical about its validity. However, since the purpose of our paper was to review approaches to the thermodynamic uncertainty relations, and not to discuss the merits of this principle, we have decided to confine our attention to Lavenda's derivation of these relations, and leave out the reference to this more contentious issue as much as we could, while taking care to mention those occasions where the principle is invoked in Lavenda's work.

However, Lavenda finds fault in this approach, stating that it shows "a complete lack of understanding of what error laws are all about", and is "tantamount to computing areas and volumes without integral calculus" . Now, surely, we will congratulate Lavenda if some day it can be shown that his principle is equally useful, innocent and devoid of empirical meaning as integral calculus. However, it seems that this day has not yet arrived, since even he leaves it to the future "practiser to be the judge of its worth".

Clearly, this so-called Gauss principle is not yet firmly established nor widely accepted. Therefore, a cautious attitude towards it is reasonable, and our decision to separate this issue from that of the thermodynamical uncertainty relations is justified.

5. Lavenda next raises the question whether the thermodynamic uncertainty relation (11) implies that temperature fluctuates. We have pointed out that, in his own Bayesian approach, the two standard deviations appearing in the relation (11) have a different interpretation. The uncertainty $\Delta\beta$ corresponds to the width of a probability distribution $\rho(\beta)$ which is epistemic, i.e. it reflects a degree of belief about an unknown, fixed temperature parameter β. (Cf. [3, p. 193]) This contrasts with the meaning of ΔU which is the width of the canonical probability distribution $\rho_\beta(U) = \frac{exp(-\beta U)}{Z(\beta)}$ and has a frequency interpretation.

In this interpretation, the uncertainty $\Delta\beta$ merely reflects one's lack of knowledge about the fixed temperature parameter β. Thus, β does not fluctuate. Lavenda's claim to the contrary conflates the distinction between the temperature parameter β and an statistical estimator $\hat{\beta}(U)$ of that parameter, and his rhetorical exclamation "uncertainty is uncertainty, whether it is 'epistemic' or not" simply equivocates the whole issue.

6. Finally, we like to reply to a point which Lavenda does not list as a separate item, but which nevertheless appears as a recurrent theme in his comments. For example, in the abstract of his comments he writes "contrary to their [i.e. our] claims, the uncertainty relations are derived from the second law." Similarly, he ends his note by saying "Uffink and van Lith would be hard pressed to find a thermodynamic inequality which did not stem from the second law and the thermodynamic uncertainty relations are no exception."

These excerpts indicate that Lavenda believes that our paper contains a

claim concerning the relationship between the thermodynamic uncertainty relation and the second law. This is most curious because the second law is not addressed in our paper at all . In fact, the phrase 'second law' occurs only once, when we report Lavenda's position on this issue.

What we have shown is that the argument presented by Lavenda that thermodynamic uncertainty relations follow from the second law is flawed. This means only that a valid demonstration of this claim has not been delivered. However, it has not been the purpose of our paper to argue for the opposite view that thermodynamic uncertainty does *not* stem from the second law. This would indeed be a tricky enterprise since the second law has many inequivalent formulations. (See e.g. [5].) It is therefore pointless to press us "to find a thermodynamic inequality that did not stem from the second law", since this is obviously not the concern of our paper.

Even so, we note that this challenge is also easy to answer. Beside Lavenda, our paper provides a review of many other approaches to the thermodynamic uncertainty relations, for instance by Mandelbrot [6] and Schlögl [7]. In the work of both authors, derivations of thermodynamic inequalities are provided in a purely statical (i.e. time-independent) context. Here, there is no need to assume the existence of irreversible processes and, hence, these inequalities are independent of the second law.

References

[1] B.H. Lavenda *Found. Phys. Lett.* **13**, 487 (2000).

[2] J. Uffink and J. van Lith *Found. Phys.* **29**, 655, (1999).

[3] B.H. Lavenda, *Statistical Physics: a Probabilistic Approach* (Wiley, New York, 1991).

[4] B.H. Lavenda, *J. Phys. Chem. Sol.* **49**, 685 (1988).

[5] J. Uffink "Bluff your way in the second law of thermodynamics" *Stud. Hist. Phil. Mod. Phys.* (to appear).

[6] B. Mandelbrot, *IRE Trans. Inform. Theory* **IT-2**, 190 (1956).

[7] F. Schlögl, *J. Phys. Chem. Sol.* **49** , 679 (1988).