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Operational approach to fluctuations of thermodynamic variables in finite quantum systems

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In this paper we present a quantum approach to the old problem of temperature fluctuations. We start by observing that according to quantum thermodynamics, fluctuations of intensive parameters like temperature cannot exist. Furthermore, such parameters are not observables, so their estimation has to be done indirectly. The respective temperature estimate based on quantum measurements of the energy is shown to fluctuate according to the well-known formula $\Delta T^2 = \frac{k_B T^2}{C}$, but only within a certain temperature range and if the system is not too small. We also calculate the fourth-order correction term, becoming important at higher temperatures. Finally we illustrate our results with a concrete model of n spins.

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I. INTRODUCTION

Fluctuations within a thermodynamical setting have long since attracted considerable interest [1]. These refer to extensive and intensive thermodynamic variables [1,2] as well as work and heat along certain thermodynamic processes [3–5]. The nature and operational accessibility of such fluctuations, however, often lack clarity. In part this is due to the fact that neither intensive variables nor heat and work are observables in the strict sense (see the following discussion).

In statistical mechanics a system might be described by a canonical ensemble. In this case the ensemble average of the energy variance ΔE could—under the ergodic hypothesis—be identified with the corresponding time average associated with the spontaneous exchange of energy between system and environment.

On the other hand, from the point of view of quantum thermodynamics [6], fluctuations proper cannot exist for an individual system appropriately embedded in a large environment, since the environment enforces a quasistationary state on the system, implying that energy and temperature should be constant.

The concept of temperature fluctuations has caused longstanding controversies [7,8] that have not been resolved satisfactorily to this day [9]. Under exactly what conditions should one be able to test or confirm the well-known relation for the temperature variance [1,10],

$$\Delta T^2 = \frac{T^2}{C}, \tag{1}$$

with C being the heat capacity of the respective system (the Boltzmann constant k_B is set to unity)? It is fairly obvious that any attempt to do so will have to be based on data resulting from some measurement scenario. Only then can one hope to give fluctuations a well-defined, that is, operational meaning.

In a previous paper [11] we have shown how including measurements in a quantum thermodynamical setting leads to a situation in accordance with statistical mechanics. Here we will show that with respect to fluctuations, the essential link is also provided by measurement: While implemented as a well-controlled act, its result is quantum-mechanically undetermined. We argue that although the temperature itself does not fluctuate, there will be fluctuations for the temperature estimate based on energy measurements. Formula (1) is recovered for modular systems within a certain temperature window; possible deviations from this formula will be discussed. Finally, we consider a system consisting of n spins to illustrate our general considerations.

II. TEMPERATURE ESTIMATION

Temperature is not an observable, that is, it can only be measured indirectly (for example, by measuring energy). We assume the mean energy to be a bijective function of temperature,

$$\langle E\rangle = f(T), \tag{2}$$

which thus can be inverted to give $T = f^{-1}(\langle E\rangle)$. However, the average energy on the right-hand side can only be obtained by carrying out (in principle infinitely) many measurements. Hence, the question of how to get an estimate for temperature after a single energy measurement arises. Since the best guess for a random variable is its average [12], an obvious estimate for temperature in the case of having measured energy E_m is

$$T_{\text{est}} = f^{-1}(E_m). \tag{3}$$

At this point it is already clear that the so-defined temperature estimate T_{est} will fluctuate, since a quantum measurement of energy will cause the system to collapse into one of the energy eigenstates E_m, implying different values T_{est}. Thus, fluctuations of energy and the estimated temperature are directly correlated.

We now want to calculate the expectation value of the estimated temperature and its fluctuations. To do so, the first step is to make an approximation for the occupation probabilities $\omega(E)$. In general, $\omega(E)$ is given by the Boltzmann distribution $\omega(E) = g(E)e^{-E/T}$, where $g(E)$ is the degeneracy (we set k_B to unity). Let us assume that our system is modular, or composed of many identical parts. Such a modular structure is typical in nature as discussed in [6]. This allows us to apply the so-called central limit theorem, which states that a random variable, which is the sum of n identically distributed random variables, is in good approximation normally distributed if n is sufficiently large. In our case, this means that the total

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energy E, which is the sum of the energies of the subsystems, will be approximately Gaussian distributed if the number of subsystems is large enough:

$$\omega(E) \approx \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{E-\langle E\rangle}{\sigma}\right)^2}. \tag{4}$$

With this, the expectation value for the temperature estimate is given by

$$\langle T_{\text{est}}\rangle = \int_{-\infty}^{\infty} \omega(E) T_{\text{est}}(E) dE. \tag{5}$$

In general, this integral cannot be solved analytically. However, since the distribution (4) is peaked at $\langle E\rangle$, we can perform a Taylor expansion of $T_{\text{est}}(E) = f^{-1}(E)$ around this point in energy space. Therefore, we use the fact that the derivative of the inverse function can be expressed as

$$\frac{d}{dE} f^{-1}(E) = \frac{1}{f'[f^{-1}(E)]}, \tag{6}$$

and that $f^{-1}(\langle E\rangle) = T$. This leads to the expansion up to fourth order:

$$\begin{aligned} T_{\text{est}}(E) = {} & T + \frac{1}{f'(T)}(E - \langle E\rangle) - \frac{f''(T)}{2[f'(T)]^3}(E - \langle E\rangle)^2 \\ & + \frac{3[f''(T)]^2 - f'(T)f'''(T)}{6[f'(T)]^5}(E - \langle E\rangle)^3 \\ & + \frac{-15[f''(T)]^3 + 10 f'(T)f''(T)f'''(T) - [f'(T)]^2 f^{(4)}(T)}{24[f'(T)]^7}(E - \langle E\rangle)^4 \\ & + \mathcal{O}[(E - \langle E\rangle)^5]. \end{aligned} \tag{7}$$

Plugging this into (5) leads to analytically solvable integrals of the form

$$\begin{aligned} I_a &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} (x-\mu)^a e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} dx \\ &= \frac{1}{\sqrt{\pi}} 2^{\frac{a}{2}-1}[1 + (-1)^a]\sigma^a \Gamma\left(\frac{a+1}{2}\right), \end{aligned} \tag{8}$$

which are zero for odd a. The nonvanishing integrals in our expansion read $I_0 = 1$, $I_2 = \sigma^2$, $I_4 = 3\sigma^4$.

Here σ can be expressed by the heat capacity $C(T) = f'(T)$ according to

$$\sigma^2 = \Delta E^2 = \langle E^2\rangle - \langle E\rangle^2 = T^2 C(T), \tag{9}$$

which can be easily shown by standard methods of statistical mechanics using the partition sum. This finally leads to the expectation value for the temperature estimate

$$\langle T_{\text{est}}\rangle = T - T^2 \frac{C'(T)}{2[C(T)]^2} - T^4 \frac{15[C'(T)]^3 - 10C(T)C'(T)C''(T) + [C(T)]^2 C'''(T)}{8[C(T)]^5} + \cdots. \tag{10}$$

As one can see, the expectation value of T_{est} would equal the true temperature T in the case of a constant heat capacity. Otherwise, there will be deviations that increase with increasing temperature and decreasing subsystem number n since C is extensive (i.e., the first correction term is of the order $1/n$, the second one is of the order $1/n^2$, etc.). The higher-order terms typically become more important for higher temperatures because of the factors $T^2, T^4, \ldots$. However, this is no systematic expansion in T, since the heat capacity C also depends on the temperature.

Let us now turn to the fluctuations of the estimated temperature characterized by $\Delta T_{\text{est}}^2 = \langle T_{\text{est}}^2\rangle - \langle T_{\text{est}}\rangle^2$. $\langle T_{\text{est}}^2\rangle$ can be calculated in the same way as described for $\langle T_{\text{est}}\rangle$. We obtain

$$\begin{aligned} \langle T_{\text{est}}^2\rangle = {} & T^2 + \frac{T^2 f'(T) - T^3 f''(T)}{[f'(T)]^2} \\ & - \frac{15T^5[f''(T)]^3 - 5T^4 f'(T)f''(T)[3f''(T) + 2Tf'''(T)] - T^4[f'(T)]^2[4f'''(T) + Tf^{(4)}(T)]}{4[f'(T)]^5} + \cdots. \end{aligned} \tag{11}$$

This finally leads us to

$$\Delta T_{\text{est}}^2 = \frac{T^2}{C(T)} + T^4\left(\frac{7[C'(T)]^2}{2[C(T)]^4} - \frac{C''(T)}{[C(T)]^3}\right) + \cdots. \tag{12}$$

Thus, in lowest order, we confirm Eq. (1). This means this formula is valid for sufficiently large systems as well as not too high temperatures. Moreover, the formula would be exact if the heat capacity $C(T)$ were independent of temperature, since all higher-order terms contain derivatives of $C(T)$.

Combining (9) and (12) we recover a kind of "thermodynamic uncertainty relation" [13,14]:

$$\Delta E^2 \Delta T_{\mathrm{est}}^2 = T^4 + \mathcal{O}\left(\frac{1}{n}\right). \tag{13}$$

For fixed temperature this uncertainty product is also fixed and thus appears to leave no room for variations. But the relation indicates that any increase of fluctuations in energy (e.g., by increasing the size of the thermometer system and thus of C) has to be counterbalanced by a reduction of the fluctuations of the temperature estimate.

Looking at the expansion, one may expect the formulas (10)–(13) to be valid for arbitrary low temperatures. This is not the case, though, since at low temperatures the approximation (4) breaks down for finite systems: Below a certain temperature the occupation probabilities can no longer be described by a normal distribution.

How can we get an estimate for the lower bound? Let us set the energy of the ground state to zero. Then occupation probabilities for $E < 0$ following from (4) should be negligibly small, if the normal distribution should be a good approximation. To achieve this, we demand the expectation value of the distribution to be larger than three times the standard deviation: $\langle E\rangle \geqslant 3\sigma$. This guarantees that 99.87% of the occupation probability is at $E > 0$. Expressing this condition in terms of the heat capacity yields

$$3T_{\mathrm{min}}\sqrt{C(T_{\mathrm{min}})} = \int_0^{T_{\mathrm{min}}} C(T')\,dT' \tag{14}$$

as a criterion for the minimal temperature T_{min} below which the fluctuation formula (1) may break down.

Until now, the discussion has been based on a single measurement. If one wants to improve the estimate of temperature (e.g., for small systems, where the fluctuations of T_{est} tend to become large), one has to perform more measurements. It is clear that for modular systems with n parts the probability of measuring the total energy E after j independent measurements equals the probability for measuring energy E for a system of jn parts after a single measurement: $\omega^{(n,j)}(E) = \omega^{(jn,1)}(E)$. This means that calculating the temperature by averaging over several measurements amounts to an effective increase of system size, thus reducing the fluctuations. In turn, this demonstrates that the formula (1) can be applicable only for a single measurement; whenever an average over more measurements is used, the number of measurements will modify the fluctuations of estimated temperature.

III. EXAMPLE: THE *n* SPIN MODEL

In this section, we want to apply our general considerations to a concrete model. The quantum system we consider here is a set of n spins, with energy splitting ε each, which we first suppose to be without mutual interaction. Energy levels are indexed by $r = 0,\dots,n$, with $E_r = r\varepsilon$ and degeneracy $g(E_r) = \binom{n}{r}$. This system is prepared in a canonical state by coupling with a bath at T so that its mean energy is

$$\langle E\rangle_T = f(T) = \frac{n\varepsilon}{1+\exp\left(\frac{\varepsilon}{T}\right)}. \tag{15}$$

According to (3) the temperature estimate is inferred from

$$T_{\mathrm{est}}(E_m) = \frac{\varepsilon}{\ln\left(\frac{n\varepsilon}{E_m} - 1\right)} \tag{16}$$

after energy E_m has been measured.

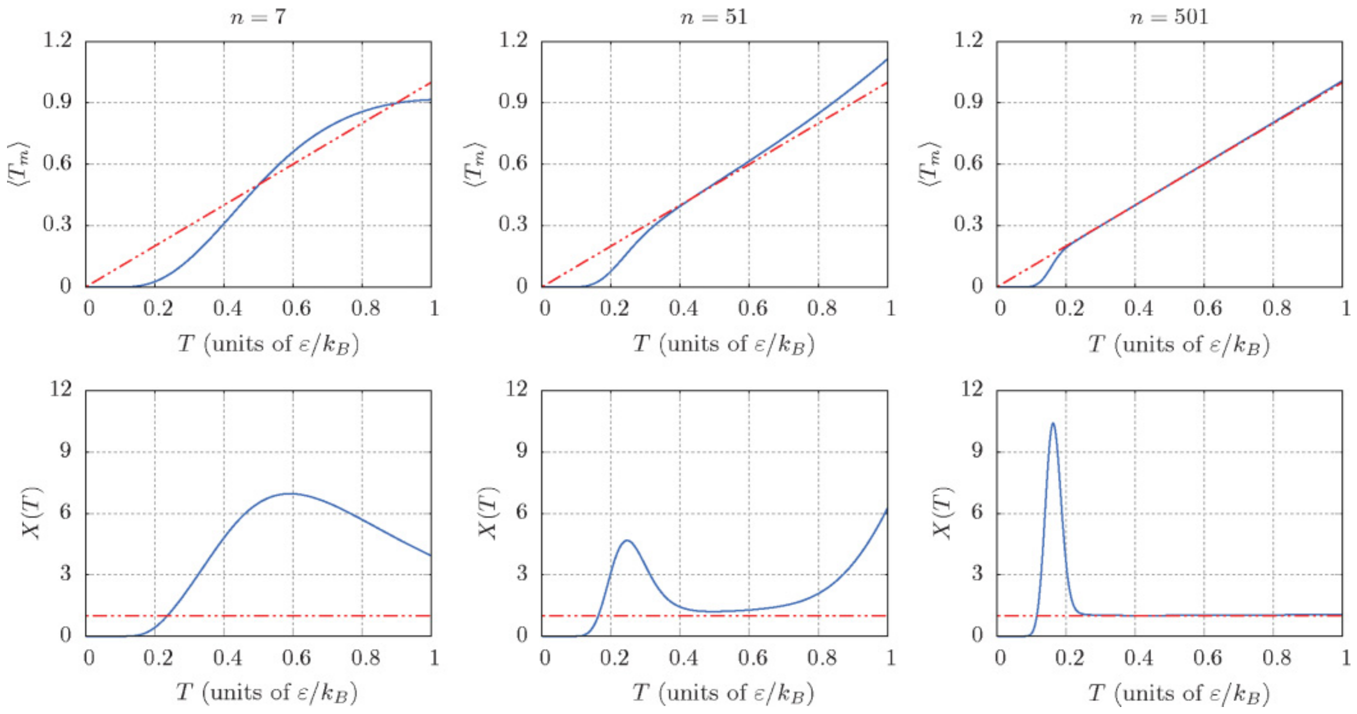

FIG. 1. (Color online) $\langle T_{\mathrm{est}}\rangle_T$ as compared to $\langle T_{\mathrm{est}}\rangle_T = T$ (dash-dotted line) and $X(T) = \frac{\Delta T_{\mathrm{est}}^2}{\Delta^2}$ as compared to $X(T) = 1$, both as a function of T for $n = 7, 51$, and 501.

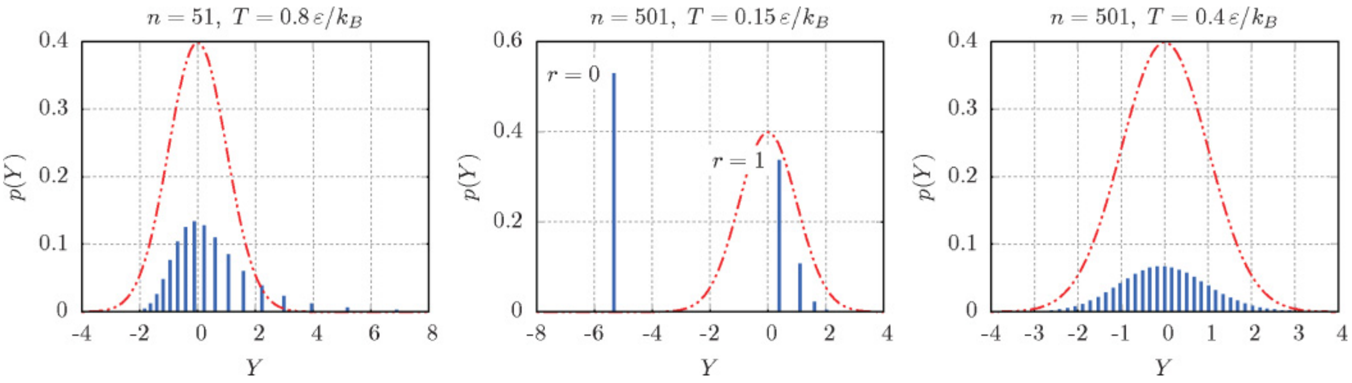

FIG. 2. (Color online) Discrete probability distribution of $Y = \frac{T_{\text{est}} - T}{\Delta}$ compared with the Gaussian form assumed by fluctuation theory, $p(Y) = \frac{1}{\sqrt{2\pi}} \exp(-Y^2/2)$ (dash-dotted line).

Obviously, T_{est} defined this way is singular at $E_m = \frac{n\varepsilon}{2}$. To avoid inconsistencies we introduce a cutoff temperature T^{cut} redefining $T_{\text{est}}(E_m)$ for $E_m > \langle E \rangle_{T^{\text{cut}}}$ by $T_{\text{est}}(E_m) = T^{\text{cut}}$. If we choose T^{cut} large enough (note that we are interested in low temperatures), the probability of measuring $E_m > \langle E \rangle_{T^{\text{cut}}}$ is negligible, ensuring that the results will not depend on T^{cut}.

We now compare the (exact) fluctuations of the estimated temperature ΔT_{est}^2 based on

$$\Delta T_{\text{est}}^2 = \frac{1}{Z(T)} \sum_{r=0}^{n} \binom{n}{r} \exp\left(-\frac{E_r}{T}\right) T_{\text{est}}^2(E_r) - \left[\frac{1}{Z(T)} \sum_{r=0}^{n} \binom{n}{r} \exp\left(-\frac{E_r}{T}\right) T_{\text{est}}(E_r)\right]^2 \tag{17}$$

with the fluctuation formula [the lowest order of (12)]

$$\Delta^2 = \frac{T^2}{C} = \frac{T^4[1 + \exp(\varepsilon/T)]^2}{n\varepsilon^2 \exp(\varepsilon/T)}. \tag{18}$$

In the second step in Eq. (18), we have used the analytical form for the heat capacity $C(T) = \frac{\partial}{\partial T}\langle E \rangle_T$ derived from Eq. (15). As discussed in the preceding section, this formula should be valid in a temperature window bounded from below by condition (14), which reads for the present model,

$$T_{\min} = \frac{\varepsilon}{\log(n/9)}, \tag{19}$$

and from above by the fact that higher-order terms in (12) should still be negligible, which is roughly the case for $T < T_{\max} = 0.05\sqrt{n}\,\varepsilon$. It is clear that if the lower bound $T_{\min}$ becomes larger than the upper bound $T_{\max}$, the fluctuation formula should no longer apply. This turns out to be the case for small systems of less then 82 spins.

The curves of $X(T) = \frac{\Delta T_{\text{est}}^2}{\Delta^2}$ as a function of T for $n = 7$, 51, and 501 are given in Fig. 1 together with those of $\langle T_{\text{est}} \rangle_T$ (which is, as said, not necessarily equal to T). As expected, $X(T) = 1$ (dash-dotted line) is definitively unsuitable below n of the order of about 100 spins. For bigger systems there is a range of temperatures where $X(T) = 1$ becomes valid. This domain of system size and temperature coincides with the conditions for the measurement protocol to be considered acceptable, with $\langle T_{\text{est}} \rangle_T \approx T$.

Figure 2 shows the probability distribution of T_{est} for different values of n and T. As one can see, the Gaussian approximation breaks down at low temperatures as well as for small systems, which explains the deviations form $X(T) = 1$ in these areas.

Interactions between the spins will influence the present results. It can be shown that for weak interactions the initial peak in the curves $X(T)$ (see Fig. 1) slightly shifts toward higher temperature.

IV. CONCLUSION

In this paper we have tried to shed new light on the old debate about fluctuations of thermodynamic variables, in particular of temperature. We have argued that according to quantum thermodynamics, temperature is a fixed parameter T determined by the large environment. Thus, there are no fluctuations "when nobody looks."[1]

However, if one wants to estimate temperature from a single energy measurement, the estimated temperature, indeed, will fluctuate. These fluctuations are based neither on mere formal calculation nor on experimental error but actually represent a fundamental limit for the instantaneous determination of temperature. The fluctuations of T_{est} are directly connected with the energy fluctuations due to the measurement and therefore with the measurement postulate of quantum mechanics. This connection can be expressed by the thermodynamic uncertainty relation (13).

We found that T_{est} fluctuates according to the well-known fluctuation formula (1), subject, however, to some conditions: On the one hand, the actual temperature T has to be not too low, since otherwise the occupation probabilities will no longer be Gaussian distributed, which was assumed for deriving the formula. This deviation from the Gaussian distribution typically also leads to a deviation of the fluctuations from formula (1), as shown for the concrete model of n spins. On the other hand, for too high temperatures, higher-order correction terms will become important. The range of temperatures in

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[1] This statement is a reminder of D. Mermin's seminal paper entitled "Is the moon there when nobody looks? Reality and the quantum theory", Physics Today, April 1985, pp 38–47. The question points to the fact that "observations not only disturb what has to be measured, they produce it".

which the formula is valid becomes larger and larger for increasing size of the system. Therefore, it is not surprising that this formula can be confirmed already for mesoscopic systems, as done in [15].

The fluctuations of T_{est} can be reduced at will by averaging over more and more (independent) measurements [16]. Formula (1), therefore, is valid only if temperature is estimated via a single measurement, which is, in a sense, local in time.

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[16] Independence requires that the quantum system has enough time to recover its equilibrium state before the next measurement.