QUANTUM THERMOMETRY

Lecture notes Quantum thermodynamics Summer School

Main topics and relevant references → (biased selection!)

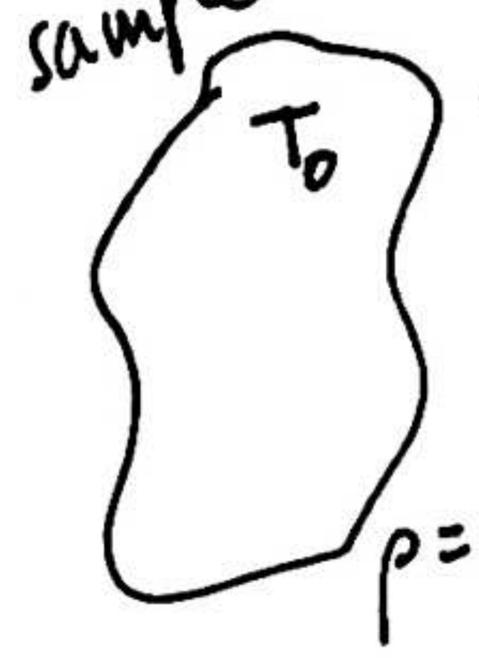
1. Motivation (review q. thermometry: arxiv. 1811.03988)
2. Crámer - Rao bound (e.g. ~~or~~ see arxiv: 1804.10048)
3. Quantum Fisher Information (see e.g. arxiv:0804.2981)
4. Energy - Temperature uncertainty relation: $\Delta\beta\Delta H \geq 1$.
5. Low - temperature thermometry (arxiv: 1711.09827)
6. Optimal thermometers and critically - enhanced thermometry (arxiv: 1411.2437, arxiv: 2108.05932)

Motivation

Q. Thermometry: an applied science, with fundamental implications.

applied ↓
- cold atomic ensembles
- nanoresonators
- black body radiation

fundamental ↓
- nature of temperature & entropy
- equivalence of ensembles
- third law of thermodynamics



$$\rho = \frac{e^{-H/k_B T_0}}{Z}$$

but also microcanonical ensemble, pure state ...

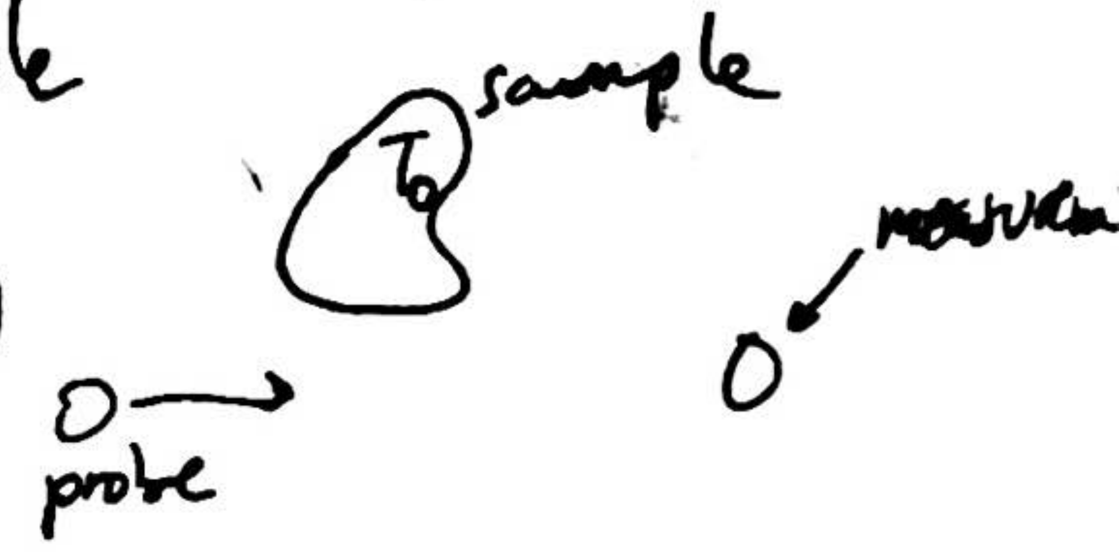
* Temperature is not an observable, it needs to be indirectly inferred

Basic steps in an estimation process:

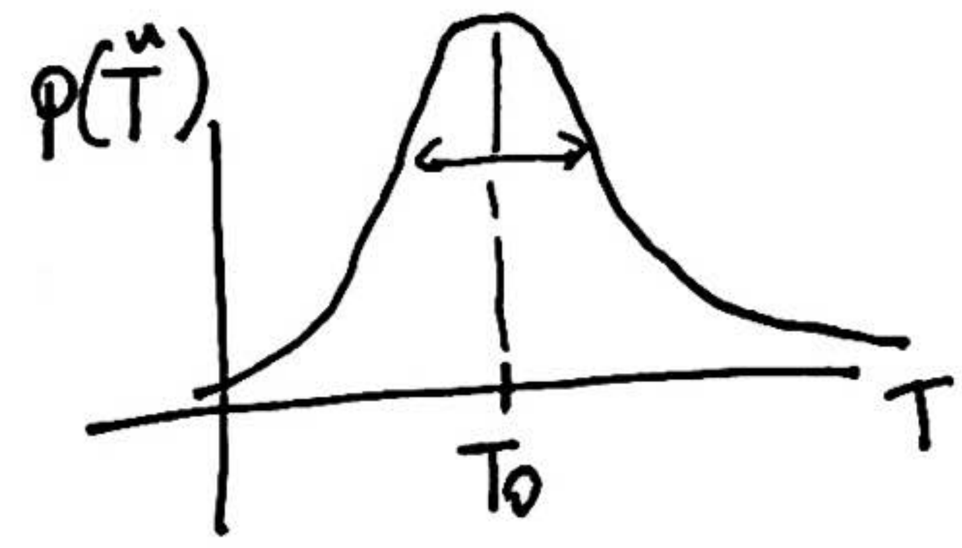
"m" independent measurements μ_j i.i.d. → In this lecture!! (not general)

Data acquisition $\{\mu_1, \mu_2, \dots, \mu_m\} \equiv \vec{\mu}$ → Data processing $\hat{T}(\vec{\mu})$ → estimator: $\vec{\mu} \to \hat{T}(\vec{\mu})$, temperature estimate

→ - direct measurements of the sample
- probe-based thermometry



→ When "m" is finite, and due to thermal and quantum fluctuations, ~~[illegible]~~ $\hat{T}$ will usually fluctuate.



* → Explain Frameworks here.

→ What makes a good estimation process?

* Accurate (unbiased)

$$\langle \text{Bias} \rangle \equiv \langle \hat{T} \rangle - T_0 = \left(\sum_{\vec{\mu}} p(\vec{\mu}|T_0)\, \hat{T}(\vec{\mu})\right) - T_0$$

the sum extends over all possible outcomes for a given "m"

- unbiased: $\langle \text{Bias} \rangle = 0 \quad \forall T_0$ → great, but typically not the case.
- locally unbiased $\left[\langle \hat{T} \rangle = T_0 \text{ for a given } T_0 \quad \frac{d(\langle \hat{T} \rangle - T)}{dT}\Big|_{T=T_0} = 0 \right.$

* Precise (small fluctuations)

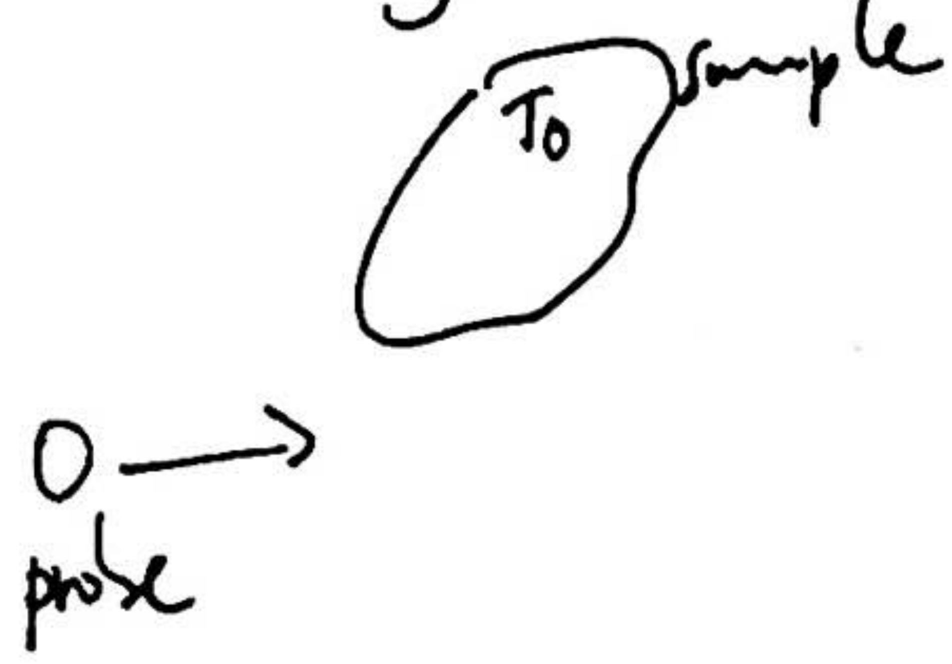
mean squared error ← $$M.S.E \equiv \langle (\hat{T} - T_0)^2 \rangle = \sum_{\vec{\mu}} p(\vec{\mu}|T_0) \left(\hat{T}(\vec{\mu}) - T_0\right)^2$$

as small as possible.

$\boxed{MSE \to 0}$ guarantees both accurate and precise → main figure of merit.

"Bonus"

* minimally - invasive estimation processes



* optimal use of <u>resources</u>: | number of probes/measurements "m"
| time, "t"

$$M.S.E. \sim f(m, t)$$

→ * Frameworks
→ gen before

| Frequentist → applicable to any "m" but most useful for $m \gg 1$. (and given identical repeated measurements)
→ this lecture.

| Bayesian → useful for any "m". (and for correlated/adaptive measurements)
→ needs the notion of a prior/posterior

↓

see arxiv: 2011.13018, arxiv: 2108.05932

$\boxed{\text{Cramér - Rao bound}}$

$$\rightarrow \quad M.S.E_{T_0} = \Delta^2 \check{T} + \big(\overbrace{\langle \check{T} \rangle_{T_0} - T_0}^{\text{Bias}}\big)^2$$

$$\Delta^2 \check{T} \equiv \langle (\check{T} - \langle \check{T} \rangle_{T_0})^2 \rangle_{T_0} \qquad \text{with} \quad \langle \dots \rangle_{T_0} \equiv \sum_{\vec{\mu}} p(\mu|T_0)(\dots)$$

$$\rightarrow \quad \left(\frac{d \langle T_{est} \rangle_T}{dT} \right)^2 = \left(\sum_{\vec{\mu}} \frac{d\, p(\vec{\mu}|T)}{dT} \check{T}(\vec{\mu}) \right)^2$$

$$= \left[\sum_{\vec{\mu}} \frac{dp(\vec{\mu}|T)}{dT} \left(\check{T}(\vec{\mu}) - \langle \check{T} \rangle \right) \right]^2$$

$\sum_{\vec{\mu}} \frac{d\,p(\vec{\mu}|T)}{dT} = 0$

$$= \Bigg[\sum_{\vec{\mu}} \underbrace{\frac{1}{\sqrt{p(\vec{\mu}|T)}} \frac{dp(\vec{\mu}|T)}{dT}}_{\vec{X}_j} \underbrace{\sqrt{p(\vec{\mu}|T)} \left(\check{T}(\vec{\mu}) - \langle \check{T} \rangle \right)}_{Y_j} \Bigg]^2$$

Cauchy-Schwarz

$|\langle \vec{X}, \vec{Y} \rangle|^2 \leq \langle \vec{X}, \vec{X} \rangle \langle \vec{Y}, \vec{Y} \rangle$

$$\leq \sum_{\vec{\mu}} \frac{1}{p(\vec{\mu}|T)} \left(\frac{dp(\vec{\mu}|T)}{dT} \right)^2 \sum_{\vec{\mu}'} p(\vec{\mu}'|T) \left(\check{T}(\vec{\mu}) - \langle \check{T} \rangle \right)^2$$

identical, uncorrelated "m" measurements:

$p(\vec{\mu}|T) = \prod_{i=1}^{m} p(\mu_i|T)$

$$= m \underbrace{\boxed{\sum_{\mu} \frac{1}{p(\mu|T)} \left(\frac{dp(\mu|T)}{dT} \right)^2}}_{\text{Fisher information } F_c} \Delta^2 \check{T}$$

$\rightarrow$ For locally unbiased estimators: $\left(\frac{d \langle T_{est} \rangle_T}{dT} \Big|_{T=T_0} = 1, \quad \Delta^2 \check{T} = M.S.E. \right)$

$$\boxed{M.S.E \geq \frac{1}{m F_c}}$$

→ Examples of estimators and asymptotic unbiasedness

"m" qubits at temperature T_0

$$q_0 = \frac{e^{-E/k_B T_0}}{1+e^{-E/k_B T_0}} \rightarrow \text{excitation probability}$$

$\ominus \quad \ominus \quad \dots \quad \ominus \updownarrow E$

measure energy (in the computational basis)

data set: (example) $\vec{\mu} = \underbrace{\{0, 1, 1, \dots, 0\}}_{\boxed{\substack{k \to 1\text{'s} \\ m-k \to 0\text{'s}}}}$.

$$p(\vec{\mu}\,|\,T_0) \longrightarrow p(k\,|\,q_0) = q_0^{\,k}\,(1-q_0)^{m-k}\,\frac{m!}{k!\,(m-k)!}$$

$q_0 \leftrightarrow T_0$

→ maximum likelihood estimator

$$\check{q}_0(k) = \underset{q_0}{\arg\max}\; p(k\,|\,q_0) \Rightarrow \boxed{\check{q}_0(k) = \frac{k}{m}}$$

from here we compute $\check{T}_0(k)$

→ mean estimator

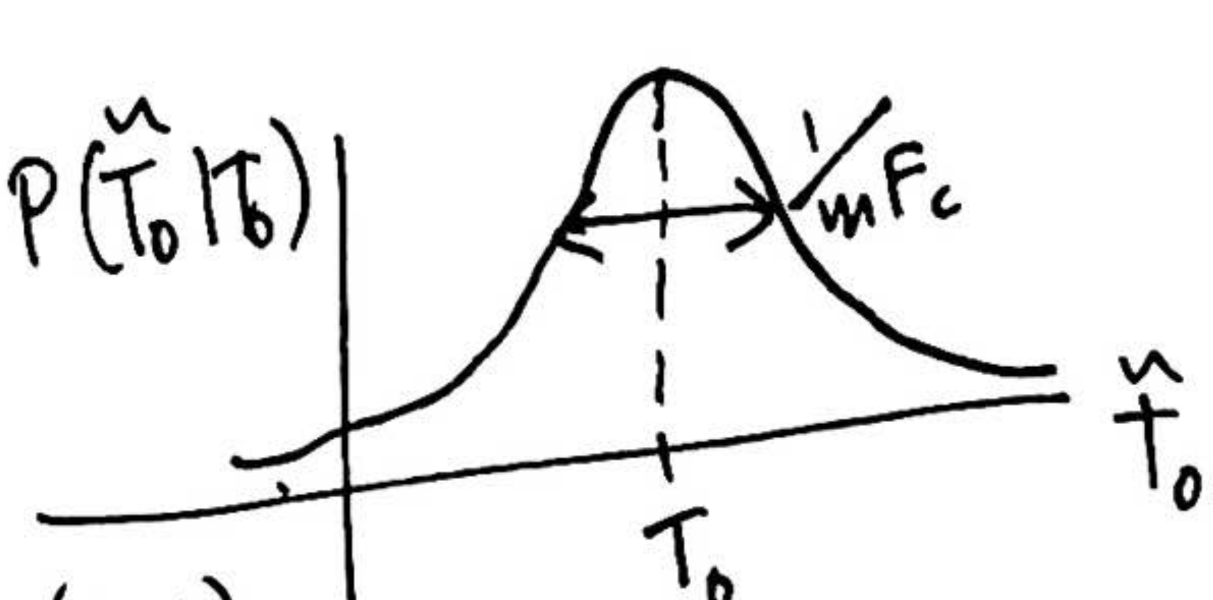
→ For sufficiently large $m \gg 1$, we obtain (using the central limit theorem)

$$\boxed{p\left(\check{T}_0\,|\,T_0\right) = \sqrt{\frac{m\,F_c}{2\pi}}\; e^{-\frac{mF_c}{2}\left(T_0-\check{T}_0\right)^2}}$$

unbiased estimator with $\Delta\check{T}^2 = \frac{1}{mF_c}$

$\langle \check{T}_0\rangle = T_0$

⚠



Exercise: reproduce calculations of Jahnke, Lanéry, Mahler, PRE 83, 011109 (2011)

Quantum Fisher Information

$\to$ POVM.

In Quantum mechanics: $p(\mu | T) = \mathrm{Tr}\left(\Pi_\mu \rho_T\right)$

- let us introduce: $\dfrac{\partial \rho_T}{\partial T} = \dfrac{L_T \rho_T + \rho_T L_T}{2}$ $\to$ symmetric logarithmic derivative.

$$\partial_T p(\mu | T) = \mathrm{Tr}\left(\partial_T \rho_T \Pi_\mu\right) = \mathrm{Re}\left(\mathrm{Tr}\left[\rho_T \Pi_\mu L_T\right]\right)$$

- Fisher information:

$$F_c = \sum_\mu \frac{1}{p_\mu}\left(\frac{dp_\mu}{dT}\right)^2 = \sum_\mu \frac{\mathrm{Re}\left(\mathrm{Tr}\left[\rho_T \Pi_\mu L_T\right]\right)^2}{\mathrm{Tr}\left(\rho_T \Pi_\mu\right)}$$

saturated when $\mathrm{Tr}(\rho_T \Pi_\mu L_T)$ is real

$$\leq \sum_\mu \left|\frac{\mathrm{Tr}\left[\rho_T \Pi_\mu L_T\right]}{\sqrt{\mathrm{Tr}\left(\rho_T \Pi_\mu\right)}}\right|^2 = \sum_\mu \left|\mathrm{Tr}\left[\frac{\sqrt{\rho_T}\sqrt{\Pi_\mu}}{\sqrt{\mathrm{Tr}(\rho_T \Pi_\mu)}} \sqrt{\Pi_\mu} L_T \sqrt{\rho_T}\right]\right|^2$$

Cauchy-Schwartz $|\mathrm{Tr}[A^\dagger B]|^2 \leq \mathrm{Tr}[A^\dagger A]\,\mathrm{Tr}[B^\dagger B]$

$$\leq \sum_\mu \mathrm{Tr}\left[\Pi_\mu L_T \rho_T L_T\right]$$

$\sum_\mu \Pi_\mu = \mathbb{1}$

$$= \mathrm{Tr}\left[\rho_T L_T^2\right]$$

$$\boxed{F_c \leq \mathrm{Tr}\left[\rho_T L_T^2\right]}$$

Quantum Fisher information

$$\boxed{F_Q = \mathrm{Tr}\left[\rho_T L_T^2\right]}$$

it depends only on ρ_T, independent of the measurement

$$\boxed{\max_{\text{all measurements}}\left(F_c\right) = F_Q}$$

Optimal measurement

$\Downarrow$

$$L_\lambda = \sum_k q_k \hat{\Pi}_k$$

for this POVM C-S is tight:

$$\frac{\sqrt{\hat{\Pi}_k}\sqrt{\rho_T}}{\sqrt{\rho_T}} \propto \sqrt{\hat{\Pi}_k} L_T \sqrt{\rho_T} \quad \forall k$$

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Quantum Fisher Information in Thermometry

$$\rho_T = \frac{e^{-H/T}}{\mathrm{Tr}\left(e^{-H/T}\right)} \qquad \text{(in what follows } k_B = 1\text{)}$$

$$\frac{\partial \rho_T}{\partial T} = \frac{e^{-H/T} H}{Z\, T^2} - \frac{e^{-H/T}\,\mathrm{Tr}\left(H e^{-H/T}\right)}{Z^2\, T^2}$$

$$= \frac{H \rho_T}{T^2} - \frac{\rho_T \langle H \rangle_{\rho_T}}{T^2} \qquad \langle A \rangle_{\rho_T} \equiv \mathrm{Tr}\left(A \rho_T\right)$$

$$= \rho_T \underbrace{\left(\frac{H - \langle H \rangle_{\rho_T}}{T^2} \right)}_{L_T}$$

$$F_Q = \mathrm{Tr}\left(\rho_T L_T^2\right) = \frac{1}{T^4} \mathrm{Tr}\left(\rho_T \left(H - \langle H \rangle_{\rho_T}\right)^2\right)$$

$$\boxed{F_Q = \frac{1}{T^4} \Delta H^2}$$

Recap:

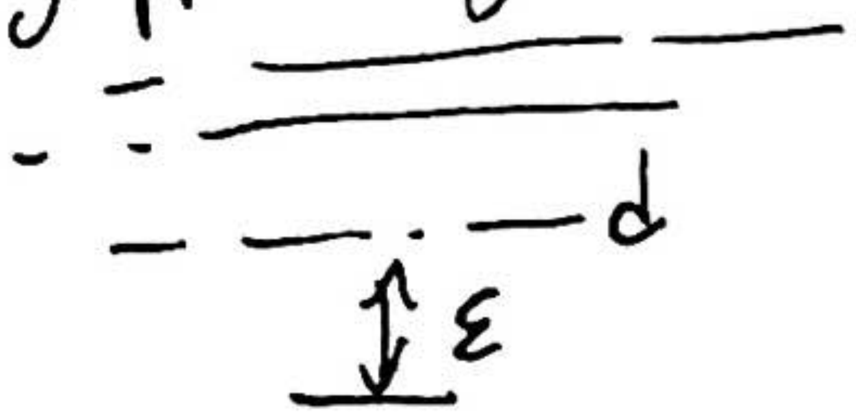
$$\boxed{\underset{\Delta \tilde{T}^2}{\underset{\approx}{\text{M.S.E}}} \underset{\substack{\uparrow \\ \text{locally} \\ \text{unbiased} \\ \text{estimators}}}{\geq} \frac{1}{m F_C} \underset{\substack{\uparrow \\ \text{projective} \\ \text{energy} \\ \text{measurements}}}{\geq} \frac{T^4}{m \Delta H^2}} \leftarrow \text{MAIN TAKE-HOME MESSAGE.}$$

Remark: for $n=1$ (this is justified because $p(\vec{\mu}|T)$ belongs to the exponential family see e.g. arxiv: 1409.0535)

$$\boxed{\Delta \tilde{T}^2 \geq \frac{T^4}{\Delta H^2}} \quad \text{Energy - temperature uncertainty relation}$$

low-temperature thermometry: ~~why so hard?~~ why is it so hard?

→ gapped systems



assume $k_B T \ll \varepsilon$, then population is found in the first two levels (up to exponential corrections)

$$p \simeq \frac{d\, e^{-\varepsilon/T}}{1 + d\, e^{-\varepsilon/T}}$$

$$\Delta H^2 = \varepsilon^2 p(1-p) \simeq \varepsilon^2 p \simeq \varepsilon^2 d\, e^{-\varepsilon/T}$$

$$\Delta H^2 = \varepsilon^2 d\, e^{-\varepsilon/T} + \mathcal{O}(e^{-2\varepsilon/T})$$

$$\Delta \tilde{T}^2 \geq \frac{k_B T^4\, e^{\varepsilon/T}}{m d \varepsilon^2},$$

diverges exponentially!

$$\boxed{\frac{\Delta T^2}{T^2} \geq \frac{k_B T^2\, e^{\varepsilon/T}}{m d \varepsilon^2}}$$

→ gapless systems

Remark: $C = \frac{\Delta H^2}{T^2}$;

↑ heat capacity!

$$C = T \frac{\partial S_{th}}{\partial T} = \frac{\partial \langle H \rangle_\beta}{\partial T}$$

$$\langle H \rangle_T = \mathrm{Tr}\left(H \frac{e^{-\beta H}}{Z}\right)$$

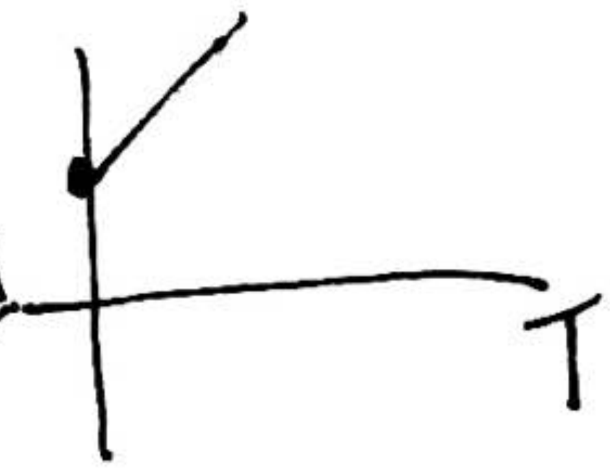
$$S = -\mathrm{Tr}(\rho_T \ln \rho_T)$$

$$\frac{\Delta T^2}{T^2} \geq \frac{1}{C} = \frac{1}{T \partial_T S_{th}} \Rightarrow \boxed{\frac{\Delta T^2}{T^2} \sim \frac{1}{T}}$$

non-exponential divergence! see e.g. arxiv: 1711.09827

Third law of thermodynamics: $S_{th} = \text{ctnt}$ at $T = 0$.

$\partial_T S_{th} = \text{ctnt}'$ → also often assumed



Criticality-enhanced thermometry

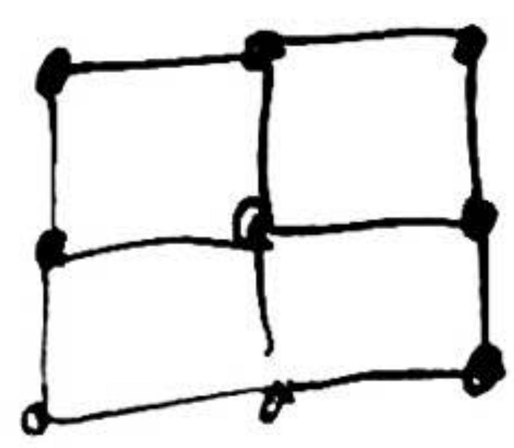
$$\frac{\Delta T^2}{T^2} \geq \frac{1}{mC} \qquad C = \frac{\Delta H^2}{T^2}$$

↑ heat capacity

→ imagine our sample is ~~a set~~ set of "n" ~~parts~~ systems

$\ominus \ \ominus \ -- \ \ominus \qquad C = n \cdot C_{syst.}$

→ our sample is a ~~set~~ composed of "n" interacting systems but away from a phase transition (recall Alvaro's talk)



$C = n \, \hat{C}_{syst}$ → same scaling, different slope.

→ However, in a phase transition : $C \propto n^{1+x}$ with $0 \leq x \leq 1$

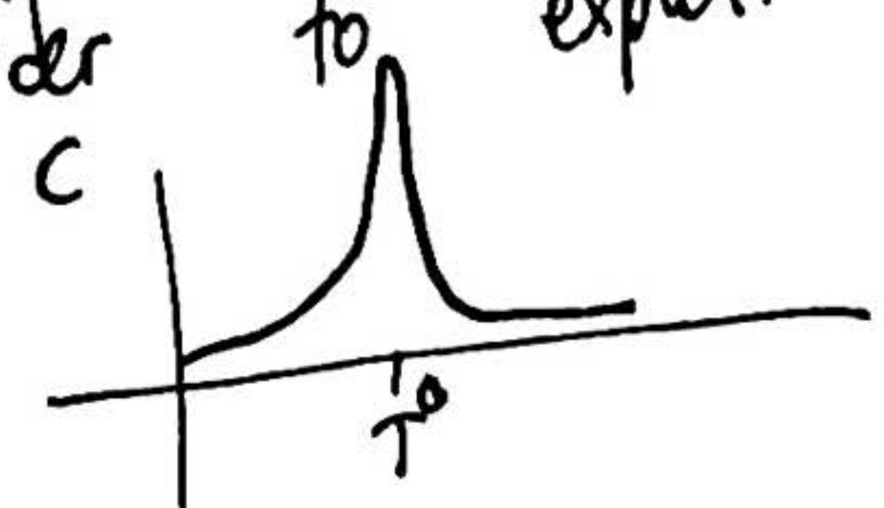
It turns out that the maximum C satisfies

$$\boxed{\max_{\text{all } H} C \simeq \frac{n^2}{4}}$$

arxiv: 1411.2437

But: * it requires highly non-local interactions — with two body interactions it is possible to achieve $\simeq \frac{C_{max}}{2}$

* it requires very precise prior knowledge of the estimated temperature in order to exploit criticality



This can be ~~overcome~~ ~~via~~ overcomed via *adaptive strategies*

arxiv: 2108.05932