Title: Computational difficulty of simulation methods: Density Functional Theory, DMRG, and beyond

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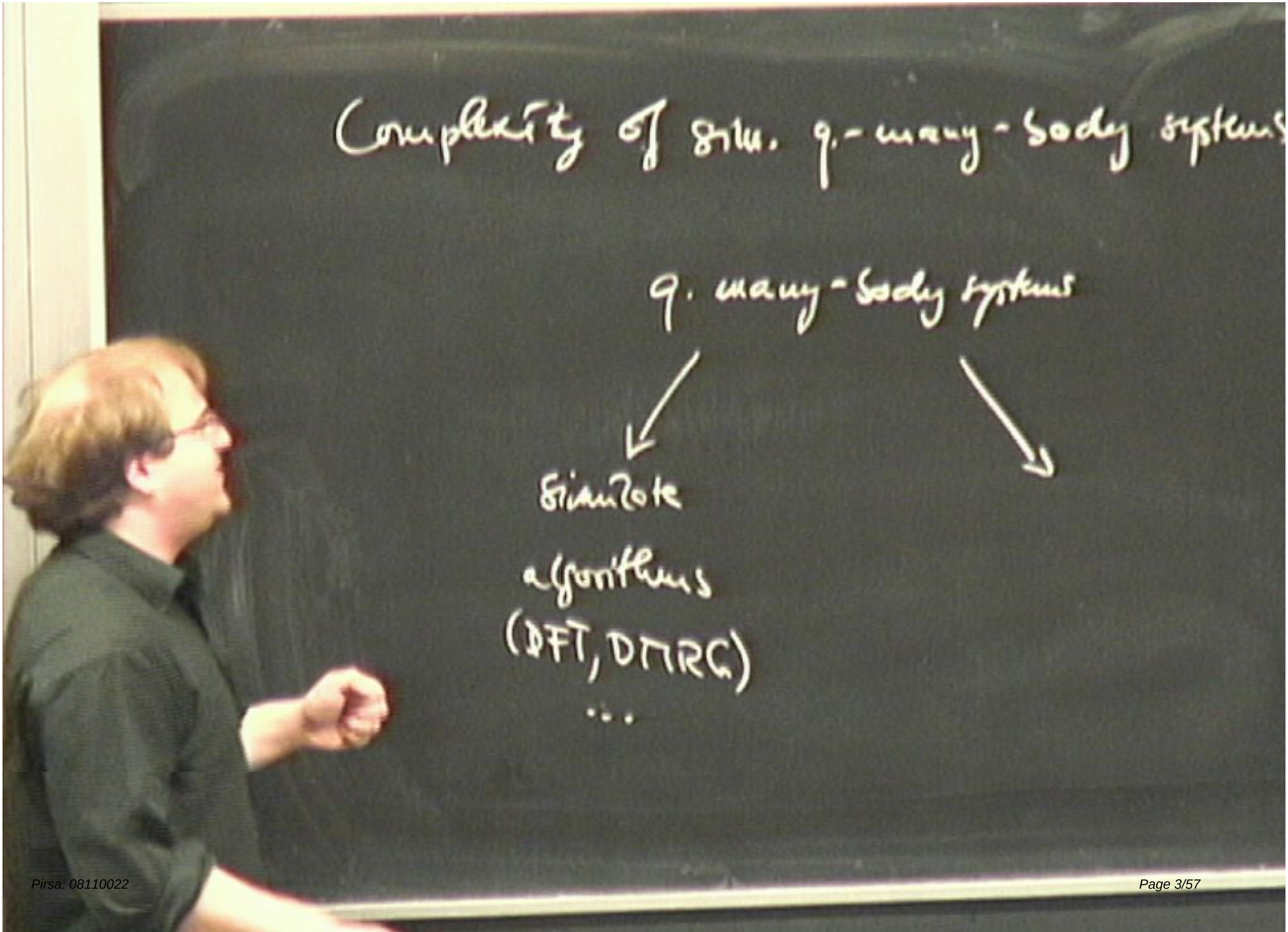
Abstract: We analyze how quantum complexity poses bounds to the simulation of quantum systems. While methods as Density Functional Theory (DFT) and the Density Matrix Renormalization Group (DMRG) work very well in practice, essentially nothing on the formal requirements is known. In this talk, we consider these methods from a quantum complexity perspective: First, we discuss DFT which encapsulates the difficulty of solving the Schroedinger equation in a universal functional and show that this functional cannot be efficiently computed unless several complexity classes collapse. Second, we consider DMRG, a method to deal with quantum spin chains, and show that even under reasonable assumptions -- a polynomial gap and matrix product ground states -- finding the ground state is still a computationally hard problem. Beyond pinpointing the limitations of the methods, this helps us to understand under which assumptions we might be able to prove their convergence.

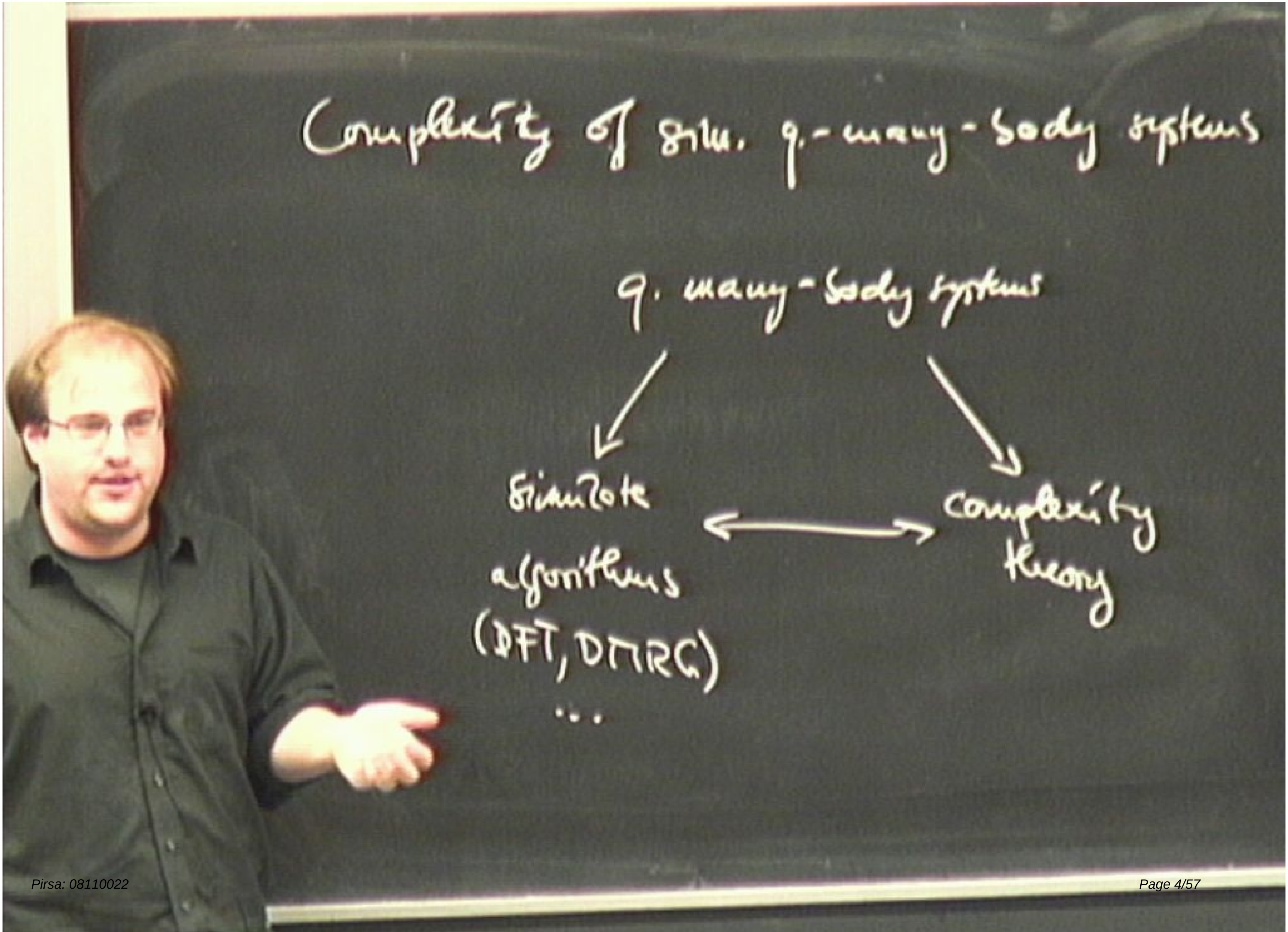
Complexity of sim. q.-many-body systems

q. many-body systems

$\swarrow$

simulate


Complexity of sim. q.-many-body systems
q. many-body systems
simulate
algorithms
(DFT, DMRG)
...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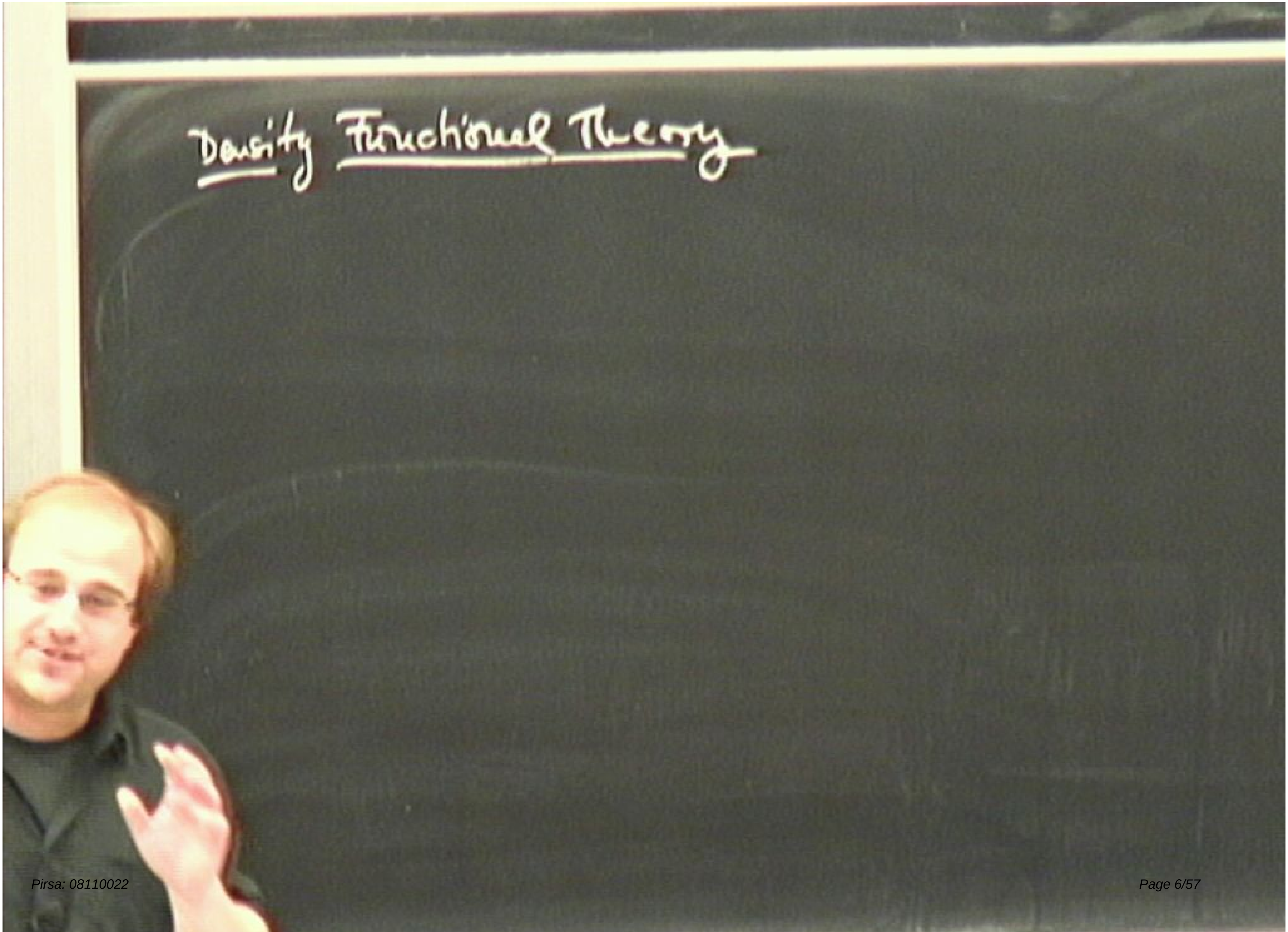
complexity theory

Complexity of sim. q.-many-body systems

q. many-body systems

simulate algorithms (DFT, DMRG) ... $\longleftrightarrow$ complexity theory

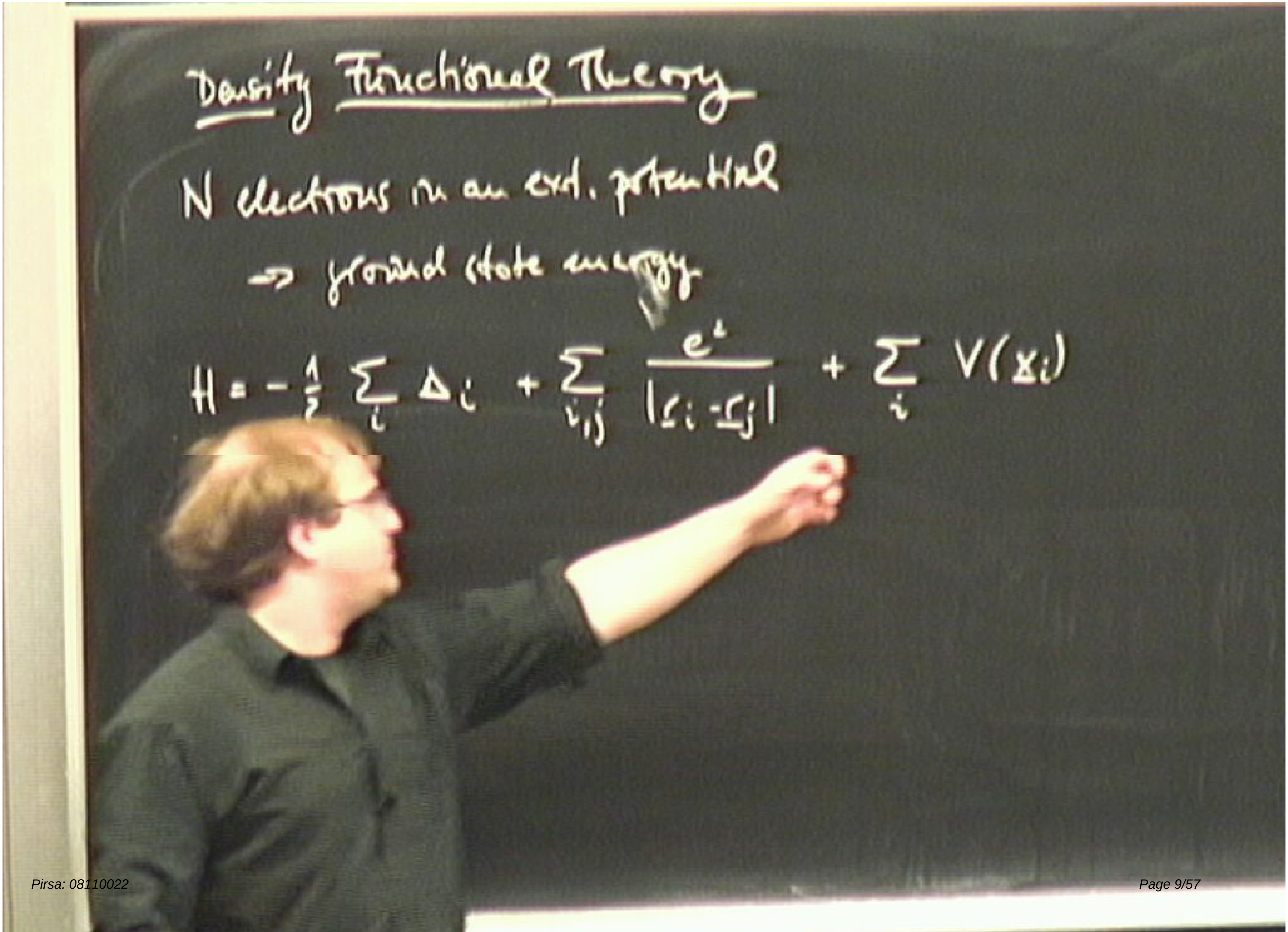

Density Functional Theory

Density Functional Theory

Density Functional Theory

N electrons in an ext. potential

→ ground state energy


Density Functional Theory
N electrons in an ext. potential
→ ground state energy
$H = -\frac{1}{2}\sum_i \Delta_i + \sum_{i,j} \frac{e^2}{|\underline{r}_i - \underline{r}_j|} + \sum_i V(\underline{x}_i)$

Density Functional Theory

N electrons in an ext. potential

→ ground state energy

$$H = \underbrace{-\frac{1}{2}\sum_i \Delta_i}_{=:T} + \underbrace{\sum_{i,j} \frac{e^2}{|r_i - r_j|}}_{=:I} + \underbrace{\sum_i V(x_i)}_{=:V}$$

$$H = \min$$

Density Functional Theory

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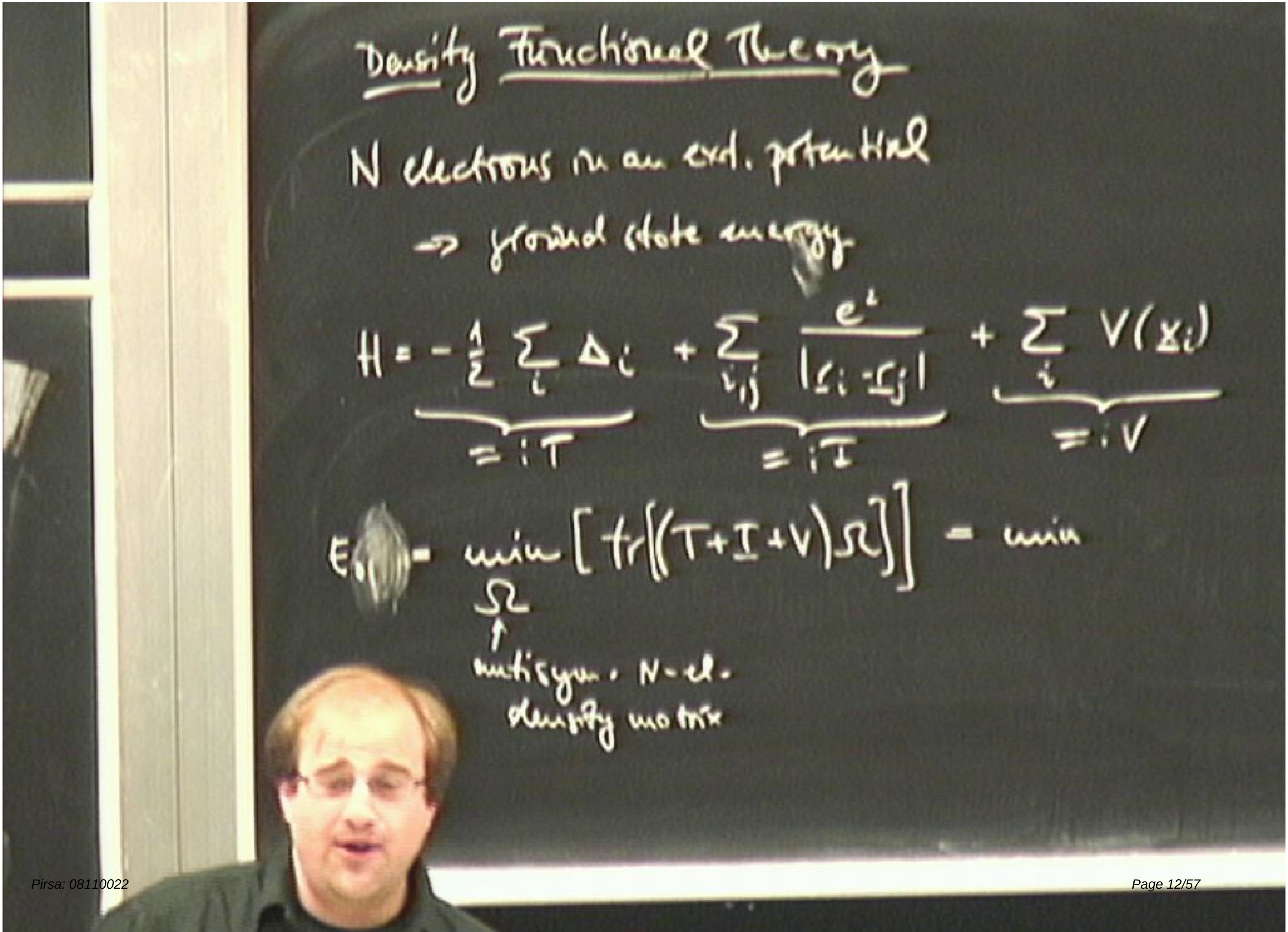
$$\min_{\Omega} \left[\mathrm{tr}\left[(T+I+V)\Omega\right]\right]$$

Ω: antisym. N-el. density matrix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$=: T$
$=: I$
$=: V$
$E_0 = \min_{\Omega} \left[tr\left((T+I+V)\Omega\right)\right] = \min$
antisym. N-el. density matrix

Density Functional Theory

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Density Functional Theory

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$\Rightarrow$ ground state energy

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$$E_0 = \min_{\Omega} \Big[\mathrm{tr}\big((T+I+V)\Omega\big)\Big] = \min_{\rho(r)} \min_{\Omega \to \rho}$$

symm. N-el. density matrix

$$\rho(r_1, r_1') = \int \Omega(r_1, r_1', r_2 r_2', \ldots, r_N r_N')\, dr_2, \ldots, dr_N$$

(DFT, DMRG)

Density Functional Theory

N electrons in an ext. potential

$\Rightarrow$ ground state energy

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Ω ↑ antisym. N-el. density matrix

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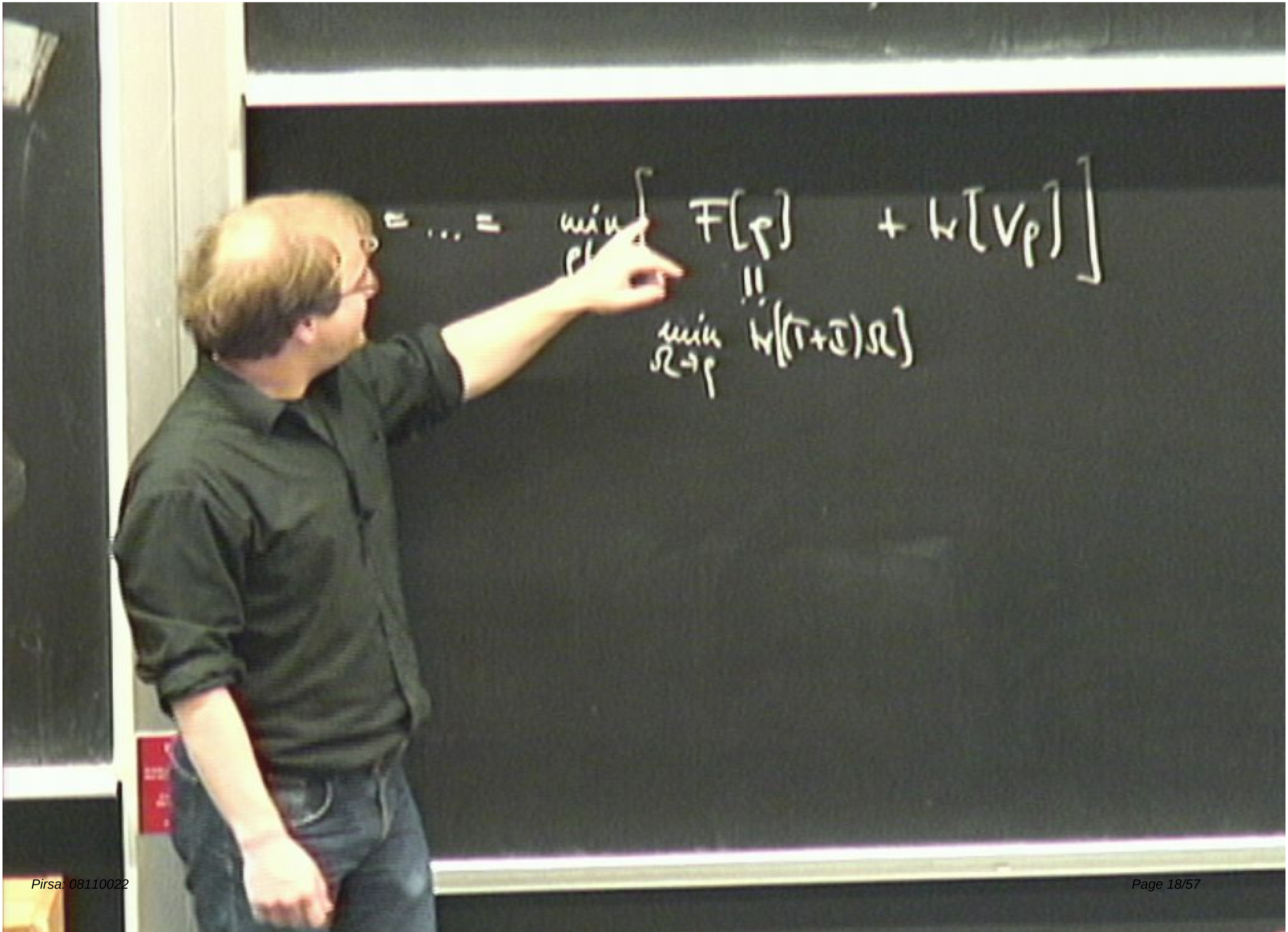
...


= ... = min [F[ρ] + tr[Vρ]]
min tr[(T+I)Ω]

$$E_0 = \dots = \min_{\rho(r)} \Big[\underbrace{F[\rho]}_{\min\limits_{\Omega \to \rho} \mathrm{tr}[(T+I)\Omega]} + \mathrm{tr}[V\rho] \Big]$$

„universal functional"

$$E_0 = \ldots = \min_{\rho(r)} \Big[\underbrace{F[\rho]}_{=\ \min_{\Omega \to \rho} \operatorname{tr}[(T+I)\Omega]} + \operatorname{tr}[V\rho] \Big]$$

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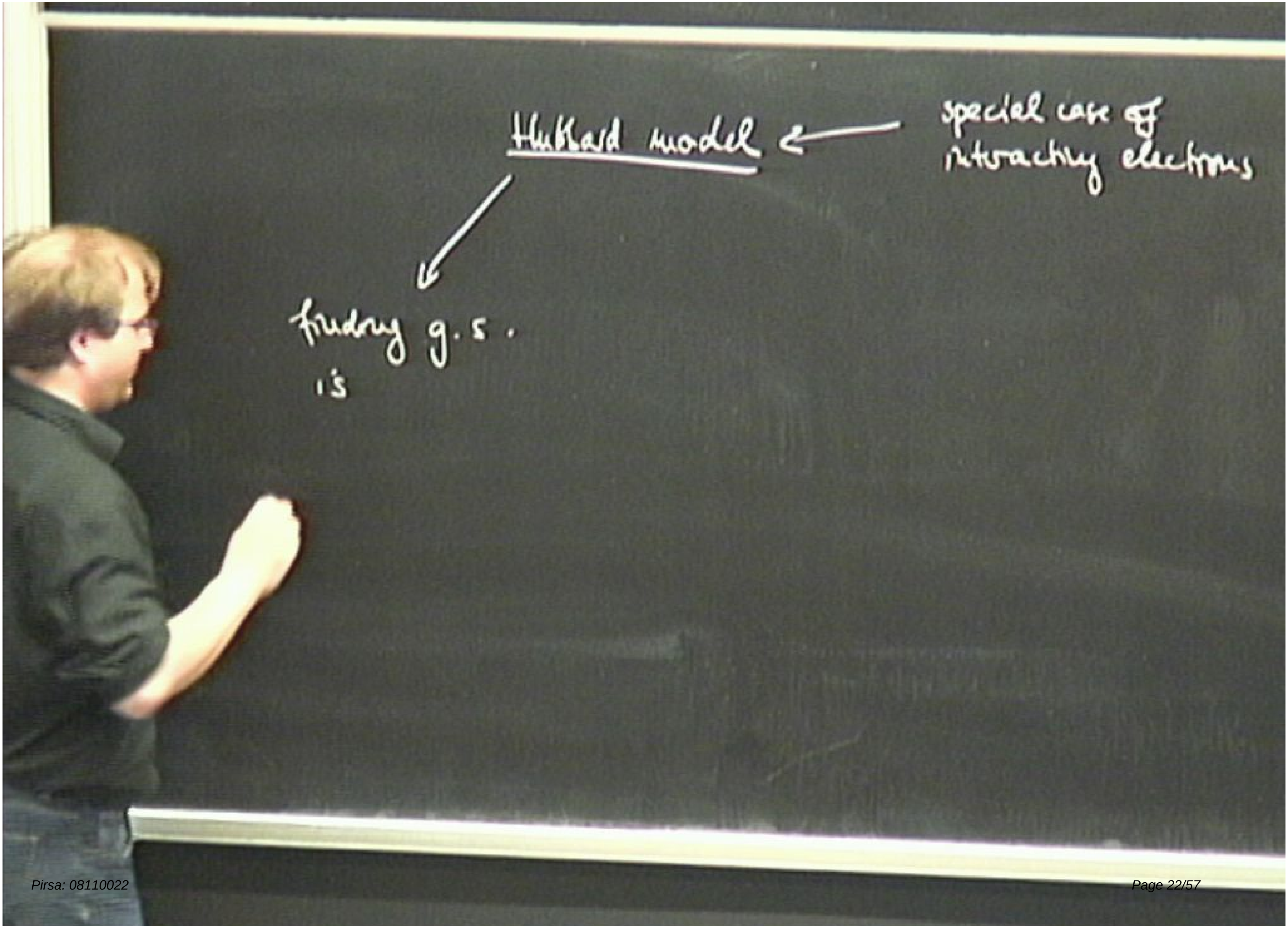
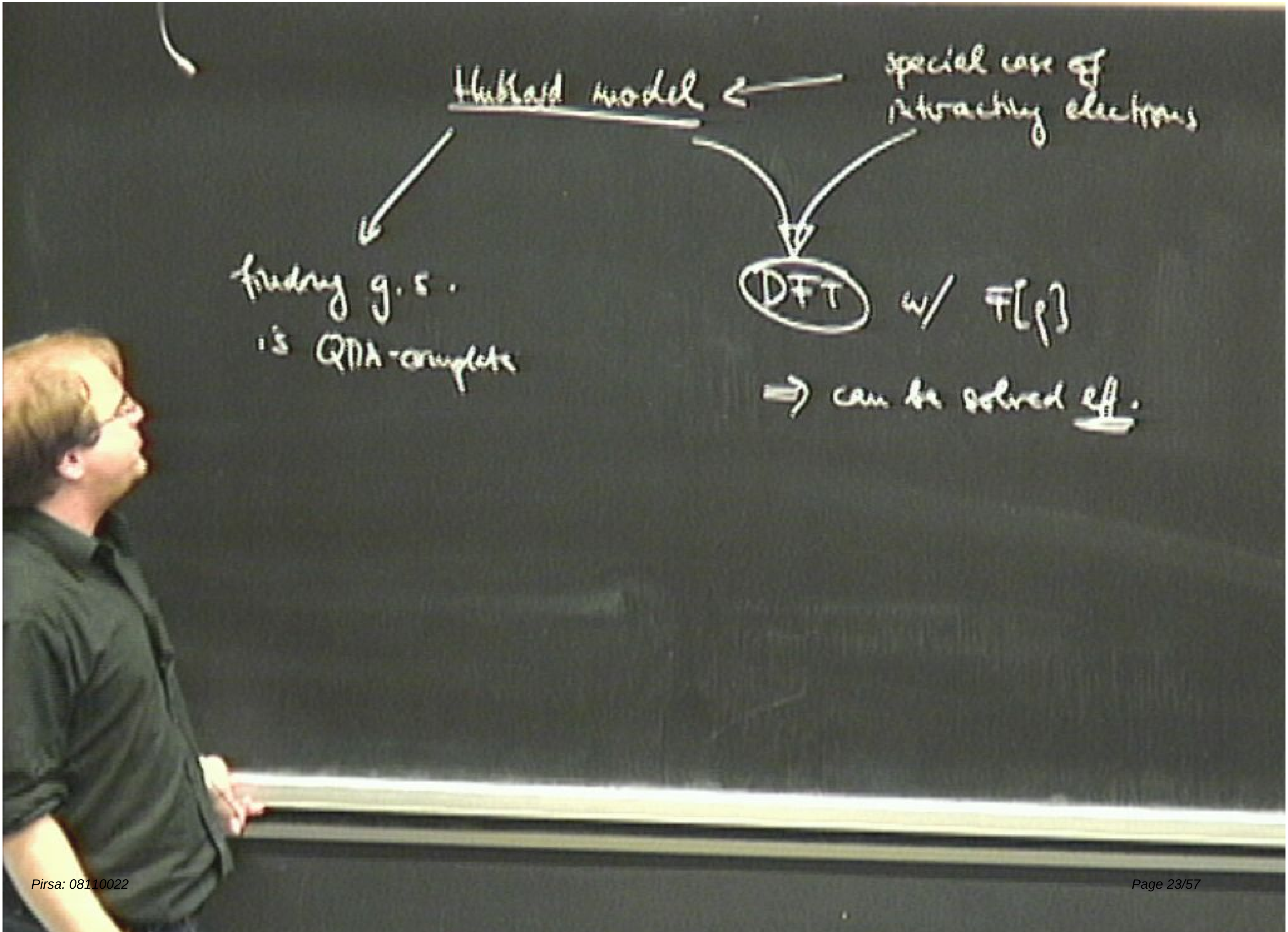

Hubbard model
special case of
interacting electrons
finding g.s.
is


Hubbard model
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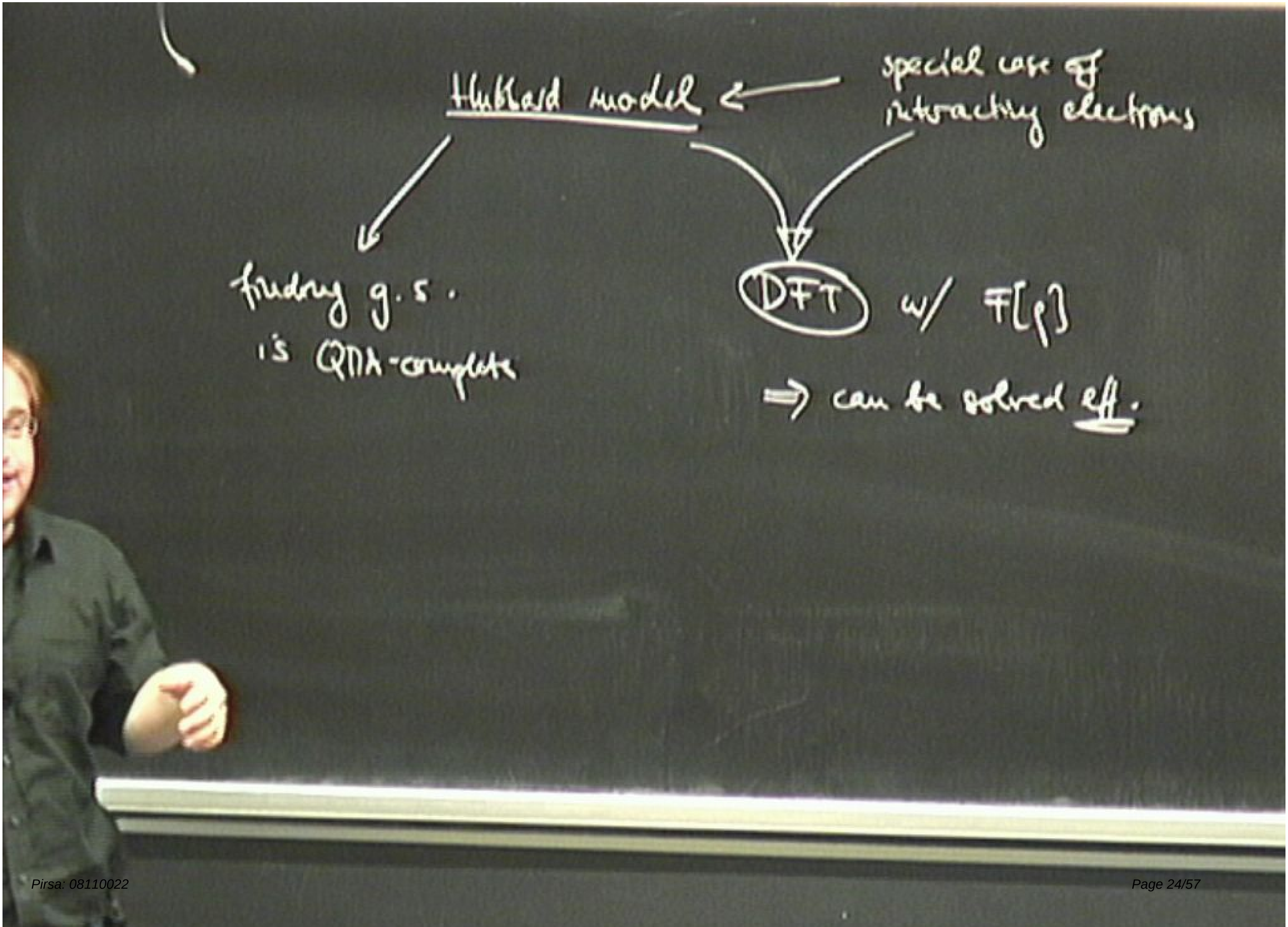
is QMA-complete
DFT w/ F[ρ]
⇒ can be solved eff.


Hubbard model
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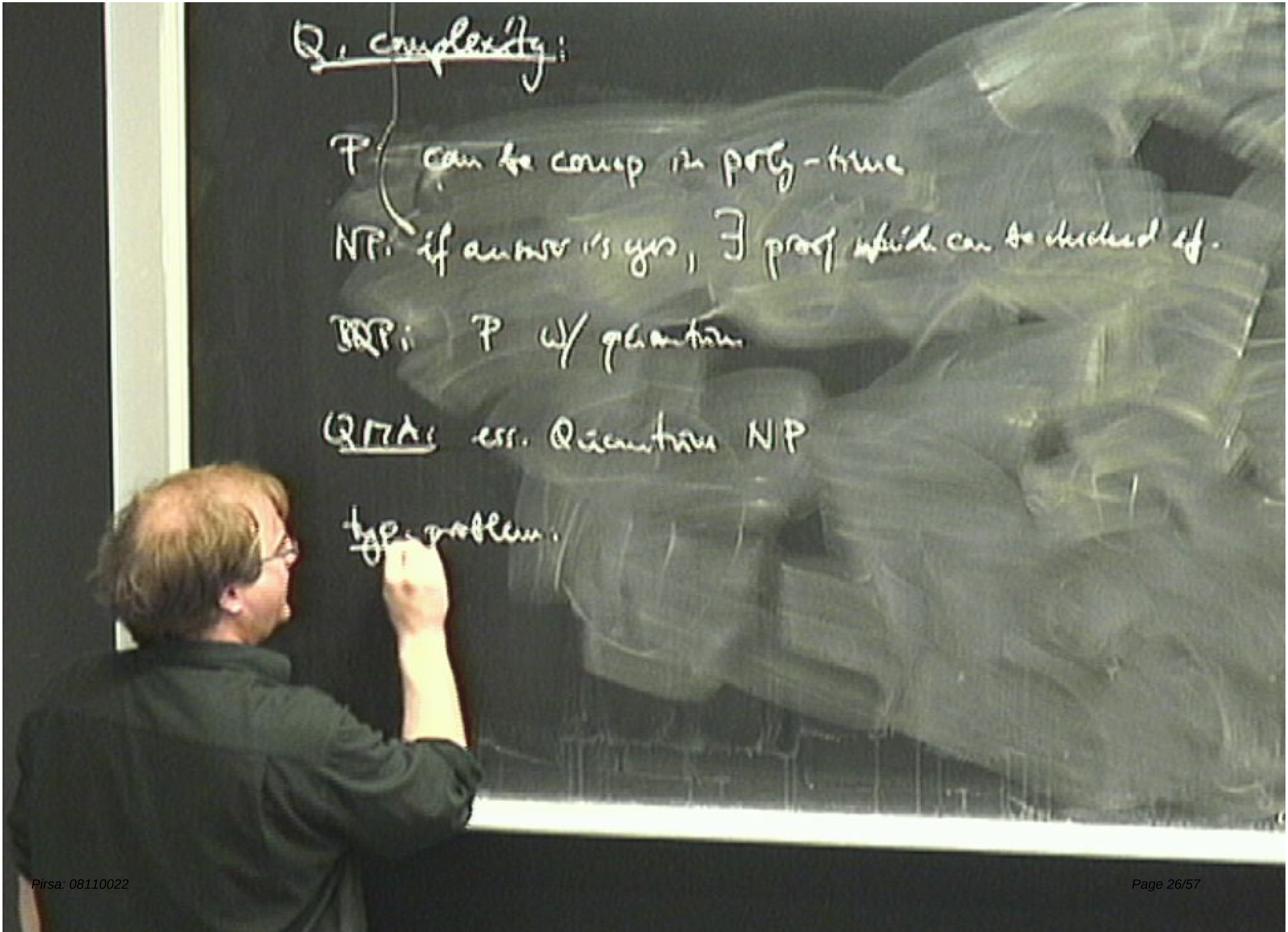
Q. complexity:

P: can be comp in poly-time

NP: if answer is yes, $\exists$ proof which can be checked eff.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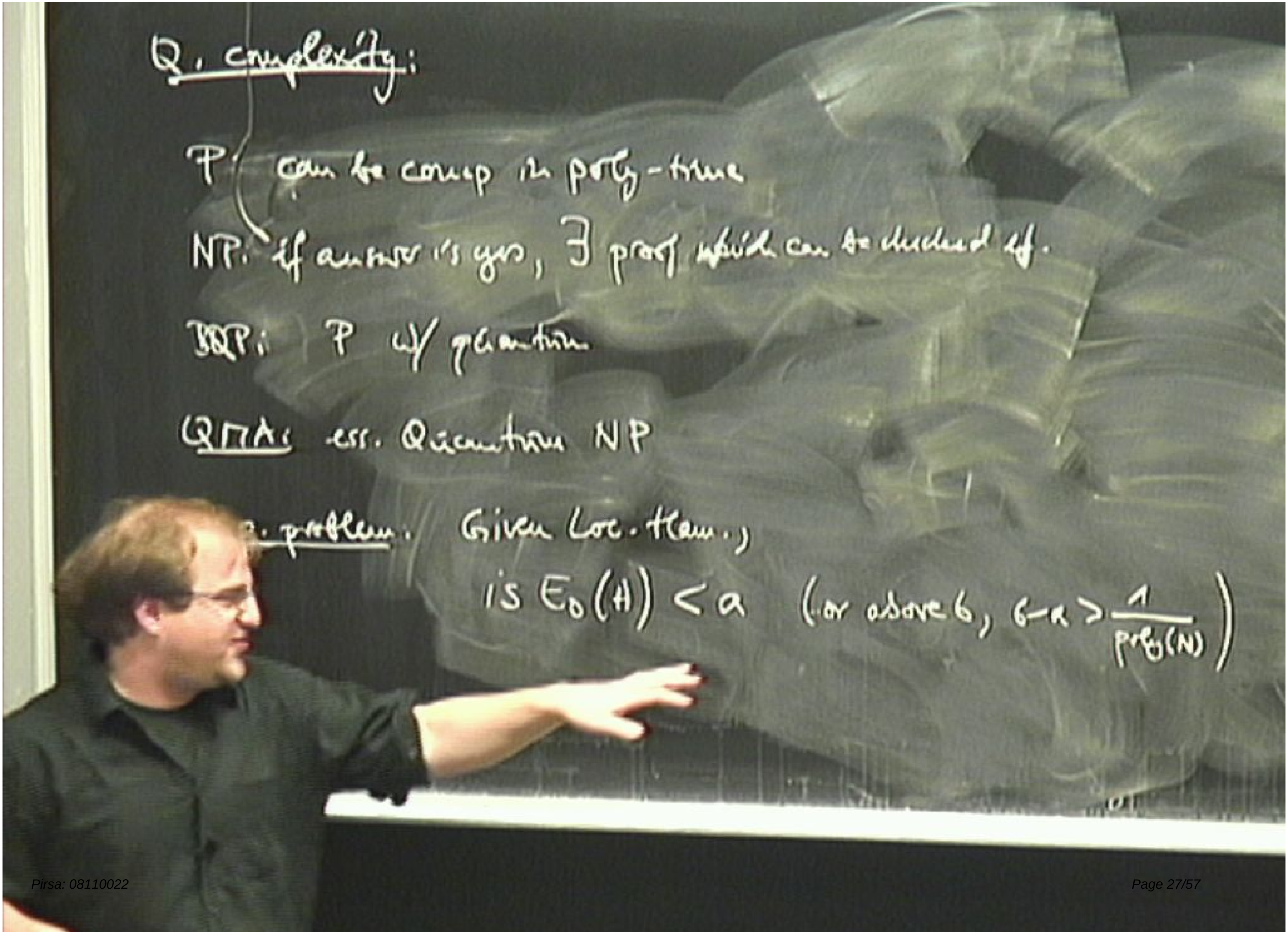
BQP: P w/ quantum
QMA: ess. Quantum NP
type problem..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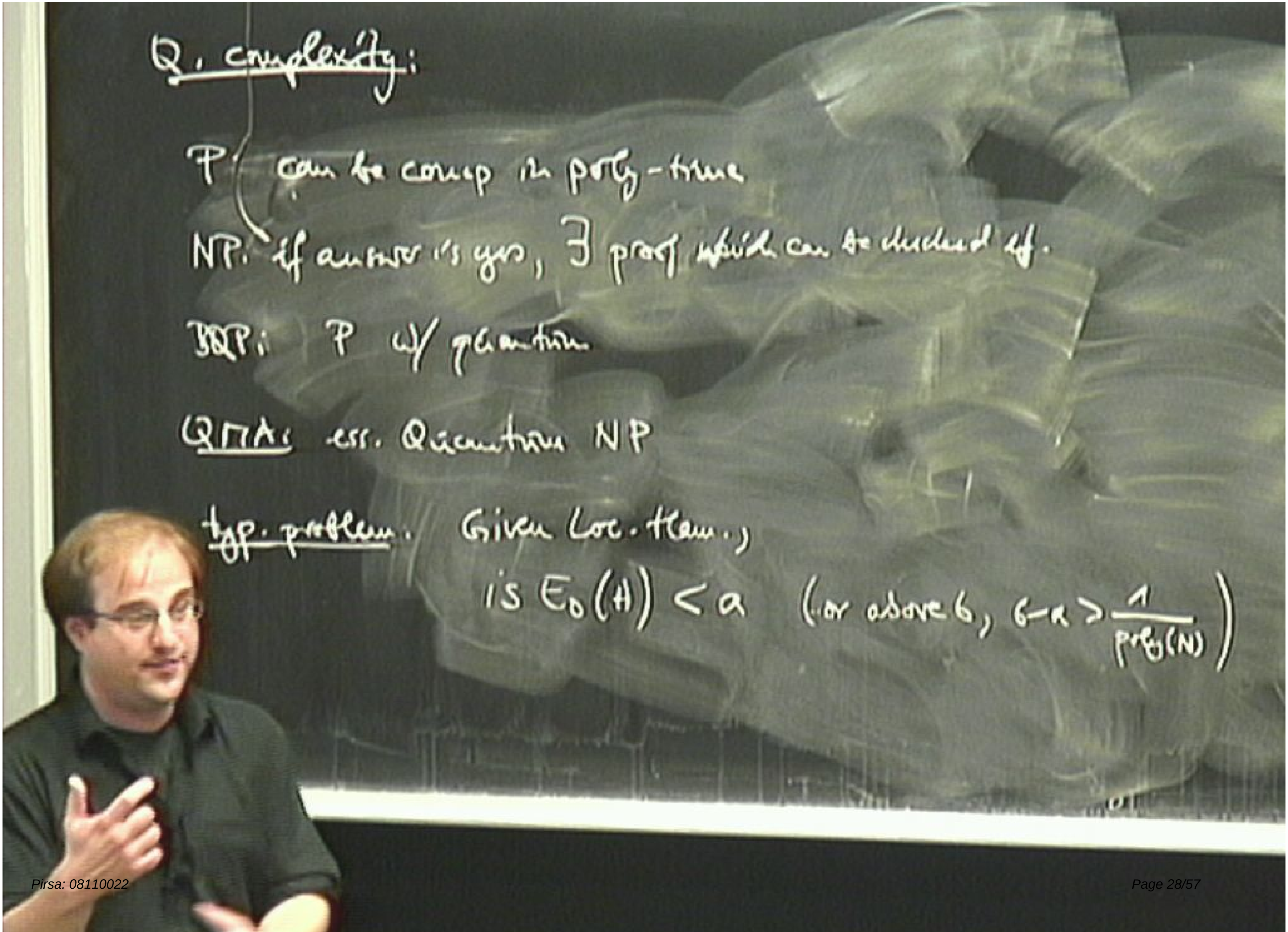
problem: Given Loc. Ham.,
is $E_0(H) < a$ (or above b, $b-a > \frac{1}{\mathrm{poly}(N)}$)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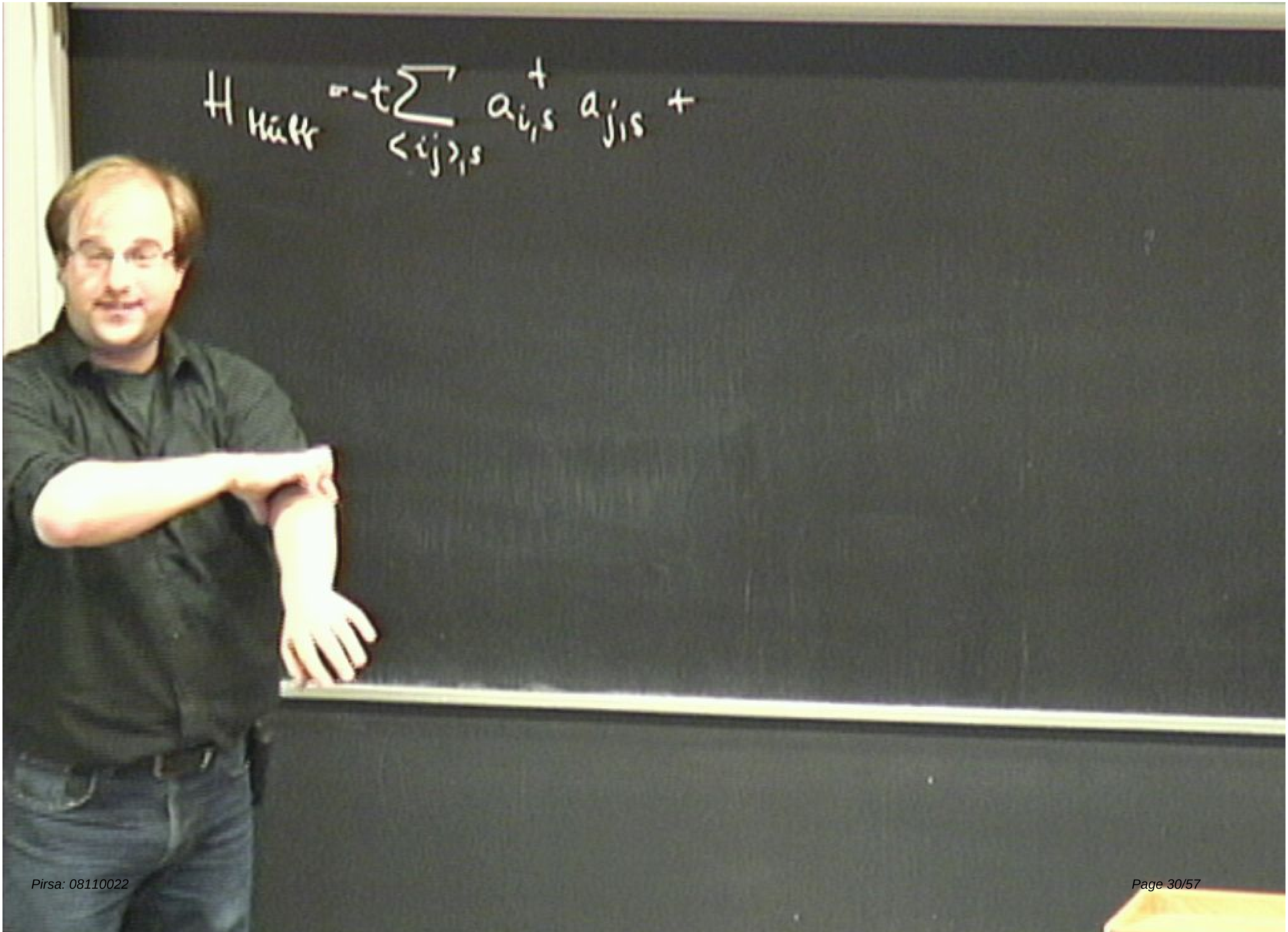
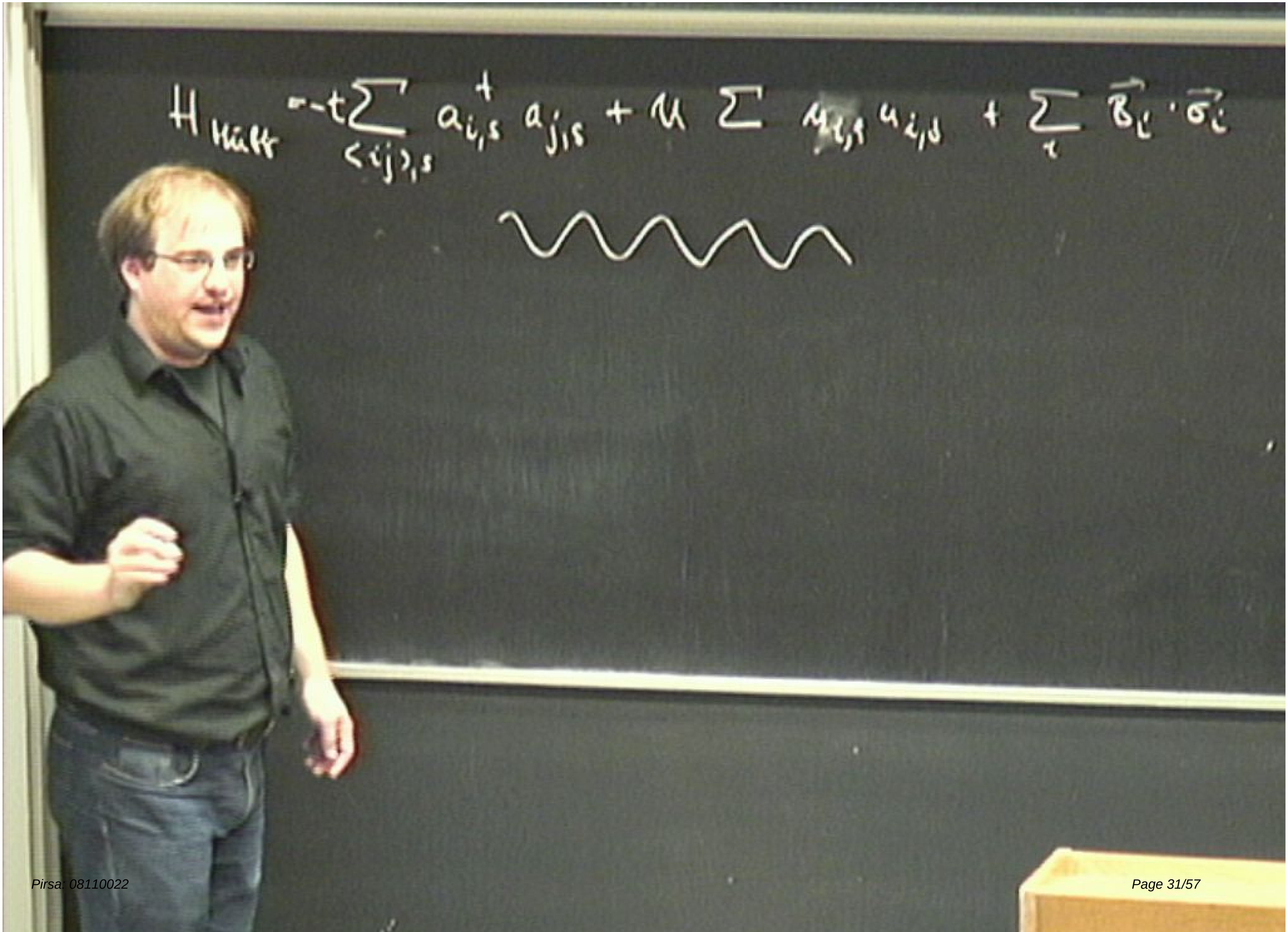
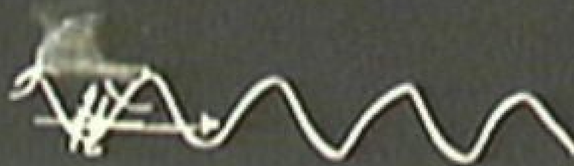
Proof: g.s.

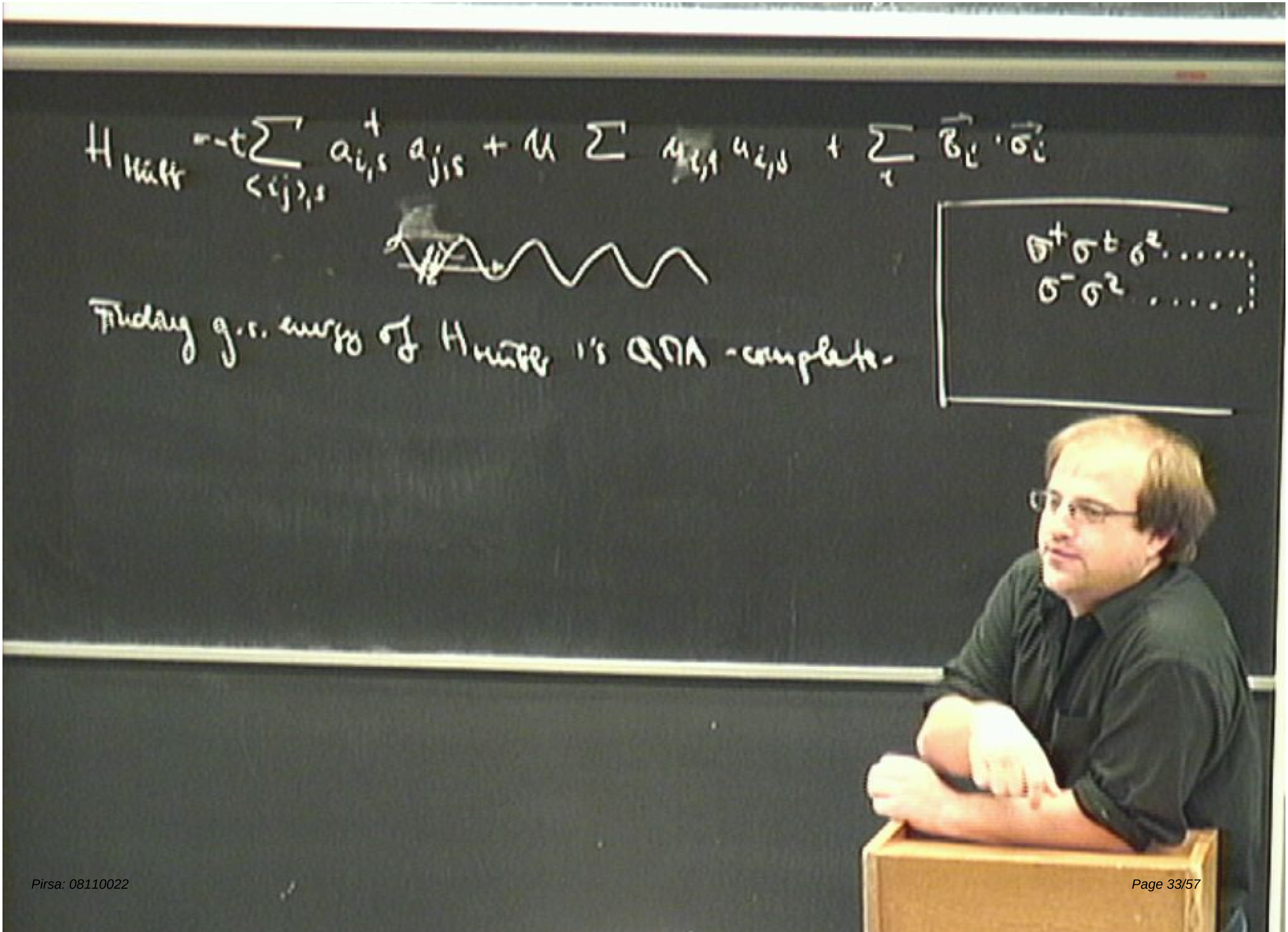

$H_{Hubb} = -t \sum_{\langle ij \rangle, s} a_{i,s}^{\dagger} a_{j,s} +$


$H_{Hubb} = -t \sum_{\langle ij \rangle, s} a^{\dagger}_{i,s} a_{j,s} + U \sum n_{i,\uparrow} n_{i,\downarrow} + \sum_{i} \vec{B}_i \cdot \vec{\sigma}_i$

$$H_{\text{Hubb}} = -t \sum_{\langle ij\rangle, s} a_{i,s}^{\dagger} a_{j,s} + U \sum n_{i,\uparrow} n_{i,\downarrow} + \sum_{i} \vec{B}_i \cdot \vec{\sigma}_i$$



finding g.s. energy of H_{Hubb} is QMA-complete.



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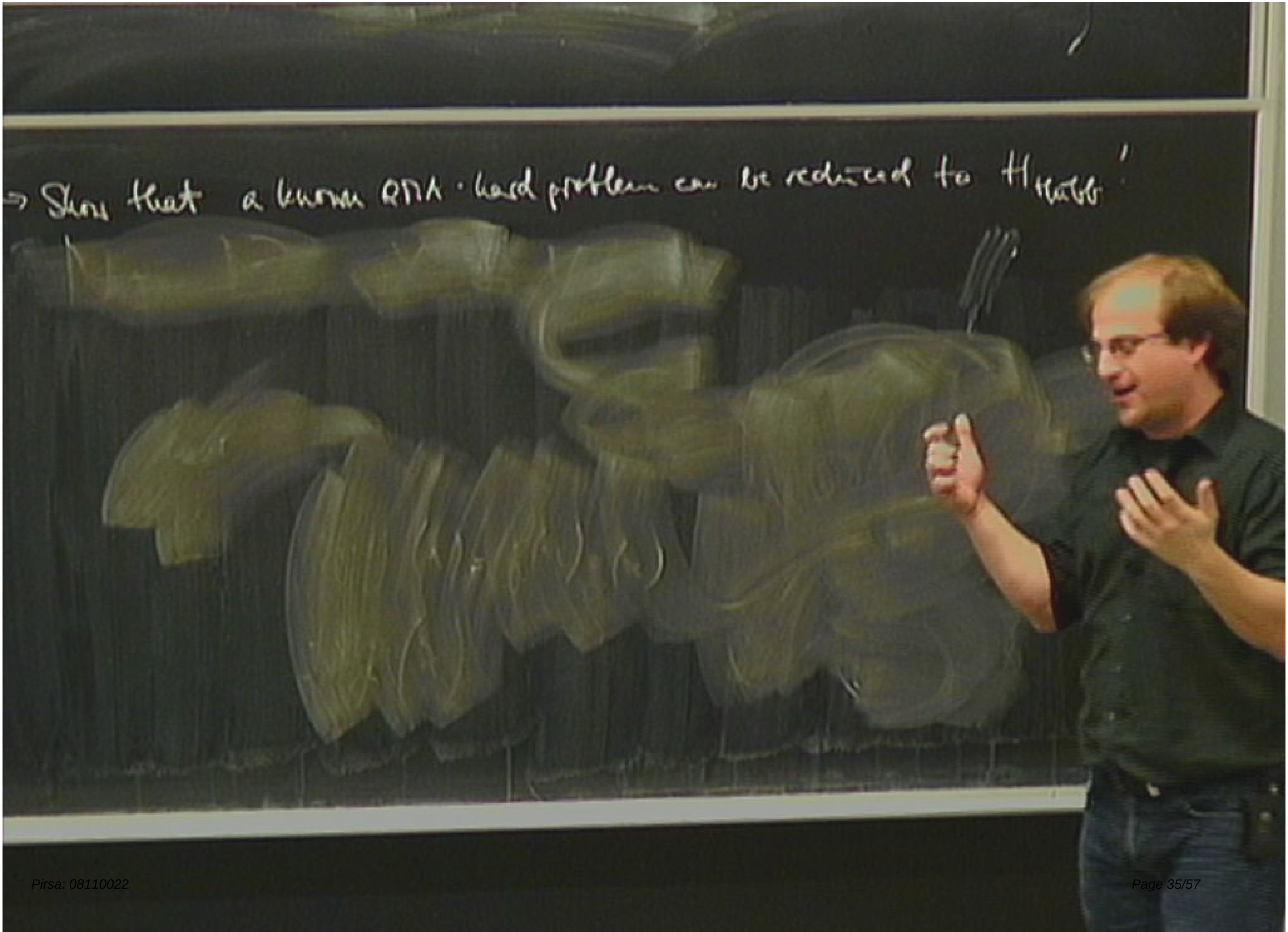
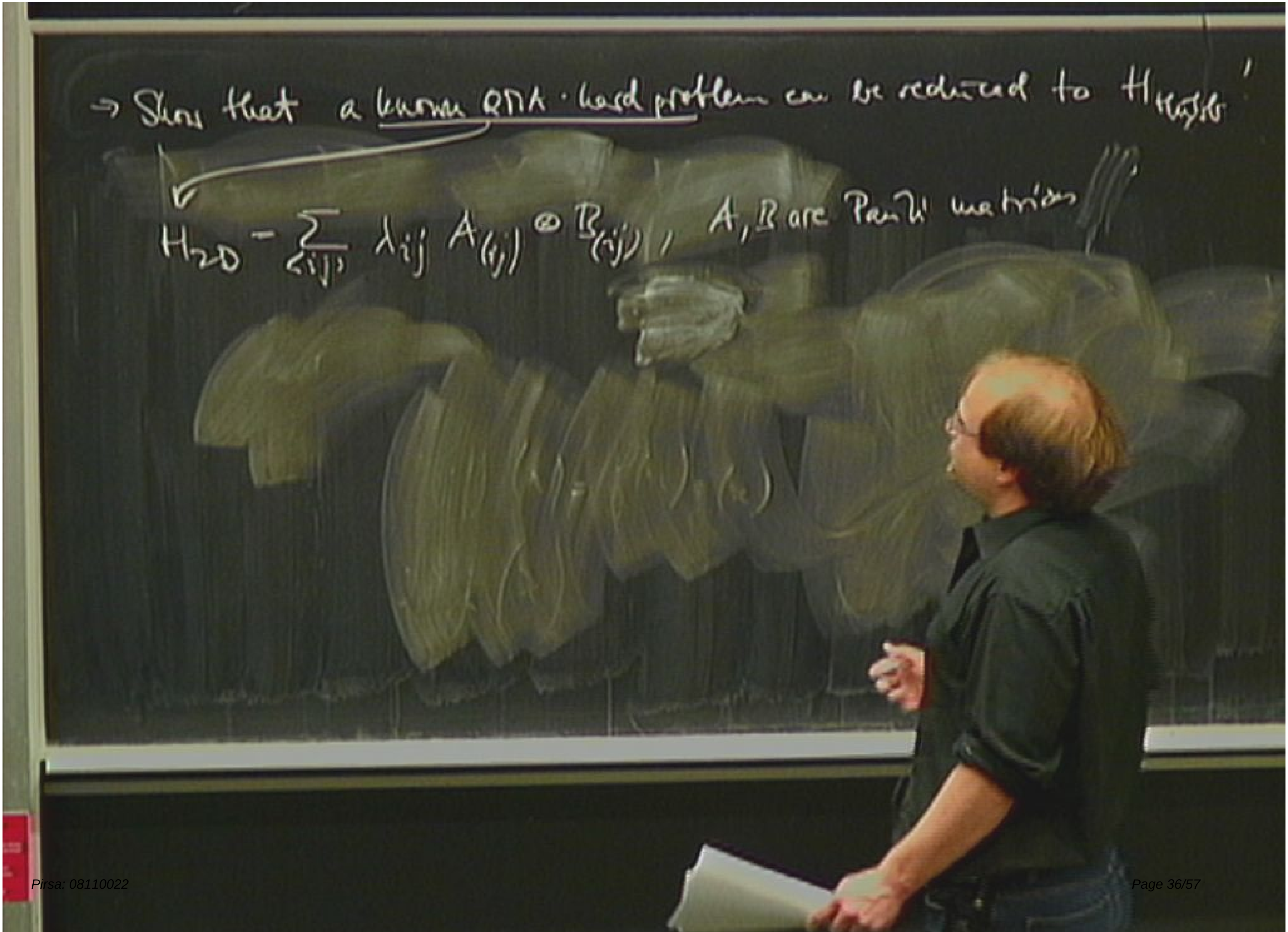
Finding g.s. energy of H_{Hubb} is QMA-complete.

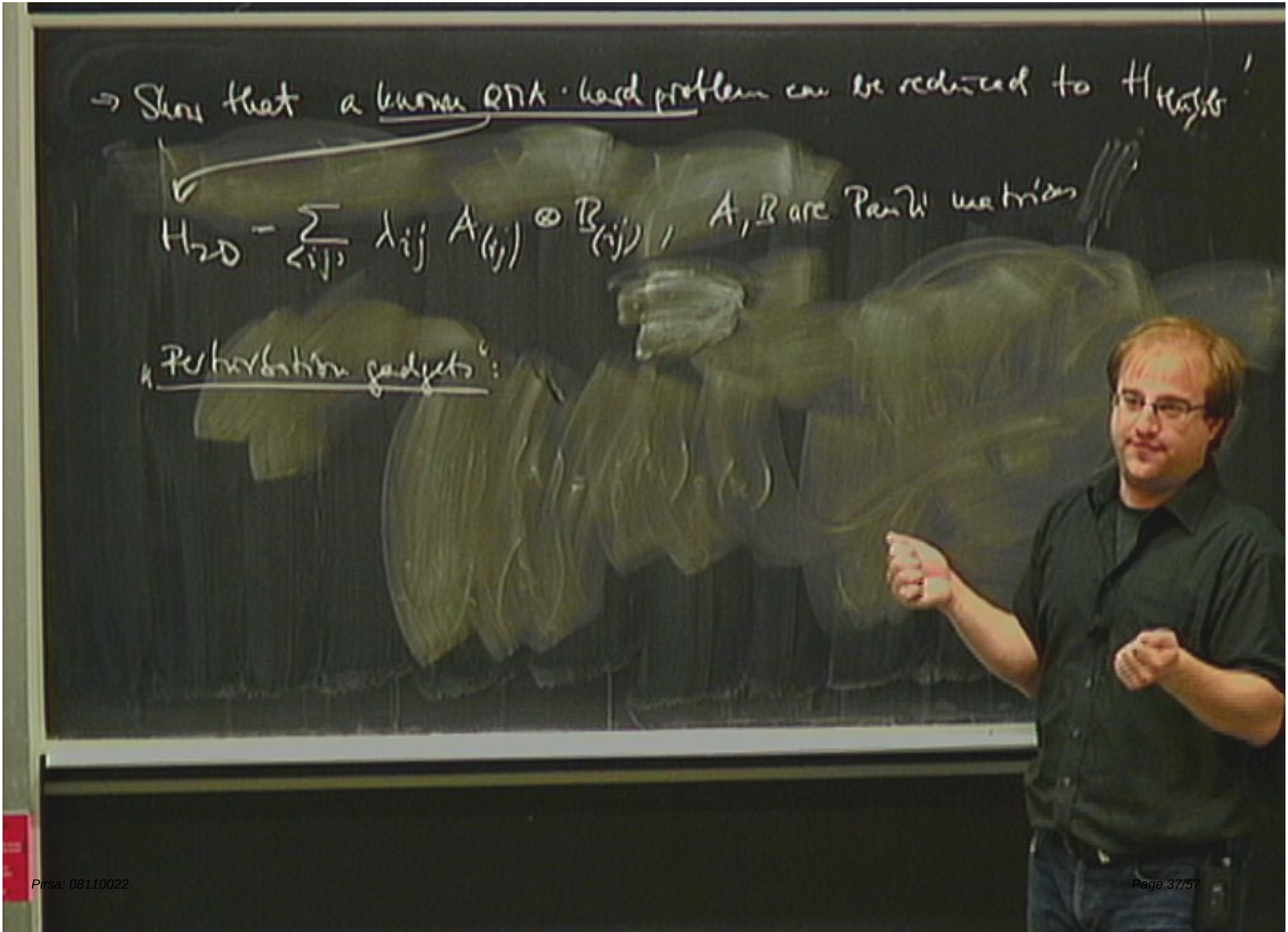
- In QMA ✓
- hard for QMA ?

$\sigma^+ \sigma^{\pm} \sigma^z \ldots\ldots$

$\sigma^- \sigma^z \ldots\ldots$


⇒ Show that a known QMA-hard problem can be reduced to H_{Hubb}!


→ Show that a known QMA-hard problem can be reduced to H
H2D = Σ⟨ij⟩ λij A(ij) ⊗ B(ij), A, B are Pauli matrices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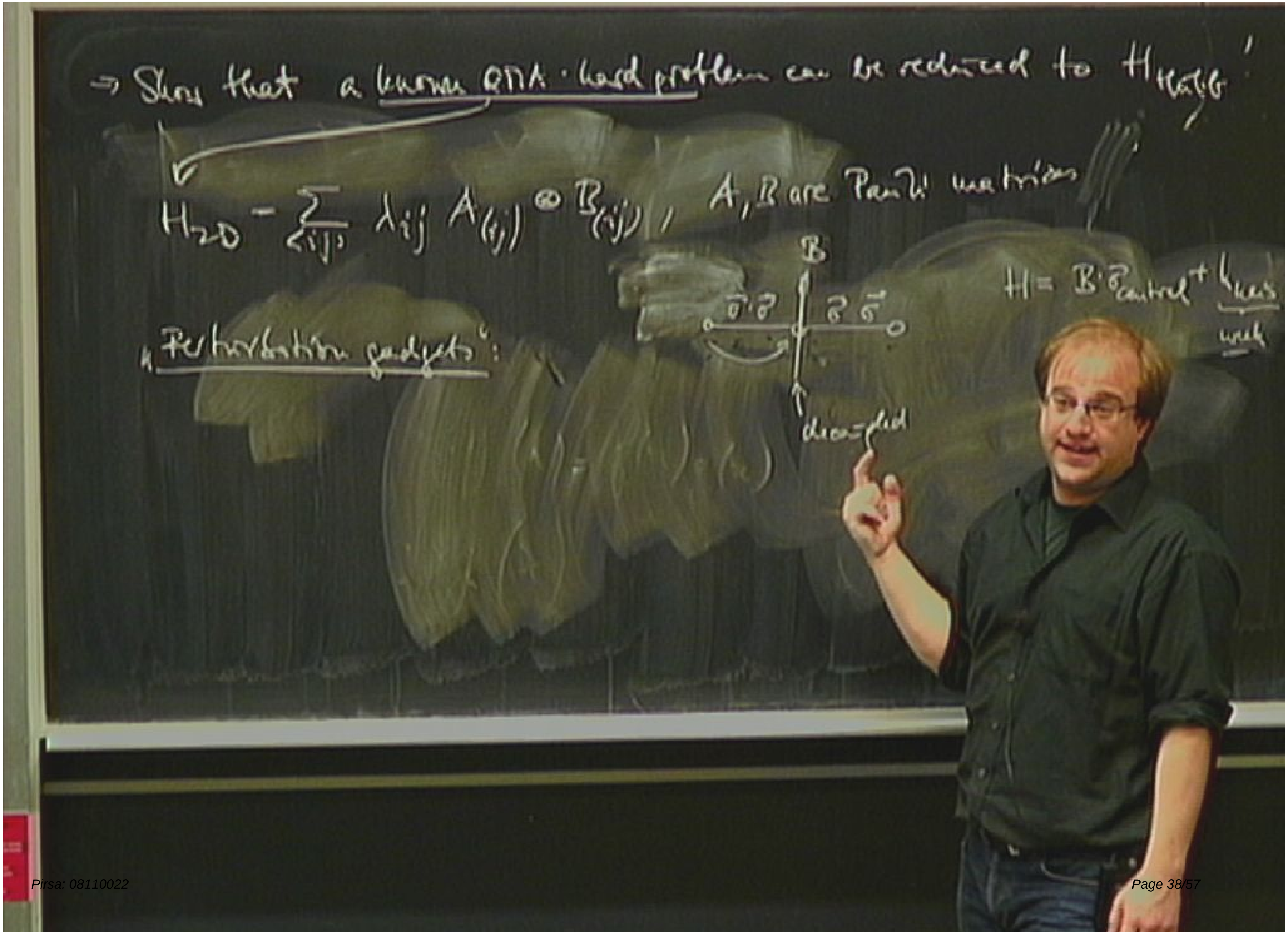
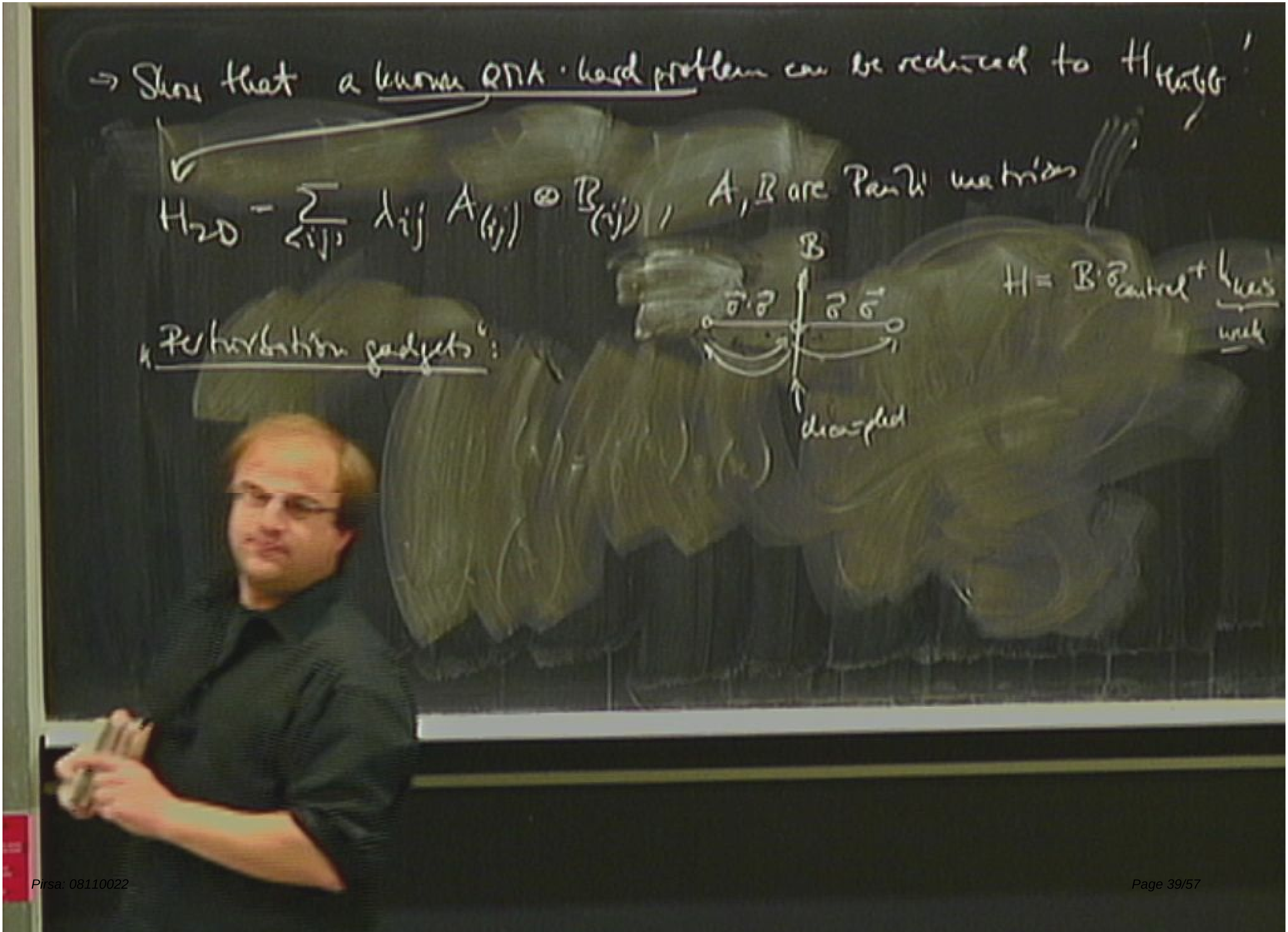
„Perturbation gadgets":


⇒ Show that a known QMA-hard problem can be reduced to
H2D = Σ λij A(ij) ⊗ B(ij) , A, B are Pauli matrices
B
H = B·σcontrol + hrest
weak
Perturbation gadgets:
decoupled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H_2D = Σ_⟨ij⟩ λ_ij A_(ij) ⊗ B_(ij) , A, B are Pauli matrices
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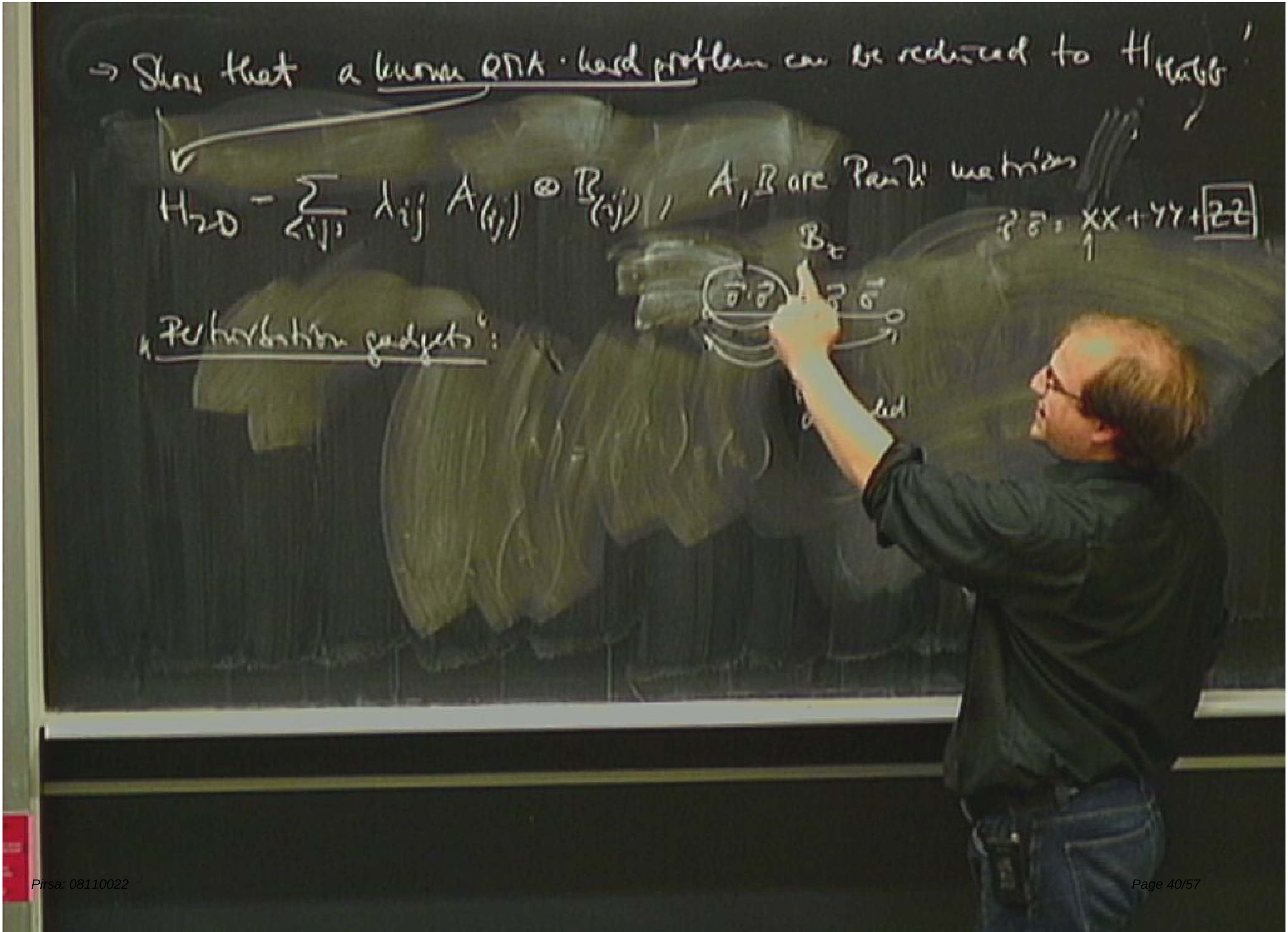
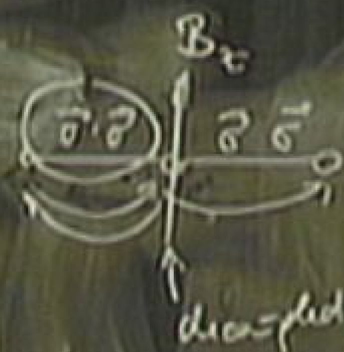

→ Show that a known QMA-hard problem can be reduced to H
H_2D = Σ_⟨ij⟩ λ_ij A_(ij) ⊗ B_(ij), A, B are Pauli matrices
σ·σ = XX + YY + ZZ
B_z
σ·σ
"Perturbation gadgets":

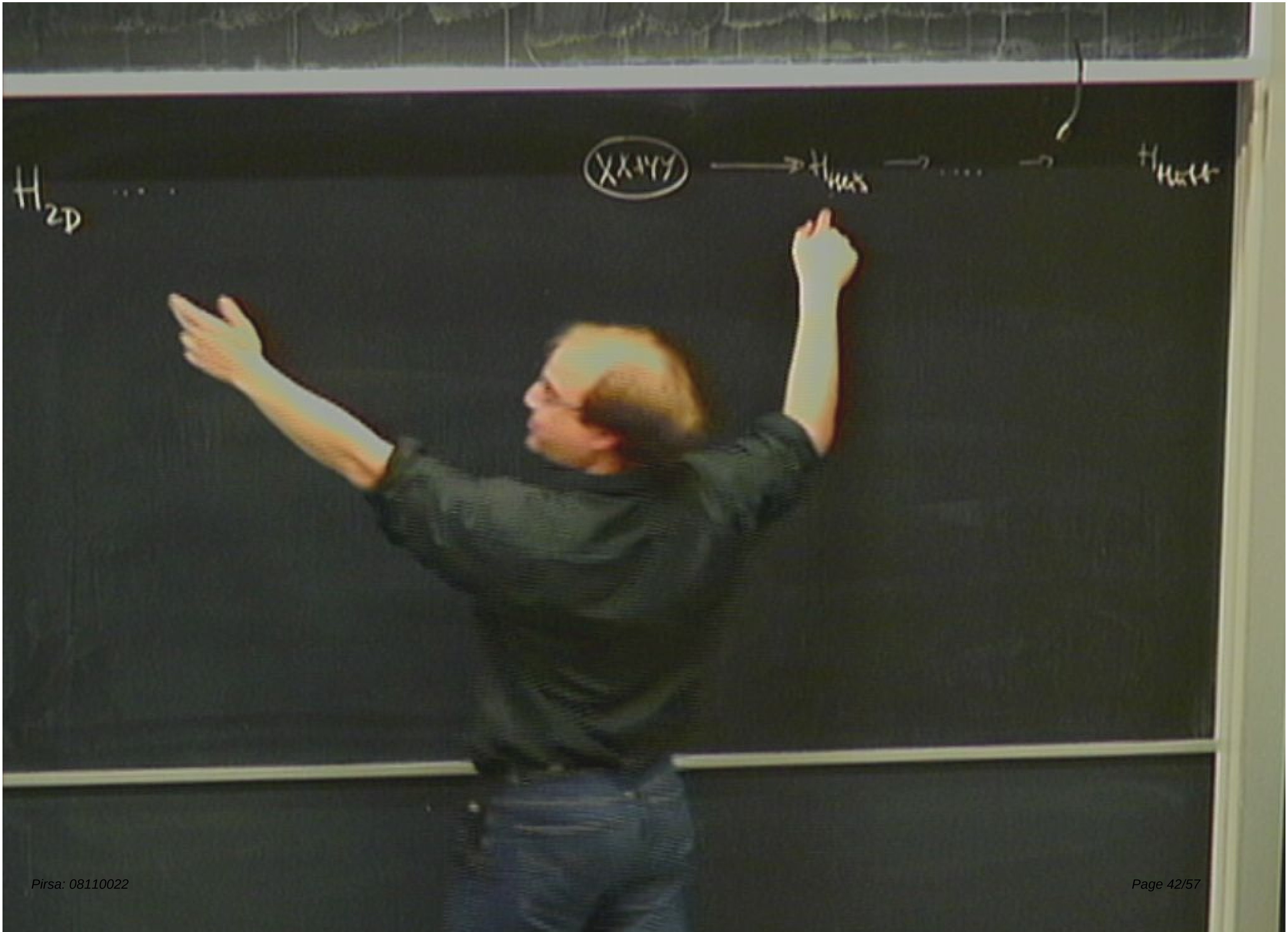
→ Show that a known QMA-hard problem can be reduced to H_{Heis}!

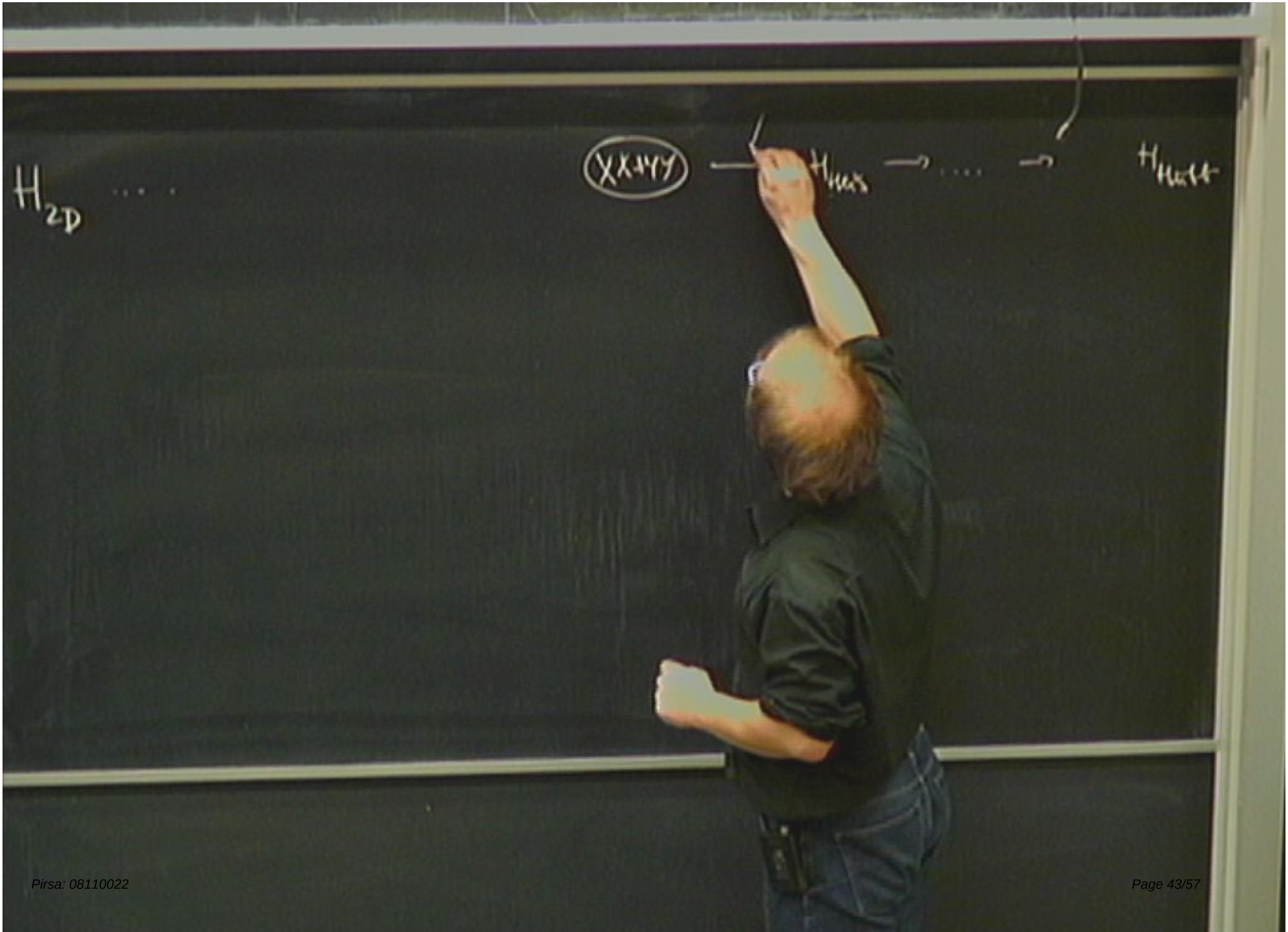
$$H_{2D} = \sum_{\langle ij \rangle} \lambda_{ij} A_{(ij)} \otimes B_{(ij)}, \quad A, B \text{ are Pauli matrices}$$

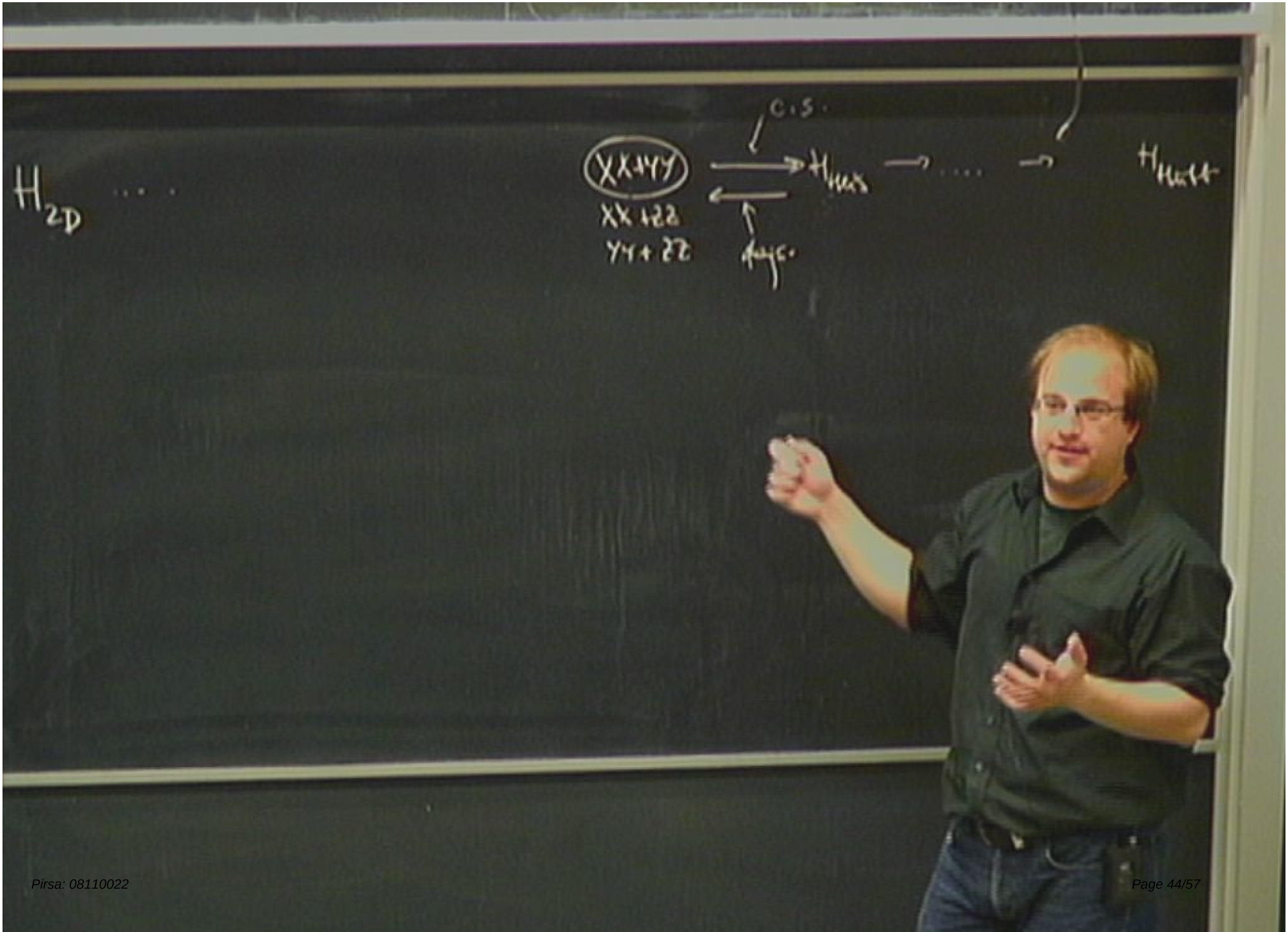
$$\vec{\sigma}\cdot\vec{\sigma} = XX + YY + \cancel{ZZ}$$

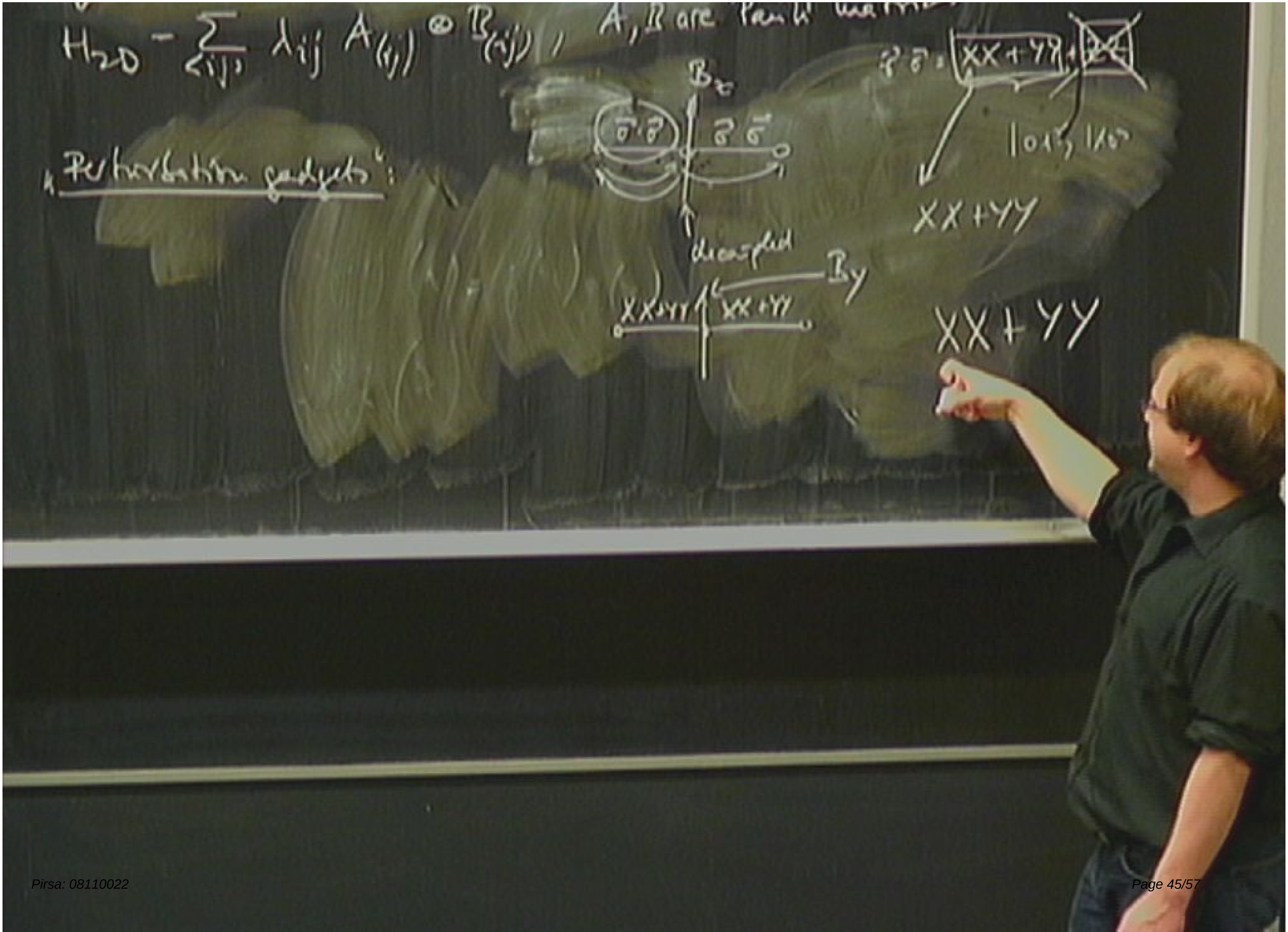


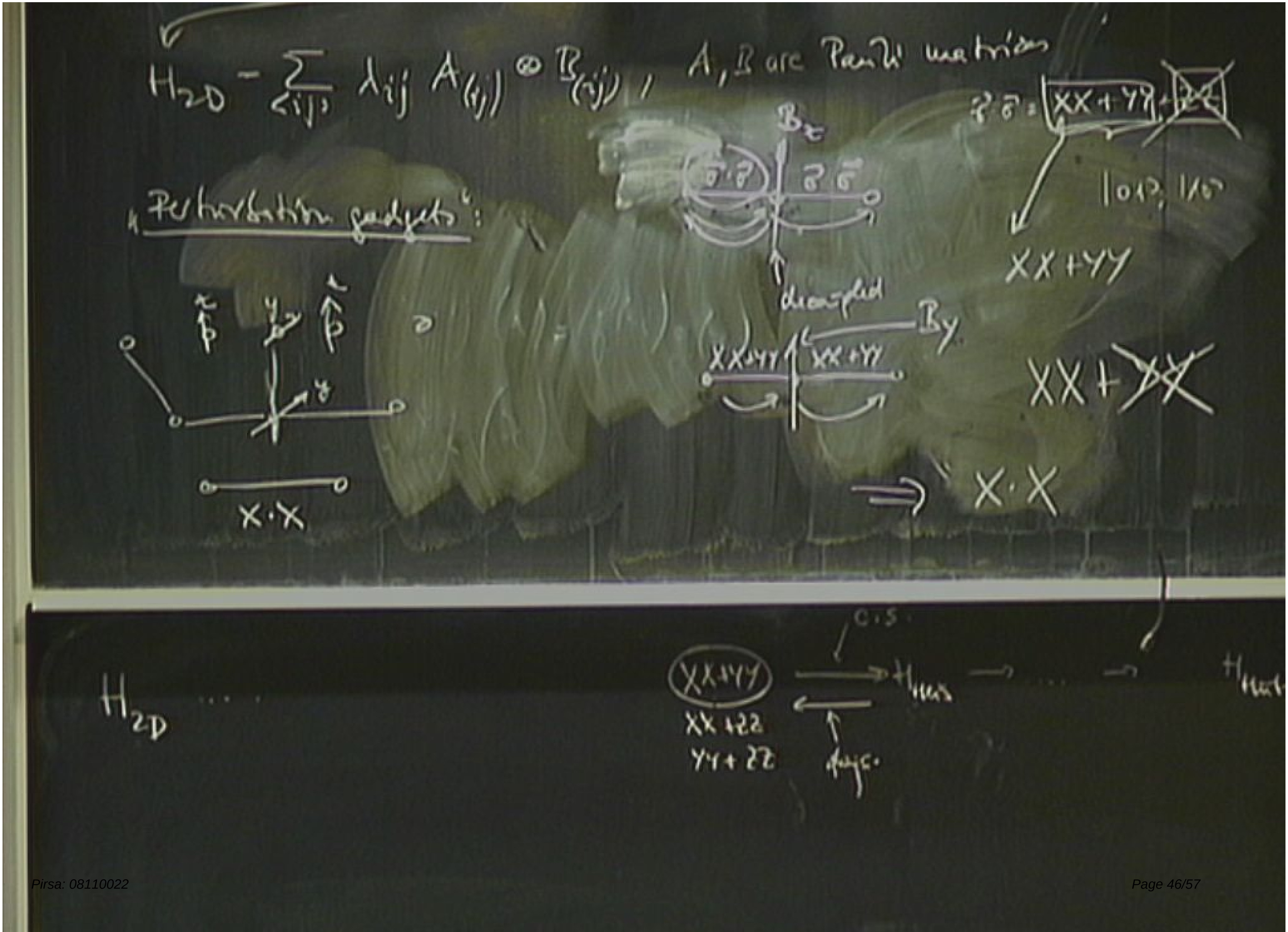
„Perturbation gadgets“:


H2D
XXYY

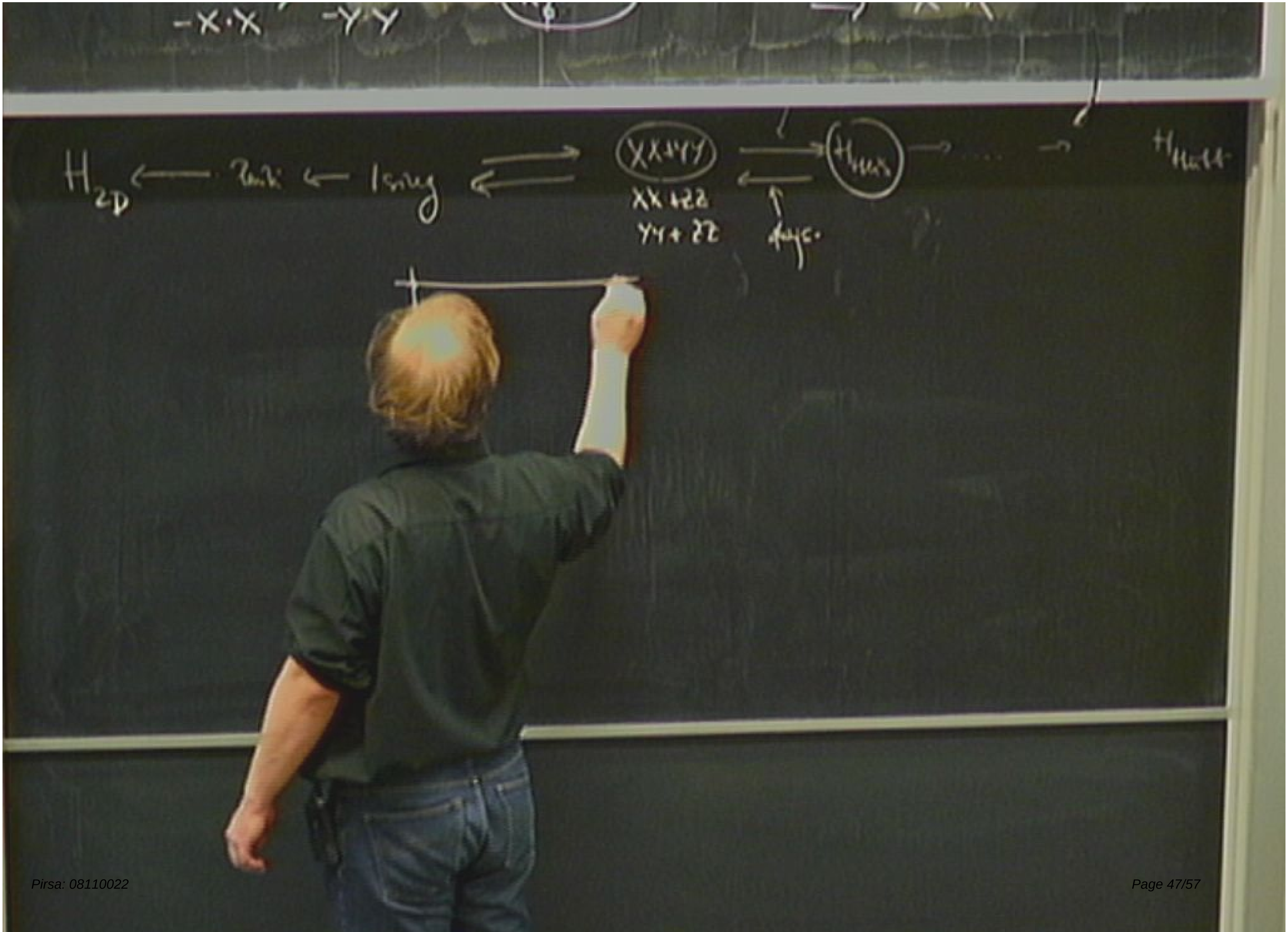

H_{2D} ....
XX+YY

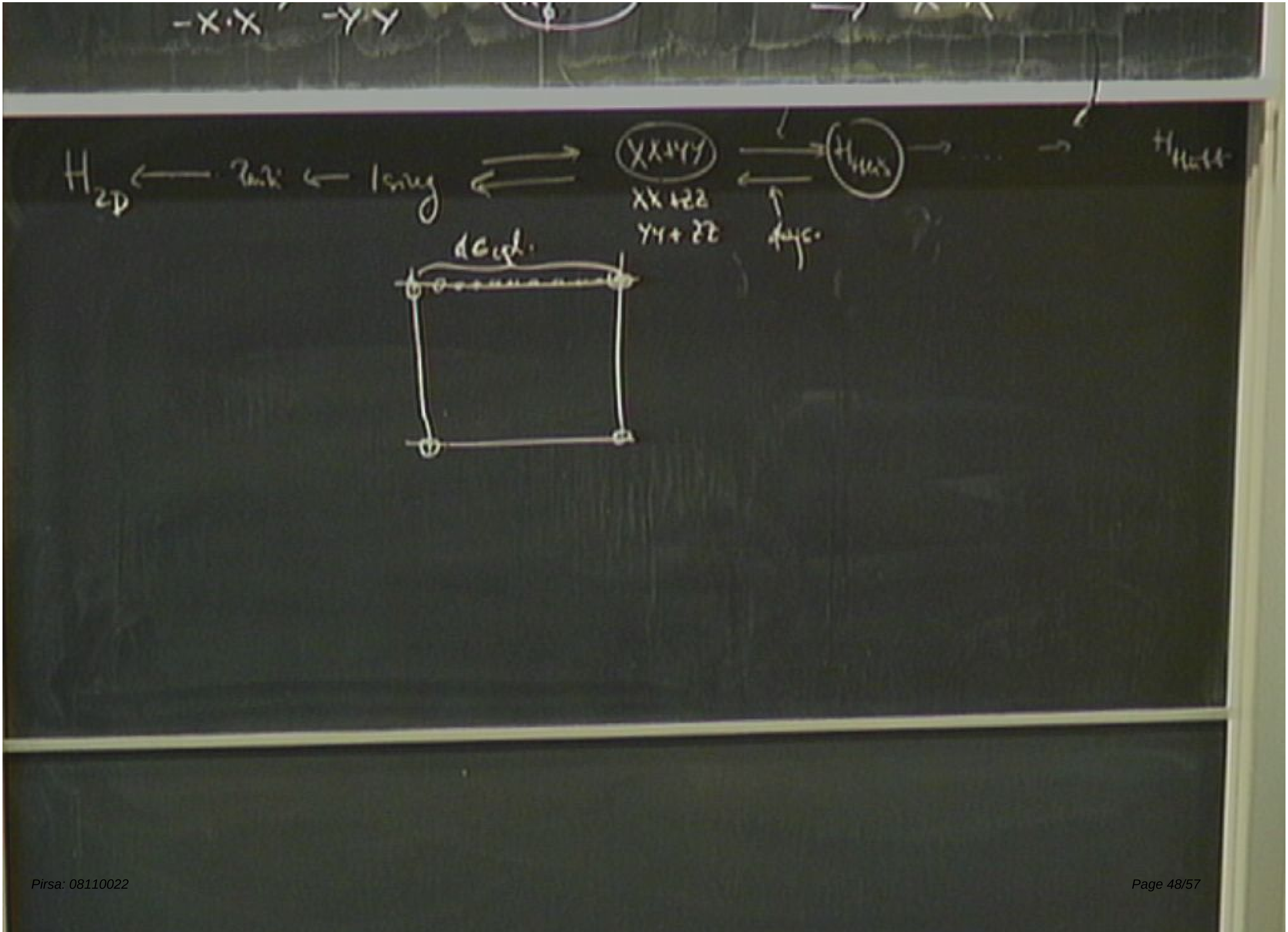

c.s.
XX+YY
XX+ZZ
YY+ZZ

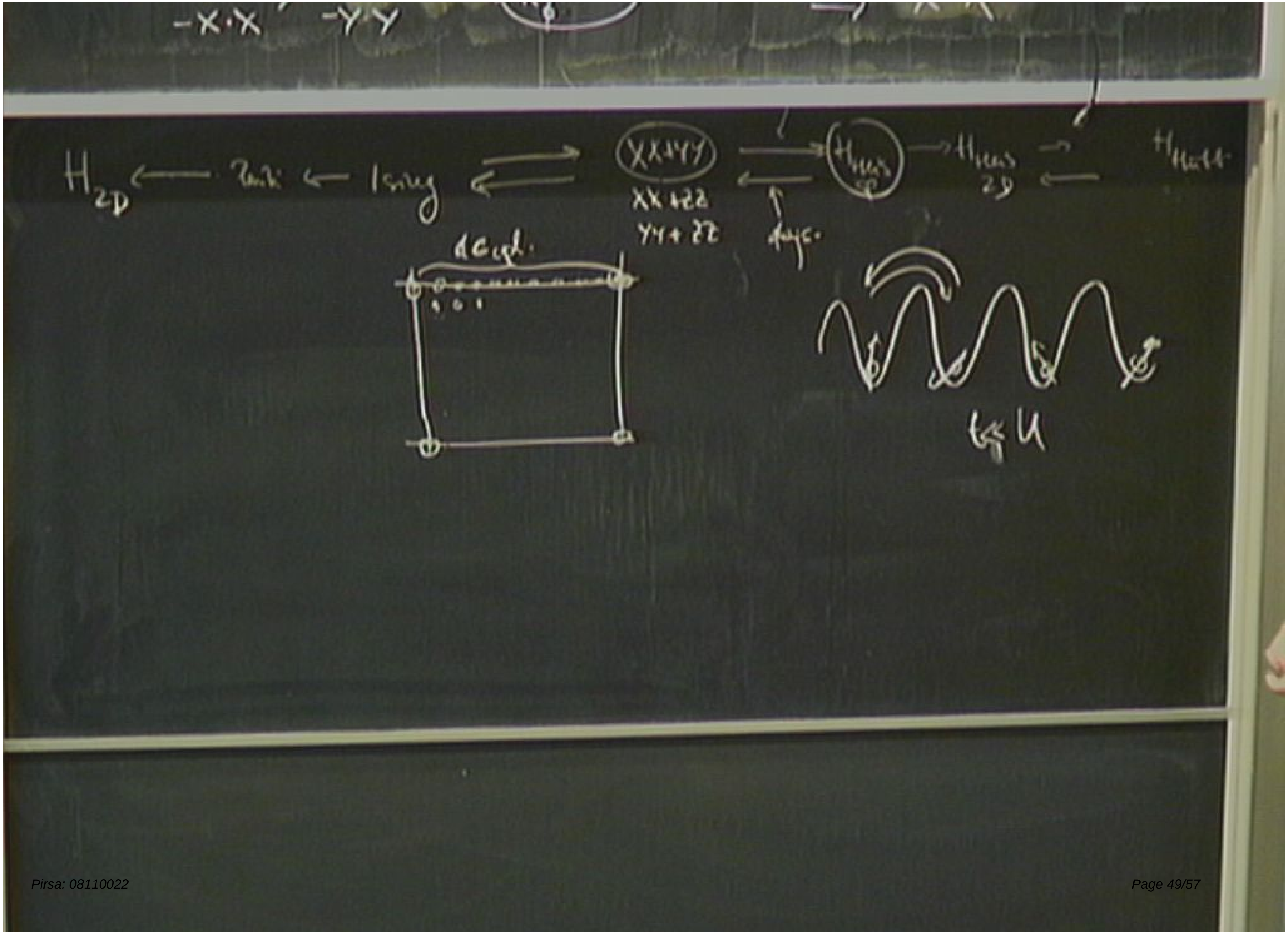

$H_{2D} = \sum_{\langle i,j \rangle} \lambda_{ij} A_{(i)} \otimes B_{(j)}$, A, B are
"Perturbation gadgets":
B_x
decoupled
B_y
XX+YY
|01⟩, |10⟩
XX+YY
XX+YY

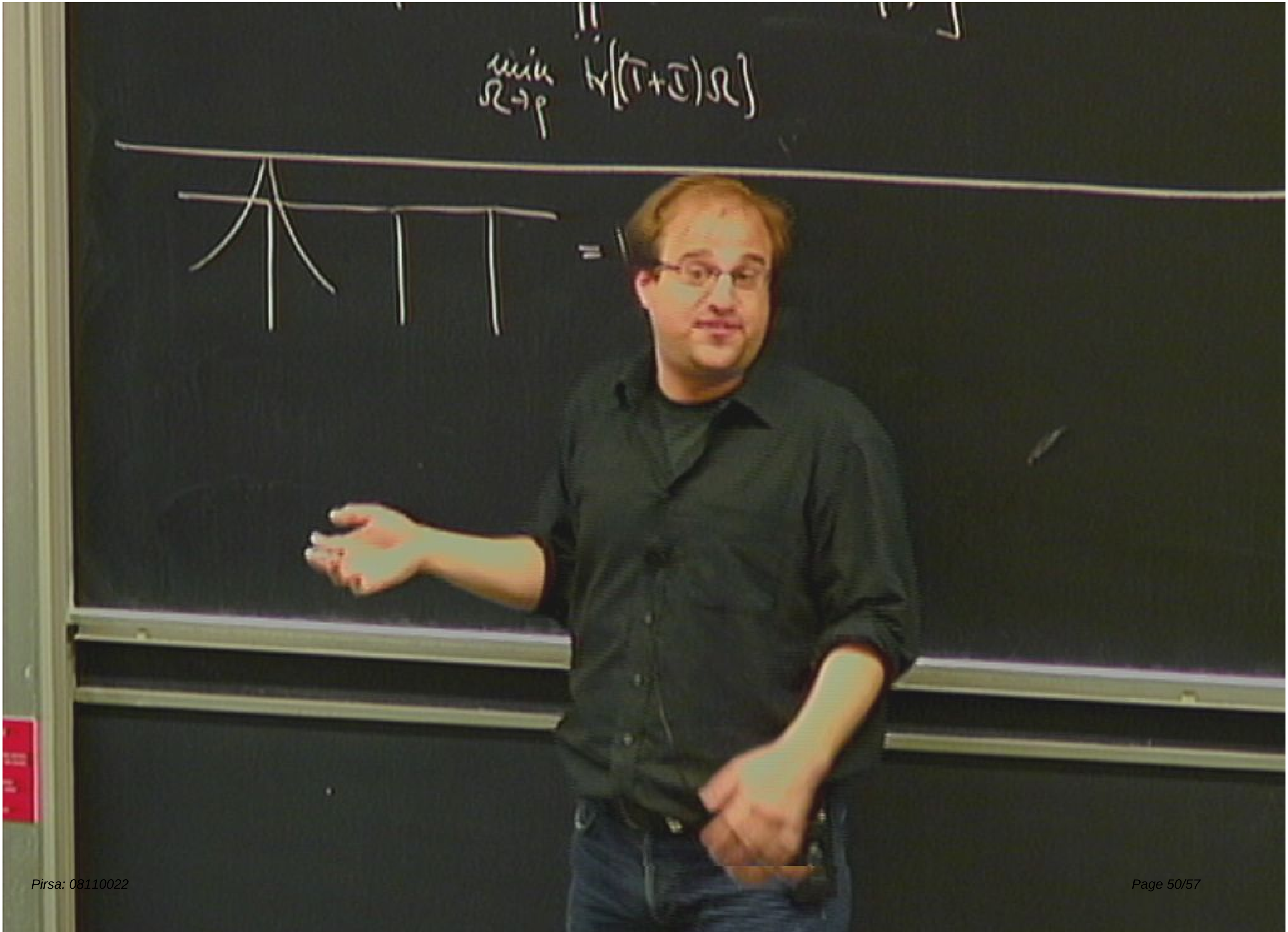


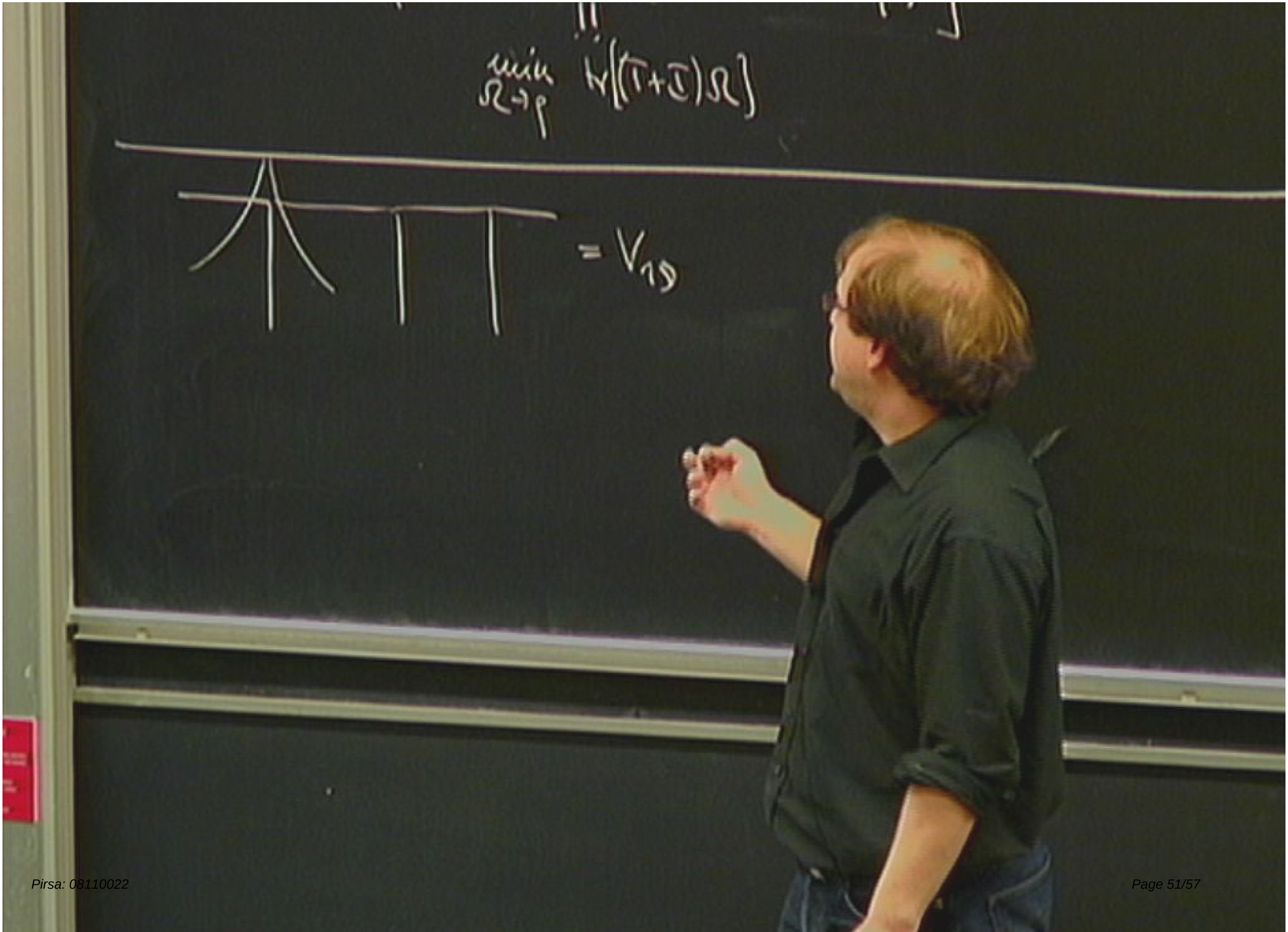
H_2D = Σ_⟨ij⟩ λ_ij A_(ij) ⊗ B_(ij) , A, B are Pauli matrices
Perturbation gadgets:
X·X
B_z
decoupled
B_y
XX+YY
XX+YY
XX+YY
X·X
|01⟩, |10⟩
XX+YY
XX+ZZ
YY+ZZ
H_2D
H_heis


-X·X
-Y Y
H2D
Ising
XX+YY
XX+ZZ
YY+ZZ

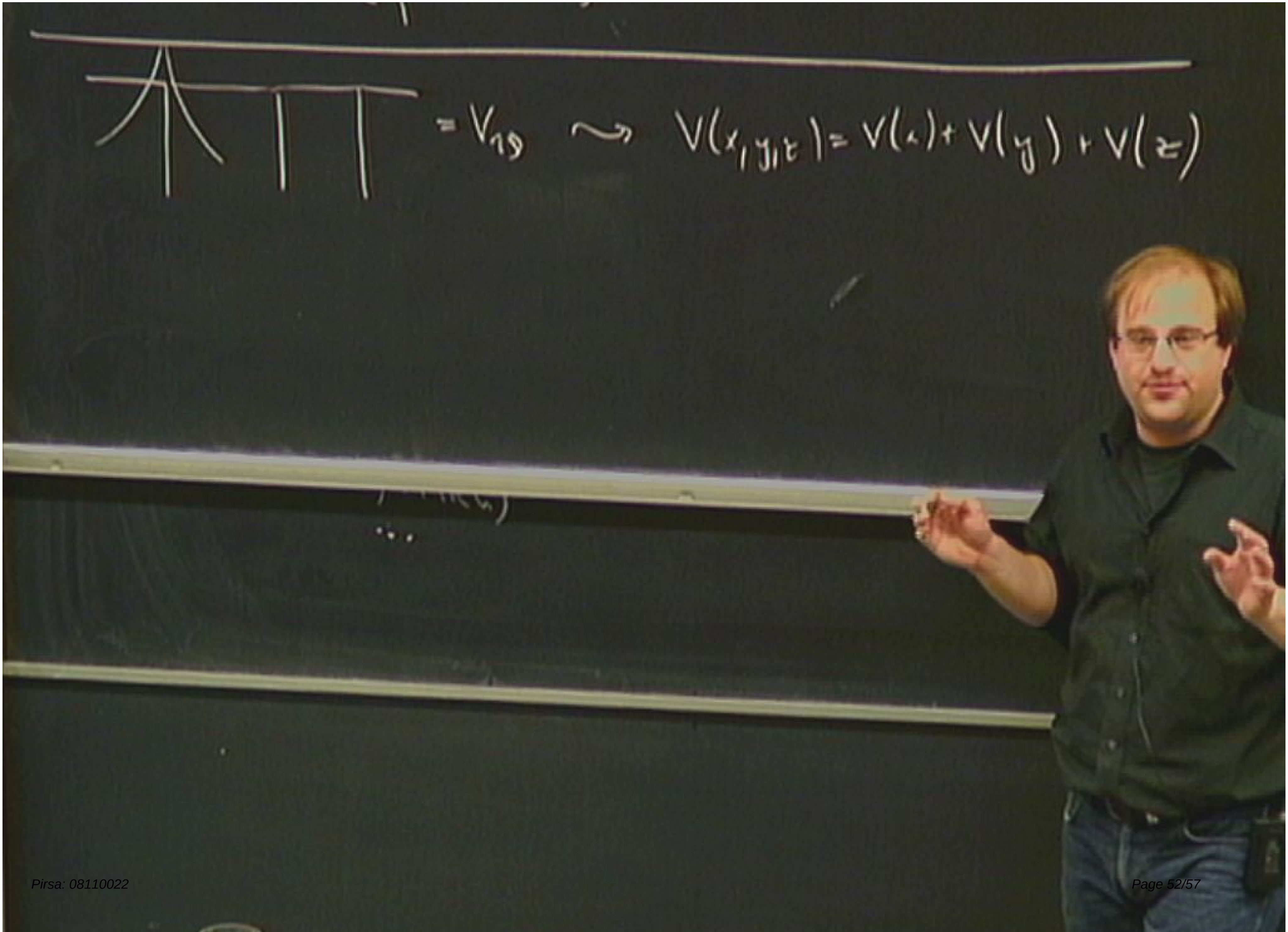

-X·X
-Y Y
Ising
XX+YY
XX+ZZ
YY+ZZ

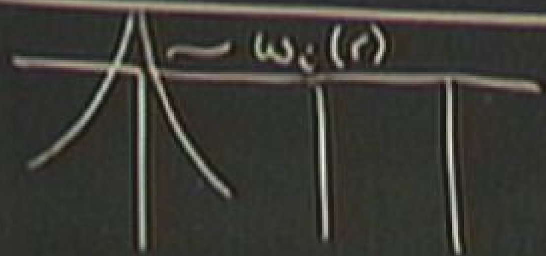

-X·X
-Y·Y
H 2D
Ising
XX+YY
XX+ZZ
YY+ZZ
H Heis
H Heis 2D
t ≪ U





min_{Ω→ρ} tr[(T+I)Ω]
= V_{1D}


= V_19 ⇝ V(x, y, z) = V(x) + V(y) + V(z)

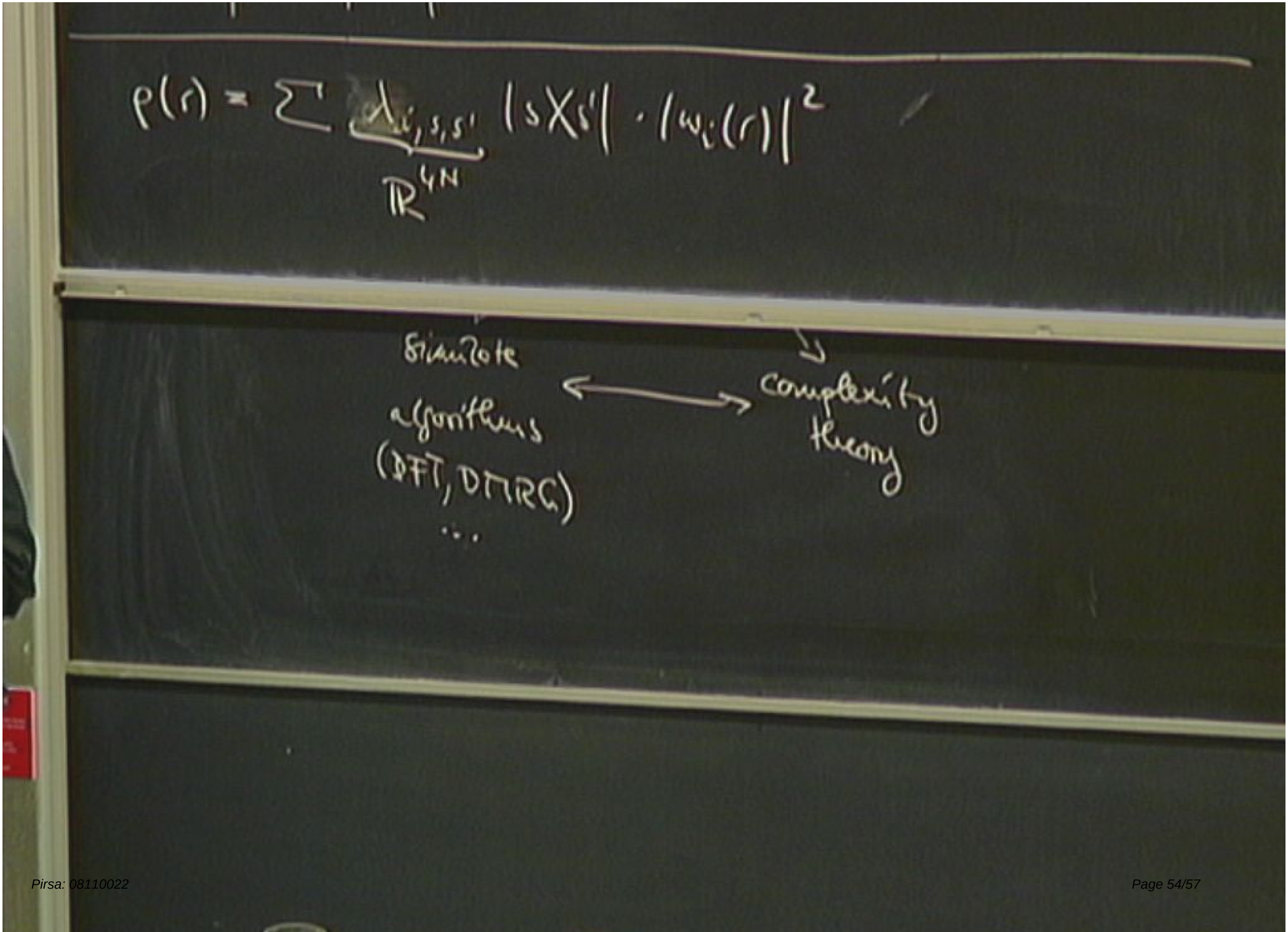


$$= V_{1B} \rightsquigarrow V(x,y,z) = V(x) + V(y) + V(z)$$

$$\rho(r) = \sum{}' \underline{\lambda_{i,s,s'}} \, |s\rangle\langle s'| \cdot |w_i(r)|^2$$

(…, DMRG)

…


$\rho(r) = \sum' \underbrace{\lambda_{i,s,s'}}_{\mathbb{R}^{4N}} |s\rangle\langle s'| \cdot |\omega_i(r)|^2$
simulate
algorithms
(DFT, DMRG)
...
complexity
theory

C.S.

XX+YY → H_{XXX} → H_{XXZ} →

$F[\rho]$ is <u>convex</u>!

c.s.

$XX+YY \longrightarrow H$

$F[\rho]$ is <u>convex</u>!

$$E(\rho) = F[\rho] + \mathrm{tr}[V\rho] \quad \text{is convex!}$$

$F[\rho]$ is convex!

$$E(\rho) = F[\rho] + \mathrm{tr}[V\rho] \text{ is convex!}$$

$\longrightarrow$ can be done efficiently!

Hubb. model QMA-complete.