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PAPER

Conditional quantum thermometry—enhancing precision by measuring less

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Abstract

Taking accurate measurements of the temperature of quantum systems is a challenging task. The mathematical peculiarities of quantum information make it virtually impossible to measure with infinite precision. In the present paper, we introduce a generalize thermal state, which is conditioned on the pointer states of the available measurement apparatus. We show that this conditional thermal state outperforms the Gibbs state in quantum thermometry. The origin for the enhanced precision can be sought in its asymmetry quantified by the Wigner–Yanase–Dyson skew information. This additional resource is further clarified in a fully resource-theoretic analysis, and we show that there is a Gibbs-preserving map to convert a target state into the conditional thermal state. We relate the quantum J-divergence between the conditional thermal state and the same target state to quantum heat.

1. Introduction

Quantum metrology is a task to utilize the peculiar properties of quantum systems, such as quantum coherence and entanglement, to achieve parameter estimation at precision beyond the classical limit [1–4]. Hence, the quest to identify quantum states that are uniquely suited for metrological tasks with limited resources [5, 6] is of crucial practical relevance. In the following, we address this issue and impose the plausible and realistic condition that only the observable *eigenstates* of the measurement apparatus, aka pointer states [7–11] are available.

One of the most prominent metrological tasks is quantum thermometry of stationary states. In fact, quantum thermometry with Gibbs states has been well studied [12–20]. In this simplest scenario it is easy to see that the optimal measurement for estimating the inverse temperature β is the Hamiltonian. However, when the system size is very large and supports quantum correlations, even energy measurements are a challenging task [14, 15]. Therefore, it is desirable to find *better* states whose corresponding optimal measurements are experimentally implementable, and which ideally even outperform Gibbs states in the low-temperature limit [21–23].

In this paper, we discuss a quantum state, that indeed fulfills the aforementioned 'wishlist'. The *conditional thermal state* (CTS) is constructed as Gibbsian-distributed quantum state of the pointer basis corresponding to the available measurement apparatus. The CTS originally appeared in the one-time measurement approach to quantum work [24–29] and correspondingly tighter maximum work theorems. In the following, we demonstrate that the CTS outperforms the Gibbs state in quantum thermometry. To elucidate its properties further we then show that it can be understood as a non-passive state with useful resources [30–34]. To this end, we first relate its asymmetry, which is quantified by the Wigner–Yanase–Dyson (WYD) skew information [35–40], to its QFI. Then, focusing on a system undergoing unitary evolution, we discuss the state convertibility between the exact final state and the CTS constructed by the pointer states given by the evolved post-measurement state. Finally, we demonstrate that their symmetric

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divergence, also known as quantum J-divergence, can be interpreted as quantum heat [41]. Our results demonstrate the usefulness of the CTS as a resource state from both fundamental and practical perspectives.

2. Conditional thermal state

We begin by establishing notions and notations. For the ease of the presentation, and to avoid clutter in the formulas, we work in units for which the Boltzmann constant k_{B} and the reduced Planck constant $\hbar$ are $k_{\mathrm{B}} = \hbar = 1$.

The concept of the CTS is illustrated in figure 1. In a d-dimensional Hilbert space $\mathcal{H}$, given a Hamiltonian H and the pointer states $\{|\psi_k\rangle\}_{k=1}^{d}$ of an implementable measurement M, the CTS is defined as

$$\rho_\beta \equiv \sum_{k=1}^{d} \frac{e^{-\beta\langle\psi_k|H|\psi_k\rangle}}{Z_\beta} |\psi_k\rangle\langle\psi_k| \,. \tag{1}$$

Here, Z_β is the normalization factor

$$Z_\beta \equiv \sum_{k=1}^{d} e^{-\beta\langle\psi_k|H|\psi_k\rangle} \,, \tag{2}$$

which can be interpreted as a generalized partition function [24–28]. The CTS is defined as the thermal state conditioned on the choice of the measurement implementable in the laboratory. The CTS maximizes the von Neumann entropy [42] under the constraint that the ensemble average of the Hamiltonian is fixed (see appendix A). Note that when $\{|\psi_k\rangle\}_{k=1}^{d}$ are the pointer states of H, ρ_β becomes the Gibbs state $\rho_\beta^{\mathrm{eq}} \equiv e^{-\beta H}/Z_\beta^{\mathrm{eq}}$, where $Z_\beta^{\mathrm{eq}} \equiv \mathrm{tr}\left\{e^{-\beta H}\right\}$ is the standard canonical partition function. Therefore, the CTS can be regarded as a generalized thermal state.

For later convenience, we also define the following conditional thermal separable state in a composite Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$

$$\widetilde{\rho}_\beta \equiv \sum_{k=1}^{d} \frac{e^{-\beta\langle\psi_k|H|\psi_k\rangle}}{Z_\beta} |\psi_k\rangle\langle\psi_k|_1 \otimes |\phi_k\rangle\langle\phi_k|_2 \,, \tag{3}$$

where $\{|\phi_k\rangle\}_{k=1}^{d}$ are the arbitrary orthogonal eigenstates of $\mathcal{H}_2$. From these definitions, we also have $\rho_\beta = \mathrm{tr}_2\{\widetilde{\rho}_\beta\}$, which will become important in our discussion of the relation between the quantum Fisher information (QFI) for quantum thermometry and the asymmetry measure of ρ_β.

3. Quantum thermometry

3.1. Quantum Fisher information

An important figure of merit in quantum metrology is the QFI. Given a quantum state ρ_θ parameterized by a certain parameter $\theta \in \mathbb{R}$, the variance of an unbiased estimator $(\delta\theta)^2$ is bounded by the quantum Cramér–Rao bound (QCRB), $(\delta\theta)^2 \geqslant 1/\mathcal{I}(\rho_\theta;\theta)$, where $\mathcal{I}(\rho_\theta;\theta)$ is the QFI defined by $\mathcal{I}(\rho_\theta;\theta) \equiv -2\lim_{\epsilon\to 0}\partial_\epsilon^2 \mathcal{F}(\rho_\theta,\rho_{\theta+\epsilon})$ [43–48]. The definition stems from the relation between the Bures distance and the symmetric logarithmic derivative. Thus, the QFI can be obtained by optimizing the classical Fisher information over all possible measurements, as detailed in [45]. Here, $\mathcal{F}(\rho,\sigma) \equiv ||\sqrt{\rho}\sqrt{\sigma}||_1^2$ is the quantum fidelity between two quantum states ρ and σ [49], and $||A||_1 \equiv \mathrm{tr}\{\sqrt{A^\dagger A}\}$ is the trace norm. We denote $\partial^m/\partial x^m$ simply by ∂_x^m.

3.2. Quantum thermometry with the CTS

For our present purposes we now analyze the precision, with which the inverse temperature β can be estimated from the CTS. This will also allow us to relate the QFI of the CTS to the WYD skew information $I_\alpha(\rho_\beta, H)$ contained by ρ_β with respect to the Hamiltonian H, which quantifies the asymmetry of ρ_β.

The QFI $\mathcal{I}(\rho_\beta;\beta)$ of the CTS ρ_β is given by (see appendix B for the proof.)

$$\mathcal{I}(\rho_\beta;\beta) = \partial_\beta^2 \ln Z_\beta \,, \tag{4}$$

and the optimal measurement achieving the quantum Cramér–Rao bound is

$$G = \sum_{k=1}^{d} \langle\psi_k|H|\psi_k\rangle |\psi_k\rangle\langle\psi_k| \,. \tag{5}$$

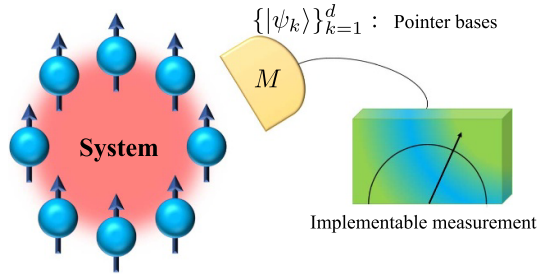

Figure 1. Illustration of the concept: The *conditional thermal state* (CTS) describes state of a thermal quantum system conditioned on the measurable pointer basis $\{|\psi_k\rangle\}_{k=1}^d$ of an implementable measurement M. The CTS maximizes the von Neumann entropy under the constraint that the ensemble average of the Hamiltonian is fixed.

To compare the sensitivity of the CTS ρ_β and the Gibbs state ρ_β^{eq}, we define the QFI difference as $\Delta\mathcal{I}_\beta \equiv \mathcal{I}(\rho_\beta;\beta) - \mathcal{I}(\rho_\beta^{\mathrm{eq}};\beta)$. We have

$$\Delta\mathcal{I}_\beta = -\partial_\beta^2 S\left(\rho_\beta || \rho_\beta^{\mathrm{eq}}\right) = \partial_\beta^2\left(\ln\frac{Z_\beta}{Z_\beta^{\mathrm{eq}}}\right), \tag{6}$$

where $S(\rho_\beta||\rho_\beta^{\mathrm{eq}}) \equiv \mathrm{tr}\{\rho_\beta \ln\rho_\beta\} - \mathrm{tr}\left\{\rho_\beta \ln\rho_\beta^{\mathrm{eq}}\right\}$ denotes the quantum relative entropy [50] of ρ_β with respect to ρ_β^{eq}. The relative entropy measures the distinguishability of ρ_β and ρ_β^{eq}. Therefore, the condition that the CTS outperforms the Gibbs state in quantum thermometry at a certain temperature β_0 is

$$\partial_\beta^2 S\left(\rho_\beta||\rho_\beta^{\mathrm{eq}}\right)\Big|_{\beta=\beta_0} < 0. \tag{7}$$

Therefore, the curvature of the quantum relative entropy $S(\rho_\beta||\rho_\beta^{\mathrm{eq}})$ with respect to β can be regarded as the criteria quantifying the performance of the CTS for quantum thermometry.

4. Single-qubit example

As a pedagogical example, we show the single-qubit case. Let σ_x, σ_y and σ_z be the Pauli matrices. The Hamiltonian is $H = \omega\sigma_z$, so that the eigenstates of H are $|0\rangle = \begin{pmatrix}1 & 0\end{pmatrix}^T$ and $|1\rangle = \begin{pmatrix}0 & 1\end{pmatrix}^T$. Therefore, $Z_\beta^{\mathrm{eq}} = \mathrm{tr}\left\{e^{-\beta H}\right\} = 2\cosh(\beta\omega)$. Considering the pointer states $|\psi_0(\theta)\rangle = e^{i\frac{\theta}{2}\sigma_x}|0\rangle$ and $|\psi_1(\theta)\rangle = e^{i\frac{\theta}{2}\sigma_x}|1\rangle$ with $\theta \in \mathbb{R}$, the normalization factor of the CTS becomes $Z_\beta(\theta) = 2\cosh(\beta\omega\cos(\theta))$.

Therefore, we obtain from equation (6),

$$\Delta\mathcal{I}_\beta(\theta) = \omega^2\left(-1 + \frac{\cos^2(\theta)}{\cosh^2(\beta\omega\cos(\theta))} + \tanh^2(\beta\omega)\right). \tag{8}$$

In the low-temperature limit ($\beta\omega \gg 1$), we have

$$\Delta\mathcal{I}_\beta(\theta) \simeq \left(\frac{\omega\cos(\theta)}{\cosh(\beta\omega\cos(\theta))}\right)^2 \geqslant 0 \quad \forall\theta \in \mathbb{R}. \tag{9}$$

This means that the CTS can outperform the Gibbs state for any choice of pointer states in the low-temperature limit. As an example, choose $\theta = \pi/4$ and $\omega = 1$, which is illustrated in figure 2.

5. Asymmetry

The natural question arises, where exactly this enhanced performance of the CTS in thermometry originates. To this end, we now analyze the relation between the QFI of ρ_β and the asymmetry measure, which is quantified by the WYD skew information $I_\alpha(\rho_\beta, H)$ contained by ρ_β with respect to the Hamiltonian H.

The asymmetry of quantum state is related to its quantum coherence, which is regarded as a resource of breaking the symmetry of a group. This is characterized by the *resource theory of asymmetry* (RTA) [30–34], whose development has also contributed to exploring quantum thermodynamic resources [51–56]. In particular, when we consider time translations $\{\exp(-iHt), |, t \in \mathbb{R}\}$, a state ρ is symmetric if and only if $[\rho, H] = 0$, and asymmetric if and only if $[\rho, H] \neq 0$. Here, the symmetric state is considered the free state,

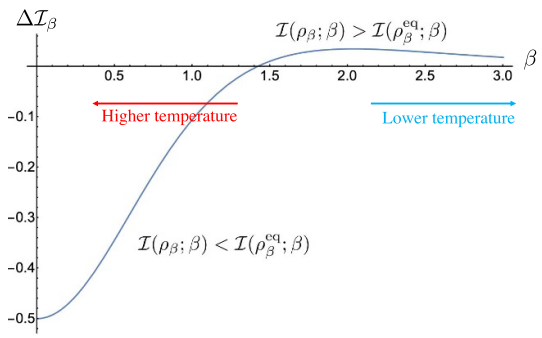

Figure 2. Relation between ΔI_β and β: We choose $\omega = 1$ and $\theta = \pi/4$. In the low-temperature limit, we have $\mathcal{I}(\rho_\beta;\beta) \geqslant \mathcal{I}(\rho_\beta^{\rm eq};\beta)$, meaning that the CTS outperforms the Gibbs state in thermometry.

while the asymmetric state is regarded as the resource state. Covariant operations [57], which are the relevant set of free operations, cannot generate an asymmetric state from a symmetric one or convert one asymmetric state into another. An asymmetry measure must satisfy two conditions: (i) it vanishes if and only if the state is symmetric, and (ii) it does not increase under all covariant operations. One quantity satisfying these conditions is the skew information [35–40].

For a quantum state ρ, the WYD skew information is defined as $I_\alpha(\rho,H) \equiv \mathrm{tr}\left\{\rho H^2\right\} - \mathrm{tr}\left\{\rho^\alpha H \rho^{1-\alpha} H\right\}$ with $0 < \alpha < 1$. With $\mathrm{Var}_\rho\{H\} \equiv \mathrm{tr}\left\{\rho H^2\right\} - (\mathrm{tr}\{\rho H\})^2$ the variance of H with respect to ρ, we can define the general variance (covariance) $Q_\alpha(\rho,H)$ as $Q_\alpha(\rho,H) \equiv \mathrm{Var}_\rho\{H\} - I_\alpha(\rho,H)$ [58–60].

Hence, the QFI of ρ_β can be alternatively written as the covariance of the Hamiltonian $H_{12} \equiv H \otimes \mathbb{1}_2$ with respect to the conditional thermal separable state $\widetilde{\rho}_\beta$ (3). By using the fact that $\mathrm{Var}_{\widetilde{\rho}_\beta}\{H_{12}\} = \mathrm{Var}_{\rho_\beta}\{H\}$ and the asymmetry monotone of WYD skew information $I_\alpha(\widetilde{\rho}_\beta, H_{12}) \geqslant I_\alpha(\rho_\beta, H)$ [35–37], we obtain (see appendix C for the proof.)

$$\mathcal{I}\left(\rho_\beta;\beta\right) = Q_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right) \leqslant Q_\alpha\left(\rho_\beta, H\right). \tag{10}$$

Note that when the chosen basis comprises the pointer states of the Hamiltonian, i.e. $\rho_\beta = \rho_\beta^{\rm eq}$, we have $I_\alpha(\rho_\beta^{\rm eq}, H) = 0$ because of $[\rho_\beta^{\rm eq}, H] = 0$. In this case, the upper bound becomes $\mathrm{Var}_{\rho_\beta}\{H\}$, which is exactly the QFI of ρ_β for estimating β, and equation (10) saturates.

These results demonstrate that the asymmetry of the CTS quantifies the maximum ultimate precision limit of the quantum thermometry. In our scenario, since the asymmetry resource contains the quantum coherence over the eigenstates of the Hamiltonian [35], from equation (10), the quantum coherence of the conditional thermal separable state $\widetilde{\rho}_\beta$ can be engineered by choosing appropriate pointer states maximizing the QFI of ρ_β.

6. State preparation of the CTS

In the preceding section we have shown that the inherent asymmetry of the CTS can be exploited as a resource. Hence, we now continue with a more formal analysis of the resource-theoretic properties of the CTS arising from the state distinguishability with the Gibbs state. To this end, we consider a quantum system, which is initially prepared in a Gibbs state, $\rho_\beta^{\rm eq}(0)$, and evolves under a time-dependent Hamiltonian H_t from $t = 0$ to $t = \tau$ with a corresponding unitary U_τ. Our main interest is the state convertibility of the exact final state into the CTS by considering the information-theoretic properties of the averaged excess work.

Let us write $\rho(\tau)$ as the exact final state $\rho(\tau) = U_\tau \rho_\beta^{\rm eq}(0) U_\tau$. In this case, the exact averaged work $\langle W\rangle$ is given by $\langle W\rangle = \mathrm{tr}\{\rho(\tau)H_\tau\} - \mathrm{tr}\left\{\rho_\beta^{\rm eq}(0)H_0\right\}$. When $\Delta F^{\rm eq}$ is the equilibrium free energy difference $\Delta F^{\rm eq} \equiv -\beta^{-1}\ln(Z_\beta^{\rm eq}(\tau)/Z_\beta^{\rm eq}(0))$, the excess work is given by [61, 62]

$$\langle W_{\rm ex}\rangle \equiv \langle W\rangle - \Delta F^{\rm eq} = \beta^{-1} S\left(\rho(\tau)\,||\rho_\beta^{\rm eq}(\tau)\right). \tag{11}$$

We initially measure the system with $H_0 \equiv \sum_{k=1}^d E_k |E_k\rangle\langle E_k|$, where $\{|E_k\rangle\}_{k=1}^d$ are the eigenstates of H_0. The post-measurement state of the system after the evolution is $U_\tau|E_k\rangle$. Thus, the CTS constructed from the

post-measurement state for the final Hamiltonian $H_\tau \equiv \sum_{k=1}^{d} E'_k |E'_k\rangle\langle E'_k|$ is given by [24]

$$\rho_\beta(\tau) = \sum_{k=1}^{d} \frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} U_\tau |E_k\rangle\langle E_k| U_\tau^\dagger , \tag{12}$$

where $Z_\beta(\tau)$ is again the conditional partition function.

In [24] it was shown that the excess work is lower bounded by

$$\langle W_{\rm ex}\rangle \geqslant \beta^{-1} S\left(\rho_\beta(\tau)||\rho_\beta^{\rm eq}(\tau)\right) . \tag{13}$$

Therefore, from equations (11) and (13), we have

$$S\left(\rho(\tau)||\rho_\beta^{\rm eq}(\tau)\right) \geqslant S\left(\rho_\beta(\tau)||\rho_\beta^{\rm eq}(\tau)\right) . \tag{14}$$

From [63–65], equation (14) becomes tight if and only if there exists a sufficiently large n_0 and there exists a Gibbs-preserving map $\mathcal{E}_n : \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes n}$ for $n \geqslant n_0$ such that

$$\mathcal{E}_n\left(\rho_\beta^{\rm eq}(\tau)^{\otimes n}\right) = \rho_\beta^{\rm eq}(\tau)^{\otimes n} , \ \mathcal{E}_n\left(\rho(\tau)^{\otimes n}\right) = \Xi_n , \tag{15}$$

where for any $\epsilon > 0$, the quantum state Ξ_n satisfies

$$T_n \equiv \frac{1}{2}||\rho_\beta(\tau)^{\otimes n} - \Xi_n||_1 < \epsilon . \tag{16}$$

This means that the CTS is not just a mathematical object but can be prepared, allowing for an arbitrarily small error via the Gibbs-preserving map with an *asymptotic* number of copies of the state.

Also, from the quantum relative entropy of the exact final state $\rho(\tau)$ with respect to the CTS $\rho_\beta(\tau)$ $S(\rho(\tau)||\rho_\beta(\tau))$, we obtain (see appendix D for the proof.)

$$S(\rho(\tau)||\rho_\beta(\tau)) + S\left(\rho_\beta(\tau)||\rho_\beta^{\rm eq}(\tau)\right) = S\left(\rho(\tau)||\rho_\beta^{\rm eq}(\tau)\right) , \tag{17}$$

which we call *thermodynamic triangle equality*. Therefore, when $S(\rho(\tau)||\rho_\beta^{\rm eq}(\tau)) = S(\rho_\beta(\tau)||\rho_\beta^{\rm eq}(\tau))$, we must have $\rho(\tau) = \rho_\beta(\tau)$ (i.e. $U_\tau^\dagger H_\tau U_\tau = H_0$).

To analyze the scaling of the required number of copies n given an arbitrarily small error ϵ, we employ the inequality $S(\rho_\beta(\tau)^{\otimes n}||\Xi_n) \leqslant (T_n + \lambda_n)\ln(1 + T_n/\lambda_n)$ [66], where λ_n denotes the minimum non-zero eigenvalue of Ξ_n. Since $d = {\rm rank}(\rho_\beta(\tau))$, we can write $\lambda_n \sim 1/d^n$ [66]. Therefore, when $T_n < \epsilon \ll 1$, we have

$$\begin{aligned} S\left(\rho_\beta(\tau)^{\otimes n}||\Xi_n\right) &\lesssim \left(\epsilon + \frac{1}{d^n}\right)\ln(1 + \epsilon d^n) \\ &= \epsilon\left(1 + \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k(k+1)} \epsilon^k d^{kn}\right) \\ &= \epsilon\left(1 + \frac{d^n}{2}\epsilon + O\left(\epsilon^2 d^{2n}\right)\right) . \end{aligned} \tag{18}$$

To guarantee $\lim_{n\to 0} S(\rho_\beta(\tau)^{\otimes n}||\Xi_n) = 0$, the simplest condition is $\epsilon d^n \sim 1$. Therefore, the required number of copies of $\rho_\beta(\tau)$ can be approximately given by

$$n \sim \log_d\left(\frac{1}{\epsilon}\right) . \tag{19}$$

Here, we note that this state preparation protocol inherently depends on an unknown parameter. Therefore, in the context of thermometry, this protocol remains limited. We need to further explore state preparation protocols that are independent of such parameters.

7. Quantum heat from the CTS

Furthermore, the symmetric divergence between $\rho(\tau)$ and $\rho_\beta(\tau)$, i.e. the quantum J-divergence defined as [67],

$$J(\rho(\tau),\rho_\beta(\tau)) \equiv S(\rho(\tau)||\rho_\beta(\tau)) + S(\rho_\beta(\tau)||\rho(\tau)), \tag{20}$$

is related to the concept of quantum heat [41]. This becomes obvious when the quantum J-divergence is written as (see appendix E for the proof.)

$$J(\rho(\tau),\rho_\beta(\tau)) = \beta(\langle W\rangle - \mathcal{W}_0(\rho_\beta(\tau)) - \Delta E(\rho_\beta(\tau))). \tag{21}$$

Here, the internal energy change of $\rho_\beta(\tau)$ is $\Delta E(\rho_\beta(\tau)) \equiv \mathrm{tr}\{\rho_\beta(\tau)(H_\tau - H_0)\}$, and the quantum ergotropy of $\rho_\beta(\tau)$ with respect to H_0 is $\mathcal{W}_0(\rho_\beta(\tau)) \equiv \mathrm{tr}\{\rho_\beta(\tau)H_0\} - \mathrm{tr}\{\Gamma\rho_\beta(\tau)\Gamma^\dagger H_0\}$, where $\Gamma \equiv \sum_{k=1}^d |E_k\rangle\langle E_k|U_\tau^\dagger = U_\tau^\dagger$ is the ergotropic transformation [68]. From the first law of thermodynamics, $\beta^{-1}J(\rho(\tau),\rho_\beta(\tau))$ can be regarded as a heat, particularly the *quantum heat*, which has been discussed in the literature as the heat induced by the measurement [41]. In essence, the CTS $\rho_\beta(\tau)$ is conditioned on the first energy measurement outcome; therefore, its relation to the quantum heat is consistent in this context. Also, note that when U_τ is a adiabatic passage, then $\rho(\tau) = \rho_\beta(\tau) = \rho_\beta^{\mathrm{eq}}(\tau)$, so that $\beta^{-1}J(\rho(\tau),\rho_\beta(\tau)) = 0$, which is consistent with zero heat exchange in the adiabatic process.

8. Conclusion

In conclusion, we have introduced a conditional thermal state, which is a thermal state conditioned on the pointer states, and demonstrated that this conditional thermal state can outperform the Gibbs state in the quantum thermometry as a useful resource state. We also have explored its resource-theoretic properties in terms of the asymmetry, state convertibility and its relation to the quantum heat. As an application, these results could help experimentalists to achieve a better sensitivity in quantum thermometry under the constraints in the implementable measurements. From the fundamental point of view, these results provide insightful perspective on the implications of the conditional thermal state in the thermodynamic protocols in the quantum systems in a resource-theoretic approach. Finally, the present analysis also provides an additional *a posteriori* motivation and justification for the one-time energy measurement approach to quantum work [24–29]. Future work will involve further exploration of concrete state preparation protocols for generating the conditional thermal state.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgments

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Appendix A. Derivation of conditional thermal state

Consider a density matrix ρ with the following spectral decomposition

$$\rho = \sum_{k=1}^d p_k|\psi_k\rangle\langle\psi_k|, \tag{A1}$$

where $\{|\psi_k\rangle\}_{k=1}^d$ are the pointer states of a given measurement M. Let H be the Hamiltonian of the system. Then, we want to maximize the von Neumann entropy

$$S(\rho) \equiv -\mathrm{tr}\{\rho\ln\rho\} \tag{A2}$$

under the conditions

$$\mathrm{tr}\{\rho\} = 1 \quad \text{and} \quad E(\rho) \equiv \mathrm{tr}\{\rho H\} = \text{Const.} \tag{A3}$$

By using the optimization method of Lagrange multipliers with constraints, we have:

$$\delta\left(S(\rho) - \gamma E(\rho) - \alpha\right) = -\sum_{k=1}^{d} \delta p_k \left(\ln p_k + \beta\langle\psi_k|H|\psi_k\rangle + \alpha + 1\right) = 0\,. \tag{A4}$$

For any δp_k, equation (A4) has to be valid so that each term has to be independently 0. Therefore, we must have $p_k \propto e^{-\beta\langle\psi_k|H|\psi_k\rangle}$. From the requirement of $\sum_{k=1}^{d} p_k = 1$, we obtain the CTS ρ_β.

Appendix B. Detailed derivations of equations (4)–(7)

From the definition of QFI, we have

$$\mathcal{I}(\rho_\theta;\theta) = -2\lim_{\epsilon\to 0}\partial_\epsilon^2 \mathcal{F}(\rho_\theta, \rho_{\theta+\epsilon}) \tag{B1}$$

where

$$\begin{aligned}\mathcal{F}(\rho_\beta, \rho_{\beta+\epsilon}) &\equiv ||\sqrt{\rho_\beta}\sqrt{\rho_{\beta+\epsilon}}||_1^2 \\ &\equiv \left(\mathrm{tr}\left\{\sqrt{\rho_\beta^{1/2}\rho_{\beta+\epsilon}\rho_\beta^{1/2}}\right\}\right)^2 \\ &= \frac{1}{Z_\beta Z_{\beta+\epsilon}}\left(\sum_{k=1}^{d} e^{-\left(\beta+\frac{\epsilon}{2}\right)\langle\psi_k|H|\psi_k\rangle}\right)^2 \\ &= \frac{Z_{\beta+\epsilon/2}^2}{Z_\beta Z_{\beta+\epsilon}}\,.\end{aligned} \tag{B2}$$

Before calculating the quantum Fisher information, let us show the following fact:

$$\begin{aligned}\lim_{\epsilon\to 0}\partial_\epsilon Z_{\beta+\epsilon} &= -\sum_{k=1}^{d} e^{-\beta\langle\psi_k|H|\psi_k\rangle}\langle\psi_k|H|\psi_k\rangle = \partial_\beta Z_\beta \\ \lim_{\epsilon\to 0}\partial_\epsilon^2 Z_{\beta+\epsilon} &= \sum_{k=1}^{d} e^{-\beta\langle\psi_k|H|\psi_k\rangle}\langle\psi_k|H|\psi_k\rangle^2 = \partial_\beta^2 Z_\beta \\ \lim_{\epsilon\to 0}\partial_\epsilon Z_{\beta+\epsilon/2} &= -\frac{1}{2}\sum_{k=1}^{d} e^{-\beta\langle\psi_k|H|\psi_k\rangle}\langle\psi_k|H|\psi_k\rangle = \frac{1}{2}\partial_\beta Z_\beta \\ \lim_{\epsilon\to 0}\partial_\epsilon^2 Z_{\beta+\epsilon/2} &= \frac{1}{4}\sum_{k=1}^{d} e^{-\beta\langle\psi_k|H|\psi_k\rangle}\langle\psi_k|H|\psi_k\rangle^2 = \frac{1}{4}\partial_\beta^2 Z_\beta\,.\end{aligned} \tag{B3}$$

For two functions $f(x)$ and $g(x)$, where $g(x) \neq 0$, we have:

$$\partial_x^2\left(\frac{f^2}{g}\right) = 2\left(\partial_x^2 f\right)\frac{f}{g} + \frac{2}{g}\left(\partial_x f\right)^2 - \frac{4f}{g^2}\left(\partial_x f\right)\left(\partial_x g\right) - \left(\partial_x^2 g\right)\frac{f^2}{g^2} + \frac{2f^2}{g^3}\left(\partial_x g\right)^2.$$

Therefore, if we define $x = \epsilon$, $f = Z_{\beta+\epsilon/2}$ and $g = Z_{\beta+\epsilon}$, we can obtain:

$$\begin{aligned}\lim_{\epsilon\to 0}\partial_\epsilon^2 F(\rho_\beta, \rho_{\beta+\epsilon}) &= \lim_{\epsilon\to 0}\partial_\epsilon^2\left(\frac{Z_{\beta+\epsilon/2}^2}{Z_\beta Z_{\beta+\epsilon}}\right) \\ &= \frac{1}{2}\frac{\partial_\beta^2 Z_\beta}{Z_\beta} + \frac{1}{2}\left(\frac{\partial_\beta Z_\beta}{Z_\beta}\right)^2 - 2\left(\frac{\partial_\beta Z_\beta}{Z_\beta}\right)^2 - \frac{\partial_\beta^2 Z_\beta}{Z_\beta} + 2\left(\frac{\partial_\beta Z_\beta}{Z_\beta}\right)^2 \\ &= \frac{1}{2}\left(\frac{\partial_\beta Z_\beta}{Z_\beta}\right)^2 - \frac{1}{2}\frac{\partial_\beta^2 Z_\beta}{Z_\beta} \\ &= \frac{1}{2}\left((\partial_\beta \ln Z_\beta)^2 - Z_\beta^{-1}\partial_\beta^2 Z_\beta\right).\end{aligned} \tag{B4}$$

Therefore, from equation (B1), we can obtain

$$\mathcal{I}(\rho_\beta;\beta) = Z_\beta^{-1}\partial_\beta^2 Z_\beta - (\partial_\beta \ln Z_\beta)^2 = \partial_\beta^2 \ln Z_\beta\,. \tag{B5}$$

For the optimal measurement, we need to prove that the uncertainty of the unbiased estimator with the measurement

$$G = \sum_{k=1}^{d} \langle\psi_k|H|\psi_k\rangle |\psi_k\rangle\langle\psi_k| \tag{B6}$$

achieves the quantum Cramér–Rao bound. The uncertainty is given by

$$(\delta\beta)_G^2 \equiv \frac{\mathrm{Var}_{\rho_\beta}\{G\}}{|\partial_\beta \mathrm{tr}\{\rho_\beta G\}|^2}\,. \tag{B7}$$

Here, we have

$$\mathrm{tr}\{\rho_\beta G\} = \sum_{k=1}^{d} \frac{e^{-\beta\langle\psi_k|H|\psi_k\rangle}}{Z_\beta}\langle\psi_k|H|\psi_k\rangle = \mathrm{tr}\{\rho_\beta H\} = -\partial_\beta \ln Z_\beta \tag{B8}$$

and

$$\begin{aligned}\mathrm{Var}_{\rho_\beta}\{G\} &\equiv \mathrm{tr}\left\{\rho_\beta H^2\right\} - (\mathrm{tr}\{\rho_\beta H\})^2\\ &= \sum_{k=1}^{d} \frac{e^{-\beta\langle\psi_k|H|\psi_k\rangle}}{Z_\beta}\langle\psi_k|H|\psi_k\rangle^2 - (\partial_\beta \ln Z_\beta)^2\\ &= Z_\beta^{-1}\partial_\beta^2 Z_\beta - (\partial_\beta \ln Z_\beta)^2\\ &= \partial_\beta^2 \ln Z_\beta\,.\end{aligned} \tag{B9}$$

From equations (B5) and (B7), we can obtain

$$(\delta\beta)_G^2 = \frac{1}{\partial_\beta^2 \ln Z_\beta} = \frac{1}{\mathcal{I}(\rho_\beta;\beta)}\,, \tag{B10}$$

which is the quantum Cramér–Rao bound; therefore, equation (B6) is the optimal measurement for the quantum thermometry.

From equation (B5), we can write

$$\Delta\mathcal{I}_\beta \equiv \mathcal{I}(\rho_\beta;\beta) - \mathcal{I}\left(\rho_\beta^{\mathrm{eq}};\beta\right) = \partial_\beta^2 \ln \frac{Z_\beta}{Z_\beta^{\mathrm{eq}}}\,. \tag{B11}$$

Since the von Neumann entropy $S(\rho_\beta) \equiv -\mathrm{tr}\{\rho_\beta \ln \rho_\beta\}$ is

$$S(\rho_\beta) = \beta\,\mathrm{tr}\{\rho_\beta H\} + \ln Z_\beta\,, \tag{B12}$$

the quantum relative entropy $S(\rho_\beta||\rho_\beta^{\mathrm{eq}})$ becomes

$$S\left(\rho_\beta||\rho_\beta^{\mathrm{eq}}\right) = -S(\rho_\beta) - \mathrm{tr}\left\{\rho_\beta \ln \rho_\beta^{\mathrm{eq}}\right\} = -\ln \frac{Z_\beta}{Z_\beta^{\mathrm{eq}}}\,. \tag{B13}$$

Therefore, we can write

$$\Delta\mathcal{I}_\beta = -\partial_\beta^2 S\left(\rho_\beta||\rho_\beta^{\mathrm{eq}}\right)\,. \tag{B14}$$

When the CTS outperforms the Gibbs state for the quantum thermometry at $\beta = \beta_0$, i.e.

$$\Delta\mathcal{I}_{\beta_0} > 0\,, \tag{B15}$$

we must have

$$\partial_\beta^2 S\left(\rho_\beta||\rho_\beta^{\mathrm{eq}}\right)\Big|_{\beta=\beta_0} < 0\,. \tag{B16}$$

Appendix C. Proof of equation (10)

First, let us prove $\mathcal{I}(\rho_\beta;\beta) = Q_\alpha(\widetilde{\rho}_\beta, H_{12})$, where

$$H_{12} \equiv H \otimes \mathbb{1}_2 \,. \tag{C1}$$

Since

$$\widetilde{\rho}_\beta \equiv \sum_{k=1}^{d} \frac{e^{-\beta\langle\psi_k|H|\psi_k\rangle}}{Z_\beta} |\psi_k\rangle\langle\psi_k|_1 \otimes |\phi_k\rangle\langle\phi_k|_2 \tag{C2}$$

and

$$\rho_\beta = \mathrm{tr}_2\left\{\widetilde{\rho}_\beta\right\}, \tag{C3}$$

we have

$$\mathrm{tr}\left\{\widetilde{\rho}_\beta H_{12}\right\} = \mathrm{tr}\left\{\rho_\beta H\right\} = -\partial_\beta \ln Z_\beta \tag{C4}$$

and

$$\mathrm{tr}\left\{\widetilde{\rho}_\beta H_{12}^2\right\} = \mathrm{tr}\left\{\rho_\beta H^2\right\}, \tag{C5}$$

so that

$$\mathrm{Var}_{\widetilde{\rho}_\beta}\left\{H_{12}\right\} = \mathrm{Var}_{\rho_\beta}\left\{H\right\}. \tag{C6}$$

Next, let us compute the WYD skew information $I_\alpha(\widetilde{\rho}_\beta, H)$ contained by $\widetilde{\rho}_\beta$ with respect to H_{12}. By using the fact that for a pure state $|\varphi\rangle$ we have $|\varphi\rangle\langle\varphi|^\alpha = |\varphi\rangle\langle\varphi|$ for any α, we can obtain

$$\begin{aligned} I_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right) &= \mathrm{tr}\left\{\widetilde{\rho}_\beta H_{12}^2\right\} - \mathrm{tr}\left\{\widetilde{\rho}_\beta^\alpha H_{12} \widetilde{\rho}_\beta^{1-\alpha} H_{12}\right\} \\ &= \mathrm{tr}\left\{\widetilde{\rho}_\beta H_{12}^2\right\} - \sum_{k=1}^{d} \frac{e^{-\beta\langle\psi_k|H|\psi_k\rangle}}{Z_\beta} \langle\psi_k|H|\psi_k\rangle^2 \\ &= \mathrm{tr}\left\{\widetilde{\rho}_\beta H_{12}^2\right\} - Z_\beta^{-1}\partial_\beta^2 Z_\beta \,. \end{aligned} \tag{C7}$$

Therefore, we can obtain

$$\begin{aligned} Q_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right) &\equiv \mathrm{Var}_{\widetilde{\rho}_\beta}\left\{H\right\} - I_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right) \\ &= Z_\beta^{-1}\partial_\beta^2 Z_\beta - \left(\partial_\beta \ln Z_\beta\right)^2 \\ &= \partial_\beta^2 \ln Z_\beta \,. \end{aligned} \tag{C8}$$

From equation (B5), we can finally write

$$\mathcal{I}\left(\rho_\beta;\beta\right) = Q_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right). \tag{C9}$$

Next, let us prove $I(\rho_\beta;\beta) \leqslant Q_\alpha(\rho_\beta, H)$. The WYD skew information has asymmetry monotone [36]

$$I_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right) \geqslant I_\alpha\left(\rho_\beta, H\right). \tag{C10}$$

From equation (C6), we can obtain

$$Q_\alpha\left(\widetilde{\rho}_\beta, H_{12}\right) \leqslant Q_\alpha\left(\rho_\beta, H\right) = \mathrm{Var}_{\rho_\beta}\left\{H\right\} - I_\alpha\left(\rho_\beta, H\right). \tag{C11}$$

Because of equation (C9), we can obtain

$$\mathcal{I}\left(\rho_\beta;\beta\right) \leqslant Q_\alpha\left(\rho_\beta, H\right). \tag{C12}$$

Appendix D. Proof of equation (17)

The quantum relative entropy $S(\rho(\tau)||\rho_\beta(\tau))$ can be written as

$$\begin{aligned} S(\rho(\tau)||\rho_\beta(\tau)) &= -S(\rho(\tau)) - \mathrm{tr}\{\rho(\tau)\ln\rho_\beta(\tau)\} \\ &= -S(\rho(\tau)) + \beta\sum_{k=1}^{d}\langle E_k|U_\tau^\dagger\rho(\tau)U_\tau|E_k\rangle\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle + \ln Z_\beta(\tau)\,. \end{aligned} \tag{D1}$$

Because

$$\rho(\tau) = U_\tau\rho_\beta^{\mathrm{eq}}(0)U_\tau^\dagger = \sum_{k=1}^{d}\frac{e^{-\beta E_k}}{Z_\beta^{\mathrm{eq}}(0)}U_\tau|E_k\rangle\langle E_k|U_\tau^\dagger\,, \tag{D2}$$

we have

$$\sum_{k=1}^{d}\langle E_k|U_\tau^\dagger\rho(\tau)U_\tau|E_k\rangle\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle = \mathrm{tr}\left\{U_\tau\rho_\beta^{\mathrm{eq}}(0)U_\tau^\dagger H_\tau\right\} = \mathrm{tr}\{\rho(\tau)H_\tau\}\,. \tag{D3}$$

Therefore,

$$S(\rho(\tau)||\rho_\beta(\tau)) = -S(\rho(\tau)) + \beta\mathrm{tr}\{\rho(\tau)H_\tau\} + \ln Z_\beta(\tau)\,. \tag{D4}$$

From the unitary invariance of the von Neumann entropy, we can write

$$\begin{aligned} S(\rho(\tau)||\rho_\beta(\tau)) &= -S\left(\rho_\beta^{\mathrm{eq}}(0)\right) + \ln Z_\beta(\tau) + \beta\mathrm{tr}\{\rho(\tau)H_\tau\} \\ &= \beta\left(\mathrm{tr}\{\rho(\tau)H_\tau\} - \mathrm{tr}\left\{\rho_\beta^{\mathrm{eq}}(0)H_0\right\}\right) + \ln\frac{Z_\beta(\tau)}{Z_\beta^{\mathrm{eq}}(0)} \\ &= \beta\langle W\rangle + \ln\frac{Z_\beta(\tau)}{Z_\beta^{\mathrm{eq}}(0)}\,, \end{aligned} \tag{D5}$$

where

$$\langle W\rangle \equiv \mathrm{tr}\{\rho(\tau)H_\tau\} - \mathrm{tr}\left\{\rho_\beta^{\mathrm{eq}}(0)H_0\right\} \tag{D6}$$

is the exact averaged work. Because

$$\ln\frac{Z_\beta(\tau)}{Z_\beta^{\mathrm{eq}}(0)} = \ln\frac{Z_\beta(\tau)}{Z_\beta^{\mathrm{eq}}(\tau)} + \ln\frac{Z_\beta^{\mathrm{eq}}(\tau)}{Z_\beta^{\mathrm{eq}}(0)}\,, \tag{D7}$$

from [24], we have

$$\ln\frac{Z_\beta(\tau)}{Z_\beta^{\mathrm{eq}}(0)} = -S\left(\rho_\beta(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right) - \beta\Delta F^{\mathrm{eq}}\,. \tag{D8}$$

Therefore, we have

$$S(\rho(\tau)||\rho_\beta(\tau)) + S\left(\rho_\beta(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right) = \beta(\langle W\rangle - \Delta F^{\mathrm{eq}})\,. \tag{D9}$$

Because the exact excess work is [62]

$$\langle W_{\mathrm{ex}}\rangle = \langle W\rangle - \Delta F^{\mathrm{eq}} = \beta^{-1}S\left(\rho(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right)\,, \tag{D10}$$

we can obtain the thermodynamic triangle equality

$$S(\rho(\tau)||\rho_\beta(\tau)) + S\left(\rho_\beta(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right) = S\left(\rho(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right)\,. \tag{D11}$$

Appendix E. Proof of equation (21)

The quantum J-divergence of $\rho(\tau)$ and $\rho_\beta(\tau)$ is defined as

$$J(\rho(\tau),\rho_\beta(\tau)) \equiv S(\rho(\tau)||\rho_\beta(\tau)) + S(\rho_\beta(\tau)||\rho(\tau)) . \tag{E1}$$

In equations (D9) and (D11), we have already proved the thermodynamic triangle equality. Next, let us consider the quantum relative entropy $S(\rho_\beta(\tau)||\rho(\tau))$, which is given by

$$S(\rho_\beta(\tau)||\rho(\tau)) = -S(\rho_\beta(\tau)) - \mathrm{tr}\{\rho_\beta(\tau)\ln\rho(\tau)\} . \tag{E2}$$

The von Neumann entropy of $\rho_\beta(\tau)$ is

$$S(\rho_\beta(\tau)) = \beta\mathrm{tr}\{\rho_\beta(\tau)H_\tau\} + \ln Z_\beta(\tau) . \tag{E3}$$

Also

$$\begin{aligned}\mathrm{tr}\{\rho_\beta(\tau)\ln\rho(\tau)\} &= -\beta\sum_{k=1}^{d}E_k\langle E_k|U_\tau^\dagger\rho_\beta(\tau)U_\tau|E_k\rangle - \ln Z_\beta^{\mathrm{eq}}(0)\\ &= -\beta\sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} - \ln Z_\beta^{\mathrm{eq}}(0) .\end{aligned} \tag{E4}$$

Therefore,

$$S(\rho_\beta(\tau)||\rho(\tau)) = \beta\left(\sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} - \mathrm{tr}\{\rho_\beta(\tau)H_\tau\}\right) - \ln\frac{Z_\beta(\tau)}{Z_\beta^{\mathrm{eq}}(0)} . \tag{E5}$$

From equation (D8), we can obtain

$$S(\rho_\beta(\tau)||\rho(\tau)) - S\left(\rho_\beta(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right) - \beta\Delta F_\beta^{\mathrm{eq}} = \beta\left(\sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} - \mathrm{tr}\{\rho_\beta(\tau)H_\tau\}\right) . \tag{E6}$$

By using $\mathrm{tr}\{\rho_\beta(\tau)H_0\}$, we can write

$$\begin{aligned}&\sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} - \mathrm{tr}\{\rho_\beta(\tau)H_\tau\}\\ &\quad= \sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} - \mathrm{tr}\{\rho_\beta(\tau)H_0\} - \mathrm{tr}\{\rho_\beta(\tau)(H_\tau - H_0)\} .\end{aligned} \tag{E7}$$

Let Γ be the ergotropic transformation

$$\Gamma \equiv \sum_{k=1}^{d}|E_k\rangle\langle E_k|U_\tau^\dagger = U_\tau^\dagger . \tag{E8}$$

Then, we have

$$\mathrm{tr}\{\Gamma\rho_\beta(\tau)\Gamma^\dagger H_0\} = \sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} . \tag{E9}$$

The ergotropy of $\rho_\beta(\tau)$ with respect to the Hamiltonian H_0 is defined as [68]

$$\mathcal{W}_0(\rho_\beta(\tau)) \equiv \mathrm{tr}\{\rho_\beta(\tau)H_0\} - \mathrm{tr}\{\Gamma\rho_\beta(\tau)\Gamma^\dagger H_0\} = \mathrm{tr}\{\rho_\beta(\tau)H_0\} - \sum_{k=1}^{d}E_k\frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} . \tag{E10}$$

Therefore, by defining

$$\Delta E(\rho_\beta(\tau)) \equiv \mathrm{tr}\{\rho_\beta(\tau)(H_\tau - H_0)\} , \tag{E11}$$

we can write

$$\sum_{k=1}^{d} E_k \frac{e^{-\beta\langle E_k|U_\tau^\dagger H_\tau U_\tau|E_k\rangle}}{Z_\beta(\tau)} - \mathrm{tr}\{\rho_\beta(\tau)H_\tau\} = -\mathcal{W}_0(\rho_\beta(\tau)) - \Delta E(\rho_\beta(\tau)) . \tag{E12}$$

Therefore,

$$S(\rho_\beta(\tau)||\rho(\tau)) - S\left(\rho_\beta(\tau)||\rho_\beta^{\mathrm{eq}}(\tau)\right) = \beta(\Delta F^{\mathrm{eq}} - \mathcal{W}_0(\rho_\beta(\tau)) - \Delta E(\rho_\beta(\tau))) . \tag{E13}$$

From equations (E1), (D9) and (E13), we can obtain

$$J(\rho(\tau), \rho_\beta(\tau)) = \beta(\langle W\rangle - \mathcal{W}_0(\rho_\beta(\tau)) - \Delta E(\rho_\beta(\tau))) . \tag{E14}$$

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