

Letter

Achieving the Landau bound to precision of quantum thermometry in systems with vanishing gap

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Abstract

We address estimation of temperature for finite quantum systems at thermal equilibrium and show that the Landau bound to precision $\delta T^2 \propto T^2$, originally derived for a classical *not too small* system being a portion of a large isolated system at thermal equilibrium, may be also achieved by energy measurement in microscopic *quantum* systems exhibiting vanishing gap as a function of some control parameter. On the contrary, for any quantum system with a non-vanishing gap Δ , precision of any temperature estimator diverges as $\delta T^2 \gtrsim T^4 e^{\Delta/T}$.

Keywords: quantum thermometry, quantum estimation, Landau bound

(Some figures may appear in colour only in the online journal)

1. Introduction

In the last decades, we have seen a constant improvement in the generation and control of engineered quantum systems, either to test quantum mechanics in a mesoscopic or macroscopic setting, or for the implementation of quantum-enhanced technologies. More recently, controlled quantum systems have become of interest to test and explore thermodynamics in the quantum regime, e.g. for the characterization of work and energy statistics. Indeed experiments in several optical and material systems have been suggested and implemented, with the aim of understanding relaxation, thermalization, and fluctuations properties in systems exhibiting explicit quantum features or being at the classical-quantum boundary [1–21].

In this framework, it has become increasingly relevant to have a precise determination of temperature for quantum systems [22–28], and to understand the ultimate bounds to precision in the estimation of temperature posed by quantum mechanics itself [29–39]. The problem

cannot be addressed in elementary terms since, as a matter of fact, for a quantum system in equilibrium with a thermal bath, there is no linear operator that acts as an observable for temperature and we cannot write down any uncertainty relation involving temperature. In turn, this is somehow connected with the fact that temperature, thought as a macroscopic manifestation of random energy exchanges between particles, *does not*, in fact, fluctuate for a system at thermal equilibrium. Therefore, in order to retain the operational definition of temperature, one is led to argue that although the temperature itself does not fluctuate, there will be fluctuations for any temperature estimate, which is based on the measurement of some proper observable of the systems, e.g. energy or population.

This line of thought has been effectively pursued in classical statistical mechanics where, upon considering temperature as a function of the exact and fluctuating values of the other state parameters, Landau and Lifshitz derived a relation for the temperature fluctuations of a finite system [40, 41]. This is given by $\delta T^2 = T^2/C$ where C is the heat capacity of the system itself. In turn, this appears as a fundamental bound to the precision of any temperature estimation. However, the relation has been derived for a system which represents a small portion (but not too small) of a large, isolated, system in thermal equilibrium. Besides, it has been derived assuming the absence of any quantum fluctuation. Overall, its validity is thus questionable if the temperature is low enough or the system is known to exhibit quantum features [42].

A first attempt to establish the Landau bound for finite quantum systems has been pursued by inverting the energy dependence on temperature [43], however still assuming that the system is large enough. Earlier, the concept of temperature fluctuations had caused longstanding controversies [44–51], which have not really solved to date, at least in fundamental terms [52]. In particular, it is not clear whether, and under which conditions, the Landau bound may be confirmed for quantum systems at low temperature (where quantum fluctuations become relevant), and whether the corresponding precision may be achieved in practice.

2. The Landau bound in quantum systems with vanishing gap

Our starting point is to recall that temperature is not an observable and therefore its value should be estimated through an indirect detection scheme, i.e. by measuring something else, say the observable X on M repeated preparations of the system, and then suitably processing the data sample x_1, \dots, x_M in order to infer the value of temperature. The function $\hat{T}(x_1, \dots, x_M)$ is usually referred to as an *estimator* and provide an operational definition of temperature for the system under investigation. However, as firstly noticed by Mandelbrot for closed systems [44, 48], different inference strategies may be employed, e.g. by starting from different observables, or just by using different estimators (say, the mean or the mode) on the same data sample, thus leading to different, and perfectly acceptable, definitions of temperature. In other words, temperature for a thermodynamic system cannot uniquely defined, and no specific definition can give rise to consensus.

On the other hand, we may give proper and unique definition to the notion of temperature fluctuations. In fact, the variance of *any* unbiased estimator of temperature is bounded by the Cramer–Rao theorem [53], stating that

$$\delta T^2 \geq \frac{1}{MF(T)}, \quad (1)$$

where $\delta T^2 \equiv \text{Var}(\hat{T}) = \langle (\hat{T} - T)^2 \rangle$, M is the number of repeated measurements and $F(T)$ is the so-called Fisher information, given by

$$F(T) = \int dx p(x|T) [\partial_T \log p(x|T)]^2, \quad (2)$$

being X the quantity measured to infer the temperature and $p(x|T)$ the conditional distribution of its outcomes given the true, fixed, value of temperature. The overall picture arising from the Cramer–Rao theorem is that the notion of temperature may be indeed imperfectly defined whereas, at the same time, the notion of temperature fluctuations may be given an unique meaning.

We will fully exploit this approach to establish whether, and in which regimes, the Landau bound to thermometry may be established for quantum systems. To this aim, the crucial observation is that the quantum version of the Cramer–Rao theorem [54–59] provides tools to individuate an *optimal* strategy to infer the value of temperature, i.e. to define a privileged observable related to temperature, which allows one to determine temperature with the ultimate precision. This is done in two steps: (i) find the observable that maximizes the Fisher information and (ii) find an estimator that saturate the Cramer–Rao bound. The first step may be solved in a *system-independent* way, upon considering the observable defined by the spectral measure of the so-called *symmetric logarithmic derivative*, i.e. the self-adjoint operator L_T obtained by solving the Lyapunov-like equation

$$\partial_T \varrho_T = \frac{1}{2} (L_T \varrho_T + \varrho_T L_T), \quad (3)$$

where ϱ_T is the density operator of the system under investigation. The second step is, in general, dependent on the system under investigation, though general solutions may be found in the asymptotic regime of large data samples, where Bayesian or maximum-likelihood estimators are known to saturate the Cramer–Rao bound.

In approaching the issue of temperature fluctuation, one often assumes that the quantity that should be measured is the energy of the system. The first thing we can prove using quantum estimation theory is that energy measurement is, in fact, the optimal one for any quantum systems. The only assumption needed to prove this statement is that the system under examination may be described in the canonical ensemble. Let us denote by \mathcal{H} the Hamiltonian of the quantum system under investigation and by $\mathcal{H}|e_n\rangle = E_n|e_n\rangle$ its eigenvalues and eigenvectors. At thermal equilibrium the density operator of the system is

$$\varrho_T = \frac{1}{Z} \exp\{-\beta\mathcal{H}\} = \frac{1}{Z} \sum_n e^{-\beta E_n} |e_n\rangle\langle e_n|, \quad (4)$$

where $\beta = T^{-1}$, being the Boltzmann’s constant set to one, and $Z = \text{Tr}[\exp\{-\beta\mathcal{H}\}]$ is the partition function of the system. Inserting equation (4) in equation (3) we have a solvable equation, leading to

$$L_T = \sum_n \frac{E_n - \langle \mathcal{H} \rangle}{T^2} |e_n\rangle\langle e_n|, \quad (5)$$

where $\langle \mathcal{H} \rangle$ is the average energy of the system. Equation (5) shows that the optimal measurement is diagonal in the Hamiltonian basis, i.e. it may be achieved by measuring the energy of the system. The corresponding Fisher information is given by $F(T) \propto \langle \delta \mathcal{H}^2 \rangle / T^4 = c_V(T) / T^2$, $c_V(T)$ being the specific heat at temperature T . In turn, this relation reveals that when the specific heat increases then the same happens to the Fisher information associated to temperature, e.g. temperature may be effectively estimated at the classical phase transitions with diverging specific heat [60, 61]. On the other hand, if the

specific heat is bounded from above than precision of temperature estimation is bounded from below.

We now proceed to investigate whether the Landau bound for quantum systems holds also in the low temperature regime. In doing this, we analyze the microscopic origin of the behavior of the specific heat *without* making any assumptions of the size of the system. To this aim we assume that only the two lowest energy levels of the system are populated (we are in the low temperature regime). The density operator may be written as

$$\varrho_T = \frac{1}{Z} (|e_0\rangle\langle e_0| + e^{-\Delta(\lambda)/T} |e_1\rangle\langle e_1|), \quad (6)$$

where the partition function reads as follows $Z = 1 + e^{-\Delta(\lambda)/T}$ and $\Delta \equiv \Delta(\lambda) = E_1 - E_0$ is the energy gap between the two levels. In writing (6) we also assumed that the energy levels of the systems do depend on some external control parameter λ , e.g. an internal coupling or an external field, which may be exploited to tune the energy gap $\Delta(\lambda)$ between the two levels. Using equation (2) and the fact that energy measurement is optimal, the Cramer–Rao bound (1) for temperature estimation says that the variance of any temperature estimator is bounded by

$$\delta T^2 \geq T^2 g(\Delta/T)$$

where

$$g(x) = \frac{2}{x^2} (1 + \cosh x).$$

The function $g(x)$ is depicted in the left panel of figure 1. It diverges as e^x/x^2 for $x \rightarrow \infty$ and as $4/x^2$ for $x \rightarrow 0$, whereas it shows a minimum $g(x_m) \simeq 2.27$ located at $x_m \simeq 2.4$. It follows that in systems where the gap Δ may be tuned to arbitrarily small values by tuning the external control λ , such that $\Delta/T \simeq x_m$ remains finite, optimal estimation of temperature with precision at the Landau bound $\Delta T^2 \propto T^2$ may be achieved by measuring energy and a suitable data processing. On the contrary, in system where the gap has a minimum, temperature may be estimated efficiently only down to a threshold, below which the variance of any estimators starts to increase as

$$\delta T^2 \gtrsim T^4 e^{\Delta/T}.$$

The above results are valid for arbitrarily small systems at low temperature and do not depend on the specific structure of the system Hamiltonian, nor on the size of the system. The only requirement is that the system exhibits vanishing gap between its lowest energy levels as a function of some external control parameter. Results are also independent on any specific features of the two-level approximation, assuming that a gap above the first excited level is present in order to make sense of the two-level description. The range of temperature where the results holds corresponds to the range of validity of the two-level approximation, roughly speaking T of the order of the gap above the first excited level. Results are however robust against this parameter. To confirm this statement, let us consider a three-level approximation where

$$\varrho_T = \frac{1}{Z} (|e_0\rangle\langle e_0| + e^{-\Delta_1(\lambda)/T} |e_1\rangle\langle e_1| + e^{-\Delta_2(\lambda)/T} |e_2\rangle\langle e_2|)$$

and $Z = 1 + e^{-\Delta_1(\lambda)/T} + e^{-\Delta_2(\lambda)/T}$, $\Delta_k = E_k - E_0$. The resulting Cramer–Rao bound, for energy measurement, is given by

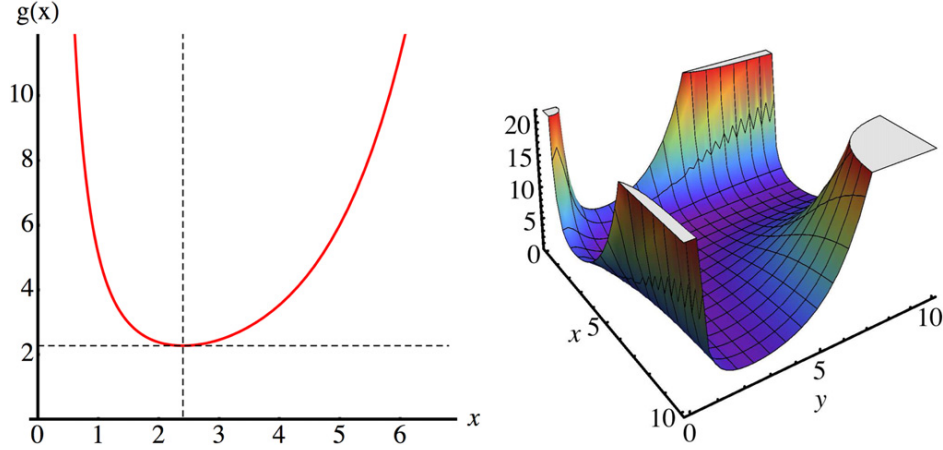


Figure 1. The functions $g(x)$ and $h(x, y)$ governing the variance of temperature estimators in the low temperature regime.

$$\Delta T^2 \geq T^2 h\left(\frac{\Delta_1}{T}, \frac{\Delta_2}{T}\right),$$

where

$$h(x, y) = \frac{e^{-x-y}(e^x + e^y + e^{x+y})^2}{(1 + e^y)x^2 - 2xy + (1 + e^x)y^2}.$$

The function $h(x, y)$ is depicted in right left panel of figure 1. It is symmetric and shows a global minimum $h_m \simeq 1.31$ located at $x_h = y_h \simeq 2.66$. It also shows local minima at $x_m \simeq 2.4$ for increasing y . Upon tuning the gap Δ_1 to arbitrarily small values such that $\Delta/T \simeq x_m$ remains finite, we have $y = \Delta_2/T \rightarrow \infty$. On the other hand, $h(x, y)$ approaches $g(x)$ for increasing y and we are thus smoothly back to the two-level case.

2.1. Remarks

Estimation theory has been also used to address properties of thermometers, rather than intrinsic properties of the system under investigation. In particular, the role of the numbers N of particles has been analyzed, showing that performing energy measurement on a non thermalizing thermometer made of two-level atoms allows one to improve scaling of precision from $N^{-1/2}$ to N^{-1} [30]. The analysis has been also extended to thermometer made of multilevel atoms [35], either fully or partly thermalizing, showing that the sensitivity grows significantly with the number of levels, with the optimization over their energy spectrum playing a crucial role. We emphasize that this results pertain to properties of quantum thermometers, i.e. quantum systems used to probe the temperature of an external bath, whereas our focus has been on establishing intrinsic bounds to precision, thus providing benchmarks to assess any detection scheme. It should be also mentioned that upon employing arguments similar to those used in [30] the analysis of the previous section may be extended to degenerate systems, where Δ now represents the average energy per particle.

Another remark concerns a possible, alternative, explanation introduced to account for fluctuations in temperature measurements. The argument is based on the idea that an intrinsic distribution of temperatures may exists, which is consistent with a given thermodynamic

state, without implying dynamical fluctuations of the temperature(s) themselves. The argument is usually referred to as the polythermal ensemble hypothesis [41], and it has been somehow criticized [49] since it requires more hypothesis than just assuming the canonical ensemble.

Finally, it should be mentioned the use of a Hamiltonian control parameter to improve thermometric strategies has been already implemented experimentally, e.g. for strongly interacting Fermi gases [62, 63].

3. Conclusions

In the recent years, schemes for temperature estimation involving the interaction of the system with an individual quantum probe have received attention [30–37, 64, 65] mostly because they provide temperature estimate by adding the minimal disturbance. Our results, which have been obtained with basically no assumptions on the structure of the system under investigation and on the measurement performed to extract information, provide a general benchmark to assess this schemes, and to design effective thermometers for quantum systems.

Our results also provide a framework to reconcile the different approaches to temperature fluctuations. As a matter of fact, temperature itself does not fluctuate, however, there are fluctuations for the temperature estimate based on any indirect measurement. In other words, temperature is a classical parameter which do not correspond to a quantum observable and estimation of temperature necessarily involves the measurement of another quantity, corresponding to a proper observable. In turn, quantumness in temperature estimation is in the measurement stage and in the nature of fluctuations of the measured observable.

The optimal strategy to estimate temperature of a small quantum system turns out to be measuring the energy of the system and suitably process data, e.g. by Bayesian analysis [66, 67], in order to achieve the Cramer–Rao bound to precision. In this way, we have shown that the classical Landau bound to precision is recovered, in the low temperature regime, for systems exhibiting a vanishing gap as a function of some control parameter. On the contrary, in systems with a non-vanishing gap Δ between the lowest energy levels, temperature may be effectively estimated only down to a threshold, below which the variance of any estimator starts to increase as $\delta T^2 \gtrsim T^4 e^{\Delta/T}$. Notice that this is true independently on the use of an external ancillary system to probe the temperature of the system under investigation. In other words, rather than being a property of the ‘thermometer’ (i.e. of the chosen ancillary system and of the probing interaction scheme), the ultimate precision in temperature estimation is an intrinsic property of the quantum system itself. Our analysis shows the optimality of quantum thermometry based on energy measurements, and provides quantum benchmarks for high precision temperature measurement, as well as an efficient operational quantification of temperature for quantum mechanical systems lying arbitrary close to their ground state.

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