

– Supplementary Information –

Energy-temperature uncertainty relation in quantum thermodynamics

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SUPPLEMENTARY NOTE 1: DERIVATION OF UPPER BOUND ON THE QUANTUM FISHER INFORMATION

We begin by considering an exponential state $\hat{\rho}_\theta$ dependent on smooth parameter θ of the form $\hat{\rho}_\theta = e^{-\hat{A}_\theta}/Z_\theta$, where $Z_\theta = \text{tr}[e^{-\hat{A}_\theta}]$ and $\hat{A}_\theta$ is some positive hermitian operator. Suppressing the dependence on θ for now, let us denote the spectral decomposition by $\hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$ where the eigenstates satisfy $\hat{A}|\psi_n\rangle = \lambda_n|\psi_n\rangle$. We arrange the sum in decreasing order, so that $p_n \geq p_m$ if $n < m$. The quantum Fisher information (QFI) with respect to θ is then $F(\theta) := \text{tr}[\hat{\rho}_\theta \hat{L}_\theta^2]$, where $\hat{L}_\theta$ is the operator satisfying

$$\partial_\theta \hat{\rho}_\theta = \frac{1}{2} \{\hat{\rho}_\theta, \hat{L}_\theta\}. \quad (1)$$

By expanding both sides of (1) in the basis of $\hat{\rho}_\theta$, one may show that the QFI can be written as follows [1]:

$$F(\theta) = 2 \sum_{n,m} \frac{|\langle\psi_n|\partial_\theta \hat{\rho}_\theta|\psi_m\rangle|^2}{p_n + p_m}. \quad (2)$$

We define the operator $\hat{B}_\theta = \partial_\theta \hat{A}_\theta$ and note that $\text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] = \text{tr}[(\delta\hat{B}_\theta)^2 \hat{\rho}_\theta]$, where $\delta\hat{B}_\theta = \hat{B}_\theta - \text{tr}[\hat{B}_\theta \hat{\rho}_\theta]$ and $\text{tr}[\hat{B}_\theta \hat{\rho}_\theta] = -\partial_\theta \ln Z_\theta$. Given the exponential form of $\hat{\rho}_\theta$, we use the following integral expression to expand the derivative [2]:

$$\partial_\theta [e^{-\hat{A}_\theta}] := - \int_0^1 da e^{-(1-a)\hat{A}_\theta} \partial_\theta [\hat{A}_\theta] e^{-a\hat{A}_\theta}, \quad (3)$$

where $a \in \mathbb{R}$ is a real number. Using this the QFI becomes

$$\begin{aligned} F(\theta) &= 2 \sum_{n,m} \frac{|\langle\psi_n|\partial_\theta e^{-(\hat{A}_\theta + \ln Z_\theta)}|\psi_m\rangle|^2}{p_n + p_m}, \\ &= \frac{2}{Z_\theta^2} \sum_{n,m} \frac{1}{p_n + p_m} \left| \langle\psi_n| \int_0^1 da e^{-(1-a)\hat{A}_\theta} \delta\hat{B}_\theta e^{-a\hat{A}_\theta} |\psi_m\rangle \right|^2, \\ &= \sum_n p_n |\langle\psi_n|\delta\hat{B}_\theta|\psi_n\rangle|^2 + \frac{4}{Z_\theta^2} \sum_{n < m} \frac{1}{p_n + p_m} |\langle\psi_m|\hat{B}_\theta|\psi_n\rangle|^2 \left[\int_0^1 da e^{-(a\lambda_m + (1-a)\lambda_n)} \right]^2, \\ &= \sum_n p_n |\langle\psi_n|\delta\hat{B}_\theta|\psi_n\rangle|^2 + 4 \sum_{n < m} \frac{(p_n - p_m)^2}{p_n + p_m} |\langle\psi_n|\hat{B}_\theta|\psi_m\rangle|^2 \frac{1}{(\ln p_n - \ln p_m)^2}. \end{aligned} \quad (4)$$

Let us now use the following expression for the variance:

$$\begin{aligned} \text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] &= \sum_{n,m} \frac{p_n + p_m}{2} |\langle\psi_n|\delta\hat{B}_\theta|\psi_m\rangle|^2, \\ &= \sum_n p_n |\langle\psi_n|\delta\hat{B}_\theta|\psi_n\rangle|^2 + \sum_{n \neq m} \frac{p_n + p_m}{2} |\langle\psi_n|\delta\hat{B}_\theta|\psi_m\rangle|^2, \\ &= \sum_n p_n |\langle\psi_n|\delta\hat{B}_\theta|\psi_n\rangle|^2 + \sum_{n < m} (p_n + p_m) |\langle\psi_n|\delta\hat{B}_\theta|\psi_m\rangle|^2. \end{aligned} \quad (5)$$

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Following this we now substitute (5) into (4), which gives the following expression for the QFI:

$$F(\theta) = \text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] + \sum_{n < m} \left[\left(\frac{2(p_n - p_m)}{\ln(p_n/p_m)} \right) \left(\frac{2(p_n - p_m)}{(p_n + p_m) \ln(p_n/p_m)} \right) - (p_n + p_m) \right] |\langle \psi_n | \hat{B}_\theta | \psi_m \rangle|^2. \quad (6)$$

We now turn to the average WYD skew information of observable $\hat{B}_\theta$, which is given by

$$Q[\hat{\rho}_\theta, \hat{B}_\theta] = -\frac{1}{2} \int_0^1 da \, \text{tr}[[\hat{B}_\theta, \hat{\rho}_\theta^a][\hat{B}_\theta, \hat{\rho}_\theta^{1-a}]]. \quad (7)$$

It follows from the analysis of [3] that for a full-rank state $Q[\hat{\rho}_\theta, \hat{B}_\theta]$ can also be expanded in the eigenbasis of $\hat{\rho}_\theta$, yielding

$$Q[\hat{\rho}_\theta, \hat{B}_\theta] = \sum_{n < m} \left(p_n + p_m - \frac{2(p_n - p_m)}{\ln p_n - \ln p_m} \right) |\langle \psi_n | \hat{B}_\theta | \psi_m \rangle|^2. \quad (8)$$

We now bound the QFI following on from (6):

$$\begin{aligned} F(\theta) &= \text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] + \sum_{n < m} \left[\left(\frac{2(p_n - p_m)}{\ln(p_n/p_m)} \right) \left(\frac{2(p_n - p_m)}{(p_n + p_m) \ln(p_n/p_m)} \right) - (p_n + p_m) \right] |\langle \psi_n | \hat{B}_\theta | \psi_m \rangle|^2, \\ &\leq \text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] + \sum_{n < m} \left[\frac{2(p_n - p_m)}{\ln(p_n/p_m)} - (p_n + p_m) \right] |\langle \psi_n | \hat{B}_\theta | \psi_m \rangle|^2, \\ &= \text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] - Q[\hat{\rho}_\theta, \hat{B}_\theta], \end{aligned} \quad (9)$$

where in the second line we used the fact that $(p_n - p_m)/\ln(p_n/p_m) \geq 0$ since $p_n \geq p_m$ for $n < m$, and the inequality

$$\frac{x-1}{x+1} \leq \ln \sqrt{x}; \quad x \geq 1, \quad (10)$$

identifying $x = p_n/p_m \geq 1$. This allowed us to use

$$\left(\frac{2(p_n - p_m)}{(p_n + p_m) \ln(p_n/p_m)} \right) \leq 1, \quad (11)$$

for each term inside the sum. In the third line we used the expression (8) for the skew information. Finally we recall that $\text{Var}[\hat{\rho}_\theta, \hat{B}_\theta] - Q[\hat{\rho}_\theta, \hat{B}_\theta] = K[\hat{\rho}_\theta, \hat{B}_\theta]$, and so we arrive at the bound on the QFI stated in the main text:

$$F(\theta) \leq K[\hat{\rho}_\theta, \hat{B}_\theta]. \quad (12)$$

SUPPLEMENTARY NOTE 2: DERIVATION OF THE MODIFIED FLUCTUATION-DISSIPATION RELATION

Denote the operator $\delta \hat{E}_s^* := \hat{E}_s^*(T) - \langle \hat{E}_s^*(T) \rangle$ as the deviation in internal energy and $\Delta U_s^2 = \text{tr}[\hat{\pi}_s(T)(\delta \hat{E}_s^*)^2]$ as the energy variance, dropping the temperature dependence for now. We now evaluate the average WYD skew information of the internal energy:

$$\begin{aligned} Q[\hat{\pi}_s, \hat{E}_s^*] &= \Delta U_s^2 - K[\hat{\pi}_s, \hat{E}_s^*], \\ &= \Delta U_s^2 - \int_0^1 da \, \text{tr}[\hat{\pi}_s^{1-a} \delta \hat{E}_s^* \hat{\pi}_s^a \delta \hat{E}_s^*], \\ &= \Delta U_s^2 - \int_0^1 da \, \text{tr}[e^{-(1-a)(\beta \hat{H}_s^* + \ln Z_s^*)} \delta \hat{E}_s^* e^{-a(\beta \hat{H}_s^* + \ln Z_s^*)} \delta \hat{E}_s^*], \\ &= \Delta U_s^2 + \text{tr}[\delta \hat{E}_s^* \partial_\beta \hat{\pi}_s], \\ &= \Delta U_s^2 + \text{tr}[\hat{E}_s^* \partial_\beta \hat{\pi}_s], \\ &= \Delta U_s^2 - T^2 \text{tr}[\hat{E}_s^* \partial_T \hat{\pi}_s], \\ &= \Delta U_s^2 - T^2 \partial_T \text{tr}[\hat{E}_s^* \hat{\pi}_s] + T^2 \text{tr}[\partial_T \hat{E}_s^* \hat{\pi}_s], \\ &= \Delta U_s^2 - T^2 C_s(T) + T^2 \langle \partial_T \hat{E}_s^* \rangle, \end{aligned} \quad (13)$$

where we used the relation $\delta \hat{E}_s^* = \partial_\beta(\beta \hat{H}_s^* + \ln Z_s^*)$ and (3) in the fourth line, and the fact that the operator $\partial_\beta \hat{\pi}_s$ is traceless in the fifth line. Rearranging both sides yields the modified fluctuation-dissipation relation:

$$C_s(T) = \frac{\Delta U_s^2}{T^2} - \frac{Q[\hat{\pi}_s, \hat{E}_s^*]}{T^2} + \langle \partial_T \hat{E}_s^* \rangle. \quad (14)$$

SUPPLEMENTARY NOTE 3: CALCULATIONS FOR THE DAMPED HARMONIC OSCILLATOR

As stated in the main text the mean force Hamiltonian of the probe is given by $\hat{H}_s^*(T) = \omega_T(\hat{n}_T + \frac{1}{2})$, with $\hat{n}_T = \hat{a}_T^\dagger \hat{a}_T$ and $\hat{a}_T = \sqrt{\frac{A_T}{2}}(\hat{x} + i\frac{\hat{p}}{A_T})$. We will set $\hbar = 1$ throughout and A_T is given by $A_T = \sqrt{\langle \hat{p}^2 \rangle / \langle \hat{x}^2 \rangle}$, where the effective mass and frequency are given respectively by

$$M_T = \omega_T^{-1} \sqrt{\frac{\langle \hat{p}^2 \rangle}{\langle \hat{x}^2 \rangle}}, \quad (15)$$

$$\omega_T = 2T \operatorname{arccoth}(2\sqrt{\langle \hat{p}^2 \rangle \langle \hat{x}^2 \rangle}). \quad (16)$$

We can diagonalise the state of the probe in terms of the number states of $\hat{n}_T$, so $\hat{\pi}_s(T) = e^{-\beta \hat{H}_s^*(T)} / Z_s^* = \sum_{n=0}^{\infty} p_n |n\rangle \langle n|$ where

$$p_n = \frac{e^{-\beta \epsilon_n}}{Z_s^*}, \quad Z_s^* = 2 \sinh^{-1} \left(\frac{\beta \omega_T}{2} \right), \quad (17)$$

and $\epsilon_n = \omega_T(n + \frac{1}{2})$. Furthermore, from the main text the internal energy operator is given by

$$\hat{E}_s^*(T) = \alpha_T \hat{H}_s^*(T) - g_T \frac{\hat{a}_T^2 + (\hat{a}_T^\dagger)^2}{2}, \quad (18)$$

with $\alpha_T = 1 - \frac{\omega'_T}{\omega_T} T$ and $g_T = \omega_T T \frac{A'_T}{A_T}$. The functions g_T and α_T are determined by the effective mass and frequency of the oscillator defined above, so we need to calculate $\langle \hat{x}^2 \rangle$ and $\langle \hat{p}^2 \rangle$. In the continuum limit $N \rightarrow \infty$ the exact expressions for the quadratures are found to be [4]:

$$\langle \hat{x}^2 \rangle = \frac{1}{M\beta\omega^2} + \frac{\hbar}{M\pi} \sum_{i=1}^3 \left[\frac{(\lambda_i - \omega_D)\Gamma(1 + \frac{\beta\hbar\lambda_i}{2\pi})}{(\lambda_{i+1} - \lambda_i)(\lambda_{i-1} - \lambda_i)} \right], \quad (19)$$

$$\langle \hat{p}^2 \rangle = M\omega^2 \langle \hat{x}^2 \rangle + \frac{\hbar M \gamma \omega_D}{\pi} \sum_{i=1}^3 \left[\frac{\lambda_i \Gamma(1 + \frac{\beta\hbar\lambda_i}{2\pi})}{(\lambda_{i+1} - \lambda_i)(\lambda_{i-1} - \lambda_i)} \right], \quad (20)$$

where $\Gamma(z)$ is the digamma function and λ_i are the characteristic frequencies of the oscillator. In the limit of a large cutoff frequency, $\omega_D \gg \omega, \gamma$ the frequencies are given by

$$\lambda_1 = \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} - \omega^2}, \quad (21)$$

$$\lambda_2 = \frac{\gamma}{2} - \sqrt{\frac{\gamma^2}{4} - \omega^2}, \quad (22)$$

$$\lambda_3 = \omega_D - \gamma. \quad (23)$$

Due to the complicated dependence on T we will not present the exact analytic expressions for g_T and α_T , but we will proceed to calculate $C_s(T)$, $F_s(T)$ and $\langle \partial_T \hat{E}_s^* \rangle$. The average internal energy is found to be

$$\langle \hat{E}_s^* \rangle = \alpha_T \langle \hat{H}_s^*(T) \rangle, \quad (24)$$

$$\langle \hat{H}_s^*(T) \rangle = \frac{\omega_T}{2} \coth \left(\frac{\beta \omega_T}{2} \right). \quad (25)$$

The heat capacity can now be calculated by differentiating the average energy:

$$\begin{aligned}
C_S(T) &= \partial_T \langle \hat{E}_S^* \rangle, \\
&= \alpha'_T \frac{\omega_T}{2} \coth\left(\frac{\beta\omega_T}{2}\right) + \alpha_T \frac{\omega'_T}{2} \coth\left(\frac{\beta\omega_T}{2}\right) - \frac{\alpha_T \omega_T (\omega'_T \beta - \omega_T \beta^2)}{4 \sinh^2\left(\frac{\beta\omega_T}{2}\right)}, \\
&= \frac{1}{2} \coth\left(\frac{\beta\omega_T}{2}\right) (\alpha'_T \omega_T + \alpha_T \omega'_T) - \frac{\alpha_T \omega_T \beta (\omega'_T - \omega_T \beta)}{4 \sinh^2\left(\frac{\beta\omega_T}{2}\right)}.
\end{aligned} \tag{26}$$

In order to calculate the QFI (2) and skew information (8) we will need to obtain the elements $E_{nm} = |\langle n | \delta \hat{E}^* | m \rangle|^2$. Firstly one finds the following:

$$\begin{aligned}
\langle n | \delta \hat{E}^* | m \rangle &= \langle n | \hat{E}_S^* | m \rangle - \langle \hat{E}_S^* \rangle \delta_{n,m}, \\
&= \alpha_T \langle n | \hat{H}_S^*(T) | m \rangle - g_T \langle n | \frac{\hat{a}_T^2 + (\hat{a}_T^\dagger)^2}{2} | m \rangle - \langle \hat{E}_S^* \rangle \delta_{n,m}, \\
&= \alpha_T (\epsilon_n - \langle \hat{H}_S^*(T) \rangle) \delta_{n,m} - g_T \left(\frac{\sqrt{m} \sqrt{m-1}}{2} \delta_{n,m-2} + \frac{\sqrt{n} \sqrt{n-1}}{2} \delta_{m,n-2} \right),
\end{aligned} \tag{27}$$

where $\delta_{n,m}$ represents the Kronecker-Delta function. Squaring both sides yields

$$E_{nm} = \alpha_T^2 (\epsilon_n - \langle \hat{H}_S^*(T) \rangle)^2 \delta_{n,m} + \frac{g_T^2}{4} \left((n+2)(n+1) \delta_{n+2,m} + (m+2)(m+1) \delta_{m+2,n} \right), \tag{28}$$

The variance in internal energy is given by (5), so that

$$\begin{aligned}
\text{Var}[\hat{\pi}_S, \hat{E}_S^*] &= \sum_{n,m=0}^{\infty} p_n E_{nm}, \\
&= \alpha_T^2 \text{Var}[\hat{\pi}_S, \hat{H}_S^*] + \frac{g_T^2}{2} \sum_{n=0}^{\infty} p_n (n+1)(n+2), \\
&= \alpha_T^2 \text{Var}[\hat{\pi}_S, \hat{H}_S^*] + g_T^2 \sinh\left(\frac{\beta\omega_T}{2}\right) \sum_{n=0}^{\infty} (n+1)(n+2) e^{-\beta\omega_T(n+\frac{1}{2})}, \\
&= \alpha_T^2 \text{Var}[\hat{\pi}_S, \hat{H}_S^*] + 2g_T^2 \sinh\left(\frac{\beta\omega_T}{2}\right) \left(\frac{e^{-\frac{\beta\omega_T}{2}}}{(1 - e^{-\beta\omega_T})^3} \right), \\
&= \frac{\alpha_T^2 \omega_T^2}{4 \sinh^2\left(\frac{\beta\omega_T}{2}\right)} + 2g_T^2 \sinh\left(\frac{\beta\omega_T}{2}\right) \left(\frac{e^{-\frac{\beta\omega_T}{2}}}{(1 - e^{-\beta\omega_T})^3} \right),
\end{aligned} \tag{29}$$

where we used the series $\sum_{n=0}^{\infty} (n+1)(n+2)x^n = 2/(1-x)^3$ for $|x| < 1$ and that the variance of $\hat{H}_S^*(T)$ is

$$\text{Var}[\hat{\pi}_S, \hat{H}_S^*] = \frac{\omega_T^2}{4 \sinh^2\left(\frac{\beta\omega_T}{2}\right)}. \tag{30}$$

We now compute the QFI, using (2) and the fact that $p_n \pm p_{n+2} = p_n(1 \pm e^{-2\beta\omega_T})$:

$$\begin{aligned}
T^4 F_S(T) &= \sum_{n=0}^{\infty} p_n E_{nn} + 4 \sum_{n < m} \frac{(p_n - p_m)^2}{(p_n + p_m) \ln^2\left(\frac{p_n}{p_m}\right)} E_{nm}, \\
&= \alpha_T^2 \text{Var}[\hat{\pi}_S, \hat{H}_S^*] + \frac{g_T^2}{\beta^2 \omega_T^2} \sum_{n=0}^{\infty} \frac{(p_n - p_{n+2})^2}{p_n + p_{n+2}} (n+2)(n+1), \\
&= \alpha_T^2 \text{Var}[\hat{\pi}_S, \hat{H}_S^*] + \frac{g_T^2 (1 - e^{-2\beta\omega_T})^2}{\beta^2 \omega_T^2 (1 + e^{-2\beta\omega_T})} \sum_{n=0}^{\infty} p_n (n+2)(n+1), \\
&= \alpha_T^2 \text{Var}[\hat{\pi}_S, \hat{H}_S^*] + \frac{g_T^2}{\beta^2 \omega_T^2} \sinh\left(\frac{\beta\omega_T}{2}\right) \left(\frac{(1 - e^{-2\beta\omega_T})^2}{(1 + e^{-2\beta\omega_T})} \right) \left(\frac{e^{-\frac{\beta\omega_T}{2}}}{(1 - e^{-\beta\omega_T})^3} \right), \\
&= \frac{\alpha_T^2 \omega_T^2}{4 \sinh^2\left(\frac{\beta\omega_T}{2}\right)} + \frac{g_T^2}{\beta^2 \omega_T^2} \sinh\left(\frac{\beta\omega_T}{2}\right) \left(\frac{(1 - e^{-2\beta\omega_T})^2}{(1 + e^{-2\beta\omega_T})} \right) \left(\frac{e^{-\frac{\beta\omega_T}{2}}}{(1 - e^{-\beta\omega_T})^3} \right),
\end{aligned} \tag{31}$$

We also require the average skew information, which can be obtained using (8):

$$\begin{aligned}
Q[\hat{\pi}_S, \hat{E}_S^*] &= \sum_{n < m} \left(p_n + p_m - \frac{2(p_n - p_m)}{\ln p_n - \ln p_m} \right) E_{nm}, \\
&= \frac{g_T^2}{4} \sum_{n=0}^{\infty} \left(p_n + p_{n+2} - \frac{2(p_n - p_{n+2})}{\ln p_n - \ln p_{n+2}} \right) (n+2)(n+1), \\
&= g_T^2 \sinh\left(\frac{\beta\omega_T}{2}\right) \frac{e^{-\frac{\beta\omega_T}{2}}}{(1 - e^{-\beta\omega_T})^3} \left(1 + e^{-2\beta\omega_T} - \frac{T}{\omega_T} (1 - e^{-2\beta\omega_T}) \right). \tag{32}
\end{aligned}$$

To calculate the term $\langle \partial_T \hat{E}_S^* \rangle$ we use the fluctuation-dissipation relation (14):

$$\begin{aligned}
\langle \partial_T \hat{E}_S^* \rangle &= C_S(T) + \frac{Q[\hat{\pi}_S, \hat{E}_S^*] - \text{Var}[\hat{\pi}_S, \hat{E}_S^*]}{T^2}, \\
&= C_S(T) - \frac{g_T^2}{T\omega_T} \sinh\left(\frac{\beta\omega_T}{2}\right) \left(\frac{(1 - e^{-2\beta\omega_T})}{(1 - e^{-\beta\omega_T})^3} \right) e^{-\frac{\beta\omega_T}{2}}. \tag{33}
\end{aligned}$$

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