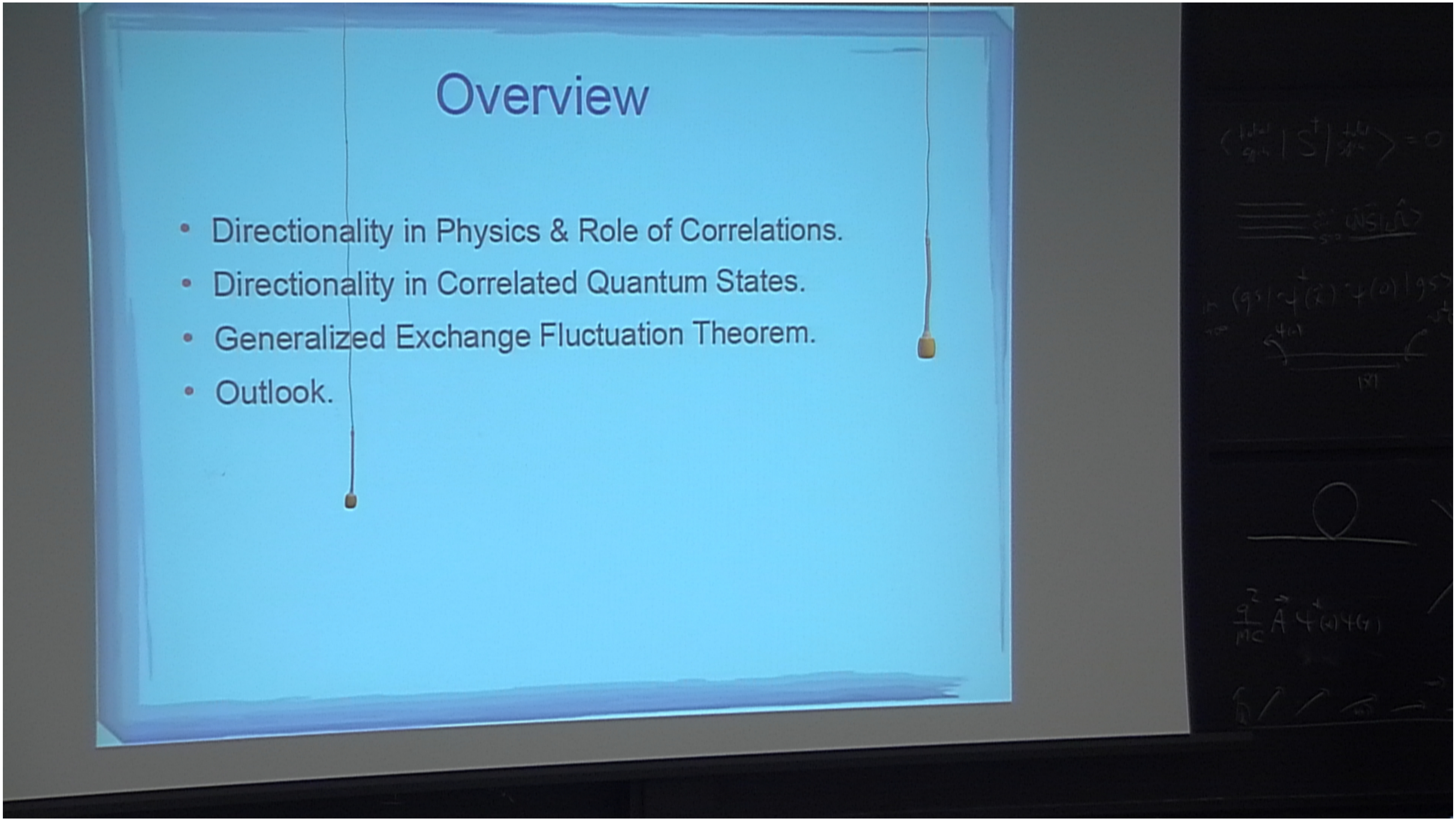
Title: Thermodynamics of correlated quantum systems and a generalized exchange fluctuation theorem.

Date: Oct 23, 2012 03:30 PM

URL: http://pirsa.org/12100105

Abstract: I will discuss the central role of correlations in thermodynamic directionality, how strong correlations can distort the thermodynamic arrow and contrast these distortions in both the classical and quantum regimes. These distortions constitute non-linear entanglement witnesses, and give rise to a rich information-theoretic structure. I shall explain how these results are then cast into the language of fluctuation theorems to derive a generalized exchange fluctuation theorem, and discuss the limitations of such a framework.


Overview
Directionality in Physics & Role of Correlations.
Directionality in Correlated Quantum States.
Generalized Exchange Fluctuation Theorem.
Outlook.

Issues of Time in Physics

- Time ⟹ Classical parameter in QM
- Relativistic QM or QFT does not help.

Wheeler de Witt equation

$$H|\Psi\rangle = 0$$

(interpretation is problematic).

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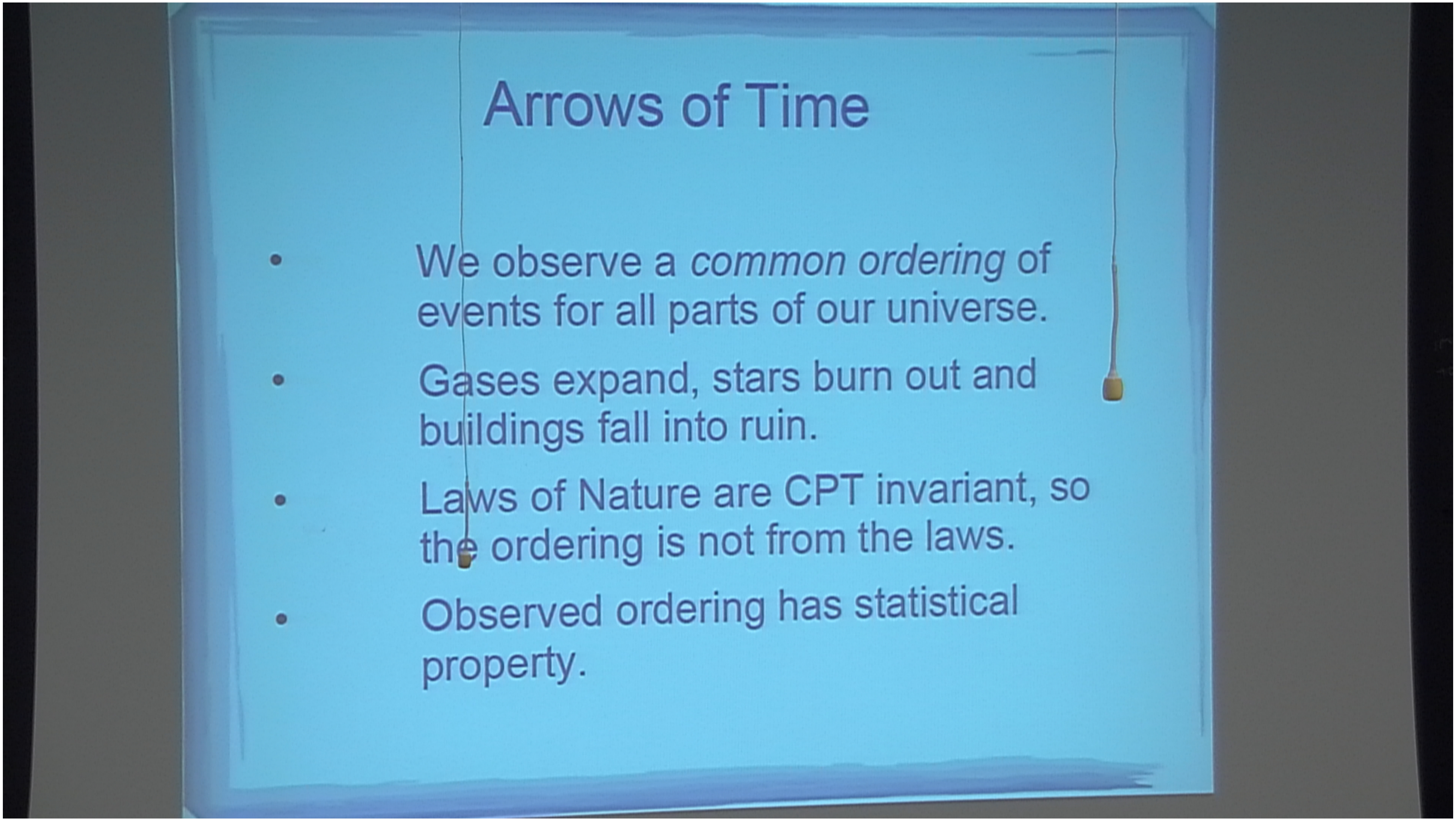
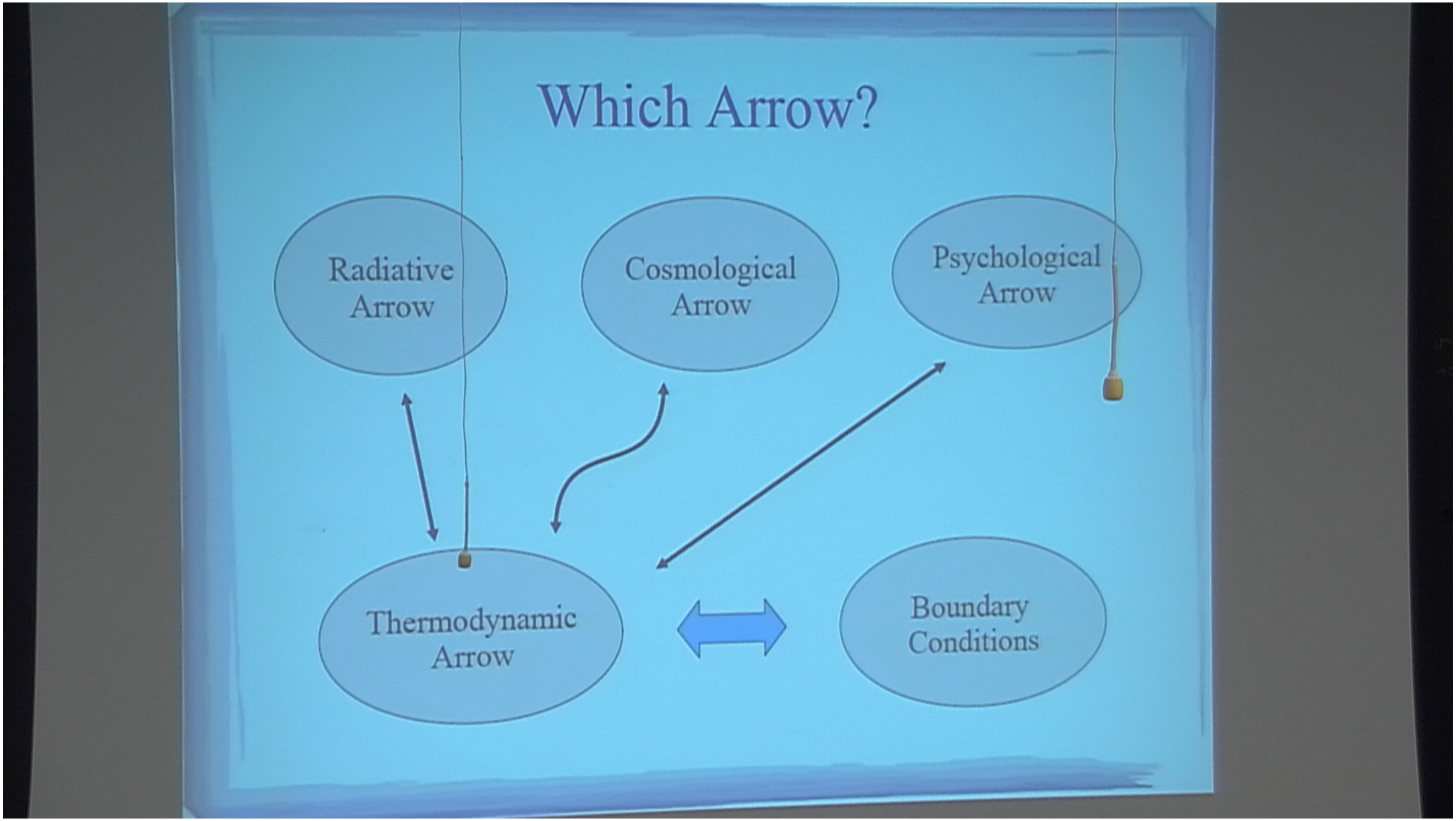

Arrows of Time
We observe a common ordering of events for all parts of our universe.
Gases expand, stars burn out and buildings fall into ruin.
Laws of Nature are CPT invariant, so the ordering is not from the laws.
Observed ordering has statistical property.


Which Arrow?
Radiative Arrow
Cosmological Arrow
Psychological Arrow
Thermodynamic Arrow
Boundary Conditions

The Thermodynamic Arrow

- Bipartite system AB in thermal states:

$\rho_A(T_A)$ $\rho_B(T_B)$

$$T_A < T_B$$

“Molecular Chaos”

- The key assumption for thermodynamic directionality.

$$\rho_{AB} = \rho_A \otimes \rho_B$$

- Entirely local “thermodynamic level of description”

Bipartite Interactions

- State of composite system AB:

$$\rho_{AB} = \rho_A \otimes \rho_B$$

- Allow AB to unitarily interact:

$$\rho_A \otimes \rho_B \rightarrow U(\rho_A \otimes \rho_B)U^\dagger$$

- Assume total energy conservation.

Key property:

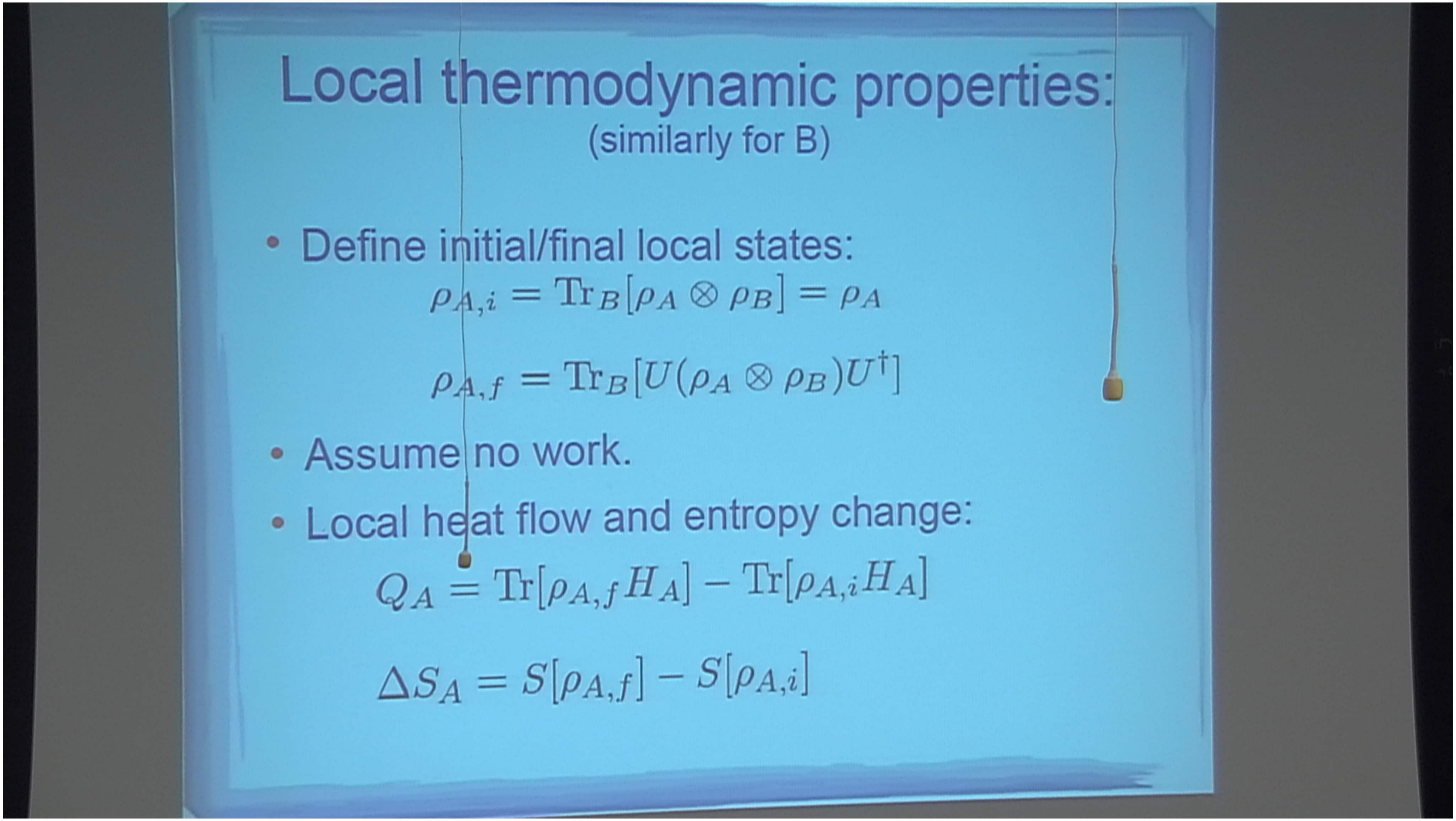
- Hamiltonian H, temperature $T = (k\beta)^{-1}$
- Free Energy Function, F:

$$F[\rho] := \mathrm{Tr}[H\rho] - S[\rho]/\beta$$

For any state ρ :

$$F[\rho] \geq F[e^{-\beta H}/Z]$$

$\Longrightarrow$ Thermal states minimize F


Local thermodynamic properties:
(similarly for B)
• Define initial/final local states:
$\rho_{A,i} = \mathrm{Tr}_B[\rho_A \otimes \rho_B] = \rho_A$
$\rho_{A,f} = \mathrm{Tr}_B[U(\rho_A \otimes \rho_B)U^\dagger]$
• Assume no work.
• Local heat flow and entropy change:
$Q_A = \mathrm{Tr}[\rho_{A,f} H_A] - \mathrm{Tr}[\rho_{A,i} H_A]$
$\Delta S_A = S[\rho_{A,f}] - S[\rho_{A,i}]$

Generalized Clausius Relation

- Applying the free energy relation to A and B gives:

$$\frac{Q_A}{T_A} + \frac{Q_B}{T_B} \geq \Delta S_A + \Delta S_B = \Delta I(A:B)$$

Where we define the quantum mutual information between A and B as:

$$I(A:B) := S[\rho_A] + S[\rho_B] - S[\rho_{AB}]$$

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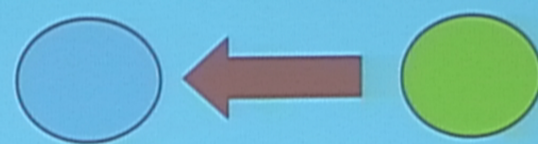
The Thermodynamic Arrow

$$\frac{Q_A}{T_A} + \frac{Q_B}{T_B} \geq 0$$



$$T_A < T_B$$

$$Q_A + Q_B = 0$$

$$T_A < T_B$$

$$\Rightarrow Q_A \geq 0$$ ☆ The predicted Thermodynamic Arrow ☆

The Thermodynamic Arrow

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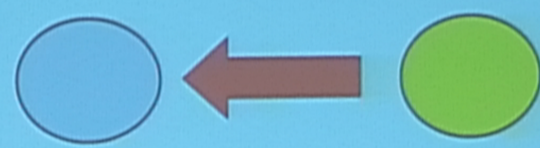


$$Q_A + Q_B = 0$$

$T_A < T_B$

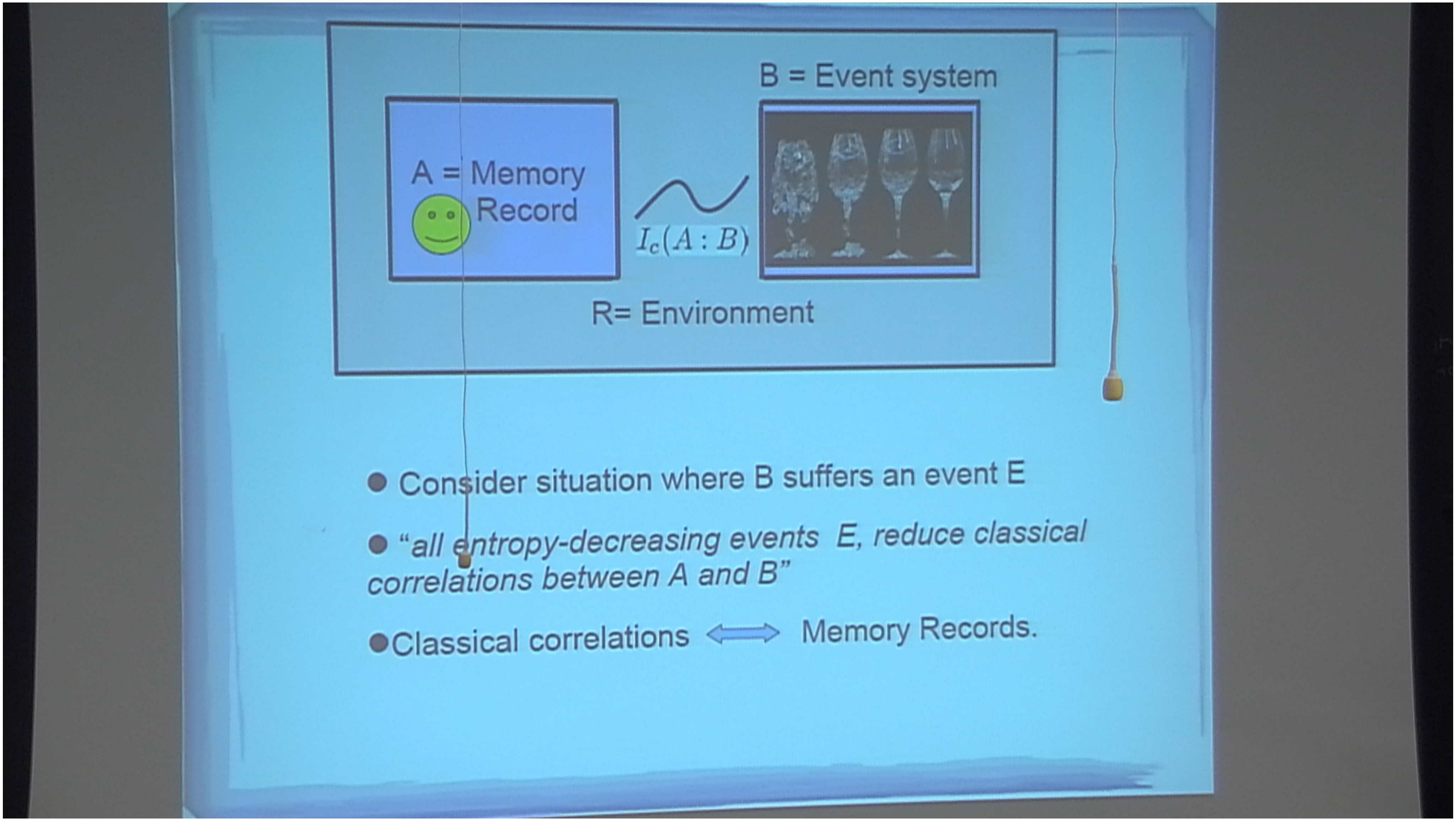
$T_A < T_B$

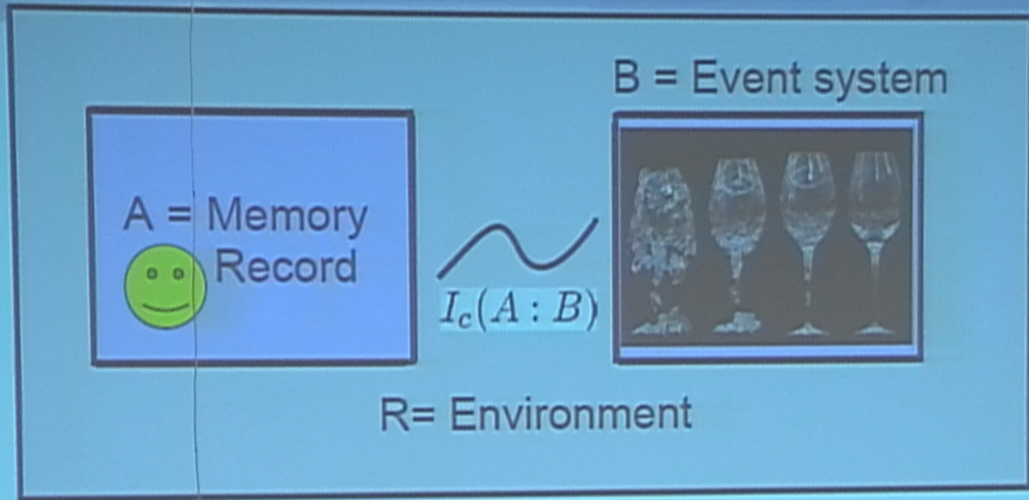
$\Rightarrow Q_A \geq 0$ ☆ The predicted Thermodynamic Arrow ☆

Correlations and Memory Records

- Proposed resolution of observed Arrow*.
- Emphasis on *Memory Records* of Entropy-decreasing events.
- *Memory Records* identified with *Classical Correlations.*
- Argument: entropy-decreasing events always coincide with memory erasure.

*(L. Maccone, PRL **103** 080401, 2009).*


B = Event system
A = Memory Record
$I_c(A:B)$
R= Environment
Consider situation where B suffers an event E
"all entropy-decreasing events E, reduce classical correlations between A and B"
Classical correlations ⟺ Memory Records.



Can construct (W-state) quantum example where:

$$\Delta S_R = 0 \qquad \Delta I_c(A:B) > 0$$

$$\Delta S_B < 0$$

The entropy of B has decreased, but the classical correlation=memory has <u>increased.</u>

Distorting the Arrow

- Recall that for an isolated interaction

$$\frac{Q_A}{T_A} + \frac{Q_B}{T_B} \geq \Delta S_A + \Delta S_B = \Delta I(A:B)$$

- System *initially correlated* it is possible to have $\Delta I(A:B) \leq 0$. Allows heat to flow from cold hot!
- A reversal of the observed thermodynamic arrow.

Distorting the Arrow

- Reversals of the Arrow tell us something about correlations.
- We can show* that

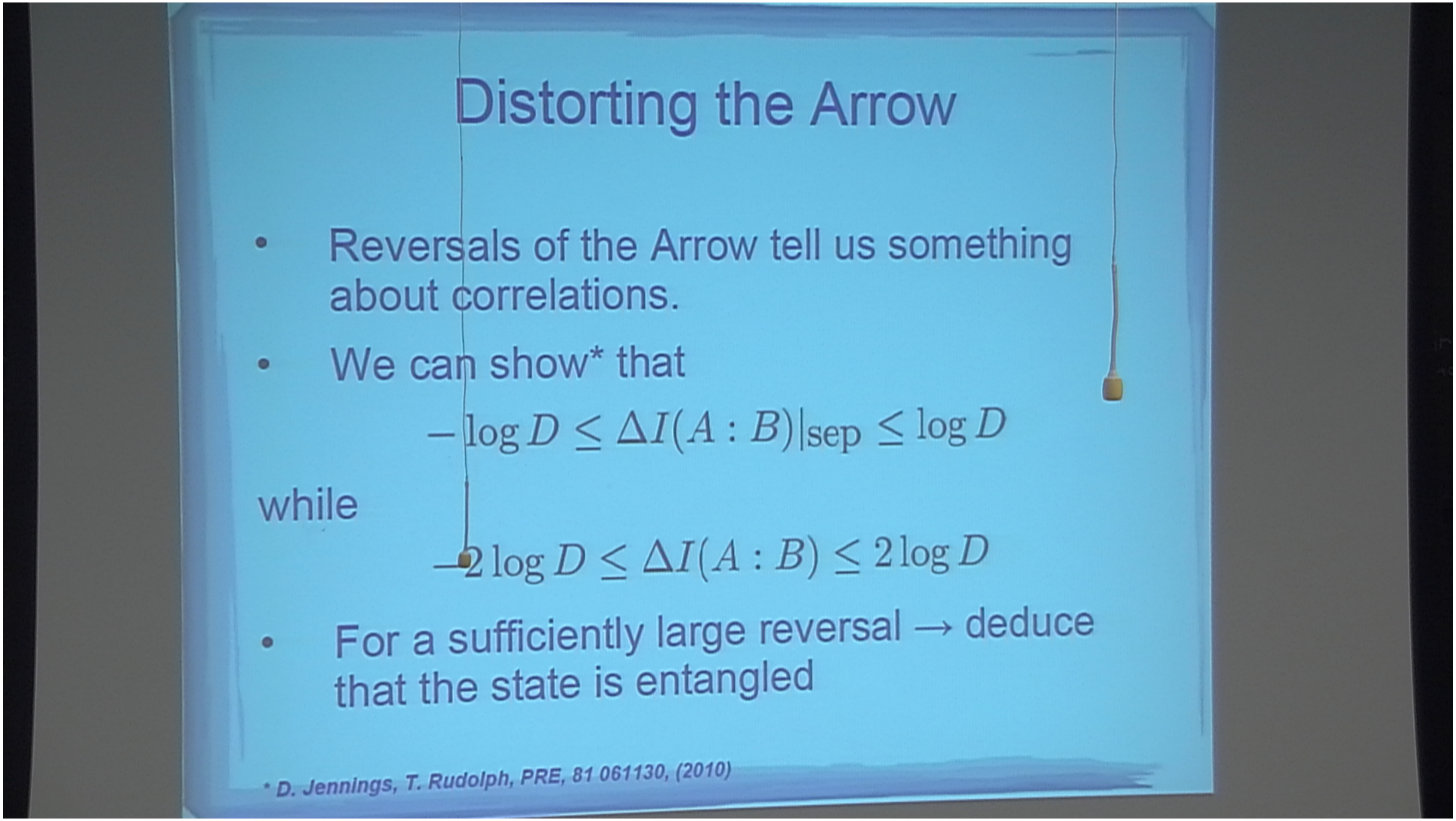
$$-\log D \leq \Delta I(A:B)|_{\text{sep}} \leq \log D$$

while

$$-2\log D \leq \Delta I(A:B) \leq 2\log D$$

- For a sufficiently large reversal → deduce that the state is entangled

* D. Jennings, T. Rudolph, PRE, 81 061130, (2010)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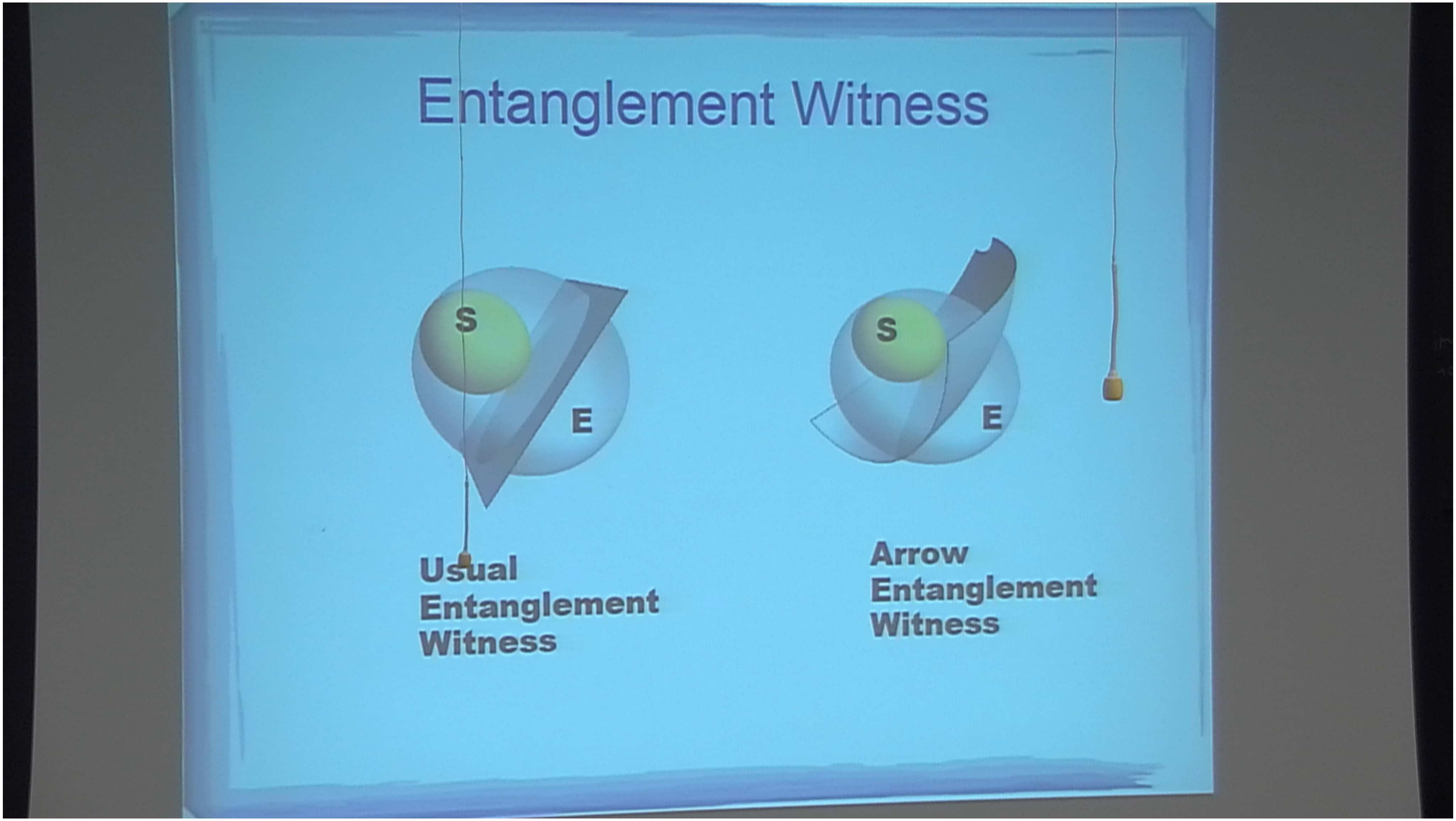
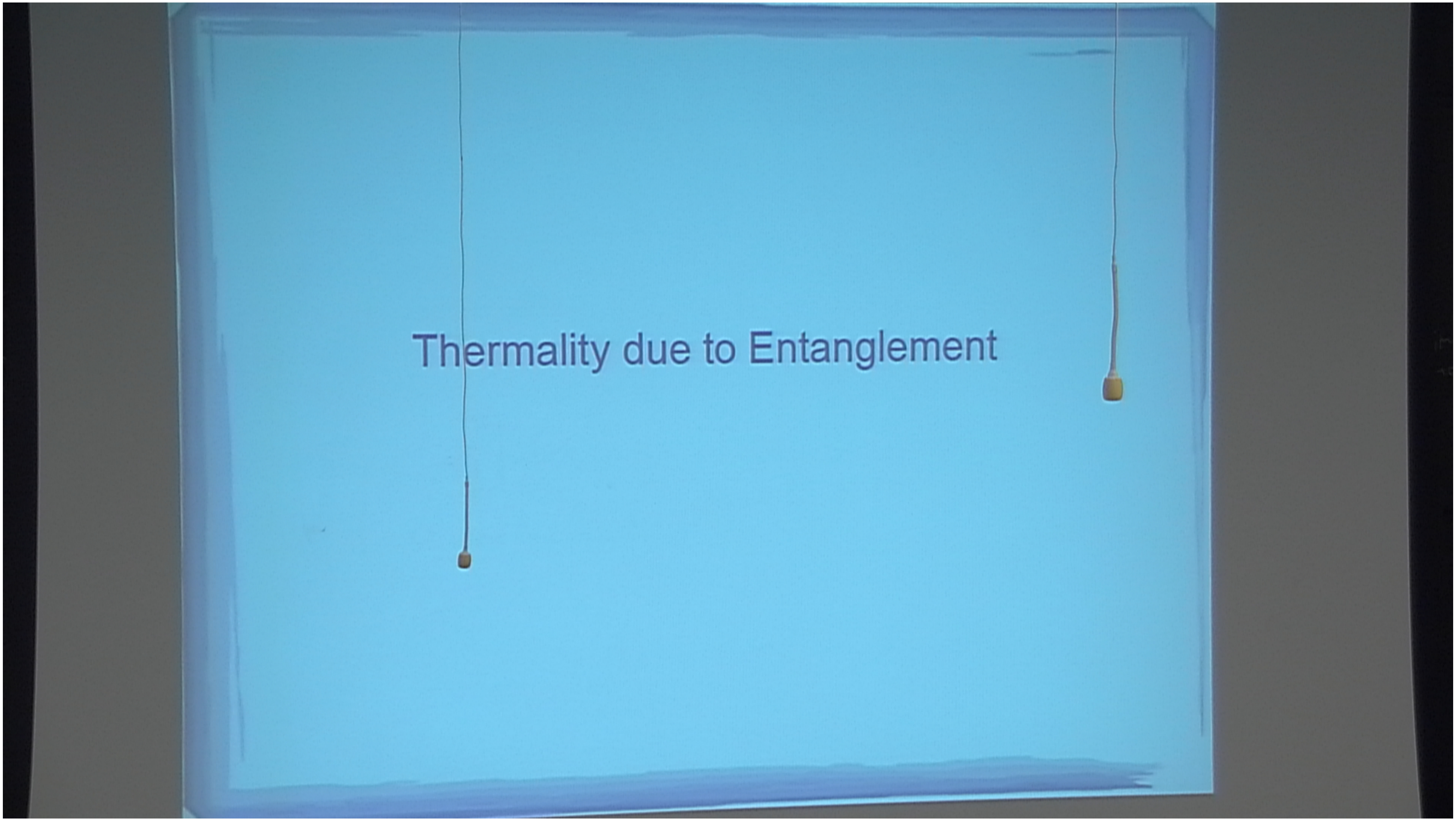

Entanglement Witness
S
E
S
E
Usual
Entanglement
Witness
Arrow
Entanglement
Witness

Entanglement Witness

- Requires only local measurements of energy.
- Transformations X → Y rather than properties of a state.
- Different from traditional 'linear witnesses'.


Thermality due to Entanglement

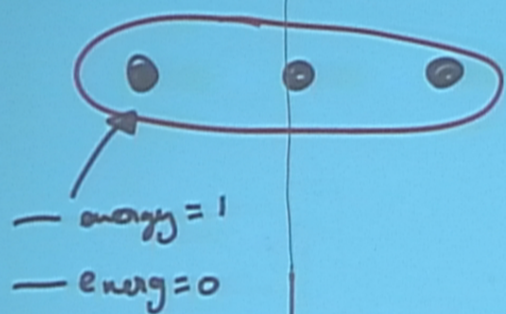
Thermality Due to Entanglement

- "Most pure states are entangled"
- "Most pure states of constant energy have subsystems close to being thermal states"*
- Concentration of measure effect.

*S. Popescu, A.J. Short, A. Winter, Nature Physics, 2 754 (2006)

Multipartite Quantum Systems.

Reversal of the Arrow: $\sum_i \frac{Q_i}{T_i} < 0$



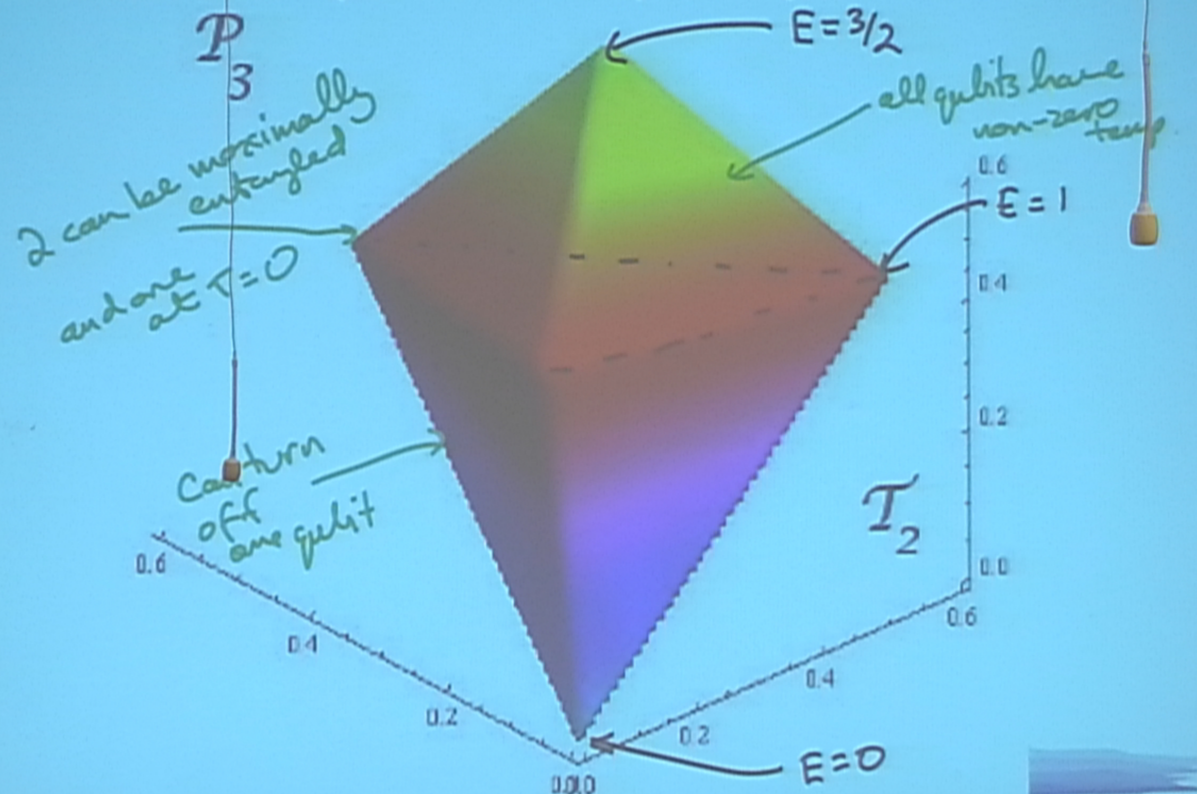
$\rho_{Thermal} = \begin{pmatrix} \frac{1}{1+e^{-\beta}} & 0 \\ 0 & \frac{e^{-\beta}}{1+e^{-\beta}} \end{pmatrix}$ ← λ_i is smallest eigenvalue

$|\psi_{ABC}\rangle$ exists iff $\lambda_i \leq \sum_{j \neq i} \lambda_j$, $0 \leq \lambda_i \leq 1/2$

Mean Energy, $E = \sum_i \lambda_i$

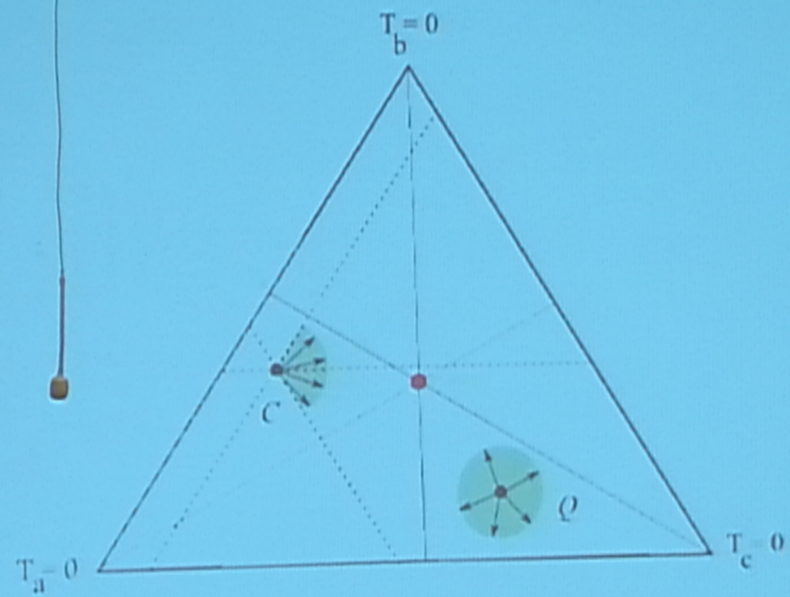
Multipartite Quantum Systems.

- Parameter Space for 3 qubit system:



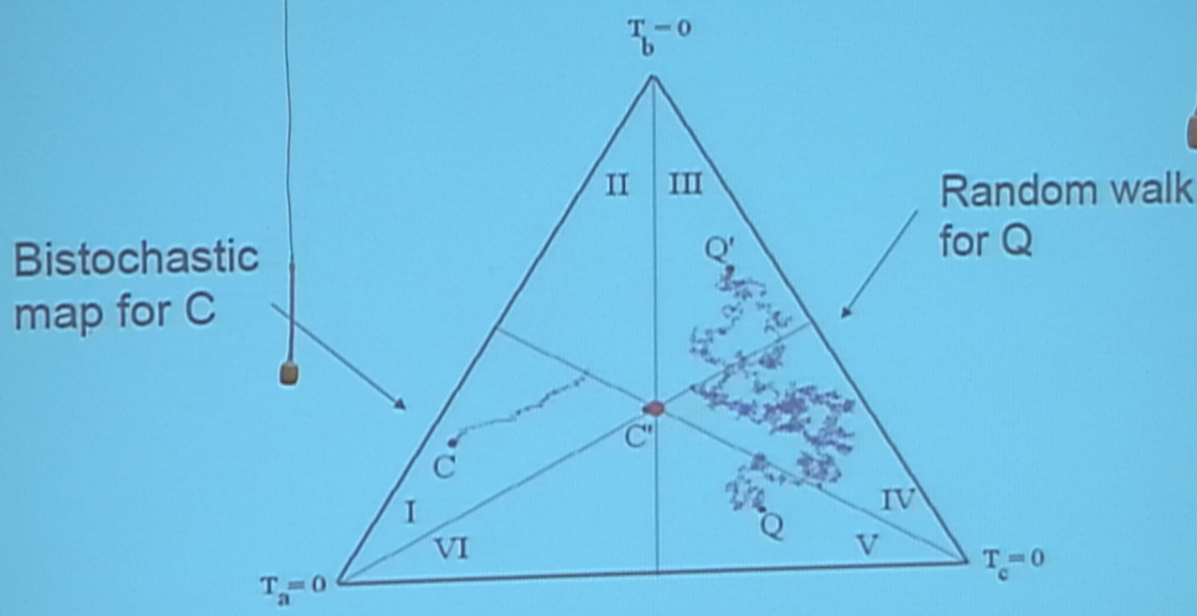
Multipartite Quantum Systems.

- Restriction to constant energy E:



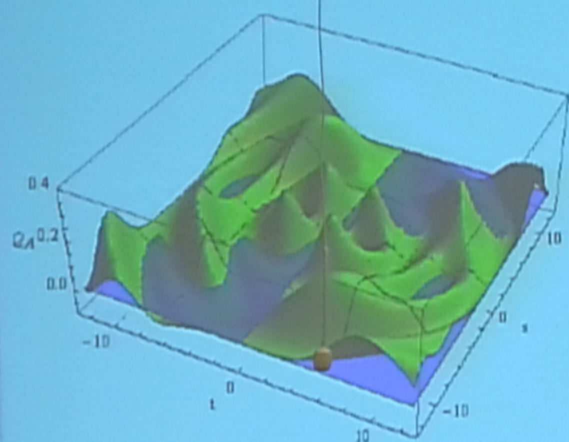
Violating the Thermodynamic Arrow with Multipartite Systems.

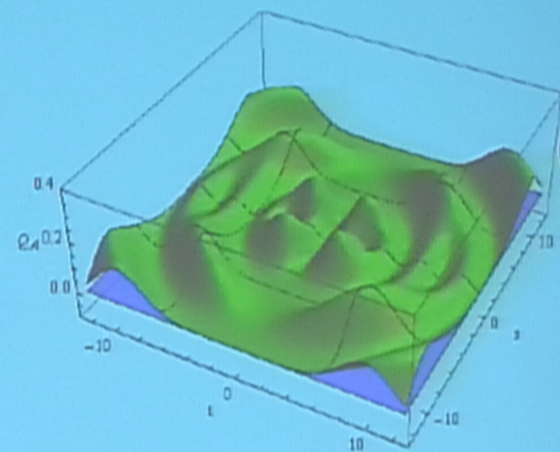
- Random energy exchanges:



With Mixed States.

- Heat flow comparison for A:





- Entangled state

No correlations

** D. Jennings, T. Rudolph, PRE, 81 061130, (2010)*

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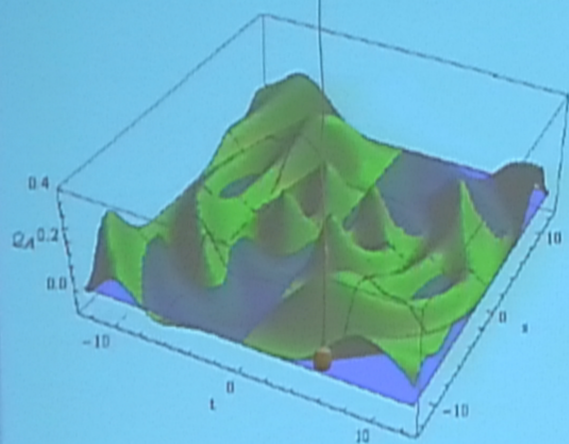

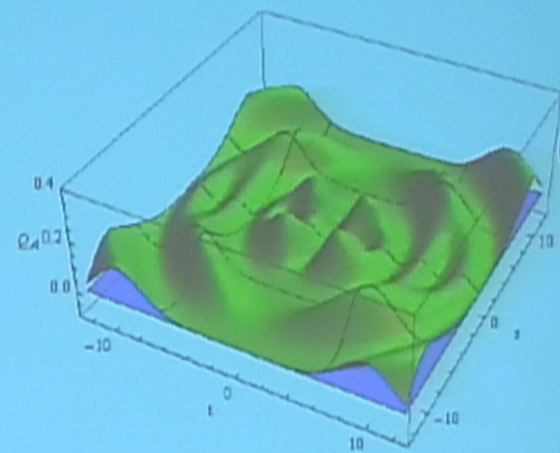

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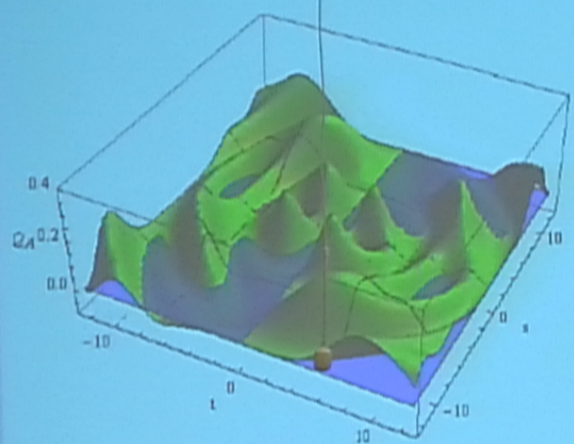

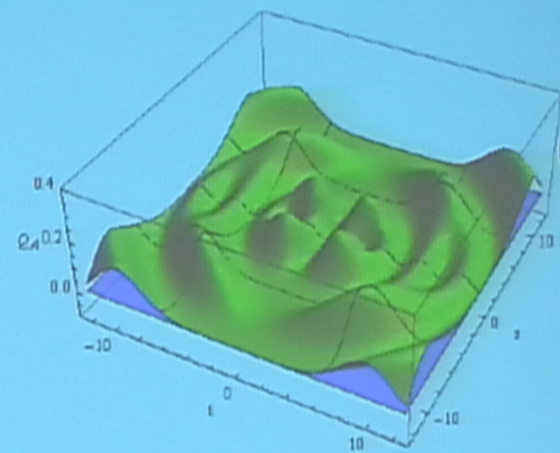

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Generating Heat Flow in the System

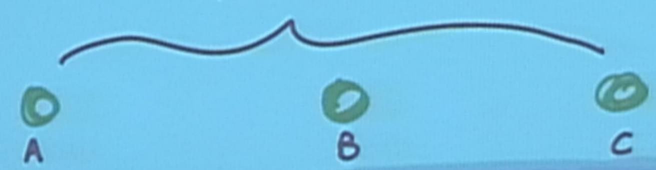
- Dynamics induced by nearest neighbour interactions:

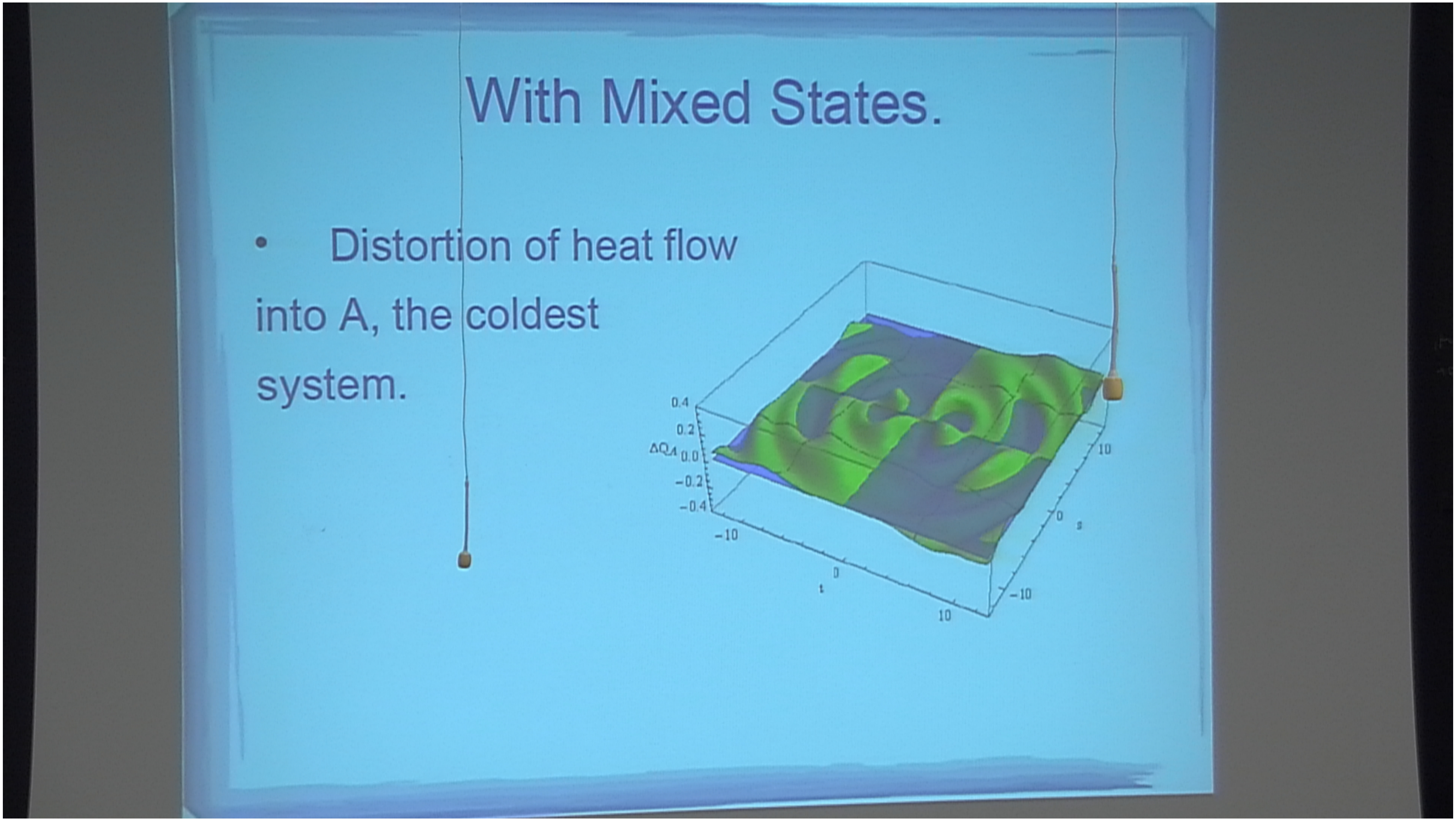
  Interaction Hamiltonian $H = tV_{AB} + sV_{BC}$

  $$V_{ij} = X_i Y_j - Y_i X_j$$

- A and C are in a correlated mixed state.

  ρ_{ABC} $\quad T_A < T_B < T_C$



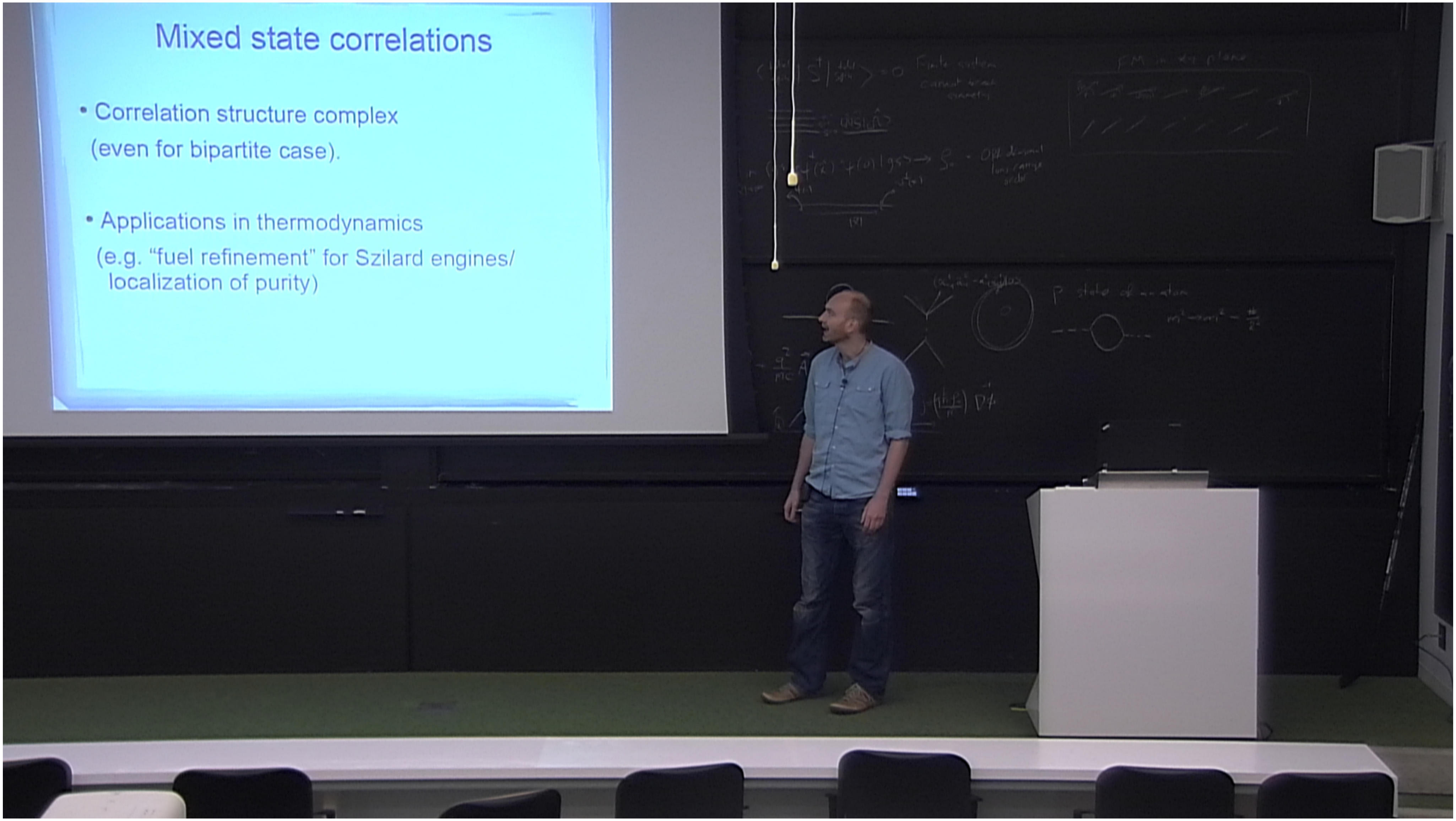

With Mixed States.
• Distortion of heat flow into A, the coldest system.
0.4
0.2
ΔQ_A 0.0
−0.2
−0.4
−10
0
t
10
10
0
s
−10

(Very) initial conditions?

Initial "Pure state of universe" $|\Psi\rangle$

Initial formation of elements in Nucleosynthesis phase relies on thermodynamic directionality.

Q. What constraint does BBN place on the allowed entanglement of $|\Psi\rangle$ *?*


Mixed state correlations
• Correlation structure complex
(even for bipartite case).
• Applications in thermodynamics
(e.g. “fuel refinement” for Szilard engines/
localization of purity)

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Correlations along Unitary Orbits*

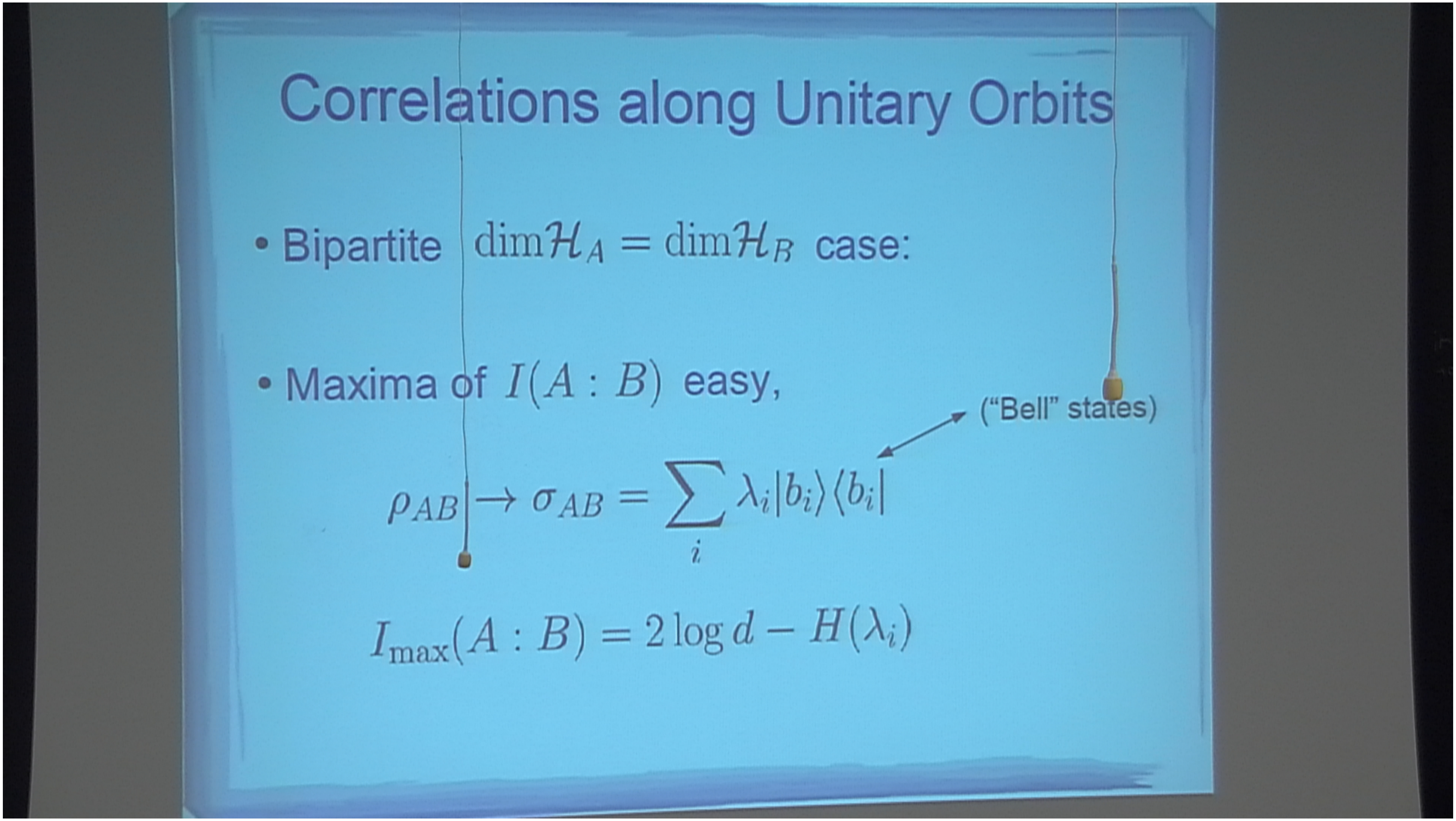
Analyse variation of the mutual information

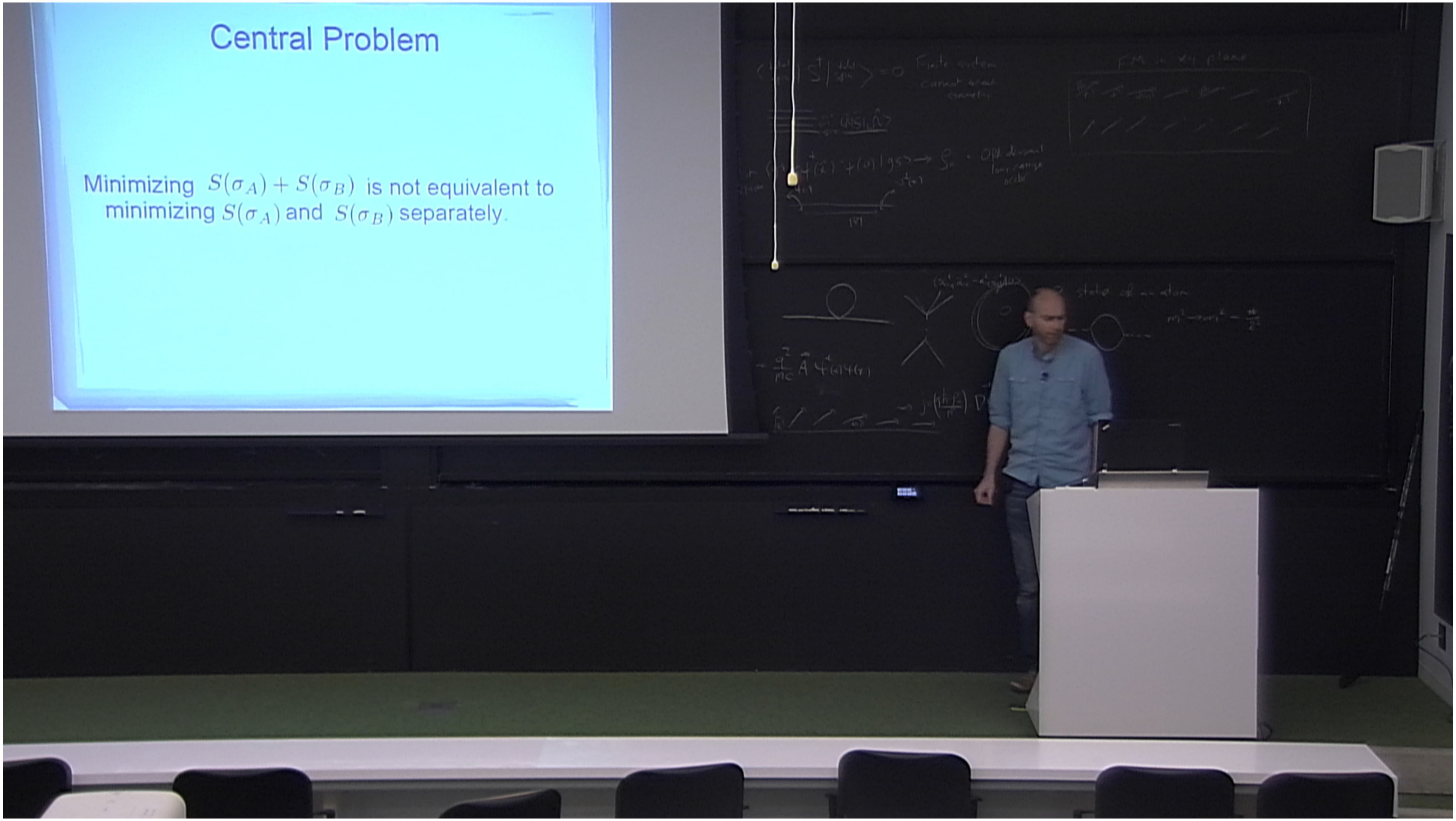
$$I(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$$

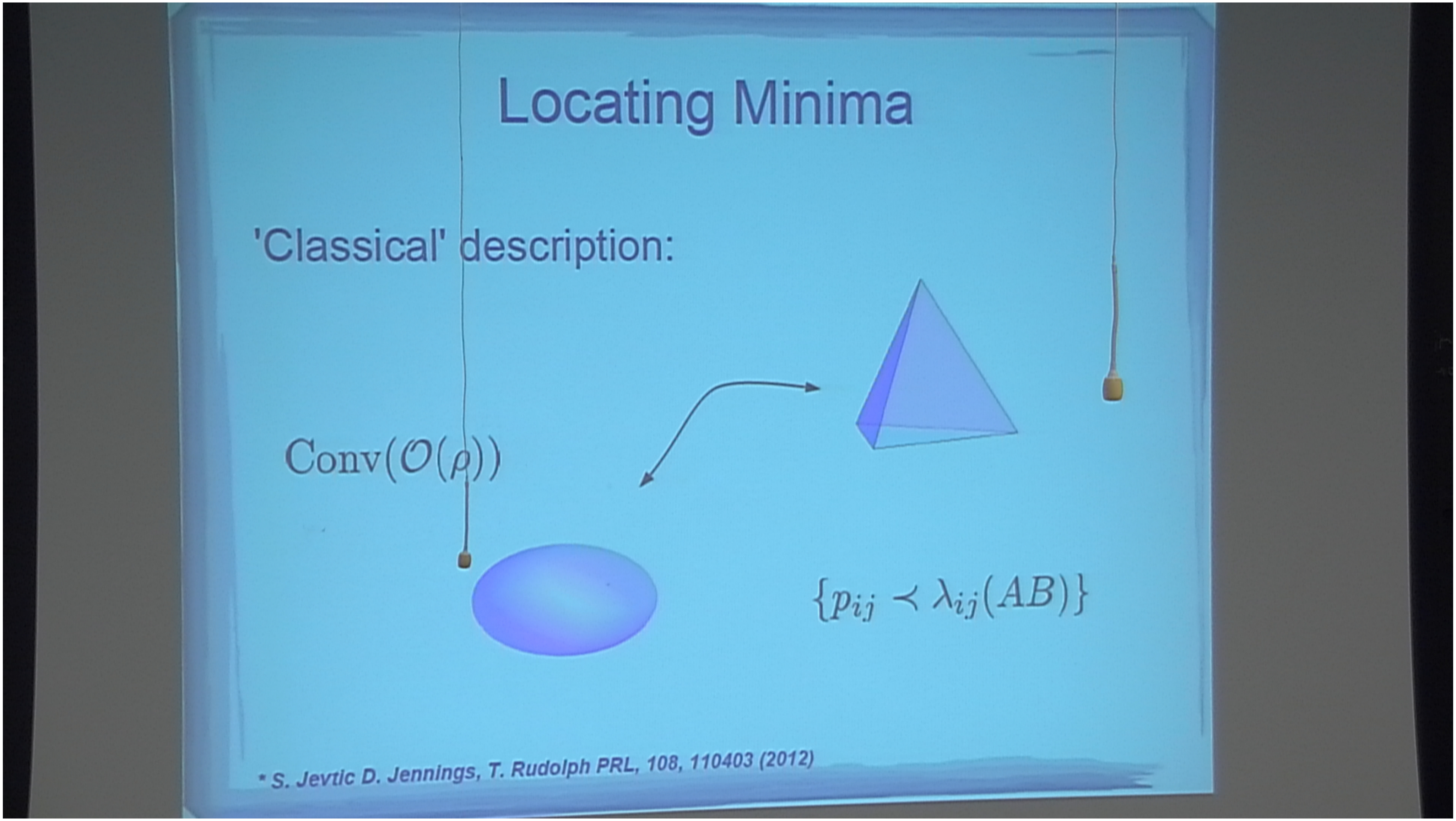
Over the set $\mathcal{O}(\rho)$

$$\mathcal{O}(\rho) := \{\sigma_{AB} = U\rho_{AB}U^\dagger : U^\dagger U = UU^\dagger = \mathbb{I}\}$$

* S. Jevtic D. Jennings, T. Rudolph PRL, 108, 110403 (2012)


Correlations along Unitary Orbits
• Bipartite $\dim\mathcal{H}_A = \dim\mathcal{H}_B$ case:
• Maxima of $I(A:B)$ easy,
("Bell" states)
$\rho_{AB} \to \sigma_{AB} = \sum_i \lambda_i |b_i\rangle\langle b_i|$
$I_{\max}(A:B) = 2\log d - H(\lambda_i)$


Central Problem
Minimizing $S(\sigma_A) + S(\sigma_B)$ is not equivalent to minimizing $S(\sigma_A)$ and $S(\sigma_B)$ separately.


Locating Minima
'Classical' description:
$\mathrm{Conv}(\mathcal{O}(\rho))$
$\{p_{ij} \prec \lambda_{ij}(AB)\}$
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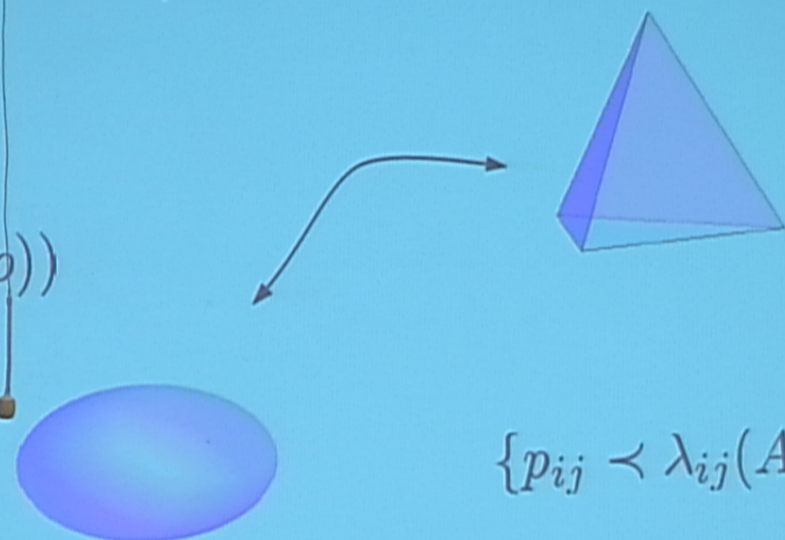
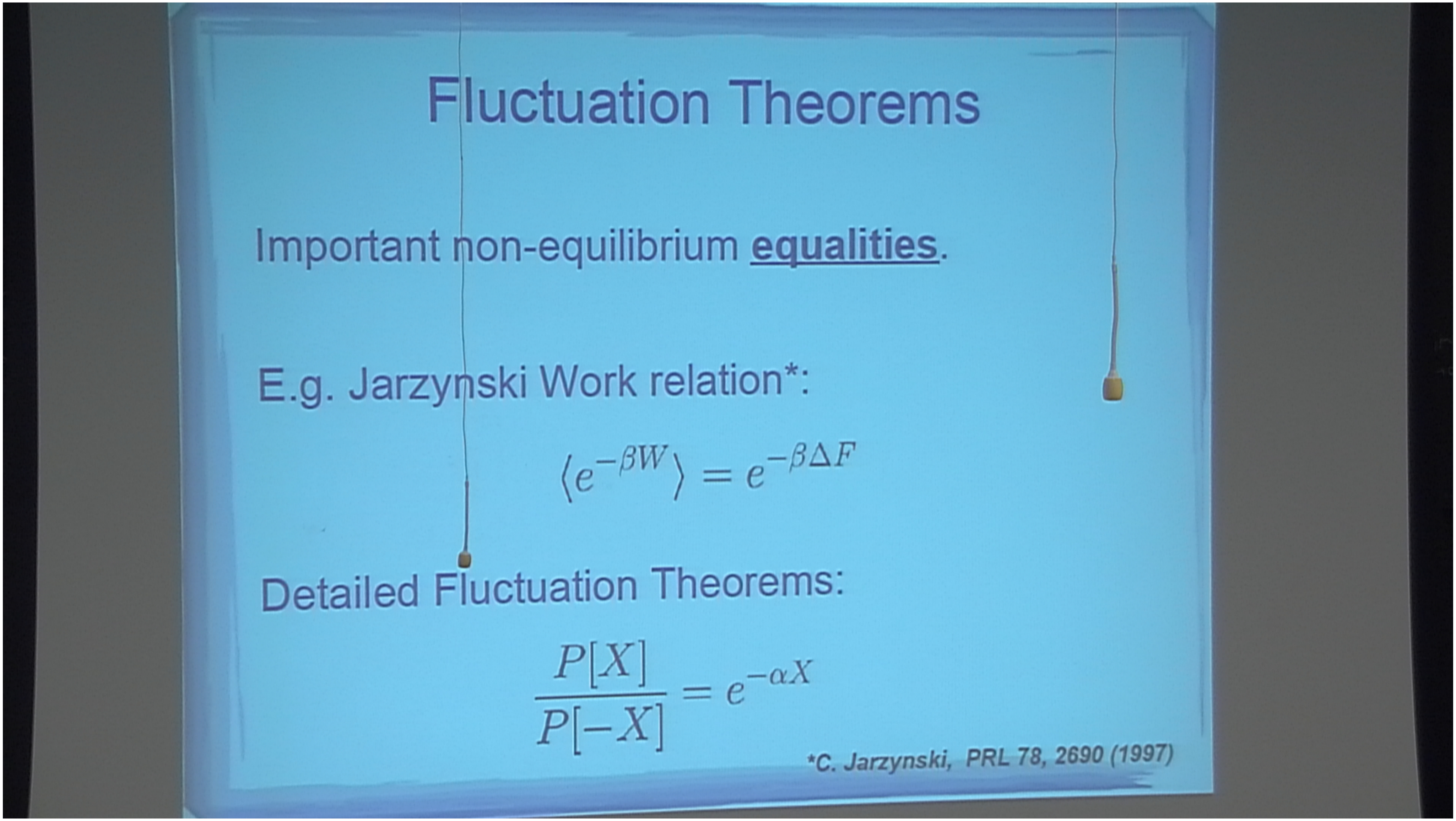
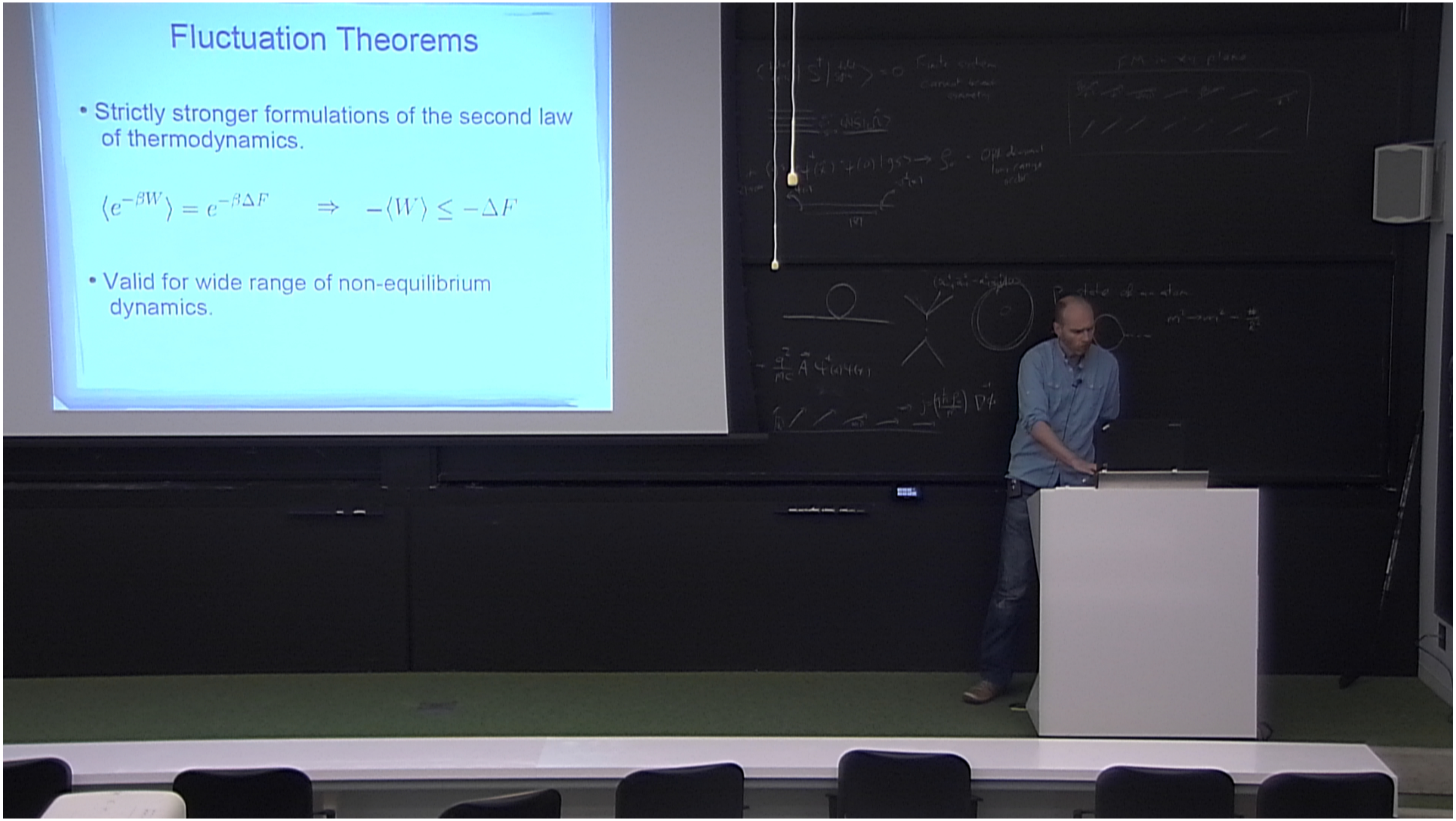


$\{p_{ij} \prec \lambda_{ij}(AB)\}$

$$\sigma_{AB}^{min} = \sum_{ij} (\Pi\lambda)_{ij} |i\rangle\langle i| \otimes |j\rangle\langle j|$$


Fluctuation Theorems
Important non-equilibrium equalities.
E.g. Jarzynski Work relation*:
$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$
Detailed Fluctuation Theorems:
$$\frac{P[X]}{P[-X]} = e^{-\alpha X}$$
*C. Jarzynski, PRL 78, 2690 (1997)


Fluctuation Theorems
• Strictly stronger formulations of the second law of thermodynamics.
$\langle e^{-\beta W}\rangle = e^{-\beta \Delta F} \quad \Rightarrow \quad -\langle W\rangle \leq -\Delta F$
• Valid for wide range of non-equilibrium dynamics.

Exchange Fluctuation Theorem

(I) Assume *Time-reversal Invariance.*

(II) Assume thermal marginals.

$$\Theta^\dagger H_\mu \Theta = H_\mu \qquad \mu = A, B, \mathrm{int}$$

where Θ is the anti-unitary time-reversal operator.

$$\Theta : (X, P) \rightarrow (X, -P)$$

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Energy Eigenstates

Convenient notation

$$|\phi^*, \chi^*\rangle := \Theta|\phi, \chi\rangle$$

If $|\phi, \chi\rangle$ an energy eigenstate of $H_A + H_B$ then so is the state $|\phi^*, \chi^*\rangle$.

Fluctuation Setting

(1) Initial thermal marginals

$$\rho_{AB}$$

$$\rho_\mu = e^{-\beta_\mu H_\mu}/\mathcal{Z}_\mu$$
$$\mathcal{Z}_\mu = \mathrm{tr}[e^{-\beta_\mu H_\mu}]$$

(2) Initial measurement

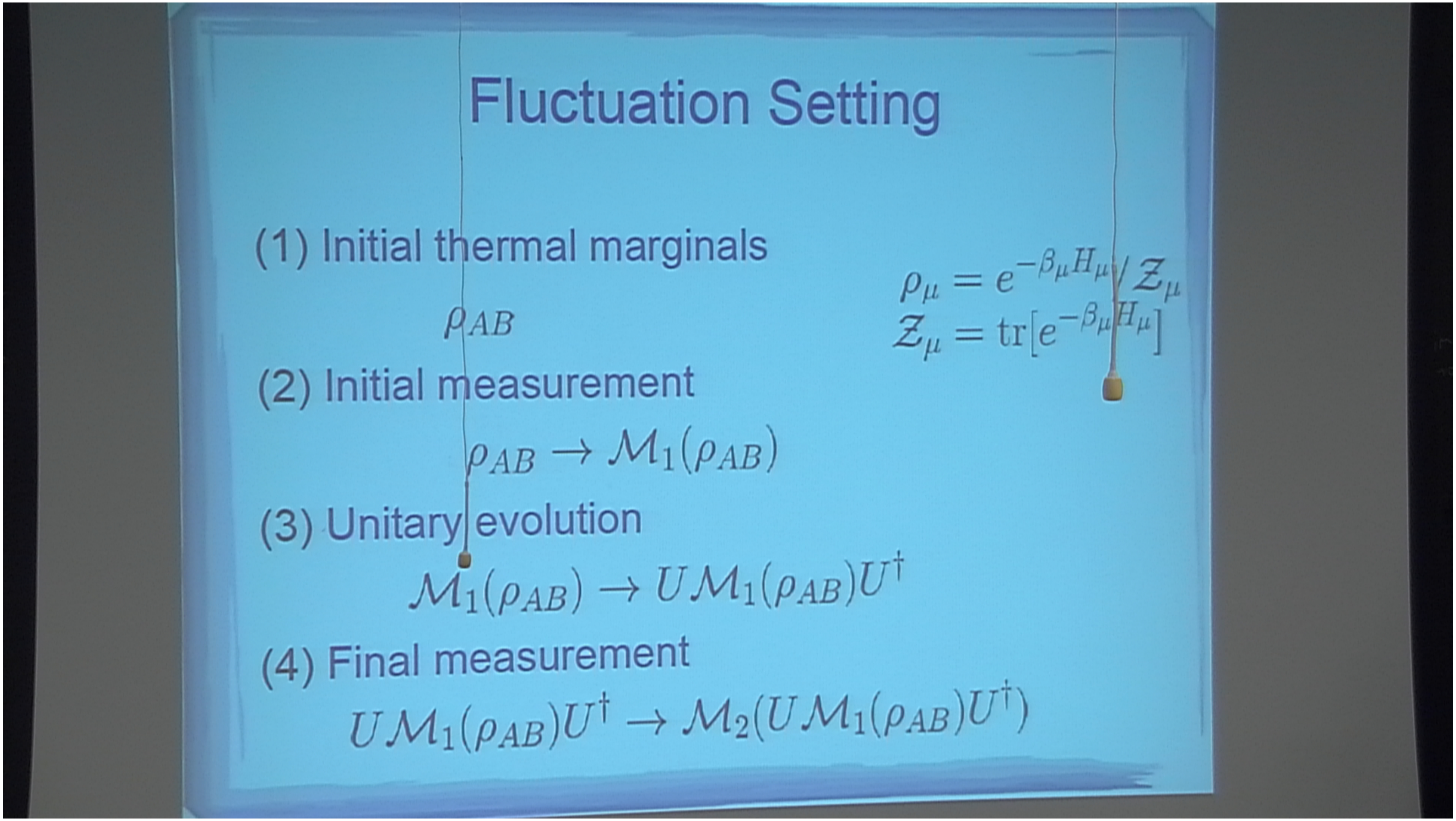
$$\rho_{AB} \to \mathcal{M}_1(\rho_{AB})$$

(3) Unitary evolution

$$\mathcal{M}_1(\rho_{AB}) \to U\mathcal{M}_1(\rho_{AB})U^\dagger$$

(4) Final measurement

$$U\mathcal{M}_1(\rho_{AB})U^\dagger \to \mathcal{M}_2(U\mathcal{M}_1(\rho_{AB})U^\dagger)$$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$\mathcal{Z}_\mu = \mathrm{tr}[e^{-\beta_\mu H_\mu}]$
(2) Initial measurement
$\rho_{AB} \to \mathcal{M}_1(\rho_{AB})$
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$\mathcal{M}_1(\rho_{AB}) \to U\mathcal{M}_1(\rho_{AB})U^\dagger$
(4) Final measurement
$U\mathcal{M}_1(\rho_{AB})U^\dagger \to \mathcal{M}_2(U\mathcal{M}_1(\rho_{AB})U^\dagger)$

Histories

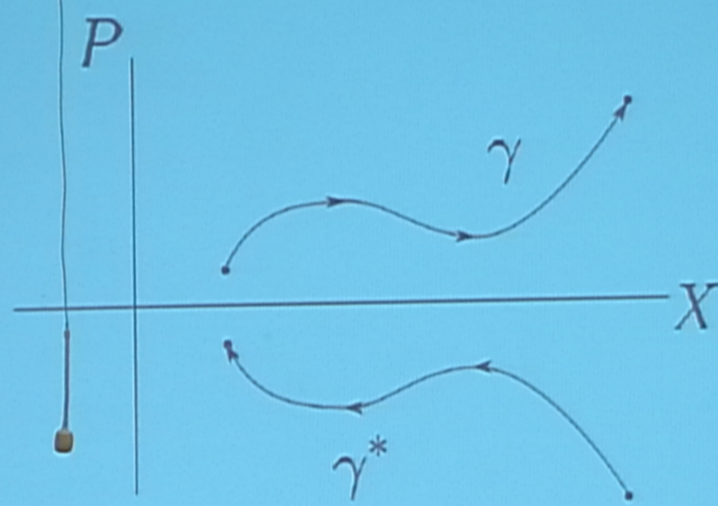
Define a ***history*** γ as

$$\gamma = (\rho_{AB}; |\phi_A, \chi_B\rangle \xrightarrow{U} |\phi'_A, \chi'_B\rangle)$$

and its time-reverse twin

$$\gamma^* = (\rho_{AB}; |\phi'^*_A, \chi'^*_B\rangle \xrightarrow{U} |\phi^*_A, \chi^*_B\rangle)$$

Histories



Set of all histories

- Consider Γ the set of all histories.
- Divide Γ in terms of energy changes:

$$\Gamma = \cup_{q,\Delta\epsilon}\Gamma(q,\Delta\epsilon)$$

$\Gamma(q,\Delta\epsilon)$: energy of A changes by q & total energy of AB changes by $\Delta\epsilon$

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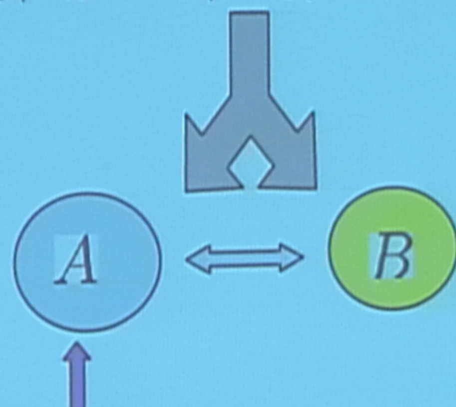
Energy Parameters

We have

$$\Delta\epsilon = \langle \phi', \chi' | H_A + H_B | \phi', \chi' \rangle - \langle \phi, \chi | H_A + H_B | \phi, \chi \rangle$$



$$q = \langle \phi' | H_A | \phi' \rangle - \langle \phi | H_A | \phi \rangle$$

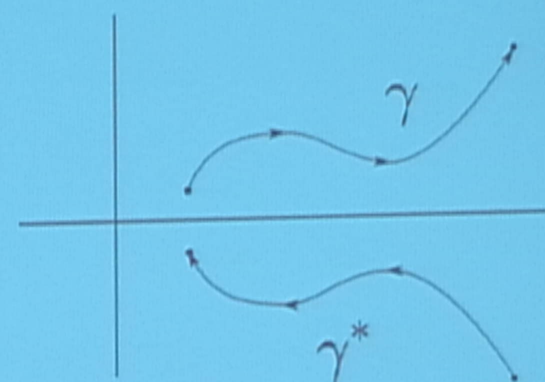
History distributions

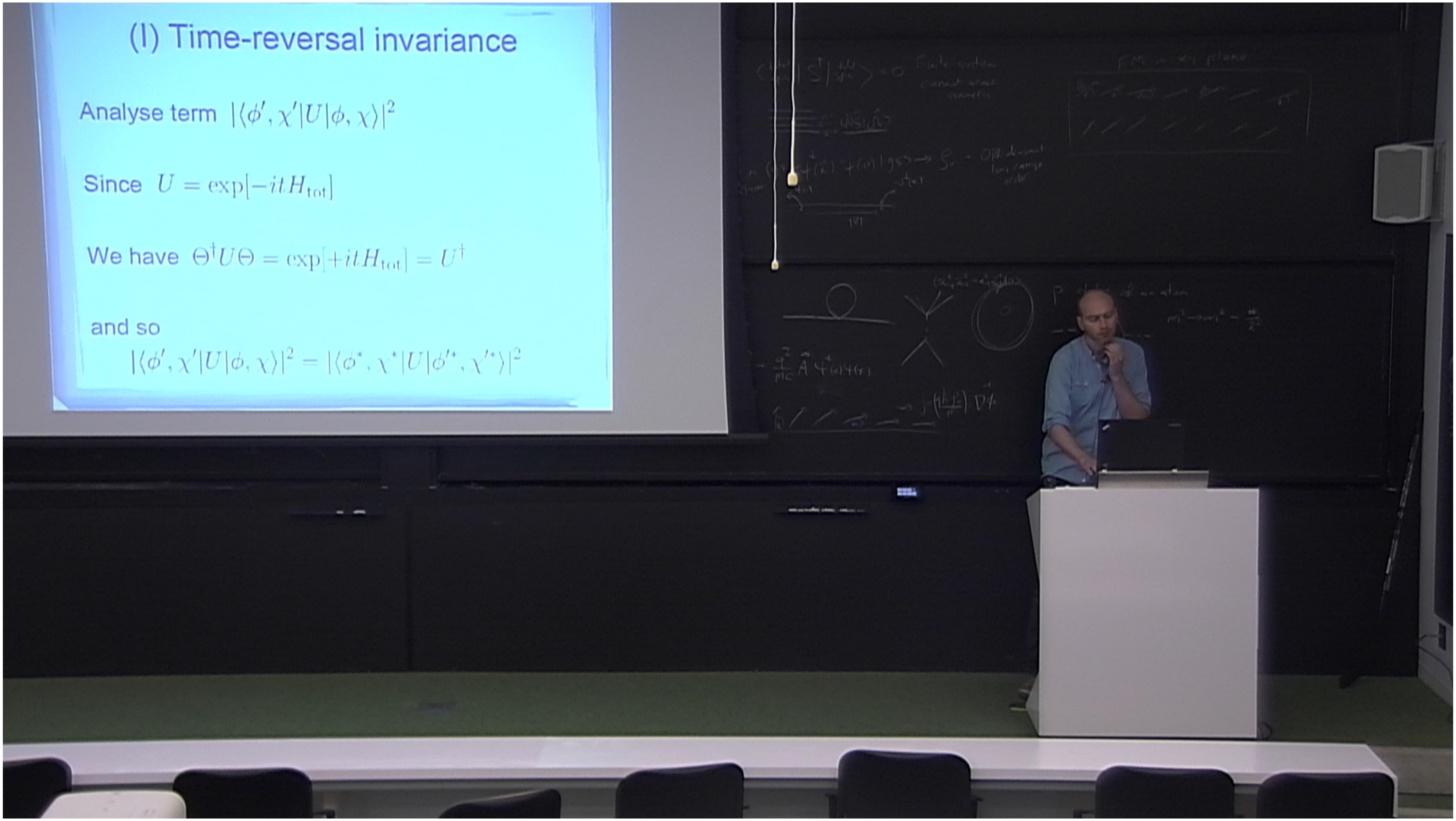
The probability of a history γ is

$$P[\gamma] = \langle \phi, \chi | \rho_{AB} | \phi, \chi \rangle | \langle \phi', \chi' | U | \phi, \chi \rangle |^2$$

Twin-pairing trick:

Compare γ with γ^*




(I) Time-reversal invariance
Analyse term $|\langle \phi', \chi' | U | \phi, \chi \rangle|^2$
Since $U = \exp[-itH_{\rm tot}]$
We have $\Theta^\dagger U \Theta = \exp[+itH_{\rm tot}] = U^\dagger$
and so
$|\langle \phi', \chi' | U | \phi, \chi \rangle|^2 = |\langle \phi^*, \chi^* | U | \phi'^*, \chi'^* \rangle|^2$

(I) Time-reversal invariance

Analyse term $|\langle \phi', \chi' | U | \phi, \chi \rangle|^2$

Since $U = \exp[-itH_{\text{tot}}]$

We have $\Theta^\dagger U \Theta = \exp[+itH_{\text{tot}}] = U^\dagger$

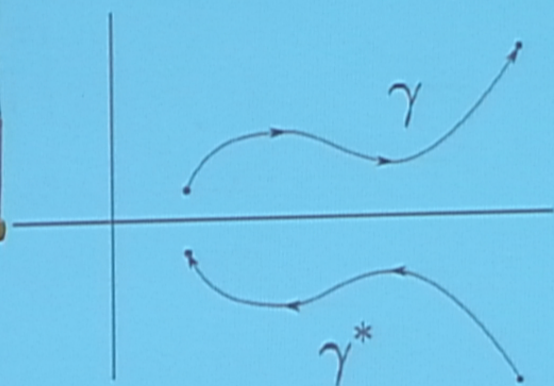
and so

$$|\langle \phi', \chi' | U | \phi, \chi \rangle|^2 = |\langle \phi^*, \chi^* | U | \phi'^*, \chi'^* \rangle|^2$$

Implication of $\Theta^\dagger H_\mu \Theta = H_\mu$

We have that

$$|\langle\phi',\chi'|U|\phi,\chi\rangle|^2 = |\langle\phi^*,\chi^*|U|\phi'^*,\chi'^*\rangle|^2$$



(II) Thermality

Now look at term $\langle \phi, \chi | \rho_{AB} | \phi, \chi \rangle$

Can re-write as

$$\langle \phi, \chi | \rho_{AB} | \phi, \chi \rangle = e^{-\beta_A H_\phi - \beta_B H_\chi - \log \mathcal{Z}_A \mathcal{Z}_B + \mathcal{I}}$$

where

$$\mathcal{I}[\rho_{AB}; \phi, \chi] := \ln \frac{\langle \phi, \chi | \rho_{AB} \ | \phi, \chi \rangle}{\langle \phi | \rho_A | \phi \rangle \langle \chi | \rho_B | \chi \rangle}$$

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Implication of (II)

We have that

$$P_{\rm init}[|\phi, \chi\rangle] \propto e^{-\beta_A E_\phi - \beta_B E_\chi + \mathcal{I}(\rho_{AB};\phi,\chi)}$$

And also

$$P_{\rm init}[|\phi'^*, \chi'^*\rangle] \propto e^{-\beta_A E_{\phi'^*} - \beta_B E_{\chi'^*} + \mathcal{I}(\rho_{AB};\phi'^*,\chi'^*)}$$

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Central expression

Combining (I) and (II):

$$|\langle \phi', \chi' | U | \phi, \chi \rangle|^2 = |\langle \phi^*, \chi^* | U | \phi'^*, \chi'^* \rangle|^2$$

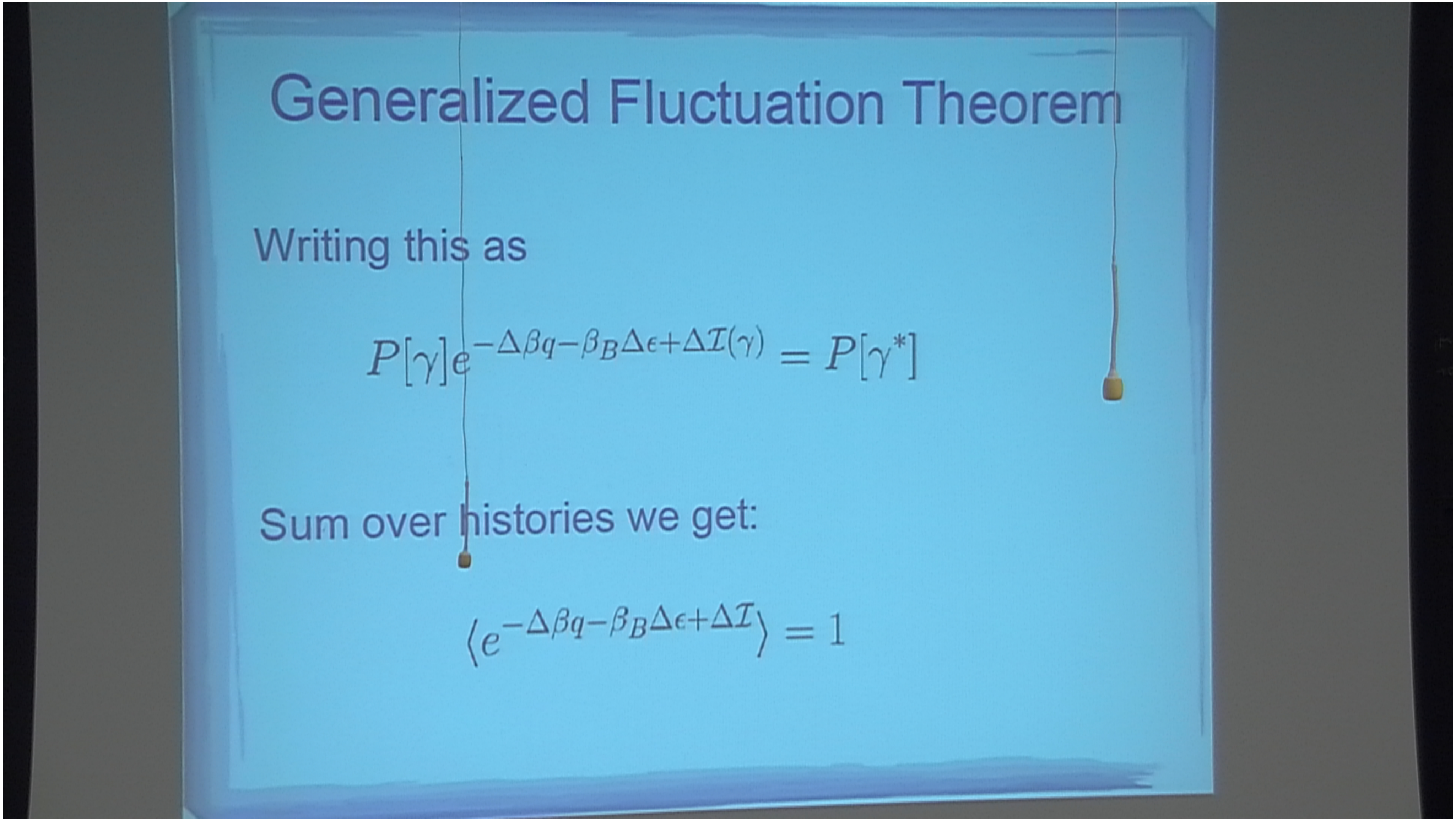
$$P_{\mathrm{init}}[|\phi, \chi\rangle] \propto e^{-\beta_A E_\phi - \beta_B E_\chi + \mathcal{I}(\rho_{AB};\phi,\chi)}$$

Central expression

Combining (I) and (II) we get:

$$\Rightarrow \quad \frac{P[\gamma]}{P[\gamma^*]} = e^{\Delta\beta q + \beta_B \Delta\epsilon - \Delta\mathcal{I}(\gamma)}$$

$$\Delta\beta = \beta_A - \beta_B$$


Generalized Fluctuation Theorem
Writing this as
$P[\gamma]e^{-\Delta\beta q-\beta_B\Delta\epsilon+\Delta\mathcal{I}(\gamma)} = P[\gamma^*]$
Sum over histories we get:
$\langle e^{-\Delta\beta q-\beta_B\Delta\epsilon+\Delta\mathcal{I}}\rangle = 1$

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Generalized Fluctuation Theorem

Of interest is ratio:

$$\frac{P[q,\Delta\epsilon]}{P[-q,-\Delta\epsilon]}$$

where

$$P[q,\Delta\epsilon] := P[\Gamma(q,\Delta\epsilon)]$$

We find

$$e^{\Delta\beta q+\beta_B\Delta\epsilon-\Delta\mathcal{I}_l} \leq \frac{P[q,\Delta\epsilon]}{P[-q,-\Delta\epsilon]} \leq e^{\Delta\beta+\beta_B\Delta\epsilon-\Delta\mathcal{I}_u}$$

Generalized Fluctuation Theorem

For case of $\Delta\epsilon = 0$ and $\Delta\mathcal{I} = 0$

we recover detailed FT

$$\frac{P[q]}{P[-q]} = e^{\Delta\beta q}$$

Generalized Clausius

$$\langle e^{-\Delta\beta q - \beta_B \Delta\epsilon + \Delta\mathcal{I}} \rangle = 1$$

Application of Jensen's inequality $\langle e^X \rangle \geq e^{\langle X \rangle}$ gives us:

$$\Delta\beta\langle q \rangle + \beta_B \langle \Delta\epsilon \rangle \geq \langle \Delta\mathcal{I} \rangle$$

Clausius Relation

$$\Delta\beta\langle q\rangle + \beta_B\langle\Delta\epsilon\rangle \geq \langle\Delta\mathcal{I}\rangle$$

For $\langle\Delta\epsilon\rangle = 0$ we obtain

$$\left(\frac{1}{kT_A} - \frac{1}{kT_B}\right)\langle q\rangle \geq \langle\Delta\mathcal{I}\rangle$$

However $\langle\Delta\mathcal{I}\rangle$ is a purely <u>classical</u> correlation.

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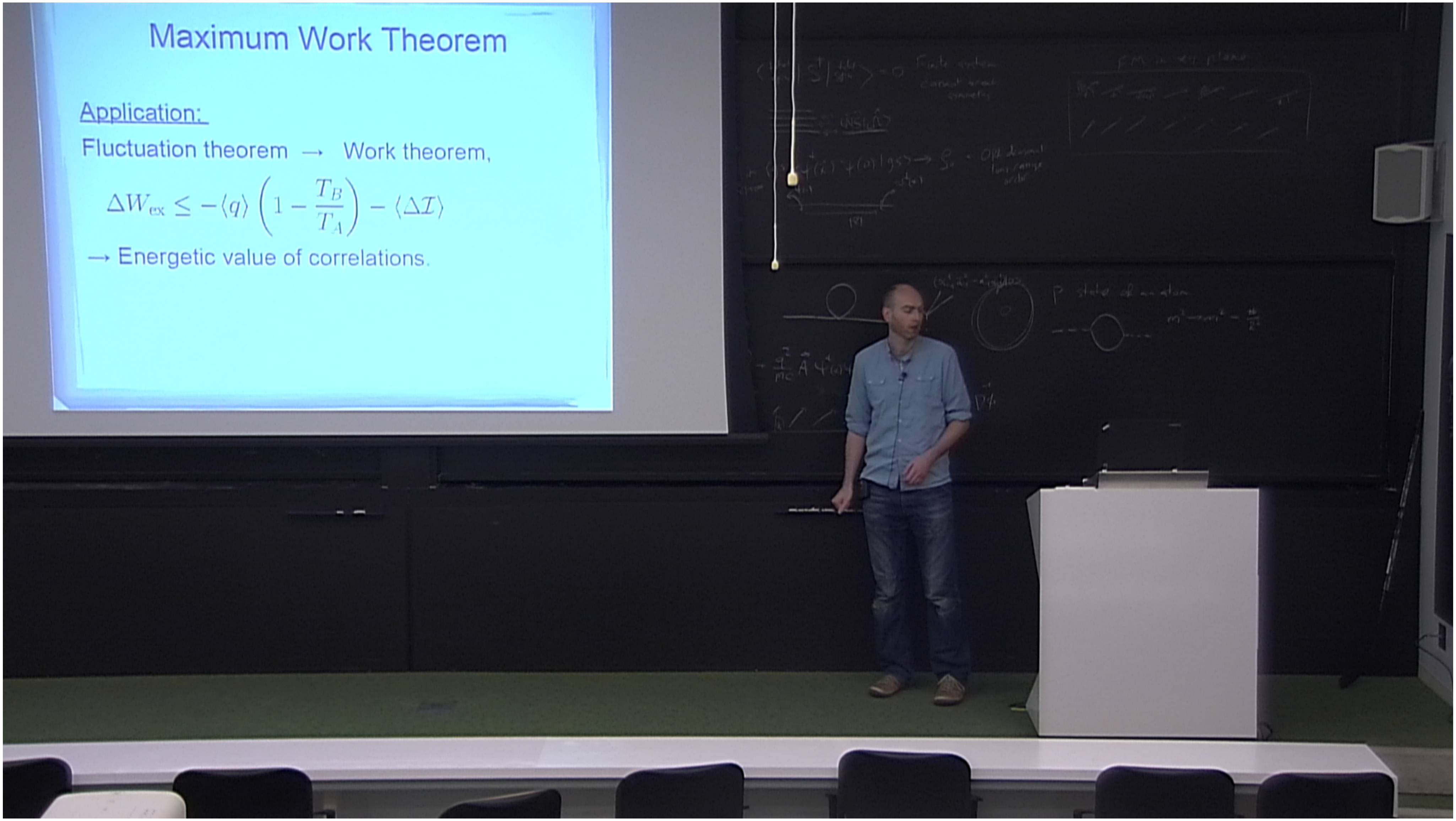
Maximum Work Theorem
Application:
Fluctuation theorem → Work theorem,
$\Delta W_{\rm ex} \leq -\langle q \rangle \left(1 - \frac{T_B}{T_A}\right) - \langle \Delta \mathcal{I} \rangle$
→ Energetic value of correlations.

Maximum Work Theorem

<u>Application:</u>

Fluctuation theorem $\rightarrow$ Work theorem,

$$\Delta W_{\text{ex}} \leq -\langle q \rangle \left(1 - \frac{T_B}{T_A}\right) - \langle \Delta \mathcal{I} \rangle$$

$\rightarrow$ Energetic value of correlations.

Classicality of XFT

- Projective measurements kill entanglement.
- POVMs?
- Time-reversal pairing trick constraint:

POVM elements of $\mathcal{M}_2$ must be same set of states prepared by $\mathcal{M}_1$

- Ways to evade this?

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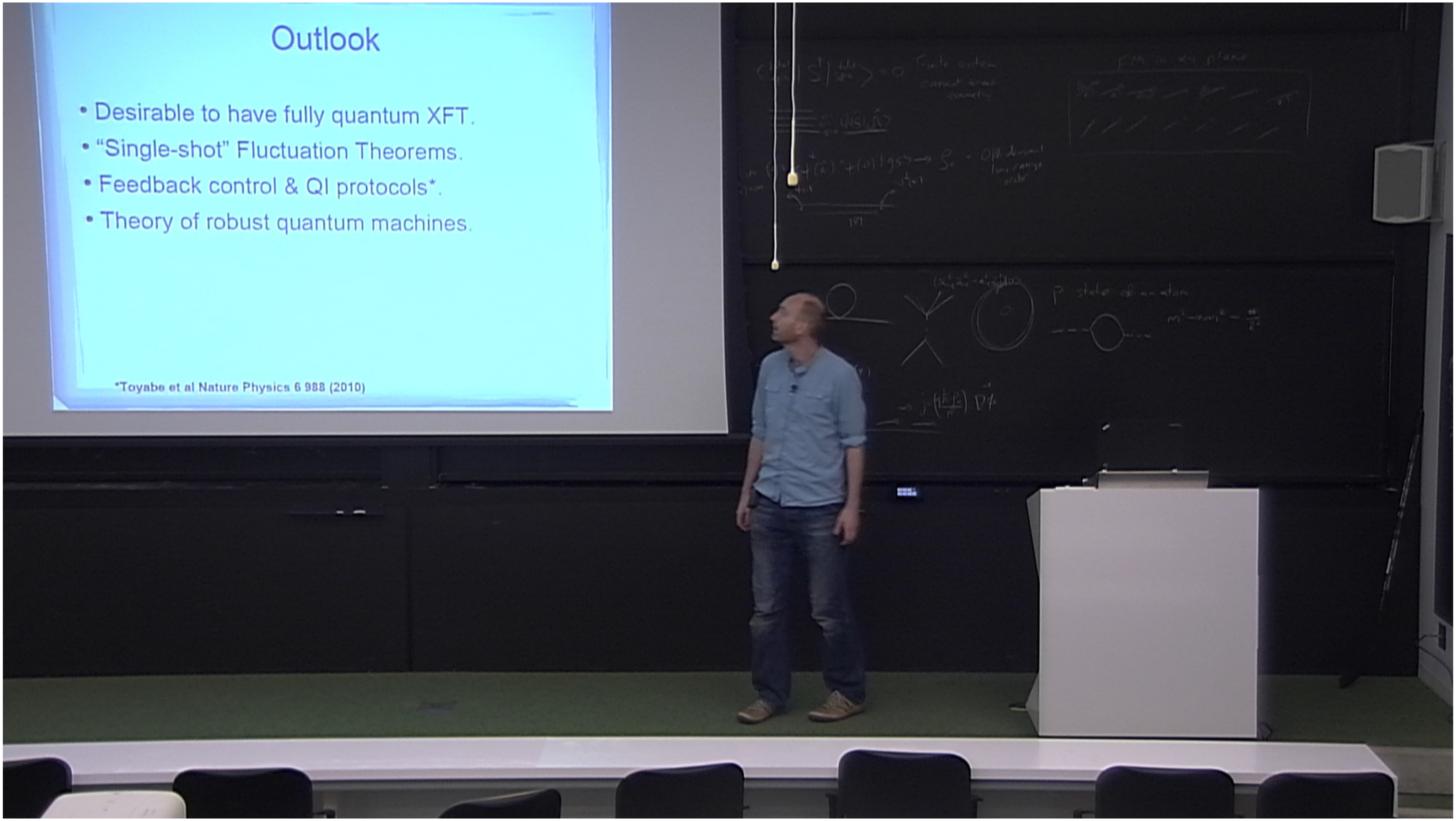
Outlook
• Desirable to have fully quantum XFT.
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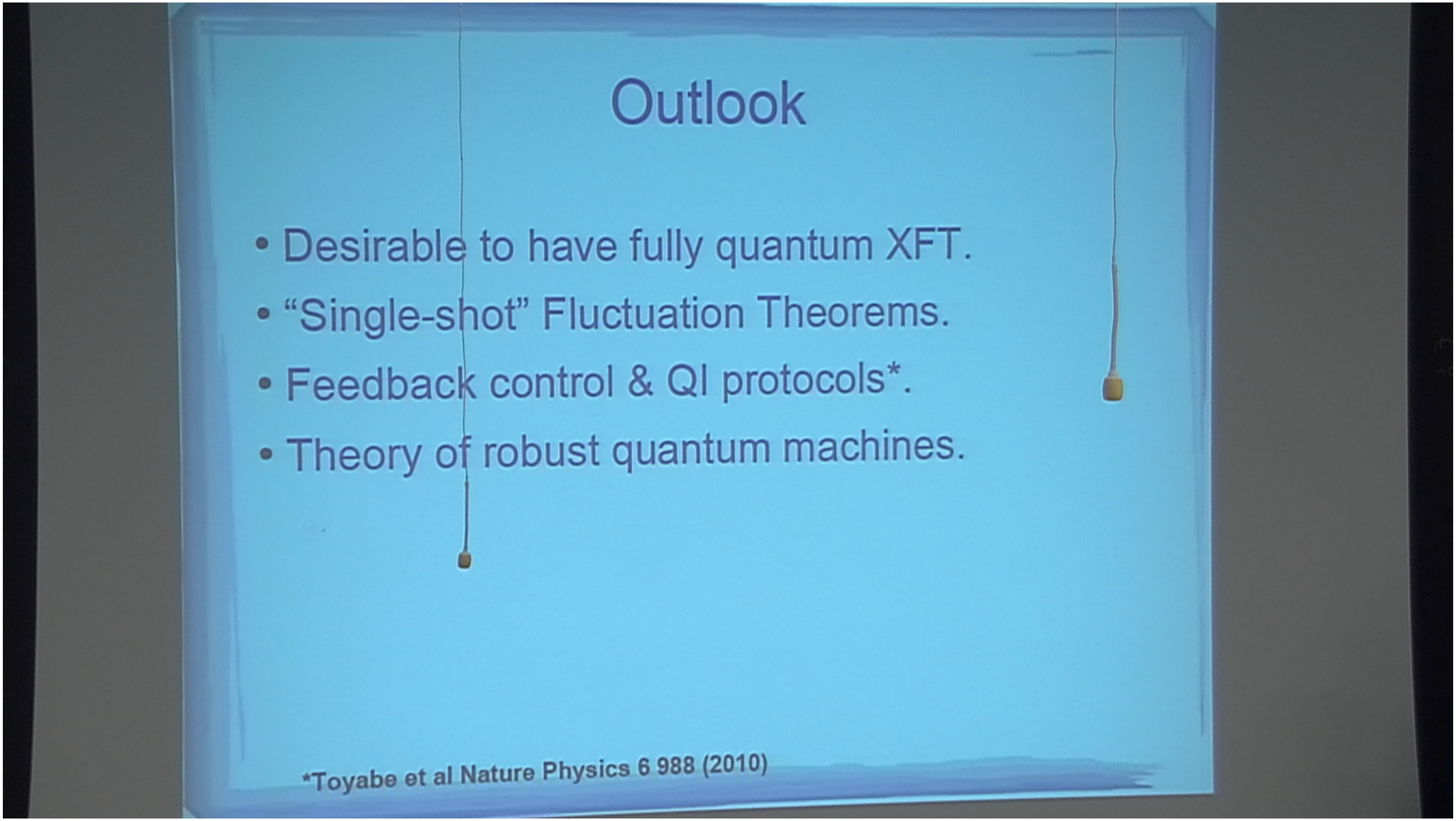
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