Title: Under what conditions quantum systems thermalize?

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Abstract: This talk presents sufficient conditions for equilibration and thermalization of subsystems within closed many body quantum systems. That is, we identify when the local properties of the equilibrium state resemble those of a thermal state. With this aim, the recent progress in this field is reviewed and we introduce a novel perturbation technique for a realistic weak coupling between the subsystem and its environment. Unlike the standard perturbation theory, our technique is robust in the thermodynamic limit. Based on our thermalization results, we construct a simple and fully general quantum algorithm for preparing Gibbs states with a certified runtime and error bonds.

Thermalization in nature and on a quantum computer

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Universität Potsdam

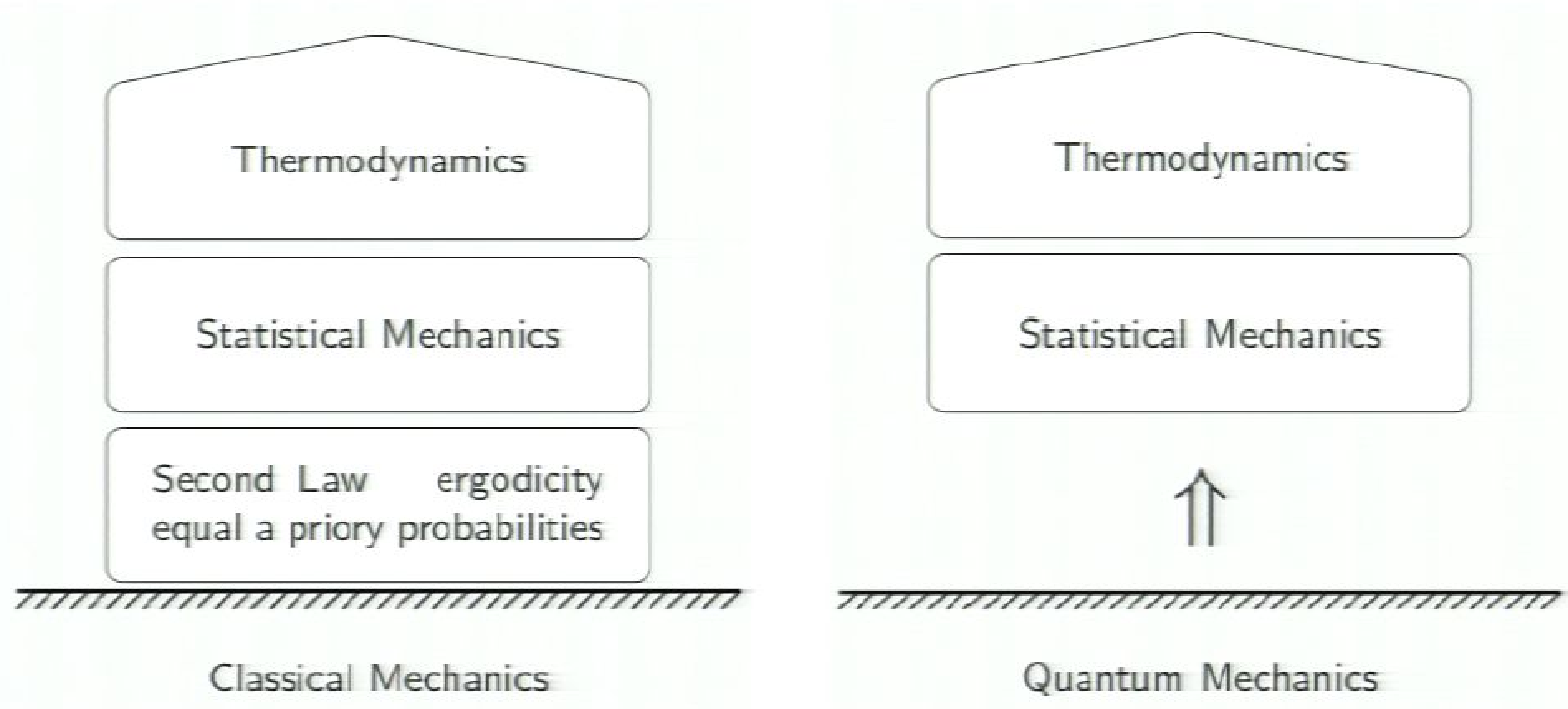
arXiv:1102.2389

April 2011

Introduction

Context and motivation

New foundation for Statistical Mechanics.



Setup

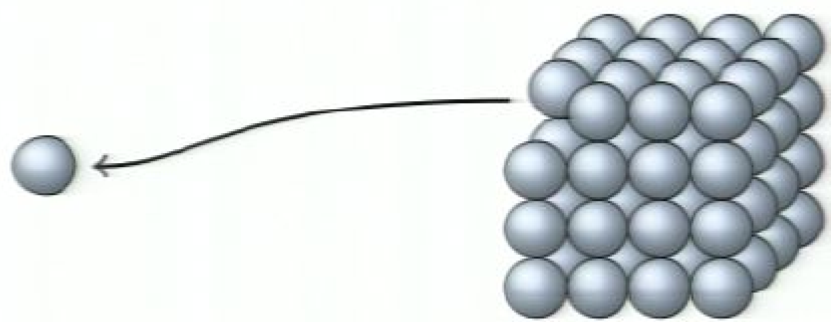
System

$d_S := \dim \mathcal{H}_S$

Bath

$d_B := \dim \mathcal{H}_B$

$$H = H_S + H_B + V$$



The whole system follows a unitary evolution $|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}Ht}|\psi(0)\rangle$

$$\rho^S(t) = \mathrm{Tr}_B\, |\psi(t)\rangle\langle\psi(t)|$$

Definition of the problem

Given the initial state and the Hamiltonian:

$$|\psi(0)\rangle = \sum_n c_n |E_n\rangle \qquad H = \sum_n E_n |E_n\rangle\langle E_n|$$

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(2) Under what conditions the system **thermalizes**?

$$\rho^S(t) \longrightarrow \boxed{\omega^S \propto \mathrm{e}^{-\beta H_S} = \sum_k \mathrm{e}^{-\beta E_k^S} |E_k^S\rangle\langle E_k^S|}$$

Gibbs state!

Conditions for equilibration

Most of initial states equilibrate

If the system **equilibrates**, it equilibrates towards its **time average**:

$$\omega^S = \langle \rho^S(t) \rangle_t = \lim_{T \to \infty} \frac{1}{T} \int_0^T \rho^S(t) \mathrm{d}t$$

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Assumption 1. The **Hamiltonian** has no degeneracies.

Then,

$$\omega^S = \sum_n |c_n|^2 \, \mathrm{Tr}_B \, |E_n\rangle\langle E_n|$$

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In Ref. [1], it is shown that **most of initial states** of the Hilbert space **equilibrate**.

[1] N. Linden, S. Popescu, A. J. Short, and A. Winter PRE 79 (2009) no. 6, 061103

Most of initial states equilibrate

What do we understand by "equilibration"?

When the **average distance** between the **state of the system** and the **equilibrium state** is small, the system must spend most of its time at the equilibrium state.

$$\text{equilibration} \quad \equiv \quad \left\langle \mathcal{D}(\rho^S(t), \omega^S) \right\rangle_t \leq \text{small}$$

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In [1], it is proven that

$$\left\langle \mathcal{D}(\rho^S(t), \omega^S) \right\rangle_t \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\text{eff}}}}$$

where $d^{\text{eff}} = \dfrac{1}{\sum_n |c_n|^4}$.

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Conditions for thermalization

Conditions for the thermal state

Under what conditions is the **equilibrium** state **thermal**?

$$\rho^S(t) \longrightarrow \omega^S = \sum_n |c_n|^2 \, \mathrm{Tr}_B \, |E_n\rangle\langle E_n| \propto \mathrm{e}^{-\beta H_S}$$

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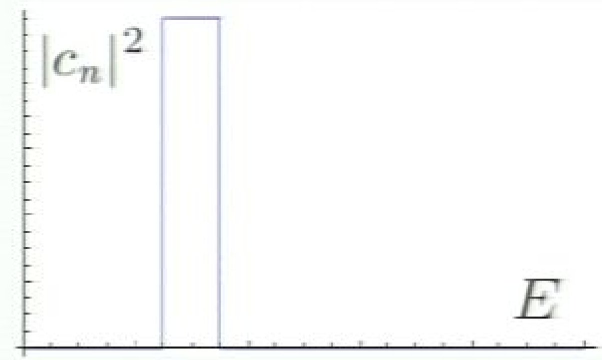
Our claim: if the dephased state of the total system is a rectangular state, it looks locally thermal.



$$|\psi(0)\rangle = \sum_n c_n |E_n\rangle$$

$$|\psi(0)\rangle \longrightarrow \omega_\sqcap = \frac{1}{\Omega_\Delta(E)} \sum_{E_n \in [E, E+\Delta]} |E_n\rangle\langle E_n|$$

$$\omega^S = \mathrm{Tr}_B \, \omega_\sqcap \propto \mathrm{e}^{-\beta H_S}$$

How this problem was addressed so far?

$$H = \underbrace{H_S + H_B}_{} + V$$
$$H = H_0 + V$$

$$\begin{cases} H_0 |E_n^{(0)}\rangle = E_n^{(0)} |E_n^{(0)}\rangle \\ |E_n^{(0)}\rangle = |E_k^S\rangle \otimes |E_q^B\rangle \end{cases}$$

It was assumed so far that $|E_n\rangle \simeq |E_n^{(0)}\rangle$

⬇

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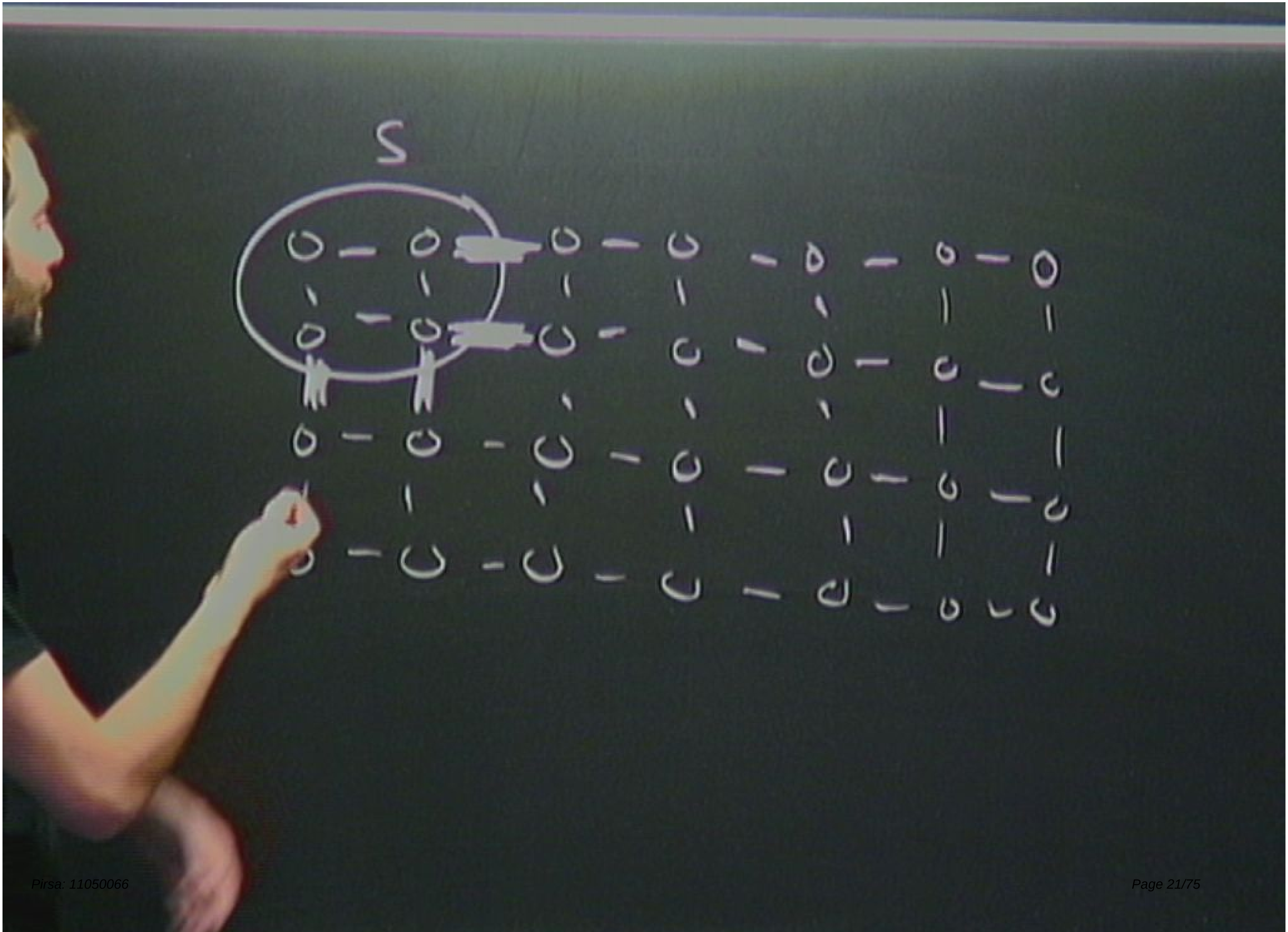
But typically the gaps decrease exponentially with the size of the system.

Example: chain of *m* non-interacting spins.

$E_{\max} = m \quad \uparrow\uparrow\uparrow \cdots \uparrow$

$E_{\min} = 0 \quad \downarrow\downarrow\downarrow \cdots \downarrow$

→ $\|H\|_\infty = m$, $d = 2^m$ → $\bar{\delta} = \frac{\|H\|_\infty}{d} = m2^{-m}$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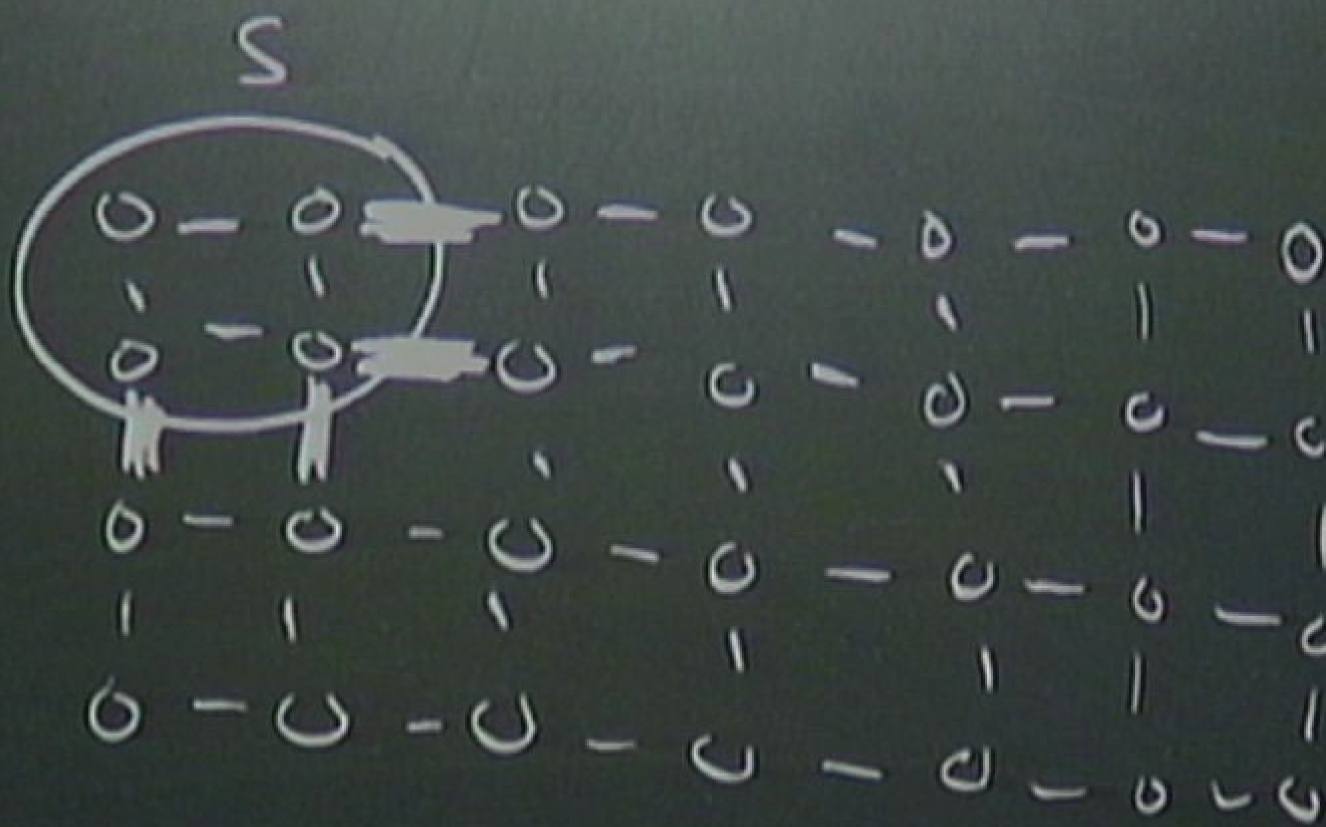
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rst condition for thermalization: a weak (but realistic) interaction

Nevertheless, a **weaker condition** is required in order to be able to compute the trace of the **rectangular state**:

$$\omega_{\sqcap} \simeq \omega_{\sqcap}^{(0)}$$

$$\sum_{E_n \in [E, E+\Delta]} |E_n\rangle\langle E_n| \simeq \sum_{E_n^{(0)} \in [E, E+\Delta]} |E_n^{(0)}\rangle\langle E_n^{(0)}|$$

heorem. *The* ***rectangular states*** *of the interacting and non-interacting* **Hamiltonians** *are indistinguishable in the following sense*

$$\mathcal{D}(\omega_{\sqcap}^{S}, \omega_{\sqcap}^{S(0)}) \leq \mathcal{D}(\omega_{\sqcap}, \omega_{\sqcap}^{(0)}) \leq \frac{3\sqrt{2}}{2}\left(\frac{\|V\|_{\infty}}{\Delta}\right)^{1/2}$$

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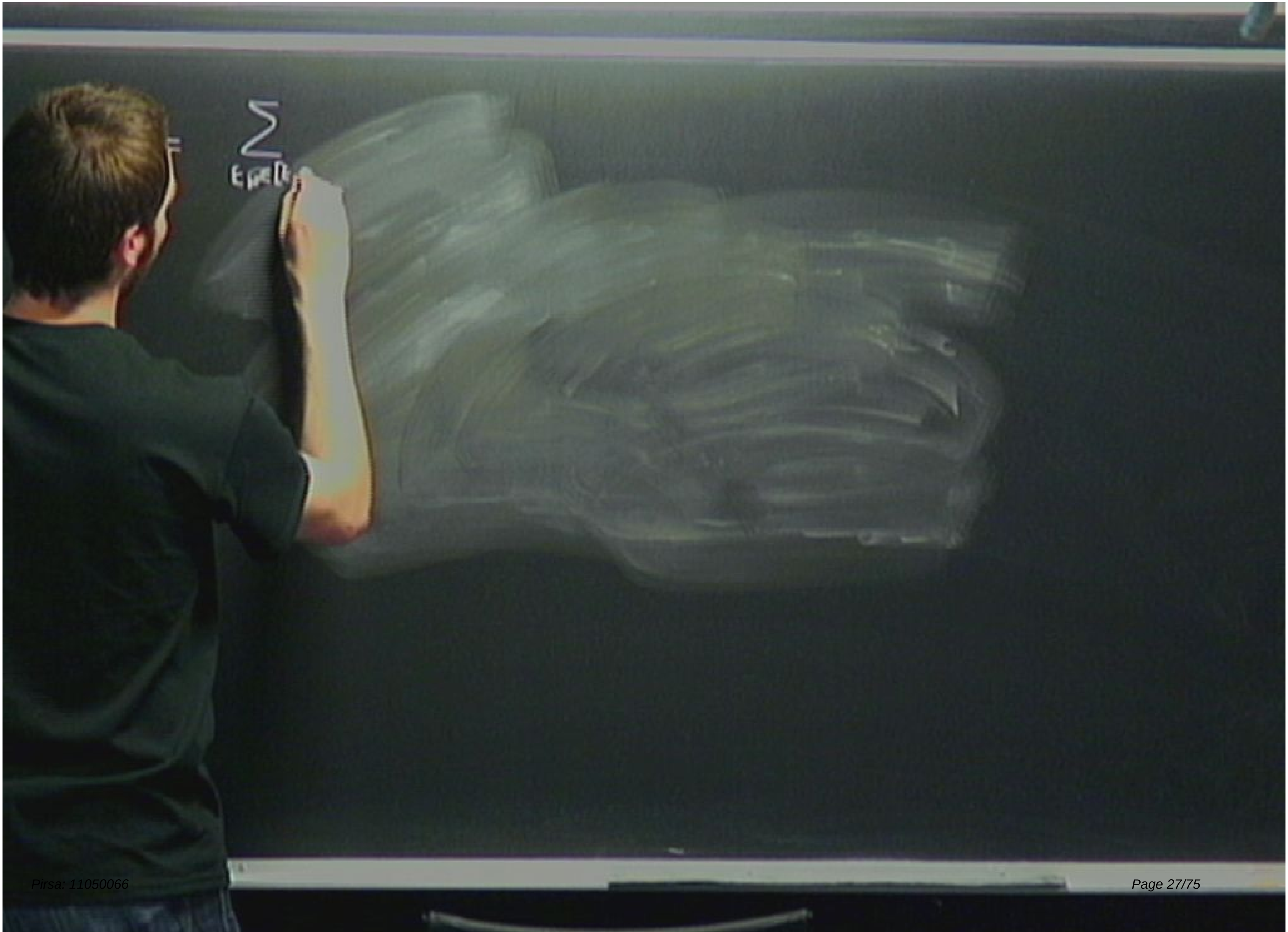
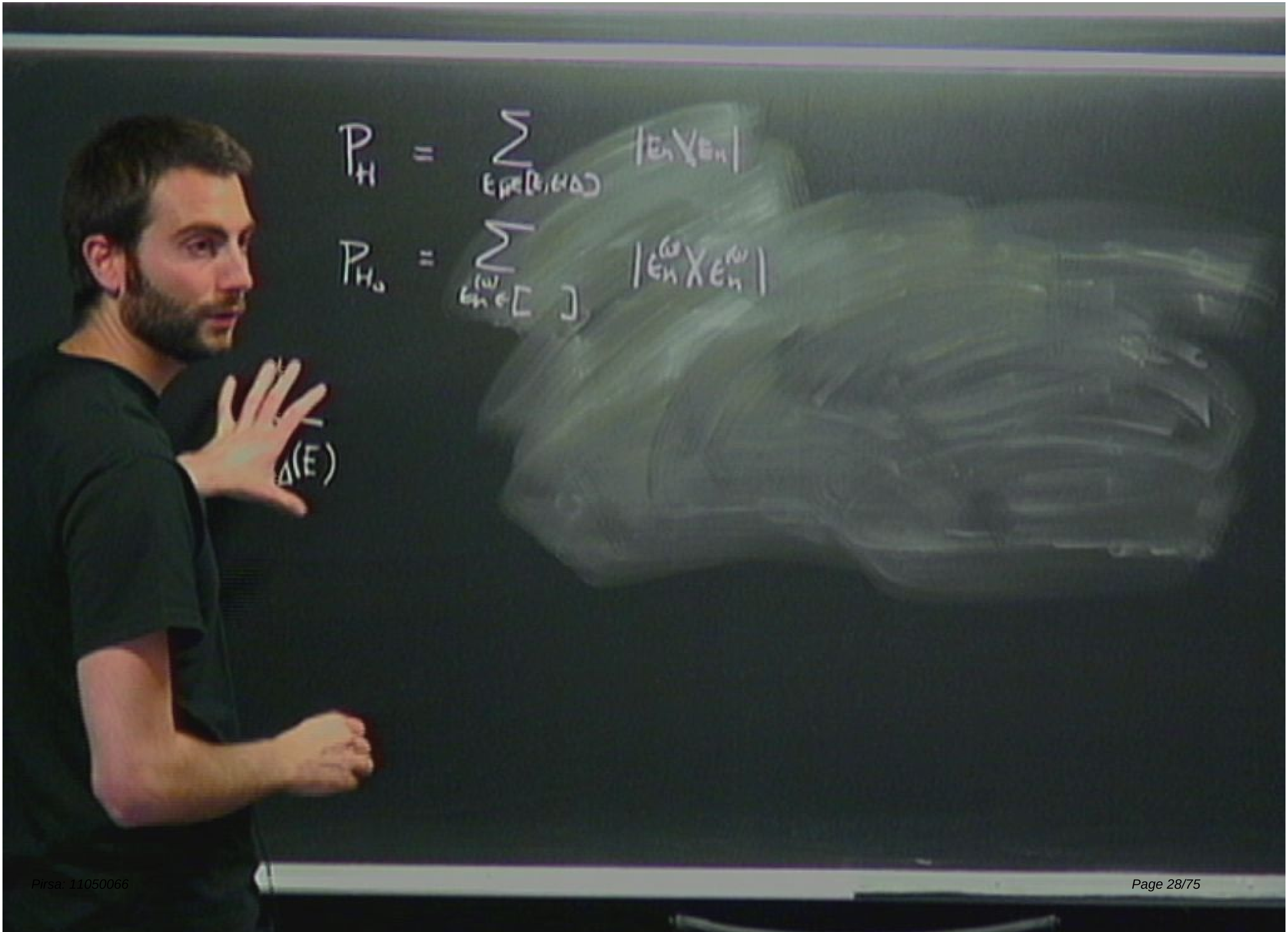
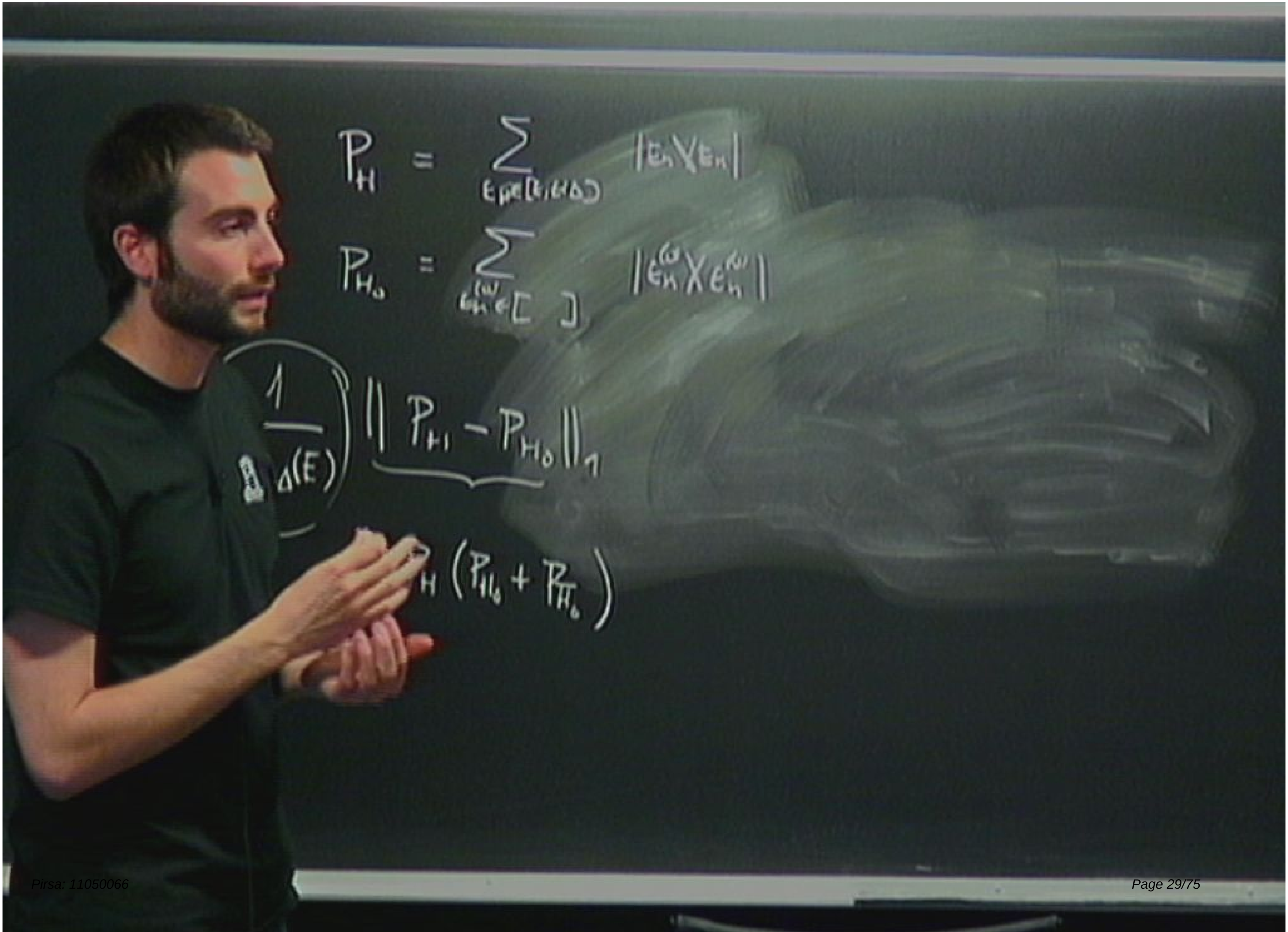
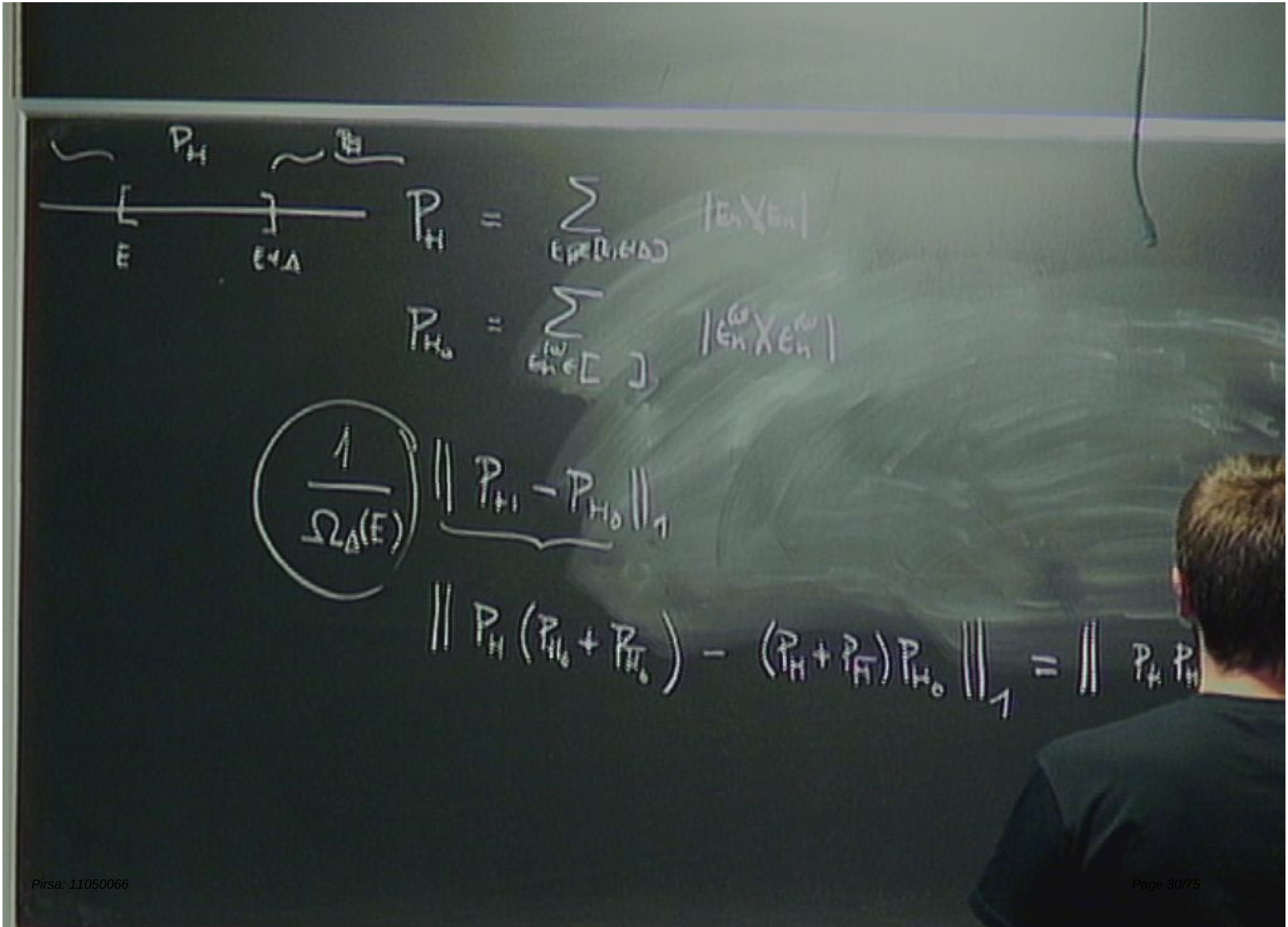
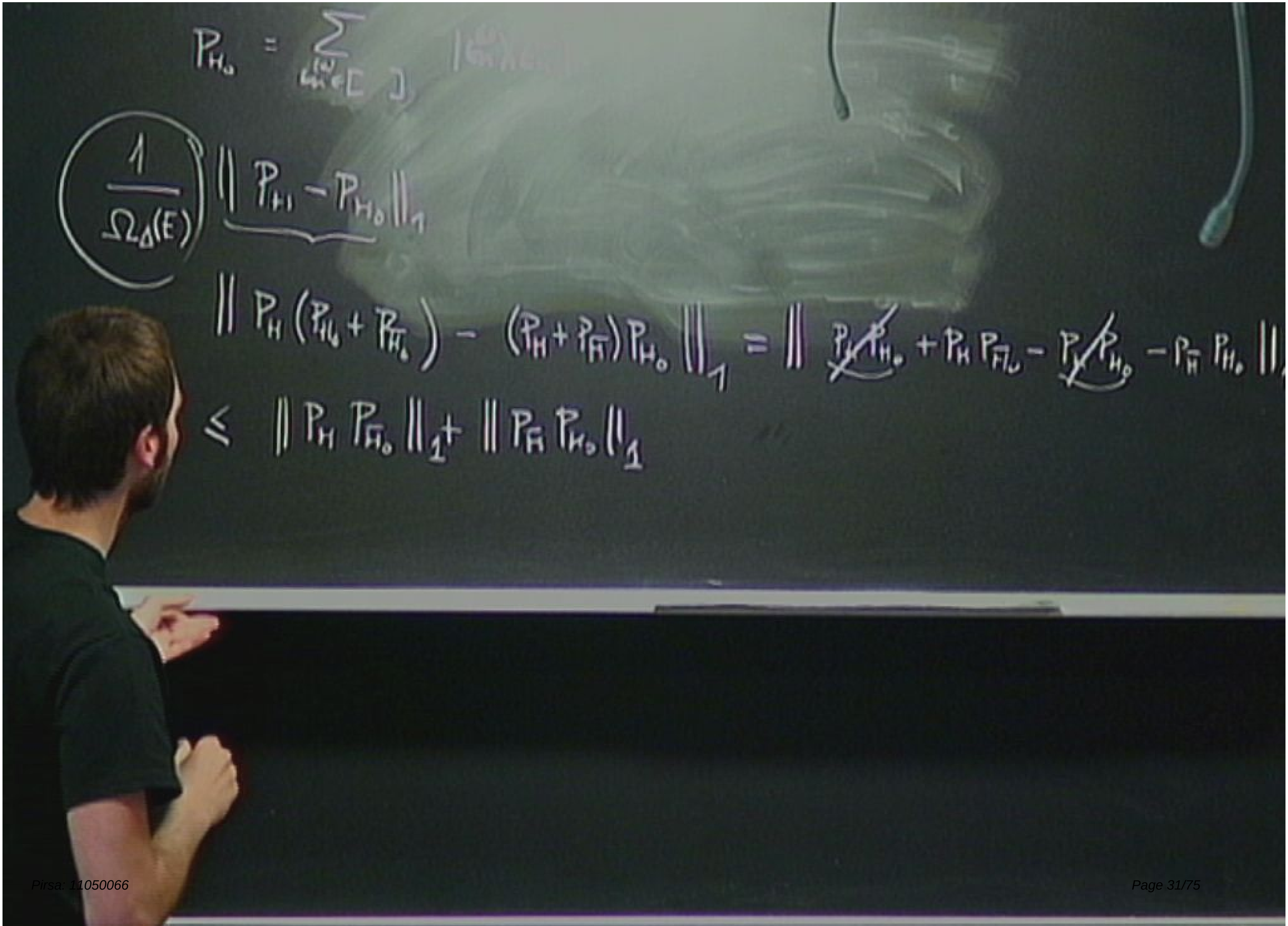


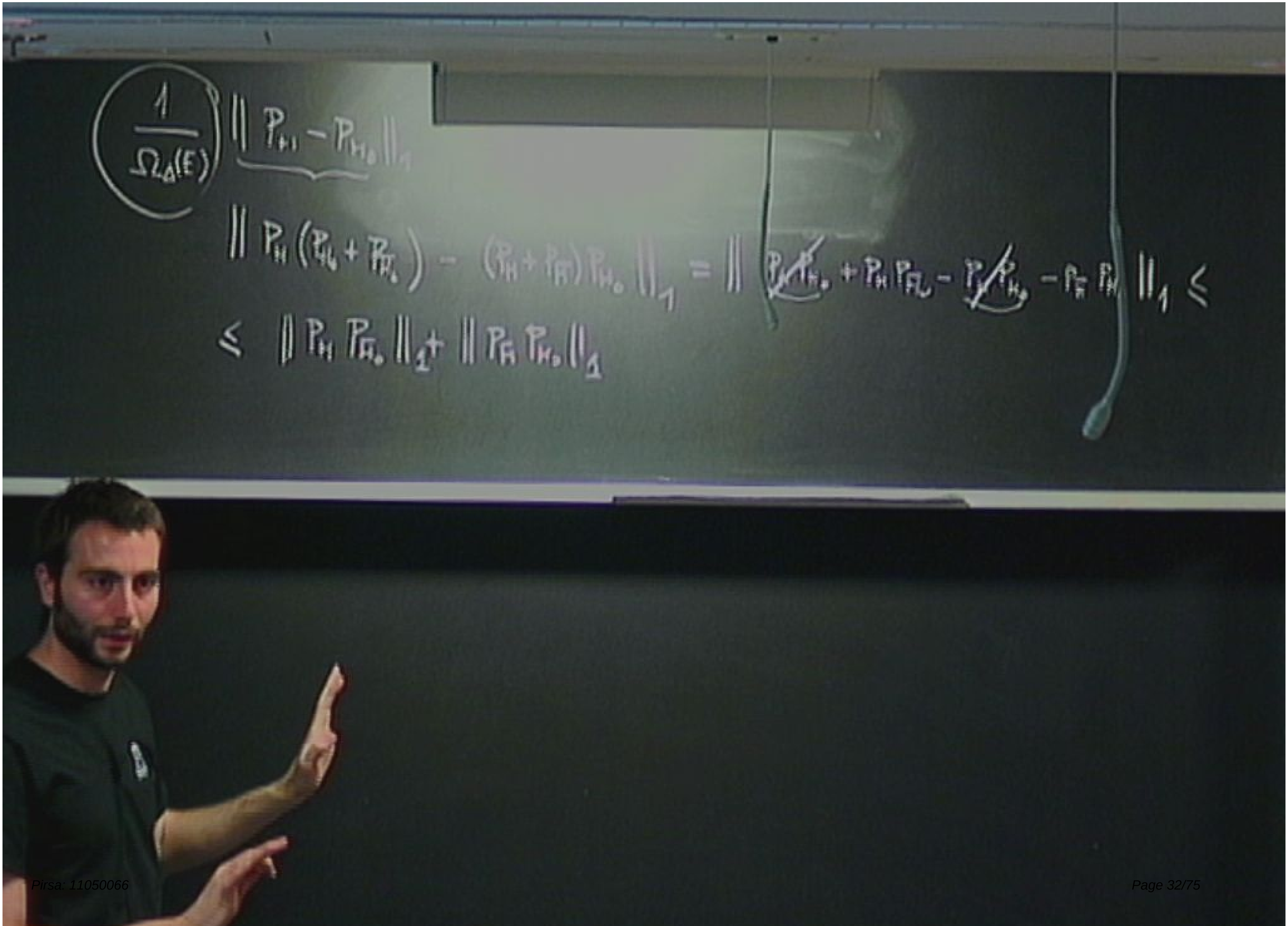


P_H = Σ |E_n⟩⟨E_n|
P_H0 = Σ |E_n^(ω)⟩⟨E_n^(ω)|
Δ(E)


P_H = Σ |E_n⟩⟨E_n|
P_{H_0} = Σ |E_n^{(0)}⟩⟨E_n^{(0)}|
1 / Δ(E)
|| P_{H} − P_{H_0} ||_1


P_H
E
$E+\Delta$
$P_H = \sum_{E_n \in [E, E+\Delta]} |E_n\rangle\langle E_n|$
$P_{H_0} = \sum_{E_n^{(\omega)} \in [\ ]} |E_n^{(\omega)}\rangle\langle E_n^{(\omega)}|$
$\frac{1}{\Omega_\Delta(E)} \| P_{H} - P_{H_0} \|_1$
$\| P_H (P_{H_0} + P_{\bar{H}_0}) - (P_H + P_{\bar{H}}) P_{H_0} \|_1 = \|$


$P_{H_0} = \sum$
$\frac{1}{\Omega_\Delta(E)} \| P_{H_1} - P_{H_0} \|_1$
$\| P_H (P_{H_0} + P_{\bar{H}_0}) - (P_H + P_{\bar{H}}) P_{H_0} \|_1 = \| P_H P_{H_0} + P_H P_{\bar{H}_0} - P_H P_{H_0} - P_{\bar{H}} P_{H_0} \|_1$
$\leq \| P_H P_{\bar{H}_0} \|_1 + \| P_{\bar{H}} P_{H_0} \|_1$



$\frac{1}{\Omega_\Delta(E)} \| P_H - P_{H_0} \|_1$
$\| P_H (P_{H_0} + P_{\bar{H}_0}) - (P_H + P_{\bar{H}}) P_{H_0} \|_1 = \| P_H P_{H_0} + P_H P_{\bar{H}_0} - P_H P_{H_0} - P_{\bar{H}} P_{H_0} \|_1 \leq$
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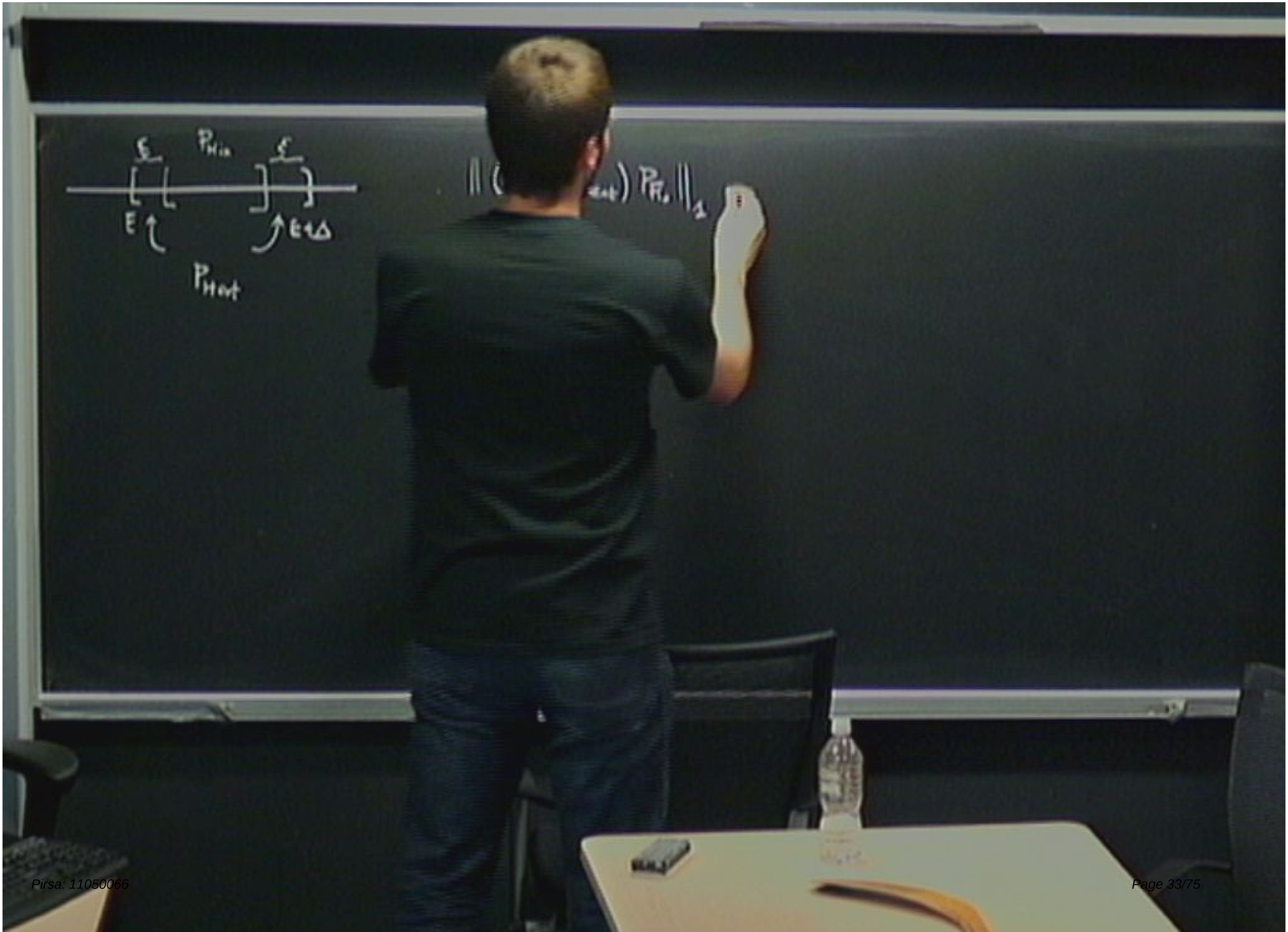
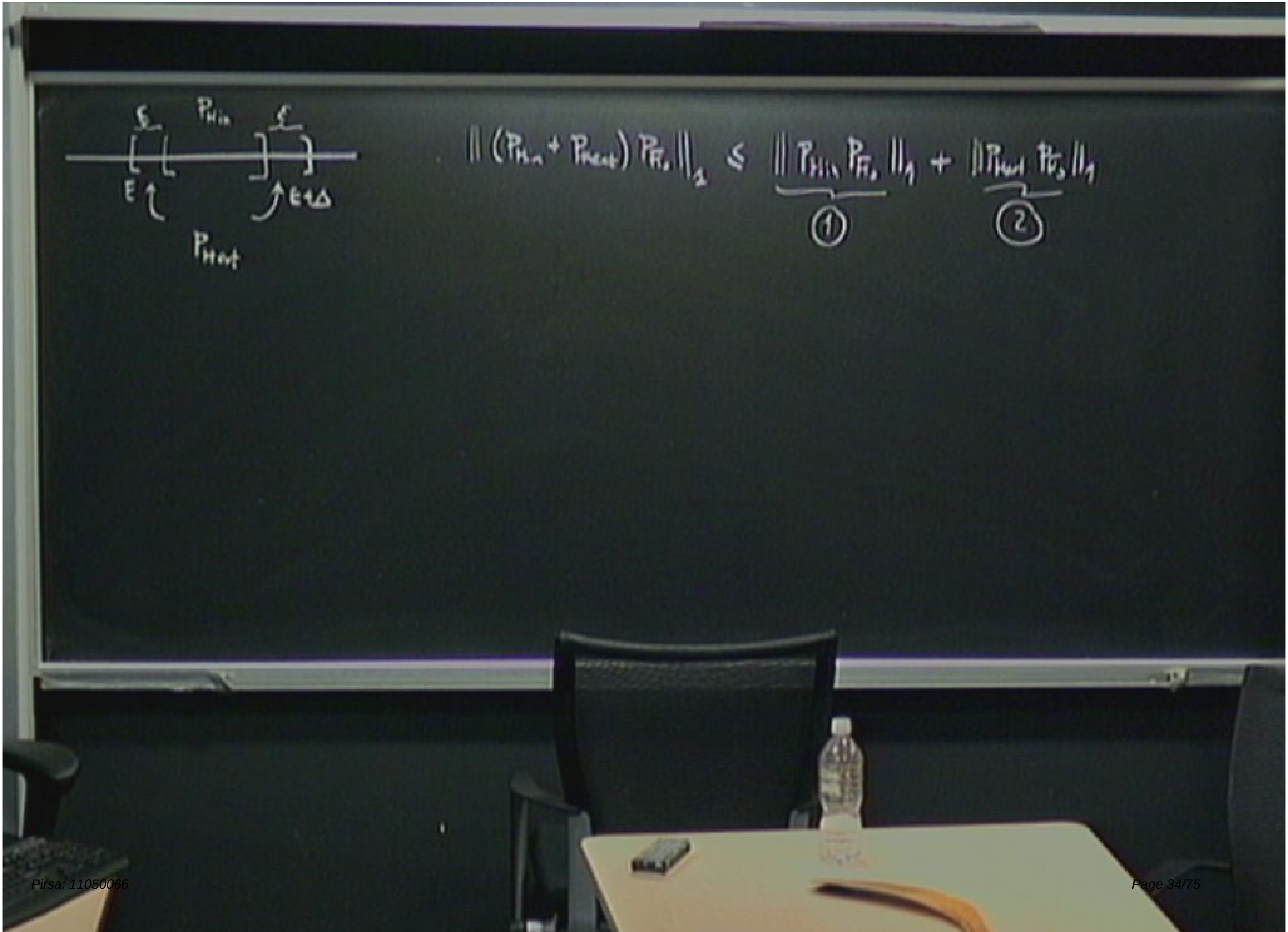


P_Hin
E
E+Δ
P_Hout


ε
P_Hin
ε
E
E+Δ
P_Hout
|| (P_Hin + P_Hout) P_H0 ||_1 ≤ || P_Hin P_H0 ||_1 + || P_Hout P_H0 ||_1
1
2

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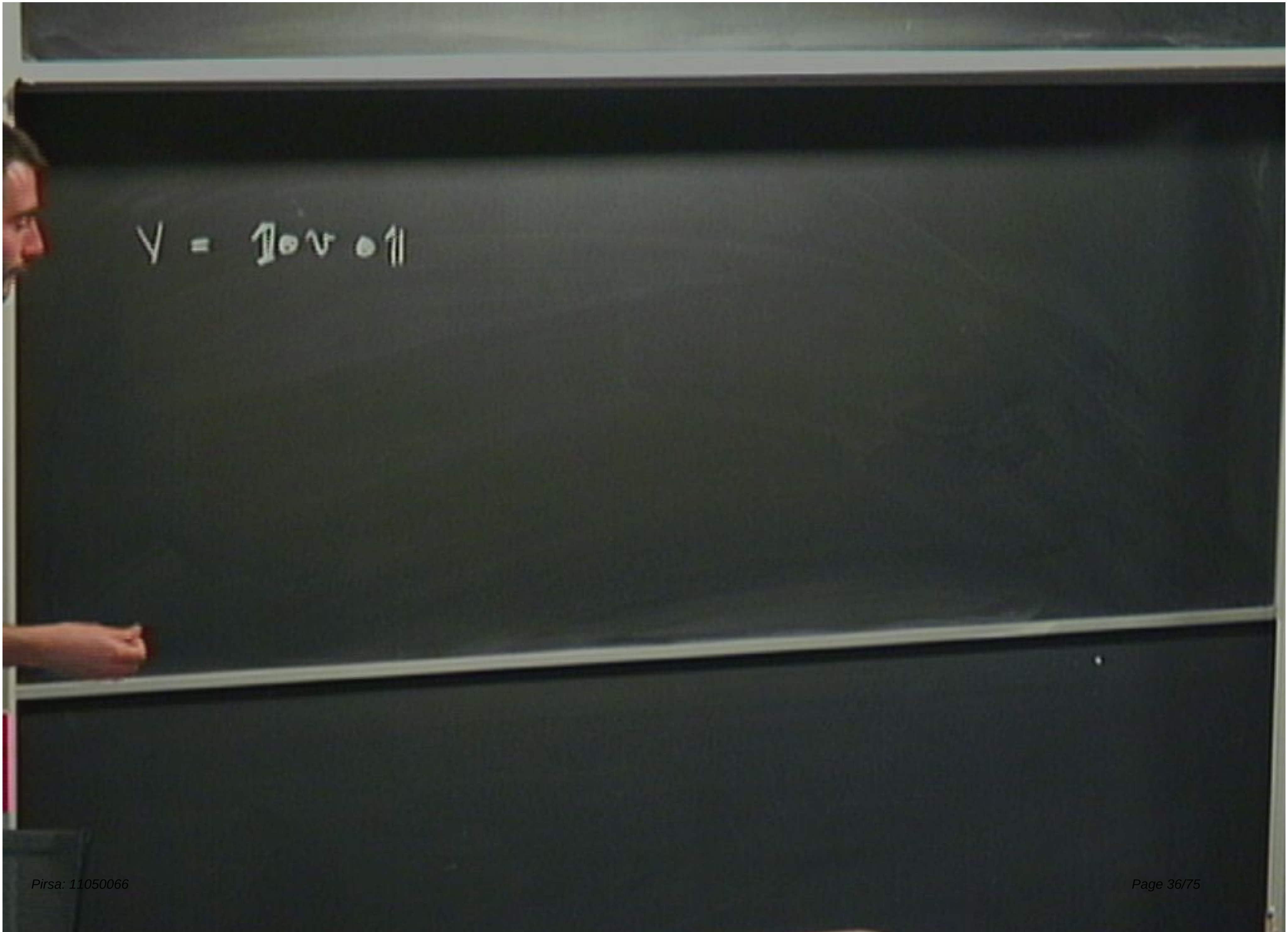
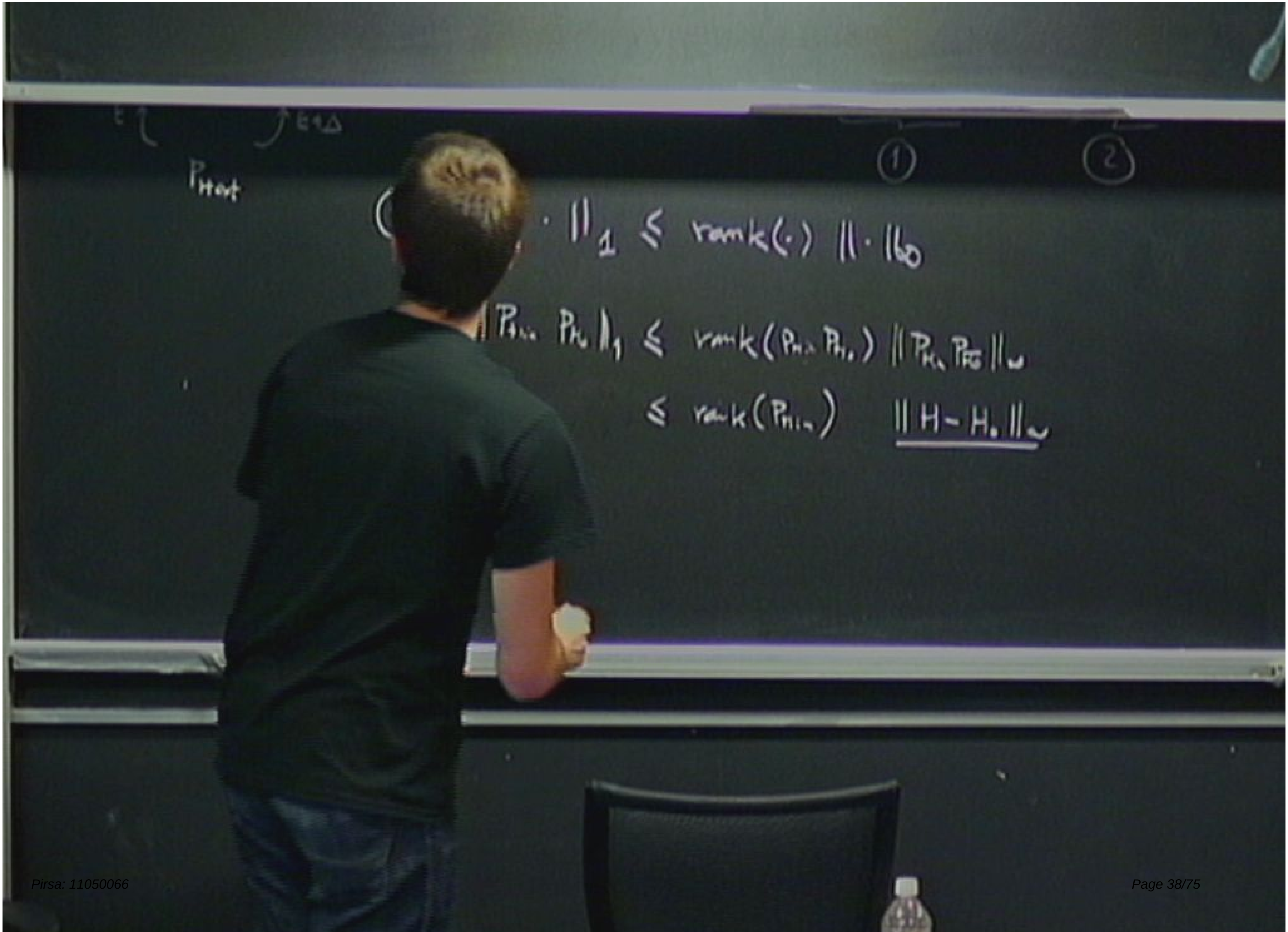
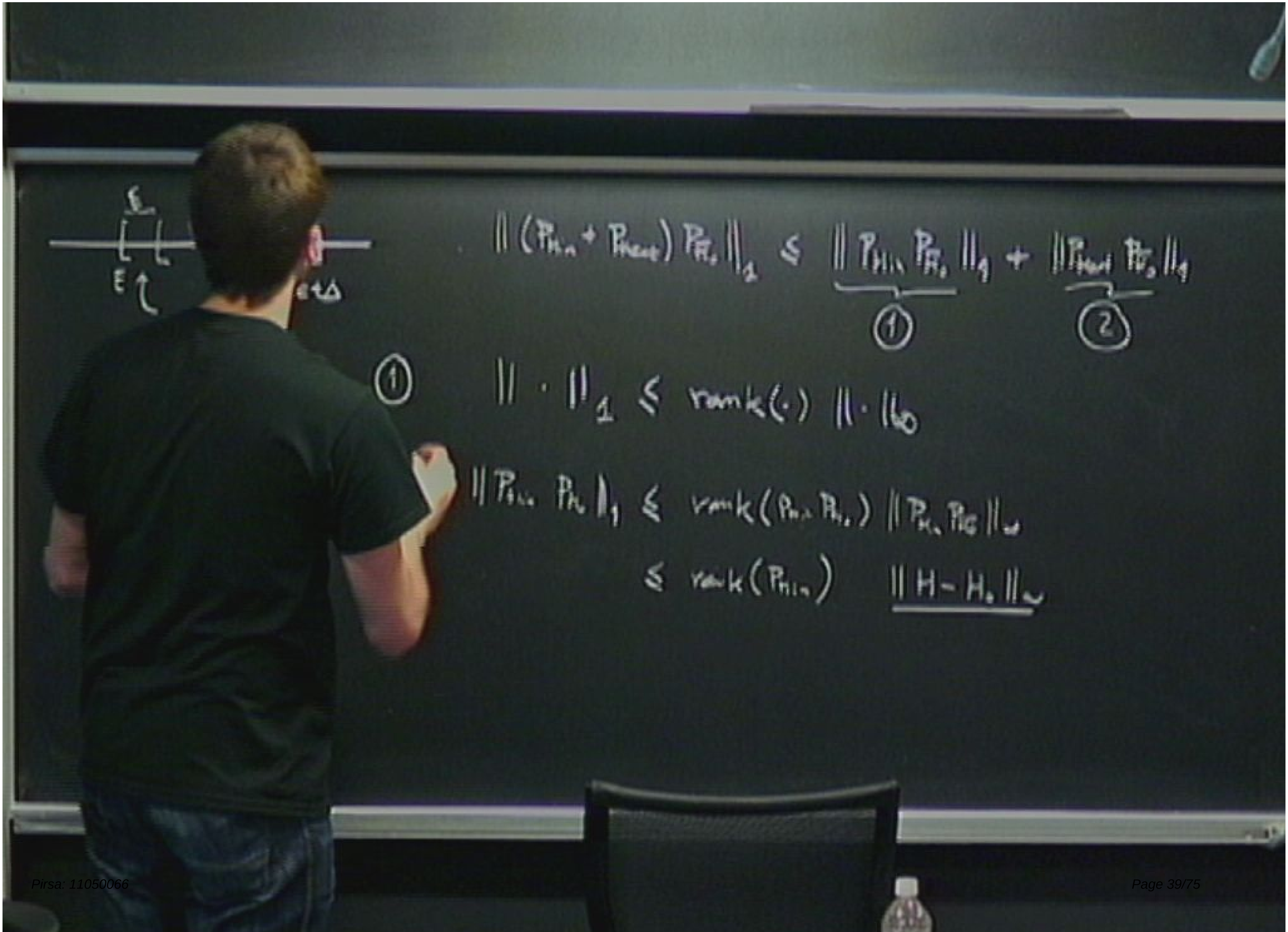

V = 1 ⊗ V ⊗ 1

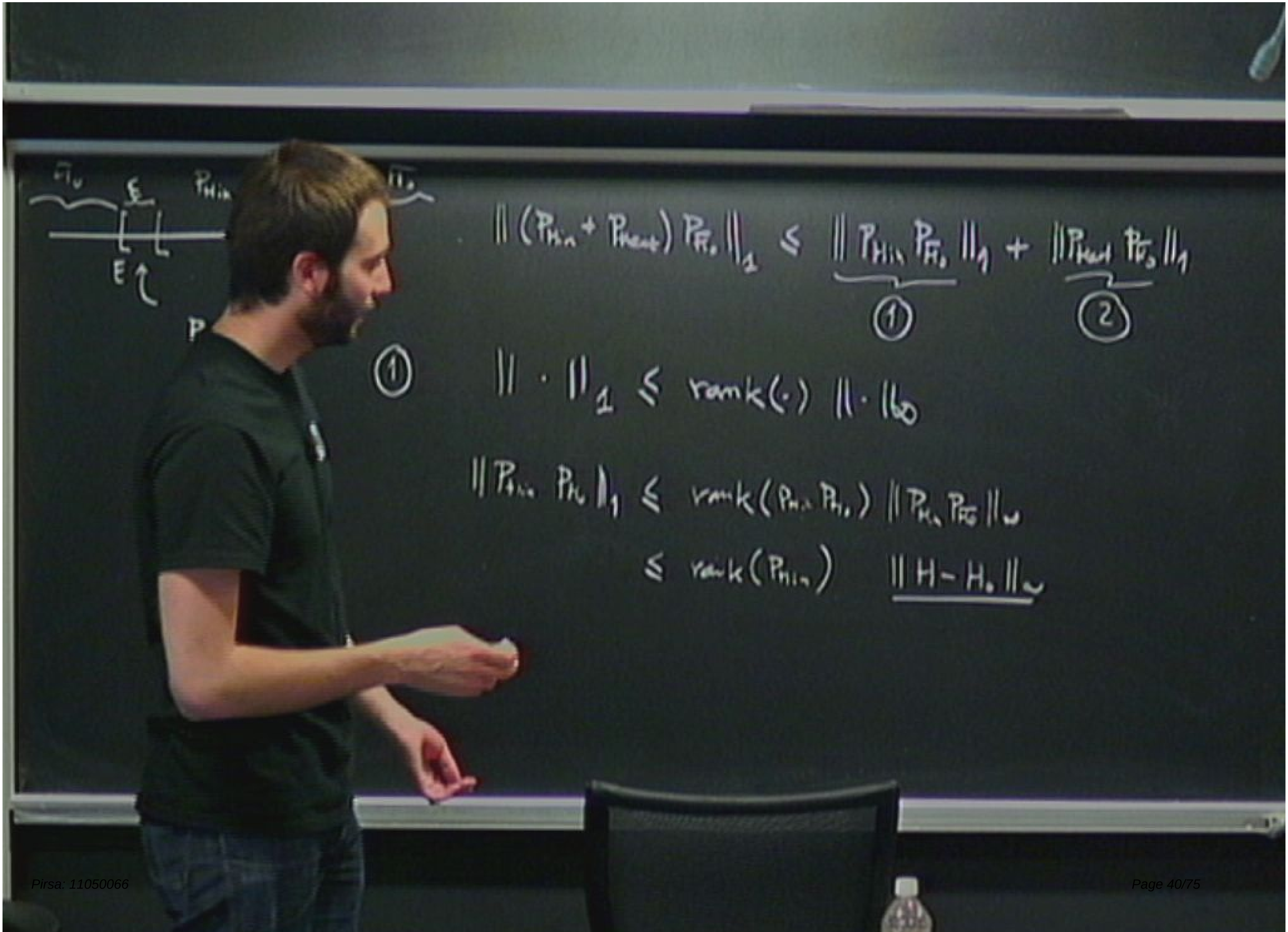
$$V = \mathbb{1} \otimes v \otimes \mathbb{1}$$

$$\|V\|_1 = \|v\|_1 \left(\|\mathbb{1}\|_1\right)^d$$


P_Hint
|| · ||_1 ≤ rank(·) || · ||_∞
||P_Hin P_H0||_1 ≤ rank(P_Hin P_H0) ||P_Hin P_H0||_∞
≤ rank(P_Hin) ||H − H_0||_∞



|| (P_Hin + P_heat) P_H0 ||_1 ≤ || P_Hin P_H0 ||_1 + || P_heat P_H0 ||_1
① ②
① || · ||_1 ≤ rank(·) || · ||_∞
|| P_Hin P_H0 ||_1 ≤ rank(P_Hin P_H0) || P_Hin P_H0 ||_∞
≤ rank(P_Hin) || H − H_0 ||_∞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||·||_1 ≤ rank(·) ||·||_∞
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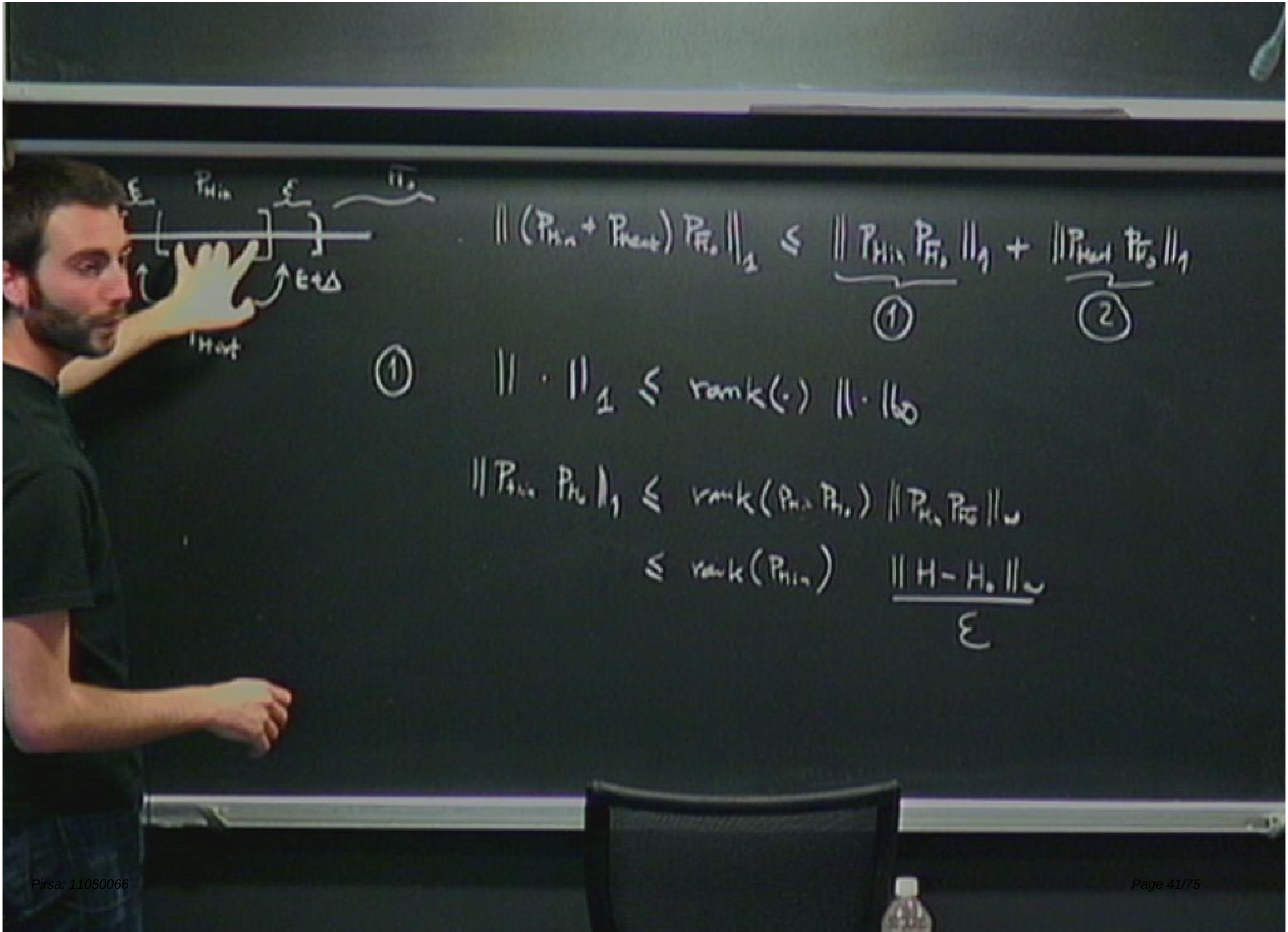
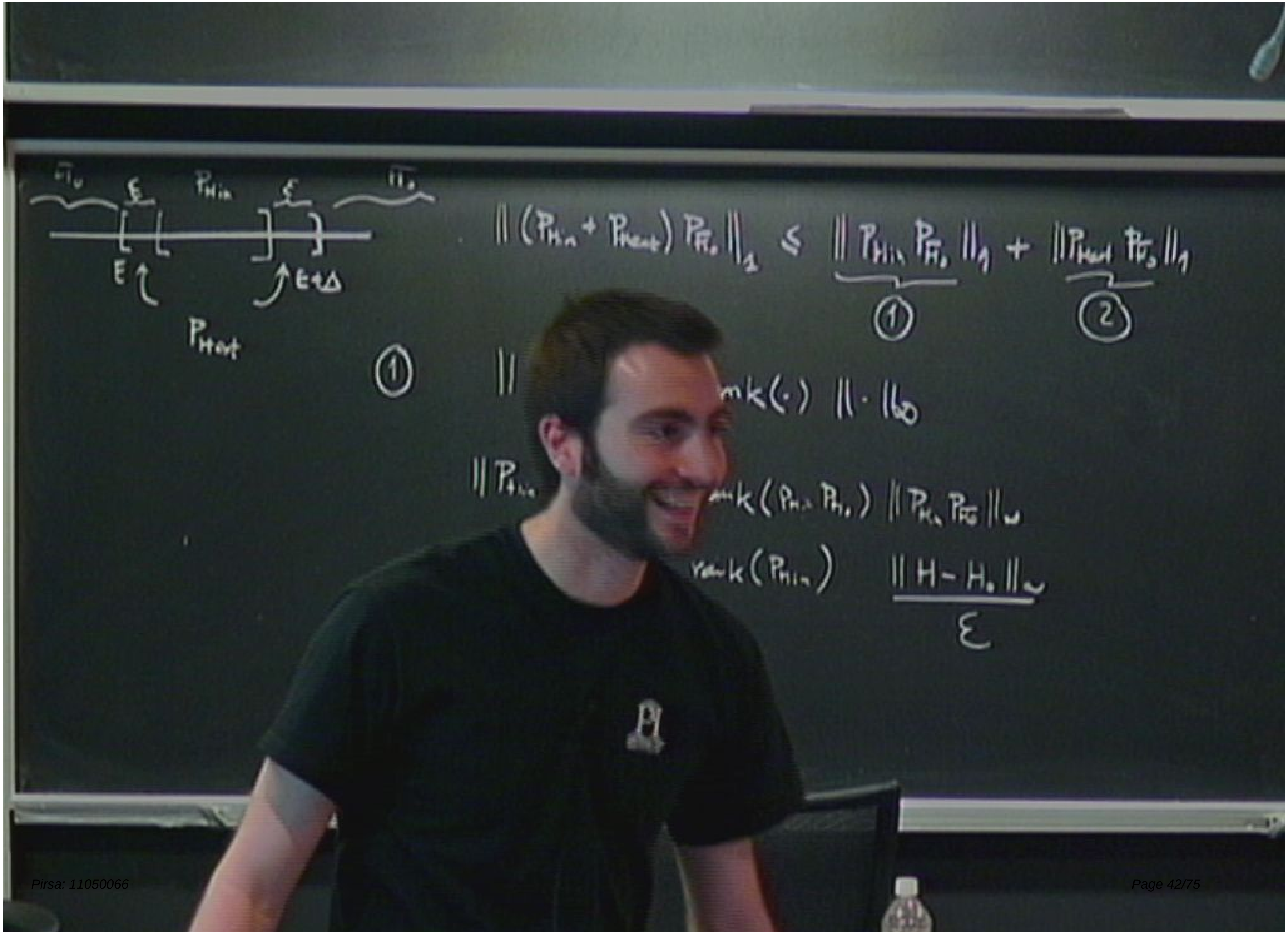

$\|(P_{H_{in}} + P_{H_{out}}) P_{\bar{H}_0}\|_1 \le \|P_{H_{in}} P_{\bar{H}_0}\|_1 + \|P_{H_{out}} P_{\bar{H}_0}\|_1$
① ②
① $\|\cdot\|_1 \le \mathrm{rank}(\cdot)\, \|\cdot\|_\infty$
$\|P_{H_{in}} P_{\bar{H}_0}\|_1 \le \mathrm{rank}(P_{H_{in}} P_{\bar{H}_0})\, \|P_{H_{in}} P_{\bar{H}_0}\|_\infty$
$\le \mathrm{rank}(P_{H_{in}})\, \frac{\|H - H_0\|_\infty}{\varepsilon}$
ε $P_{H_{in}}$ ε Π_0
$E+\Delta$
H_{out}



P_Hin
P_Hout
E
E+Δ
ε
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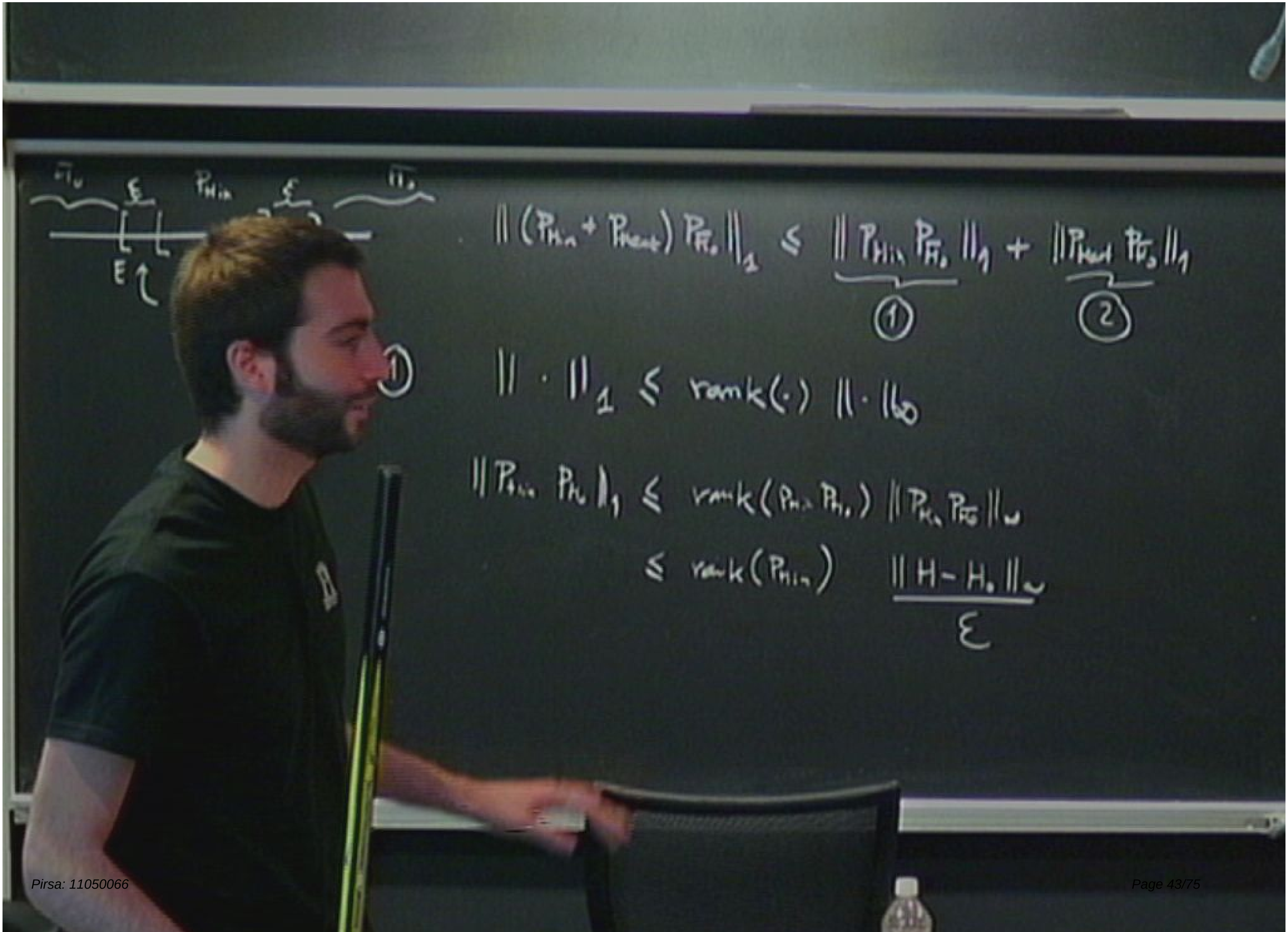
①
②
rank(·) ||·||_∞
rank(P_Hin P_H0) ||P_Hin P_H0||_∞
rank(P_Hin) ||H − H_0||_∞ / ε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① ②
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econd condition for thermalization: an exponential density of states

The **reduced density matrix** of the non-interacting **microcanonical** state reads,

$$\omega_{\sqcap}^{S(0)} = \mathrm{Tr}_B\, \omega_{\sqcap}^{(0)} \propto \sum_{E_n^{(0)} \in [E - E_n^{(0)}, E - E_n^{(0)} + \Delta]} \mathrm{Tr}_B(|E_n^{(0)}\rangle\langle E_n^{(0)}|)$$

econd condition for thermalization: an exponential density of states

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where $\Omega_{\Delta}^{B}(E)$ is the number of states in an energy interval $[E, E + \Delta]$.

Under what conditions these probabilities follow the **Gibbs distribution**?

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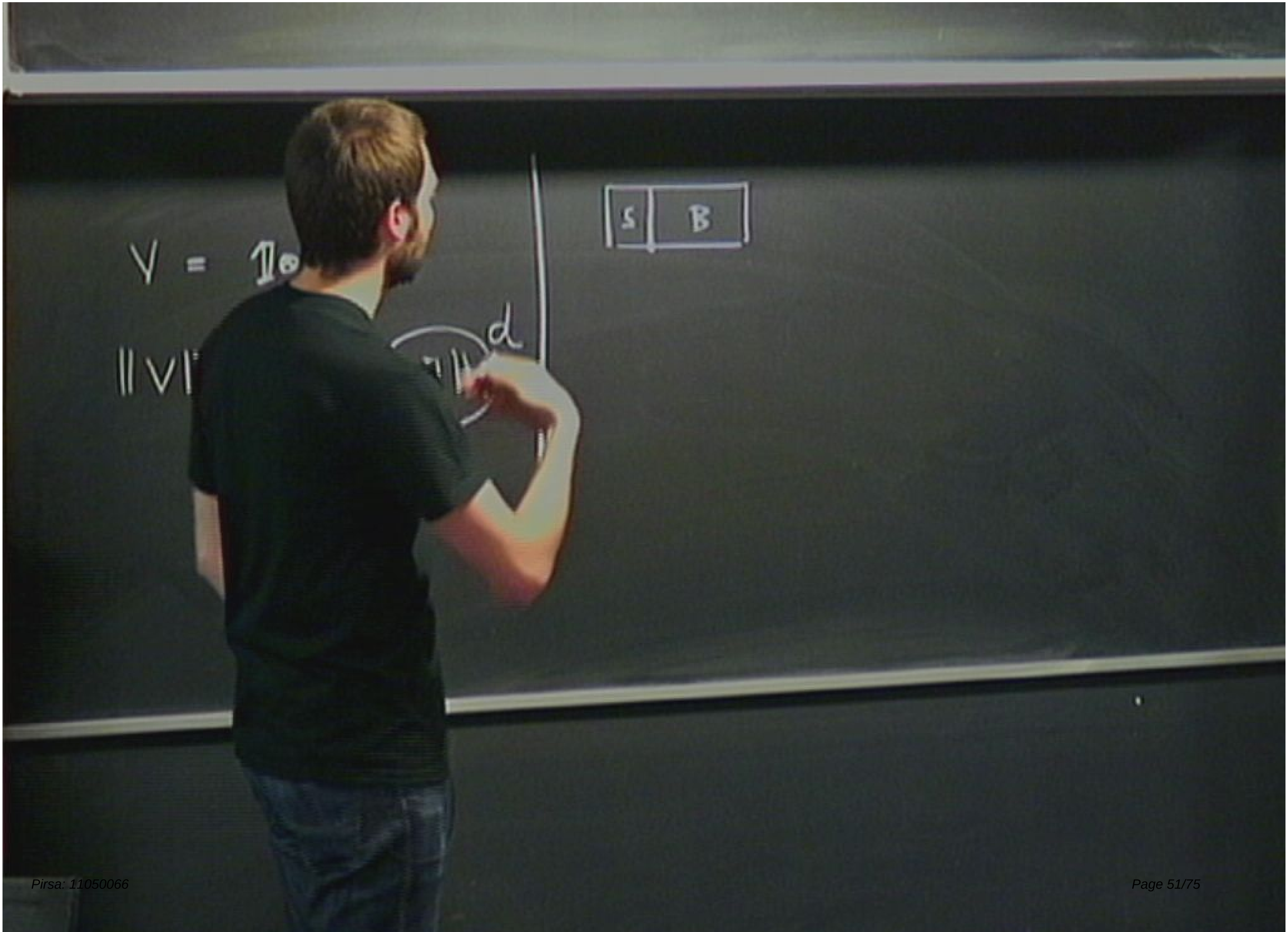
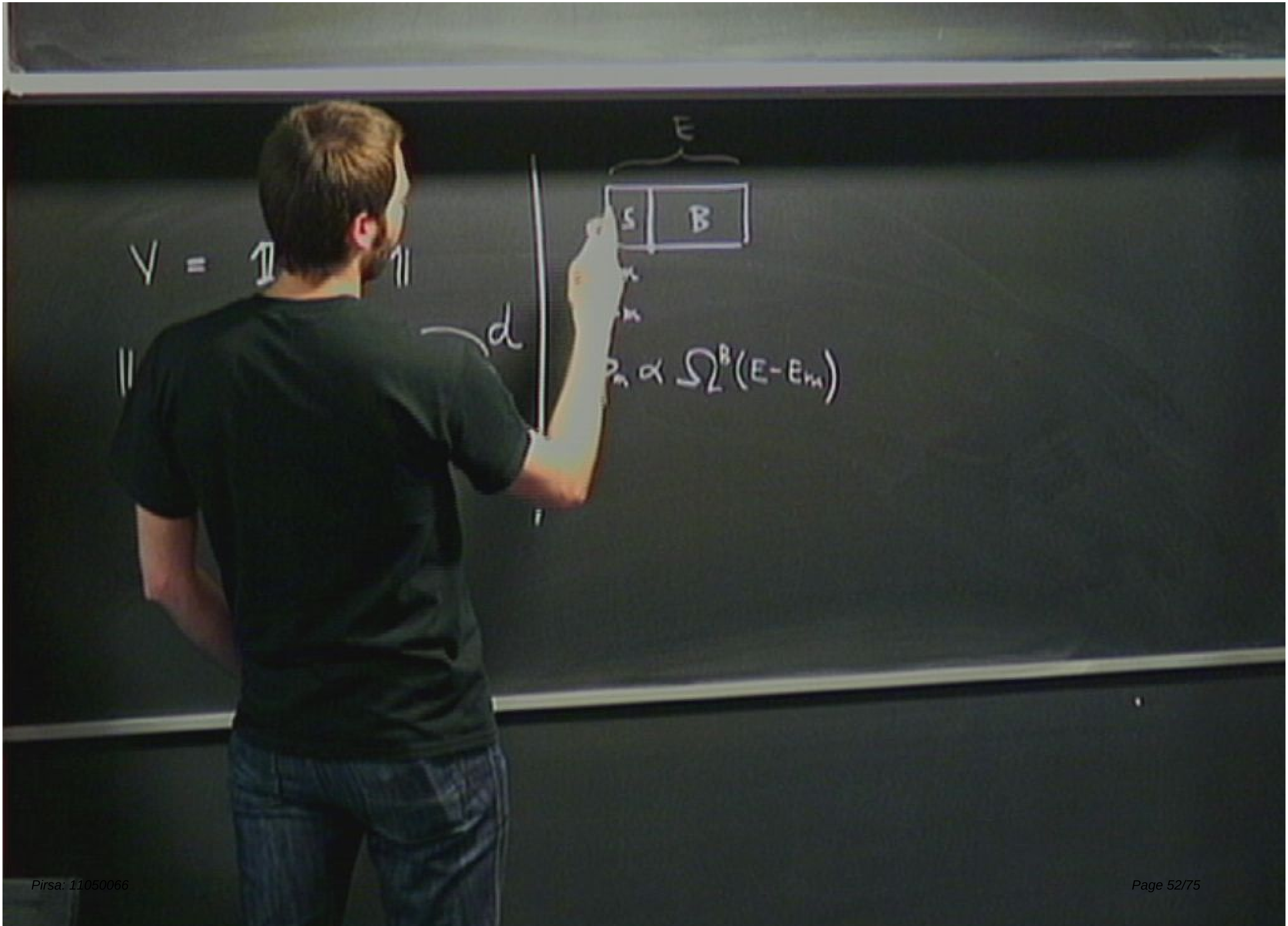
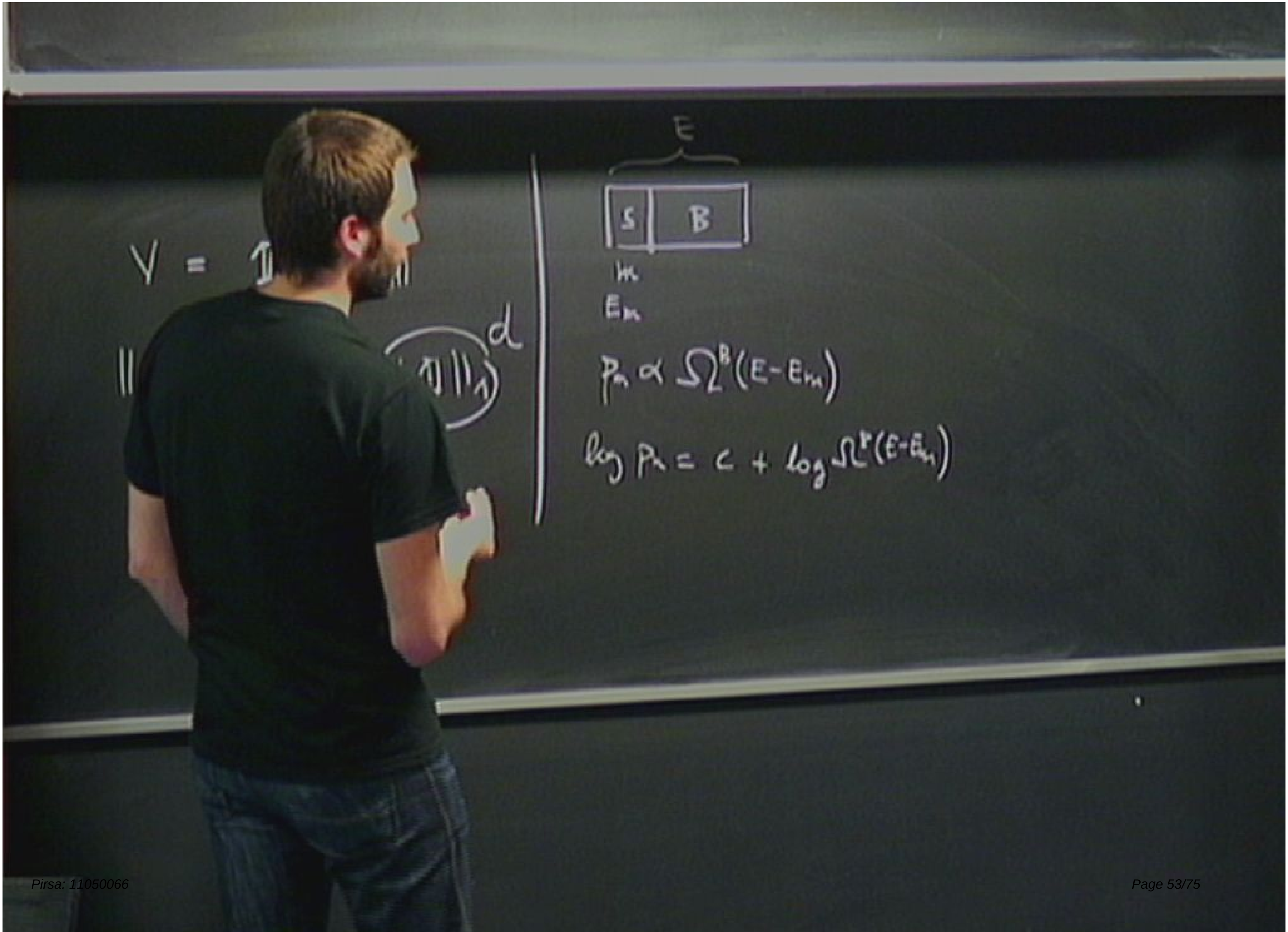
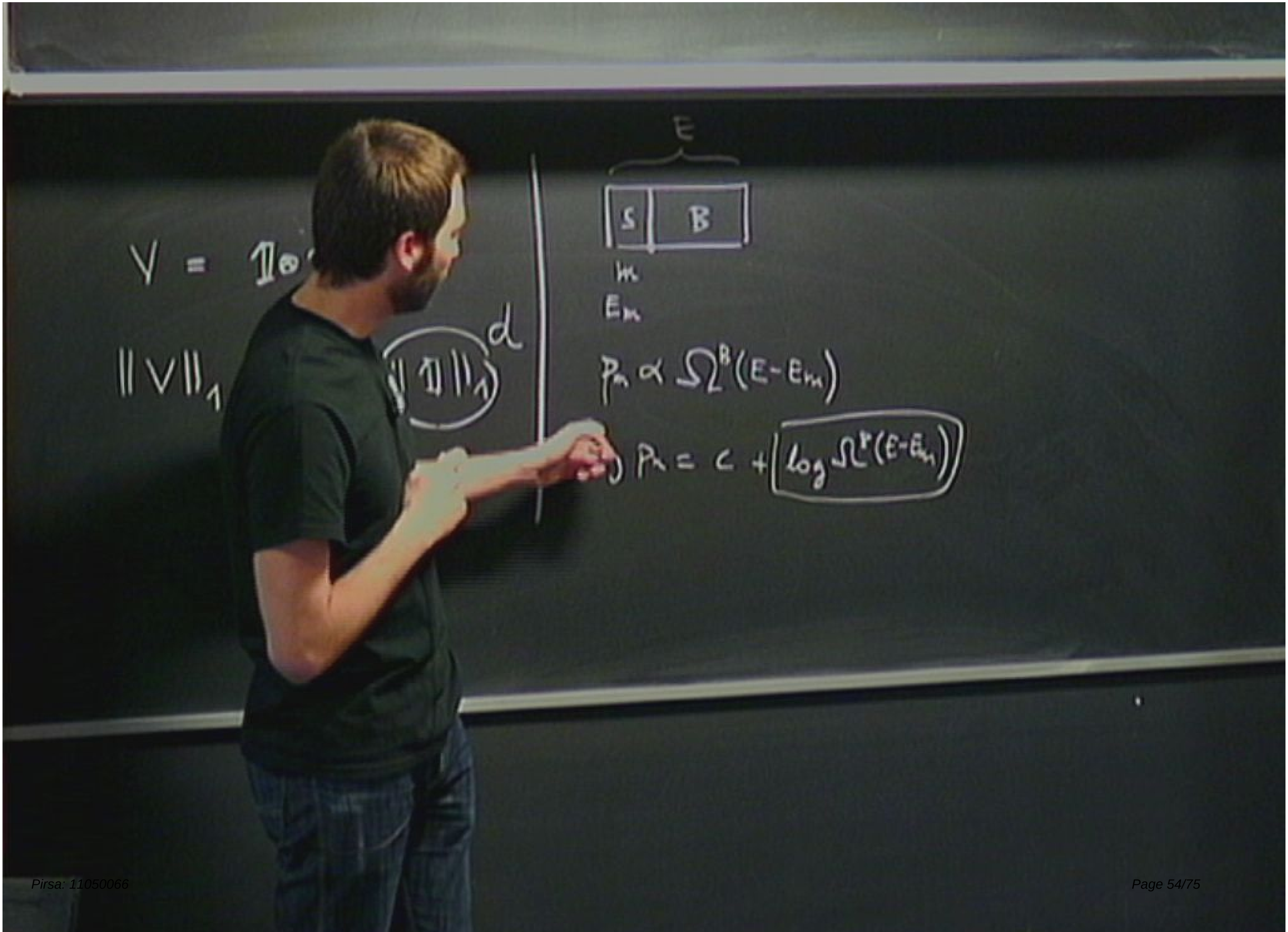
$$S(E) = \log \Omega_{\Delta}^{B}(E) \qquad \beta(E) = \frac{\partial S(E)}{\partial E}$$


S
B

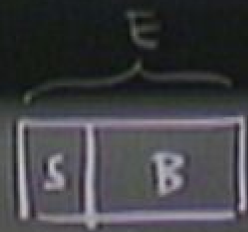

E
S
B
V =
d
ρm ∝ Ω^B(E − Em)


E
S
B
m
E_m
p_m ∝ Ω^B(E − E_m)
log p_m = c + log Ω^B(E − E_m)


E
S
B
$V = \mathbb{1} \otimes$
m
E_m
$\|V\|_1$
$\| \mathbb{1} \|_1$
d
$p_m \propto \Omega^B(E - E_m)$
$p_m = c + \log \Omega^B(E - E_m)$

$$V = \mathbb{1} \otimes v \otimes \mathbb{1}$$

$$\|V\|_1 = \|v\|_1 \left(\|\mathbb{1}\|_1\right)^d$$



n

E_n

$$p_n \propto \Omega^B(E - E_n)$$

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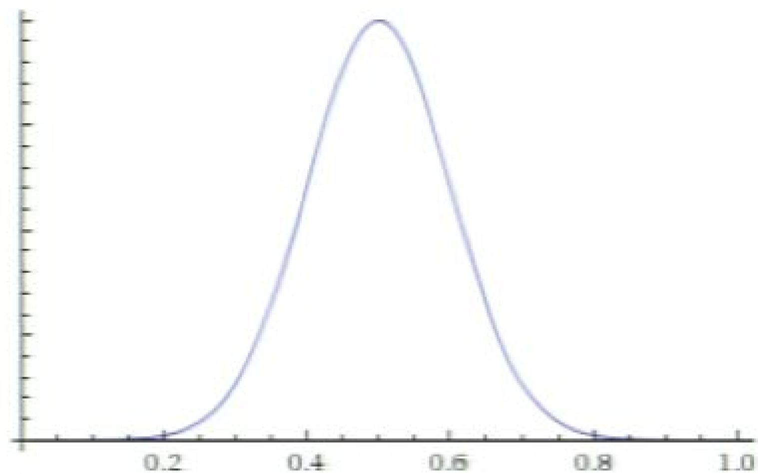
Example: chain of m non-interacting spins as bath.

$$\Omega^B_\Delta(E) \simeq \Delta 2^m \left(\frac{2}{\pi m}\right)^{1/2} \mathrm{e}^{-2m\left(\frac{E}{\eta m}-\frac{1}{2}\right)^2}$$

$$\mathcal{D}(\omega^{S(0)}_{\sqcap}, \rho^S_{\mathrm{Gibbs}}) \le \frac{1}{2}\left(\mathrm{e}^{4\frac{\|H_S\|^2_\infty}{\eta^2 m}} - 1\right)$$



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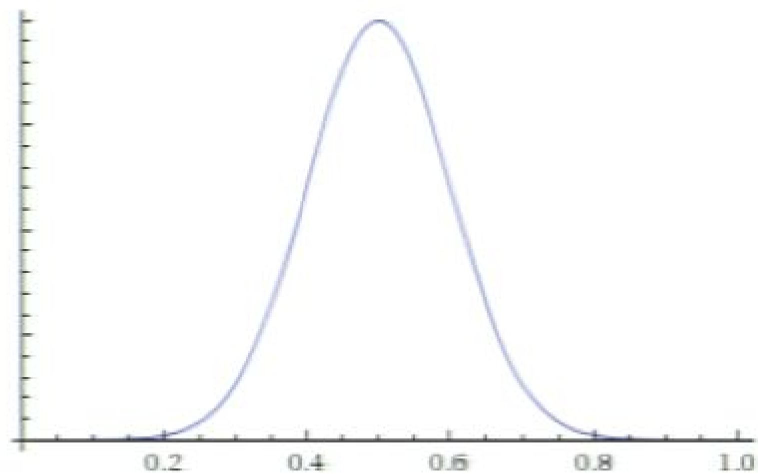

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Ups! A flaw in the argument...

Theorem. *The* ***rectangular states*** *of the interacting and non-interacting* ***Hamiltonians*** *are indistinguishable in the following sense*

$$\mathcal{D}(\omega_{\sqcap}^{S}, \omega_{\sqcap}^{S(0)}) \leq \mathcal{D}(\omega_{\sqcap}, \omega_{\sqcap}^{(0)}) \leq \frac{3\sqrt{2}}{2}\left(\frac{\|V\|_{\infty}}{\Delta}\right)^{1/2}$$

where an approximately uniform spectrum is assumed in the interval $[E, E+\Delta]$.

$$\Omega_{\Delta}^{B}(E) \propto \mathrm{e}^{\beta E} \qquad \Rightarrow \qquad p_k \propto \mathrm{e}^{-\beta E_k^S}$$

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$$\mathcal{D}(\omega_{\sqcap}^{S}, \omega_{\sqcap}^{S(0)}) \leq \mathcal{D}(\omega_{\sqcap}, \omega_{\sqcap}^{(0)}) \leq \frac{2}{1 - e^{-\beta\Delta}} (\beta \|V\|_{\infty})^{1/2}$$

where β *is the inverse temperature in the interval* $[E, E+\Delta]$.

$$\Omega_{\Delta}^{B}(E) \propto e^{\beta E} \quad \Rightarrow \quad p_k \propto e^{-\beta E_k^S}$$

Ups! A flaw in the argument...

Theorem *The* ***rectangular states*** *of the interacting and non-interacting*

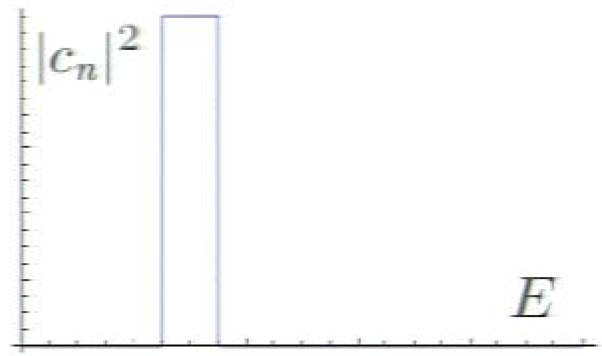
A physical intuition of when an interaction is weak

$$\|V\|_\infty \ll k_B T$$

$$\Omega^B_\Delta(E) \propto e^{\beta E} \quad \Rightarrow \quad p_k \propto e^{-\beta E^S_k}$$

Sufficient conditions for thermalization

(0) The initial state is a "*rectangular*" state.



(1) The interaction is weak in the following sense

$$\|V\|_\infty \ll k_B T$$

(2) The density of states (of the bath) can be locally approximated by an exponential

$$\Omega^B_\Delta(E) \propto e^{\beta E}$$

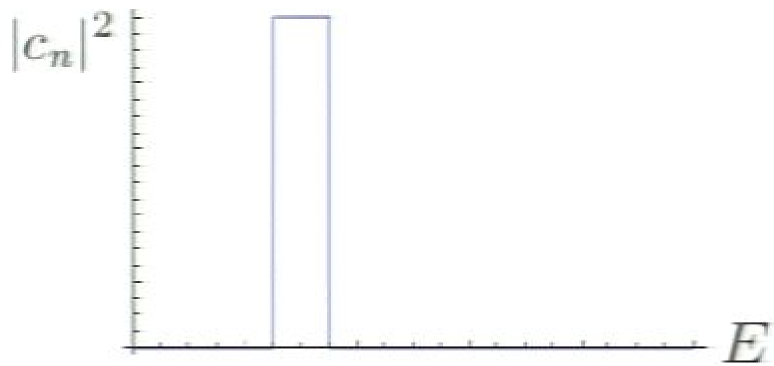
Quantum algorithm for the thermal state

Motivation, idea and requirements

Motivation. Simulation of physical system at a desired temperature.

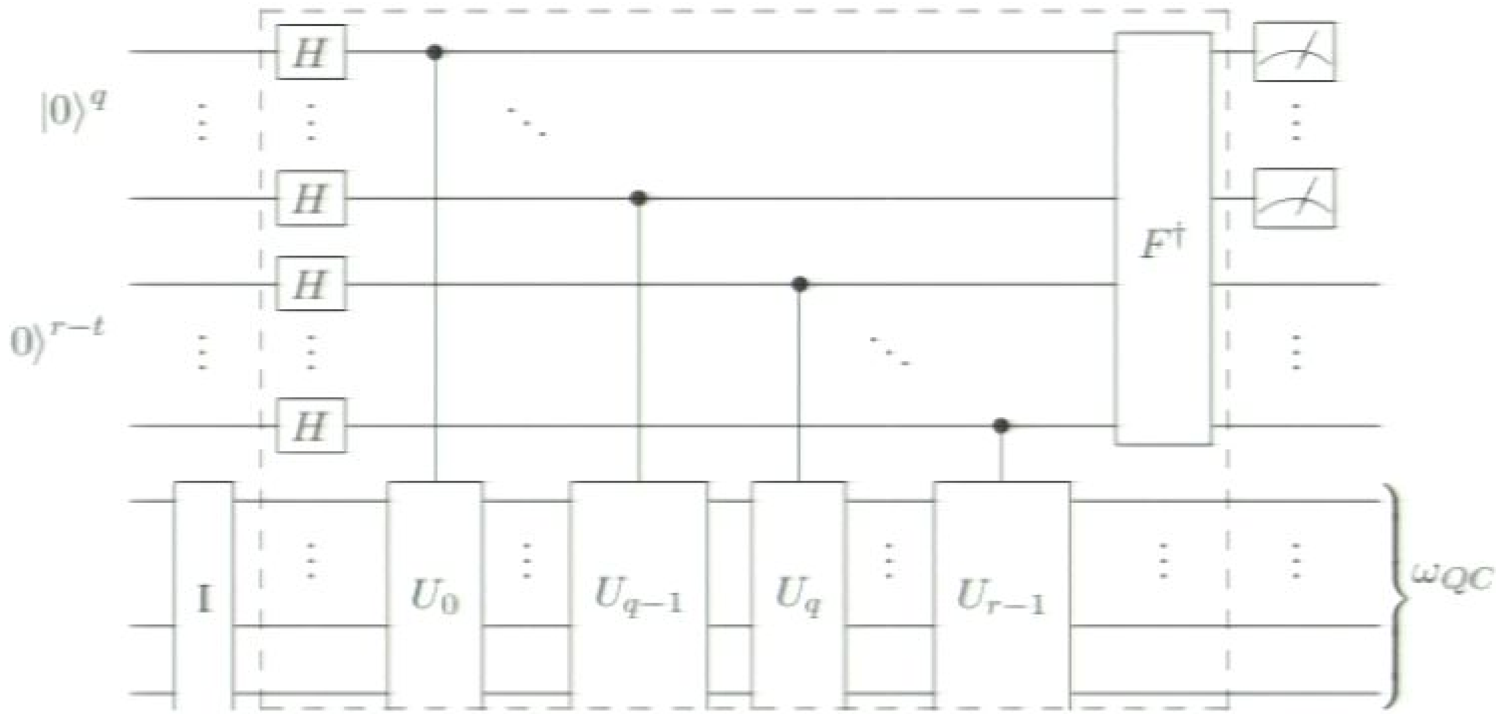
Idea: Preparation of the rectangular state.

$$H_0 = H_S + H_B$$



Requirements. The spectrum and the eigenstates of the Hamiltonian of the system are unknown. The only thing that we can do is to apply the Hamiltonian on the system as an oracle.

Algorithm



1. Initialization.

2. Partial quantum phase estimation.

3. Partial measurement.

Conclusions and outlook

Conclusions

1. For most of **Hamiltonians** and initial pure states, the reduced density matrix of a subsystem reaches **equilibrium**.

$$\rho^S(t) \longrightarrow \omega^S = \sum_n |c_n|^2 \, \mathrm{Tr}_B \, |E_n\rangle\langle E_n|$$

2. We have presented a set of sufficient conditions for thermalization.

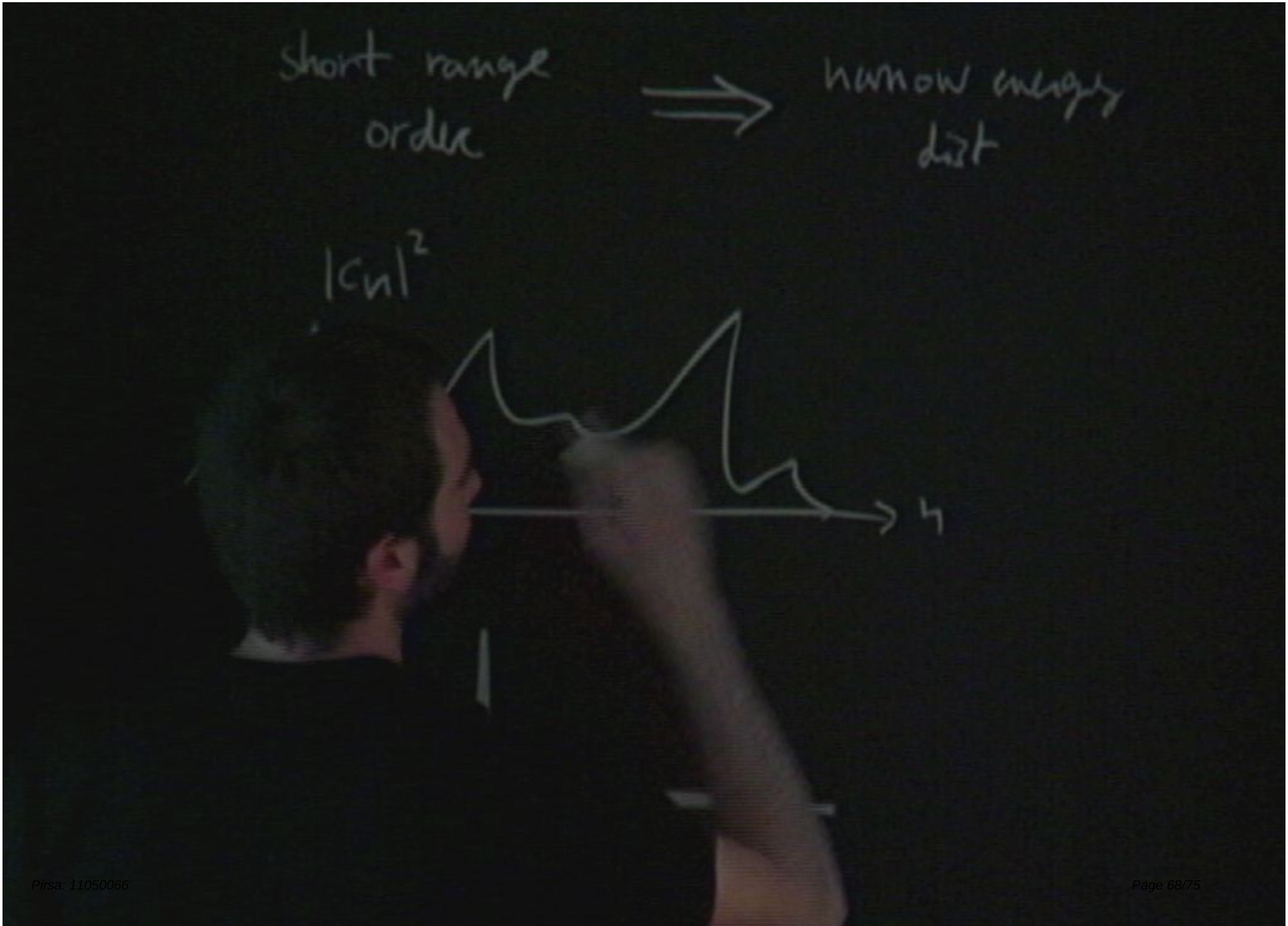
$$\rho^S(t) \longrightarrow \omega^S \propto \mathrm{e}^{-\beta H_S}$$

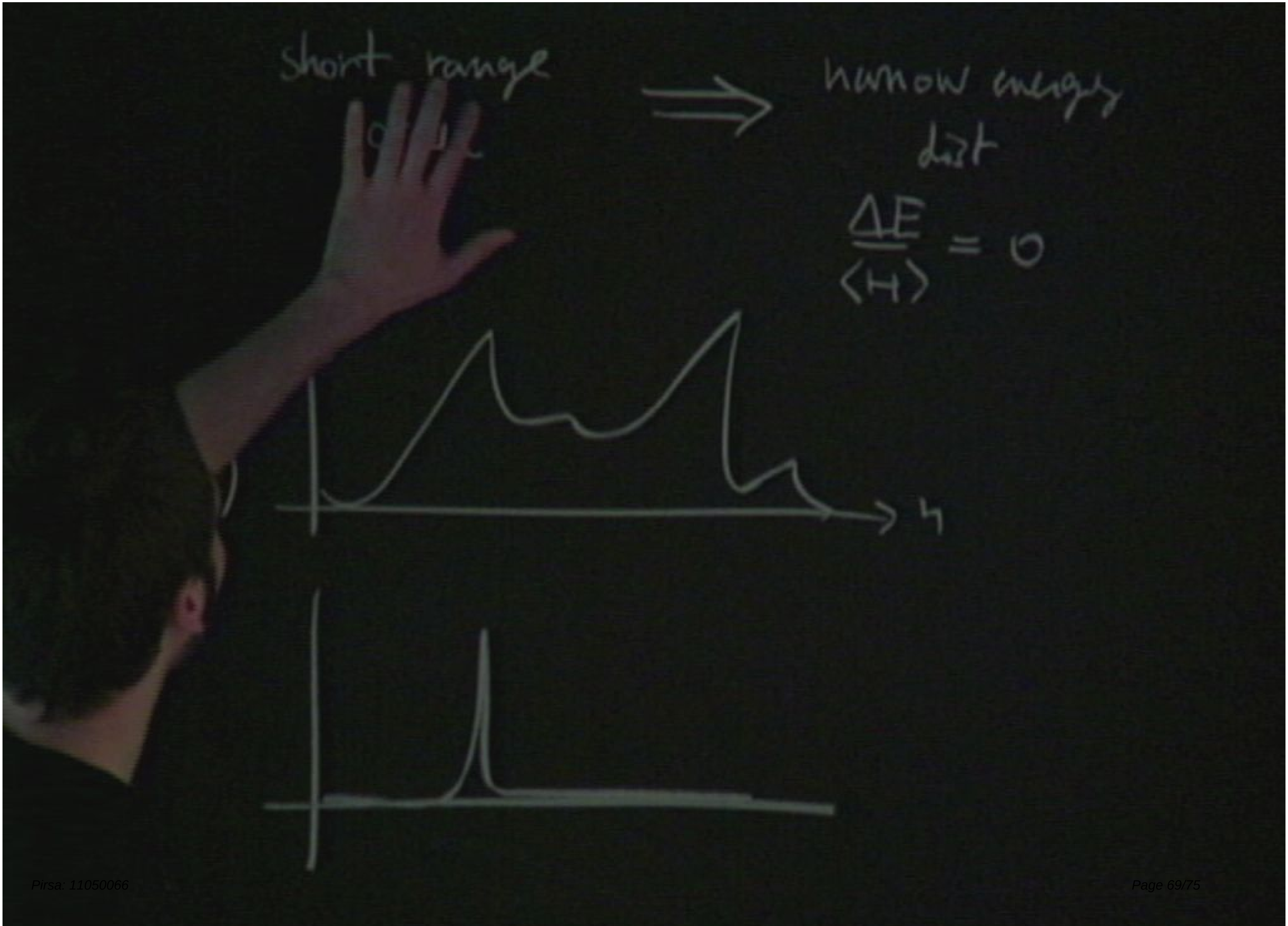
(i) Initial state -> Rectangular state.

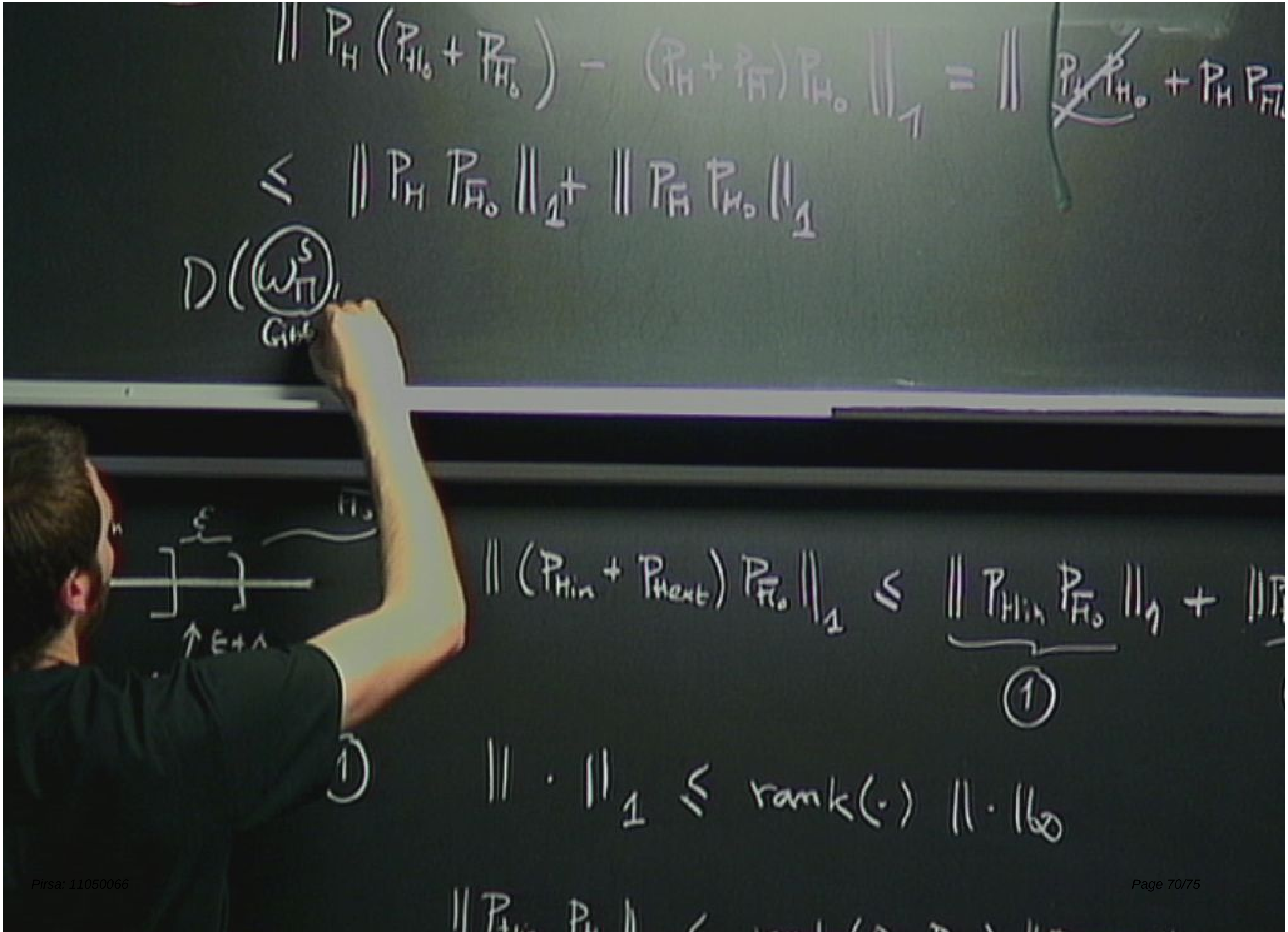
(ii) Weak interaction.

(iii) The density of states of the bath is approximated by an exponential.

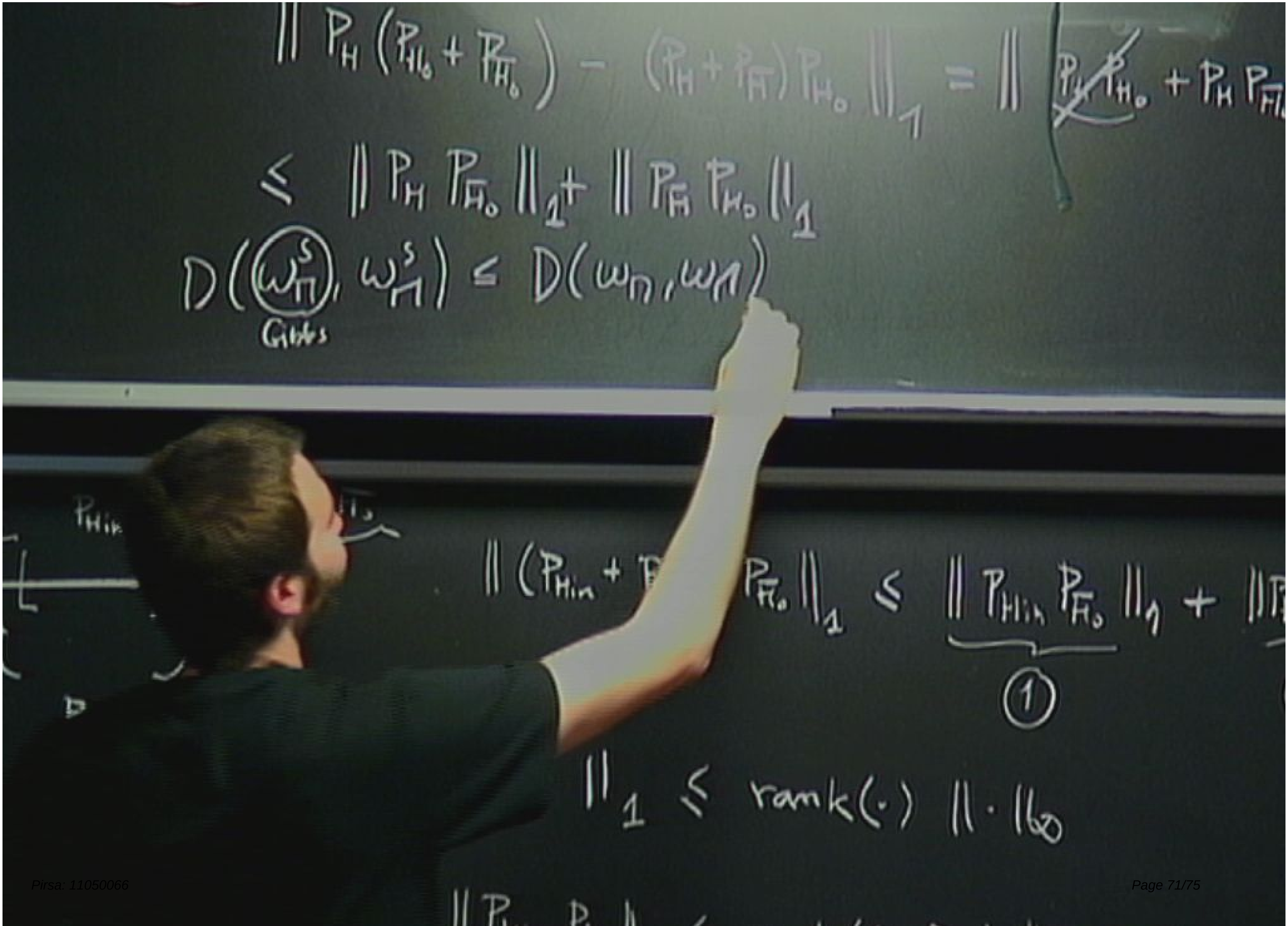
3. We finally have presented a **quantum algorithm** for preparing **thermal states** with a certified runtime.

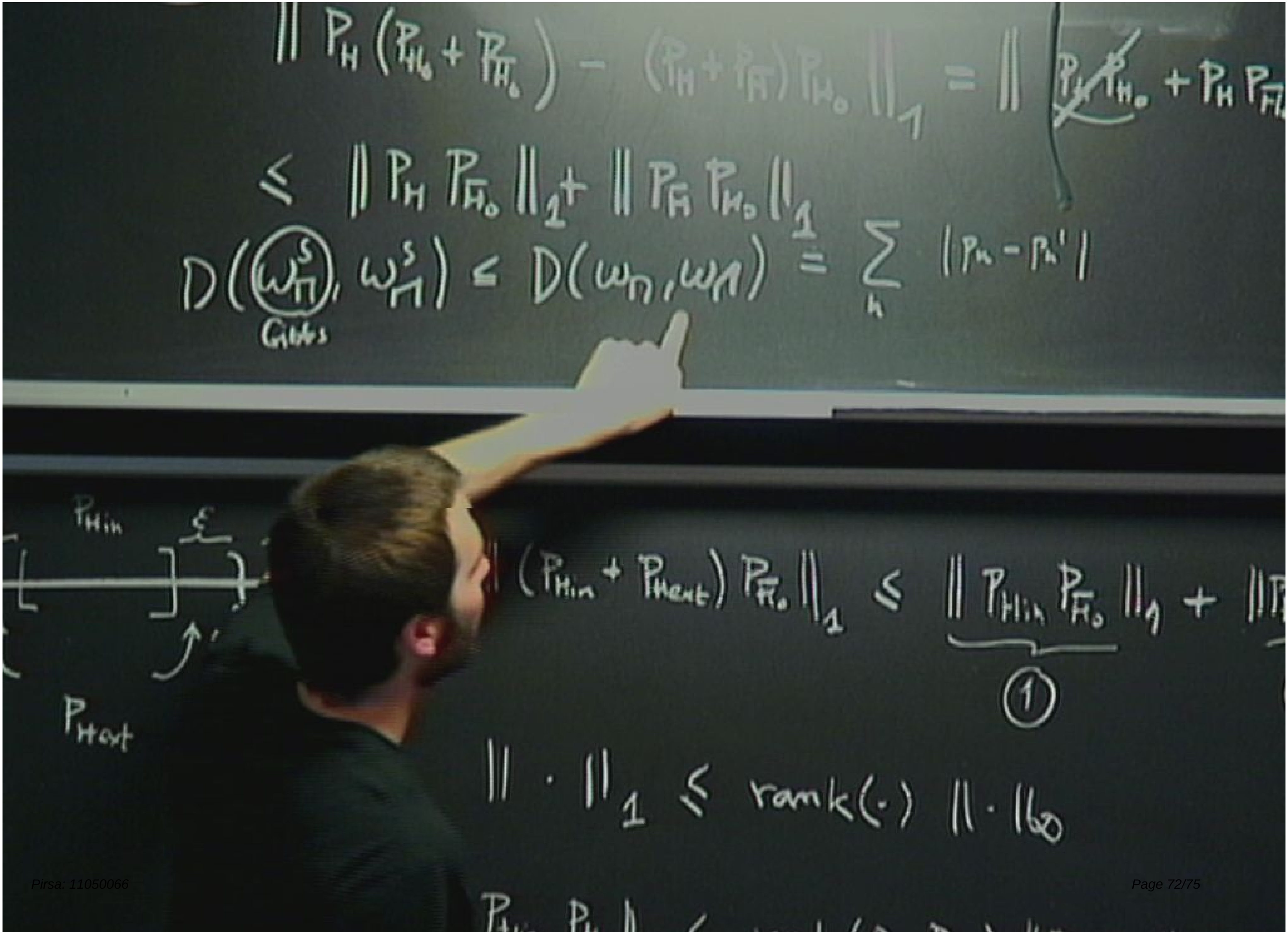

short range order ⇒ narrow energy dist
$|c_n|^2$
n


short range
⟹ narrow energy dist
ΔE / ⟨H⟩ = 0
h

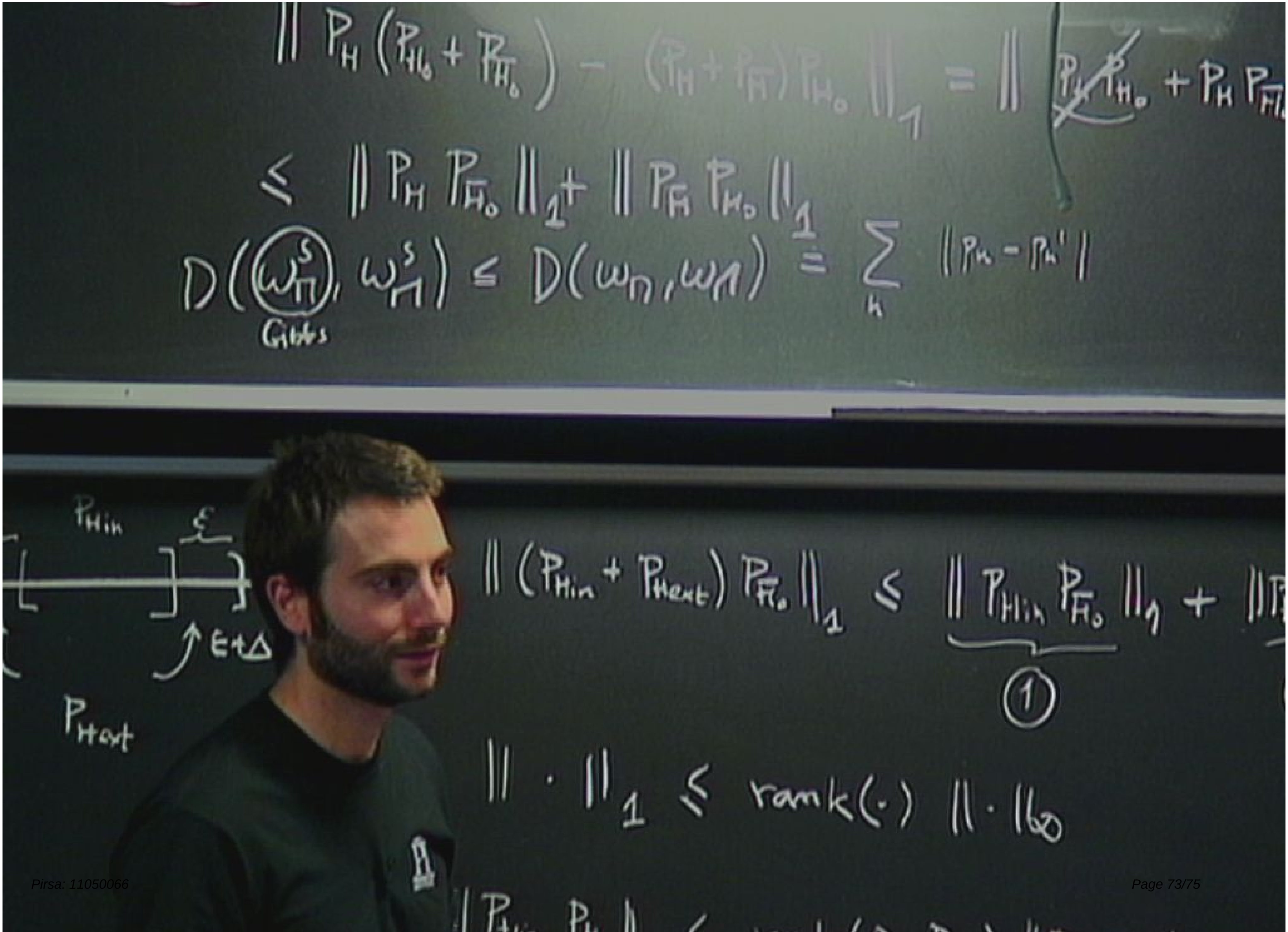


$\| P_H (P_{H_0} + P_{\bar{H}_0}) - (P_H + P_{\bar{H}}) P_{H_0} \|_1 = \| P_H P_{H_0} + P_H P_{\bar{H}_0}$
$\leq \| P_H P_{\bar{H}_0} \|_1 + \| P_{\bar{H}} P_{H_0} \|_1$
$D(\omega_\Pi^S$
$\| (P_{H_{in}} + P_{H_{ext}}) P_{\bar{H}_0} \|_1 \leq \| P_{H_{in}} P_{\bar{H}_0} \|_1 +$
$\| \cdot \|_1 \leq \mathrm{rank}(\cdot) \| \cdot \|_\infty$


Gibbs
rank(·)



‖ P_H (P_{H_0} + P_{\bar{H}_0}) − (P_H + P_{\bar{H}}) P_{H_0} ‖_1 = ‖ P_H P_{H_0} + P_H P_{\bar{H}_0}
≤ ‖ P_H P_{\bar{H}_0} ‖_1 + ‖ P_{\bar{H}} P_{H_0} ‖_1
D(ω^s_Π, ω^s_Π') ≤ D(ω_Π, ω_Π') = Σ_n | p_n − p_n' |
Gibbs
P_{H in}
ε
P_{H ext}
‖ (P_{H in} + P_{H ext}) P_{\bar{H}_0} ‖_1 ≤ ‖ P_{H in} P_{\bar{H}_0} ‖_1 +
1
‖ · ‖_1 ≤ rank(·) ‖ · ‖_∞


Gibbs
E+Δ
rank(·)

Most of initial states equilibrate

What do we understand by "equilibration"?

When the **average distance** between the **state of the system** and the **equilibrium state** is small, the system must spend most of its time at the equilibrium state.

$$\text{equilibration} \quad \equiv \quad \langle \mathcal{D}(\rho^S(t), \omega^S) \rangle_t \leq \text{small}$$

In [1], it is proven that

$$\langle \mathcal{D}(\rho^S(t), \omega^S) \rangle_t \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\text{eff}}}}$$

where $d^{\text{eff}} = \dfrac{1}{\sum_n |c_n|^4}$.

[1] N. Linden, S. Popescu, A. J. Short, and A. Winter PRE 79 (2009) no. 6, 061103