Individual quantum probes for optimal thermometry

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The unknown temperature of a sample can be estimated with minimal disturbance by putting it in thermal contact with an individual quantum probe. If the interaction time is sufficiently long so that the probe thermalizes, the temperature can be read out directly from its steady state. Here we prove that the optimal quantum probe, acting as a thermometer with maximal thermal sensitivity, is an effective two-level atom with a maximally degenerate excited state. When the total interaction time is insufficient to produce full thermalization, we optimize the estimation protocol by breaking it down into sequential stages of probe preparation, thermal contact and measurement. We observe that frequently interrogated probes initialized in the ground state achieve the best performance. For both fully and partly thermalized thermometers, the sensitivity grows significantly with the number of levels, though optimization over their energy spectrum remains always crucial.

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I. INTRODUCTION

With the advent of quantum technologies, the study of the thermodynamics of quantum devices has attracted considerable attention [1, 2]. In particular, there is a growing interest in obtaining accurate temperature readings with nanometric spatial resolution [3–5], which would pave the way towards many ground-breaking applications in medicine, biology or material science. This motivates the development of precise quantum thermometric techniques.

Recent progress in the manipulation of individual quantum systems has made it possible to use them as temperature probes, thus minimizing the undesired disturbance on the sample. Fluorescent thermometry may be implemented, for instance, on a single quantum dot to accurately estimate the temperature of fermionic [6, 7] and bosonic [8] reservoirs. Similarly, the ground state of colour centres in nano-diamonds has already been used as a fluorescent thermometer [3–5], achieving precisions down to the millikelvin scale, and a spatial resolution of few hundreds of nanometers. Thermometry applied to micro-mechanical resonators [9, 10], and nuclear spins [12] has also been subject of investigation. Other studies have focused on more fundamental questions such as the scaling of the precision of temperature estimation with the number of quantum probes [13], and the potential role played by coherence and entanglement in simple thermometric tasks [14].

In this Letter, we investigate the fundamental limitations on temperature estimation with individual quantum probes. Two complementary scenarios are considered. In the first one, we assume that the thermometer reaches thermal equilibrium with the sample. We then determine which are the optimal probes that maximize the attainable precision in the estimation of the temperature. Alternatively, we also consider the situation in which the probe does not thermalize completely due to some constraint on the total estimation time (e.g. the sample may be unstable). In this second scenario, we analyze the dissipative time evolution of the probe in order to optimize the thermometric protocol. We model it as sequence of steps of preparation, thermal contact and readout.

Our main results are the following. First, we show that a $N$-dimensional equilibrium probe with maximum heat capacity is optimal for thermometry. This is an effective two-level probe with $N-1$ degeneracy in the excited state, and some optimal gap. The maximum achievable precision grows with the dimension of the probe, yet the range of temperatures for which it operates efficiently as a thermometer becomes narrower. In contrast, a less sensitive probe with equipartition energy spectrum, such as a quantum harmonic oscillator, features wider operation ranges. On the other hand, when the estimation time is limited, we find that a frequently measured probe initialized in its ground state achieves the largest thermal sensitivity. In this case, the overall precision still scales with the dimension of the probe, even though the temperature range for efficient operation is dimension-independent.

Our results contribute not only to the theoretical advance of temperature estimation in the quantum regime, but also have potential technological impact for the development of high precision thermometry at the nanoscale.

II. FULLY THERMALIZED THERMOMETERS

In standard thermometry, a (sufficiently small) thermometer is simply allowed to equilibrate with the sample to be probed, so that the temperature of the latter is inferred from the state of the probe. In a quantum scenario, the same procedure can be applied. A first approximation to the sample temperature can be obtained by performing a suitable measurement on the steady state of the thermalized probe (ideally, the most informative one). If a large number $v$ of such independent experiments is carried out, one can refine the estimate $T$ of the sample temperature. Its corresponding uncertainty $\Delta T$ is tightly bounded from below as expressed by the quantum Cramér-
\[ \Delta T \geq \sqrt{\mathcal{F}({\hat{\Theta}})} \]  

(1)

In what follows, this minimum statistical uncertainty in the estimation of temperature will be referred to as ‘thermal sensitivity’. Here, \( \mathcal{F}({\hat{\Theta}}) \) stands for the quantum Fisher information (QFI) \( \mathcal{F} \) for temperature estimation, which reads

\[ \mathcal{F}({\hat{\Theta}}) = -2 \lim_{\delta \to 0} \delta^2 \mathbb{E}(\hat{\Theta}, \hat{\Theta} + \delta \hat{\Theta}) / \partial \delta^2, \]  

(2)

where \( \mathbb{E}(\hat{\Theta}, \hat{\Theta} + \delta \hat{\Theta}) \equiv \left( \text{tr} \sqrt{\hat{\Theta} \hat{\Theta} + \delta \hat{\Theta}} \right)^2 \) is the Uhlmann fidelity between states \( \hat{\Theta}_1 \) and \( \hat{\Theta}_2 \). The QFI thus captures the sensitivity of a state to variations in the parameter of interest. We will take its maximization as synonym of optimality \([6,10,15]\).

We write the Hamiltonian of our probe as \( \hat{H} = \sum_n \epsilon_n |\epsilon\rangle \langle \epsilon| \). A thermalization process leads to stationary states of the form \( \hat{\Theta}_T = \sum_n p_n |\epsilon\rangle \langle \epsilon| \), where the populations are \( p_n \equiv Z^{-1} e^{-\epsilon/k_BT} \) and the partition function is given by \( Z \equiv \text{tr} e^{-\hat{H}/k_BT} \). In what follows we set \( h = k_B = 1 \).

In the energy eigenbasis, eq. (2) rewrites as

\[ \mathcal{F}({\hat{\Theta}}) = 4 \sum_{mn} \frac{|\langle \epsilon_m | \hat{\Theta} | \epsilon_n \rangle|^2}{(p_m + p_n)^2} = \frac{\Delta \hat{H}^2}{\bar{T}^2}, \]  

(3)

were \( \Delta \hat{H}^2 \equiv \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 \). In this last step, we have used the identity \( \langle \hat{H} \rangle = \bar{T}^2 \partial \bar{T} \ln Z \). Interestingly, in the single shot scenario of \( v = 1 \), one can combine eqs. (1) and (2) to get the thermodynamic uncertainty relation \( \frac{\Delta}{\mathcal{F}} \Delta \hat{H} \geq 1 \). Also, note that \( \Delta \hat{H} / \bar{T} = d \langle \hat{H} \rangle / d \bar{T} \equiv C(T) \) which, in the present case, may be referred to as the ‘heat capacity’ of the probe. It thus follows that the signal-to-noise ratio \( T / \Delta T \) is lower-bounded as \( (T / \Delta T)^2 \geq C(T) \). Note as well that, since \( \hat{\Theta}_T \) is a thermal state, the most informative measurement saturating eq. (1) is just a projection onto the energy eigenbasis.

In the light of eq. (2), the maximization of the thermal sensitivity of a probe translates into finding the energy spectrum with the largest possible energy variance at thermal equilibrium, or equivalently, the \( N \)-dimensional probe with largest heat capacity. The heat capacity of the sample must be anyway much larger than that of the probe so as to minimize any disturbance arising from the estimation procedure.

For a general \( N \)-level probe, the energy variance writes simply as \( \Delta \hat{H}^2 = Z^{-1} \sum \bar{\epsilon}_n^2 e^{-\epsilon/k_BT} \), where \( \bar{\epsilon}_n \equiv \epsilon_n - \langle \hat{H} \rangle \). Imposing the extremum condition \( \partial \Delta \hat{H}^2 / \partial \bar{\epsilon}_n = 0 \) leads to the quadratic equation \( \bar{\epsilon}_n^2 - 2T \bar{\epsilon}_n - \Delta \hat{H}^2 = 0 \), from which \( \bar{\epsilon}_n \equiv \bar{\epsilon}_n = T \pm \sqrt{T^2 + \Delta \hat{H}^2} \). Therefore, in a probe with maximum thermal sensitivity, the energy levels can only take on either of these two values. In other words, the optimal spectrum is that of an effective two-level system.

For a given probe dimension \( N \), we can straightforwardly show that the maximum excited-state degeneracy \( N' = N - 1 \) provides the largest heat capacity. Defining the frequency-to-temperature ratio as \( x \equiv \Omega / T \), with \( \Omega \equiv \epsilon_+ - \epsilon_- \), one has that the equality \( \partial \bar{\epsilon}_n \Delta \hat{H}(x) \big|_{x = x_{N,N'}} = 0 \) yields an implicit expression for the optimal \( x_{N,N'} \). The fact that \( \Delta \hat{H}(x_{N,N'}) > \Delta \hat{H}(x_{N,N-1}) \) for \( N' < N - 1 \) indicates that the excited-state degeneracy must be the maximum possible at optimality. In particular, \( x_{N,N-1} \equiv x_+ \) is implicitly given by \( e^{x_+} = (N - 1) / (x_+ + 2) \). Notice that this type of effective two-level spectrum had already been acknowledged to yield the largest heat capacities in finite-dimensional systems \([19]\).

All that is left is to compute the corresponding QFI

\[ \mathcal{F}_N = \frac{x^4 e^{x_+} - (N - 1)}{\Omega^2 (N - 1 + e^{x_+})^2} \]  

(4)

which is obviously also maximal at \( x_+ \). In fig.\[1\] we plot eq. (4) for different values of \( N \). It shows that the precision in temperature estimation improves significantly by increasing the dimensionality \( N \) of the probe, albeit at the expense of reducing the specified temperature range for efficient operation of the probe as a thermometer (see inset of fig.\[1\]).

So far, we have seen that the best thermometers are effective two-level atoms with a highly degenerate excited state and a specific, temperature-dependent gap. However, these may be very hard to prepare in practice, especially if our \( a \ priori \) knowledge of the sample temperature is imprecise. For this reason we now consider more versatile sub-optimal probes with a richer spectrum, such as a single thermalized harmonic oscillator. In this case, the corresponding QFI can be easily computed from the \( 2 \times 2 \) steady-state covariance matrix \([20,21]\) of a thermal state \( \sigma_T = \text{coth} \frac{\Omega}{2} [1]_2 \) as in eq. (2). Using the fact that the Uhlmann fidelity between two single-mode Gaussian states \( \sigma_1 \) and \( \sigma_2 \) is given by \( \mathbb{F}(\sigma_1, \sigma_2) = 2 \left( \sqrt{\lambda + \Lambda} - \sqrt{\lambda - \sqrt{\Lambda}} \right) \) \([22]\), where \( \Delta \equiv \det(\sigma_1 + \sigma_2) \) and \( \Lambda \equiv \det(\sigma_1 - 1) \det(\sigma_2 - 1) \), one arrives at \( \mathcal{F}_{\text{coh}} = \frac{\Omega^2}{2 \sqrt{\lambda - \sqrt{\Lambda}}} \). This is represented in fig.\[1\] with a dashed blue line. For ease of comparison we take the oscillator frequency \( \Omega \) to be \( \epsilon_+ - \epsilon_- \). As we can see, a harmonic probe features a thermal sensitivity similar to that of a two-level probe. Even if harmonic thermometers are largely outperformed by most optimized \( N \)-level probes, they are endowed as well with a
much broader specified temperature range for efficient operation, which makes them a choice of practical interest.

This can be better understood if one observes that, in fact, the thermal sensitivity of a probe with a single energy gap may only peak when this resonates with the characteristic frequency of the equilibrium thermal fluctuations of the sample. On the contrary in a thermometer with equispaced and unbounded spectrum, there will always be some transition close to resonance, no matter how hot the sample is.

III. PARTLY THERMALIZED THERMOMETERS

All the previous analysis holds regardless of the probe-sample interactions or the spectral properties of the sample, as long as thermalization takes place. In practice, however, one may have to read out the temperature before attaining full thermalization. This would be the case, for instance, if the sample was unstable and existed only for times comparable to the dissipation time scale. In this alternative scenario, we ask ourselves about the optimal breakup of the total running time of the estimation procedure \( t_r \) into sequential stages of probe-preparation, thermal contact (during time \( \Delta_t \)), and measurement, so as to optimize the achievable precision in eq. (1). Note that the number of interrogations is now limited to \( \nu = t_r / \Delta_t \), so that the figure of merit to be maximized is the ratio \( F(\Delta_t) / \Delta_t \).

Since we must monitor the time evolution of the probe, it is necessary now to specify the sample and its coupling with the thermometer. We shall model the sample as a bosonic heat bath, linearly coupled to an arbitrary probe. The total Hamiltonian writes as \( \hat{H}_{tot} = \hat{H} + \sum_\mu \omega_\mu \hat{b}_\mu \hat{b}_\mu + \hat{X} \otimes \sum_\mu g_\mu (\hat{b}_\mu + \hat{b}_\mu^\dagger) \), where \( \hat{b}_\mu \) is the annihilation operator of mode \( \omega_\mu \) in the sample. We choose the probe-sample coupling constants to be \( g_\mu = (\gamma \omega_\mu)^{1/2} \), implying flat spectral density \( J(\omega) \sim \sum_\mu \frac{2}{\omega_\mu} \delta(\omega - \omega_\mu) \). This sets the time-scale \( \tau_D \sim \gamma^{-1} \) over which \( \hat{\rho}(t) \) varies appreciably. Tracing out the sample from the overall unitary dynamics and assuming a thermal state \( \hat{\rho}_T \) for it, leads to an effective equation of motion of the Lindblad-Gorini-Kossakovski-Sudashan type (LGKS) [26, 27], that follows from \( \dot{\hat{\rho}} = t_{eg} \frac{1}{2} e^{-i\hat{H}_{rot}} \hat{\rho}(0) e^{i\hat{H}_{rot}} \), after sequentially performing the Born, Markov and rotating-wave approximations (see [28] for a detailed derivation). Note that the Born approximation implies that no correlations are ever created between probe and sample, so the latter remains undisturbed throughout the estimation procedure. Note also that, for consistency with the Markov approximation, the temperature of the sample may not be arbitrarily low, as the thermal sensitivity of a probe with a single energy gap may only peak when this resonates with the characteristic frequency of the equilibrium thermal fluctuations of the sample. On the contrary in a thermometer with equispaced and unbounded spectrum, there will always be some transition close to resonance, no matter how hot the sample is.

In the interaction picture, the master equation can be cast as

\[
\dot{\hat{\rho}} = \Gamma_{\Omega, T} \left( \hat{A}_\Omega \hat{\rho} \hat{A}_\Omega^\dagger - \frac{1}{2} \{\hat{A}_\Omega \hat{A}_\Omega^\dagger, \hat{\rho}\} \right)
+ e^{-\Omega/T} \Gamma_{\Omega, T} \left( \hat{A}_\Omega \hat{\rho} \hat{A}_\Omega^\dagger - \frac{1}{2} \{\hat{A}_\Omega \hat{A}_\Omega^\dagger, \hat{\rho}\} \right),
\]

where \( \hat{A}_\Omega \) stands for the relaxation/excitation operator associated with the decay channel at frequency \( \Omega \). These follow from the decomposition of \( \hat{X} = \sum_\omega \hat{A}_\omega \) as sum of eigen-operators of the probe Hamiltonian (i.e. such that \( [\hat{H}, \hat{A}_\omega] = -\Omega \hat{A}_\omega \)). It is easy to show that the thermal state \( \hat{\rho} = \Omega^{-1} e^{-\hat{H}/T} \) is a fixed point of eq. (5) and, choosing a suitable coupling operator \( \hat{X} \), the open dynamics may also be ergodic, thus eventually bringing any initial state to thermal equilibrium [28].

For a two-level thermometer with Hamiltonian \( \hat{H} = \frac{\Omega}{2} \hat{\sigma}_z \), we can take, for instance, \( \hat{X} = \hat{\sigma}_x \) from which \( A_{\hat{\sigma}_z} = [-\Omega/2, \Omega/2] \), while \( \hat{A}_{\hat{\sigma}_x} = \hat{A}_{\hat{\sigma}_y} = \hat{A}_0^\dagger \). Here, \( \pm \Omega/2 \) are the corresponding energy eigenstates. Generalizing to the case of an N-level probe with eigenstates \( \{|\epsilon_i\rangle\} \), a coupling term like \( \hat{X} = \sum_\epsilon |\epsilon_i\rangle \langle \epsilon_i | \langle \epsilon_i | \langle \epsilon_i | \langle \epsilon_i \rangle \rangle \) would also thermalize any preparation, where we have labelled the ground state by \( |\epsilon_1\rangle \). The resulting relaxation operators are \( \hat{A}_{\epsilon_i \rightarrow \epsilon_1} = |\epsilon_i\rangle \langle \epsilon_1 | \). In particular, to account for our effective two-level systems with excited-state degeneracy we can take the limit \( \epsilon_1 \rightarrow \frac{\Omega}{2} \) for \( i \neq 1 \) and set \( \epsilon_i = -\frac{\Omega}{2} \) to get the desired thermalization process. Let us finally comment on the decay rates \( \Gamma_{\Omega, T} \), which follow from the power spectrum of the bath auto-correlation function \( \langle \hat{S}(t) \hat{S}(0) \rangle_T = tr(\hat{S}(t) \hat{S}(0) \hat{\rho}_T) \), where \( \hat{S} = \sum_\mu g_\mu (\hat{b}_\mu + \hat{b}_\mu^\dagger) \). In the specific case of a quantum probe coupled through dipole interaction to the quantized electromagnetic field in three dimensions, one obtains \( \Gamma_{\Omega, T} = \gamma \Omega^2 (1 - e^{-\gamma \epsilon / T})^{-1} \).

The problem now goes down to just solving eq. (5), transforming the time-evolved state \( \hat{\rho}(t) \) back into the Schrödinger picture (i.e. \( \hat{\rho} \rightarrow e^{-i\hat{H}_{rot} t} \hat{\rho} e^{i\hat{H}_{rot} t} \)), and computing the QFI according to eq. (6) [23, 29, 32]. Note that besides comparing the performance of different types of probe, we must now optimize as well over its initial state.

We will start by considering the simplest case of two-level thermometers. Extensive numerical analysis over different initial states shows that ground-state preparations display maximal thermal sensitivity. In particular, this indicates that the presence of initial quantum coherence does not provide any significant advantage for thermometry in this setting.

Thus, by choosing \( \hat{\rho}(0) = |\Omega/2\rangle \langle -\Omega/2| \) we can combine...
Eqs. (5) and (5) to compute $\mathcal{F}_2(\Delta t)$ as a function of the interrogation time $\Delta t$, starting from a ground state preparation:

$$
\mathcal{F}_2(\Delta t) = \frac{x^2 \left( e^{\Delta_t/\tau} - 1 \right) + \left( 1 + e^{\Delta_t/\tau} \right) \sqrt{\frac{2 \gamma}{\Delta_t}} \cosh \frac{\gamma}{\Delta_t} \right)^2}{(1 + e^{\Delta_t/\tau})(1 + e^{\Delta(t/\tau)}/T^2)},
$$

where $\tau^{-1} \equiv \gamma T^2 \cosh \frac{\gamma}{\Delta_t}$. Eq. (6) shows that the details of the thermal fluctuations of the sample, encoded in $\Gamma_{\Omega,T}$, only enter in the dynamics through the scaling factor $\tau$. Hence, even if our choice of a flat spectral density might seem pretty restrictive at first, changing the probe-sample coupling would just amount to a suitable rescaling of time.

In fig. 2 we plot $\mathcal{F}_2(\Delta t)/\Delta t$ for different preparations. As we can see, the sensitivity of a cold thermal probe peaks at some optimal readout time, after which it must be quickly cooled down to start over another relaxation stage in the estimation protocol. In the limiting case of a ground-state preparation, the overall maximum sensitivity is approached as $\Delta t \to 0$.

Eq. (6) can be generalized to any of our highly degenerate effective two-level probes prepared in the ground state. Just like in the two-level case, their maximum estimation precision follows from the limit

$$
\lim_{\Delta t \to 0} \mathcal{F}_2(\Delta t) = \frac{\gamma T(N-1) \sqrt{\tau}}{(e^\tau - 1)^3}.
$$

We now search for the optimal frequency-to-temperature ratio $\bar{x}$ that sets an ultimate upper bound on the thermal sensitivity in eq. (7). This can be expressed implicitly as $e^{\bar{x}} = (5 + 2\bar{x})/(5 - \bar{x})$, which is independent of $N$. Interestingly, in this case we find that the specified temperature range for efficient operation does not scale with $N$, at variance with the fully thermalized case.

For completeness, we examine again here the performance of harmonic probes. Going back to eq. (5), we will set $\hat{H} = \Omega \hat{a}^\dagger \hat{a}$ and $\hat{X} = \hat{a} + \hat{a}^\dagger$, whose corresponding relaxation and excitation operators are trivially $A_\Omega = \hat{a}$ and $A_{-\Omega} = \hat{a}^\dagger$. The total Hamiltonian is thus quadratic in positions and momenta and therefore, any Gaussian preparation will preserve its Gaussianity in time [20]. Provided that the initial state also has vanished first order moments ($\langle \hat{X} \rangle = \langle \hat{\rho} \rangle = 0$), its covariance matrix $\sigma(t)$ alone will be enough for a full description.

In this case, the dynamics may be obtained by explicitly solving the quantum master equation in phase space, to yield $\sigma(t) = e^{-i\omega t}\sigma(0) + (1 - e^{-i\omega t})\sigma_T$ [20] [33]. Computing the transient QFI is then straightforward by resorting to eq. (2). In what follows, we shall consider general (undisplaced) single-mode Gaussian states as initial preparations; these can be written as rotated, squeezed thermal states [20] [21]. As it could be expected, ground-state initialization ($\hat{\rho}(0) = |0\rangle \langle 0|$) provides once again the largest thermal sensitivity. One can ignore the temperature dependence of $\Gamma_{\Omega,T}$ in the solution to the master equation and still get a good approximation to $\lim_{\Delta t \to 0} \mathcal{F}_2(\Delta t)/\Delta t$. Surprisingly, we recover eq. (7) with $N = 2$. Indeed, this equivalence of two-level probes and harmonic thermometers extends generally beyond the limits $\Delta t \to 0$ and $\hat{\rho}(0) = |0\rangle \langle 0|$. Therefore, at variance with the fully-thermalized scenario, the specified temperature range of both oscillators and $N$-level probes in an effective two-level configuration is virtually the same, regardless of $N$.

IV. CONCLUSIONS

We have analyzed the performance and ultimate limitations of individual quantum probes for precise thermometry on a sample. Our study is based on techniques of quantum parameter estimation, and makes use of the quantum Fisher information as indicator of optimal thermal sensitivity.

First, we have considered an $N$-dimensional quantum probe that fully thermalizes with the sample. In this case, we have proven that the best possible quantum thermometer is realized by an effective two-level atom with a maximally degenerate excited state at a specific energy gap, depending non-trivially on the sample temperature. We have shown that there exists a complementary trade-off between the maximum achievable estimation precision, which grows with the dimensionality $N$, and the specified temperature range in which the estimation is efficient, which shrinks for increasing $N$. If the temperature of the sample is completely unknown, choosing a quantum harmonic oscillator as thermometer can become advantageous even though it is not optimal in terms of thermal sensitivity.

We have also considered the scenario in which e.g. due to the short lifetime of the sample, full thermalization may not take place. The thermometry protocol must then divide optimally the total estimation time into sequential steps of probe preparation, dissipative evolution and readout. Frequently interrogated probes prepared in their ground state then provide the largest thermal sensitivity. In this case, while the maximum achievable precision scales again with $N$, the specified temperature is independent of the dimensionality.

It must be emphasized that while the results concerning fully thermalized probes are completely general, we did have to set an explicit microscopic modelling for the sample and its interaction with the probe in the second part of our analysis. In particular, we have worked with a large bosonic sample in thermal equilibrium, weakly coupled to the probe through a suitable linear interaction term, ensuring ergodicity and thus, steady-state thermalization. Though this is a very general model of thermalization, it would be interesting to discuss to which extent can the estimation precision be enhanced with a suitably engineered thermal coupling. For instance, in certain systems it is possible to engineer the decay rates by externally controlling some parameter, such as the scattering length in a cold atomic gas [54]. In principle, this would allow the experimenter to directly manipulate the scaling factor $\tau$ in eq. (6).

Finally, it is worth mentioning that even though quantum coherence in the initial state of the probe may not be directly linked to the overall maximization of the precision, the potential role played by quantunmess in thermometry remains an open problem [12] [14] that deserves a study on its own.

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