Title: LECTURE: Tensor networks and quantum simulations

Speakers: Martin Ganahl

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

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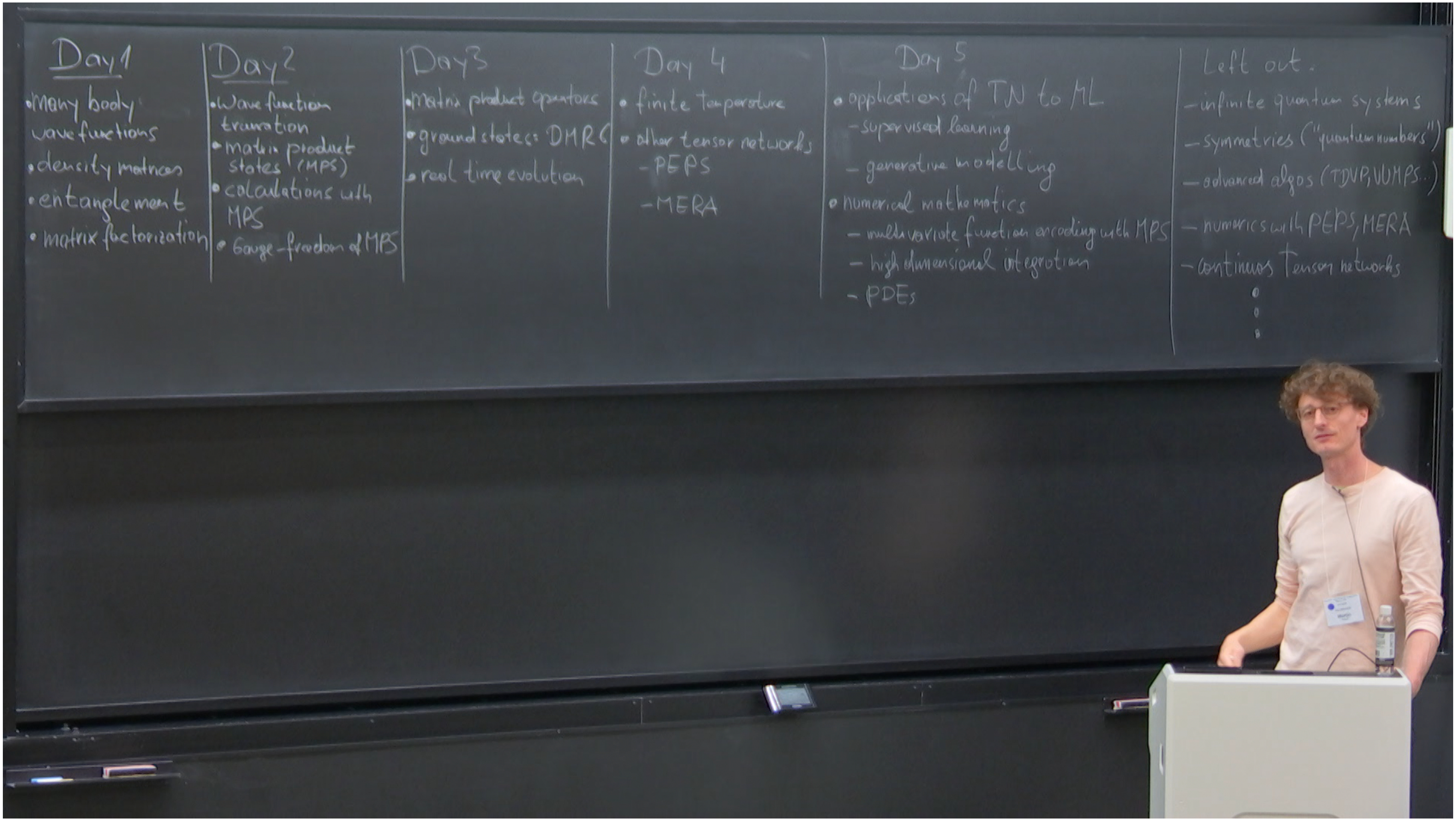
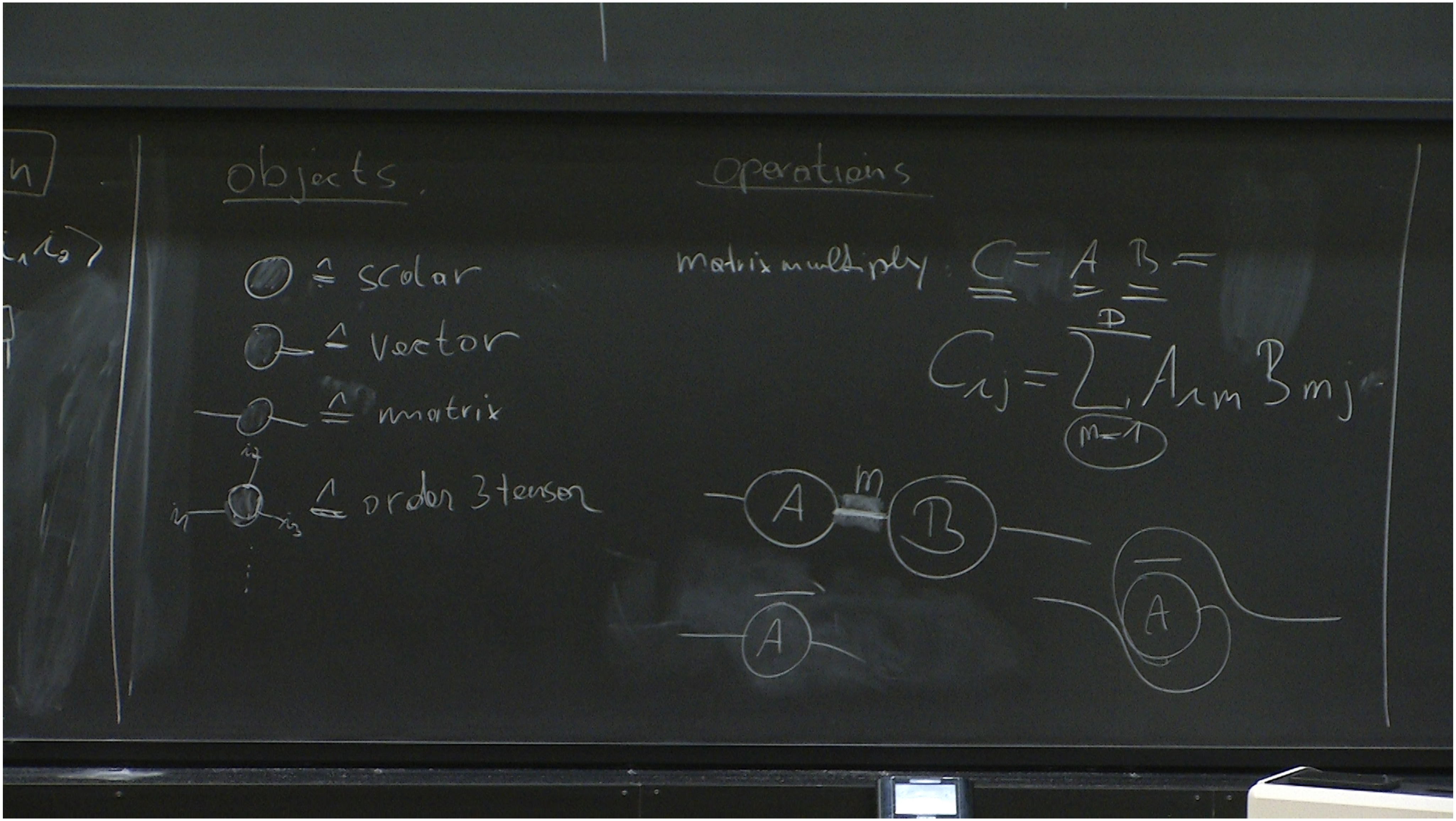
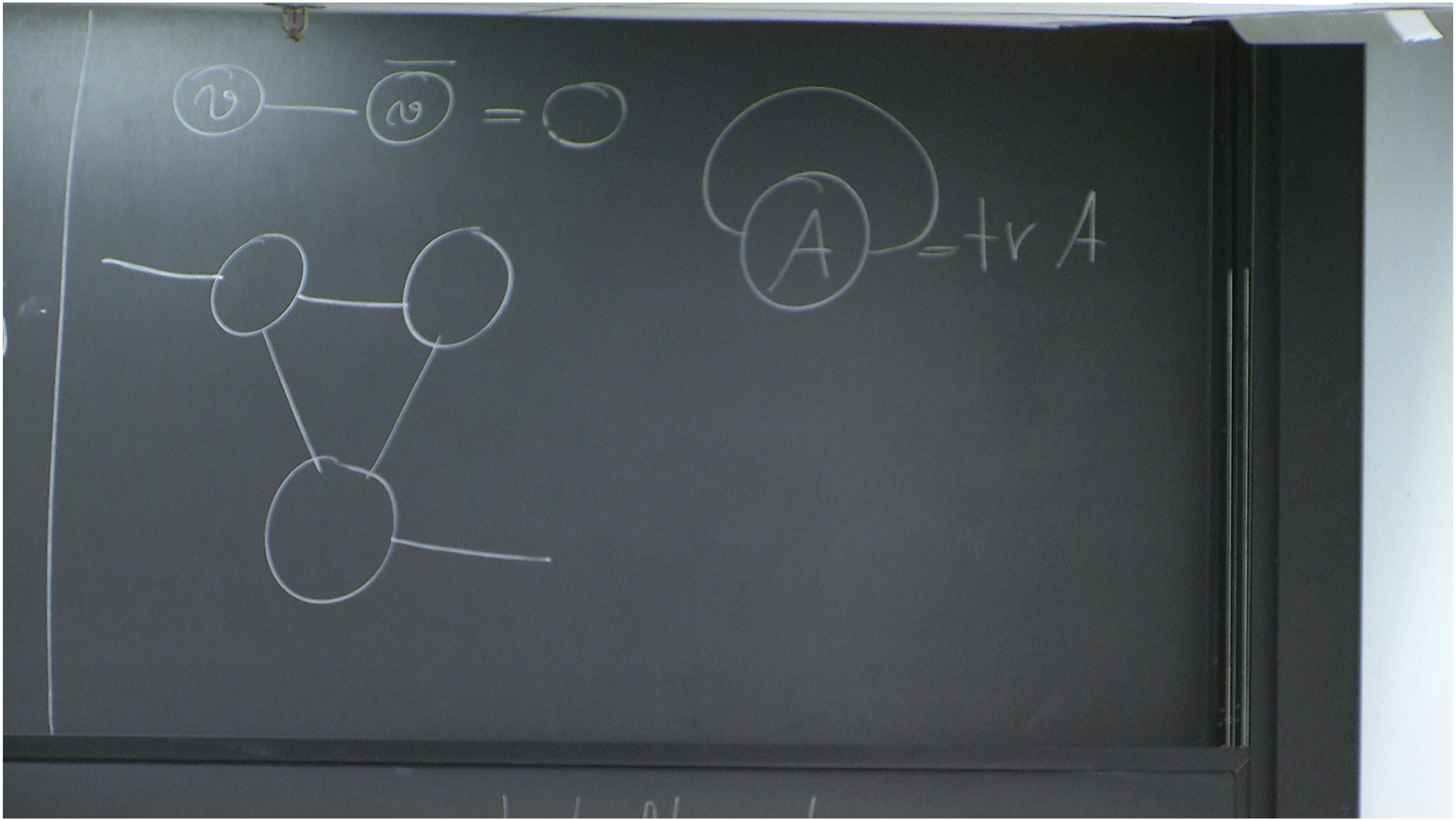
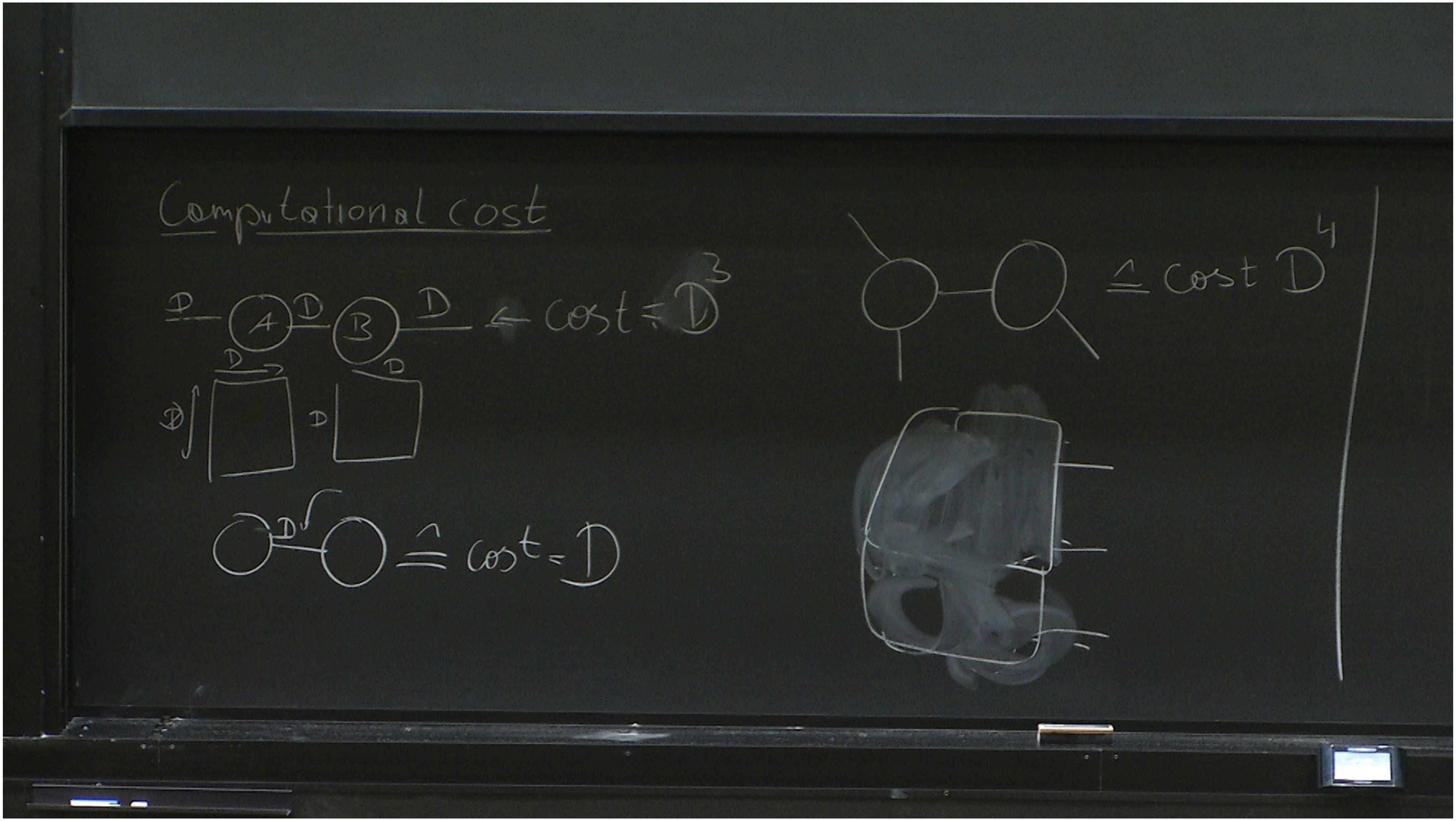
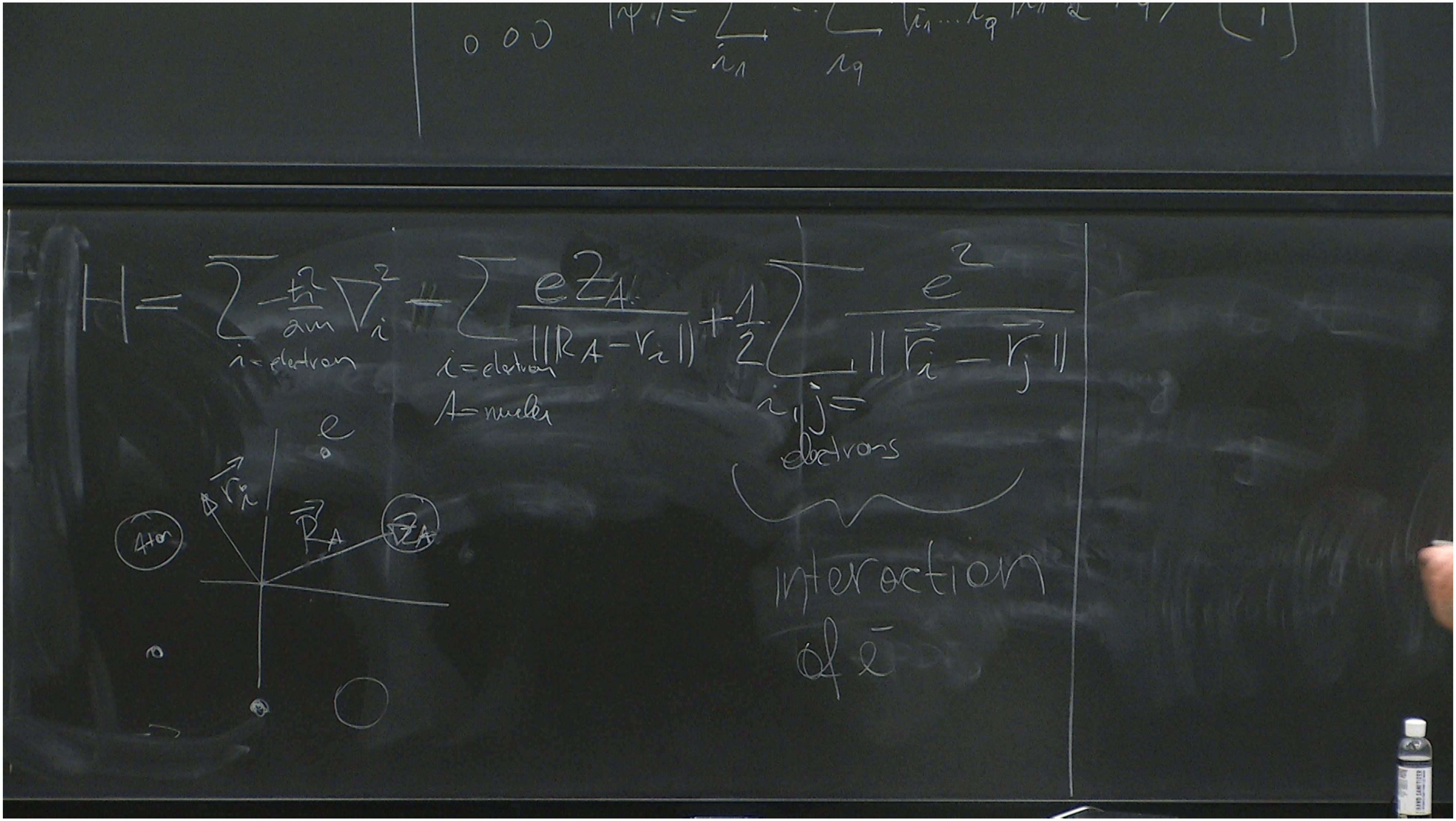
Abstract: TBC

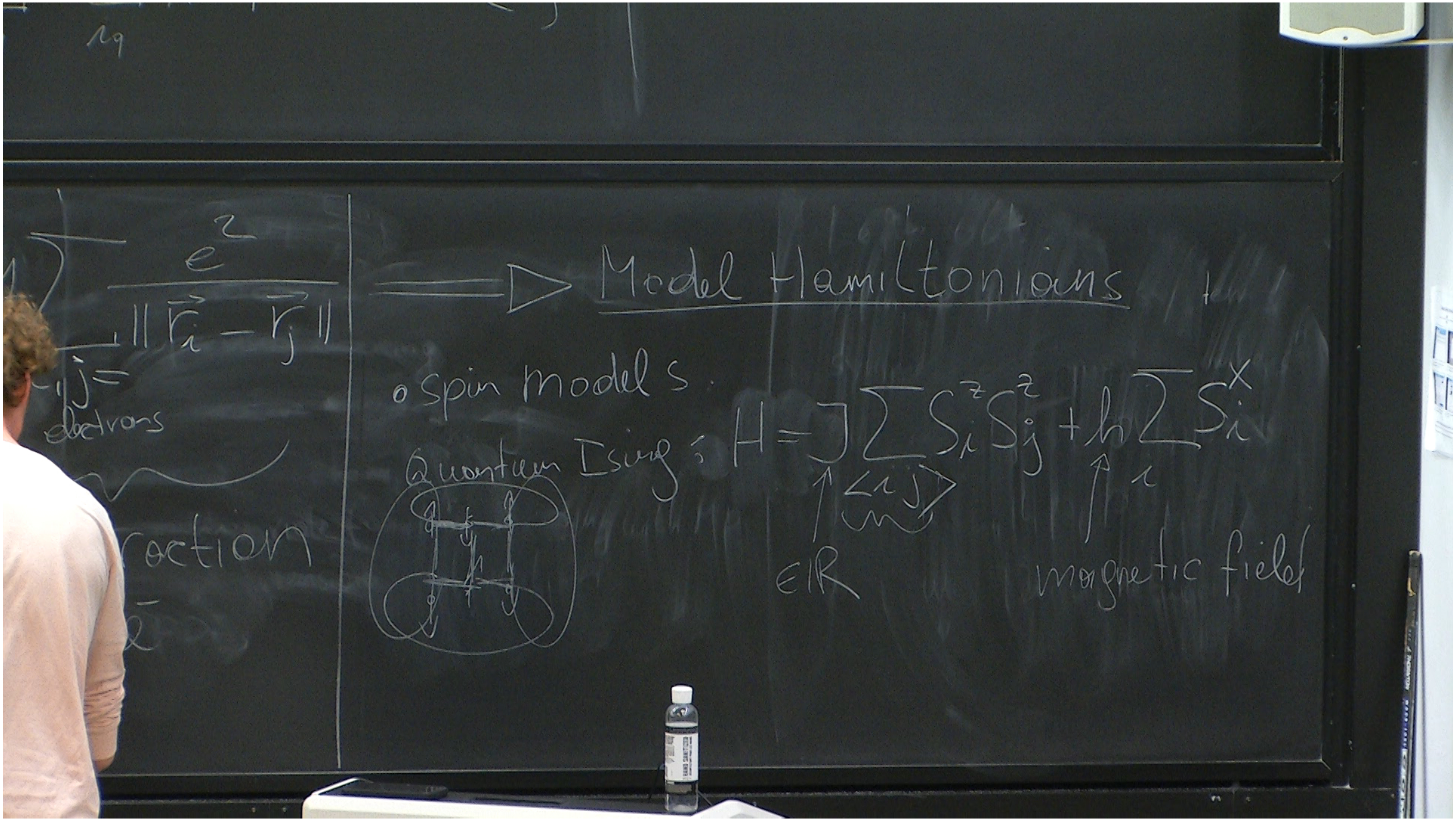

Day 1
• many body wave functions
• density matrices
• entanglement
• matrix factorization
Day 2
• Wave function truncation
• matrix product states (MPS)
• calculations with MPS
• Gauge-freedom of MPS
Day 3
• matrix product operators
• ground states: DMRG
• real time evolution
Day 4
• finite temperature
• 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

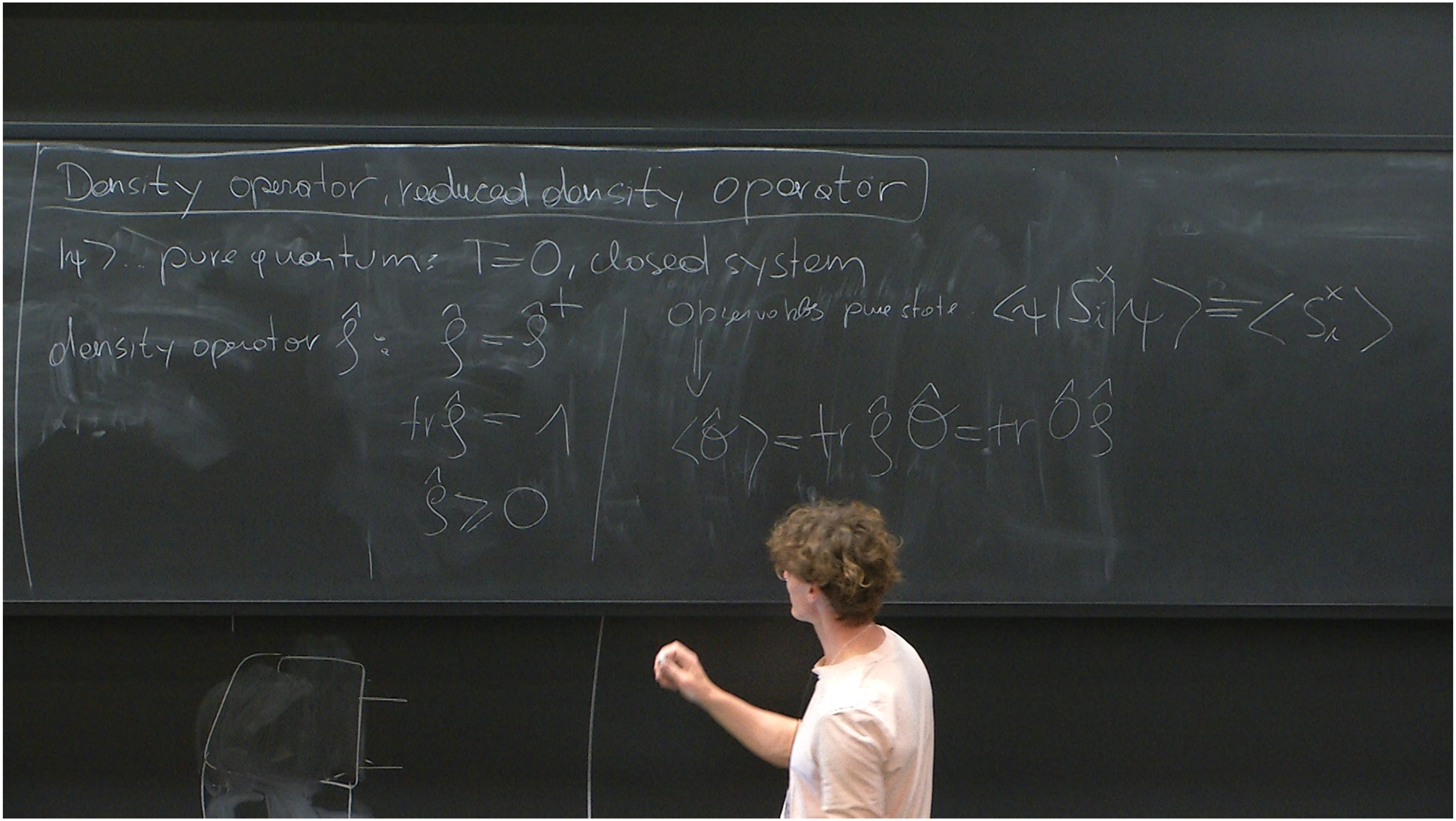

objects
≙ scalar
≙ vector
≙ matrix
≙ order 3 tensor
operations
matrix multiply: C = A B =
$C_{ij} = \sum_{m=1}^{D} A_{im} B_{mj}$
m
A
B
A
A

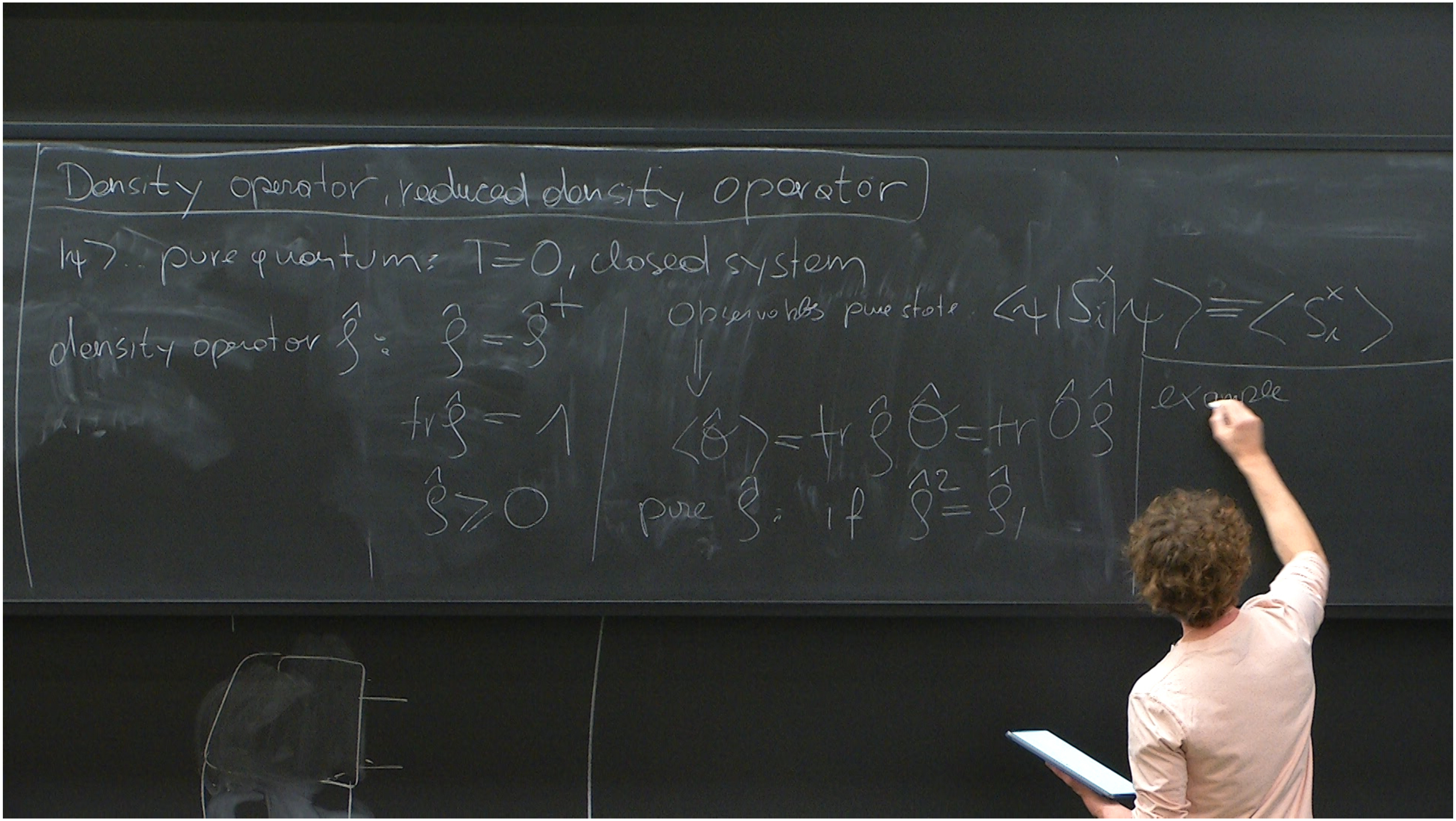

v
v
=
A
= tr A

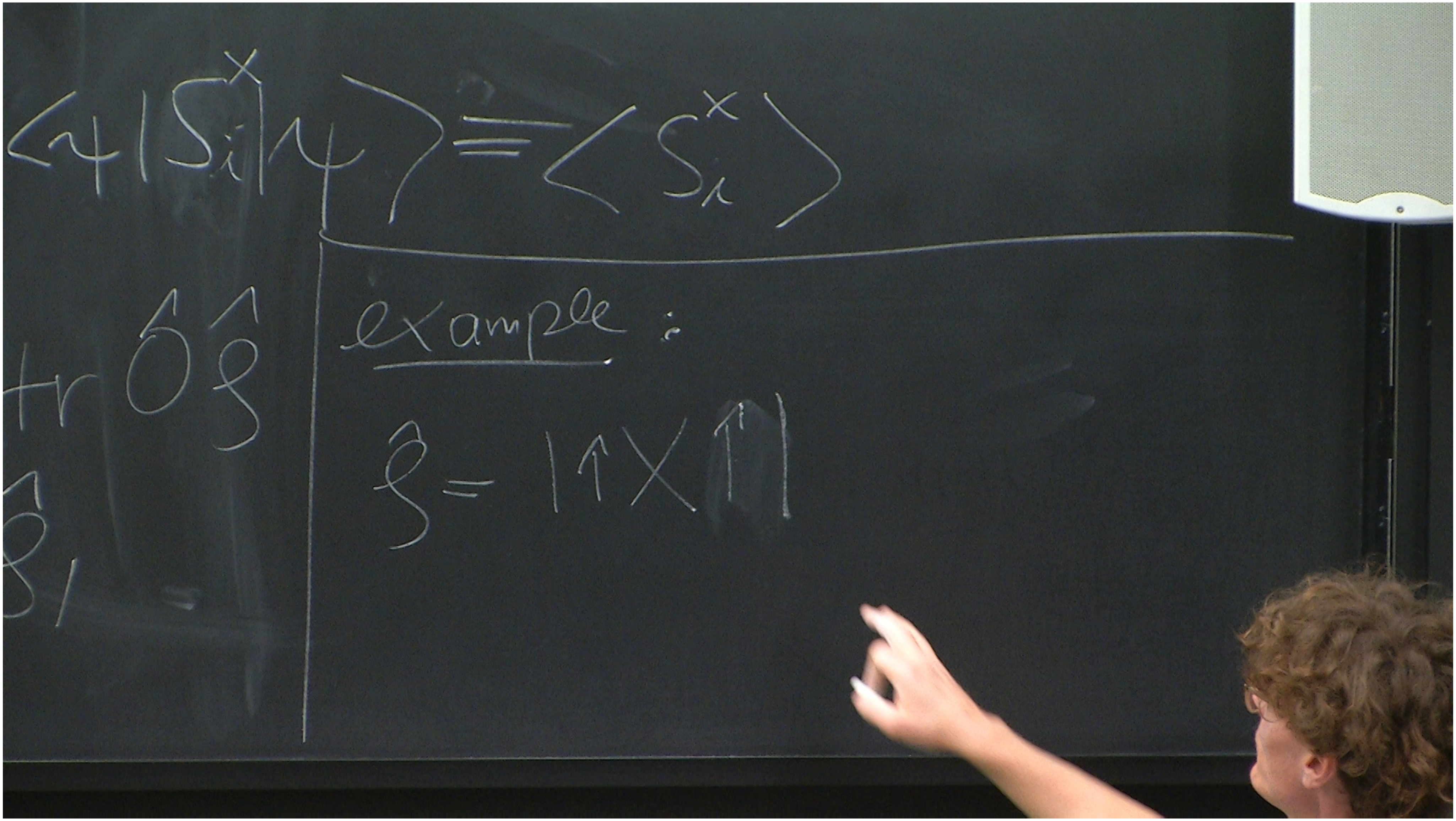

Computational cost
D A D B D ← cost = D^3
D D D D
D cost = D
cost D^4

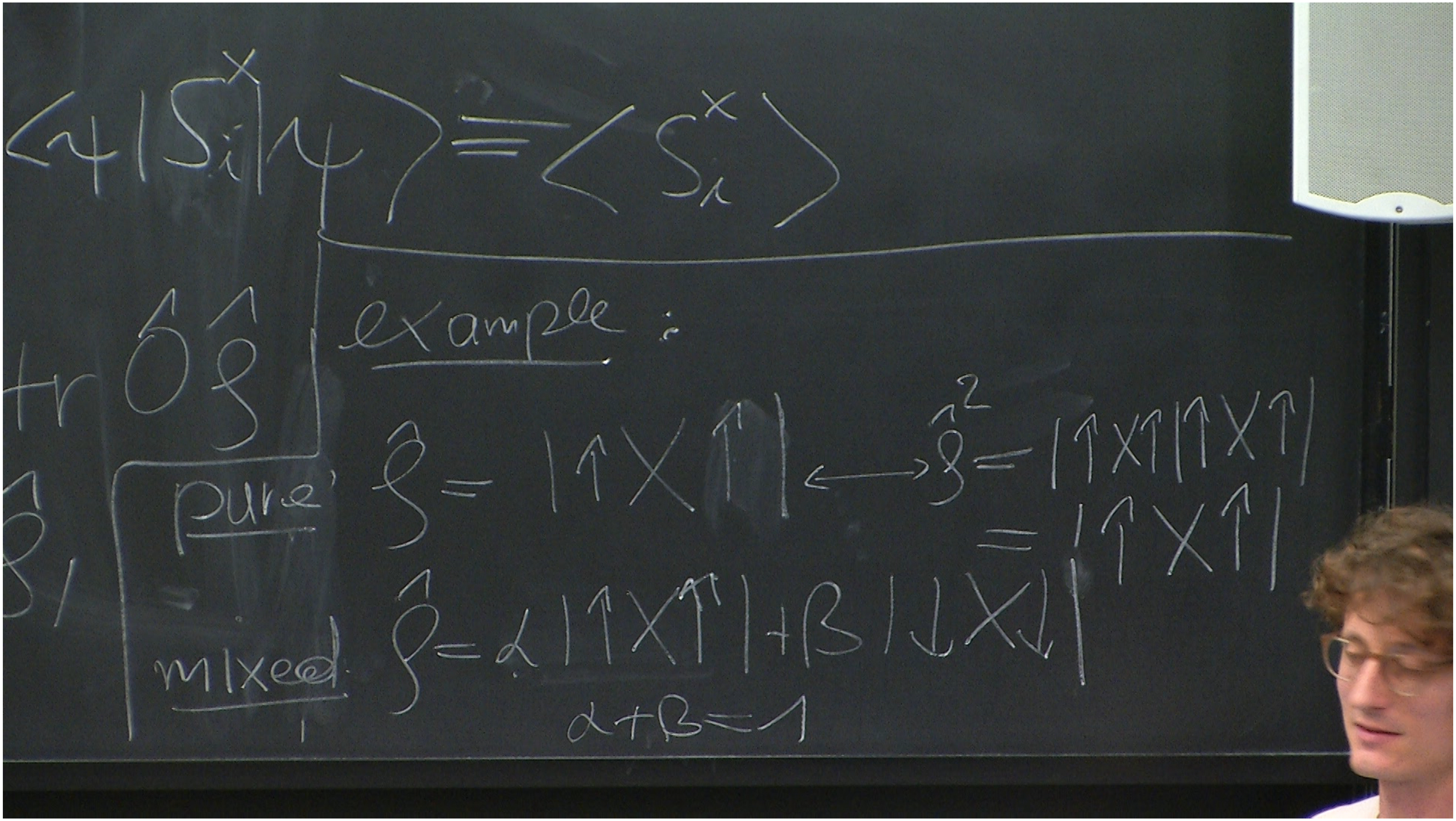

$H = \sum_{i=\text{electron}} -\frac{\hbar^2}{2m}\nabla_i^2 - \sum_{\substack{i=\text{electron}\\ A=\text{nuclei}}} \frac{e Z_A}{\|R_A - r_i\|} + \frac{1}{2}\sum_{i,j=\text{electrons}} \frac{e^2}{\|\vec{r}_i - \vec{r}_j\|}$
interaction of $\bar{e}$
e
$\vec{r}_i$
$\vec{R}_A$
Z_A
Atom

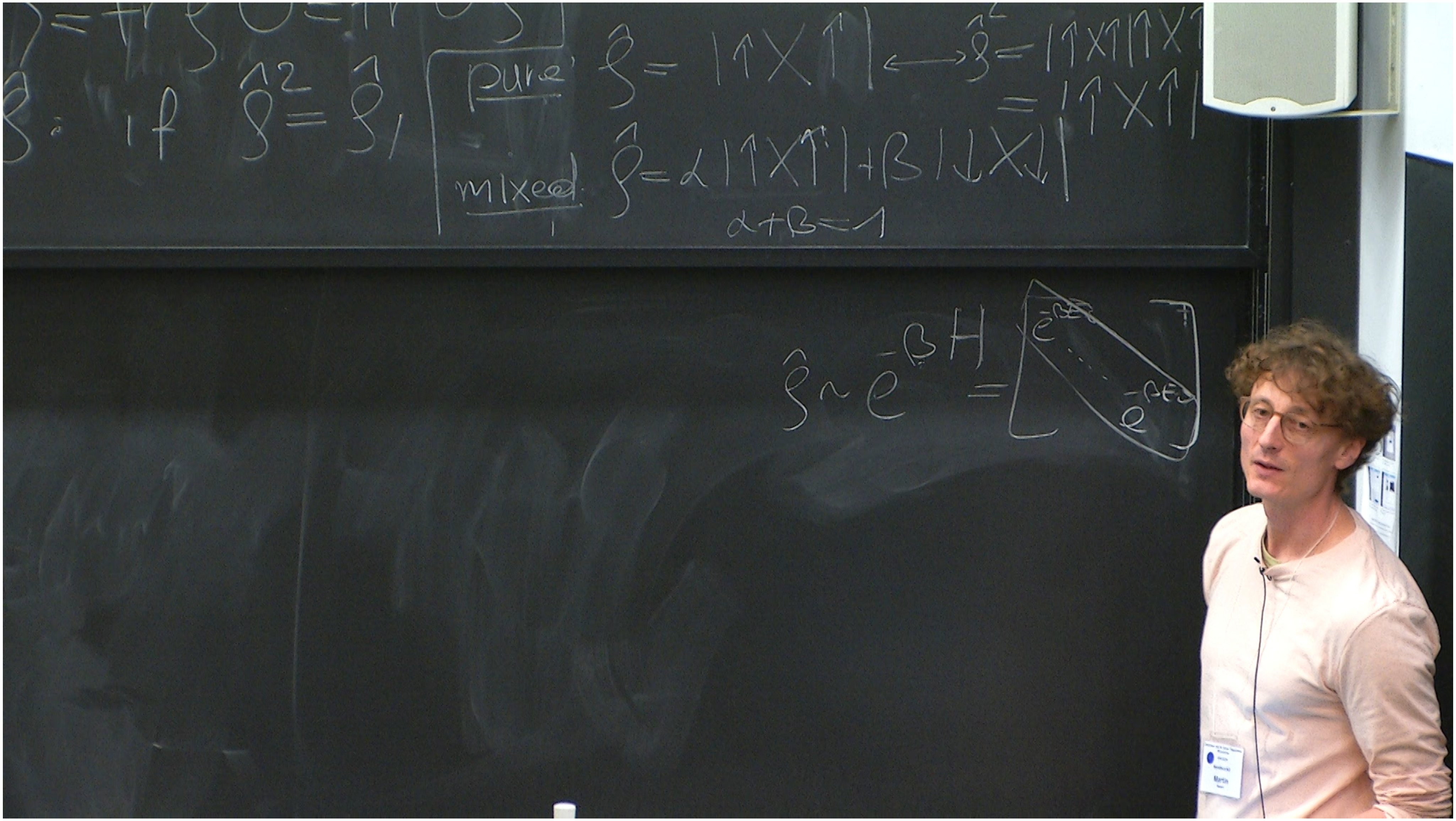

$\dfrac{e^2}{\|\vec{r}_i - \vec{r}_j\|}$
electrons
Model Hamiltonians
∘ spin models :
Quantum Ising : $H = J \sum_{\langle ij \rangle} S_i^z S_j^z + h \sum_i S_i^x$
$\in \mathbb{R}$
magnetic field

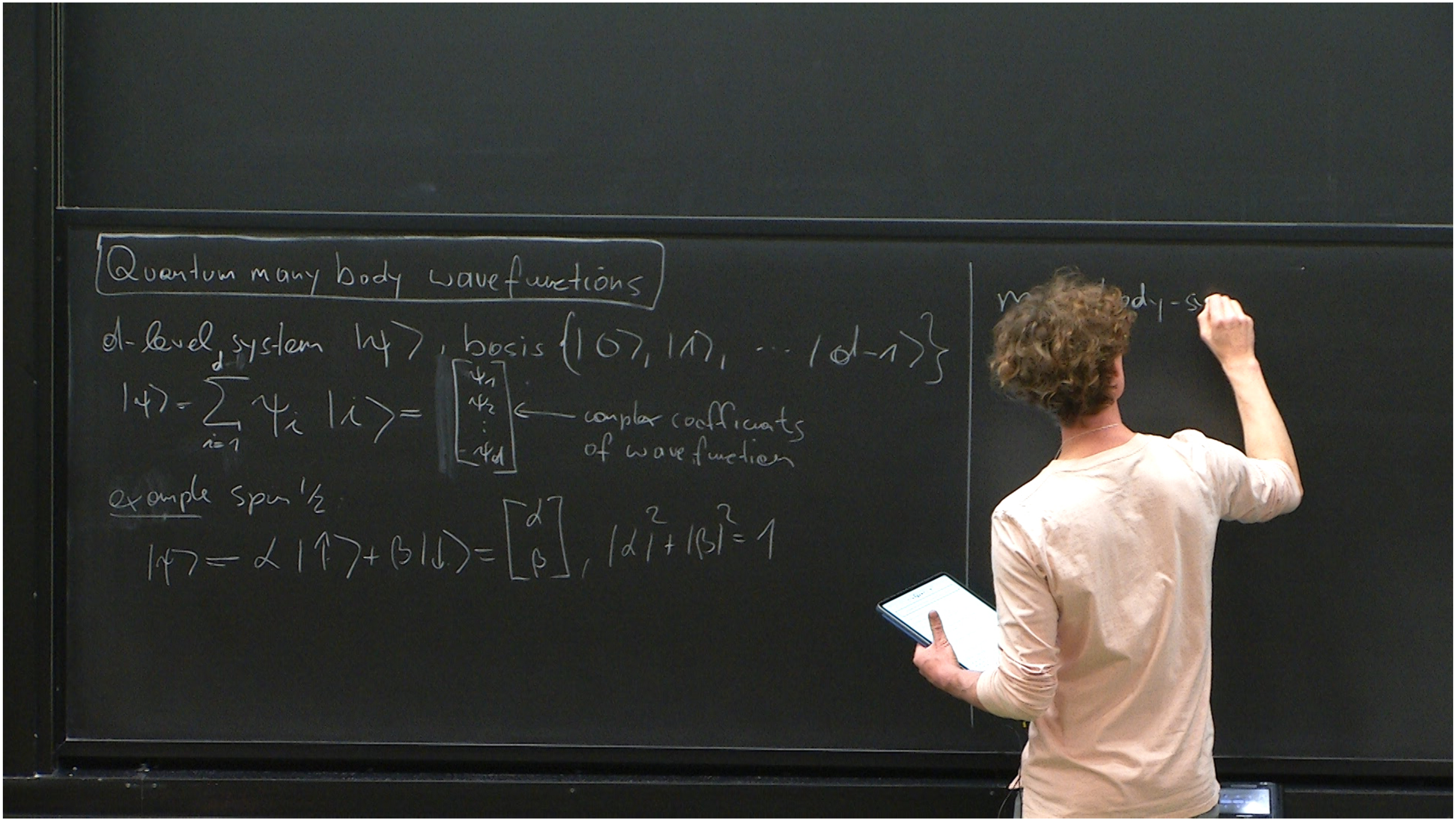

Density operator, reduced density operator
|ψ⟩: pure quantum: T=0, closed system
density operator ρ̂: ρ̂ = ρ̂†
tr ρ̂ = 1
ρ̂ ≥ 0
Observables pure state. ⟨ψ|S_i^x|ψ⟩ = ⟨S_i^x⟩
⟨Ô⟩ = tr ρ̂ Ô = tr Ô ρ̂

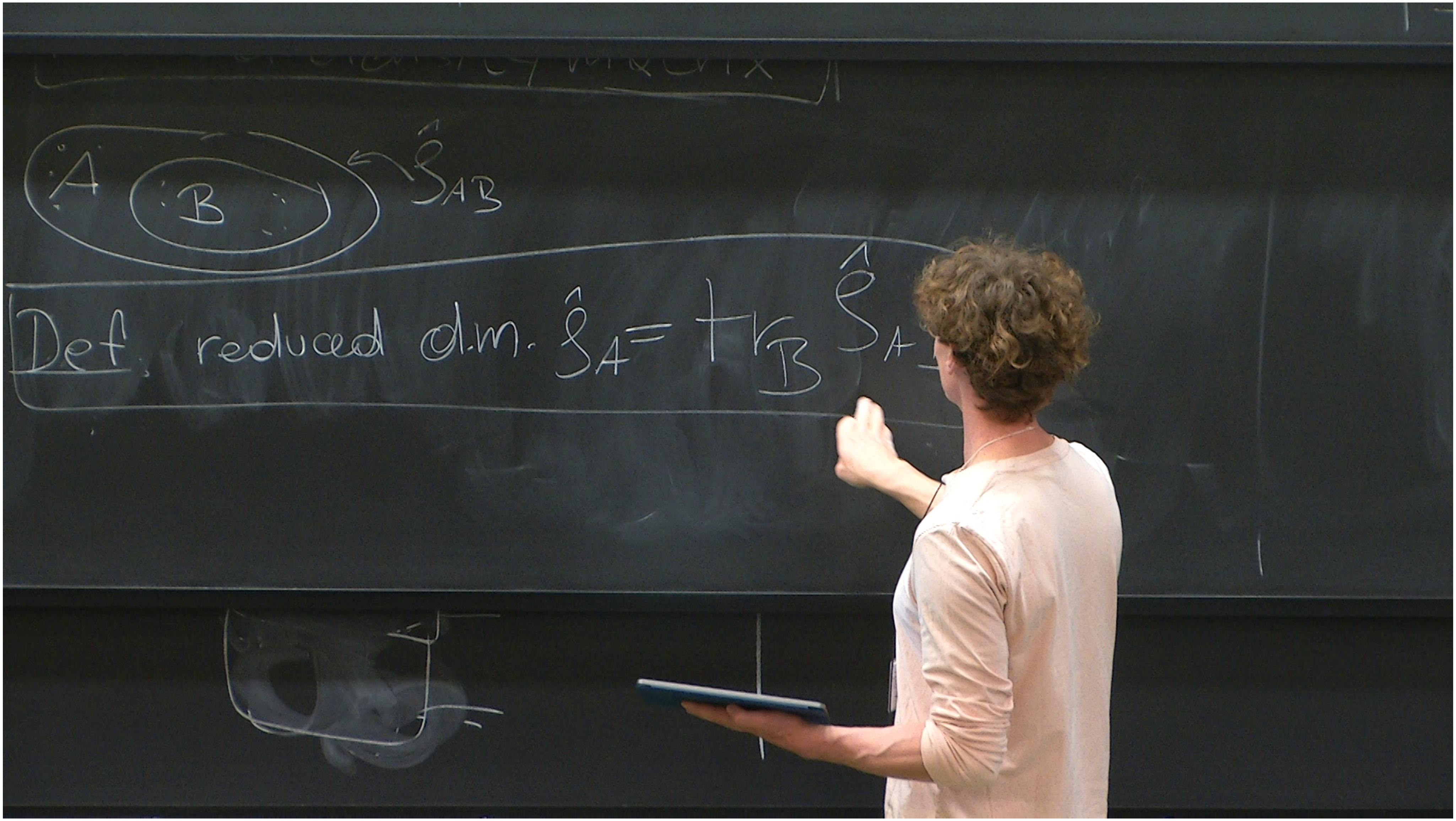

Density operator, reduced density operator
$|\psi\rangle$: pure quantum: $T=0$, closed system
density operator $\hat{\rho}$: $\hat{\rho} = \hat{\rho}^{\dagger}$
$\mathrm{tr}\,\hat{\rho} = 1$
$\hat{\rho} \geq 0$
Observables pure state: $\langle\psi|\hat{S}_i^x|\psi\rangle = \langle S_i^x\rangle$
$\langle\hat{O}\rangle = \mathrm{tr}\,\hat{\rho}\,\hat{O} = \mathrm{tr}\,\hat{O}\,\hat{\rho}$
pure $\hat{\rho}$: if $\hat{\rho}^2 = \hat{\rho}$,
example

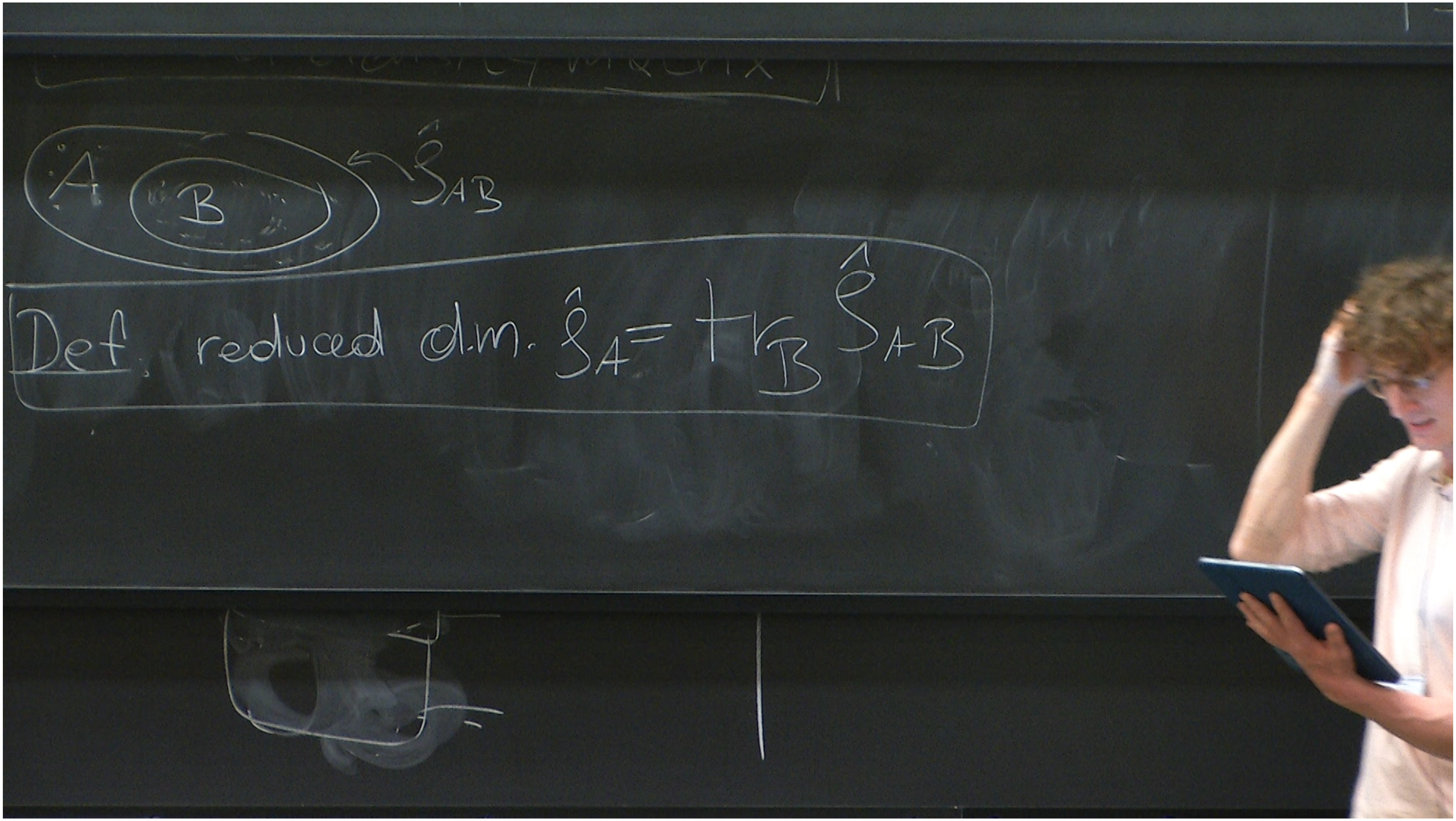

⟨ψ|S_i^x|ψ⟩ = ⟨S_i^x⟩
tr Ô ρ̂
example:
ρ = |↑⟩⟨↑|


$\langle \psi | S_i^x | \psi \rangle = \langle S_i^x \rangle$
$\mathrm{tr}\, \hat{O} \hat{\rho}$
$\hat{\rho}$,
pure
mixed
example:
$\hat{\rho} = |\uparrow\rangle\langle\uparrow| \longleftrightarrow \hat{\rho}^2 = |\uparrow\rangle\langle\uparrow|\uparrow\rangle\langle\uparrow|$
$= |\uparrow\rangle\langle\uparrow|$
$\hat{\rho} = \alpha |\uparrow\rangle\langle\uparrow| + \beta |\downarrow\rangle\langle\downarrow|$
$\alpha + \beta = 1$


if
pure
mixed
α+β=1


Quantum many body wavefunctions
d-level system |ψ⟩, basis {|0⟩, |1⟩, ··· |d-1⟩}
|ψ⟩ = Σ_{i=1}^{d} ψ_i |i⟩ = [ψ_1, ψ_2, ⋮, ψ_d]
complex coefficiants of wavefunction
example spin 1/2
|ψ⟩ = α|↑⟩ + β|↓⟩ = [α, β], |α|² + |β|² = 1


A
B
ρ̂AB
Def. reduced d.m. ρ̂A = trB ρ̂A


A
B
$\hat{\rho}_{AB}$
Def: reduced d.m. $\hat{\rho}_A = \mathrm{tr}_B \, \hat{\rho}_{AB}$

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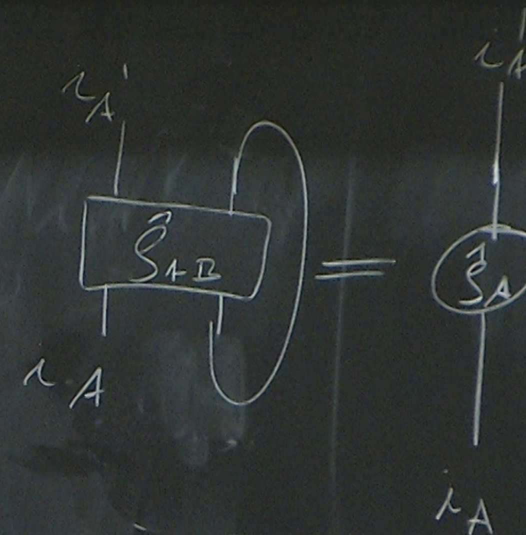
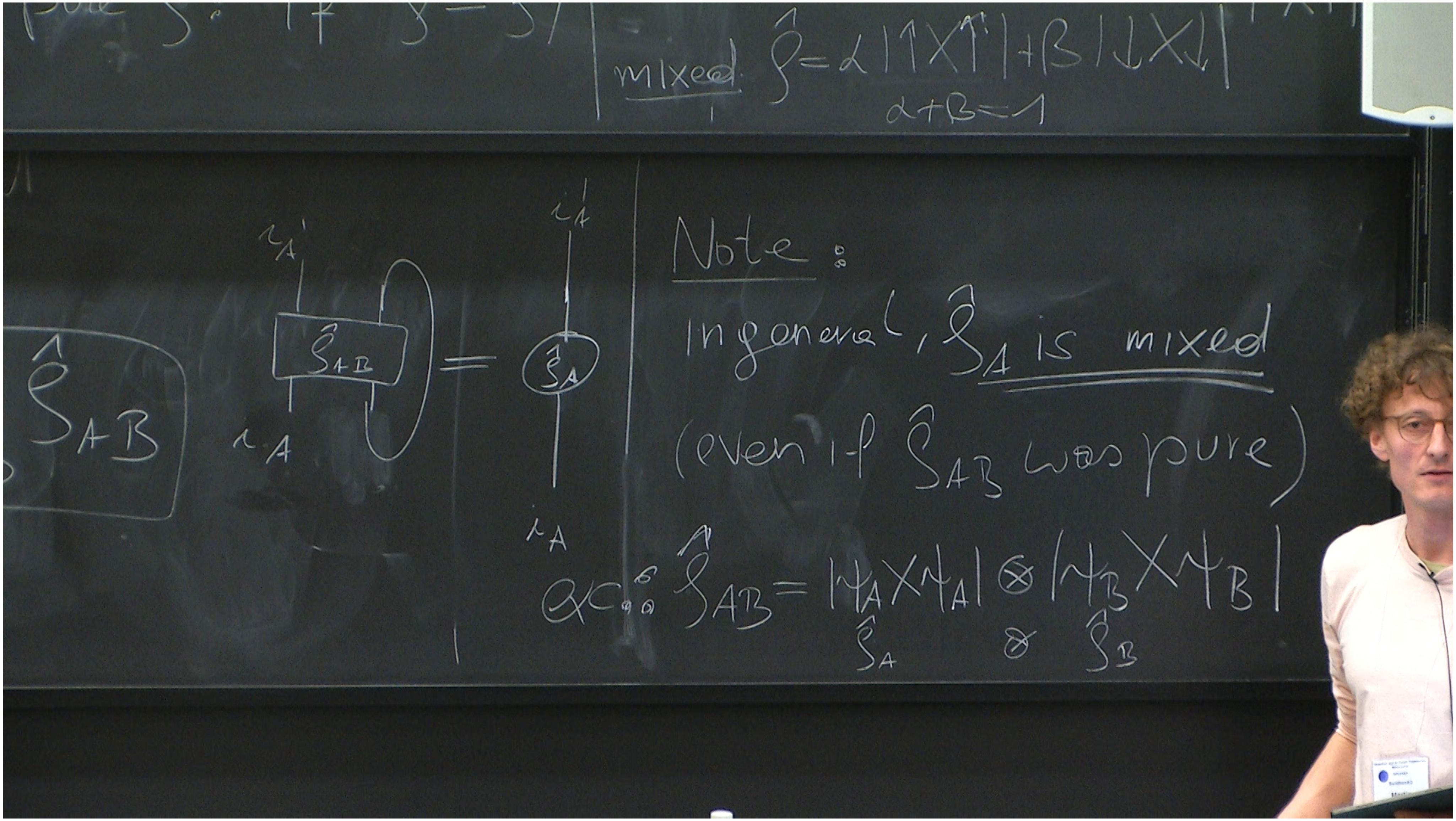
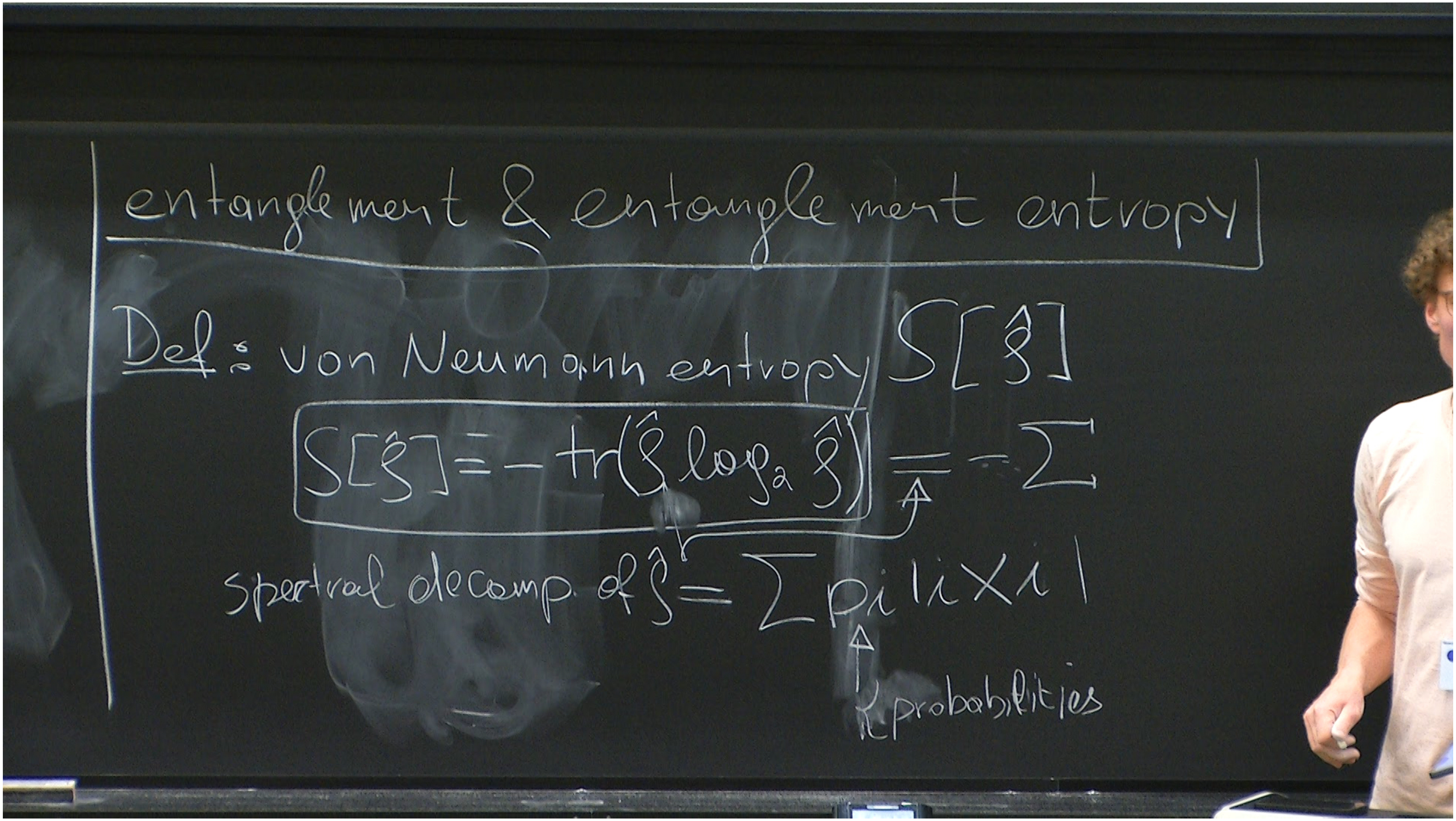




mixed: $\hat{\rho} = \alpha |\uparrow\rangle\langle\uparrow| + \beta |\downarrow\rangle\langle\downarrow|$
$\alpha + \beta = 1$
$\hat{\rho}_{AB}$
i_A'
$\hat{\rho}_{AB}$
i_A
i_A'
$\hat{\rho}_A$
i_A
Note:
in general, $\hat{\rho}_A$ is mixed
(even if $\hat{\rho}_{AB}$ was pure)
ex: $\hat{\rho}_{AB} = |\psi_A\rangle\langle\psi_A| \otimes |\psi_B\rangle\langle\psi_B|$
$\hat{\rho}_A \otimes \hat{\rho}_B$


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

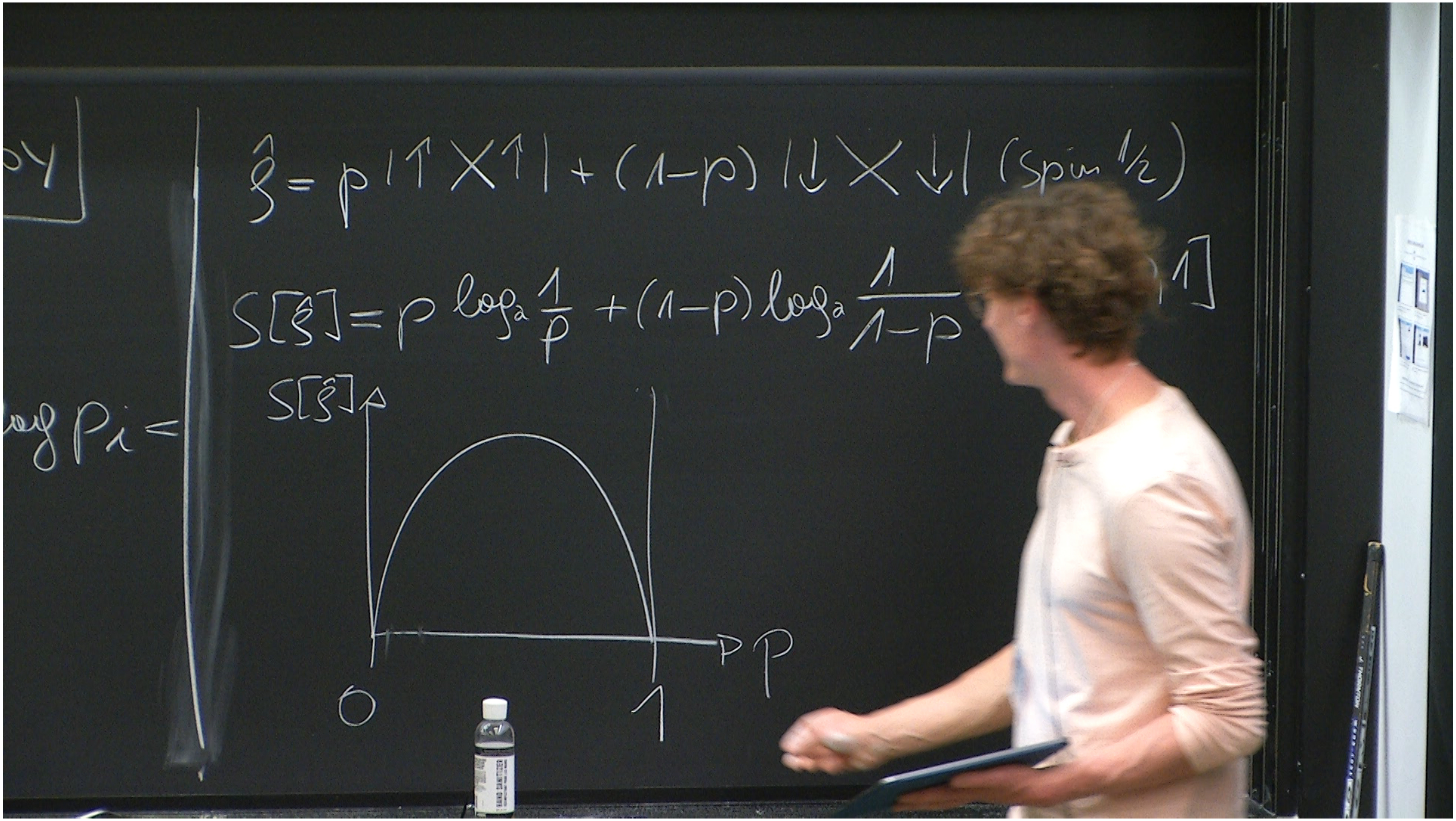
entanglement & entanglement entropy

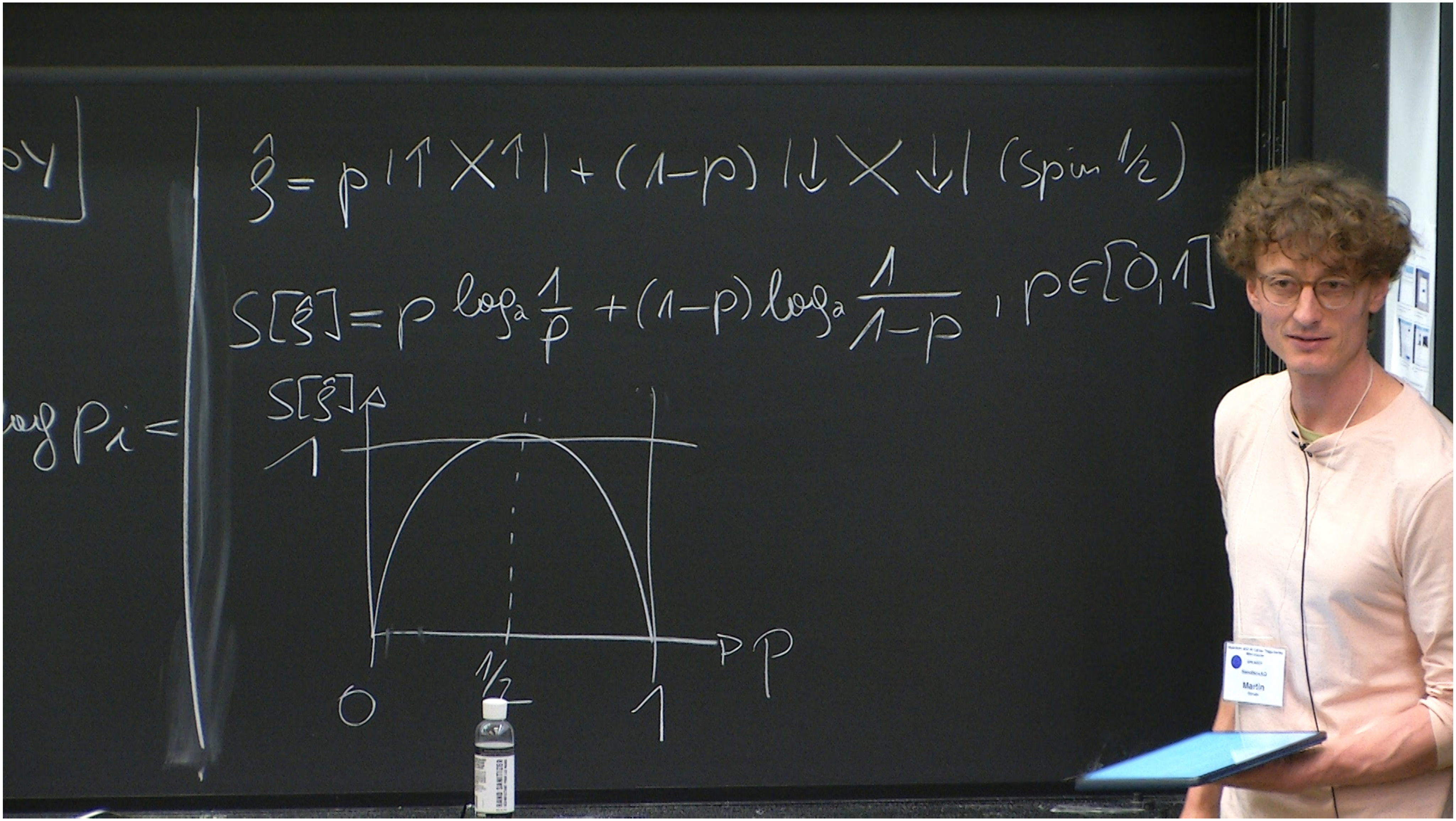
Def: von Neumann entropy $S[\hat{\rho}]$

$$\boxed{S[\hat{\rho}] = -\mathrm{tr}(\hat{\rho} \log_2 \hat{\rho})} = -\sum p_i \log p_i$$

spectral decomp. of $\hat{\rho} = \sum p_i |i\rangle\langle i|$

probabilities


$\hat{\rho} = p|\uparrow\rangle\langle\uparrow| + (1-p)|\downarrow\rangle\langle\downarrow|$ (spin 1/2)
$S[\hat{\rho}] = p \log_2 \frac{1}{p} + (1-p)\log_2 \frac{1}{1-p}$
$S[\hat{\rho}]$
0
1
p

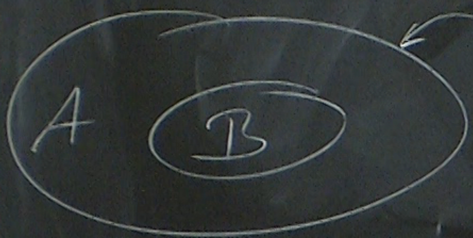


$\hat{\rho} = p |\uparrow\rangle\langle\uparrow| + (1-p) |\downarrow\rangle\langle\downarrow|$ (spin 1/2)
$S[\hat{\rho}] = p \log_2 \frac{1}{p} + (1-p) \log_2 \frac{1}{1-p}$, $p \in [0,1]$
$S[\hat{\rho}]$
1
0
1/2
1
p
Martin

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

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

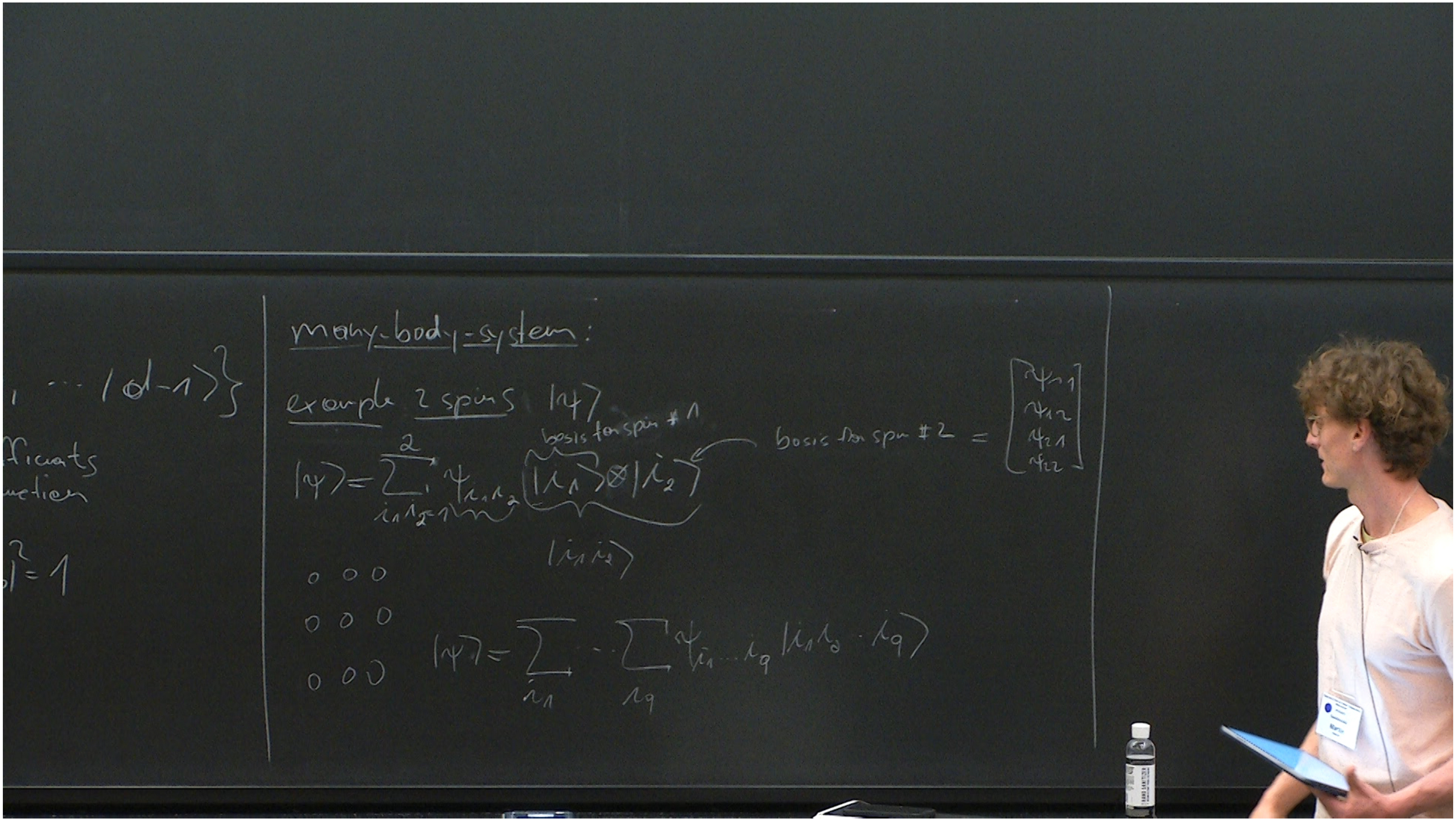
Def: entangled quantum systems



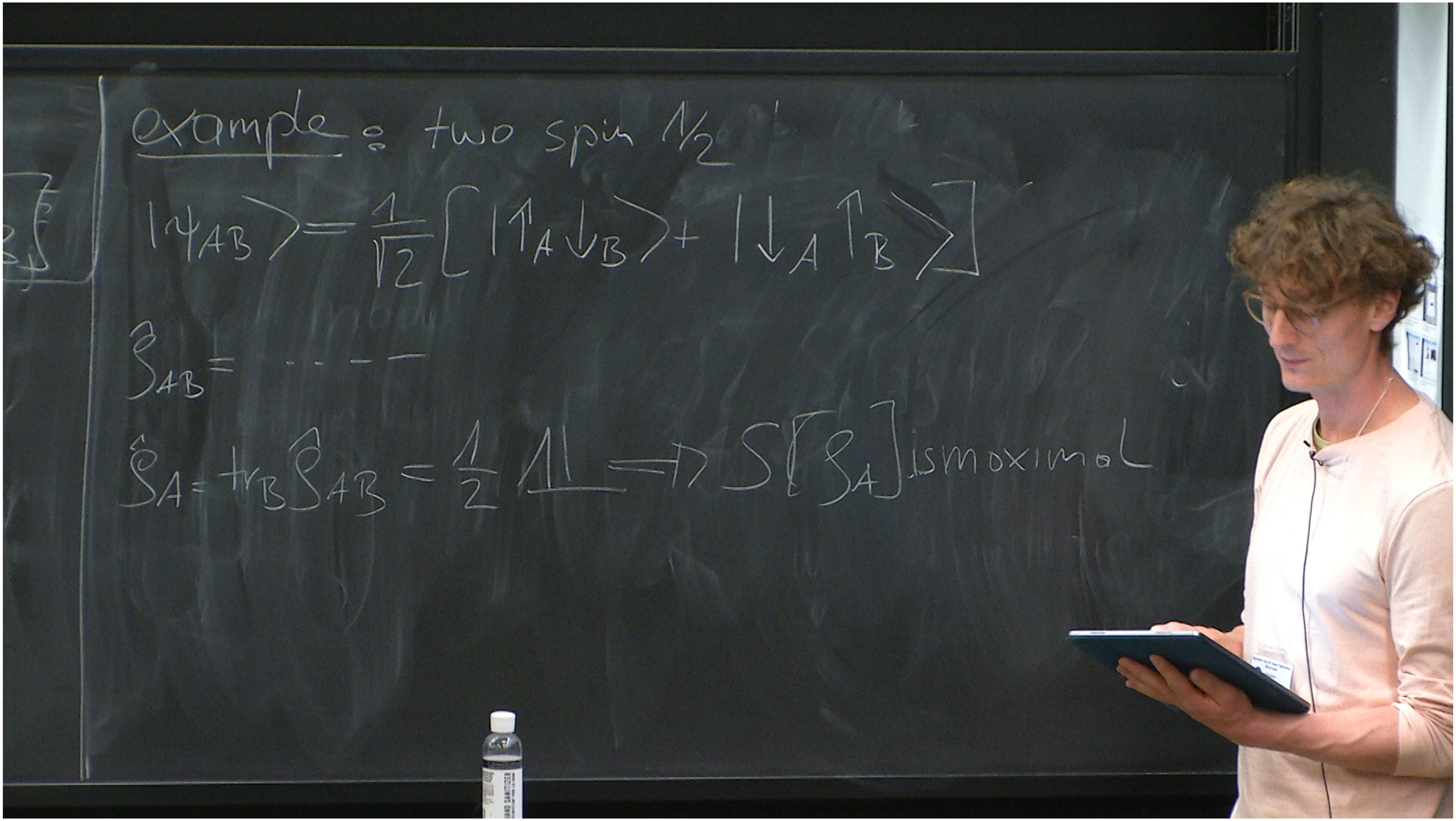
$$|\psi_{AB}\rangle \longrightarrow \hat{\rho}_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$$

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

spectral decomp. of $\rho = \sum p_i |i\rangle\langle$



many-body-system:
example 2 spins |ψ⟩
basis for spin #1
basis for spin #2
$|\psi\rangle = \sum_{i_1 i_2 = 1}^{2} \psi_{i_1 i_2} |i_1\rangle \otimes |i_2\rangle$
$|i_1 i_2\rangle$
$= \begin{bmatrix} \psi_{11} \\ \psi_{12} \\ \psi_{21} \\ \psi_{22} \end{bmatrix}$
$|\psi\rangle = \sum_{i_1} \cdots \sum_{i_q} \psi_{i_1 \cdots i_q} |i_1 i_2 \cdots i_q\rangle$


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

$\ldots, \ldots |d-1\rangle \}$

fficients

unction

$|^2 = 1$

many-body-system:

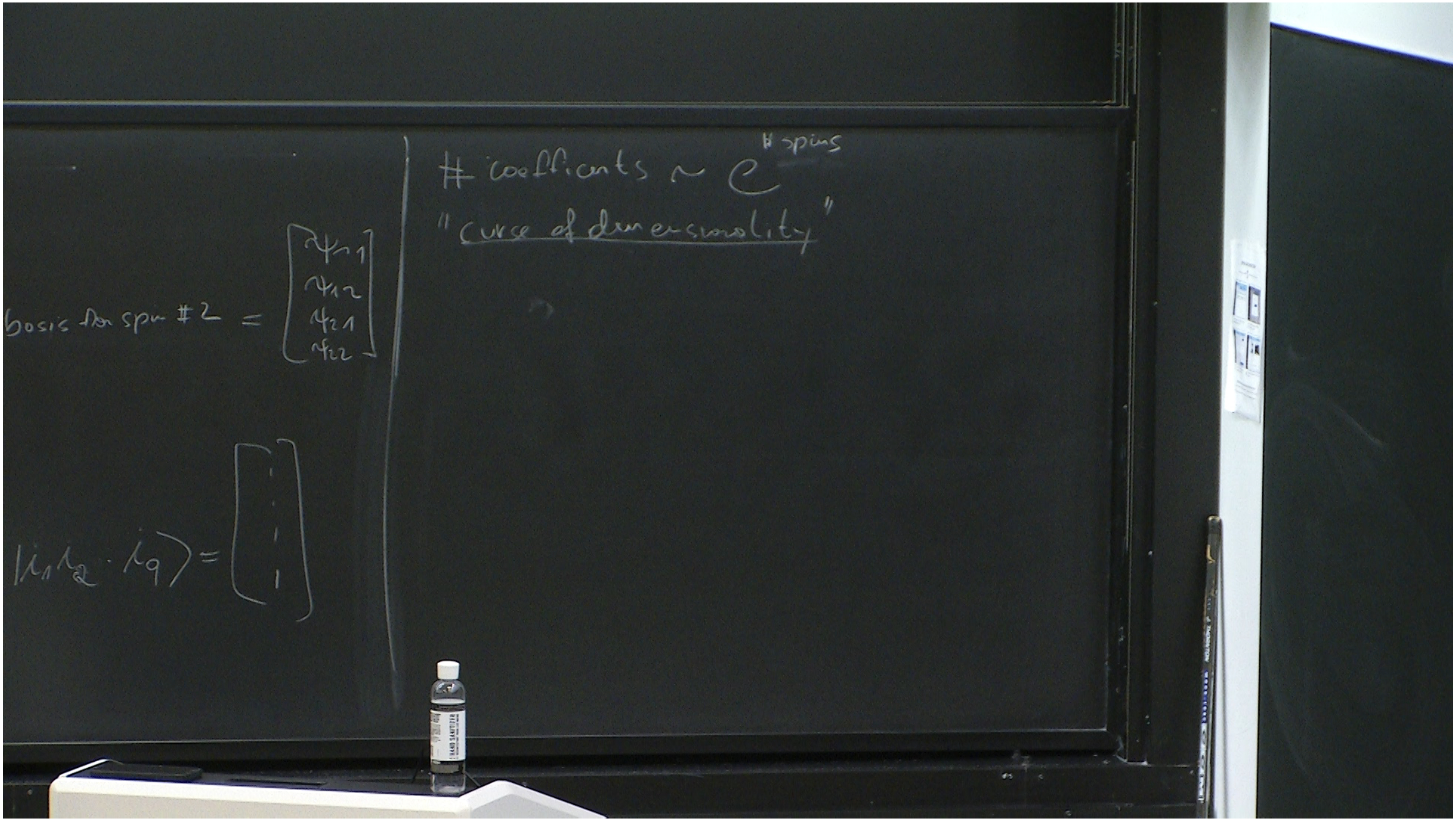
example 2 spins $|\psi\rangle$

basis for spin #1

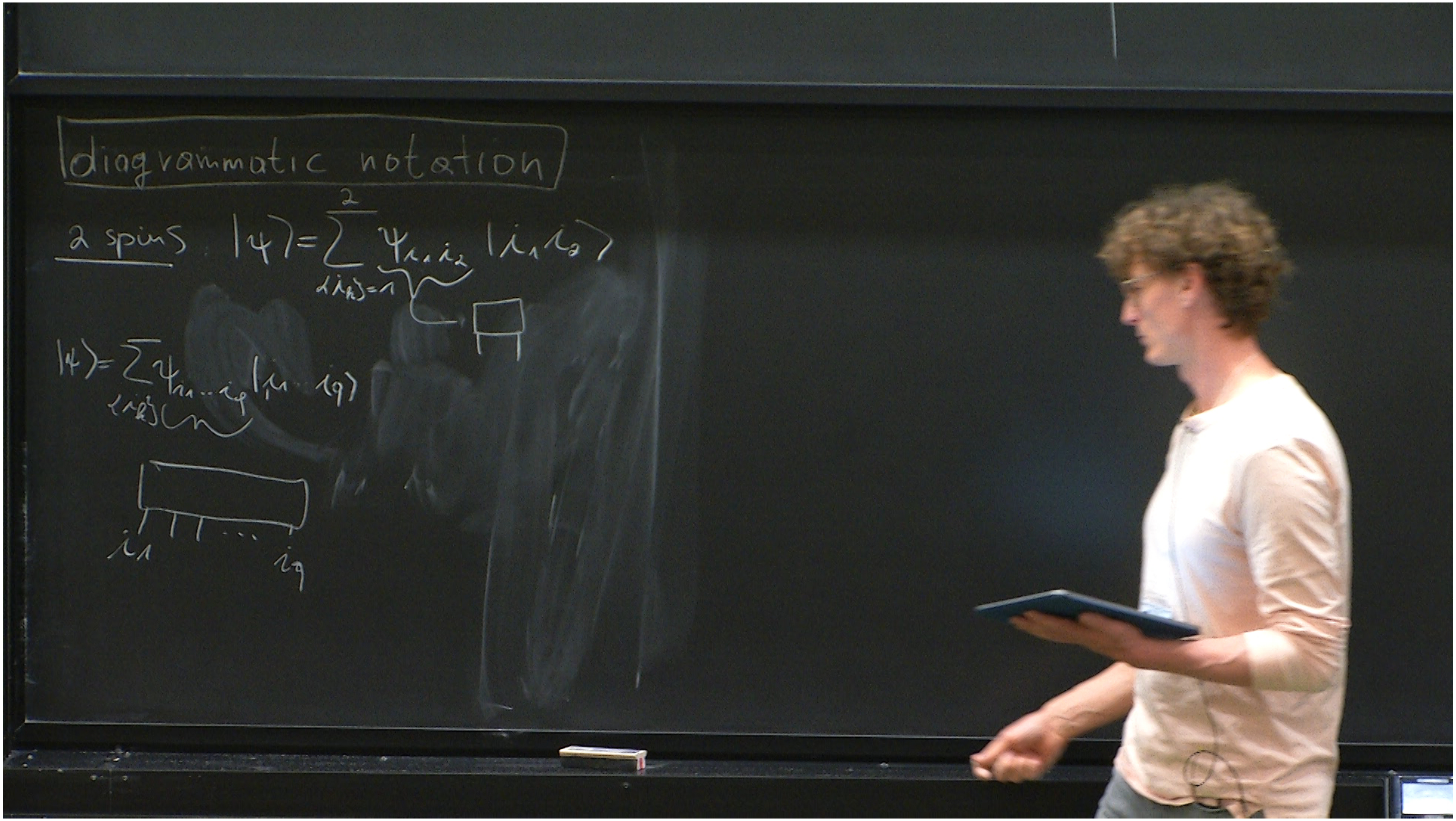
basis for spin #2

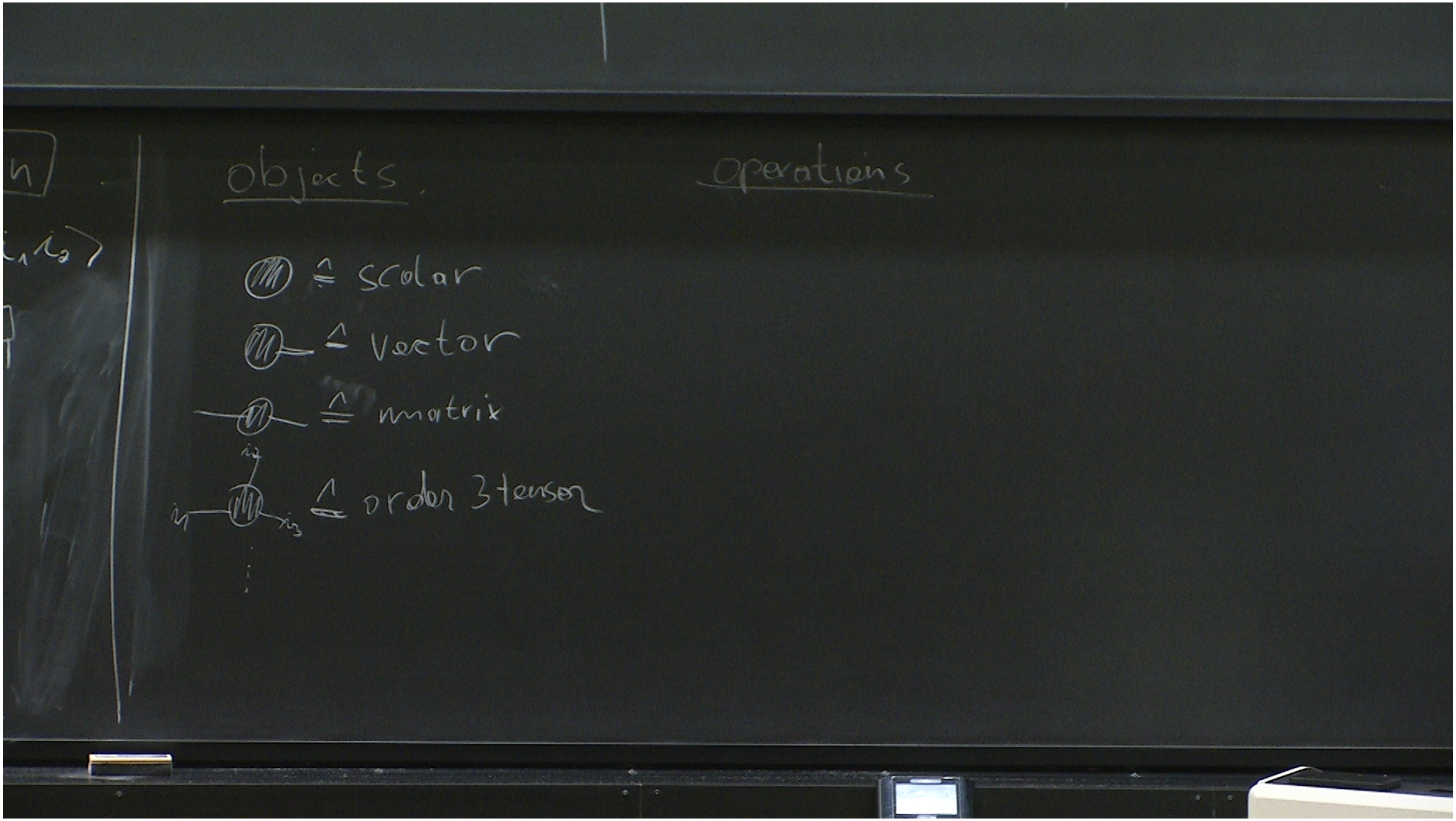
$$|\psi\rangle = \sum_{i_1 i_2 = 1}^{2} \psi_{i_1 i_2} \underbrace{|i_1\rangle \otimes |i_2\rangle}_{|i_1 i_2\rangle} = \begin{bmatrix} \psi_{11} \\ \psi_{12} \\ \psi_{21} \\ \psi_{22} \end{bmatrix}$$

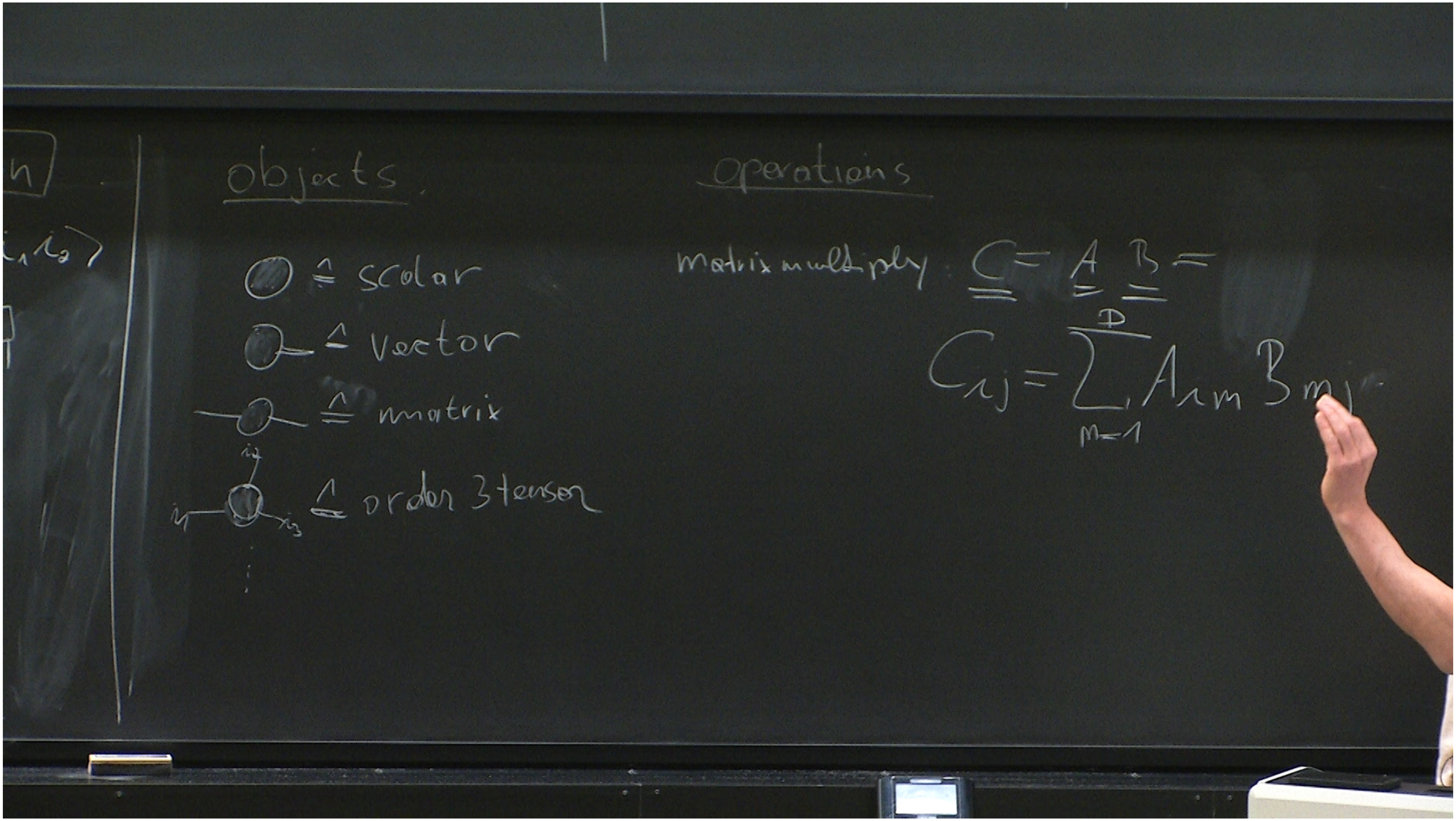
$$|\psi\rangle = \sum_{i_1} \cdots \sum_{i_q} \psi_{i_1 \ldots i_q} |i_1 i_2 \ldots i_q\rangle = \begin{bmatrix} \vdots \end{bmatrix}$$



coefficients ~ e^# spins
"curse of dimensionality"
basis for spin #2 =
ψ11
ψ12
ψ21
ψ22
|i1 i2 · i9⟩ =


diagrammatic notation
2 spins : $|\psi\rangle = \sum_{\{i_k\}=1}^{2} \psi_{i_1 i_2} |i_1 i_2\rangle$
$|\psi\rangle = \sum_{\{i_k\}} \psi_{i_1 \dots i_q} |i_1 \dots i_q\rangle$
i_1 … i_q


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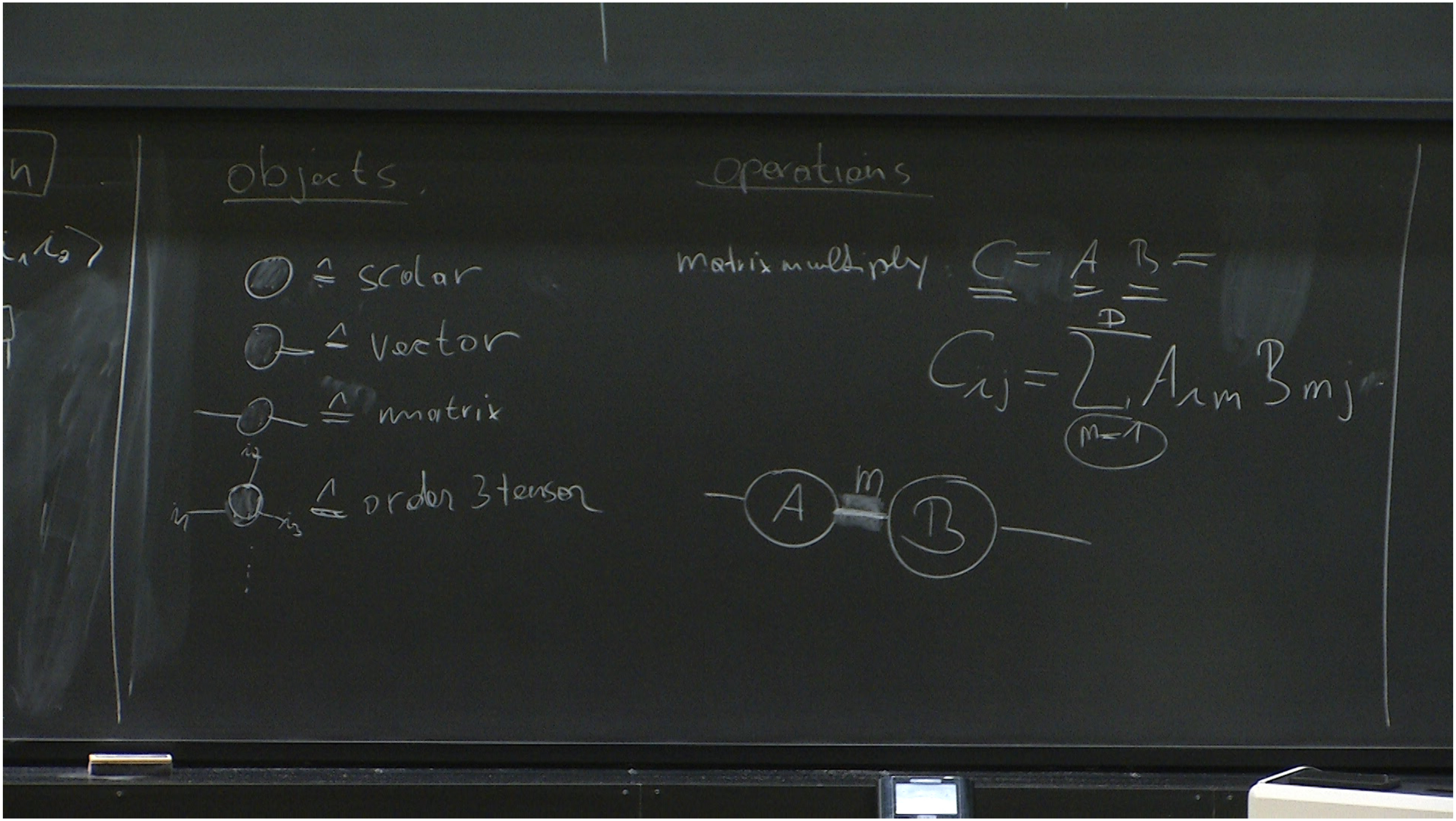
matrix multiply: C = A B =
$C_{ij} = \sum_{m=1}^{D} A_{im} B_{mj}$


objects
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matrix multiply: C = A B =
C_ij = Σ_{m=1}^{D} A_im B_mj
m
A
B


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