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

\[
\Delta E \Delta (1/T) \approx 1
\]

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

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

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 \( \beta_1 \), which satisfies

\[
E = -\frac{\partial \log Z(\beta)}{\partial \beta} \bigg|_{\beta = \beta_1}
\]

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 en
throned as a generalized "zeroth principle" of thermodynamics): "Irre
spective 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 con
tact 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 tempera
ture of a heat reservoir with which
one may assume in calculations our
system had been in contact. In
statistics, an estimate of $\beta$ is written
as $\hat{\beta}$. The meaning of the process
of estimation has been thoroughly dis
cussed in statistics and need not be
tackled from the ground up. Two
facts emerge. First, the procedure is
intrinsically and unavoidably indeter
minate: It does not allow a unique
solution. Second, its formulas follow
precisely the paths taken by Boltz
mann and Gibbs.

Many estimates identify the ob
served $E$ with some "typical value" of
a canonical energy of parameter $\beta$.
One statistician will interpret "typi
cal value" as "expectation," and he
will recommend Boltzmann's value
$\beta_1$. This value is also obtained as a
"maximum likelihood" estimate and it is
"unbiased," meaning $\langle \hat{\beta} \rangle = \beta$.
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 $\beta_2$. These two statisti
cians, 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 recommenda
tions agree. The statisticians call
them "consistent"—and Kittel may
call them "consensual." On the other
hand, for small systems, the statisti
cians 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 Cramér–Rao inequality or the
Fisher–Fréchet–Dugué–Rao–Cramér
inequality. (It is discussed, often un
der "statistical efficiency," in every
advanced book on mathematical sta
tistics.) Applied to a single sample and
to an unbiased estimator, that

is, assuming $\langle \hat{\beta} \rangle = \beta$, this theorem yields

$$\langle \hat{\beta} - \beta \rangle^2 \geq \frac{E}{\beta}$$

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 dis
tribution, $F$ happens to simplify to

$$F = \int [E + \frac{\partial \ln Z}{\partial \beta}]^2 \rho(E|\beta) dE$$

When this simplified $F$ is taken as a
function of $\beta$, 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 conceptu
al justification has been discussed
elessly, but it is now agreed 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 no
tion 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 conceptu
ally distinct are combined into one
complementarity relation. The com
bination yields

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

and

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

When a canonical system is of
extremely large size $n$, one has $E \sim n$ and $\Delta E \sim n^{1/2}$; 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 microca
nonical temperature with a well-de
fined fluctuation may at first seem
strange, but there should be no insur
mountable difficulty in achieving con
sensus on its behalf.

References

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