Energy measurements remain thermometrically optimal beyond weak coupling

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We develop a general perturbative theory of finite-coupling quantum thermometry up to second order in probe-sample interaction. By assumption the probe and sample are in thermal equilibrium, so the probe is described by the mean-force Gibbs state. We prove that the ultimate thermometric precision can be achieved—to second order in the coupling—solely by means of local energy measurements on the probe. Hence, seeking to extract temperature information from coherences or devising adaptive schemes confers no practical advantage in this regime. Additionally, we provide a closed-form expression for the quantum Fisher information, which captures the probe's sensitivity to temperature variations. Finally, we benchmark and illustrate the ease of use of our formulae with two simple examples. Our formalism is completely general and makes no assumptions about separation of dynamical timescales or the nature of either the probe or the sample. Therefore, by providing analytical insight into both the thermal sensitivity and the optimal measurement for achieving it, our results pave the way for quantum thermometry in setups where finite-coupling effects cannot be ignored.

1 Introduction

Precise measurements of low temperatures are crucial in experiments dealing with quantum phenomena. Indeed, ultra-low temperatures are routinely achieved in nanoelectronic systems [1, 2] and cold-atom based platforms [3, 4]. Applications range from the study of fundamental problems in condensed matter [5–7] to thermalisation in closed quantum systems [8–10]; and from the realisation of thermodynamic cycles [11–13] to analog quantum simulation in optical lattices [14, 15], and computation on large-scale programmable simulators [16, 17].

On the other hand, the application of estimation-theoretic methods to model thermometric protocols in the ultracold regime has consolidated into the novel field of *quantum* thermometry [18, 19]. Its central goals have been to establish fundamental scaling laws

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for the signal-to-noise ratio of low-temperature estimates [20-23] and to identify design prescriptions that can make a probe more responsive to temperature variations [23-33]. A particular focus has been recently placed on sensing applications with atomic impurities [10, 27, 34-36], which has helped to close the gap between theory and applications [35].

Specifically, the quantum Fisher information \mathcal{F} [37] has played a central role as a figure of merit for quantum thermometry. It governs the scaling of the best-case signal-to-noise ratio of unbiased temperature estimates, in the asymptotic limit a of large number of measurements both in the frequentist approach, through the Crámer–Rao bound [38, 39], and Bayesian approach, through the van Trees inequality^{*} [47, 48]. In this paper, we study equilibrium probe-based thermometry, where the temperature of the sample is inferred by measuring a small system—the probe—which is coupled to it so that both equilibrate [20, 21, 24, 27, 29, 34, 49, 50]. In this setting, we compute \mathcal{F} and investigate the most informative measurements for probes that are coupled *non-perturbatively* to the sample.

In this work, we go beyond the 'weak' probe-sample coupling, which is usually understood as being 'negligibly small', such that the equilibrium marginal of the probe is simply a Gibbs state with respect to the probe's bare Hamiltonian at the sample's temperature. In this case, temperature may be optimally inferred from energy measurements [24], which offers simplicity and universality. This is precisely the steady-state prediction of the common Gorini–Kossakowski–Lindblad–Sudarshan (GKLS) [51–53] quantum master equation describing the dynamics of the probe at time t. Importantly, however, the GKLS equation is mathematically rigorous only if the strength of the probe-sample coupling decays with time and vanishes asymptotically [54]. This means that it cannot reliably describe its own steady state, other than in the case of asymptotically vanishing dissipation. But perturbative quantum master equations may encounter even bigger problems in the context of quantum thermometry. Namely, the assumption that the probe-sample coupling is neglible tends to break down in the low-temperature regime. There, the temperature Tsets a small energy scale that can become comparable to the interaction Hamiltonian—no matter how small the latter may be next to the bare Hamiltonians of the sample and the probe [55, 56].

Here, we refer to the 'finite-coupling' regime to denote situations in which the coupling is not negligible. The probe would be then described by the marginal of the global probe– sample equilibrium state, referred-to as *mean-force Gibbs state*—this can be significantly far from 'Gibbsian' with respect to the probe's bare Hamiltonian [57–71]. While the quantum Fisher information of the probe in this regime has received considerable attention [20, 21, 27, 29, 34, 50, 72, 73], not much is known about the optimal thermometric measurement beyond some specific examples [21, 22, 34]. In this work, we show that energy measurements remain optimal up to the first two leading orders in the coupling strength. This is the first general result about the optimal thermometric measurement beyond the weak-coupling regime and has critical practical importance. Namely, it establishes that non-diagonal measurements, aimed at extracting temperature information encoded coherences, do not necessarily confer a real advantage in the finite-coupling regime, nor does any possible adaptive strategy. Furthermore, our approach provides general formulas to evaluate thermal sensitivity explicitly, to second order in the coupling, circumventing the common pitfalls of the conventional weak coupling assumption.

This paper is structured as follows: In Sec. 2 we introduce the perturbative formalism of finite-coupling quantum thermometry and present our main results. We then apply

^{*}The Bayesian framework has been considered within quantum thermometry only recently [40–46], proving particularly useful when estimating temperatures from scarce data in real experimental situations [35, 41].

our results to two standard probe–sample models in Sec. 3; namelly, quantum Brownian motion and the spin–boson model. In Sec. 4 we give detailed derivations of the formulas presented. Finally, in Sec. 5 we summarise and draw our conclusions.

2 Finite-coupling quantum thermometry

2.1 Framework

Let us consider a probe S (for 'system') coupled to a sample B (for 'bath') with Hamiltonian

$$\boldsymbol{H} = \boldsymbol{H}_{S} + \boldsymbol{H}_{B} + \boldsymbol{H}_{\text{int}}.$$
 (1)

The total system is in a Gibbs state at the inverse temperature β :

$$\tilde{\pi} = \frac{e^{-\beta H}}{\tilde{Z}},\tag{2}$$

with partition function $\tilde{Z} = \text{tr } e^{-\beta \boldsymbol{H}}$, and the goal is to determine the inverse temperature β by measuring only the probe S. In this paper, we work in the units where $\hbar = k = 1$, the latter being the Boltzmann constant. In all what follows, operators are denoted with boldface symbols. Note that, since only the probe is measured, for our forthcoming results to hold it is only required that the probe's state be given by $\text{tr}_B[\tilde{\boldsymbol{\pi}}]$ —the actual global state may differ from $\tilde{\boldsymbol{\pi}}$ and be microcanonical [74–79], pure [77, 80, 81], or neither [76, 82].

To control the magnitude of the probe-sample interaction, we will henceforth write the interaction term as $\boldsymbol{H}_{\text{int}} = \gamma \boldsymbol{V}$, where the dimensionless parameter γ is the coupling strength. The equilibrium state of the probe, from which the inverse temperature β is to be inferred,

$$\tilde{\boldsymbol{\pi}}_{S} = \frac{\operatorname{tr}_{B}\left[e^{-\beta \boldsymbol{H}}\right]}{\tilde{Z}},\tag{3}$$

is the so-called mean-force Gibbs state [64, 69], and it will only coincide with the bare thermal state of the probe,

$$\boldsymbol{\pi}_{S} = \frac{e^{-\beta \boldsymbol{H}_{S}}}{Z_{S}},\tag{4}$$

in the limit of vanishing coupling $(\gamma \to 0)$. Here the partition function is $Z_s = \operatorname{tr} e^{-\beta H_s}$.

Estimates for β , drawn from a measurement record of length N via an unbiased estimator, carry an uncertainty $\delta\beta$ such that the signal-to-noise ratio (SNR) is upper-bounded through the Cramér–Rao inequality [37–39, 83, 84] as

$$\frac{\beta}{\delta\beta} \le \sqrt{N\beta^2 \mathcal{F}_S(\beta)}.\tag{5}$$

Here, $\mathcal{F}_{s}(\beta)$ is the quantum Fisher information (QFI), which is given by [37, 83, 84]

$$\mathcal{F}_{S}(\beta) = \operatorname{tr}_{S} \left[\boldsymbol{L}_{S}^{2} \tilde{\boldsymbol{\pi}}_{S} \right], \tag{6}$$

where the symmetric logarithmic derivative L_s (SLD) is implicitly defined by

$$\partial_{\beta} \,\tilde{\boldsymbol{\pi}}_{S} = \frac{1}{2} \{ \boldsymbol{L}_{S}, \tilde{\boldsymbol{\pi}}_{S} \}, \tag{7}$$

with $\{\cdot, \cdot\}$ denoting the anticommutator. Equation (7) is a Lyapunov equation with respect to \boldsymbol{L}_{S} and, since $\tilde{\boldsymbol{\pi}}_{S}$ is a bounded positive operator, it has a unique solution, given by [85]

$$\boldsymbol{L}_{S} = 2 \int_{0}^{\infty} d\lambda \ e^{-\lambda \tilde{\boldsymbol{\pi}}_{S}} (\partial_{\beta} \, \tilde{\boldsymbol{\pi}}_{S}) e^{-\lambda \tilde{\boldsymbol{\pi}}_{S}}.$$
(8)

The optimal thermometric measurement—namely, the one that minimizes $\delta\beta$ —is the projection onto the eigenbasis of L_s [37, 83, 84]. This saturates the Cramér–Rao bound (5) in the $N \to \infty$ limit [37, 48]. For any other measurement, the best-case scaling of the SNR is given by the 'classical' Cramér–Rao bound [38, 39]. For example, when one projects onto the eigenbasis of H_s , then

$$\frac{\beta}{\delta\beta} \le \sqrt{N\beta^2 \mathcal{I}_{\boldsymbol{H}_S}(\beta)},\tag{9}$$

where $\mathcal{I}_{H_S}(\beta) \leq \mathcal{F}_S(\beta)$ is the (classical) Fisher information associated with this specific measurement. Here, the bound also becomes tight in the $N \to \infty$ limit [86]. By definition,

$$\mathcal{I}_{\boldsymbol{H}_{S}}(\beta) = \sum_{n} \tilde{p}_{n} \left(\partial_{\beta} \ln \tilde{p}_{n}\right)^{2}, \tag{10}$$

where $\tilde{p}_n := \langle \epsilon_n | \tilde{\pi}_S | \epsilon_n \rangle$ are the populations of the probe's equilibrium state in the eigenbasis $\{ |\epsilon_n \rangle \}_n$ of \boldsymbol{H}_S . Equivalently, $\mathcal{I}_{\boldsymbol{H}_S}(\beta)$ can be written as

$$\mathcal{I}_{\boldsymbol{H}_{S}}(\beta) = \operatorname{tr}_{S} \left[\mathscr{D}_{\boldsymbol{H}_{S}}(\boldsymbol{L}_{S})^{2} \mathscr{D}_{\boldsymbol{H}_{S}}(\tilde{\boldsymbol{\pi}}_{S}) \right],$$
(11)

where \mathscr{D}_{H_S} is the dephasing operation in the eigenbasis of H_S :

$$\mathscr{D}_{\boldsymbol{H}_{S}}(\boldsymbol{Q}) := \sum_{n} |\epsilon_{n}\rangle \langle \epsilon_{n} | \boldsymbol{Q} | \epsilon_{n}\rangle \langle \epsilon_{n} | .$$
(12)

The bare energy measurement defined by $\{|\epsilon_n\rangle\}_n$ is known to be optimal in the limit $\gamma \to 0$, where $\tilde{\pi}_S \to \pi_S$ and, therefore, $L_S \to \langle H_S \rangle_S - H_S$ [24]; here and throughout, $\langle \cdot \rangle_S := \operatorname{tr}_S [\pi_S \cdot]$. Furthermore, the bare energy measurement is optimal at any γ as long as $[H_{\text{int}}, H_S] = 0$, because then $[\tilde{\pi}_S, H_S] = 0$, and therefore $[L_S, H_S] = 0$, which means that $\{|\epsilon_n\rangle\}_n$ is an eigenbasis for L_S . In general, however, $\tilde{\pi}_S$, and hence L_S , will not commute with H_S , so the optimal thermometric basis will differ from $\{|\epsilon_n\rangle\}_n$. Nonetheless, as we prove below, the bare energy measurement remains as informative as the truly optimal measurement up to the first two leading orders in the perturbative expansion in the probesample coupling strength γ .

2.2 Results

2.2.1 Optimality of local energy measurements at finite coupling

Suppose $\tilde{\pi}_s$ is twice differentiable in γ . It can then be Taylor-expanded as

$$\tilde{\boldsymbol{\pi}}_{S} = \boldsymbol{\pi}_{S} + \gamma \, \boldsymbol{p}_{1} + \gamma^{2} \boldsymbol{p}_{2} + O(\gamma^{3}), \tag{13}$$

where p_1 and p_2 are some operators and O is the 'big O' as per the standard asymptotic notation. In the same manner, the SLD L_S of $\tilde{\pi}_S$ [Eq. (8)] will decompose as

$$\boldsymbol{L}_{S} = -\Delta \boldsymbol{H}_{S} + \gamma \, \boldsymbol{l}_{1} + \gamma^{2} \boldsymbol{l}_{2} + O(\gamma^{3}), \tag{14}$$

where $-\Delta \boldsymbol{H}_{s} := \langle \boldsymbol{H}_{s} \rangle_{s} - \boldsymbol{H}_{s}$ is the SLD of $\boldsymbol{\pi}_{s} = \tilde{\boldsymbol{\pi}}_{s} \Big|_{\gamma=0}$ and $\boldsymbol{l}_{1}, \boldsymbol{l}_{2}$ are some operators related to $\boldsymbol{\pi}_{s}, \boldsymbol{p}_{1}$, and \boldsymbol{p}_{2} through Eq. (8). Plugging these into Eq. (6), we obtain

$$\mathcal{F}_{S}(\beta) = \mathcal{F}_{S}^{(0)}(\beta) + \gamma \left[\operatorname{tr}(\boldsymbol{p}_{1} \Delta \boldsymbol{H}_{S}^{2}) - 2 \operatorname{tr}(\boldsymbol{l}_{1} \boldsymbol{\pi}_{S} \Delta \boldsymbol{H}_{S}) \right] + \gamma^{2} \left[\operatorname{tr}(\boldsymbol{l}_{1}^{2} \boldsymbol{\pi}_{S}) + \operatorname{tr}(\boldsymbol{p}_{2} \Delta \boldsymbol{H}_{S}^{2}) - 2 \operatorname{tr}(\boldsymbol{l}_{2} \boldsymbol{\pi}_{S} \Delta \boldsymbol{H}_{S}) - \operatorname{tr}(\{\boldsymbol{p}_{1}, \boldsymbol{l}_{1}\} \Delta \boldsymbol{H}_{S}) \right] + O(\gamma^{3}), \quad (15)$$

where $\mathcal{F}_{S}^{(0)}(\beta) := \operatorname{tr}(\boldsymbol{\pi}_{S} \Delta \boldsymbol{H}_{S}^{2}) = \partial_{\beta}^{2} \ln Z_{S}$ is the zeroth-order QFI, i.e., that of $\boldsymbol{\pi}_{S}$. Now, observing that

$$\begin{aligned} \operatorname{tr}(\boldsymbol{p}_1 \Delta \boldsymbol{H}_S^2) &= \operatorname{tr}(\mathscr{D}_{\boldsymbol{H}_S}[\boldsymbol{p}_1] \Delta \boldsymbol{H}_S^2), \\ \operatorname{tr}(\boldsymbol{l}_1 \boldsymbol{\pi}_S \Delta \boldsymbol{H}_S) &= \operatorname{tr}(\mathscr{D}_{\boldsymbol{H}_S}[\boldsymbol{l}_1] \boldsymbol{\pi}_S \Delta \boldsymbol{H}_S), \end{aligned}$$

we immediately conclude from Eq. (11) that, up to the first order in γ , $\mathcal{F}_{S}(\beta)$ and $\mathcal{I}_{\mathbf{H}_{S}}(\beta)$ coincide; that is,

$$\mathcal{I}_{\boldsymbol{H}_S}(\beta) = \mathcal{F}_S(\beta) + O(\gamma^2).$$
(16)

However, in general, $\mathscr{D}_{H_S}[\{p_1, l_1\}] \neq \{\mathscr{D}_{H_S}[p_1], \mathscr{D}_{H_S}[l_1]\}$, meaning that $\mathcal{F}_S(\beta)$ and $\mathcal{I}_{H_S}(\beta)$ do differ in the second order. Therefore, we have shown that the bare energy measurement is thermometrically optimal up to the first two leading orders (i.e., zeroth and first order), provided that the $O(\gamma)$ term in Eq. (15) is non-zero. In Appendix A we give explicit examples.

Let us now consider the case where the deviation between the mean-force Gibbs state $\tilde{\boldsymbol{\pi}}_{S}$ and the local thermal state $\boldsymbol{\pi}_{S}$ appears only at $O(\gamma^{2})$. This is relevant from the point of view of applications, since it is the situation most commonly studied in open quantum systems. Since, in this case $\boldsymbol{p}_{1} = 0$, we have that, due to Eq. (8), also $\boldsymbol{l}_{1} = 0$. As a result, the $O(\gamma)$ term in Eq. (15) vanishes, so that $\mathcal{F}_{S}(\beta)$ becomes

$$\mathcal{F}_{S}(\beta) = \mathcal{F}_{S}^{(0)}(\beta) + \gamma^{2} \left[\operatorname{tr}(\boldsymbol{p}_{2} \Delta \boldsymbol{H}_{S}^{2}) - 2 \operatorname{tr}(\boldsymbol{l}_{2} \boldsymbol{\pi}_{S} \Delta \boldsymbol{H}_{S}) \right] + O(\gamma^{3}).$$
(17)

As above, we have that

$$\begin{aligned} &\operatorname{tr}(\boldsymbol{p}_{2}\Delta\boldsymbol{H}_{S}^{2}) = \operatorname{tr}(\mathscr{D}_{\boldsymbol{H}_{S}}[\boldsymbol{p}_{2}]\Delta\boldsymbol{H}_{S}^{2}), \\ &\operatorname{tr}(\boldsymbol{l}_{2}\boldsymbol{\pi}_{S}\Delta\boldsymbol{H}_{S}) = \operatorname{tr}(\mathscr{D}_{\boldsymbol{H}_{S}}[\boldsymbol{l}_{2}]\boldsymbol{\pi}_{S}\Delta\boldsymbol{H}_{S}), \end{aligned}$$

which tells us that, according to Eq. (11), $\mathcal{F}_{s}(\beta)$ and $\mathcal{I}_{H_{s}}(\beta)$ coincide up to the second leading order in γ . Moreover, as we will show below, if one additionally imposes the generic assumption (19), the cubic term in Eq. (17) also vanishes (see Sec. 4), leaving us with

$$\mathcal{I}_{\boldsymbol{H}_S}(\beta) = \mathcal{F}_S(\beta) + O(\gamma^4). \tag{18}$$

Equations (16) and (18) constitute our first main result. Namely, the bare energy measurement is thermometrically optimal up to the first two nonzero leading orders in γ . Importantly, Eq. (18) applies to typical open quantum system scenarios, which means that, in such settings, measurement optimisation is only necessary at much stronger couplings[†].

[†]Note, however, that measurements not commuting with the probe's bare Hamiltonian can be advantageous in *nonequilibrium* thermometry even in the ultraweak coupling limit [87, 88].

2.2.2 Quantum Fisher information in finite-coupling thermometry

Having proven that energy measurements remain optimal at finite coupling, we now turn to deriving a closed-form expression for $\mathcal{F}_{s}(\beta)$ up to the second order in γ for the case of $p_{1} = 0$. Here, we outline the derivation of our formulae. For a detailed derivation one may skip directly to Sec. 4.

We begin by imposing the generic assumption of a factorised probe–sample interaction; namely,

Assumption I:
$$\boldsymbol{H}_{int} = \gamma \boldsymbol{S} \otimes \boldsymbol{B},$$
 (19)

where S and B are coupling operators belonging to probe and sample, respectively. Importantly, these are chosen such that $S \otimes B$ is of the same dimension as H_S and H_B , to ensure that γ is dimensionless.

As we will show below, under Assumption I, the condition $p_1 = 0$ is equivalent to

Assumption II:
$$\langle \boldsymbol{B} \rangle_{_{B}} = 0,$$
 (20)

where $\langle \boldsymbol{B} \rangle_B := \operatorname{tr}_B[\boldsymbol{\pi}_B \boldsymbol{B}]$, with $\boldsymbol{\pi}_B = e^{-\beta \boldsymbol{H}_B}/Z_B$ being the Gibbs state of the sample with respect to its bare Hamiltonian \boldsymbol{H}_B , and with the same β as in Eq. (2). $Z_B =$ $\operatorname{tr} e^{-\beta \boldsymbol{H}_B}$ is the corresponding partition function[‡]. Importantly, this assumption is also almost universally adopted in the theory of open quantum systems. There, Assumptions I and II are often disregarded as technical. However, they are crucial from the perspective of thermometry[§].

Our main tool is the Taylor expansion for the operator exponential function [89]. Let \boldsymbol{Q} and \boldsymbol{R} be a pair of dimensionless linear operators. Then, the function $\mathbb{R} \ni \gamma \mapsto e^{\boldsymbol{Q}+\gamma \boldsymbol{R}}$ can be cast as [90]

$$e^{\mathbf{Q}+\gamma\mathbf{R}} = \sum_{n=0}^{\infty} \mathbf{Q}_n(1)\gamma^n,$$
(21a)

where $\boldsymbol{Q}_0(s) = e^{s\boldsymbol{Q}}$ and

$$\boldsymbol{Q}_{n}(s) := \int_{0}^{s} dt_{1} \int_{0}^{t_{1}} dt_{2} \dots \int_{0}^{t_{n-1}} dt_{n} e^{(s-t_{1})\boldsymbol{Q}} \boldsymbol{R} e^{(t_{1}-t_{2})\boldsymbol{Q}} \boldsymbol{R} \cdots \boldsymbol{R} e^{t_{n}\boldsymbol{Q}}.$$
 (21b)

Applying Eq. (21) to $\tilde{\pi}_s$, we find, after some algebra, that

$$\boldsymbol{p}_{1} = -\left\langle \boldsymbol{B} \right\rangle_{B} \boldsymbol{\pi}_{S} \int_{0}^{\beta} d\beta_{1} e^{\beta_{1} \boldsymbol{H}_{S}} [\boldsymbol{S} - \left\langle \boldsymbol{S} \right\rangle_{S}] e^{-\beta_{1} \boldsymbol{H}_{S}}, \qquad (22)$$

from where it evident that, unless $\boldsymbol{S} \propto \boldsymbol{1}_{S}, \, \boldsymbol{p}_{1} = 0$ iff $\langle \boldsymbol{B} \rangle_{B} = 0$.

Hence, the application of Eq. (21) to Eq. (3) up to the second order results in

$$\tilde{\boldsymbol{\pi}}_{S} = \boldsymbol{\pi}_{S} \left(\boldsymbol{1}_{S} + \gamma^{2} \boldsymbol{X}_{S} \right) + O(\gamma^{4}), \tag{23}$$

[‡]Note that, whenever $\gamma \neq 0$, the actual reduced state of B, tr_s $[\tilde{\pi}]$, will not coincide with π_B . Both π_B and π_S are simply fictitious states that appear in our perturbative expansions.

[§]In open quantum systems theory [53], it is often argued that even when Assumption II is not met, it can be easily enforced without loss of generality, by re-defining $\boldsymbol{H} = \boldsymbol{H}'_{S}(\beta) + \boldsymbol{H}_{B} + \boldsymbol{H}'_{\text{int}}$, where $\boldsymbol{H}'_{S}(\beta) = \boldsymbol{H}_{S} + \operatorname{tr}_{B}[\boldsymbol{\pi}_{B}\boldsymbol{H}_{\text{int}}]$ and $\boldsymbol{H}'_{\text{int}} = \boldsymbol{H}_{\text{int}} - \operatorname{tr}_{B}[\boldsymbol{\pi}_{B}\boldsymbol{H}_{\text{int}}]$. Note, however, that there would be an explicit β -dependence in the modified probe Hamiltonian, which does crucially change the problem from a thermometric viewpoint.

where the matrix elements $(\boldsymbol{X}_{S})_{nm} = \langle \epsilon_{n} | \boldsymbol{X}_{S} | \epsilon_{m} \rangle$ of the traceless operator \boldsymbol{X}_{S} in the eigenbasis of $\boldsymbol{H}_{S} = \sum_{n} \epsilon_{n} | \epsilon_{n} \rangle \langle \epsilon_{n} |$ are

$$(\boldsymbol{X}_{S})_{nn} = \int_{0}^{\beta} du \ (\beta - u) \Phi_{B}(-iu) \Big(\sum_{k} \phi_{nk}(-iu) - \Phi_{S}(-iu) \Big), \tag{24a}$$

$$(\boldsymbol{X}_{S})_{n\neq m} = \frac{1}{\Delta_{mn}} \sum_{k} (\boldsymbol{S})_{nk} (\boldsymbol{S})_{km} \int_{0}^{\beta} du \, \Phi_{B}(-iu) \left(e^{u\Delta_{km}} e^{\beta\Delta_{mn}} - e^{u\Delta_{kn}} \right).$$
(24b)

We have defined

$$\phi_{nk}(x) = |(\mathbf{S})_{nk}|^2 e^{-i \, x \, \Delta_{nk}}.$$
(25)

with $\Delta_{nk} = \epsilon_k - \epsilon_n$ and $(\boldsymbol{S})_{nk} = \langle \epsilon_n | \boldsymbol{S} | \epsilon_k \rangle$. We have also introduced here the probe and sample auto-correlation functions, defined as

$$\Phi_{S}(x) \coloneqq \left\langle e^{ix\boldsymbol{H}_{S}}\boldsymbol{S} e^{-ix\boldsymbol{H}_{S}}\boldsymbol{S} \right\rangle_{S} = \operatorname{tr}_{S} \left[\boldsymbol{\pi}_{S} e^{ix\boldsymbol{H}_{S}}\boldsymbol{S} e^{-ix\boldsymbol{H}_{S}}\boldsymbol{S} \right]$$
(26a)

$$\Phi_B(x) \coloneqq \left\langle e^{ix\boldsymbol{H}_B}\boldsymbol{B} \, e^{-ix\boldsymbol{H}_B}\boldsymbol{B} \right\rangle_B = \operatorname{tr}_B \left[\boldsymbol{\pi}_B \, e^{ix\boldsymbol{H}_B}\boldsymbol{B} \, e^{-ix\boldsymbol{H}_B}\boldsymbol{B} \right].$$
(26b)

From these formulas, we see that the condition for the validity of Eq. (23), $X_s \ll \mathbf{1}_s$, is satisfied if $\gamma^2 \langle S^2 \rangle_s \langle B^2 \rangle_B \ll T^2$. This shows that, the smaller the temperature T, the weaker the coupling needs to be in order for the perturbative calculations to make sense. An analogue of Eq. (24) was derived in Ref. [61] and for the special case of linear coupling to a bosonic bath in Ref. [65].

Thus equipped with Eqs. (23) and (24), we can turn to Eq. (8) and write the SLD as

$$\boldsymbol{L}_{S}(\beta) = -\Delta \boldsymbol{H}_{S} + \gamma^{2} \sum_{nm} \alpha_{nm}(\beta) |\epsilon_{n}\rangle \langle\epsilon_{m}| + O(\gamma^{4})$$
(27a)

with $\Delta \boldsymbol{H}_{S} \coloneqq \boldsymbol{H}_{S} - \langle \boldsymbol{H}_{S} \rangle_{S}$ and coefficients

$$\alpha_{nm}(\beta) = \frac{2p_n}{p_n + p_m} \partial_\beta(\boldsymbol{X}_S)_{nm} + \frac{p_n \Delta_{nm}}{p_n + p_m} (\boldsymbol{X}_S)_{nm}.$$
 (27b)

Here, $\Delta_n \coloneqq \epsilon_n - \langle \boldsymbol{H}_S \rangle_S$. Also note that the populations appearing above are

$$p_n = \langle \epsilon_n | \boldsymbol{\pi}_S | \epsilon_n \rangle = e^{-\beta \epsilon_n} / Z_S$$
(28)

and should not be confused with the populations of the mean-force Gibbs state

$$\tilde{p}_n = \langle \epsilon_n | \, \tilde{\boldsymbol{\pi}}_S \, | \epsilon_n \rangle = p_n + \gamma^2 p_n(\boldsymbol{X}_S)_{nn} + O(\gamma^4).$$
⁽²⁹⁾

We now have the two ingredients needed to compute the QFI from Eq. (6). After some algebra, this can be compactly written as

$$\mathcal{F}_{S}(\beta) = \partial_{\beta}^{2} \ln Z_{S} + \gamma^{2} \int_{0}^{\beta} du \left[\tilde{\Phi}_{B}(-iu) \partial_{\beta}^{2} \Phi_{S}(-iu) + 2 \partial_{\beta} \tilde{\Phi}_{B}(-iu) \partial_{\beta} \Phi_{S}(-iu) \right] + O(\gamma^{4}),$$
(30)

with the modified auto-correlation function $\tilde{\Phi}_B(x) \coloneqq (\beta - ix)\Phi_B(x)$. To second order in γ the QFI can thus be expressed solely in terms of the probe and sample correlation functions. We emphasise that the validity of Eqs. (27) and (30) is not, in any way, underpinned by the Born–Markov approximation.

Equations (27) and (30) are our second main result. They can be applied directly to *any* open quantum system under finite coupling, provided that Assumptions I and II are met. And since the systems satisfying these assumptions span an exceptionally wide range, our closed-form expressions for L_s and $\mathcal{F}_s(\beta)$ open up new avenues in quantum thermometry. Note that, when Assumptions I and II are violated, the QFI will in general pick up a first-order term, as can be anticipated from Eq. (22). We provide illustrative examples of that in Appendix A.

Finally, it is often useful to talk in terms of T rather than inverse temperature β . Namely, from Eq. (5) we see that the best-case signal-to-noise ratio (SNR) for estimates of T can be cast as

$$\frac{1}{N} \left(\frac{T}{\delta T}\right)^2 \le \beta^2 \,\mathcal{F}_S(\beta) \coloneqq C_S(T) + \gamma^2 \xi(T),\tag{31}$$

with $C_s(T) = \beta^2 \partial_\beta^2 \ln Z_s = \partial_T \langle \boldsymbol{H}_s \rangle_s$ being the heat capacity of the probe when in local thermal equilibrium [24], and where $\xi(T)$ follows from the second-order term in Eq. (30).

3 Examples

We now benchmark our Eq. (30) against the exactly solvable Caldeira–Leggett model for quantum Brownian motion and then, apply it to the spin–boson problem. In both cases, we model the sample as an infinite collection of uncoupled harmonic oscillators spanning a quasi-continuum of frequencies—the most common bath model in open quantum systems. That is,

$$\boldsymbol{H}_{B} = \sum_{k} \omega_{k} \boldsymbol{b}_{k}^{\dagger} \boldsymbol{b}_{k}, \qquad (32)$$

where $\boldsymbol{b}_{k}^{\dagger}(\boldsymbol{b}_{k})$ is the creation (annihilation) operator at frequency ω_{k} . As it is also customary, we take the coupling operator \boldsymbol{B} to be

$$\boldsymbol{B} = \sum_{k} \left(g_k \, \boldsymbol{b}_k^{\dagger} + g_k^* \, \boldsymbol{b}_k \right), \tag{33}$$

Here, the coupling constants g_k encode the overall dissipation strength (note that γ still enters \boldsymbol{H}_{int}). We may collect them into the *spectral density* function

$$J(\omega) = \pi \sum_{k} |g_k|^2 \,\delta(\omega - \omega_k),\tag{34}$$

where $\delta(\cdot)$ stands here for the Dirac delta. Since we assume that the sample has a quasicontinuum spectrum, we may give some smooth functional form to $J(\omega)$.

Using this notation, the bath correlation function evaluates to

$$\Phi_B(-iu) = \frac{1}{\pi} \int_0^\infty d\omega \ J(\omega) \ \frac{\cosh\left(\beta \,\omega/2 - u \,\omega\right)}{\sinh\left(\beta \,\omega/2\right)}.$$
(35)

Furthermore, using Eq. (30) we see that the second-order correction $\xi(T)$ to the SNR from Eq. (31) is given by

$$\xi(T) = \int_0^\infty d\omega \ J(\omega) \ f_s(T,\omega), \tag{36a}$$

where

$$f_{S}(T,\omega) = \frac{\beta^{2}}{\pi \sinh \frac{\beta \omega}{2}} \int_{0}^{\beta} du \ (\beta - u) \cosh \left(\beta \omega/2 - u \,\omega\right) \\ \times \left[\partial_{\beta}^{2} \Phi_{S}(-iu) + \partial_{\beta} \Phi_{S}(-iu) \left(\frac{2}{\beta - u} - \omega \coth \frac{\beta \omega}{2} - \omega \tanh \frac{(2u - \beta) \,\omega}{2}\right)\right]. \tag{36b}$$

Eqs. (36) above hold for any spectral density $J(\omega)$, provided that the bath and the probe-bath coupling are of the standard type defined by Eqs. (32) and (33). Hence, Eq. (36) holds even where most master equations break down, e.g., when the bath correlation function happens to be long lived. As we illustrate below, Eqs. (36) are indeed very practical to quickly evaluate the finite-coupling corrections to thermal sensitivity, and provide analytic intuition about their temperature dependence. This is our third result.

Specifically, in what follows we work with a spectral density with variable Ohmicity s and exponential cutoff; namely,

$$J(\omega) = \Omega^{a-s} \,\omega^s \, e^{-\omega/\Omega},\tag{37}$$

where a controls the dimension of $J(\omega)$ and therefore depends on the choice of **S**: if $[\mathbf{S}] = [\omega]^{\mu}$, then $a = 1 - 2\mu$, where $[\cdot]$ gives the dimension of the argument.

3.1 Quantum Brownian motion

In order to put the accuracy of our second-order formula to the test, we take a single harmonic oscillator as the probe. That is,

$$\boldsymbol{H}_{S} = \frac{1}{2}\omega_{0}^{2}\boldsymbol{x}^{2} + \frac{1}{2}\boldsymbol{p}^{2}, \qquad (38)$$

while the probe operator entering in the interaction Hamiltonian[¶] in Eq. (19) is $\mathbf{S} = \mathbf{x}$. For this choice of \mathbf{S} , dimensional analysis imposes the value a = 2 for the exponent in Eq. (37). In this simple case, exact expressions can be found for the steady state of the Brownian oscillator and its thermal sensitivity [29, 34], which allows us to benchmark Eq. (30). Explicit expressions can be found in Ref. [29].

The only ingredient missing from Eqs. (36) is the probe correlation function, for which a straighforward calculation yelds

$$\Phi_{S}(-iu) = \frac{1}{2\omega_{0}}e^{-u\,\omega_{0}} + \frac{1}{\omega_{0}}\frac{\cosh\left(u\,\omega_{0}\right)}{e^{\beta\,\omega_{0}} - 1}.$$
(39)

In Fig. 1 we compare the signal-to-noise ratio according to Eq. (31) against the exact result and the thermal sensitivity of a probe in local thermal equilibrium, which is given by the heat capacity alone. We see that our second-order formula accurately captures the sensitivity for small coupling. As already advanced, at very low temperatures, β itself sets an energy-scale compared to which the coupling is no longer perturbative. This results in our second-order approximation becoming less accurate. On the other hand, the sensitivity saturates at high temperature, and is correctly approximated by the assumption of local thermal equilibrium on the probe, as expected. Hence, our formula provides substantial quantitative advantage in the range of moderately low temperatures.

To get further insight into the correction we calculate the high-temperature expansion of Eq. (36b), which gives

$$f_s(T,\omega) = -\frac{\beta^2}{6m\pi\omega} + O(\beta^4), \qquad (40)$$

[¶]Note that we are not adding a counter-term to compensate for the distortion of the harmonic potential due to the coupling to the sample. While it may be important to do so whenever such renormalisation is not expected to be physical—especially when the coupling is strong—this effect is irrelevant for us.

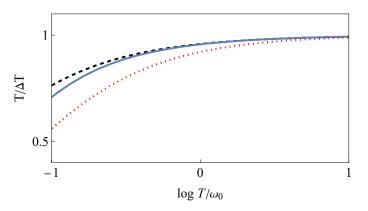


Figure 1: Benchmarking Eq. (30) for quantum Brownian motion. The plot shows the signal-tonoise ratio from our second-order formula (solid blue), the true SNR ratio from the exact mean-force Gibbs state (dashed black), and from the infinitesimal coupling limit, i.e. the local Gibbs state (dotted red). The second-order formula tracks the exact sensitivity well as long as the probe-sample coupling is the only small parameter. It starts to break down when the temperature itself becomes a small parameter as $T \rightarrow 0$. We chose $\omega_0 = 1, \gamma = 0.1, s = 1$ and $\Omega = 100$ ($\hbar = k = 1$).

doing the integral in Equation (36a) for our spectral density (37) gives

$$\xi(T) = -\frac{\Omega^2 \Gamma(s)}{3m\pi} \beta^2 + O(\beta^4), \qquad (41)$$

with $\Gamma(\cdot)$ the Euler gamma function. This is exactly the lowest-order contribution from the frequency renormalisation due to the finite interaction with the sample, i.e. the classical mean-force correction [91].

3.2 Spin-boson model

We now apply our formula to a case study for which no exact solution is available—the spin–boson model. In order to study the effects of coherence in the steady state, we focus on the ' θ -angled' spin–boson model. That is,

$$\boldsymbol{H}_{S} = \frac{\epsilon}{2} \boldsymbol{\sigma}_{z}, \tag{42a}$$

$$\boldsymbol{S} = \cos\theta\,\boldsymbol{\sigma}_z - \sin\theta\,\boldsymbol{\sigma}_x,\tag{42b}$$

where σ_{α} are Pauli operators. For this choice of S, a = 1. We thus have the probe correlation function

$$\Phi_{S}(-iu) = \cos^{2}\theta + \cosh\left(\epsilon \, u - \beta \, \epsilon/2\right) \, \operatorname{sech}\left(\beta \, \epsilon/2\right) \, \sin^{2}\theta. \tag{43}$$

In Fig. 2 we compare the the SNR ratio as per Eq. (31) for two values of θ and, once again, also against the sensitivity of a locally thermal probe. We also plot the coherence appearing in our approximation of the mean-force Gibbs state [Eq. (23)], and the coherence showing up in the symmetric logarithmic derivative, to second order in γ [Eq. (27)]. In this case, however, there is no exact SNR to compare with. We see that the two different couplings yield slightly different sensitivity, departing from the SNR of the locally thermal probe. We can also see that, at large enough temperature, the sensitivity drops to zero, as the spin populations saturate.

Rather counter-intuitively, we can see in the right panel that the $\theta = \pi/4$ coupling generates *temperature-dependent* coherences in the second-order approximation to $\tilde{\pi}_s$, and

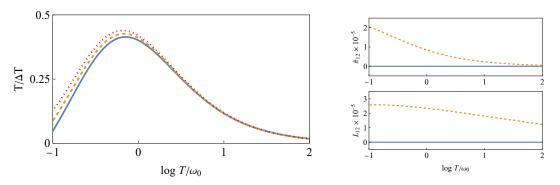


Figure 2: Applying Eq. (30) to the spin-boson model. The left panel shows the SNR from our second-order formula for two types of probe-sample coupling; namely, $\theta = 3\pi/2$, i.e. $S = \sigma_z$ (solid blue) and for $\theta = \pi/4$, i.e. the maximally coherent case (dashed orange). We compare these to the sensitivity of a locally thermal probe (dotted red). The top-right panel shows the second-order coherences of the respective mean-force Gibbs states. The same color coding applies. The bottom-right plot shows the second-order coherences of the respective symmetric logarithmic derivatives in the basis of H_s . We emphasize that diagonal energy measurements saturate the second-order precision bound despite $\tilde{\pi}_s$ and L_s acquiring temperature-dependent off-diagonal elements at second order in γ . The other parameters are the same as in Fig. 1.

in the second-order corrections to L_s . Yet, we have proven that (diagonal) measurements in the local energy basis H_s —which destroy such temperature information—do still saturate the ultimate precision bound, at least to second order in γ [cf. Eq. (18)]. In other words, temperature-dependent coherences may only improve precision at higher orders in finitecoupling quantum thermometry.

It is interesting to note that, in this case, the correction $\xi(T)$ to the optimal SNR has a definite sign—it is always negative. Indeed, the factor in brackets in Eq. (36b) is negative for all ω , while the spectral density is obviously positive for all ω . Hence, the weaker the probe–sample coupling the better for this type of probe. For completeness, we calculate the high–T limit of Eq. (36b). We get

$$f_s(T,\omega) = -\frac{2\sin^2(\theta)\,\epsilon^2}{3\pi\omega}\,\beta^3 + O(\beta^5) \tag{44}$$

which, after integration as per Eq. (36a), yields

$$\xi(T) = -\frac{4\sin^2(\theta)\,\epsilon^2\Omega\Gamma(s)}{3\pi}\,\beta^3 + O(\beta^5). \tag{45}$$

This highlights what can already be seen in Fig. 2—that here, the vanishing-coupling limit gives a far better approximation to the thermal sensitivity at moderate-to-large temperature, when compared with the quantum Brownian motion example.

4 Derivation

4.1 Mean-force Gibbs state

In this section we elaborate on the derivation of the results presented in Sec. 2. The first step in our search for an explicit expression for $\mathcal{F}_{S}(\beta)$ will be to obtain a second-order approximation of the reduced probe state $\tilde{\pi}_{S}$, following [61]. Applying Eq. (21) to $e^{-\beta H}$ leads to:

$$e^{-\beta H} = e^{-\beta (H_S + H_B)} \left(\mathbf{1} - \gamma \int_0^\beta d\beta_1 \ e^{\beta_1 (H_S + H_B)} \mathbf{V} e^{-\beta_1 (H_S + H_B)} \right) + \gamma^2 \int_0^\beta d\beta_1 \ \int_0^{\beta_1} d\beta_2 \ e^{\beta_1 (H_S + H_B)} \mathbf{V} e^{-(\beta_1 - \beta_2) (H_S + H_B)} \mathbf{V} e^{-\beta_2 (H_S + H_B)} \right) + O(\gamma^3).$$
(46)

Taking the trace yields an approximation for the total partition function

$$\tilde{Z} = Z_S Z_B - \gamma \beta \operatorname{tr}_S \left[e^{-\beta \boldsymbol{H}_S} \boldsymbol{S} \right] \operatorname{tr}_B \left[e^{-\beta \boldsymbol{H}_B} \boldsymbol{B} \right] + \gamma^2 \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \operatorname{tr}_S \left[e^{-\beta \boldsymbol{H}_S} e^{(\beta_1 - \beta_2) \boldsymbol{H}_S} \boldsymbol{S} e^{-(\beta_1 - \beta_2) \boldsymbol{H}_S} \boldsymbol{S} \right] \times \operatorname{tr}_B \left[e^{-\beta \boldsymbol{H}_B} e^{(\beta_1 - \beta_2) \boldsymbol{H}_B} \boldsymbol{B} e^{-(\beta_1 - \beta_2) \boldsymbol{H}_B} \boldsymbol{B} \right] + O(\gamma^3), \quad (47)$$

where Assumption I [Eq. (19)] has been applied. Using $(1 + x)^{-1} = 1 - x + O(x^2)$, Assumption II [Eq. (20)], and the definition of probe and sample auto-correlation functions from Eq. (26), we find

$$\frac{1}{\tilde{Z}} = \frac{1}{Z_S Z_B} \left(1 - \gamma^2 \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \Phi_S(-i(\beta_1 - \beta_2)) \Phi_B(-i(\beta_1 - \beta_2)) \right) + O(\gamma^4), \quad (48)$$

Multiplying Eqs. (46) and (48), collecting terms, and taking the partial trace over the sample, we find that the first order correction vanishes, so that

$$\tilde{\boldsymbol{\pi}}_{S} = \frac{1}{\tilde{Z}} \operatorname{tr}_{B} \left[e^{-\beta \boldsymbol{H}} \right] = \boldsymbol{\pi}_{S} \left(\boldsymbol{1}_{S} + \gamma^{2} \boldsymbol{X}_{S} \right) + O(\gamma^{4}),$$

where we have introduced the operator

$$\boldsymbol{X}_{S} = \int_{0}^{\beta} d\beta_{1} \int_{0}^{\beta_{1}} d\beta_{2} \Phi_{B}(-i(\beta_{1} - \beta_{2})) \times \left[e^{\beta_{1}\boldsymbol{H}_{S}}\boldsymbol{S}e^{-(\beta_{1} - \beta_{2}))\boldsymbol{H}_{S}}\boldsymbol{S}e^{-\beta_{2}\boldsymbol{H}_{S}} - \Phi_{S}(-i(\beta_{1} - \beta_{2}))\boldsymbol{1}_{S}\right], \quad (49)$$

Note that $\operatorname{tr}_{S} [\boldsymbol{X}_{S} \boldsymbol{\pi}_{S}] = 0$ as required by normalisation.

Writing the diagonal elements of the operator $(\boldsymbol{X}_S)_{nn} \coloneqq \langle \epsilon_n | \boldsymbol{X}_S | \epsilon_n \rangle$ in the eigenbasis of $\boldsymbol{H}_S = \sum_n \epsilon_n | \epsilon_n \rangle \langle \epsilon_n |$ gives

$$(\boldsymbol{X}_{S})_{nn} = \int_{0}^{\beta} d\beta_{1} \int_{0}^{\beta_{1}} d\beta_{2} \Phi_{B}(-i(\beta_{1} - \beta_{2})) \\ \times \Big[\sum_{k} \phi_{nk}(-i(\beta_{1} - \beta_{2})) - \Phi_{S}(-i(\beta_{1} - \beta_{2}))\Big], \quad (50)$$

which can be turned into Eq. (24) by introducing the new variables $u = \beta_1 - \beta_2$ and $v = \beta_1 + \beta_2$ and performing the integral over v; namely

$$(\mathbf{X}_{S})_{nn} = \frac{1}{2} \int_{0}^{\beta} du \int_{u}^{2\beta - u} dv \,\Phi_{B}(-iu) \Big(\sum_{k} \phi_{nk}(-iu) - \Phi_{S}(-iu)\Big) \\ = \int_{0}^{\beta} du \,(\beta - u) \Phi_{B}(-iu) \Big(\sum_{k} \phi_{nk}(-iu) - \Phi_{S}(-iu)\Big),$$

In turn, the off-diagonal elements of X_{S} are

$$(\boldsymbol{X}_{S})_{nm} = \sum_{k} (\boldsymbol{S})_{nk} (\boldsymbol{S})_{km} \int_{0}^{\beta} d\beta_{1} \ e^{\beta_{1} \Delta_{kn}} \int_{0}^{\beta_{1}} d\beta_{2} \ e^{\beta_{2} \Delta_{mk}} \Phi_{B}(-i(\beta_{1} - \beta_{2}))$$
(51)

Again, we may introduce $u = \beta_1 - \beta_2$ and $v = \beta_1 + \beta_2$ and integrate over v, which gives

$$(\boldsymbol{X}_{S})_{nm} = \frac{1}{\Delta_{mn}} \sum_{k} (\boldsymbol{S})_{nk} (\boldsymbol{S})_{km} \int_{0}^{\beta} du \, \Phi_{B}(-iu) \left(e^{u\Delta_{km}} e^{\beta\Delta_{mn}} - e^{u\Delta_{kn}} \right) \quad (n \neq m).$$
(52)

4.2 Symmetric logarithmic derivative

We now use the expression for the mean-force Gibbs state to obtain the SLD via Eq. (8). To do so, we differentiate Eq. (23) and use $\langle \boldsymbol{H}_{S} \rangle_{S} = -\partial_{\beta} \ln Z_{S}$ to get

$$\partial_{\beta} \tilde{\boldsymbol{\pi}}_{S} = -\Delta \boldsymbol{H}_{S} \boldsymbol{\pi}_{S} + \gamma^{2} \partial_{\beta} (\boldsymbol{\pi}_{S} \boldsymbol{X}_{S}) + O(\gamma^{4}).$$
(53)

Turning to the operator $e^{-\lambda \tilde{\pi}_S}$ and combining Eqs. (21) and (23) leads to

$$e^{-\lambda \tilde{\boldsymbol{\pi}}_{S}} = e^{-\lambda \boldsymbol{\pi}_{S}} \left(\mathbf{1}_{S} - \gamma^{2} \boldsymbol{\pi}_{S} \int_{0}^{\lambda} d\lambda' \ e^{\lambda' \boldsymbol{\pi}_{S}} \boldsymbol{X}_{S} \ e^{-\lambda' \boldsymbol{\pi}_{S}} \right) + O(\gamma^{4}).$$
(54)

Using this, we can finally compute the SLD. From Eqs. (53) and (54) we get

$$e^{-\lambda\tilde{\boldsymbol{\pi}}_{S}}(\partial_{\beta}\tilde{\boldsymbol{\pi}}_{S})e^{-\lambda\tilde{\boldsymbol{\pi}}_{S}} = -\Delta\boldsymbol{H}_{S}\boldsymbol{\pi}_{S}e^{-2\lambda\boldsymbol{\pi}_{S}} + \gamma^{2}\boldsymbol{\pi}_{S}\int_{0}^{\lambda}d\lambda' \ e^{-(\lambda-\lambda')\boldsymbol{\pi}_{S}}\boldsymbol{X}_{S} e^{-(\lambda+\lambda')\boldsymbol{\pi}_{S}}\Delta\boldsymbol{H}_{S}\boldsymbol{\pi}_{S}, + \gamma^{2}e^{-\lambda\boldsymbol{\pi}_{S}}\partial_{\beta}(\boldsymbol{\pi}_{S}\boldsymbol{X}_{S}) \ e^{-\lambda\boldsymbol{\pi}_{S}} + \gamma^{2}\Delta\boldsymbol{H}_{S}\boldsymbol{\pi}_{S}^{2}e^{-2\lambda\boldsymbol{\pi}_{S}}\int_{0}^{\lambda}d\lambda' \ e^{\lambda'\boldsymbol{\pi}_{S}}\boldsymbol{X}_{S} \ e^{-\lambda'\boldsymbol{\pi}_{S}} + O(\gamma^{4})$$
(55)

We can now recover Eq. (27) using Eqs. (8) and working again in the eigenbasis of H_s . Namely,

$$\boldsymbol{L}_{S}(\beta) = -\Delta \boldsymbol{H}_{S} + \gamma^{2} \sum_{nm} \alpha_{nm}(\beta) |\boldsymbol{\epsilon}_{n}\rangle \langle \boldsymbol{\epsilon}_{m}| + O(\gamma^{4}),$$

with coefficients

$$\alpha_{nm}(\beta) = \frac{2 p_n}{p_n + p_m} \,\partial_\beta(\boldsymbol{X}_S)_{nm} + \frac{p_n \Delta_{nm}}{p_n + p_m} \,(\boldsymbol{X}_S)_{nm}.$$

Here, we have used the fact that $\partial_{\beta} p_n = p_n (\langle H_S \rangle_S - \epsilon_n) = -p_n \Delta_n$ (not to be confused with the energy gaps Δ_{nk}). As long as we know the sample correlation function $\Phi_B(x)$ and the eigenstates of H_S , we will be able to obtain the elements $(X_S)_{nm}$ from Eqs. (24) and (52), and thus, the SLD as per Eq. (27).

4.3 Quantum Fisher information

The QFI can now be directly computed by using $\mathcal{F}_{S}(\beta) = \operatorname{tr}_{S} \left[\boldsymbol{L}_{S}^{2} \tilde{\boldsymbol{\pi}}_{S} \right]$. Collecting terms up to second order yields

$$\mathcal{F}_{S}(\beta) = \partial_{\beta}^{2} \ln Z_{S} + \gamma^{2} \sum_{n} \left[p_{n} \Delta_{n}^{2} (\boldsymbol{X}_{S})_{nn} - 2 p_{n} \Delta_{n} \alpha_{nn} \right] + O(\gamma^{4}),$$
(56)

where $\partial_{\beta}^2 \ln Z_s = \langle (\Delta \boldsymbol{H}_s)^2 \rangle_s$ and $\alpha_{nn} = \partial_{\beta} (\boldsymbol{X}_s)_{nn}$, by Eq. (27b).

We can still obtain the much more elegant expression (30), in terms of probe and sample auto-correlation functions alone. Noting that

$$\Phi_S(-iu) = \sum_{nk} \phi_{nk}(-iu)$$

is easy to see that

$$\sum_{n} p_n \Delta_n (\boldsymbol{X}_S)_{nn} = -\partial_\beta \Phi_S(-iu)$$
(57a)

$$\sum_{n} p_n \Delta_n^2 (\boldsymbol{X}_S)_{nn} = \partial_\beta^2 \Phi_S(-iu).$$
(57b)

Furthermore, since $\sum_{n} p_n \Delta_n = 0$, we see that $\partial_{\beta}(\boldsymbol{X}_s)_{nn}$ reduces to

$$\partial_{\beta}(\boldsymbol{X}_{S})_{nn} = -\partial_{\beta}\tilde{\Phi}_{B}(-iu)\,\partial_{\beta}\Phi_{S}(-iu),\tag{58}$$

where, recall that $\tilde{\Phi}_B(-iu) = (\beta - u) \Phi_B(-iu)$. Hence, Eq. (56) can be recast as desired:

$$\mathcal{F}_{S}(\beta) = \partial_{\beta}^{2} \ln Z_{S} + \gamma^{2} \int_{0}^{\beta} du \left[\tilde{\Phi}_{B}(-iu) \partial_{\beta}^{2} \Phi_{S}(-iu) + 2 \partial_{\beta} \tilde{\Phi}_{B}(-iu) \partial_{\beta} \Phi_{S}(-iu) \right] + O(\gamma^{4}).$$

4.4 Classical Fisher information for energy measurements

Finally, we connect with our general result in Eq. (18). To that end, we use the definition (10) of the (classical) Fisher information associated to energy measurements of $\tilde{\pi}_{s}$ on the basis of the bare Hamiltonian H_{s} . Namely,

$$\mathcal{I}_{\boldsymbol{H}_{S}}(\beta) = \sum_{n} \tilde{p}_{n} \left(\partial_{\beta} \ln \tilde{p}_{n}\right)^{2}.$$
(59)

Plugging in the mean-force Gibbs state populations from Eq. (29) gives

$$\mathcal{I}_{\boldsymbol{H}_{S}}(\beta) = \sum_{n} \tilde{p}_{n} (\partial_{\beta} \ln \tilde{p}_{n})^{2}$$

= $\partial_{\beta}^{2} \ln Z_{S} + \gamma^{2} \sum_{n} \left[p_{n} \Delta_{n}^{2} (\boldsymbol{X}_{S})_{nn} - 2\Delta_{n} \partial_{\beta} (\boldsymbol{X}_{S})_{nn} \right] + O(\gamma^{4}).$

Here, we have used the identities $\ln \tilde{p}_n = p_n + \gamma^2 (\boldsymbol{X}_S)_{nn} + O(\gamma^4)$, $\partial_\beta \ln p_n = -\Delta_n$, and the fact that $\sum_n p_n (\partial_\beta \ln p_n)^2 = \partial_\beta^2 \ln Z_S$. As expected, we thus recover Eq. (56), meaning that local energy measurements on the probe are as efficient as the truly optimal measurements in finite-coupling quantum thermometry. This statement holds generally to second order in the coupling for any thermometric setup. The only underpinning assumption is that probe and sample have a separable coupling, and that the sample operator averages to zero when in a local thermal state. This choice for the dissipative interaction is indeed widespread in open quantum systems.

5 Conclusions

We have developed a theory of finite-coupling quantum thermometry, focusing on the second-order correction terms. On the one hand, we have obtained closed-form expressions for the symmetric logarithmic derivative, which fixes the optimal basis in which to measure the probe; and the quantum Fisher information, which gauges the responsiveness of the probe to temperature fluctuations on the sample. Our formulae make minimal assumptions on the probe–bath coupling and can be readily applied to any setup by simply computing the probe and sample auto-correlation functions. In particular, we make no assumptions

on the nature of the sample, so that our framework is applicable even when standard opensystem weak-coupling tools—based on the Born–Markov approximation—break down.

On the other hand, we have proved that projective measurements in the local energy basis of the probe are always optimal to the first two leading orders in the probe–sample coupling. That is, even if temperature information may be encoded in the off-diagonal elements of the probe's marginal state, the advantage in extracting and processing such information would only show up in higher order terms. Hence, measurement optimisation is unnecessary for quantum thermometry at moderate couplings.

Finally, we have illustrated the use of our approach with two relevant examples—the exactly solvable Caldeira–Legett model (which served as benchmark) and the spin–boson model. Specifically, we have derived an explicit expression for the second-order correction to the signal-to-noise ratio for temperature estimation, suitable for any open-system model which uses a canonical linear bath with quasi-continuum spectrum; regardless of the specific spectral density. Such formula can thus be of independent interest.

Our results open up new directions in finite-coupling thermometry. Namely, our formulae can easily deal with thermometry on more realistic non-linear sample models, which remain virtually unexplored to date. They can also facilitate the treatment of complex probe–sample interactions, such as the ones appearing when modelling an atomic impurity in a Bose–Einstein condensate [34], without the need for *linearisation*. Crucially, having established the optimality of energy measurements up to second order in the coupling strength highlights the importance of directing practical efforts towards measuring the probe in its local basis. Furthermore, guaranteeing that optimal thermometry may be attained using a fixed *temperature-independent* basis also eliminates the need for more complex adaptive schemes.

Interestingly, lifting our Assumption II on the vanishing expectation value of the interaction in the stationary state of the sample would result in inhomogeneous terms, which might introduce a thermometric advantage in terms of additional temperature dependence. Studying how this may be exploited in practice will be the subject of future study.

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A Examples with $\langle \boldsymbol{B} \rangle_{\scriptscriptstyle B} \neq 0$

In this short Appendix, we give explicit examples in which Assumption II in Eq. (20) namely $\langle \boldsymbol{B} \rangle_B = 0$ —is not satisfied. Specifically, we begin by illustrating how, in this case, the QFI and SLD may pick up terms of $O(\gamma)$. To that end, let us consider the two-qubit model

$$\boldsymbol{H} = \boldsymbol{H}_{\scriptscriptstyle S} + \boldsymbol{H}_{\scriptscriptstyle B} + \boldsymbol{H}_{\rm int} = \omega \, \boldsymbol{\sigma}_{z,1} \otimes \boldsymbol{1}_2 + \omega \, \boldsymbol{1}_1 \otimes \boldsymbol{\sigma}_{z,2} + \gamma \, \boldsymbol{\sigma}_{z,1} \otimes \boldsymbol{\sigma}_{z,2},$$

where the sub-indices label the qubits, '1' being the probe and '2' being the sample. Also, in all the expressions that follow, we shall set $\omega = 1$ for simplicity.

The corresponding mean-force Gibbs state can be expanded as

$$\tilde{\boldsymbol{\pi}}_{S} = \boldsymbol{\pi}_{S} + \gamma \, p_1 \, \boldsymbol{\sigma}_{z,1} + \gamma^2 p_2 \, \boldsymbol{\sigma}_{z,1} + O(\gamma^3),$$

with $p_1 = \frac{1}{2}\beta \operatorname{sech}^2\beta \tanh\beta$ and $p_2 = \frac{1}{2}\beta^2 \operatorname{sech}^2\beta \tanh^3\beta$. As we anticipated, in this case the QFI does feature a linear term, namely

$$\mathcal{F}_{S}(\beta) = \partial_{\beta}^{2} \ln Z_{S} + \operatorname{sech}^{4} \beta \left[\beta (\cosh 2\beta - 3) - \sinh 2\beta \right] \gamma + O(\gamma^{2}),$$

and so does the symmetric logarithmic derivative

$$\boldsymbol{L}_{S} = -\Delta \boldsymbol{H}_{S} + l_{1} \boldsymbol{\sigma}_{z,1} + O(\gamma^{2}),$$

with $l_1 = 1 + \tanh \beta + \operatorname{sech}^2 \beta (\beta + 2\beta \tanh \beta - 1)$. We know from Sec. 2.2.1 that the classical Fisher information for measurements in the local energy basis and the QFI must agree in the zeroth and first order in γ . However, as noted in Sec. 2.1, due to the coupling in this toy model being 'non-dissipative', i.e., $[\boldsymbol{H}_{\text{int}}, \boldsymbol{H}] = 0, \boldsymbol{L}_S$ is diagonal in the \boldsymbol{H}_S basis at all orders. Hence, energy measurements are always optimal in this particular case.

Let us now turn to a more general scenario. Namely,

$$\boldsymbol{H} = \boldsymbol{H}_{S} + \boldsymbol{H}_{B} + \boldsymbol{H}_{\text{int}} = \omega \,\boldsymbol{\sigma}_{z,1} \otimes \boldsymbol{1}_{2} + \omega \,\boldsymbol{1}_{1} \otimes \boldsymbol{\sigma}_{z,2} + \gamma \,\boldsymbol{\Pi}_{1} \otimes \boldsymbol{\sigma}_{x,2},$$

where $\mathbf{\Pi} = |1\rangle \langle 1|$. In this case, we can see that

$$\tilde{\boldsymbol{\pi}}_{\scriptscriptstyle S} = \boldsymbol{\pi}_{\scriptscriptstyle S} + \gamma \, p_1 \, \boldsymbol{\sigma}_{x,1} + \gamma^2 \, p_2 \, \boldsymbol{\sigma}_{z,1} + O(\gamma^3),$$

with coefficients

$$p_{1} = \frac{1}{4} \tanh\beta \left(\tanh\beta - 1\right)$$
$$p_{2} = \frac{1}{8} \operatorname{sech}\beta \left(\tanh\beta - 1\right) \left(\beta \operatorname{sech}\beta - \sinh\beta\right)$$

In particular, note how the mean-force Gibbs state does feature β -dependent coherences.

The corresponding symmetric logarithmic derivative is

$$\boldsymbol{L}_{S} = -\Delta \boldsymbol{H}_{S} + \gamma \, l_{1} \, \boldsymbol{\sigma}_{x,1} + O(\gamma^{2}),$$

with $l_1 = \frac{1}{2} \operatorname{sech}^2 \beta (2 \tanh \beta - 1)$, meaning that the optimal measurement is non-diagonal in the energy basis already to first order in the coupling strength. And yet, as we proved in full generality in Sec. 2.2.1, the classical Fisher information of local energy measurements and the quantum Fisher information must agree to *second* leading order. Indeed, direct calculation shows that

$$\mathcal{F}_{S}(\beta) - \mathcal{I}_{\boldsymbol{H}_{S}}(\beta) = \frac{1}{4} \operatorname{sech}^{4} \beta \left(1 - 2 \tanh \beta\right)^{2} \gamma^{2} + O(\gamma^{3}).$$

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