Prediction, Retrodiction, and the Second Law of Thermodynamics

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About these ideas

Two papers:

- with V. Scarani. *Fluctuation relations from Bayesian retrodiction*. Phys. Rev. E (2021). arXiv:2009.02849 [quant-ph]
- with C.C. Aw and V. Scarani. *Fluctuation Theorems with Retrodiction rather than Reverse Processes*. arXiv:2106.08589 [cond-mat.stat-mech]

New physics!!

PHYSICS

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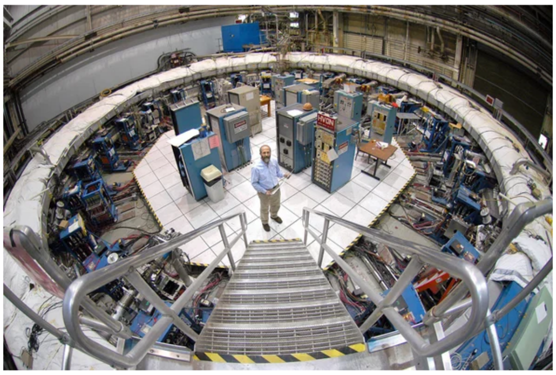
Initial data from the Muon g-2 experiment have excited particle physicists searching for undiscovered subatomic particles and forces

By Daniel Garisto on April 7, 2021 أعرض هذا باللغة العربية



Muon g-2 magnetic storage ring, seen here at Brookhaven National Laboratory in New York State before its 2013 relocation to Fermi National Accelerator Laboratory in Illinois. Credit: Alamy

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A step towards LIMITLESS energy: Loophole found in a fundamental law of physics may lead to infinite power

- **The finding may mean it's possible to create perpetual motion machines**
- **These machines can spin for eternity without losing any energy**
- **The four laws of thermodynamics set the physical rules for our universe**
- **Researchers found a way to bypass the second law of the four**
- **They have since projected a quantum system in which energy can be recycled**

By HARRY PETTIT FOR MAILONLINE
PUBLISHED: 14:00 BST, 3 November 2016 | **UPDATED:** 17:03 BST, 3 November 2016

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Einstein once boldly claimed that the Laws of Thermodynamics were the only physical theory of the universe that will 'never be overthrown'.

That all changed late last month, when scientists from the **Argonne National Laboratory** at the University of Chicago found a loophole in the system - one that allows them to break the second law of thermodynamics.

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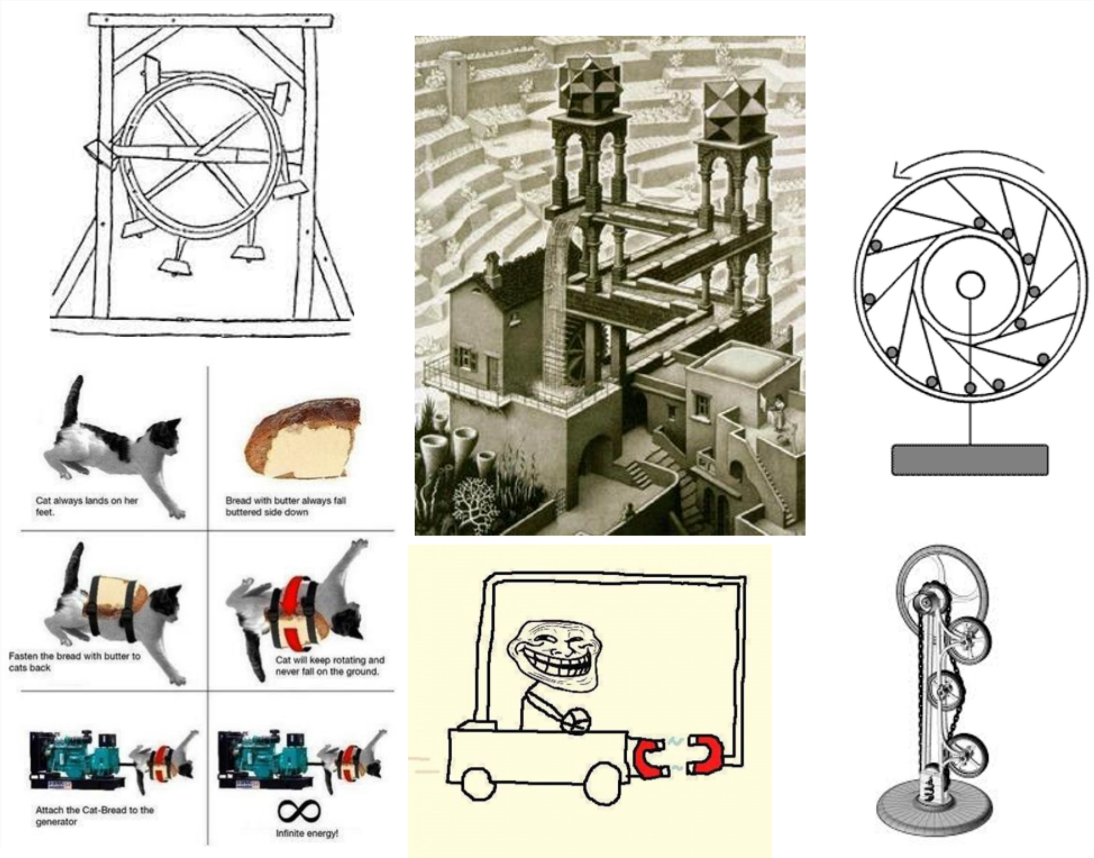
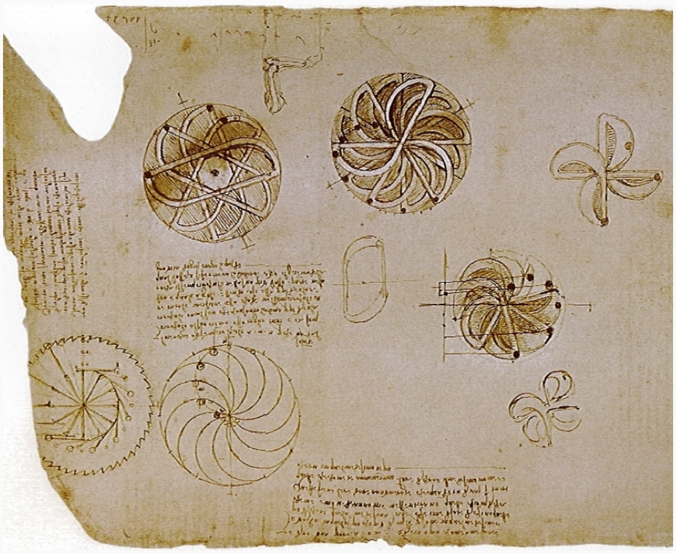


Leonardo's wheel



"Oh ye seekers after perpetual motion, how many vain chimeras have you pursued? Go and take your place with the alchemists."

Leonardo da Vinci

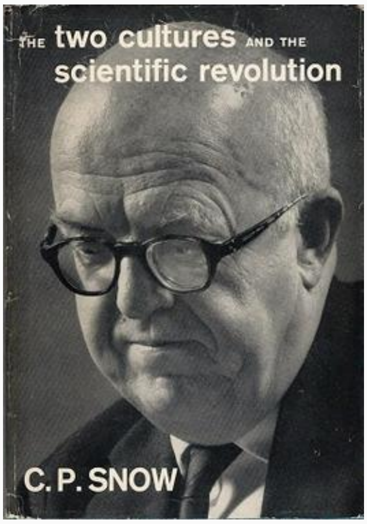
The Second Law is “special”

“The law that entropy always increases holds, I think, the supreme position among the laws of Nature. [. . .] If your theory is found to be against the Second Law of Thermodynamics I can give you no hope; there is nothing for it to collapse in deepest humiliation.”

A.S. Eddington

“[. . .] the only physical theory of universal content concerning which I am convinced that, within the framework of the applicability of its basic concepts, it will never be overthrown.” A. Einstein

Have you read a work of Shakespeare’s?



“Once or twice I have been provoked and have asked the company how many of them could describe the Second Law of Thermodynamics. The response was cold: it was also negative. Yet I was asking something which is about the equivalent of: Have you read a work of Shakespeare’s?” C.P. Snow

The “to be or not to be” of thermodynamics

The Second Axiom of Thermodynamics

A *perpetuum mobile* of the second kind is impossible; in formula,

$$\langle \Delta S_{\text{tot}} \rangle \geq 0 \ .$$

Why does the above inequality “feel” so special among physical laws?

That is the question.

Is entropy the key?

Many “explanations” of the Second Law actually amount to explanations of entropy (e.g., counting arguments).

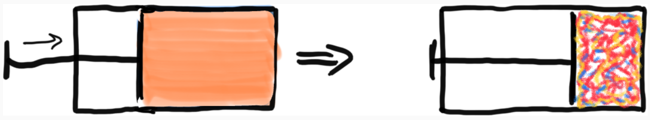
Problem is...

“ No one understands entropy very well...”

von Neumann (apocryphal)

“ ...and that’s only half of the story, anyway.” Anon

The Second Law “without entropy”

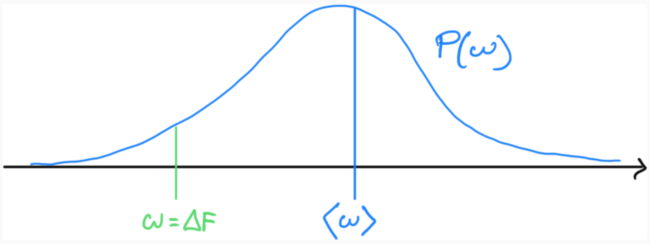


Clausius’ inequality (1865):

$$\langle W \rangle \geq \Delta F$$

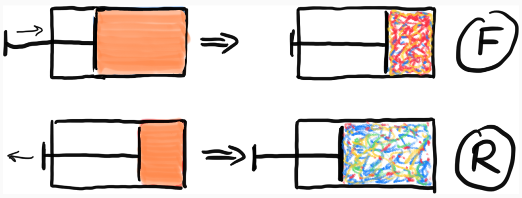
Jarzynski’s equality (1997):

$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$$



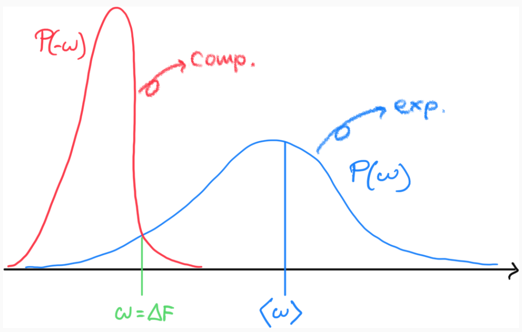
Jarzynski $\Longrightarrow$ Clausius

The Second Law and irreversibility



Crooks’ fluctation theorem (1999)

$$\frac{\mathcal{P}_F(W)}{\mathcal{P}_R(-W)} = e^{\beta(W-\Delta F)}$$



Crooks $\Longrightarrow$ Jarzynski $\Longrightarrow$ Clausius

Usual explanation

Crooks' theorem, and hence Jarzynski's relation, and hence the Second Law, all rely on two assumptions satisfied at equilibrium:

1. thermal distribution: microstate probability is $\mathcal{P}(\xi) \propto e^{-\beta\epsilon(\xi)}$
2. microscopic reversibility (cf. *detailed balance*): molecular processes and their reverses occur at the same rate

But, again: why does the Second Law feel so special then?

Is that because of some kind of "special" microscopic balancing mechanism?

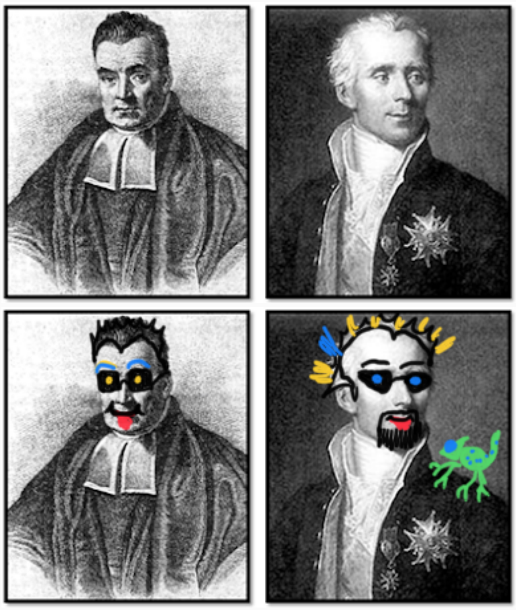
A hint from Ed Jaynes

"To understand and like thermo we need to see it, not as an example of the n-body equations of motion, but as an example of the logic of ***scientific inference****."*

E.T. Jaynes (1984)

First idea: reverse process as Bayesian retrodiction

The Bayes-Laplace Rule



Inverse Probability Formula

$$\underbrace{\mathcal{P}(H|D)}_{\text{inv. prob.}} \propto \underbrace{\mathcal{P}(D|H)}_{\text{likelihood/model}} \underbrace{\mathcal{P}(H)}_{\text{prior}}$$

where H is a hypothesis, D is the result of observation (i.e., data or evidence)

postmodern Bayesianism!

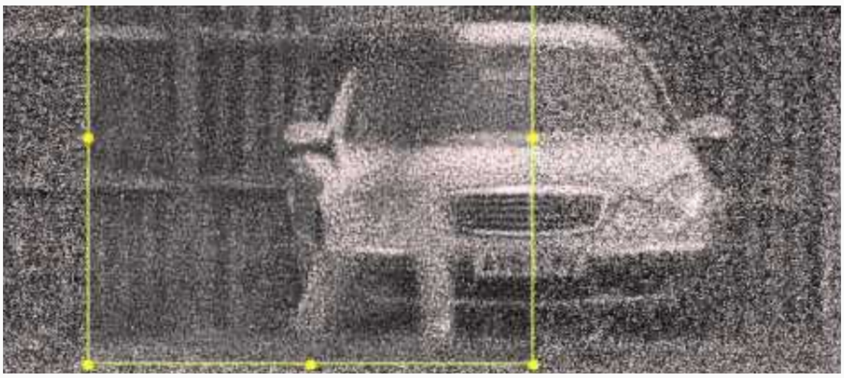
Meanings of the inverse probability

- it is the main *tool* of Bayesian statistics for problems like:
  - estimation (e.g.: how many red balls are in an urn?)
  - decision (e.g.: is ACME's stock a good investment? should I buy some? how much?)
  - inference and learning: predictive inference (e.g.: weather forecasts) and retrodictive inference (e.g.: what kind of stellar event possibly caused the Crab Nebula?)
- it measures the degree of belief that a rational agent should have in one hypothesis, among other mutually exclusive ones, given the data

Inference with noisy data or uncertain evidence

BUT! Bayes-Laplace Rule *does not* tell us how to update the prior in the face of uncertain data...

- suppose that a noisy observation suggests a probability distribution $\mathcal{Q}(D)$ for the data (e.g., the license plate no.)



- how should we update our prior $\mathcal{P}(H)$ given *uncertain evidence* in the from $\mathcal{Q}(D)$?

Jeffrey's rule of probability kinematics

Vanilla Bayes:

$$\mathcal{P}(H|D) = \mathcal{P}(D|H)\mathcal{P}(H)/\mathcal{P}(D)$$

Extended Bayes:

$$\mathcal{P}(H|\mathcal{Q}(D)) = ?$$

Jeffrey's conditioning* (1965)

$$\mathcal{P}(H|\mathcal{Q}(D)) = \sum_D \underbrace{\mathcal{P}(H|D)}_{\text{inv. prob.}} \mathcal{Q}(D)$$

$$= \sum_D \frac{\mathcal{P}(D|H)\mathcal{P}(H)}{\sum_H \mathcal{P}(D|H)\mathcal{P}(H)} \mathcal{Q}(D)$$

* Jeffrey's rule was introduced *ad hoc*, but it can be proved from Bayes-Laplace Rule and Pearl's method of virtual evidence (1988)

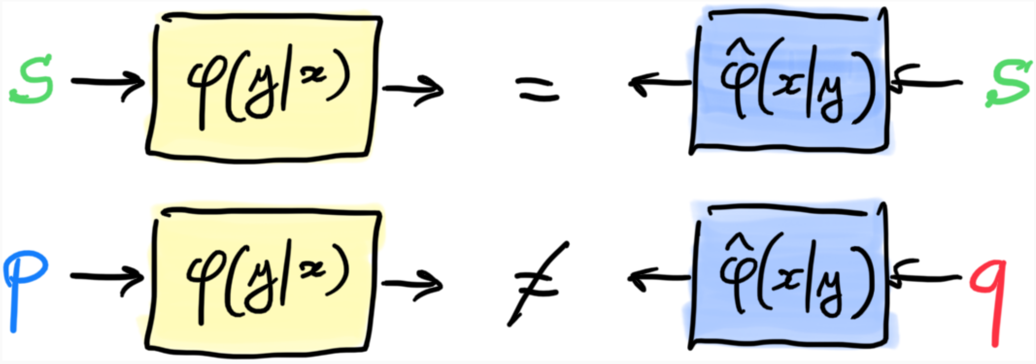
Construction of the reverse process as retrodiction

- **physical setup**:
  - a stochastic transition rule: $\varphi(y|x)$
  - a steady (viz. invariant) state: $\sum_x \varphi(y|x)s(x) = s(y)$
- **Bayesian inversion at the steady state**:

$$s(y)\hat{\varphi}(x|y) := s(x)\varphi(y|x) \iff \frac{\varphi(y|x)}{\hat{\varphi}(x|y)} = \frac{s(y)}{s(x)}$$

- **two priors**:
  - predictor's prior: $p(x)$
  - retrodictor's prior $q(y)$
- **two processes**:
  - forward process (prediction): $\mathcal{P}_F(x,y) = \varphi(y|x)p(x)$
  - reverse process (retrodiction): $\mathcal{P}_R(x,y) = \hat{\varphi}(x|y)q(y)$

A picture



- at the steady state: prediction = retrodiction
- otherwise: asymmetry (irreversibility, *irretrodictability*)

Quantifying irretrodictability

Second idea: fluctuation relations as measures of divergence between prediction and retrodiction

- relative entropy:

$$D(\mathcal{P}_F \| \mathcal{P}_R) := \left\langle -\ln \frac{\mathcal{P}_R(x,y)}{\mathcal{P}_F(x,y)} \right\rangle_F =: \langle -\ln r(x,y) \rangle_F$$

$\rightsquigarrow$ more generally, one can use $D_f(\mathcal{P}_R \| \mathcal{P}_F) := \langle f(r(x,y)) \rangle_F$

- introduce probability density functions

$\rightsquigarrow$ $\Omega(x,y) := f(r(x,y))$ (total stochastic f-entropy production)

$\rightsquigarrow$ $\mu_F(\omega) := \sum_{x,y} \delta[\omega - \Omega(x,y)]\ \mathcal{P}_F(x,y)$

$\rightsquigarrow$ $\mu_R(\omega) := \sum_{x,y} \delta[\omega - \Omega(x,y)]\ \mathcal{P}_R(x,y)$

$$\Longrightarrow \langle \omega \rangle_F = D_f(\mathcal{P}_R \| \mathcal{P}_F)$$

From f-divergences to f-fluctuation theorems

for $f : \mathbb{R}^+ \to \mathbb{R}$ invertible

f-Fluctuation Theorem

$$\mu_R(\omega) = f^{-1}(\omega)\mu_F(\omega) \qquad \Longrightarrow \qquad \langle f^{-1}(\omega)\rangle_F = 1$$

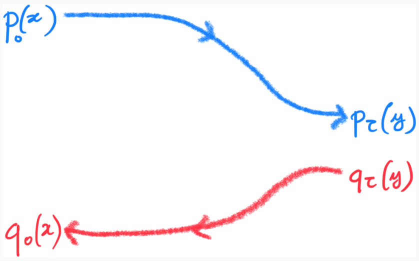
$\rightsquigarrow$ for $f(u) = -\ln u$, we have $f^{-1}(v) = e^{-v}$, that is

$$\frac{\mu_F(\omega)}{\mu_R(\omega)} = e^{\omega} \qquad \Longrightarrow \qquad \left\langle e^{-\omega}\right\rangle_F = 1$$

further discussions in `arXiv:2009.02849` and `arXiv:2106.08589`

Examples of known results recovered by retrodiction

Example: driven closed system evolution



- driving protocol: $H(0) \to H(t) \to H(\tau)$
- $H(0) = (\epsilon_x)_x$, $H(\tau) = (\eta_y)_y$
- $\varphi(y|x) = \delta_{y,y(x)}$, i.e., one-to-one
- $s(x) = d^{-1} \implies \varphi(y|x) = \hat{\varphi}(x|y)$
- $p_0(x) = e^{\beta(F-\epsilon_x)}$, $q_\tau(y) = e^{\beta(F'-\eta_y)}$

In this case, for the choice $f(u) = -\ln u$,

$$\Omega(x,y) = \ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} = \ln \frac{s(y)p(x)}{s(x)q(y)} = \ln \frac{p(x)}{q(y)}$$
$$= \beta(F - \epsilon_x + F' + \eta_y) = \beta(W - \Delta F)$$

$$\implies \frac{\mu_F(W)}{\mu_R(W)} = e^{\beta(W-\Delta F)} \implies \langle W \rangle \geq \Delta F$$

Example: nonequilibrium steady states

- stochastic process $\varphi(y|x)$ with non-thermal steady state $s(x)$
- thermal equilibrium priors: $p(x) = q(x) \propto e^{-\beta\epsilon_x}$
- fluctuation variable:
  $\omega = \ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} = \ln \frac{p(x)}{q(y)}\frac{s(y)}{s(x)} = \beta(\epsilon_y - \epsilon_x) + (\ln s(y) - \ln s(x))$
- *nonequilibrium potential*: $V(x) := -\frac{1}{\beta}\ln s(x)$ (e.g., Manzano&al 2015)
- nonequilibrium potentials (usually introduced *ad hoc*) are understood here as remnants of Bayesian inversion
- $\implies \left\langle e^{\beta(\Delta E - \Delta V)} \right\rangle_F = 1 \implies D(p\|s) - D(\varphi[p]\|s) \geq 0$

But why known relations are compatible with Bayesian inversion?

Is that a necessity?

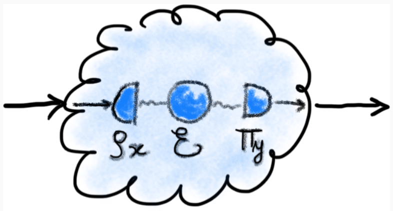
Sketch argument

- $D(\mathcal{P}_F \| \mathcal{P}_R) = \left\langle \ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} \right\rangle_F$
- let us impose that the fluctuation variable is **local**:
  $\ln \frac{\mathcal{P}_F(x,y)}{\mathcal{P}_R(x,y)} = \Omega(x,y) \overset{!}{=} G'(y) - G(x)$
  - $\implies \quad \frac{\mathcal{P}_F(y|x)}{\mathcal{P}_R(x|y)} = \frac{H'(y)}{H(x)}$
  - $\implies \quad H(x)\mathcal{P}_F(y|x) = H'(y)\mathcal{P}_R(x|y)$
  - sum over $x \implies \quad H'(y) = \sum_x H(x)\mathcal{P}_F(y|x)$
- $\implies \quad \mathcal{P}_R(x|y) = \frac{1}{\sum_x H(x)\mathcal{P}_F(y|x)} H(x)\mathcal{P}_F(y|x)$

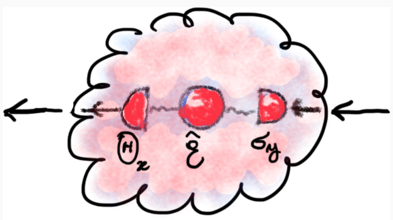
Hence, a Bayesian inverse-like form for the reverse process is **inevitable** if we want the fluctuating variable to have a local form!

Finally, what about the quantum case?

Quantum retrodiction and the Petz map



- assume $\varphi(y|x) = \mathrm{Tr}[\Pi_y\ \mathcal{E}(\rho_x)]$
- let $s(x)$ be invariant distribution
- according to the formalism of *quantum retrodiction*:
    - $\Sigma := \sum_x s(x)\rho_x$
    - $\hat{\rho}_y := \frac{1}{s(y)}\sqrt{\mathcal{E}(\Sigma)}\Pi_y\sqrt{\mathcal{E}(\Sigma)}$
    - $\hat{\Pi}_x := s(x)\frac{1}{\sqrt{\Sigma}}\rho_x\frac{1}{\sqrt{\Sigma}}$
    - $\hat{\mathcal{E}}(\cdot) := \sqrt{\Sigma}\left\{\mathcal{E}^\dagger\left[\frac{1}{\sqrt{\mathcal{E}(\Sigma)}}(\cdot)\frac{1}{\sqrt{\mathcal{E}(\Sigma)}}\right]\right\}\sqrt{\Sigma}$



- Bayesian inversion works seamlessly $\hat{\varphi}(x|y) = \mathrm{Tr}[\hat{\Pi}_x\ \hat{\mathcal{E}}(\hat{\rho}_y)]$

Some remarks about quantum retrodiction

- the Petz recovery map reduces to Bayes–Laplace rule when operators commute
- to a unique Bayes–Laplace rule there correspond infinite possible Petz maps ("rotated" Petz maps)
- retrodiction (both classical and quantum) depends on the choice of reference prior
- exceptions are unitary (i.e., "bilateral deterministic") channels, for which:
  1. there is a unique Petz reverse (the retrodiction is independent of the choice of prior, and all rotated Petz maps coincide)
  2. retrodiction and (linear) inversion coincide

Conclusion

Final messages

1. predictive and retrodictive inference provide the logical foundations of fluctuation theorems
2. while fluctuation relations measure the divergence between predictor and retrodictor, the Second Law states that they won't get further apart as a result of their inferences
3. so, the Second Law is special among the laws of physics, because it is in fact a law about the logic of inference
4. a clear distinction between mechanical *(ir)reversibility* and logical *(ir)retrodictability* avoids unnecessary paradoxes
5. quantum retrodiction and quantum fluctuation relations follow seamlessly using Petz recovery map

thank you