Local quantum thermal susceptibility

Antonella De Pasquale[1], Davide Rossini[1], Rosario Fazio[1,2,3] & Vittorio Giovannetti[1]

Thermodynamics relies on the possibility to describe systems composed of a large number of constituents in terms of few macroscopic variables. Its foundations are rooted into the paradigm of statistical mechanics, where thermal properties originate from averaging procedures which smoothen out local details. While undoubtedly successful, elegant and formally correct, this approach carries over an operational problem, namely determining the precision at which such variables are inferred, when technical/practical limitations restrict our capabilities to local probing. Here we introduce the local quantum thermal susceptibility, a quantifier for the best achievable accuracy for temperature estimation via local measurements. Our method relies on basic concepts of quantum estimation theory, providing an operative strategy to address the local thermal response of arbitrary quantum systems at equilibrium. At low temperatures, it highlights the local distinguishability of the ground state from the excited sub-manifolds, thus providing a method to locate quantum phase transitions.

[1] NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, Piazza dei Cavalieri 7, I-56126 Pisa, Italy. [2] ICTP, Strada Costiera 11, I-34151 Trieste, Italy. [3] Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, Singapore 117543, Singapore. Correspondence and requests for materials should be addressed to A.D.P. (email: antonella.depasquale@sns.it).

The measurement of temperature is a key aspect in science, technology and in our daily life. Many ingenious solutions have been designed to approach different situations and required accuracies[1]. What is the ultimate limit to the precision at which the temperature of a macroscopic state can be determined? An elegant answer to this question is offered by estimation theory[2–4]: The precision is related to the heat capacity of the system[5,6].

In view of the groundbreaking potentialities offered by present-day nanotechnologies[7–12] and the need to control the temperature at the nano-scale, it is highly relevant to question whether the heat capacity is still the relevant (fundamental) precision limit to small-scale thermometry. The extensivity of the heat capacity is a consequence of the growing volume-to-surface ratio with the size[13]. However, at a microscopic level such construction may present some limitations[14,15]. Moreover a series of theoretical efforts recently concentrated on a self-consistent generalization of the classical thermodynamics to small-scale physics, where quantum effects become predominant[16–22]. In particular, a lot of attention has been devoted to the search for novel methods of precision nanothermometry that could exploit the essence of quantum correlations[23–28]. In this context, the possibility to correctly define the thermodynamical limit, and therefore the existence of the temperature in the quantum regime, has been thoroughly investigated. It has been shown that the minimal subset of an interacting quantum system, which can be described as a canonical ensemble, with the same temperature of the global system, depends not only on the strength of the correlations within the system, but also on the temperature itself[29–31]. Using a quantum information-oriented point of view, this phenomenon has also been highlighted in Gaussian fermionic and bosonic states, by exploiting quantum fidelity as the figure of merit[32,33]. Furthermore, the significant role played by quantum correlations has been recently discussed with specific attention to spin- and fermionic-lattice systems with short-range interactions[34].

In this paper, we propose a quantum-metrology approach to thermometry, through the analysis of the local sensitivity of generic quantum systems to their global temperature. Our approach does not

An explicit evaluation of the limit in equation (1) can be obtained via the Uhlmann's theorem[38] (see the 'Methods' section for details). A convenient way to express the final result can be obtained by introducing an ancillary system $\mathcal{A}'\mathcal{B}'$ isomorphic to $\mathcal{A}\mathcal{B}$ and the purification of ρ_β defined as

$$|\rho_\beta\rangle = \sum_i \frac{e^{-\beta E_i/2}}{\sqrt{\mathcal{Z}_\beta}} |E_i\rangle_{\mathcal{A}\mathcal{B}} \otimes |E_i\rangle_{\mathcal{A}'\mathcal{B}'}, \qquad (4)$$

where $H = \sum_i E_i |E_i\rangle_{\mathcal{A}\mathcal{B}}\langle E_i|$ is the spectral decomposition of the system Hamiltonian. It can then be proved that

$$\mathfrak{S}_{\mathcal{A}}[\rho_\beta] = \mathfrak{S}_{\mathcal{A}\mathcal{B}}[\rho_\beta] - \sum_{j<k} \frac{(\lambda_j - \lambda_k)^2}{\lambda_j + \lambda_k} |\langle e_j|H|e_k\rangle|^2, \qquad (5)$$

where $\{|e_j\rangle\}$ are the eigenvectors of the reduced density matrix $\mathrm{Tr}_{\mathcal{A}'}[|\rho_\beta\rangle\langle\rho_\beta|]$ living on $\mathcal{A}\mathcal{B}\mathcal{B}'$, obtained by taking the partial trace of $|\rho_\beta\rangle$ with respect to the ancillary system $\mathcal{A}'$, while $\{\lambda_j\}$ are the corresponding eigenvalues (which, by construction, coincide with the eigenvalues of $\rho_\beta^{\mathcal{A}}$).

Equation (5) makes it explicit the ordering between $\mathfrak{S}_{\mathcal{A}}[\rho_\beta]$ and $\mathfrak{S}_{\mathcal{A}\mathcal{B}}[\rho_\beta]$: the latter is always greater than the former due to the negativity of the second contribution appearing on the right hand side. Furthermore, if H does not include interaction terms (that is, $H_{\mathcal{A}\mathcal{B}}^{(\mathrm{int})}=0$), one can easily verify that $\mathfrak{S}_{\mathcal{A}}[\rho_\beta]$ reduces to the variance of the local Hamiltonian of $\mathcal{A}$, and is given by the heat capacity of the Gibbs state $e^{-\beta H_{\mathcal{A}}}/\mathcal{Z}_\beta^{\mathcal{A}}$ which, in this special case, represents $\rho_\beta^{\mathcal{A}}$, that is, $\mathfrak{S}_{\mathcal{A}}[\rho_\beta] = \mathrm{Tr}[\rho_\beta^{\mathcal{A}} H_{\mathcal{A}}^2] - \mathrm{Tr}[\rho_\beta^{\mathcal{A}} H_{\mathcal{A}}]^2 = -\frac{\partial^2}{\partial\beta^2}\ln\mathcal{Z}_\beta^{\mathcal{A}}$. Finally we observe that in the high-temperature regime ($\beta\to 0$) the expression (5) simplifies yielding

$$\mathfrak{S}_{\mathcal{A}}[\rho_\beta] = \frac{1}{d_{\mathcal{A}}}\mathrm{Tr}\left[\tilde{H}_{\mathcal{A}}^2 - 2\beta\tilde{H}_{\mathcal{A}}\frac{\mathrm{Tr}_{\mathcal{B}}[H^2]}{d_{\mathcal{B}}} + \beta\tilde{H}_{\mathcal{A}}^3\right] + \mathcal{O}(\beta^2), \qquad (6)$$

where $d_{\mathcal{A}}$ and $d_{\mathcal{B}}$ denote the Hilbert space dimensions of $\mathcal{A}$ and $\mathcal{B}$ respectively, and we defined $\tilde{H}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}[H]/d_{\mathcal{B}}$ having set, without loss of generality, $\mathrm{Tr}[H] = 0$.

A measure of state distinguishability. In the low-temperature regime, the LQTS can be used to characterize how much the ground state of the system $\mathcal{A}\mathcal{B}$ differs from the first excited subspaces when observing it locally on $\mathcal{A}$. This is a direct consequence of the fact that the QFI (which we used to define our functional) accounts for the degree of statistical distinguishability between two quantum states (in our case the reduced density matrices $\rho_\beta^{\mathcal{A}}$ and $\rho_{\beta+\varepsilon}^{\mathcal{A}}$) differing by an infinitesimal change in the investigated parameter (in our case the inverse temperature β). Therefore for $\beta\to\infty$, the LQTS can be thought as a quantifier of the local distinguishability among the lowest energy levels in which the system is frozen.

To clarify this point, let us consider the general scenario depicted in Fig. 2, where we only discuss the physics of the ground state (with energy $E_0 = 0$) and of the lowest excited levels with energy E_i bounded by twice the energy of the first excited level, $E_i \leq 2E_1$. The degeneracy of each considered energy eigenstate is denoted by n_i. From equation (5), it then follows that up to first order in the parameter $e^{-\beta E_1}$ we get

$$\mathfrak{S}_{\mathcal{A}}[\rho_\beta] = \sum_i \frac{n_i}{n_0} E_i^2 e^{-\beta E_i}(1 - \mathrm{Tr}[P_0^{\mathcal{A}}\Pi_i^{\mathcal{A}}]) + \mathcal{O}(e^{-2\beta E_1}). \qquad (7)$$

Here $\Pi_i^{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}[\Pi_i]$, where Π_i is the normalized projector on the degenerate subspace of energy E_i. Moreover, $P_0^{\mathcal{A}}$ is the span of the local subspace associated to the ground state, that is,

$P_0^{\mathcal{A}} = \sum_{j=1}^{n_0^{\mathcal{A}}} |\phi_j\rangle_{\mathcal{A}}\langle\phi_j|$ with $\Pi_0^{\mathcal{A}} = \sum_{j=1}^{n_0^{\mathcal{A}}} p_j|\phi_j\rangle_{\mathcal{A}}\langle\phi_j|$ and $n_0^{\mathcal{A}}$ being the number of non-zero eigenvalues ($p_j > 0$) of $\Pi_0^{\mathcal{A}}$.

Equation (7) can be interpreted as follows. Our capability of measuring β relies on the distinguishability between the states $\rho_\beta^{\mathcal{A}}$ and $\rho_{\beta+\varepsilon}^{\mathcal{A}}$, with $\varepsilon \ll \beta$. In the zero-temperature limit, the system lies in the ground state and locally reads as $\Pi_0^{\mathcal{A}}$, while at small temperatures, the lowest energy levels start to get populated. If their reduced projectors $\Pi_i^{\mathcal{A}}$ ($i\geq 1$) are not completely contained in the span of $\Pi_0^{\mathcal{A}}$, that is $\mathrm{Tr}[P_0^{\mathcal{A}}\Pi_i^{\mathcal{A}}] \neq 1$, there exist some local states whose population is null for $T=0$ and greater than zero at infinitesimal temperatures. Such difference implies that the first order in $\mathfrak{S}_{\mathcal{A}}$ does not vanish. On the contrary, if the reduced projectors $\Pi_i^{\mathcal{A}}$ are completely contained in the span of $\Pi_0^{\mathcal{A}}$, that is $\mathrm{Tr}[P_0^{\mathcal{A}}\Pi_i^{\mathcal{A}}]=1$, we can distinguish $\rho_\beta^{\mathcal{A}}$ from $\rho_{\beta+\varepsilon}^{\mathcal{A}}$ only thanks to infinitesimal corrections $\mathcal{O}(\exp(-2\beta E_1))$ to the finite-valued populations of the lowest energy levels (see the 'Methods' section for an explicit evaluation of the latter). In conclusion, the quantity $\mathfrak{S}_{\mathcal{A}}[\rho_{\beta\to\infty}]$ acts as a thermodynamical indicator of the degree of distinguishability between the ground-state eigenspace and the lowest energy levels in the system Hamiltonian.

LQTS and phase estimation. A rather stimulating way to interpret equation (5) comes from the observation that, in the extended scenario where we have purified $\mathcal{A}\mathcal{B}$ as in equation (4), the global variance (3) formally coincides with the QFI $\mathfrak{F}_{\mathcal{A}\mathcal{B}\mathcal{A}'\mathcal{B}'}(|\rho_\beta^{(\varphi)}\rangle)$ associated with the estimation of a phase φ which, for given β, has been imprinted into the system $\mathcal{A}\mathcal{B}\mathcal{A}'\mathcal{B}'$ by a unitary transformation $e^{-iH'\varphi/2}$, with H' being the analogous of H on the ancillary system $\mathcal{A}'\mathcal{B}'$, that is, $\mathfrak{S}_{\mathcal{A}\mathcal{B}}[\rho_\beta] = \mathfrak{F}_{\mathcal{A}\mathcal{B}\mathcal{A}'\mathcal{B}'}(|\rho_\beta^{(\varphi)}\rangle)$ where $|\rho_\beta^{(\varphi)}\rangle = e^{-iH'\varphi/2}|\rho_\beta\rangle$ (refs 4,35,39). Interestingly enough, a similar connection can be also established with the second term appearing in the right hand side of equation (5): indeed the latter coincides with the QFI $\mathfrak{F}_{\mathcal{B}\mathcal{A}'\mathcal{B}'}(|\rho_\beta^{(\varphi)}\rangle)$ that defines the Cramér–Rao bound for the estimation of the phase φ of $|\rho_\beta^{(\varphi)}\rangle$, under the constraint of having access only on the subsystem $\mathcal{B}\mathcal{A}'\mathcal{B}'$ (that is, that part of the global system which is complementary to $\mathcal{A}$). Accordingly, we can thus express the LQTS as the difference between these two QFI phase estimation terms, the global one versus the local one or, by a simple rearrangement of the various contributions, construct the following identity

$$\mathfrak{S}_{\mathcal{A}}[\rho_\beta] + \mathfrak{F}_{\mathcal{B}\mathcal{A}'\mathcal{B}'}\left(|\rho_\beta^{(\varphi)}\rangle\right) = \langle\Delta H^2\rangle_\beta \qquad (8)$$

that establishes a complementarity relation between the temperature estimation on $\mathcal{A}$ and the phase estimation on its complementary counterpart $\mathcal{B}\mathcal{A}'\mathcal{B}'$, by forcing their corresponding accuracies to sum up to the energy variance $\langle\Delta H^2\rangle_\beta$ of the global system (3).
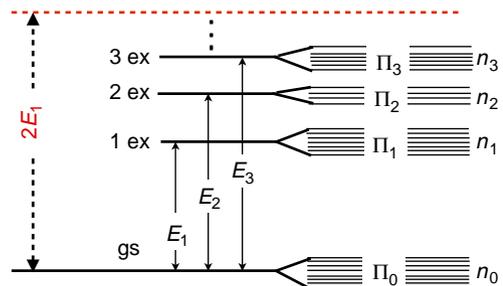
Figure 2 | Energy spectrum of a quantum system. The figure provides a schematic representation of the low-energy spectrum for a generic many-body quantum system. For simplicity the ground-state (gs) energy E_0 is set to zero. Here Π_i denotes the normalized projector on the eigenspaces of energy E_i, which can be n_i-fold degenerate.

Local thermometry in many-body systems. We have tested the behaviour of our functional on two models of quantum spin chains, with a low-energy physics characterized by the emergence of quantum phase transitions (QPTs) belonging to various universality classes[40].

Specifically, we consider the quantum spin-1/2 Ising and Heisenberg chains, in a transverse magnetic field h and with a z axis anisotropy Δ respectively,

$$H_{\text{Ising}} = -J \sum_i \left[\sigma_i^x \sigma_{i+1}^x + h \sigma_i^z \right], \tag{9}$$

$$H_{\text{XXZ}} = J \sum_i \left[\left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y \right) + \Delta \sigma_i^z \sigma_{i+1}^z \right]. \tag{10}$$

Here σ_i^α denotes the usual Pauli matrices ($\alpha = x, y, z$) on the i-th site, and periodic boundary conditions have been assumed. We set $J = 1$ as the system's energy scale. At zero temperature, the model (9) presents a $\mathbb{Z}_2$-symmetry breaking phase transition at $|h_c| = 1$ belonging to the Ising universality class. The Hamiltonian (10) has a critical behaviour for $-1 \leq \Delta \leq 1$, while it presents a ferromagnetic or antiferromagnetic ordering elsewhere. In the latter case, the system exhibits a first-order QPT in correspondence to the ferromagnetic point $\Delta_f = -1$, and a continuous QPT of the Kosterlitz–Thouless type at the antiferromagnetic point $\Delta_{af} = 1$.

Figure 3 displays the small-temperature limit of $\mathfrak{S}_{\mathcal{A}}[\rho_\beta]$ for the two models above, numerically computed by exploiting expression (21) in the 'Methods' section. We first observe that, as expected, for all the values of h and Δ, the LQTS monotonically increases with increasing the number $n_{\mathcal{A}}$ of contiguous spins belonging to the measured subsystem $\mathcal{A}$. More interestingly, we find that even when $\mathcal{A}$ reduces to two or three sites, its thermal behaviour qualitatively reproduces the same features of the global system (represented in both models by the uppermost curve). In particular, even at finite temperatures and for systems composed

of 12 sites, the LQTS is sensitive to the presence of critical regions where quantum fluctuations overwhelm thermal ones. The reminiscence of QPTs at finite temperatures has been already discussed via a quantum-metrology approach, through the analysis of the Bures metric tensor in the parameter space associated with the temperature and the external parameters[41]. The diagonal element of such tensor referring to infinitesimal variations in temperature, corresponds to the thermal susceptibility of the whole system. The latter quantity has been recently studied for the XY model[28], showing its sensitivity to critical points of Ising universality class.

In the low-temperature regime, such global sensitivity can be understood within the Landau–Zener (LZ) formalism[42]. This consists of a two-level system, whose energy gap ΔE varies with respect to an external control parameter Γ, and presents a minimum $\Delta E_{\min}$ in correspondence to some specific value Γ_c. Conversely, the global heat capacity (3) may exhibit a maximum or a local minimum at Γ_c, according to whether $\Delta E_{\min}$ is greater or lower than the value of $\Delta E^\star$ at which the expression $\mathfrak{S}_{\mathcal{AB}}[\rho_\beta] \equiv \langle \Delta H^2 \rangle_\beta$ is maximum in ΔE, respectively. Indeed it can be shown that $\langle \Delta H^2 \rangle_\beta$ for a two-level system exhibits a non-monotonic behaviour as a function of ΔE, at fixed β (see the 'Methods' section). Quite recently, an analogous mechanism has also been pointed out for the global heat capacity in the Lipkin–Meshkov–Glick model[27]. The LZ formalism represents a simplified picture of the mechanism underlying QPTs in many-body systems. However, by definition, the temperature triggers the level statistics and the equilibrium properties of physical systems. Therefore, both the heat capacity of the global system[5,6] and the LQTS of its subsystems are expected to be extremely sensitive to the presence of critical regions in the Hamiltonian parameter space.

In the Supplementary Note 1, we performed a finite-size scaling analysis of $\mathfrak{S}_{\mathcal{A}}[\rho_\beta]$ as a function of the size of the measured subsystem. For slightly interacting systems, one expects the LQTS
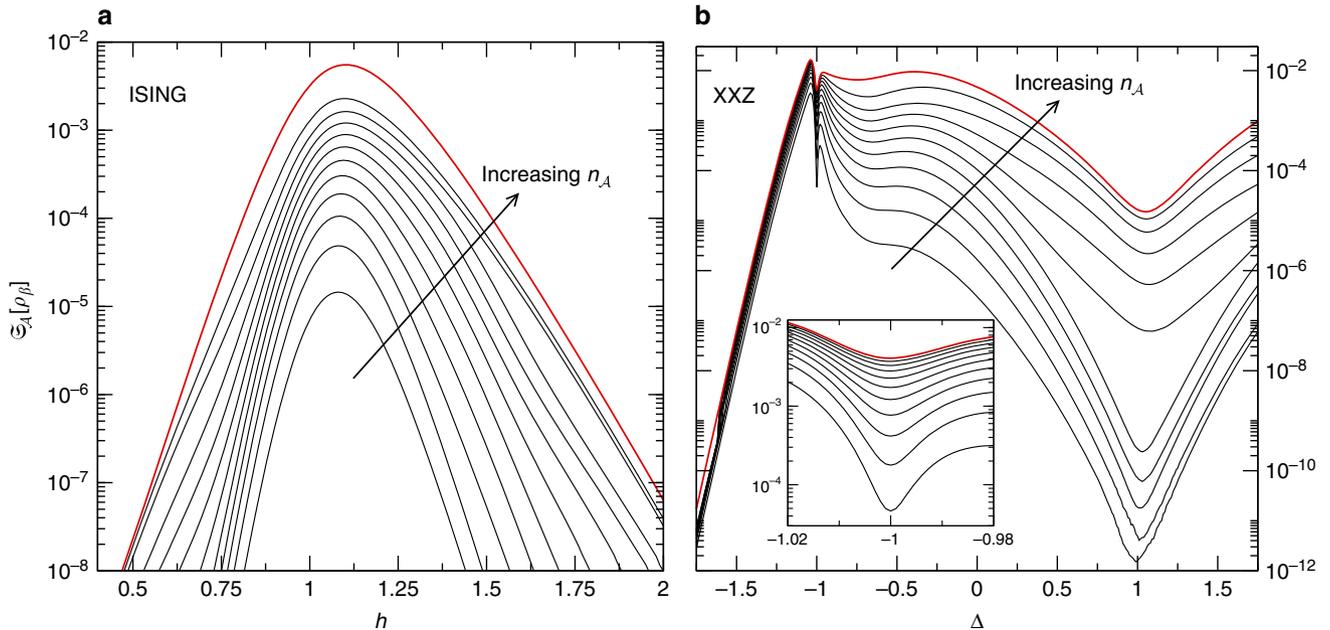
Figure 3 | The LQTS in the Ising and the Heisenberg models at low temperature. We numerically computed the LQTS of equation (1) in the low-temperature limit for a chain with $L = 12$ sites in the following two cases: (**a**) the Ising model as a function of the adimensional transverse field h; (**b**) the Heisenberg XXZ chain as a function of the anisotropy Δ. The uppermost (red) curve corresponds to the global quantum thermal susceptibility, that is the heat capacity. The other curves stand for different sizes $n_{\mathcal{A}}$ of the measured subsystem $\mathcal{A}$ of $\mathcal{AB}$ ($n_{\mathcal{A}}$ increases along the direction of the arrow). The inset in **b** magnifies the data around $\Delta = -1$. In the XXZ model, the LQTS with $n_{\mathcal{A}} = 1$ can be proved to rigorously vanish. The inverse temperature has been fixed in both cases at $\beta = 9$.

to be well approximated by the heat capacity of $\mathcal{A}$ (at least when this subsystem is large enough). The latter quantity should scale linearly with its size $n_{\mathcal{A}}$. This is indeed the case for the Ising model (9), where a direct calculation of $\langle\Delta H^2\rangle_\beta$ can be easily performed[28]. Our data for the scaling of the stationary points of $\mathfrak{S}_{\mathcal{A}}[\rho_\beta]$ close to QPTs suggest that significant deviations from a linear growth with $n_{\mathcal{A}}$ are present (see the Supplementary Fig. 1). This indicates that correlations cannot be neglected for the sizes and the systems considered here. A similar behaviour has been detected for the XXZ model, as shown in the Supplementary Fig. 2.

Discussion

We have proposed a theoretical approach to temperature locality based on quantum estimation theory. Our method deals with the construction of the local quantum thermal susceptibility, which operationally highlights the degree at which the thermal equilibrium of the global system is perceived locally, avoiding any additional hypothesis on the local structure of the system. This functional corresponds to the highest achievable accuracy up to which it is possible to recover the system temperature at thermal equilibrium via local measurements. Let us remark that, even if in principle, the Cramér–Rao bound is achievable, from a practical perspective it represents a quite demanding scenario, as it requires the precise knowledge of the Hamiltonian, the possibility to identify and perform the optimal measurements on its subsystems, and eventually a large number of copies of the system. However, in this manuscript, we have adopted a more theoretical perspective, and focused on the geometrical structure of the quantum statistical model underlying local thermalization.

In the low-temperature regime, our functional admits an interpretation as a measure of the local state distinguishability between the spaces spanned by the Hamiltonian ground state and its first energy levels. Furthermore, we established a complementarity relation between the highest achievable accuracy in the local estimation of temperature and of a global phase, by showing that the corresponding accuracies associated with complementarity subsystems sum up to heat capacity of the global system. Finally, we considered two prototypical many-body systems featuring quantum phase transitions, and studied their thermal response at low temperatures. On one hand, we found that optimal measurements on local systems provide reliable predictions on the global heat capacity. On the other hand, our functional is sensitive to the presence of critical regions, even though the total system may reduce to a dozen of components and the measured subsystem to one or two sites.

Let us remark that most of the results presented herewith do not refer to any specific choice of the interaction Hamiltonian, $H_{\mathcal{AB}}^{(\text{int})}$ between $\mathcal{A}$ and $\mathcal{B}$. As an interesting implementation of our scheme, we foresee the case of non-thermalizing interactions[43,44], whose potentialities for precision thermometry have been already unveiled.

We conclude by noticing that, while in this article we focused on temperature, the presented approach can be extended to other thermodynamic variables (like entropy, pressure, chemical potential and so on), or functionals[45]. In the latter case, quantum-estimation-based strategies, not explicitly referred to a specific quantum observable, but rather bearing the geometrical traits of the Hilbert space associated to the explored systems, may provide an effective route.

Methods

Derivation of useful analytical expressions for the LQTS. Let us recall the definition of the LQTS for a given subsystem $\mathcal{A}$ of a global system $\mathcal{AB}$ at thermal equilibrium:

$$\mathfrak{S}_{\mathcal{A}}\big[\rho_\beta\big] = 8\lim_{\varepsilon\to 0}\frac{1-\mathcal{F}\big(\rho_\beta^{\mathcal{A}},\rho_{\beta+\varepsilon}^{\mathcal{A}}\big)}{\varepsilon^2} \tag{11}$$

where $\mathcal{F}(\rho,\sigma)=\text{Tr}\big[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\big]$ is the fidelity between two generic quantum states ρ and σ. According to the Uhlmann's theorem[38], we can compute $\mathcal{F}$ as

$$\mathcal{F}\big(\rho_\beta^{\mathcal{A}},\rho_{\beta+\varepsilon}^{\mathcal{A}}\big) = \max_{|\rho_\beta^{\mathcal{A}}\rangle,|\rho_{\beta+\varepsilon}^{\mathcal{A}}\rangle}\big|\big\langle\rho_\beta^{\mathcal{A}}\big|\rho_{\beta+\varepsilon}^{\mathcal{A}}\big\rangle\big|, \tag{12}$$

where the maximization involves all the possible purifications $|\rho_\beta^{\mathcal{A}}\rangle$ and $|\rho_{\beta+\varepsilon}^{\mathcal{A}}\rangle$ of $\rho_\beta^{\mathcal{A}}$ and $\rho_{\beta+\varepsilon}^{\mathcal{A}}$, respectively through an ancillary system a. A convenient choice is to set $a=\mathcal{BA}'\mathcal{B}'$, with $\mathcal{A}'\mathcal{B}'$ isomorphic to $\mathcal{AB}$. We then observe that, by construction, the vector $|\rho_\beta\rangle$ of equation (4), besides being a purification of ρ_β, is also a particular purification of $\rho_\beta^{\mathcal{A}}$. We can now express the most generic purification of the latter as

$$\big|\rho_\beta^{\mathcal{A}}\big\rangle = (\mathbb{1}_{\mathcal{A}}\otimes V)|\rho_\beta\rangle = (\mathbb{1}_{\mathcal{A}}\otimes V)\frac{e^{-\beta H/2}}{\sqrt{\mathcal{Z}_\beta}}|\mathbb{1}_{\mathbb{E}}\rangle, \tag{13}$$

where V belongs to the set of unitary transformations on a, where $\mathbb{1}_{\mathcal{X}}$ represents the identity operator on a given system $\mathcal{X}$, and where in the last equality we introduced the vector $|\mathbb{1}_{\mathbb{E}}\rangle = \sum_i|E_i\rangle_{\mathcal{AB}}|E_i\rangle_{\mathcal{A}'\mathcal{B}'}$, $|E_i\rangle_{\mathcal{AB}}$ being the eigenvectors of H. We can thus write the fidelity (12) as

$$\mathcal{F} = \sqrt{\frac{\mathcal{Z}_\beta}{\mathcal{Z}_{\beta+\varepsilon}}}\max_V\big|\big\langle\rho_\beta\big|\big[(\mathbb{1}_A\otimes V)\big(e^{-\varepsilon H/2}\otimes\mathbb{1}_{\mathcal{A}'\mathcal{B}'}\big)\big]\big|\rho_\beta\big\rangle\big|. \tag{14}$$

Since we are interested in the small-ε limit, without loss of generality we set $V=\exp(i\,\varepsilon\,\Omega)$, with Ω being an Hermitian operator on the ancillary system a. It comes out that, up to corrections of order $\mathcal{O}(\varepsilon^3)$, the LQTS reads

$$\mathfrak{S}_{\mathcal{A}}[\rho_\beta] = \mathfrak{S}_{\mathcal{AB}}\big[\rho_\beta\big] + 4\min_{\Omega}\Big\{\text{Tr}\big[\rho_\beta^a\Omega^2\big] - \text{Tr}\big[\rho_\beta^a\Omega\big]^2 \\ + \frac{i}{2}\big\langle\rho_\beta\big|[\Omega,H]\big|\rho_\beta\big\rangle\Big\}, \tag{15}$$

where we have defined $\rho_\beta^a = \text{Tr}_{\mathcal{A}}\big[|\rho_\beta\rangle\langle\rho_\beta|\big]$. By differentiating the trace with respect to Ω, we determine the minimization condition for it, yielding

$$(\Omega-\omega)\rho_\beta^a + \rho_\beta^a(\Omega-\omega) = Q, \tag{16}$$

with $\omega=\text{Tr}[\rho_\beta^a\Omega]$ and $Q = -\frac{i}{2}[H',\rho_\beta^a]$, H' being the analogous of H which acts on $\mathcal{A}'\mathcal{B}'$ (by construction $H\,|\rho_\beta\rangle = H'|\rho_\beta\rangle$). Equation (16) explicitly implies that Ω does not depend on ω, which, without loss of generality, can be set to zero. Moreover, it enables to rewrite the LQTS in equation (15) as

$$\mathfrak{S}_{\mathcal{A}}\big[\rho_\beta\big] = \mathfrak{S}_{\mathcal{AB}}\big[\rho_\beta\big] - 4\,\text{Tr}\big[\rho_\beta^a\Omega^2\big]. \tag{17}$$

The solution of the operatorial equation (16) can be found by applying Lemma 1 presented at the end of this section, yielding

$$\begin{aligned}\Omega = &\;\Omega_0 + \frac{i}{2}\big(PH'R - RH'P\big) \\ &+ \frac{i}{2}\Big[\sum_{n=1}^{+\infty}(-1)^n\Big(P\rho_\beta^{a\,\ominus n}H'\rho_\beta^{a\,n} - h.c.\Big)\Big],\end{aligned} \tag{18}$$

with Ω_0 being an operator which anti-commutes with Ω, $\rho_\beta^{a\,\ominus n}$ being the Moore–Penrose pseudoinverse of ρ_β^a to the power n, R being the projector on kernel of ρ_β^a, $P=\mathbb{1}_a - R$ being its complementary counterpart, and with $h.c.$ denoting the hermitian conjugate term. By substituting this expression in equation (17), we finally get

$$\mathfrak{S}_{\mathcal{A}}\big[\rho_\beta\big] = 2\sum_{j,k}\frac{\lambda_j\lambda_k}{\lambda_j+\lambda_k}\big|\langle e_j|H'|e_k\rangle\big|^2 - \text{Tr}\big[\rho_\beta H\big]^2 \tag{19}$$

where $\rho_\beta^a = \sum_i\lambda_i|e_i\rangle\langle e_i|$ is the spectral decomposition of ρ_β^a, sharing the same spectrum with $\rho_\beta^{\mathcal{A}}$. The expression above holds for both invertible and not invertible ρ_β^a. To the latter scenario belongs the case in which $H = H_{\mathcal{A}} + H_{\mathcal{B}}$, where one can easily prove that the LQTS reduces to the variance of the local Hamiltonian $H_{\mathcal{A}}$, that is, $\mathfrak{S}_{\mathcal{A}} = \text{Tr}[\rho_\beta H_{\mathcal{A}}^2] - \text{Tr}[\rho_\beta H_{\mathcal{A}}]^2$ (notice that the non-zero eigenvalues of ρ_β^a are $\lambda_i = e^{-\beta E_i^A}/\mathcal{Z}_\beta^{\mathcal{A}}$ which correspond to $|e_i\rangle = |E_i^A\rangle\otimes|\rho_\beta^{\mathcal{B}}\rangle$, being $H_{\mathcal{A}} = \sum_i E_i^A|E_i^A\rangle\langle E_i^A|$, $\mathcal{Z}_\beta^{\mathcal{A}} = \text{Tr}[e^{-\beta H_{\mathcal{A}}}]$ and $|\rho_\beta^{\mathcal{B}}\rangle$ the purification of $\rho_\beta^{\mathcal{B}}$ through the ancillary system $\mathcal{B}'$). The expression above can also be rewritten as

$$\mathfrak{S}_{\mathcal{A}}\big[\rho_\beta\big] = \mathfrak{S}_{\mathcal{AB}}\big[\rho_\beta\big] - \sum_{j<k}\frac{(\lambda_j-\lambda_k)^2}{\lambda_j+\lambda_k}\big|\langle e_j|H'|e_k\rangle\big|^2 \tag{20}$$

which can be cast into equation (5) by simply exploiting the fact that the system is symmetric with respect to the exchange of $\mathcal{AB}$ with $\mathcal{A}'\mathcal{B}'$.

It is finally useful to observe that LQTS can be also expressed in terms of the eigenvectors of $\mathcal{A}$, $\rho_\beta^{\mathcal{A}} = \sum_i\lambda_i|g_i\rangle\langle g_i|$ as:

$$\mathfrak{S}_{\mathcal{A}}\big[\rho_\beta\big] = 2\sum_{j,k}\frac{\big|\text{Tr}\big[\rho_\beta H|g_j\rangle\langle g_k|\big]\big|^2}{\lambda_j+\lambda_k} - \text{Tr}\big[\rho_\beta H\big]^2, \tag{21}$$

where we have used the Schmidt decomposition of $|\rho_\beta\rangle$, with respect to bipartition $\mathcal{A}a$,

$$|\rho_\beta\rangle = \sum_i\sqrt{\lambda_i}|g_i\rangle|e_i\rangle. \tag{22}$$

In particular, expression (21) can be exploited to numerically compute the LQTS, for instance when dealing with quantum many-body systems (see Fig. 3 and the discussion in the Supplementary Note 1).

Lemma 1: For any assigned operators X, Y satisfying the equation

$$XW + WX = Y, \tag{23}$$

the following solution holds

$$\begin{aligned} W &= W_0 + X^{\ominus 1}YR + RYX^{\ominus 1} \\ &+ \sum_{n=0}^{+\infty}(-1)^n X^n PY\left(X^{\ominus(n+1)} - R\right), \end{aligned} \tag{24}$$

where $X^{\ominus 1}$ is the Moore Penrose pseudoinverse of X, R is the projector on kernel of X, $P = \mathbb{1} - R$ ($\mathbb{1}$ indicates the identity matrix) and W_0 is a generic operator which anti-commutes with Y (see also ref. 46). Furthermore if X and Y are Hermitian, equation (23) admits solutions which are Hermitian too: the latter can be expressed as

$$\begin{aligned} W &= W_0 + X^{\ominus 1}YR + RYX^{\ominus 1} \\ &+ \frac{1}{2}\left[\sum_{n=0}^{+\infty}(-1)^n X^n PY\left(X^{\ominus(n+1)} - R\right) + h.c.\right], \end{aligned} \tag{25}$$

where now W_0 is an arbitrary Hermitian operator which anti-commutes with Y.

Proof: Since (23) is a linear equation, a generic solution can be expressed as the sum of a particular solution plus a solution W_0 of the associated homogeneous
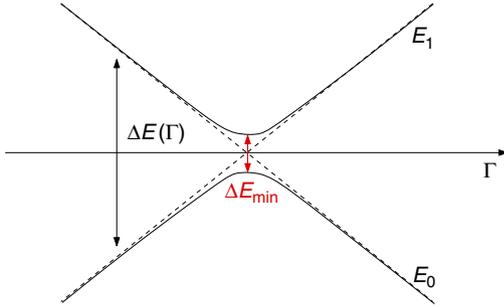
Figure 4 | The two-level Landau–Zener model. A sketch of the behaviour of the two eigenenergies (E_1, E_2) as a function of some control parameter Γ. The gap $\Delta E = E_2 - E_1$ displays a pronounced minimum in correspondence of a given Γ_c value.
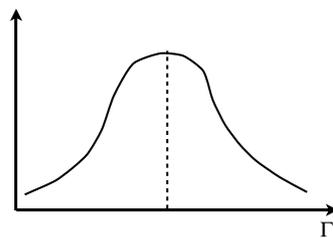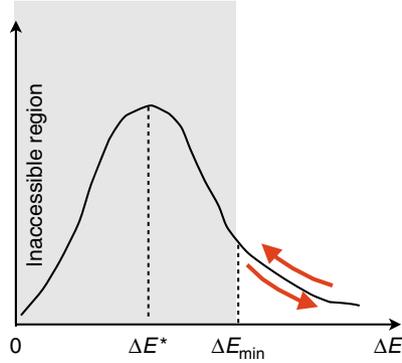
equation, that is, an operator which anti-commute with X,

$$XW_0 + W_0 X = 0. \tag{26}$$

A particular solution W of equation (23) can be always decomposed as

$$W = RWR + RWP + PWR + PWP. \tag{27}$$

Notice that by definition, $RX = XR = O$, where O identifies the null operator. Multiplying (23) on both sides by R, one gets the condition $RYR = O$. The operator W, solution of equation (23), is defined up to its projection on the kernel subspace, that is

$$W' = W + RWR \Rightarrow XW' + W'X = Y. \tag{28}$$

Therefore, without loss of generality we can set

$$RWR = O. \tag{29}$$

Multiplying equation (23) by $X^{\ominus 1}$ on the right side and repeating the same operation on the left side, we get:

$$RWP = RYX^{\ominus 1}, \tag{30}$$

$$PWR = X^{\ominus 1}YR. \tag{31}$$

On the other hand, PWP satisfies the relation

$$PWP = PYX^{\ominus 1} - PYR - X(PWP)X^{\ominus 1}. \tag{32}$$

This equation can be solved recursively in PWP and gives

$$PWP = \sum_{n=0}^{\infty}(-1)^n X^n PY\left(X^{\ominus(1+n)} - R\right), \tag{33}$$

thus concluding the first part of the proof. The second part of the proof follows simply by observing that, if X and Y are Hermitian, and if W solves equation (23), then also its adjoint counterpart does. Therefore, for each solution W of the problem, we can construct an Hermitian one by simply taking $(W + W^\dagger)/2$.

Second-order term corrections to LQTS. In the low-temperature regime ($\beta \to \infty$), we have computed the second-order correction term to the LQTS, that is of $\mathfrak{S}_A[\rho_\beta]$ in equation (1), and found:

$$\begin{aligned} &\left(\frac{E_1 n_1}{n_0}\right)^2 e^{-2\beta E_1}\Big\{ -2 + \mathrm{Tr}\big[P_0^A \Pi_1^A + \Pi_1^A \Pi_0^{A\ominus 1}\Pi_1^A\big(1 + P_0^A\big)\big] \\ &- 2\sum_{n=0}^{+\infty}(-1)^n \mathrm{Tr}\Big[\Pi_1^A \Pi_0^{A\ominus(n+2)}\Pi_1^A \Pi_0^{An+1}\Big]\Big\}, \end{aligned}$$

with $E_k \geq E_1$ and where the series in n is meant to converge to $1/2$ when
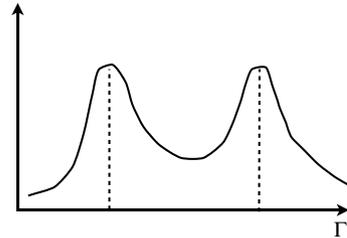
$\text{Tr}[\Pi_1^{\mathcal{A}}\Pi_0^{\mathcal{A} \ominus (n+2)}\Pi_1^{\mathcal{A}}\Pi_0^{\mathcal{A}n+1}]=1$, that is, $\sum_{n=0}^{+\infty}(-1)^n \equiv \lim_{x \to -1} \sum_{n=0}^{+\infty} x^n = \frac{1}{2}$. To vanish, this second-order correction term requires a stronger condition with respect to one necessary to nullify the first-order term in the LQTS, equation (7). It is given by $\Pi_1^{\mathcal{A}}=\Pi_0^{\mathcal{A}}$, and corresponds to the requirement that the system ground state must be locally indistinguishable from the first excited level.

Heat capacity in the two-level LZ scheme. Here we discuss the simplified case in which only the ground state (with energy E_0) and the first excited level (with energy E_1) of the global system Hamiltonian H play a role. In particular, we are interested in addressing a situation where the ground-state energy gap $\Delta E \equiv E_1 - E_0$ may become very small, as a function of some external control parameter Γ (for example, the magnetic field or the system anisotropy). A sketch is depicted in Fig. 4, and refers to the so-called LZ model[42]. This resembles the usual scenario when a given many-body system is adiabatically driven, at zero temperature, across a quantum phase transition point.

In correspondence of some critical value Γ_c, the gap is minimum. For a typical quantum many-body system, such minimum value ΔE_{min} tends to close at the thermodynamic limit and a quantum phase transition occurs (notice that Γ_c may depend on the system size). Hereafter, without loss of generality, we will assume $E_0 = 0$ and take $E_1 = \Delta E$ so that the system heat capacity (3) reduces to:

$$\mathfrak{S}_{\mathcal{AB}}[\rho_\beta] = \frac{n_1(\Delta E)^2 e^{-\beta\Delta E}}{n_0 + n_1 e^{-\beta\Delta E}} - \left(\frac{n_1 \Delta E e^{-\beta\Delta E}}{n_0 + n_1 e^{-\beta\Delta E}}\right)^2. \quad (34)$$

Here n_0 and n_1 are the degeneracy indexes associated to the levels E_0 and E_1, respectively. Notice that $\mathfrak{S}_{\mathcal{AB}}[\rho_\beta]$ is always non-negative and exhibits a non-monotonic behaviour as a function of ΔE, at fixed β. Indeed it is immediate to see that $\mathfrak{S}_{\mathcal{AB}}[\rho_\beta] \to 0$ in both limits $\Delta E \to 0$ and $\Delta E \to +\infty$. For fixed β, n_0 and n_1, the heat capacity displays a maximum in correspondence of the solution of the transcendental equation

$$\frac{\partial \mathfrak{S}_{\mathcal{AB}}[\rho_\beta]}{\partial \Delta E} = 0 \Longleftrightarrow e^{\beta\Delta E} = \frac{n_1}{n_0}\frac{(2+\beta\Delta E)}{(\beta\Delta E - 2)}. \quad (35)$$

In particular, for $n_0 = n_1 = 1$, the latter relation is fulfilled for $\Delta E^* \approx 2.3994/\beta$, while for $n_0 = 2$, $n_1 = 1$, it is fulfilled for $\Delta E^* \approx 2.2278/\beta$.

It turns out that the behaviour of the heat capacity as a function of increasing Γ in a two-level LZ scheme depends on the relative sizes of ΔE^* and ΔE_{min}, as pictorially shown in Fig. 5: (a) if $\Delta E_{min} > \Delta E^*$, then $\mathfrak{S}_{\mathcal{AB}}[\rho_\beta]$ will exhibit a maximum in correspondence of Γ_c; (b) if $\Delta E_{min} < \Delta E^*$, a maximum at Γ_1^* corresponding to $\Delta E = \Delta E^*$ will appear, followed by a local minimum at Γ_c and eventually by another maximum at Γ_2^* where the former condition occurs again. Since ΔE^* is a function of β, and ΔE_{min} depends on the system size, the point of minimum gap can be signalled by a maximum or by a local minimum depending on the way the two limits $L \to +\infty$ (thermodynamic limit) and $\beta \to +\infty$ (zero-temperature limit) are performed. In the Supplementary Note 2, we explicitly address the two many-body Hamiltonians considered in the last subsection of the 'Results' section, namely the Ising and the XXZ model (see the Supplementary Figs 3 and 4). Here in particular, we discussed the possible emergence of corrections to the low-temperature energy variance (34) when one takes into account the presence of the low-lying energy levels beyond the first excited one.

Data availability. The data that support the findings of this study are available from the corresponding author upon request.

References

1. Giazotto, F., Heikkilä, T. T., Luukanen, A., Savin, A. M. & Pekola, J. P. Opportunities for mesoscopics in thermometry and refrigeration: Physics and applications. *Rev. Mod. Phys.* **78,** 217–274 (2006).
2. Cramér, H. *Mathematical Methods of Statistics* (Princeton Univ. Press, 1946).
3. Paris, M. G. A. & Řeháček, J. *Quantum State Estimation*. Lecture Notes in Physics vol. 649 (Springer, 2004).
4. Paris, M. G. A. Quantum estimation for quantum technology. *Int. J. Quant. Inf.* **7,** 125–137 (2009).
5. Zanardi, P., Giorda, P. & Cozzini, M. Information-theoretic differential geometry of quantum phase transitions. *Phys. Rev. Lett.* **99,** 100603 (2007).
6. Zanardi, P., Paris, M. G. A. & Campos Venuti, L. Quantum criticality as a resource for quantum estimation. *Phys. Rev. A* **78,** 042105 (2008).
7. Gao, Y. & Bando, Y. Nanotechnology: carbon nanothermometer containing gallium. *Nature* **415,** 599 (2002).
8. Weld, D. M. et al. Spin gradient thermometry for ultracold atoms in optical lattices. *Phys. Rev. Lett.* **103,** 245301 (2009).
9. Neumann, P. et al. High-precision nanoscale temperature sensing using single defects in diamond. *Nano Lett.* **13,** 2738–2742 (2013).
10. Kucsko, G. et al. Nanometre-scale thermometry in a living cell. *Nature* **500,** 54–58 (2013).
11. Haupt, F., Imamoglu, A. & Kroner, M. Single quantum dot as an optical thermometer for Millikelvin temperatures. *Phys. Rev. Appl.* **2,** 024001 (2014).
12. Seilmeier, F. et al. Optical thermometry of an electron reservoir coupled to a single quantum dot in the Millikelvin range. *Phys. Rev. Appl.* **2,** 024002 (2014).
13. Huang, K. *Statistical Mechanics* 2nd edition (Wiley, 1987).
14. Hill, T. L. *Thermodynamics of Small Systems* (Dover, 1994).
15. Hill, T. L. A different approach to nanothermodynamics. *Nano Lett.* **1,** 273–275 (2001).
16. Gemmer, J., Michel, M. & Mahler, G. *Quantum Thermodynamics*. Lecture Notes in Physics vol. 657 (Springer, 2004).
17. Allahverdyan, A. E. & Nieuwenhuizen, Th. M. Extraction of work from a single thermal bath in the quantum regime. *Phys. Rev. Lett.* **85,** 1799–1802 (2000).
18. Allahverdyan, A. E. & Nieuwenhuizen, Th. M. Testing the violation of the Clausius inequality in nanoscale electric circuits. *Phys. Rev. B* **66,** 115309 (2002).
19. Nieuwenhuizen, Th. M. & Allahverdyan, A. E. Statistical thermodynamics of quantum Brownian motion: construction of perpetuum mobile of the second kind. *Phys. Rev. E* **66,** 036102 (2002).
20. Hilt, S. & Lutz, E. System-bath entanglement in quantum thermodynamics. *Phys. Rev. A* **79,** 010101 (R) (2009).
21. Williams, N. S., Le Hur, K. & Jordan, A. N. Effective thermodynamics of strongly coupled qubits. *J. Phys. A: Math. Theor* **44,** 385003 (2011).
22. Horodecki, M. & Oppenheim, J. Fundamental limitations for quantum and nanoscale thermodynamics. *Nat. Commun* **4,** 2059 (2013).
23. Brunelli, M., Olivares, S. & Paris, M. G. A. Qubit thermometry for micromechanical resonators. *Phys. Rev. A* **84,** 032105 (2011).
24. Brunelli, M., Olivares, S., Paternostro, M. & Paris, M. G. A. Qubit-assisted thermometry of a quantum harmonic oscillator. *Phys. Rev. A* **86,** 012125 (2012).
25. Marzolino, U. & Braun, D. Precision measurements of temperature and chemical potential of quantum gases. *Phys. Rev. A* **88,** 063609 (2013).
26. Correa, L. A., Mehboudi, M., Adesso, G. & Sanpera, A. Individual quantum probes for optimal thermometry. *Phys. Rev. Lett.* **114,** 220405 (2015).
27. Salvatori, G., Mandarino, A. & Paris, M. G. A. Quantum metrology in Lipkin-Meshkov-Glick critical systems. *Phys. Rev. A* **90,** 022111 (2014).
28. Mehboudi, M., Moreno-Cardoner, M., De Chiara, G. & Sanpera, A. Thermometry precision in strongly correlated ultracold lattice gases. *New J. Phys.* **17,** 055020 (2015).
29. Hartmann, M., Mahler, G. & Hess, O. Existence of temperature on the nanoscale. *Phys. Rev. Lett.* **93,** 080402 (2004).
30. Hartmann, M., Mahler, G. & Hess, O. Local versus global thermal states: correlations and the existence of local temperatures. *Phys. Rev. E* **70,** 066148 (2004).
31. Hartmann, M. & Mahler, G. Measurable consequences of the local breakdown of the concept of temperature. *Europhys. Lett.* **70,** 579–585 (2005).
32. García-Saez, A., Ferraro, A. & Acín, A. Local temperature in quantum thermal states. *Phys.Rev. A* **79,** 052340 (2009).
33. Ferraro, A., García-Saez, A. & Acín, A. Intensive temperature and quantum correlations for refined quantum measurements. *Europhys. Lett.* **98,** 10009 (2012).
34. Kliesch, M., Gogolin, C., Kastoryano, M. J., Riera, A. & Eisert, J. Locality of temperature. *Phys. Rev. X* **4,** 031019 (2014).
35. Giovannetti, V., Lloyd, S. & Maccone, L. Advances in quantum metrology. *Nat. Photon.* **5,** 222–229 (2011).
36. Peres, A. Stability of quantum motion in chaotic and regular systems. *Phys. Rev. A* **30,** 1610–1615 (1984).
37. Jozsa, R. Fidelity for mixed quantum states. *J. Mod. Opt.* **41,** 2315–2323 (1994).
38. Uhlmann, A. The 'transition probability' in the state space of a *-algebra. *Rep. Math. Phys.* **9,** 273–279 (1976).
39. Braunstein, S. L. & Caves, C. M. Statistical distance and the geometry of quantum states. *Phys. Rev. Lett.* **72,** 3439–3443 (1994).
40. Sachdev, S. *Quantum Phase Transitions* (Cambridge Univ. Press, 1999).
41. Zanardi, P., Campos Venuti, L. & Giorda, P. Bures metric over thermal state manifolds and quantum criticality. *Phys. Rev. A* **76,** 062318 (2007).
42. Zener, C. Non-adiabatic crossing of energy levels. *Proc. R. Soc. A* **137,** 696–702 (1932).
43. Stace, T. M. Quantum limits of thermometry. *Phys. Rev. A* **82,** 011611 (R) (2010).
44. Jarzyna, M. & Zwierz, M. Quantum interferometric measurements of temperature. *Phys. Rev. A* **92,** 032112 (2015).
45. Campisi, M., Hänggi, P. & Talkner, P. Colloquium: quantum fluctuation relations—foundations and applications. *Rev. Mod. Phys.* **83,** 771–791 (2011).
46. Bhatia, R. *Matrix Analysis* (Springer, 1997).

Acknowledgements

Author contributions

Additional information

Supplementary Information accompanies this paper at http://www.nature.com/naturecommunications

Competing financial interests: The authors declare no competing financial interests.

Reprints and permission information is available online at http://npg.nature.com/reprintsandpermissions/

How to cite this article: De Pasquale, A. *et al.* Local quantum thermal susceptibility. *Nat. Commun.* 7:12782 doi: 10.1038/ncomms12782 (2016).