TEMPERATURE FLUCTUATION: A WELL-DEFINED AND UNAVOIDABLE NOTION

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In the May issue of PHYSICS TODAY (page 93), Charles Kittel published an Opinion piece in which he asserted that "the consistent and consensual definition of temperature admits no fluctuations." He was responding (without quite saying so) to an earlier Reference Frame by Herman Feshbach (PHYSICS TODAY, November 1987, page 9) and implicitly criticizing the early editions of the classic treatise by Lev Landau and Evgenii Lifshitz.[1] Kittel also warned us against "fiddling" with "mature concepts."

Such games are indeed seldom effective. However, it has often happened in the history of science that a concept that appears intuitively desirable to many but makes no sense in a given consensual context eventually finds a clear-cut meaning in a context that has been suitably broadened; the redefined concept then in its turn deserves gaining consensus. My goal here is to describe an argument I made in the early 1960s that asserts (turning Kittel's own words to a different purpose) that for closed thermodynamical systems it is the notion of *temperature* that is imperfectly defined and cannot give rise to informed consensus.[2] In contrast, the notion of *temperature fluctuation* $\Delta(1/T)$ is perfectly well defined, *not* as the standard deviation of a random quantity, but rather in a novel way to be described. This approach appears to yield the simplest and fullest possible conceptual justification for the desirable and familiar complementarity relation[1]

$$\Delta E \Delta(1/T) \approx 1$$

Stated differently, I asserted that in a microcanonical system temperature is defined only up to a well-defined indeterminacy that one should be allowed to call fluctuation. This last notion, however, lies one step beyond core probability theory, and belongs to the theory of estimation of statistical parameters.

The main point of my argument is very simple, and this is a good opportunity to explain it to a wide audience.

In a canonical thermodynamical system, the temperature is a parameter that is, of course, determined exactly and is a characteristic of the heat reservoir. The energy E is a canonical random variable whose probability takes the form

$$P(E|\beta) = \sigma(E)\, e^{-E\beta} Z^{-1}(\beta)$$

where $\sigma(E)$ is the density of states, $\beta = 1/kT$ (with k the Boltzmann constant and T the absolute temperature) and $Z(\beta)$ is the partition function. In this case the energy fluctuation is usefully measured by its variance, namely its second moment centered on the first moment. Now consider a closed microcanonical system, that is, a system whose energy E is fixed. As the outcome of an approximate calculation, whose motivation and details do not matter, Ludwig Boltzmann attached to this system the inverse temperature we shall denote by $\hat{\beta}_1$, which satisfies

$$E = \left. \frac{-\partial \log Z(\beta)}{\partial \beta} \right|_{\beta = \hat{\beta}_1}$$

The approximate calculation of Josiah Willard Gibbs, on the other hand, attached a different inverse temperature to a closed system, namely

$$\hat{\beta}_2 = \frac{\partial \log \sigma(E)}{\partial E}$$

For increasingly large systems, the disagreement between Boltzmann and Gibbs becomes asymptotically negligible. This can be shown, for example, by a Darwin–Fowler steepest-descent argument. I proposed to accept the disagreement for small systems as an irreducible part of thermodynamics, and to interpret a quantity of the order of magnitude of the disagreement—it could be the "error term" in the Darwin–Fowler argument—as a new kind of fluctuation. I'll now elaborate on this "error term" by showing how one can interpret it in terms of mathematical statistics.

For a closed system in equilibrium (that must not split into noninteracting parts), one aspect of the notion of

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thermodynamic equilibrium is as follows (in reference 2 this aspect is enthroned as a generalized "zeroth principle" of thermodynamics): "Irrespective of how such a system was actually prepared, its future behavior will be exactly the same." For example, it will behave exactly as if it had been taken away from being in contact and in equilibrium with some heat reservoir, in which case the system's fixed energy is a sample value of a canonical random variable. I argued that to define a temperature for such a closed system is to make an estimate (that is, an informed guess) of the value of the canonical temperature of a heat reservoir with which one may assume in calculations our system had been in contact.[2] In statistics, an estimate of β is written as $\hat{\beta}$. The meaning of the process of estimation has been thoroughly discussed in statistics and need not be tackled from the ground up. Two facts emerge. First, the procedure is intrinsically and unavoidably indeterminate: It does not allow a unique solution. Second, its formulas follow precisely the paths taken by Boltzmann and Gibbs.

Many estimates identify the observed E with some "typical value" of a canonical energy of parameter β. One statistician will interpret "typical value" as "expectation," and he will recommend Boltzmann's value $\hat{\beta}_1$. This value is also obtained as a "maximum likelihood" estimate and it is "unbiased," meaning $\langle\hat{\beta}_1\rangle = \beta$. But a second statistician will instead interpret "typical value" as "the most likely value," also called the "mode." He will recommend as the estimate Gibbs's value $\hat{\beta}_2$. These two statisticians, and others who would give different recommendations, will also tell the physicist something that we know he expects: that in an infinitely large system, all sensible recommendations agree. The statisticians call them "consistent"—and Kittel may call them "consensual." On the other hand, for small systems, the statisticians grant that a fog of uncertainty is simply unavoidable.

In a canonical system, $\hat{\beta}_1$ and $\hat{\beta}_2$ are functions of E. Hence they are random variables, and each has a well-defined variance. It turns out that there is a lower bound to this variance, given by a theorem called the Cramèr–Rao inequality[3] or the Fisher-Fréchet-Dugué-Rao-Cramèr inequality. (It is discussed, often under "statistical efficiency," in every advanced book on mathematical statistics.) Applied to a single sample and to an unbiased estimator, that is, assuming $\langle\hat{\beta}\rangle = \beta$, this theorem yields

$$\langle(\hat{\beta} - \beta)^2\rangle \geqslant F^{-1}$$

The factor F is called Fisher's information (after Ronald Fisher); hence the alternative term "information inequality" for this formula (see the first book listed in reference 3). In the present, special case, the Gibbs distribution, F happens to simplify to

$$F = \int\left(E + \frac{\partial \log Z}{\partial \beta}\right)^2 P(E|\beta)\,\mathrm{d}E$$

When this simplified F is taken as a function of β, it simply reduces to the variance $\langle E^2\rangle$. What statisticians do next is to "invert" and take F as a function of E. The inversion's conceptual justification has been discussed endlessly, but it is now agreed[3] that inversion does *not* reduce statistical fluctuation to probabilistic variance. To achieve such a reduction would have been nice—but it cannot be done. Statistical fluctuation is a notion that is one step beyond core probability, which is perhaps why it has worried Kittel. Nevertheless a physicist should not mind if two notions of fluctuation that are conceptually distinct are combined into one complementarity relation. The combination yields

$$\Delta E \Delta(\beta) = 1$$

and

$$\Delta E \Delta(1/T) \geqslant k$$

When a canonical system is of extremely large size n, one has $E \propto n$ and $\Delta E \propto n^{1/2}$; hence the relative energy fluctuations $\Delta E/E$ and the inverse temperature fluctuations both are proportional to $n^{-1/2}$ and are negligibly small.

An imperfectly defined microcanonical temperature with a well-defined fluctuation may at first seem strange, but there should be no insurmountable difficulty in achieving consensus on its behalf.

References

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3. See, for example, P. J. Bickel, K. A. Doksum, *Mathematical Statistics*, Holden-Day, San Francisco (1977), section 4.3, p. 126; H. Cramèr, *Mathematical Methods of Statistics*, Princeton U. P., Princeton (1946), section 32.3, p. 477; C. R. Rao, *Linear Statistical Inference*, Wiley, New York (1973); S. S. Wilks, *Mathematical Statistics*, Wiley, New York (1962), section 12.2(b), p. 351. ■

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