Title: LECTURE: Tensor networks and quantum simulations

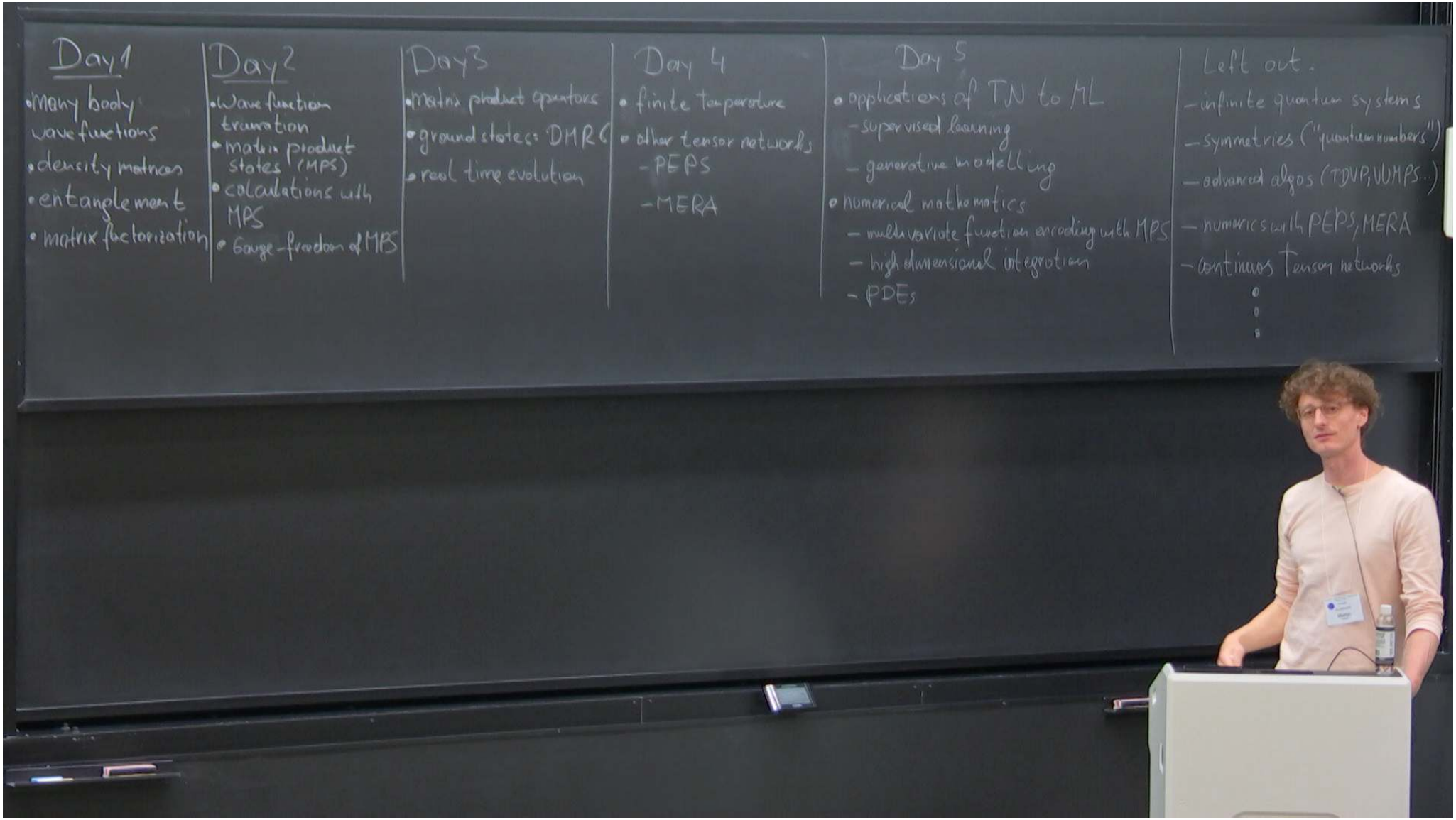
Speakers: Martin Ganahl

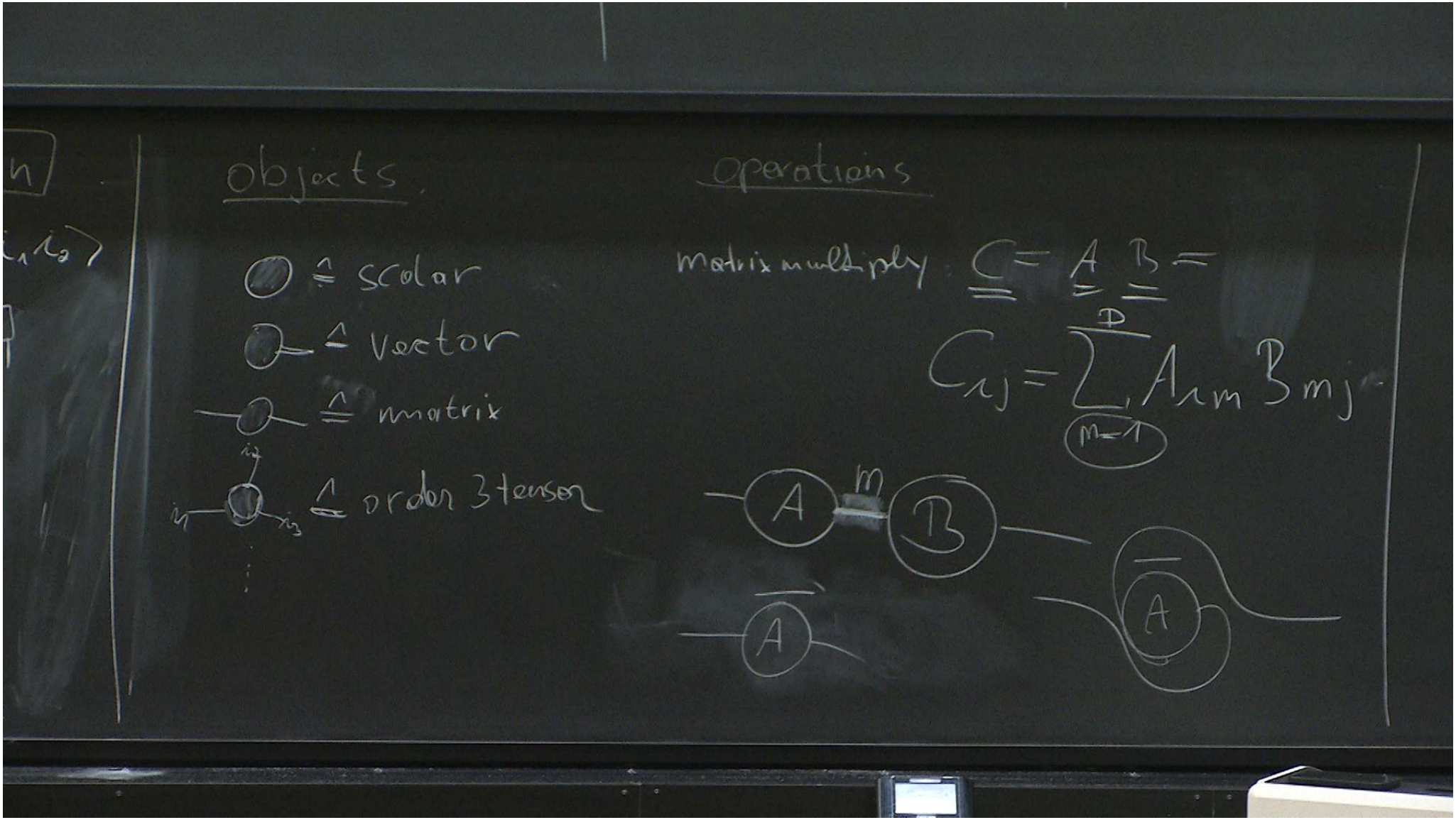
Collection: Quantum and AI Career Trajectories Mini-Course: Computational Methods and their Applications

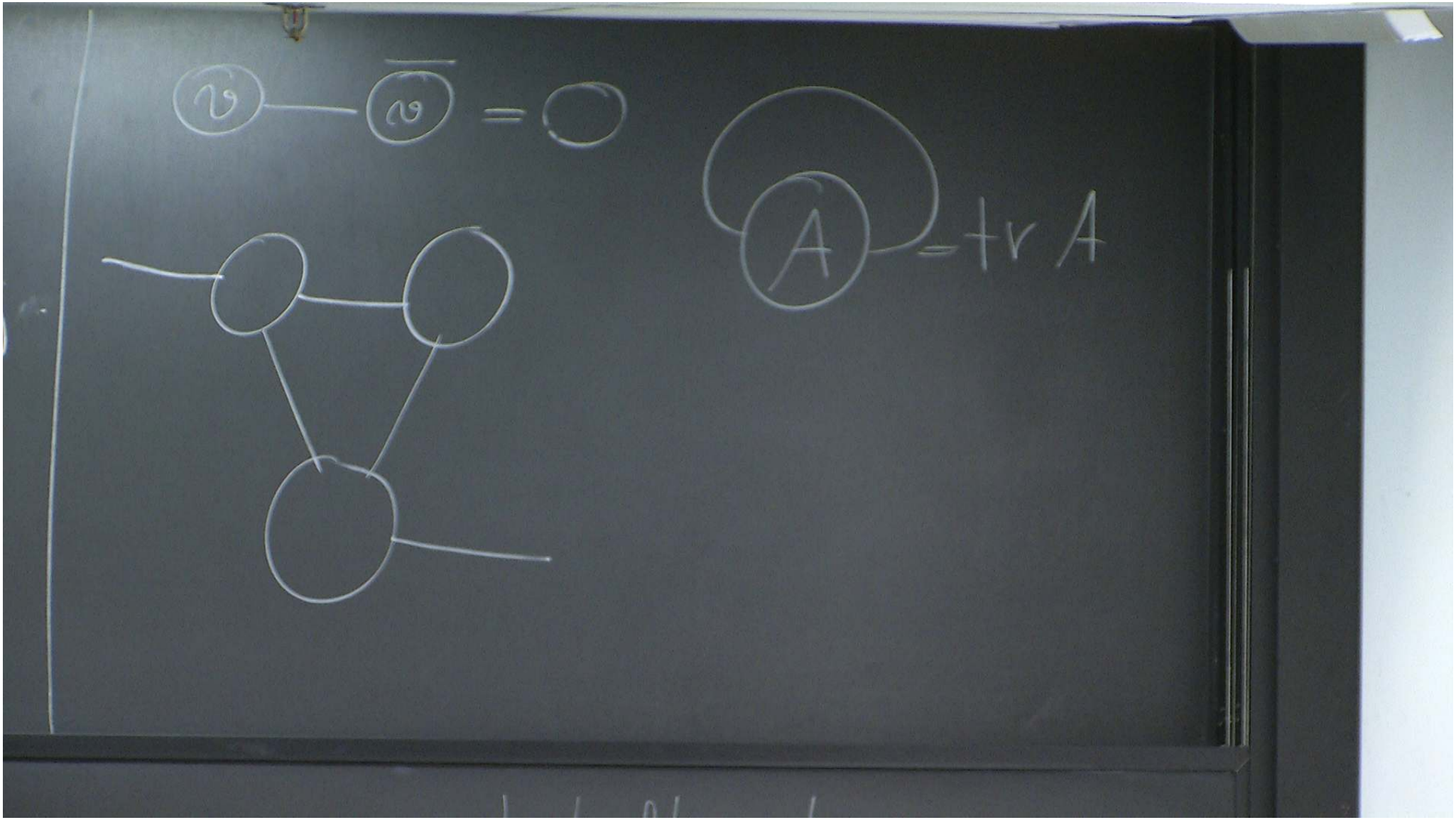
Date: May 08, 2023 - 9:30 AM

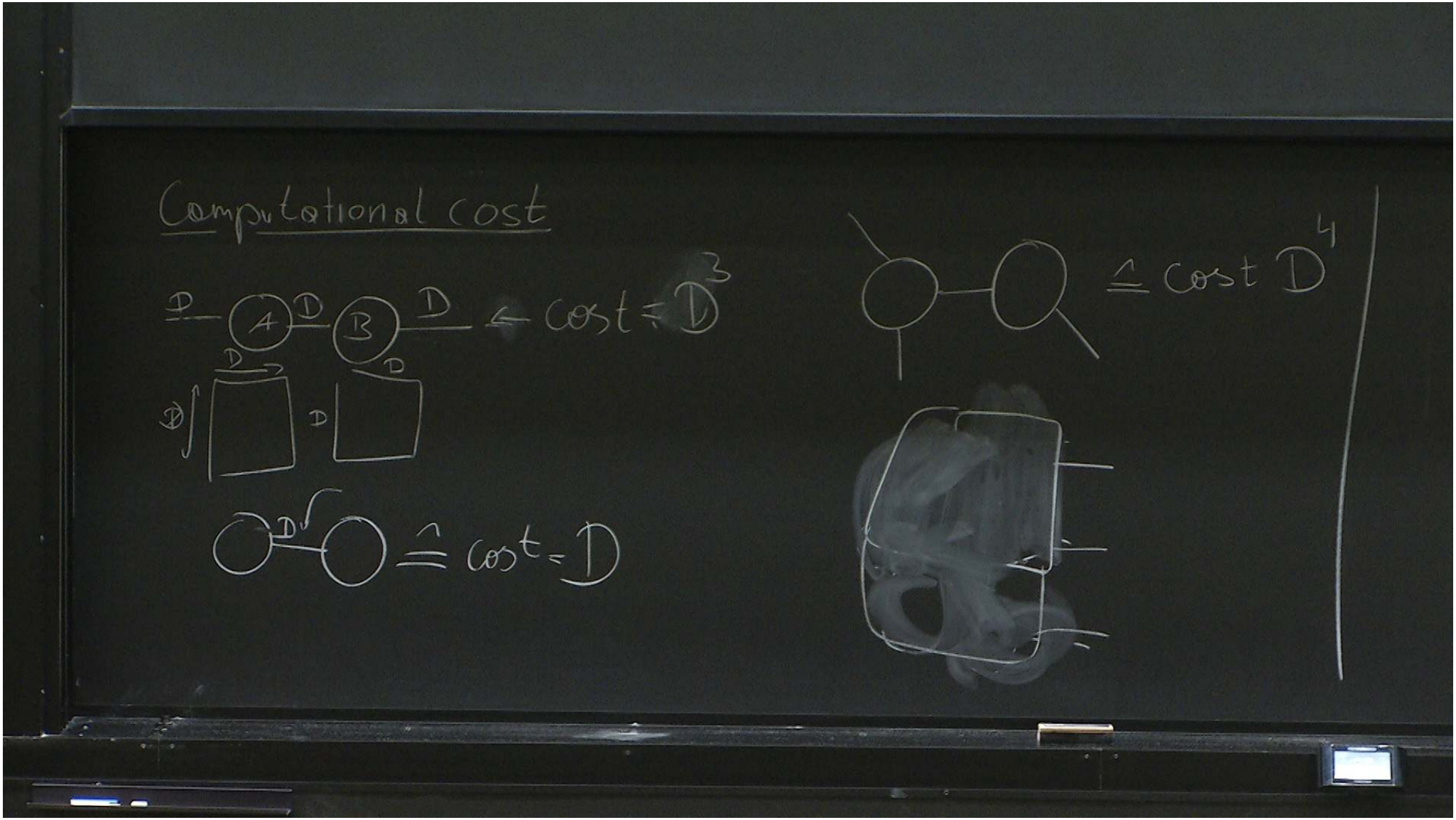
URL: https://pirsa.org/23050139

Abstract: TBC


Day 1
• many body wave functions
• density matrices
• entanglement
• matrix factorization
Day 2
• wave function truncation
• matrix product states (MPS)
• calculations with MPS
• Gauge-freedom of MPS
Day 3
• matrix product operators
• ground states: DMRG
• real time evolution
Day 4
• finite temperature
• other tensor networks
- PEPS
- MERA
Day 5
• applications of TN to ML
- supervised learning
- generative modelling
• numerical mathematics
- multivariate function encoding with MPS
- high dimensional integration
- PDEs
Left out.
- infinite quantum systems
- symmetries ("quantum numbers")
- advanced algos (TDVP, VUMPS...)
- numerics with PEPS, MERA
- continuous tensor networks

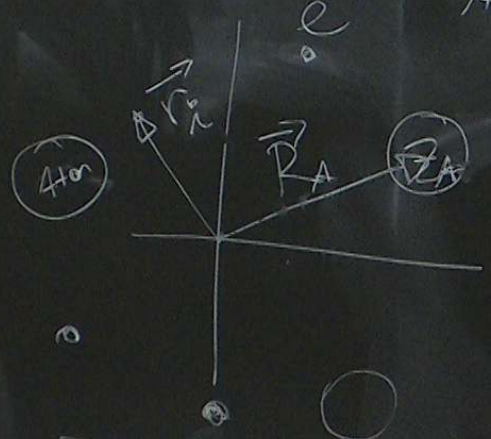

objects
≙ scalar
≙ vector
≙ matrix
≙ order 3 tensor
operations
matrix multiply: C = A B
$C_{ij} = \sum_{m=1}^{D} A_{im} B_{mj}$
A
m
B
A
A

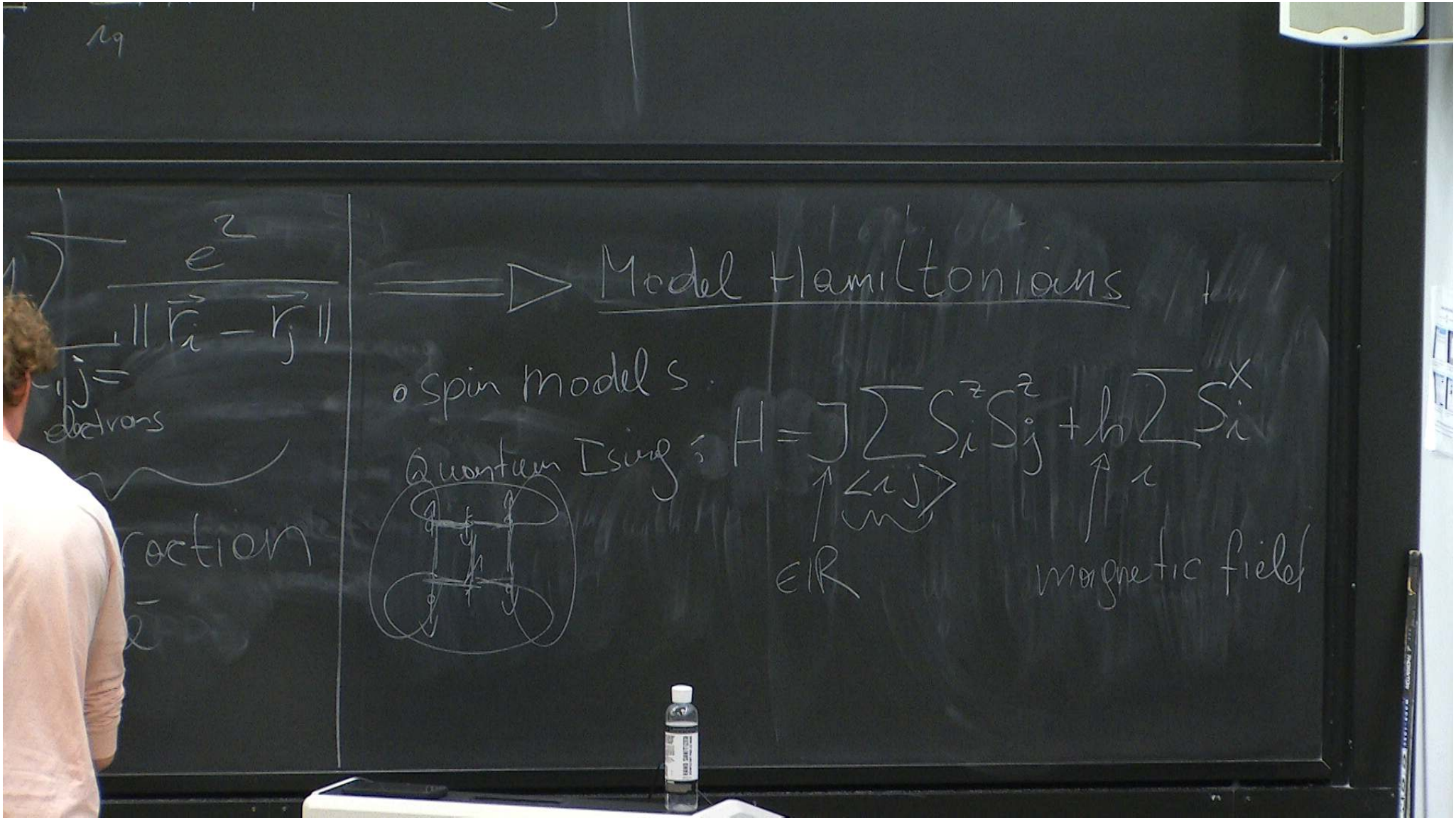

A
= tr A

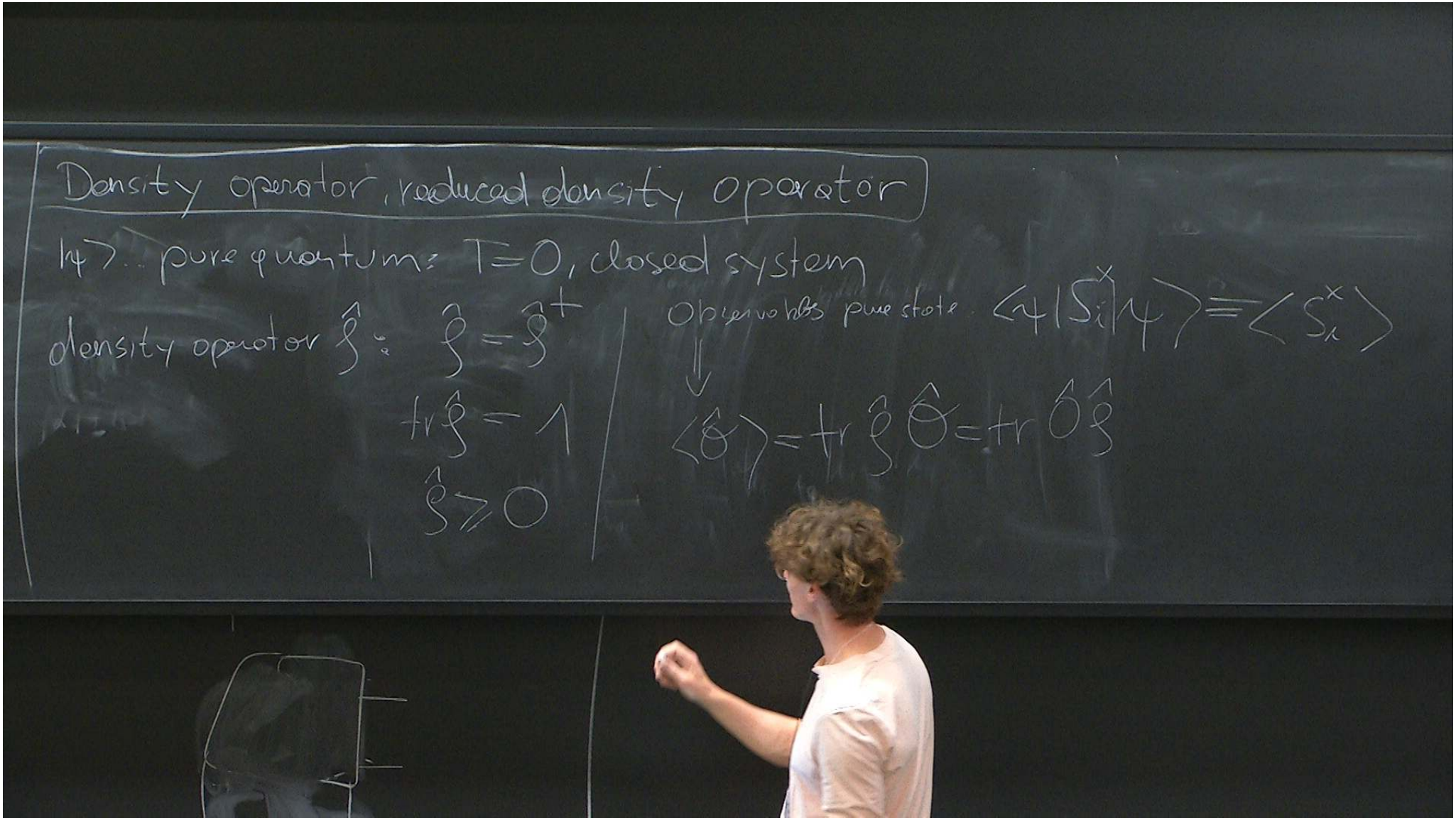

Computational cost
D
A
D
B
D
≤ cost · D³
D
D
D
D
≅ cost · D
≅ cost D⁴

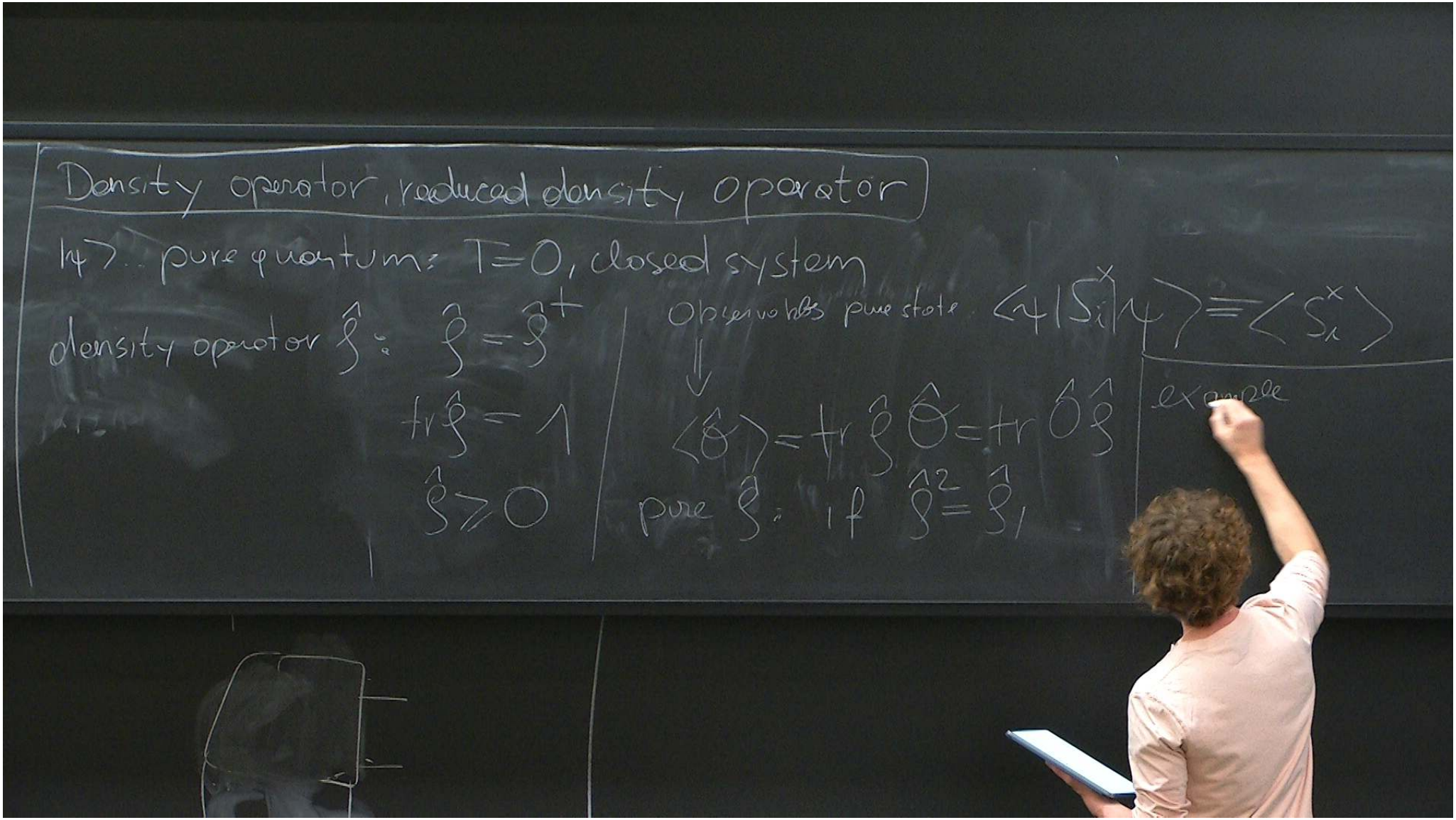
$$H = \sum_{i=\text{electron}} -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{\substack{i=\text{electron}\\ A=\text{nuclei}}} \frac{eZ_A}{\|R_A - r_i\|} + \frac{1}{2}\sum_{\substack{i,j=\\ \text{electrons}}} \frac{e^2}{\|\vec{r}_i - \vec{r}_j\|}$$

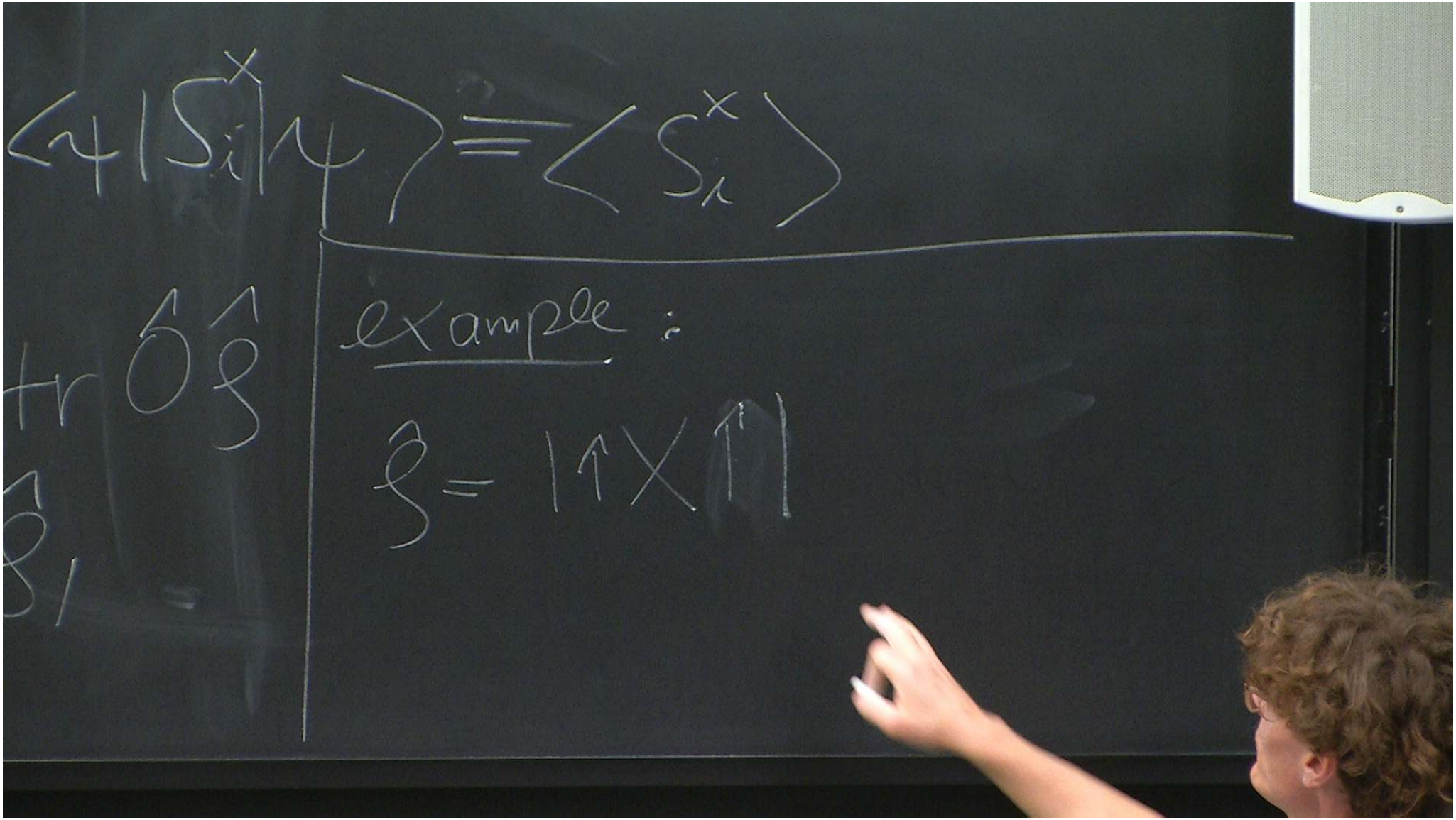
interaction of $\bar{e}$

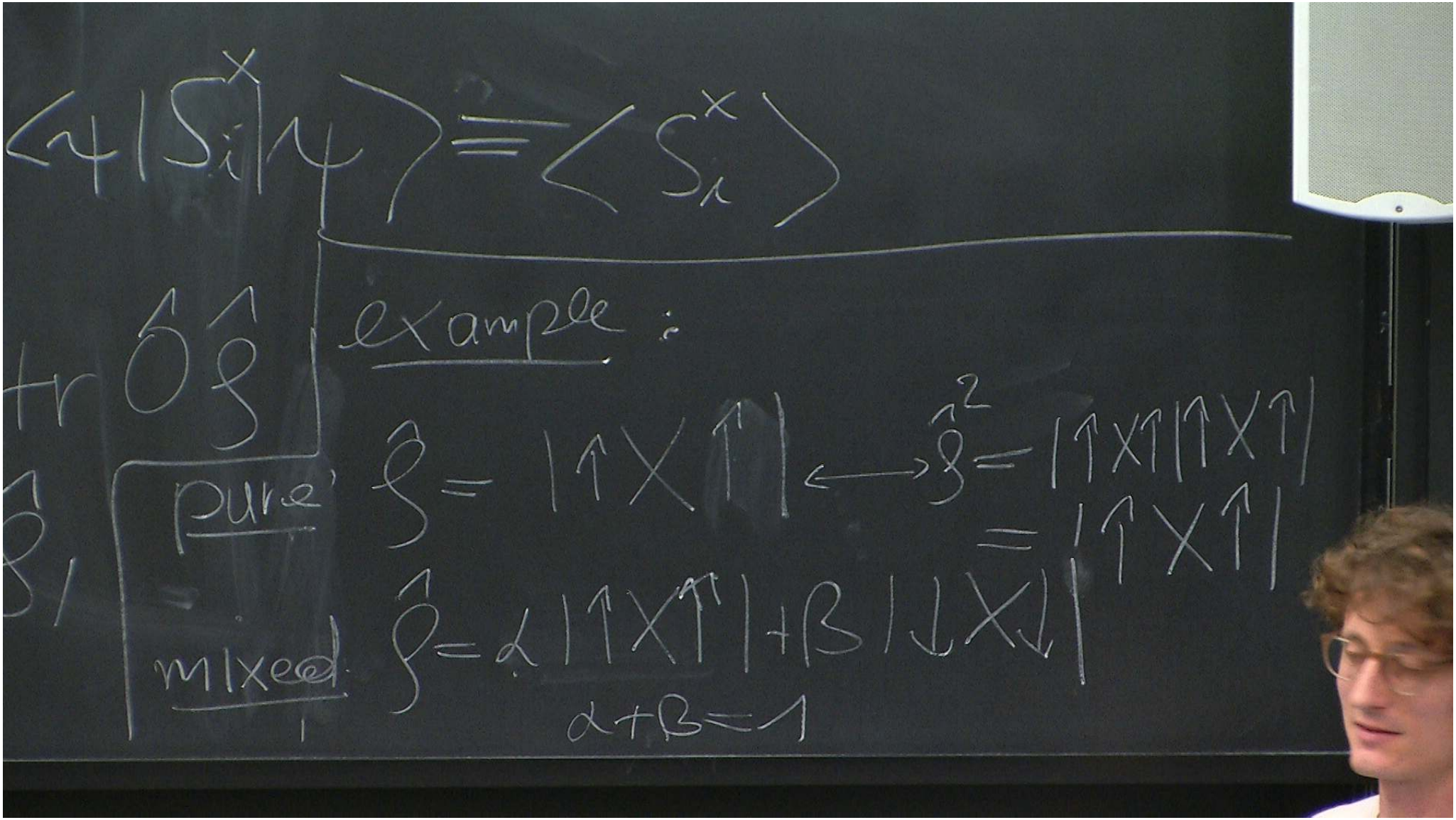


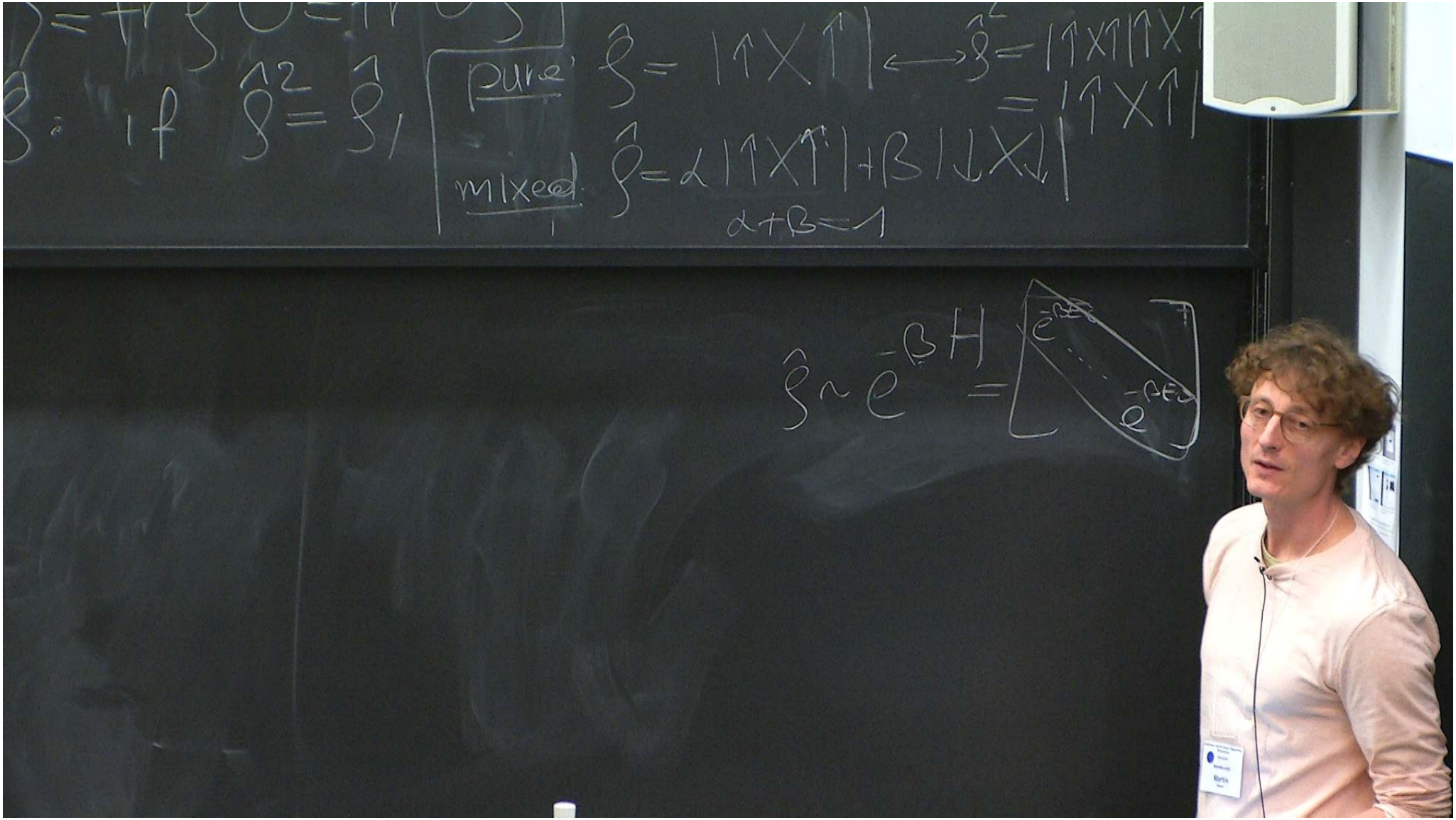

$\frac{e^2}{\|\vec{r}_i - \vec{r}_j\|}$
electrons
Model Hamiltonians
spin models.
Quantum Ising: $H = J\sum S_i^z S_j^z + h\sum S_i^x$
$\in \mathbb{R}$
magnetic field

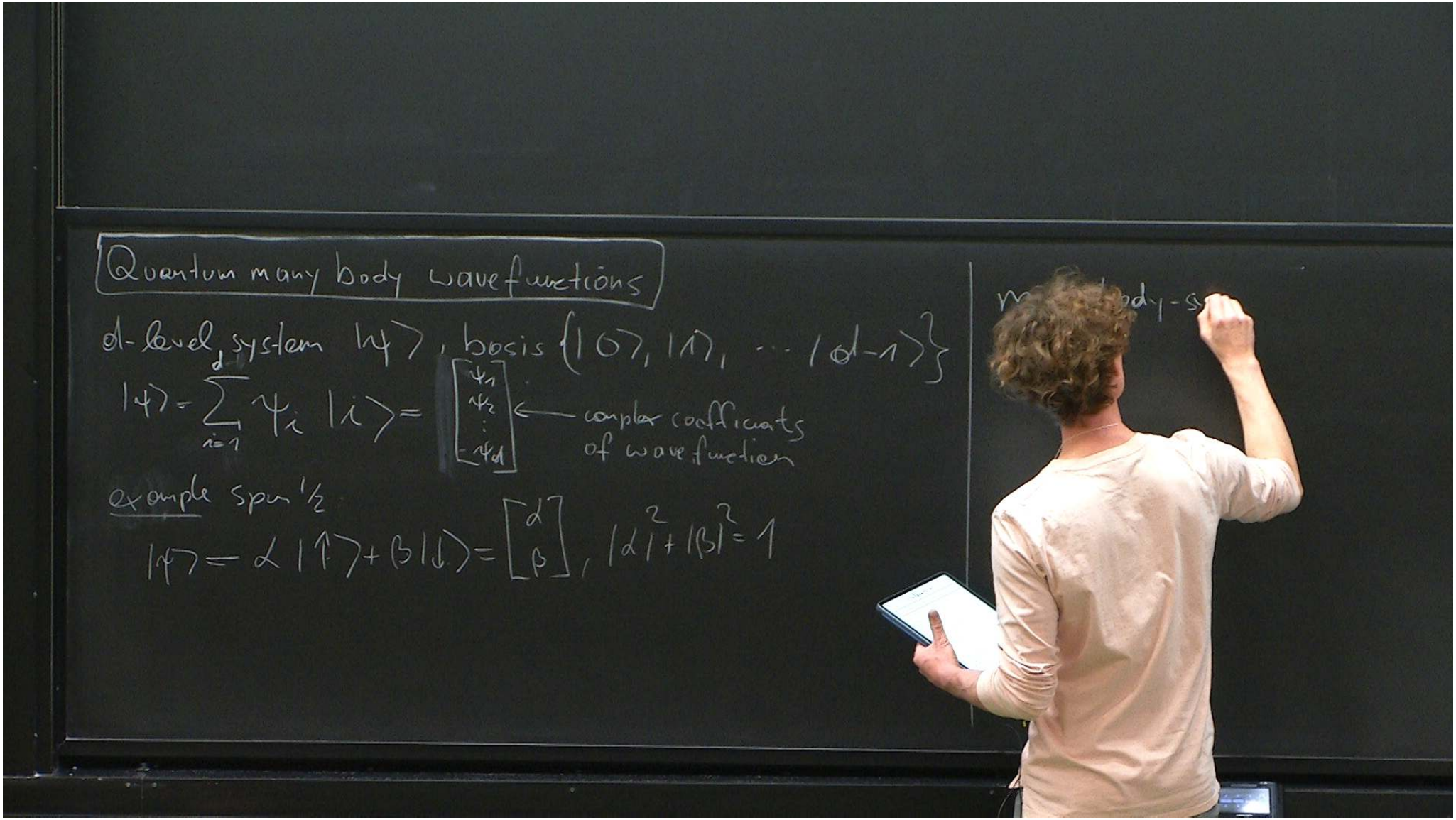

Density operator, reduced density operator
|ψ⟩ .. pure quantum: T=0, closed system
density operator $\hat{\rho}$: $\hat{\rho} = \hat{\rho}^+$
$\mathrm{tr}\hat{\rho} = 1$
$\hat{\rho} \geq 0$
observables pure state $\langle\psi|\hat{S}_i|\psi\rangle \equiv \langle S_i \rangle$
$\langle\hat{O}\rangle = \mathrm{tr}\,\hat{\rho}\hat{O} = \mathrm{tr}\,\hat{O}\hat{\rho}$

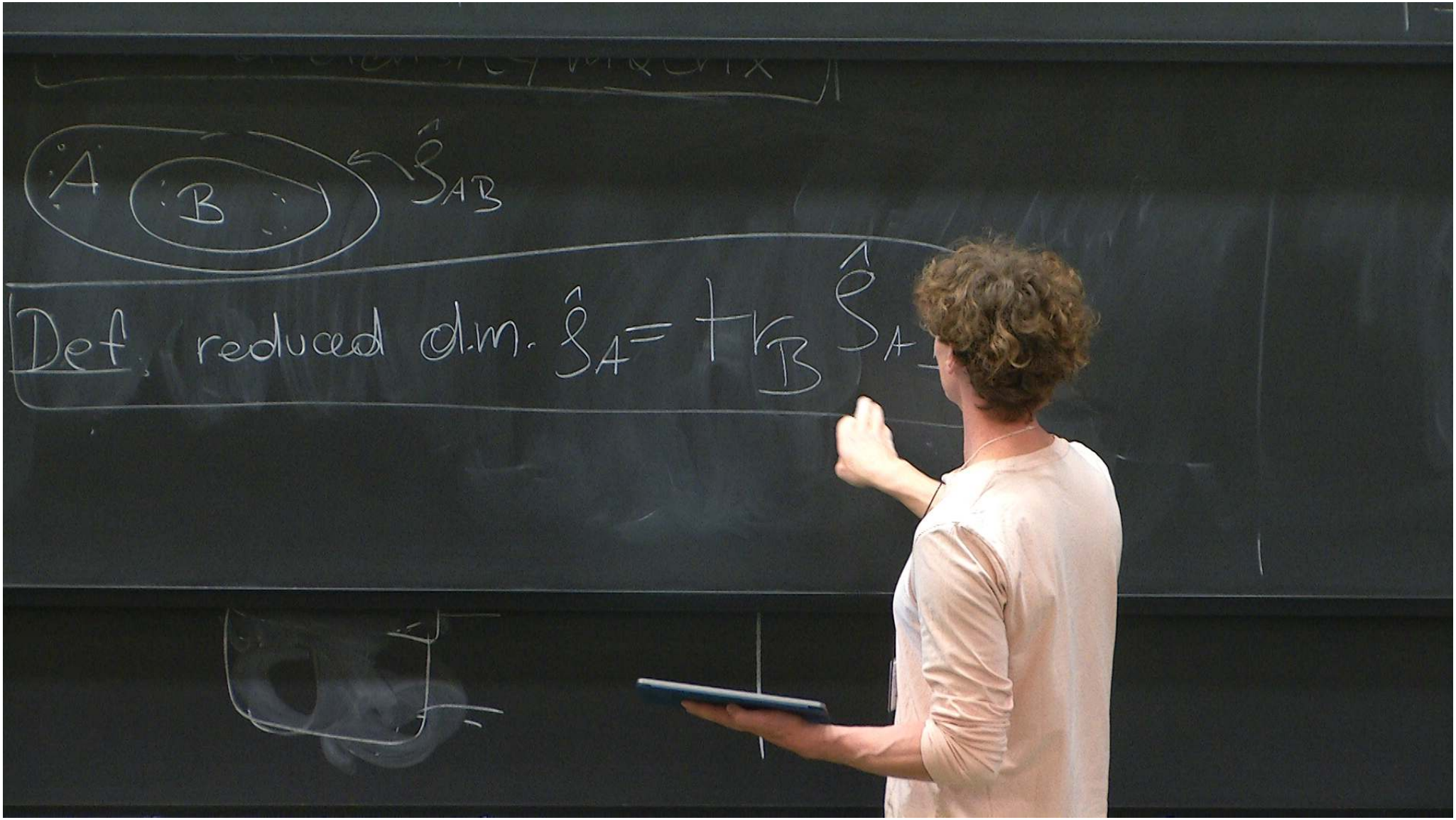

Density operator, reduced density operator
|ψ⟩ .. pure quantum: T=0, closed system
density operator ρ̂: ρ̂ = ρ̂†
tr ρ̂ = 1
ρ̂ ≥ 0
observables pure state ⟨ψ|Ŝ_i^x|ψ⟩ ≡ ⟨S_x^x⟩
⟨Ô⟩ = tr ρ̂ Ô = tr Ô ρ̂
pure ρ̂: if ρ̂² = ρ̂
example

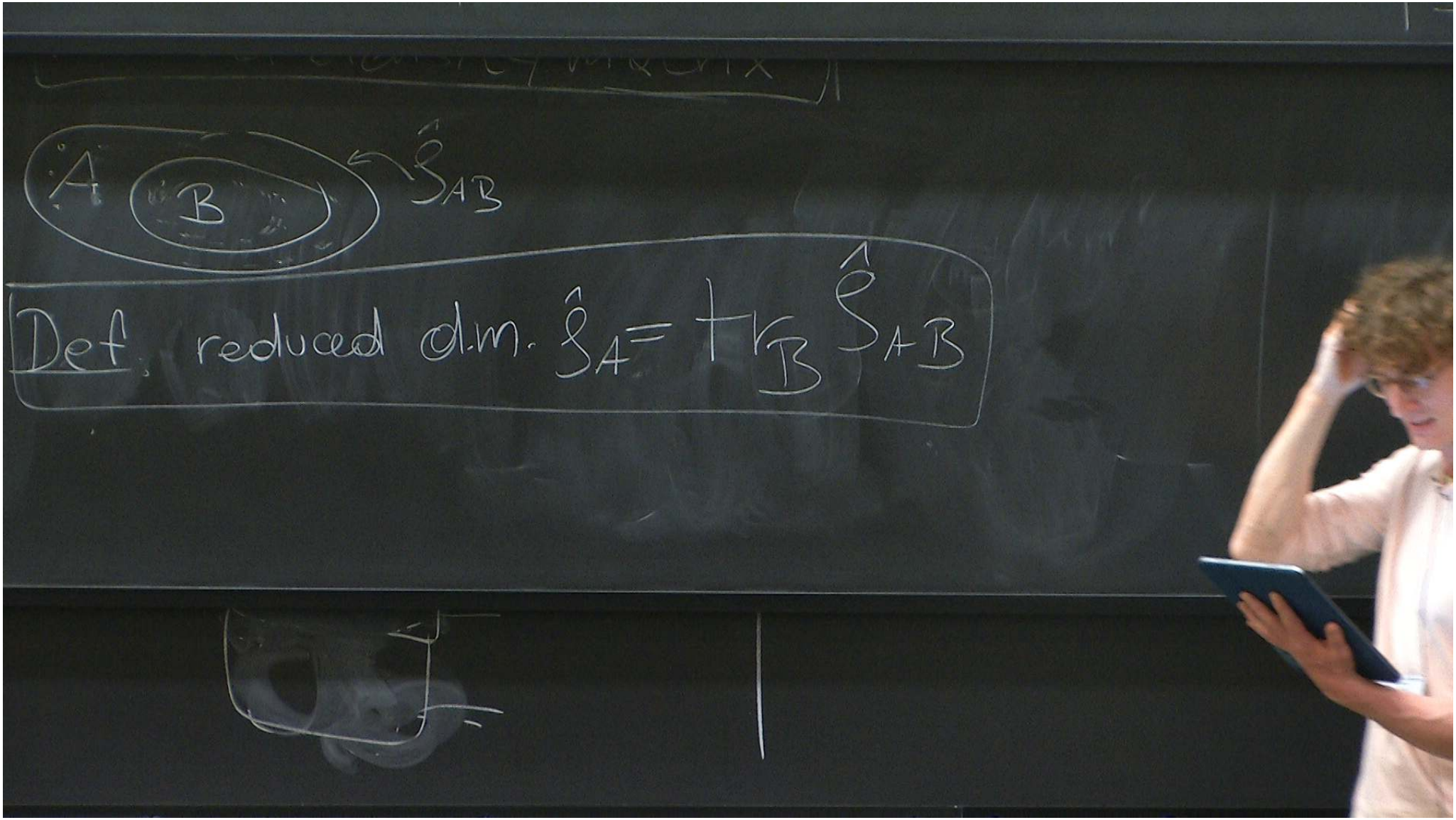

$\langle \psi | S_i^x | \psi \rangle \equiv \langle S_i^x \rangle$
$\mathrm{tr}\,\hat{O}\hat{\rho}$
example :
$\rho = |\uparrow\rangle\langle\uparrow| \otimes |\uparrow\rangle\langle\uparrow|$

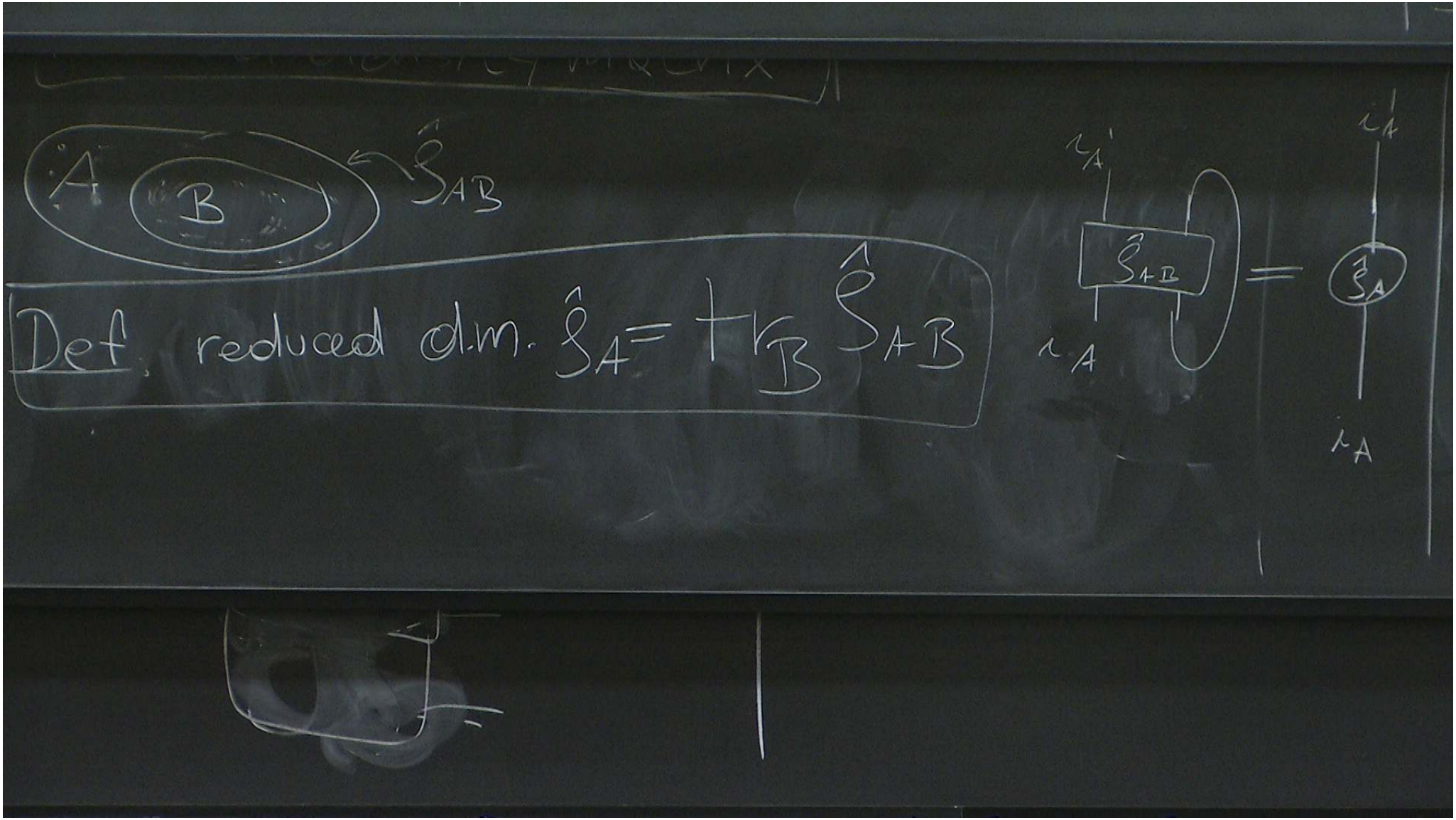

$\langle \psi | \hat{S}_x | \psi \rangle \equiv \langle S_x \rangle$
$\mathrm{tr}\,\hat{\rho}\hat{S}_x$
example :
pure
$\hat{\rho} = |\uparrow\rangle\langle\uparrow| \longleftrightarrow \hat{\rho}^2 = |\uparrow\rangle\langle\uparrow|\uparrow\rangle\langle\uparrow| = |\uparrow\rangle\langle\uparrow|$
mixed
$\hat{\rho} = \alpha\,|\uparrow\rangle\langle\uparrow| + \beta\,|\downarrow\rangle\langle\downarrow|$
$\alpha + \beta = 1$

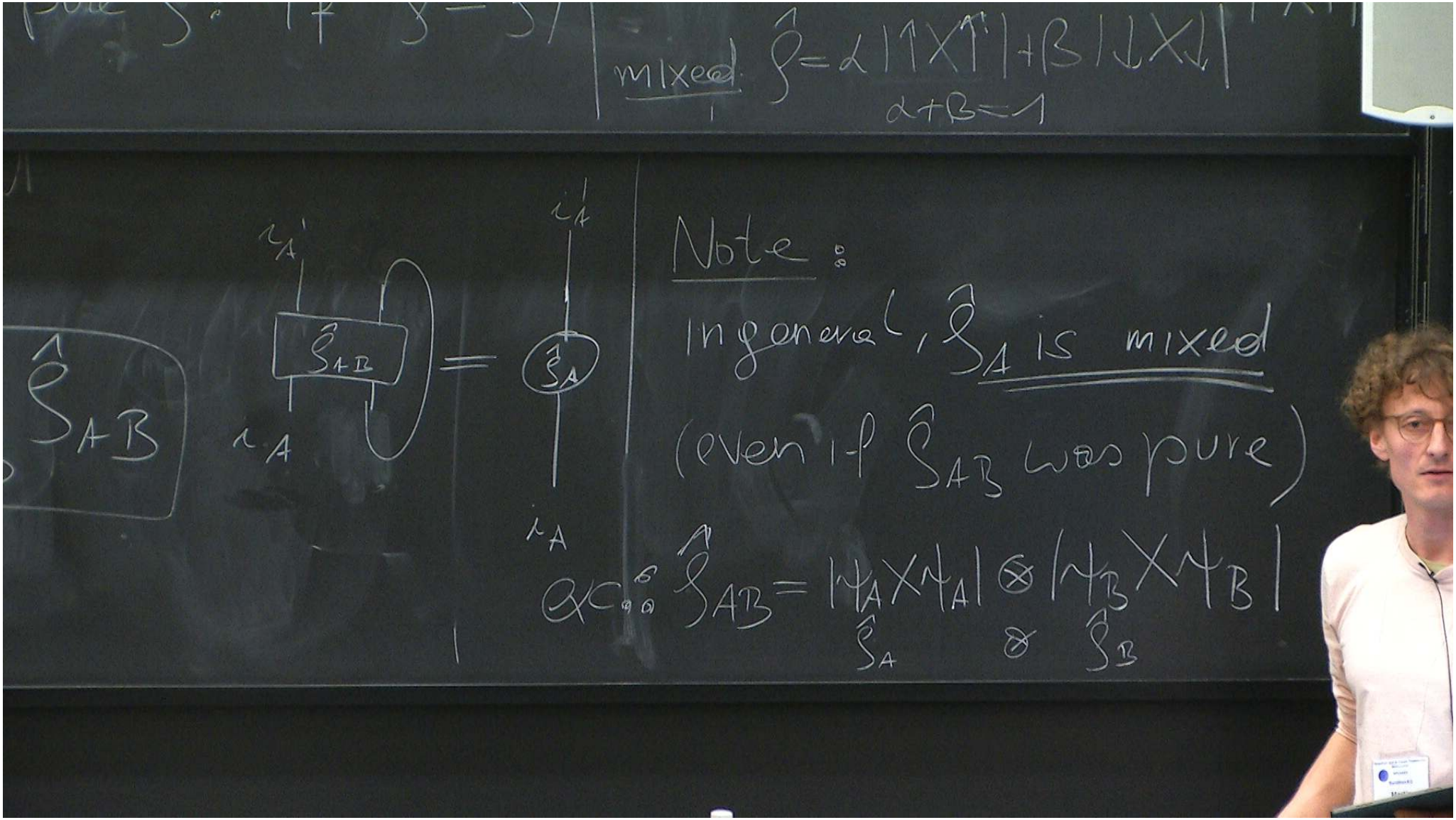

pure
mixed
α+β=1

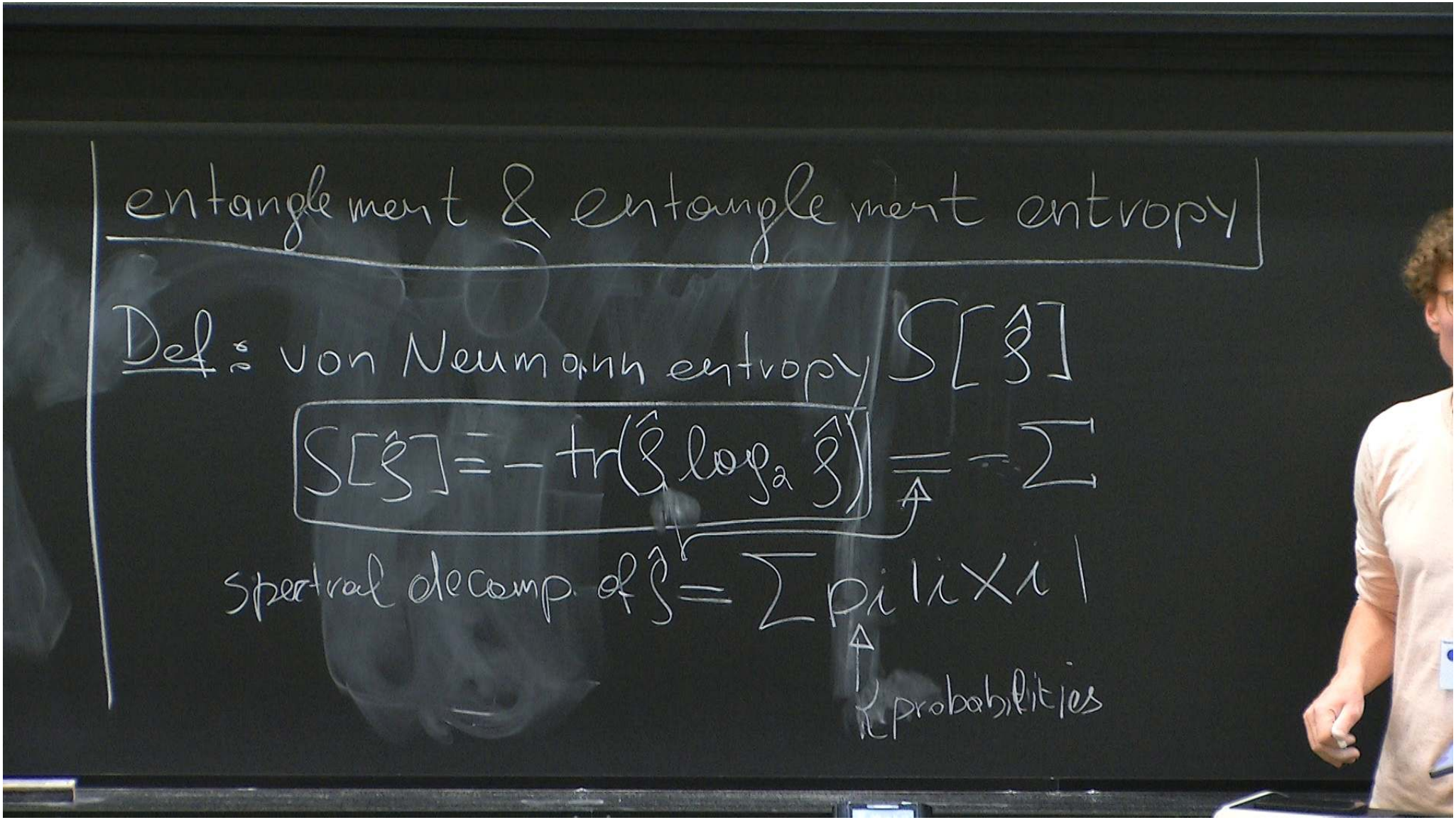

Quantum many body wavefunctions
d-level system $|\psi\rangle$, basis $\{|0\rangle, |1\rangle, \dots |d-1\rangle\}$
$|\psi\rangle = \sum_{i=1}^{d} \psi_i |i\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_d \end{bmatrix}$ ← complex coefficients of wavefunction
example spin 1/2
$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$, $|\alpha|^2 + |\beta|^2 = 1$

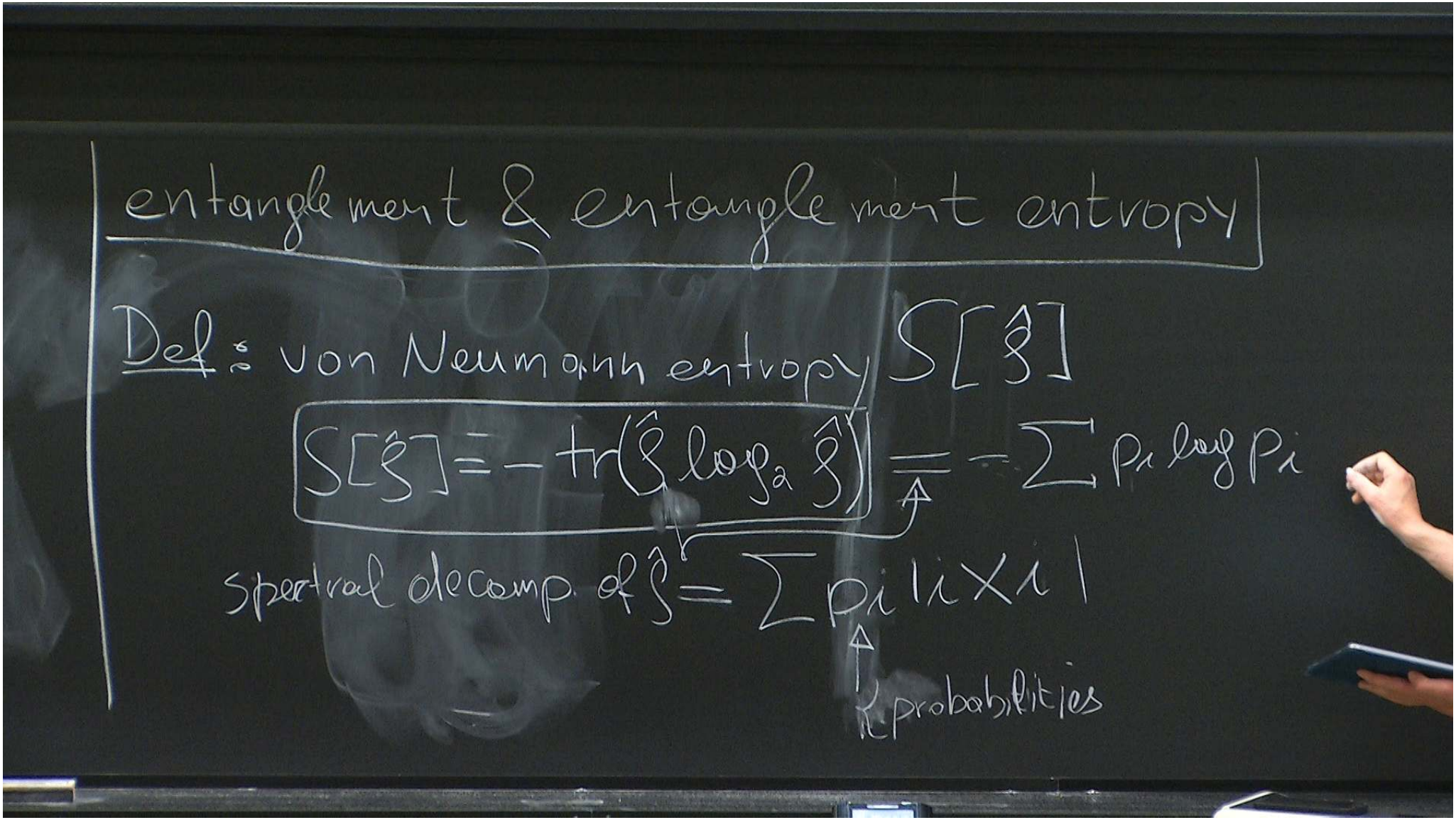

A
B
$\hat{\rho}_{AB}$
Def. reduced d.m. $\hat{\rho}_A = tr_B \hat{\rho}_{AB}$

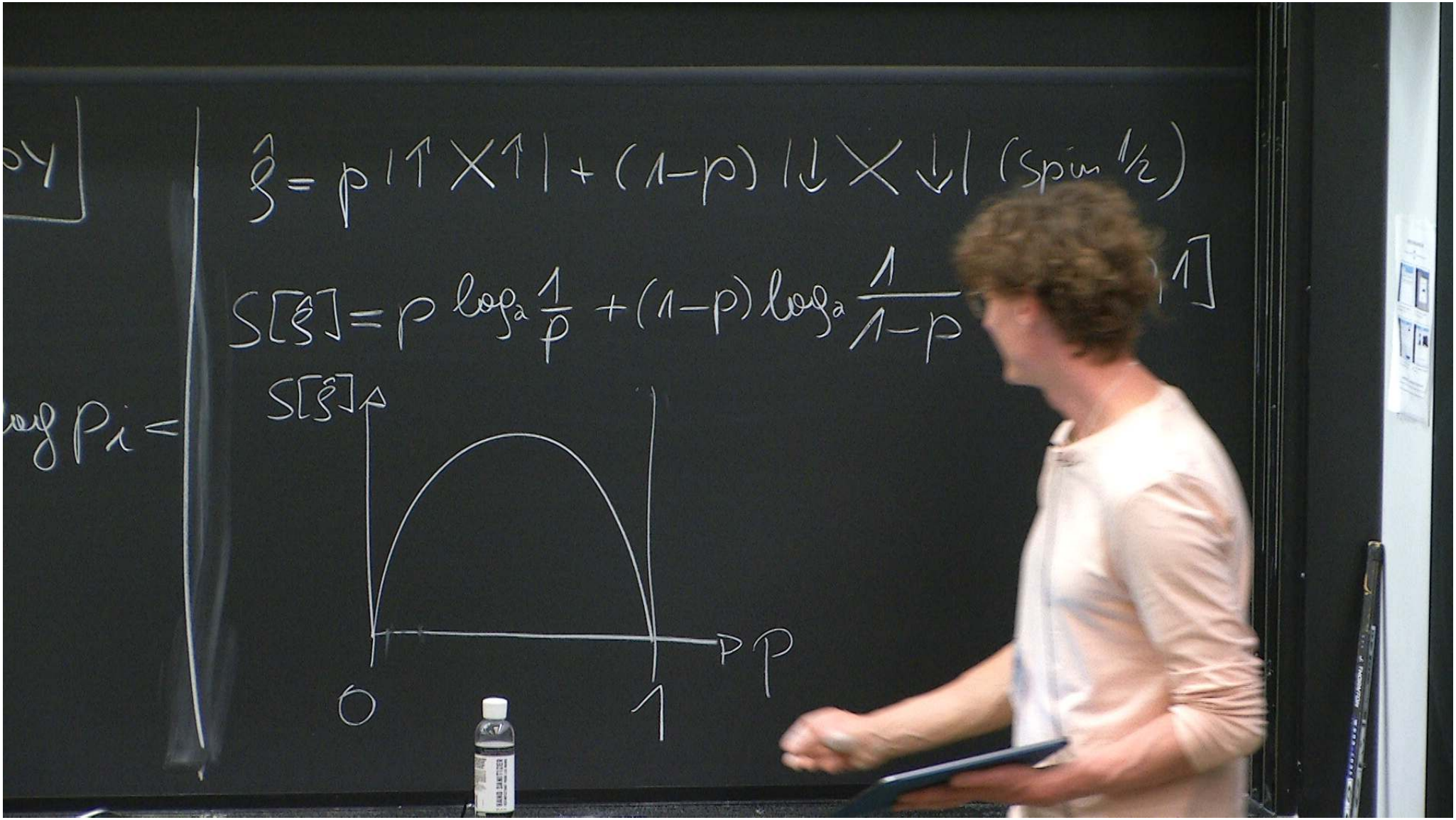

A
B
$\hat{\rho}_{AB}$
Def. reduced d.m. $\hat{\rho}_A = tr_B \hat{\rho}_{AB}$

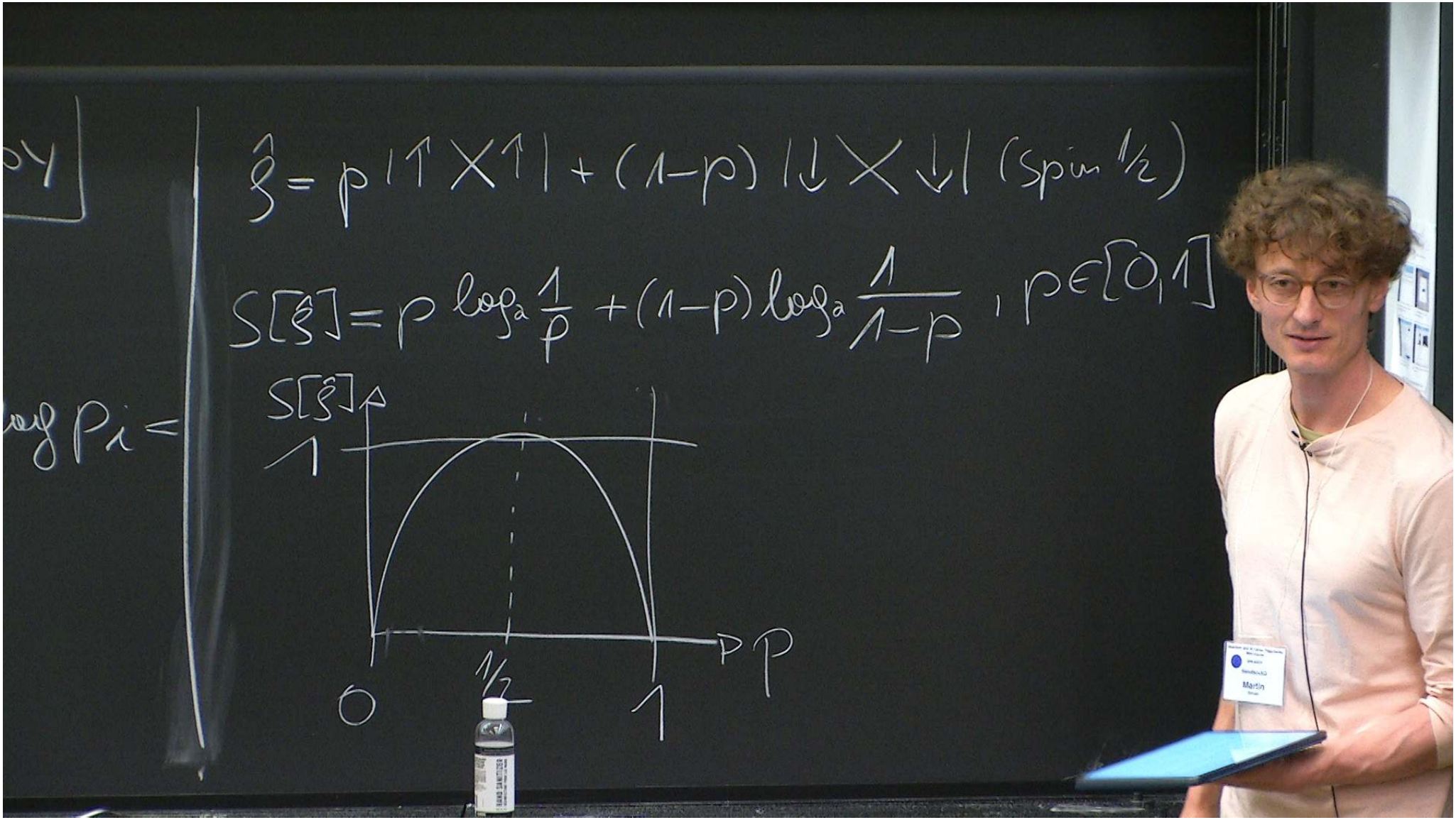

A
B
$\hat{\rho}_{AB}$
Def. reduced d.m. $\hat{\rho}_A = tr_B \hat{\rho}_{AB}$
$\mathcal{L}_A$
$\mathcal{L}_A$
$\hat{\rho}_{AB}$
=
$\mathcal{L}_A$
$\hat{\rho}_A$
$\mathcal{L}_A$

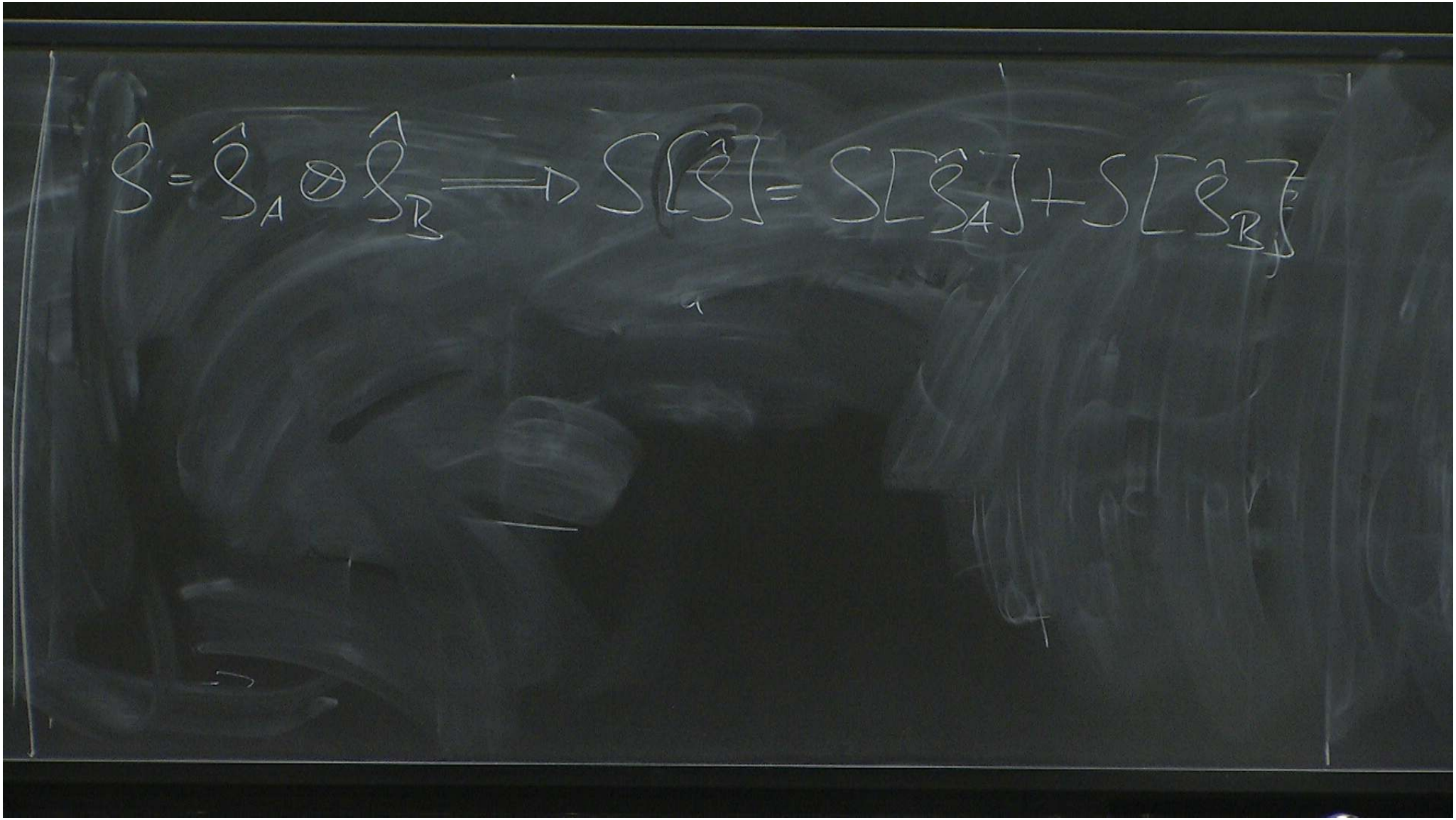

mixed: $\hat{\rho} = \alpha |\uparrow\rangle\langle\uparrow| + \beta |\downarrow\rangle\langle\downarrow|$
$\alpha + \beta = 1$
$\hat{\rho}_{AB}$
$\hat{\rho}_{AB}$
$\hat{\rho}_A$
$\hat{\rho}_A$
Note:
In general, $\hat{\rho}_A$ is mixed
(even if $\hat{\rho}_{AB}$ was pure)
e.g.: $\hat{\rho}_{AB} = |\psi_A\rangle\langle\psi_A| \otimes |\psi_B\rangle\langle\psi_B|$
$\hat{\rho}_A$ & $\hat{\rho}_B$


entanglement & entanglement entropy
Def: von Neumann entropy S[ρ̂]
S[ρ̂] = − tr(ρ̂ log₂ ρ̂) = − Σ
spectral decomp. of ρ̂ = Σ pᵢ |iᵢ⟩⟨iᵢ|
pᵢ probabilities


entanglement & entanglement entropy
Def: von Neumann entropy $S[\hat{\rho}]$
$S[\hat{\rho}] = -\mathrm{tr}(\hat{\rho}\log_2\hat{\rho}) = -\sum_i p_i \log p_i$
spectral decomp. of $\hat{\rho} = \sum_i p_i |i\rangle\langle i|$
p_i probabilities

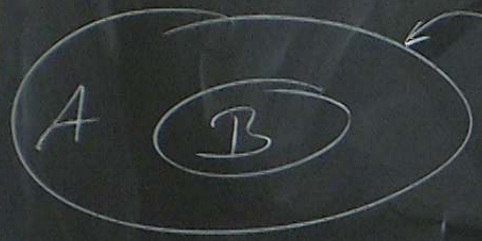

$\hat{\rho} = p\,|\uparrow\rangle\langle\uparrow| + (1-p)\,|\downarrow\rangle\langle\downarrow|$ (Spin 1/2)
$S[\hat{\rho}] = p \log_a \frac{1}{p} + (1-p) \log_a \frac{1}{1-p}$
$S[\hat{\rho}]$
p
0
1


$\hat{\rho} = p\,|\uparrow\rangle\langle\uparrow| + (1-p)\,|\downarrow\rangle\langle\downarrow|$ (spin 1/2)
$S[\hat{\rho}] = p \log_a \frac{1}{p} + (1-p) \log_a \frac{1}{1-p}$; $p \in [0,1]$
$S[\hat{\rho}]$
1
0
1/2
1
p
p


$\hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B \Longrightarrow S[\hat{\rho}] = S[\hat{\rho}_A] + S[\hat{\rho}_B]$

$\hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B \Longrightarrow S[\hat{\rho}] = S[\hat{\rho}_A] + S[\hat{\rho}_B]$

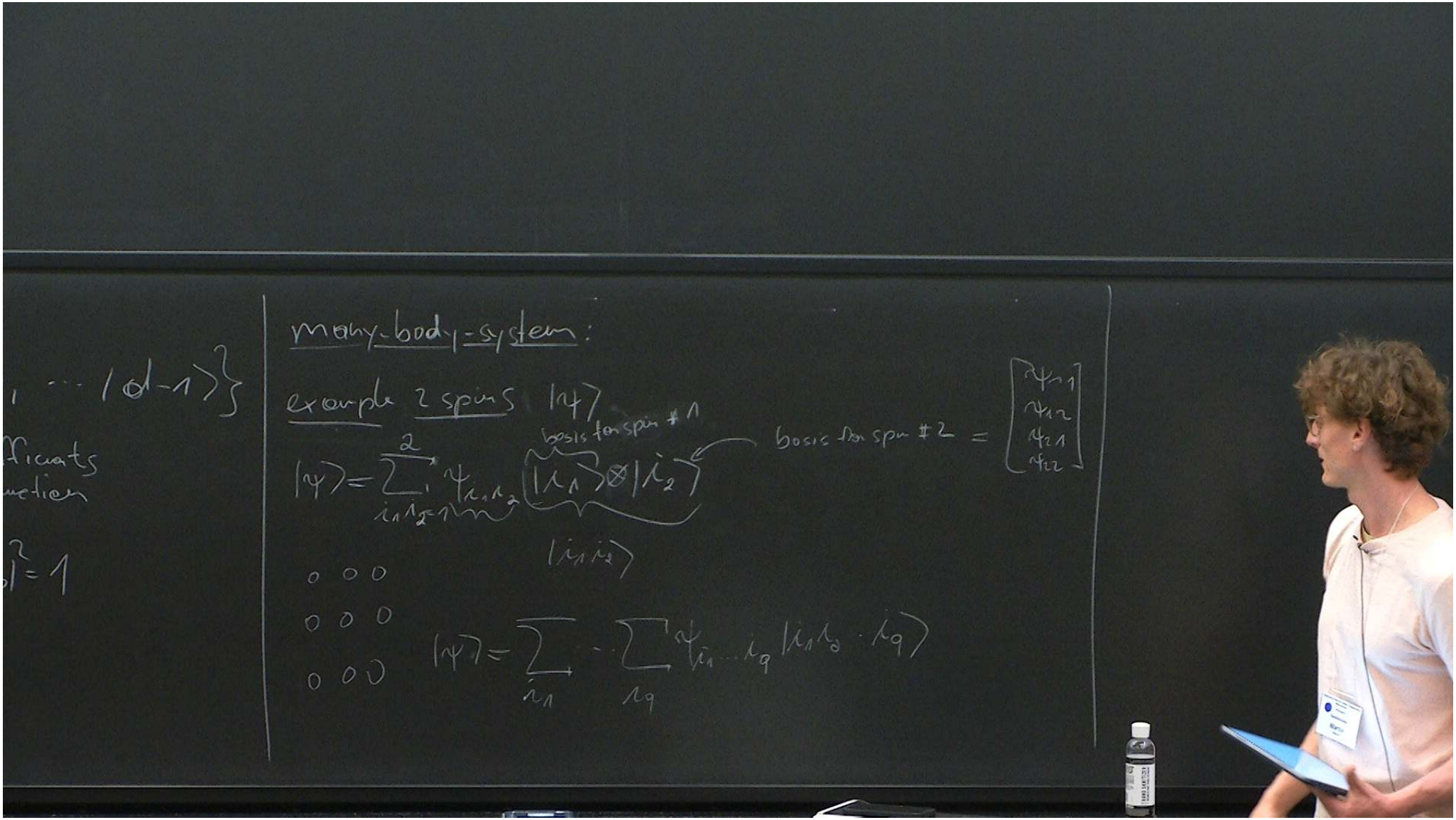
Def: entangled quantum systems

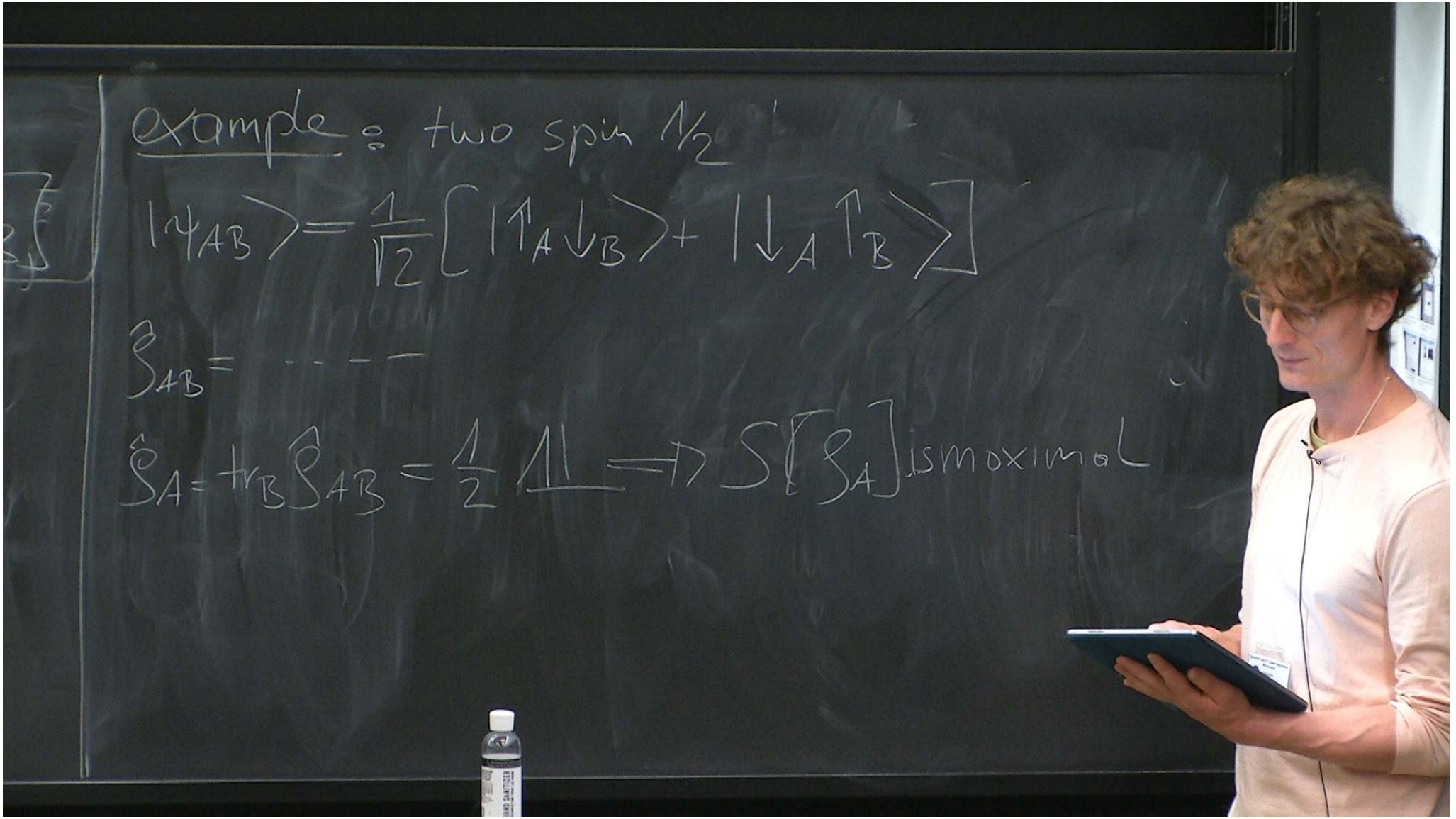


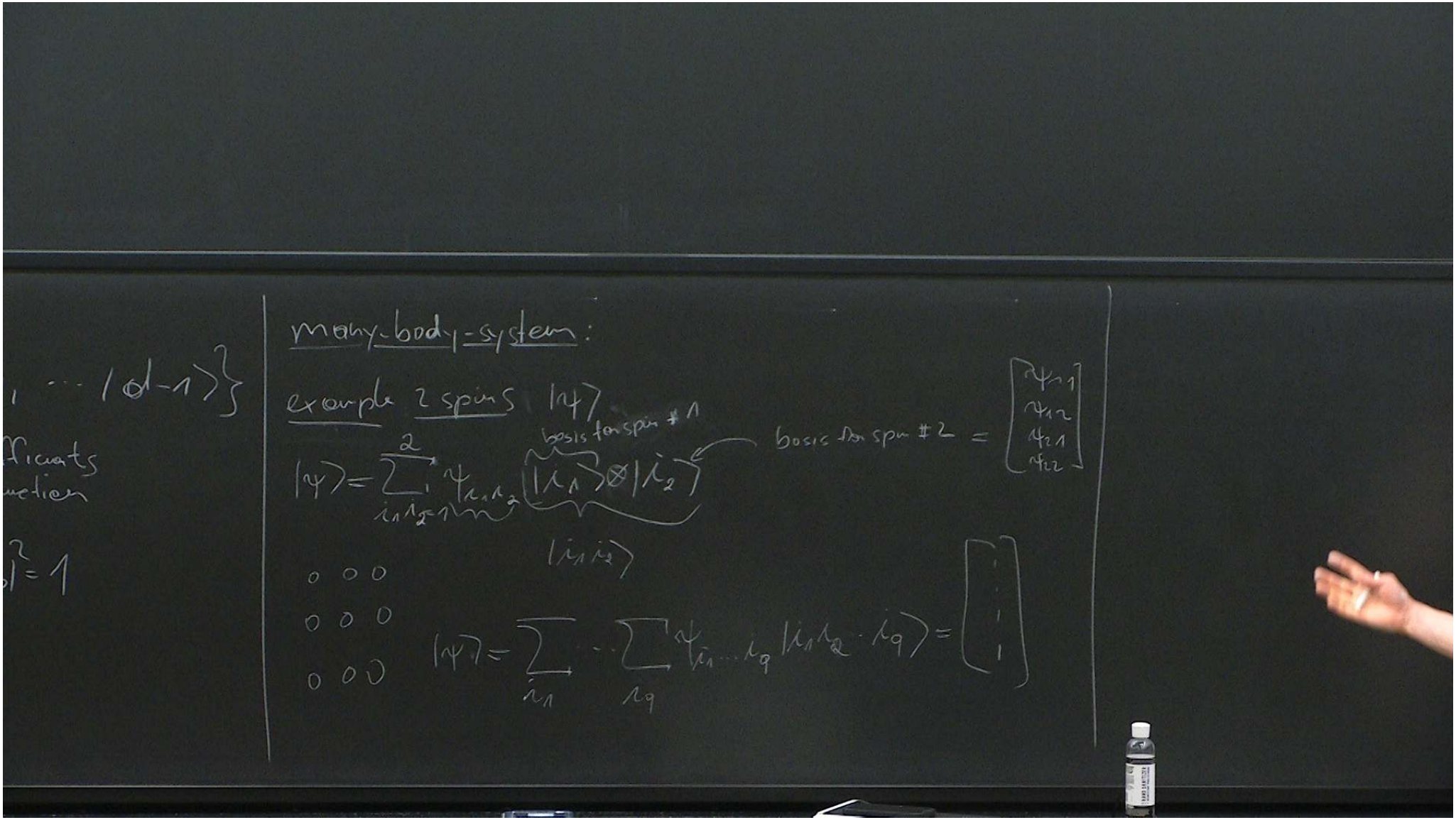
$|\psi_{AB}\rangle \Longrightarrow \hat{\rho}_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$

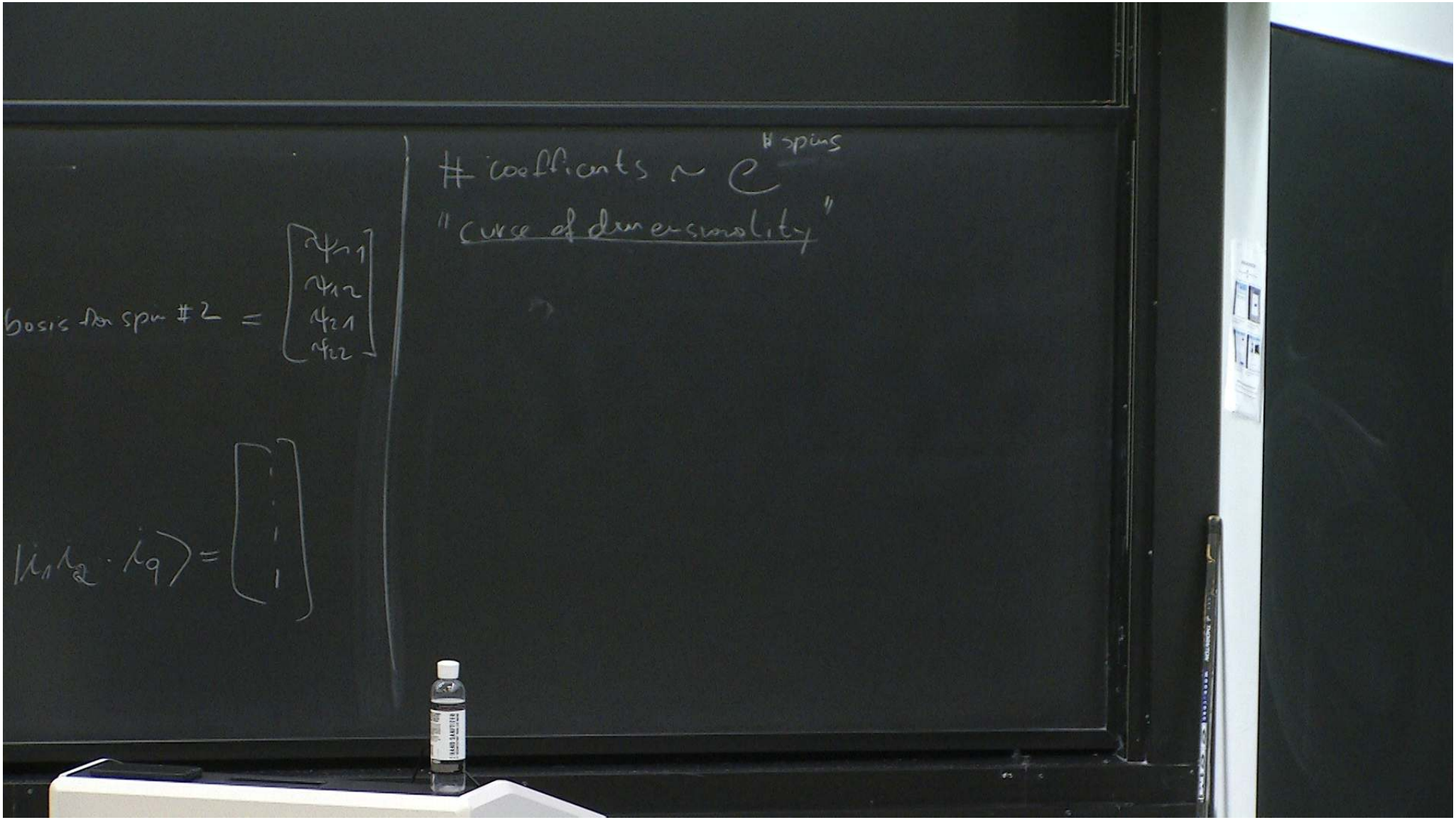
$\mathrm{tr}_B \hat{\rho}_{AB} = \hat{\rho}_A$, compute $S[\hat{\rho}_A] > 0$

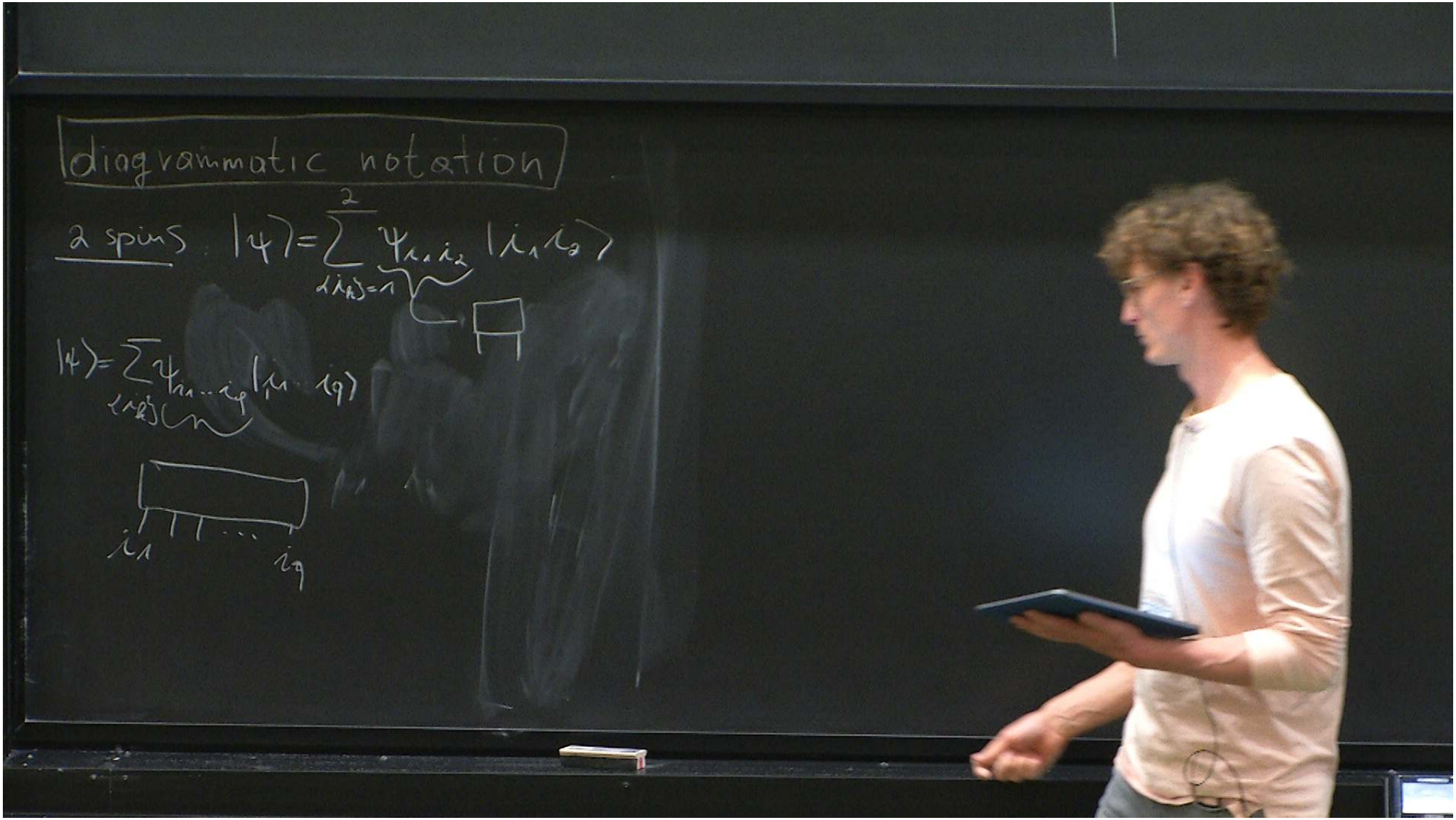
spectral decomp. of $\hat{\rho}_A = \sum_k p_k |k\rangle\langle k|$


many-body-system:
example 2 spins
basis for spin #1
basis for spin #2


example: two spin 1/2
$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow_A\downarrow_B\rangle + |\downarrow_A\uparrow_B\rangle\right]$
$\rho_{AB} = \ldots$
$\rho_A = \mathrm{tr}_B \rho_{AB} = \frac{1}{2}\mathbb{1} \Rightarrow S[\rho_A]$ is maximal


many-body-system:
example 2 spins
basis for spin #1
basis for spin #2


coefficients ~ e^(# spins)
"curse of dimensionality"
basis for spin #2 =
|↓↓⋯↓⟩ =


diagrammatic notation
2 spins
$|\psi\rangle = \sum_{\lambda_1,\lambda_2=1}^{2} \psi_{\lambda_1,\lambda_2} |\lambda_1,\lambda_2\rangle$
$|\psi\rangle = \sum_{\lambda_1,\ldots,\lambda_q=1}^{n} \psi_{\lambda_1\ldots\lambda_q} |\lambda_1 \ldots \lambda_q\rangle$
i_1
i_q

objects

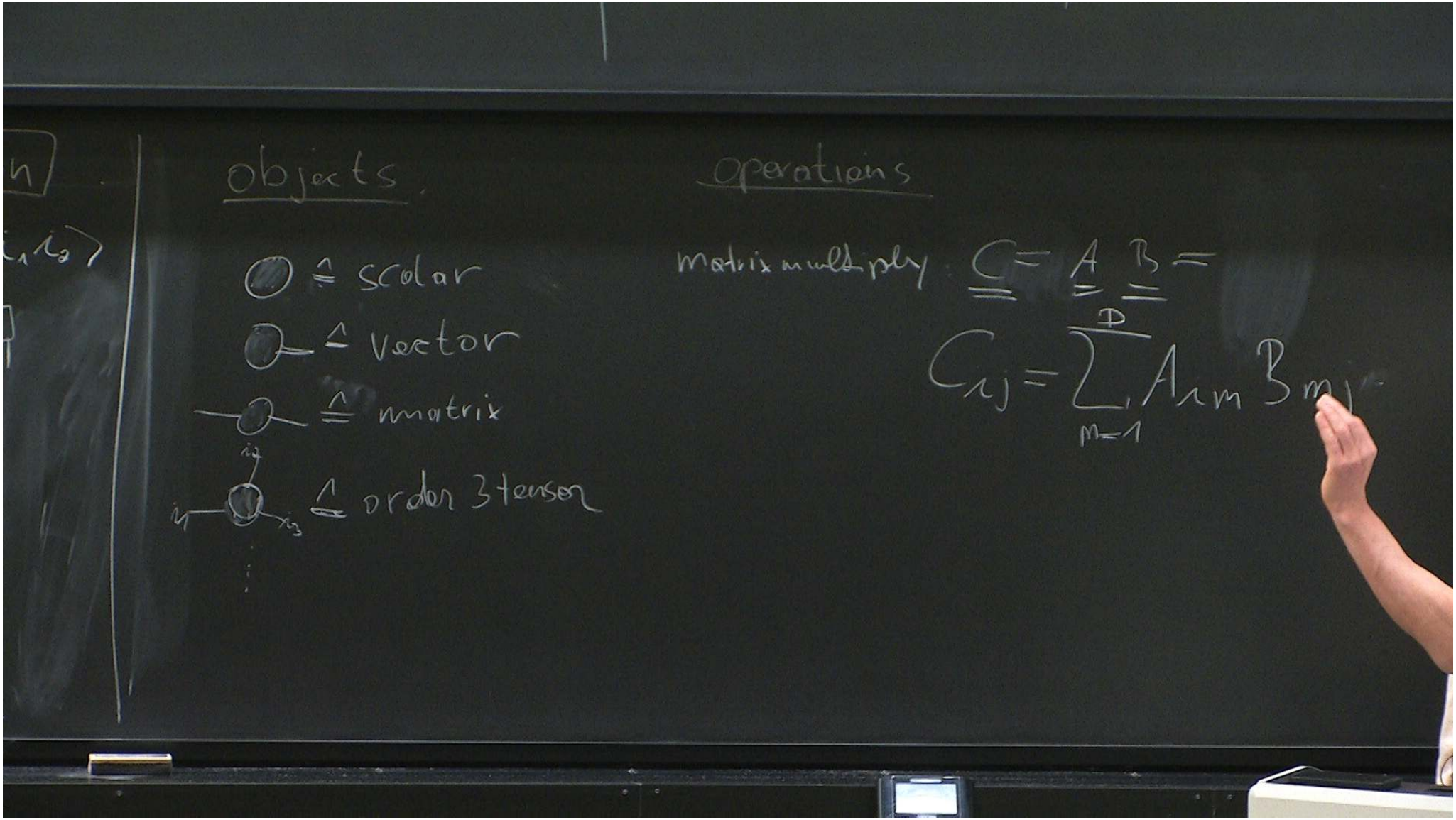
operations

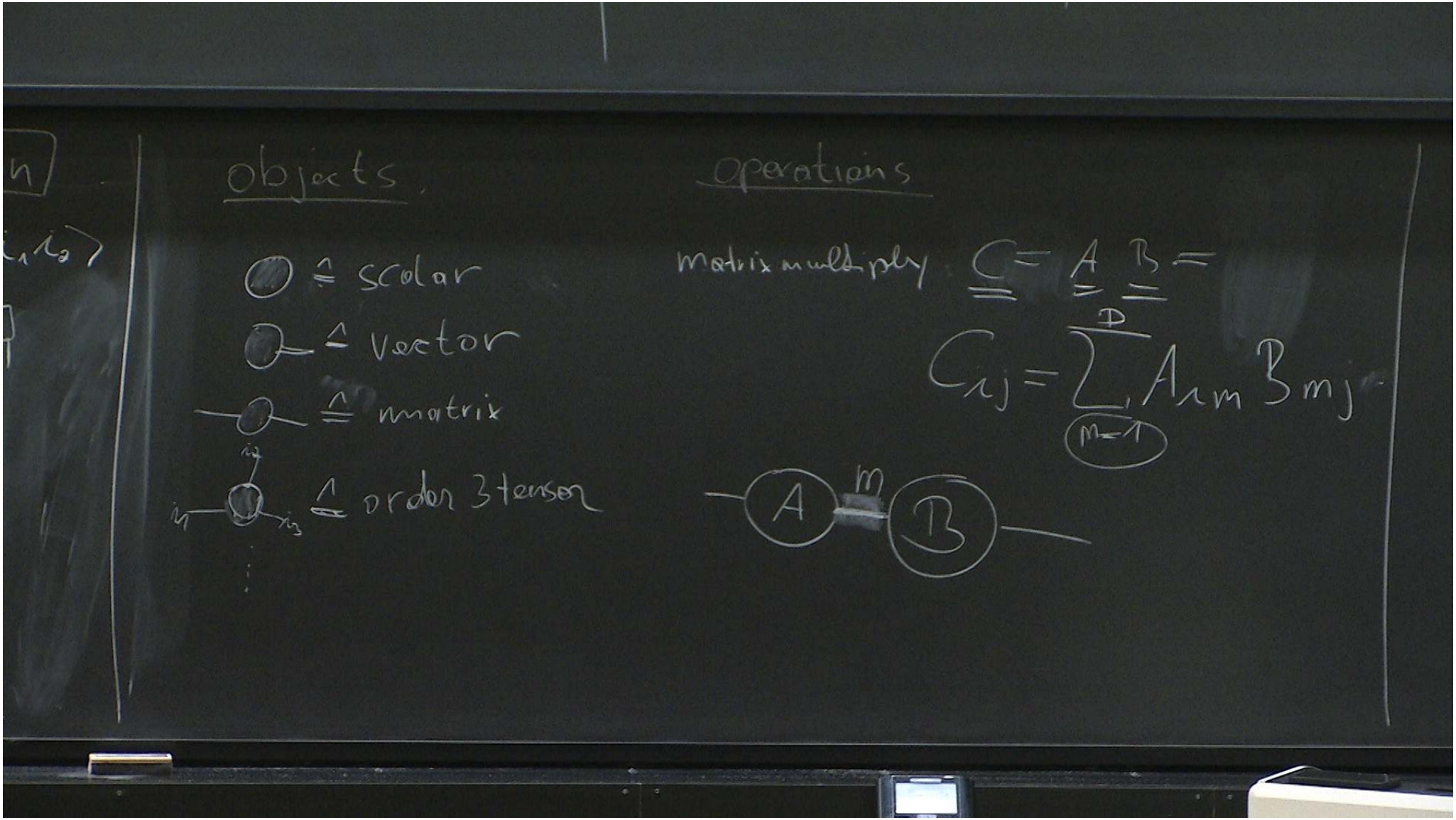
≙ scalar

≙ vector

≙ matrix

≙ order 3 tensor


objects
operations
≙ scalar
≙ vector
≙ matrix
≙ order 3 tensor
matrix multiply
$\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}}$
$C_{ij} = \sum_{m=1}^{D} A_{im} B_{mj}$


objects
operations
≙ scalar
≙ vector
≙ matrix
≙ order 3 tensor
matrix multiply
$\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}}$
$C_{ij} = \sum_{m=1}^{D} A_{im} B_{mj}$
A
m
B

MERA
Numerical Mathematics
– multivariate function encoding with MPS
– high dimensional integration
– PDEs
– numerics with PEPS, MERA
– continuous Tensor networks