Title: Non-Gaussian fermionic ansatzes from many-body correlation measures

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Series: Quantum Matter

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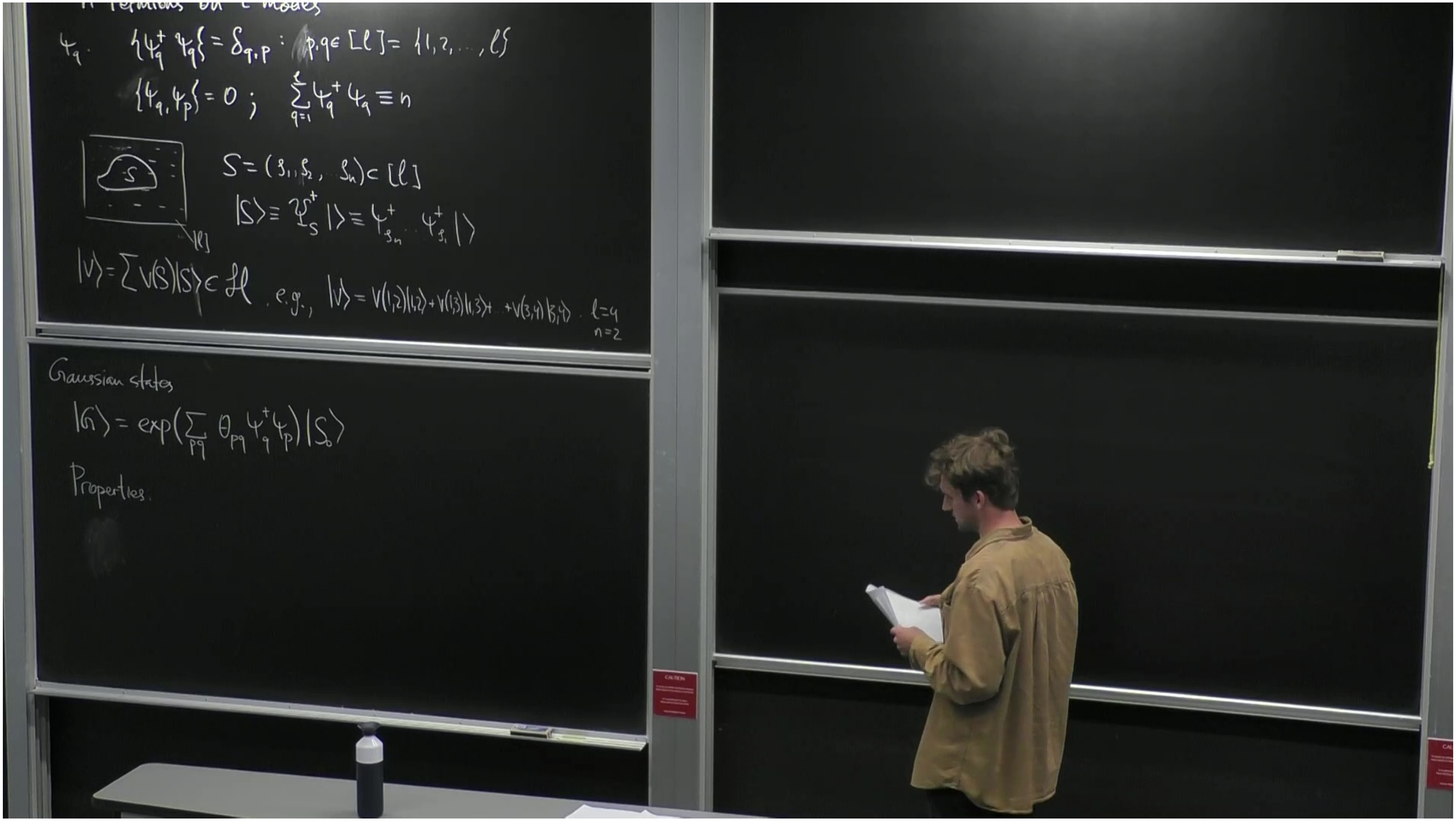
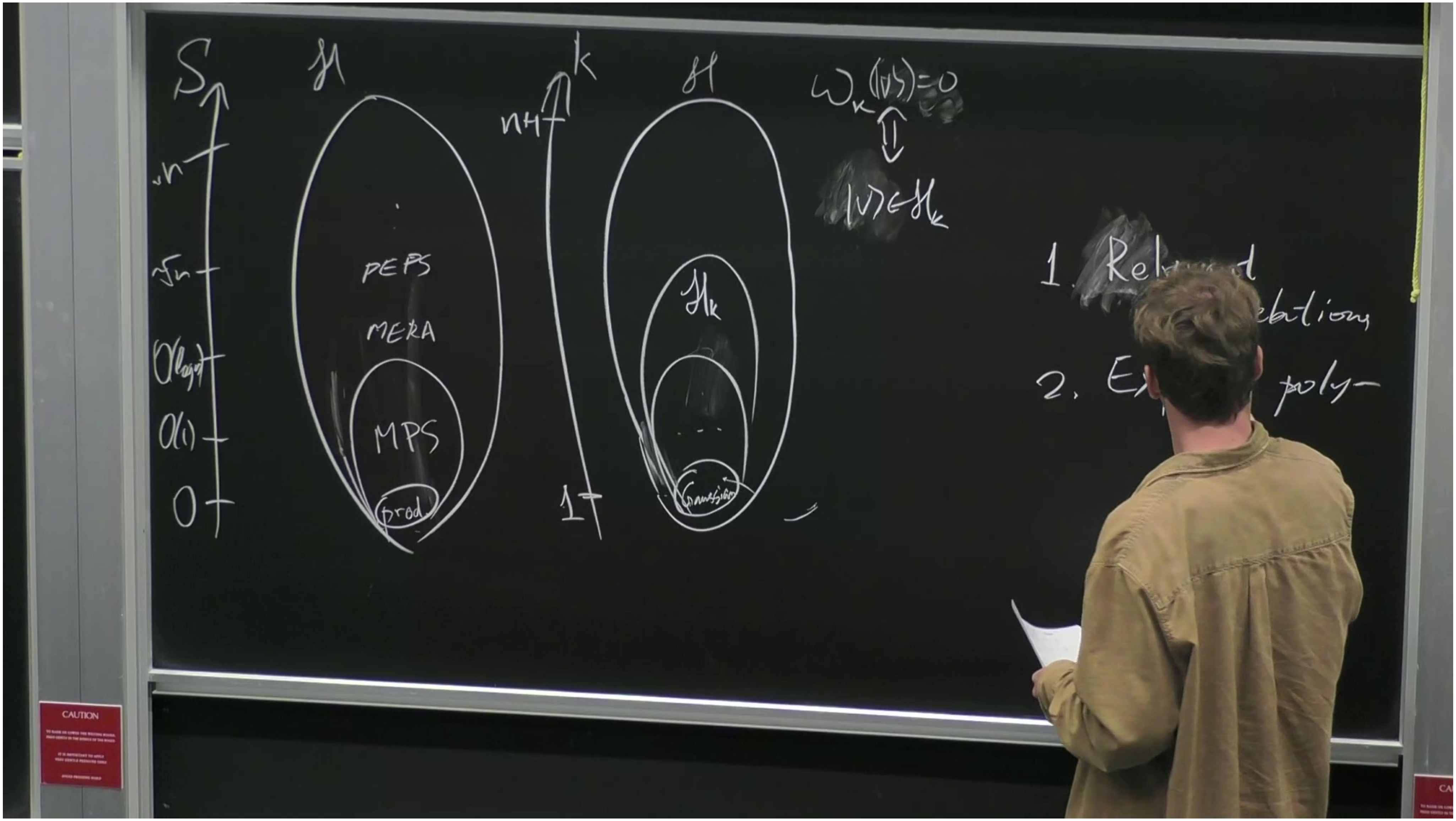
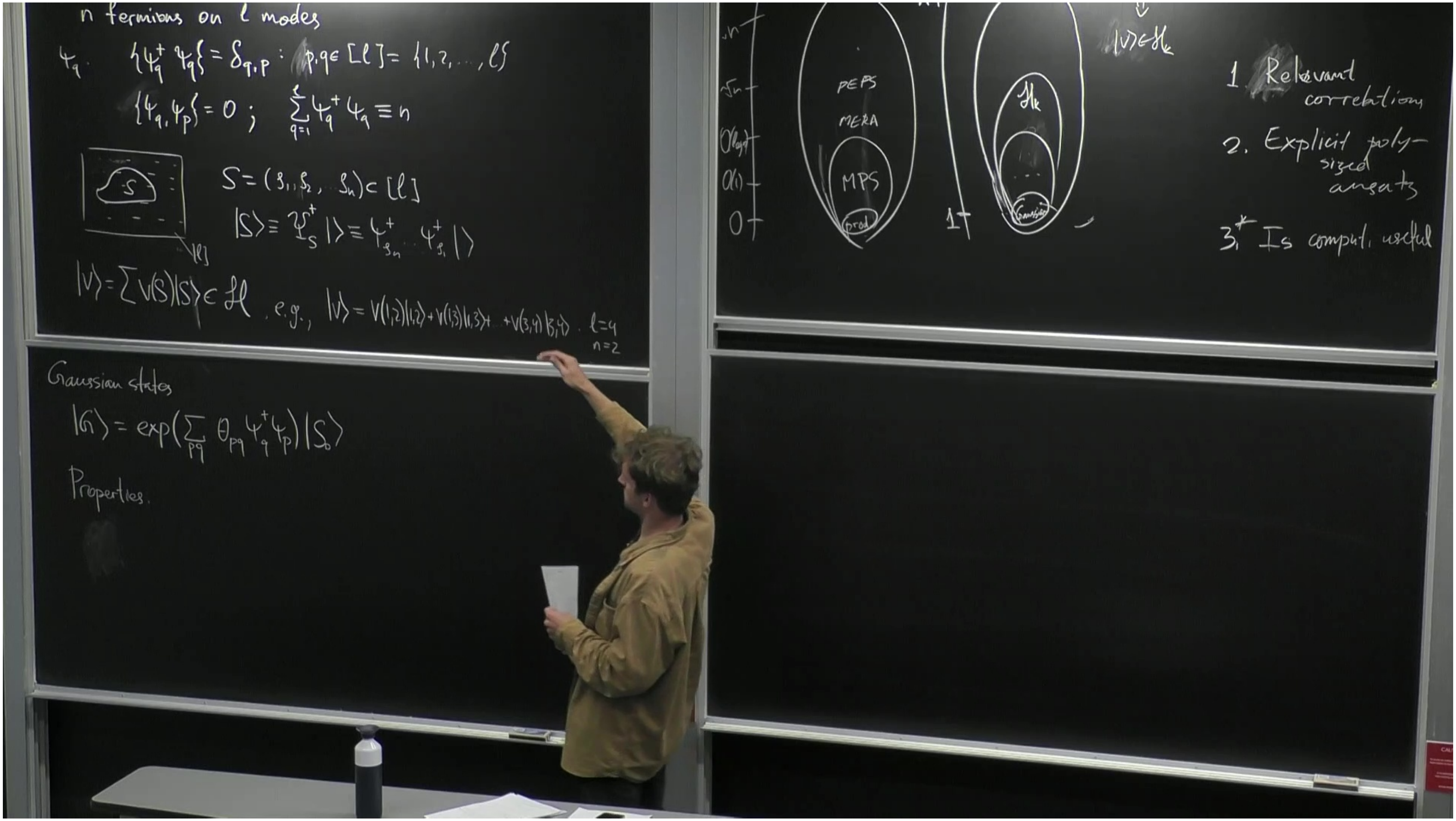
Abstract: The notorious exponential complexity of quantum problems can be avoided for systems with limited correlations. For example, states of one-dimensional systems with bounded entanglement are approximable by matrix product states. We consider fermionic systems, where correlations can be defined as deviations from Gaussian states. Heuristically, one expects a link between compact non-Gaussian ansatzes and bounded fermionic correlations. This connection, however, has not been rigorously demonstrated. Our work resolves this conceptual gap.

We focus on pure states with a fixed number of fermions. Generalizing the so-called Plücker relations, we introduce k-particle correlation measures ?_k. The vanishing of ?_k at a constant k defines a class H_k of states with limited correlations. These sets H_k are nested, ranging from Gaussian for k=1 to the full n-fermion Hilbert space H for k=n+1. States in H_{k=O(1)} can be represented using a non-Gaussian ansatz of polynomial size. Classes H_k have physical meaning, containing all truncated perturbation series around Gaussian states. We also identify non-perturbative examples of states in H_{k=O(1)}, by a numerical study of excited states in the 1D Hubbard model. Finally, we discuss the information-theoretic implications of our results for the widely used coupled-cluster ansatz.

Zoom Link: TBD


n fermions on ℓ modes
ψ_q : $\{\psi_q^+ \psi_q\} = \delta_{q,p}$: $p,q \in [\ell] = \{1,2,\dots,\ell\}$
$\{\psi_q, \psi_p\} = 0$; $\sum_{q=1}^{\ell} \psi_q^+ \psi_q \equiv n$
$S = (s_1, s_2, \dots s_n) \subset [\ell]$
$|S\rangle \equiv \Psi_S^+ |\rangle \equiv \psi_{s_n}^+ \dots \psi_{s_1}^+ |\rangle$
$|v\rangle = \sum v(S)|S\rangle \in \mathcal{H}$ e.g., $|v\rangle = v(1,2)|1,2\rangle + v(1,3)|1,3\rangle + \dots + v(3,4)|3,4\rangle$. $\ell=4$ $n=2$
Gaussian states
$|G\rangle = \exp(\sum_{pq} \theta_{pq} \psi_q^+ \psi_p)|S_0\rangle$
Properties.


S
PEPS
MERA
MPS
prod
k
$\omega_k(|\psi\rangle)=0$
$|\psi\rangle \in \mathcal{H}_k$
$\mathcal{H}_k$
1. Relaxed
2. poly-


n fermions on l modes
Gaussian states
Properties.
PEPS
MERA
MPS
prod
1. Relevant correlations
2. Explicit poly-sized ansatz
3. Is comput. useful

$$|V\rangle = \sum V(S)|S\rangle \in \mathcal{H}$$

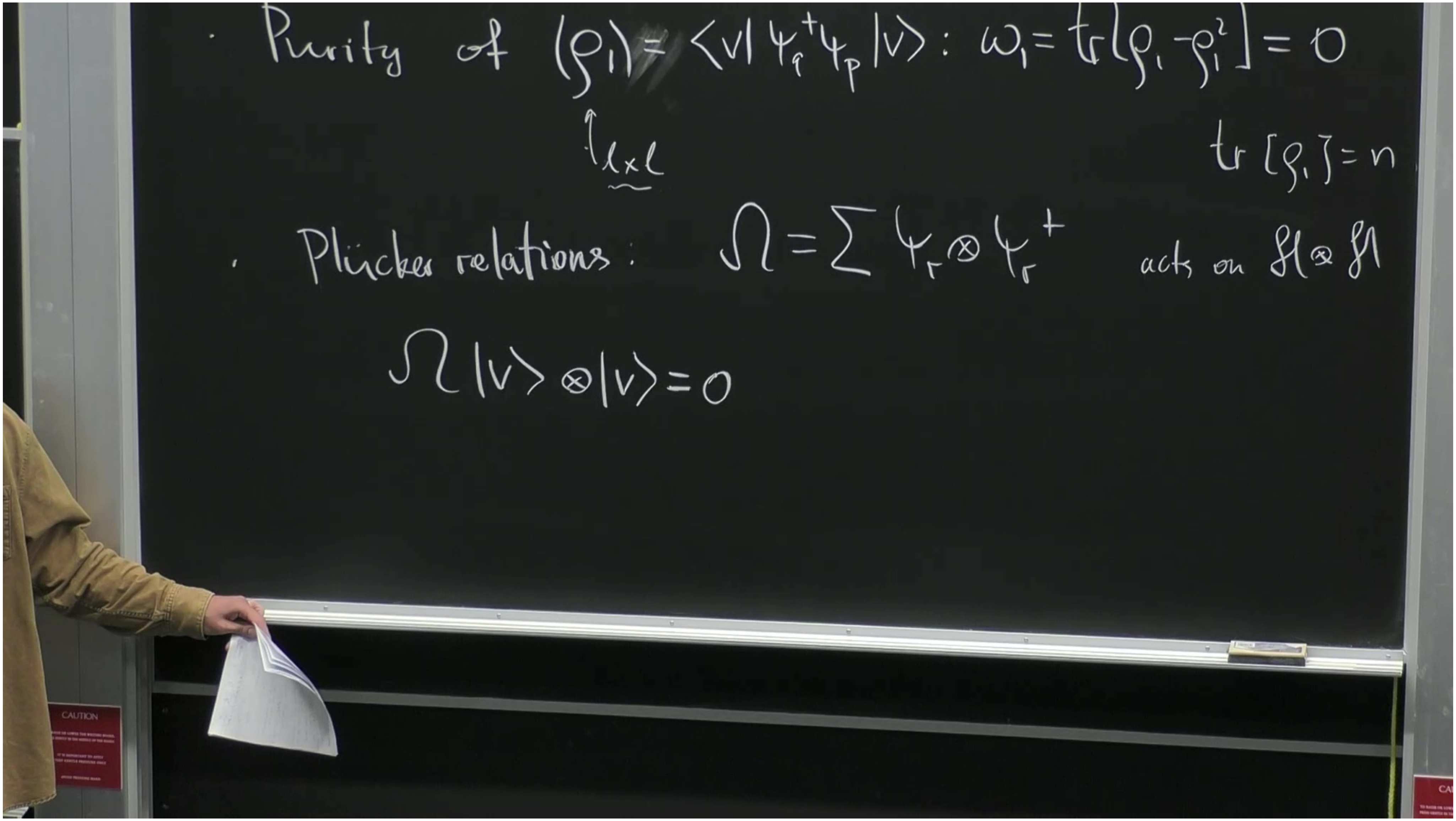
e.g., $|V\rangle = V(1,2)|1,2\rangle + V(1,3)|1,3\rangle + \ldots + V(3,4)|3,4\rangle$: $l=4$, $n=2$

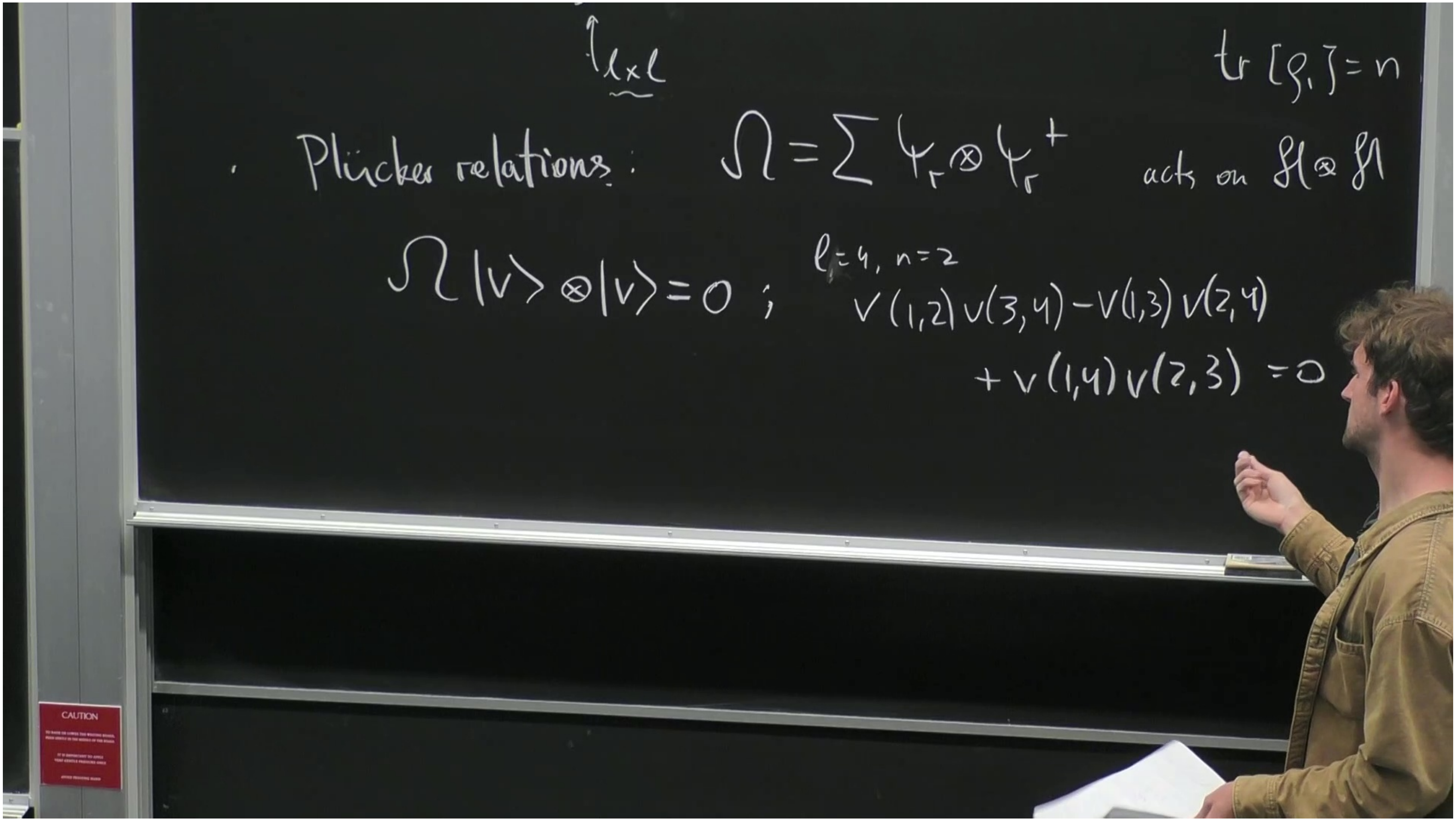
Gaussian states

$$|G\rangle = \exp\Big(\sum_{pq} \theta_{pq} \psi_q^\dagger \psi_p\Big)|S_0\rangle$$

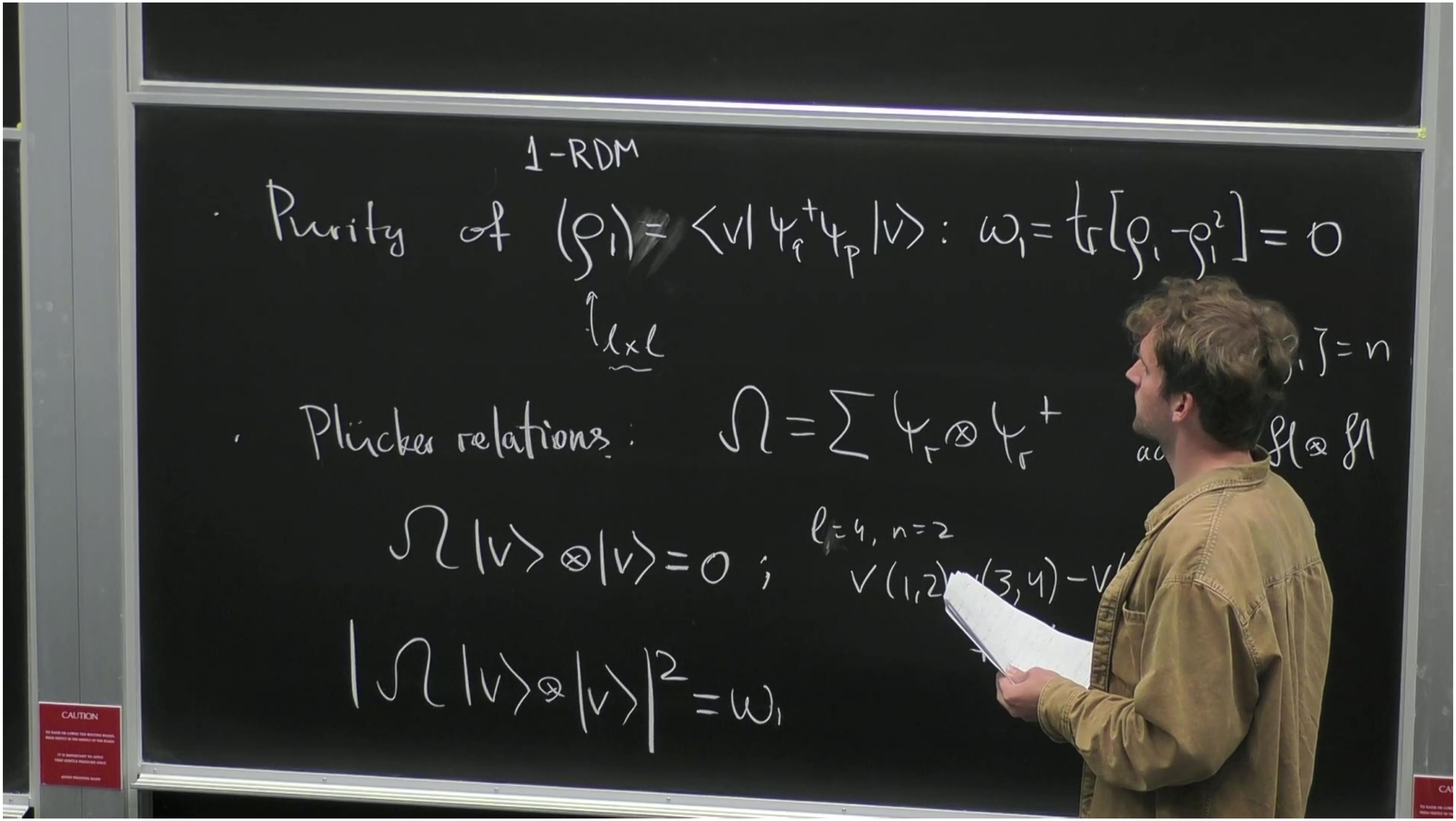
Properties:

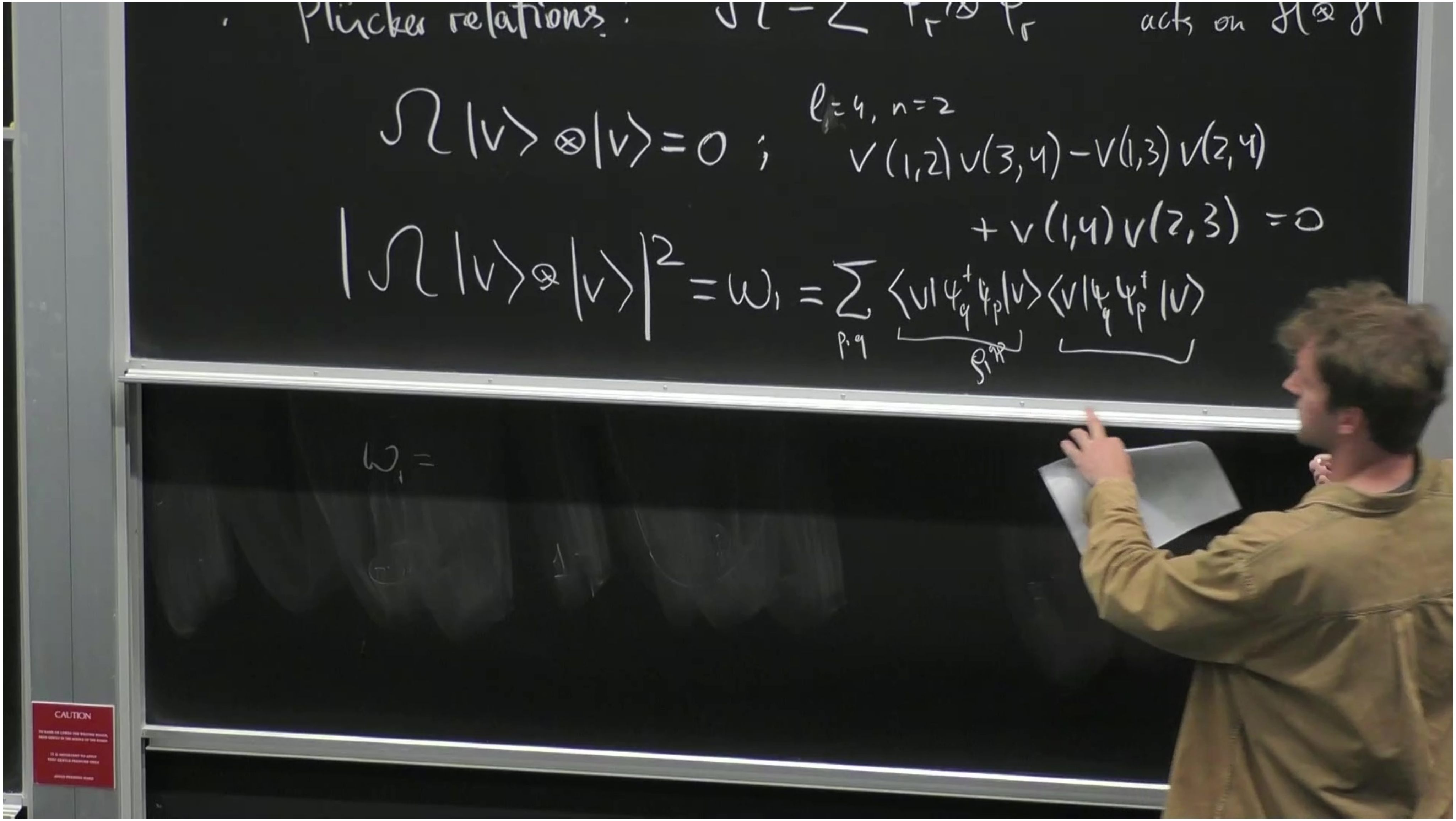
- Eigs of $H = \sum h_{pq} \psi_q^\dagger \psi_q$
- Wick's rule: $\langle G| \prod \psi_q^\dagger \prod \psi_p |G\rangle = \det\big(\langle G|\psi_q^\dagger \psi_p|G\rangle\big)$

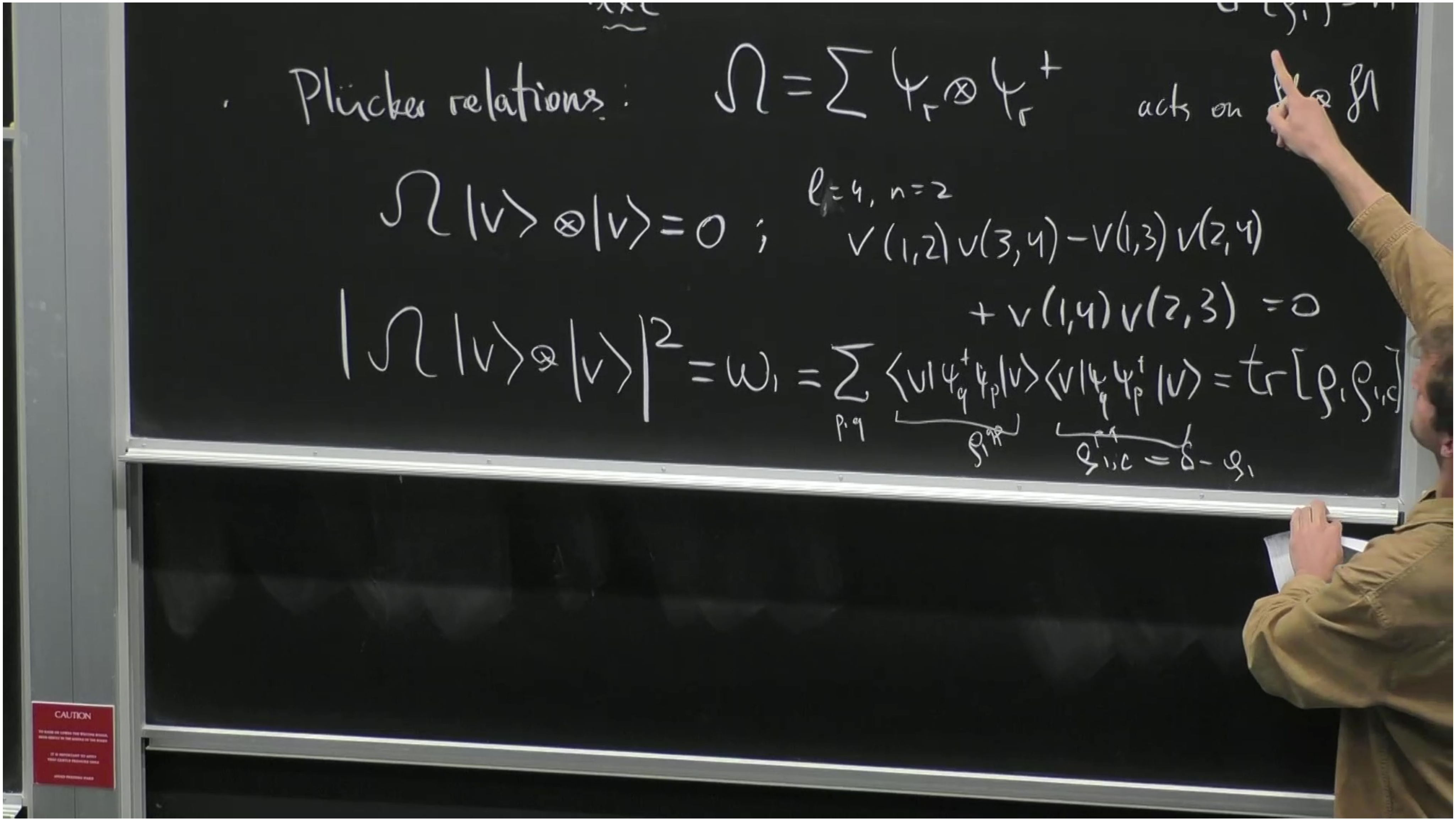

· Purity of (ρ₁) = ⟨v| ψ_q^+ ψ_p |v⟩ : ω₁ = tr[ρ₁ − ρ₁²] = 0
l×l
tr[ρ₁] = n
· Plücker relations: Ω = Σ ψ_r ⊗ ψ_r^+ acts on H⊗H
Ω |v⟩ ⊗ |v⟩ = 0
CAUTION



$1_{l \times l}$
$tr[\rho_1] = n$
· Plücker relations: $\Omega = \sum \psi_r \otimes \psi_r^+$ acts on $\mathcal{H} \otimes \mathcal{H}$
$\Omega |v\rangle \otimes |v\rangle = 0$;
$l = 4, n = 2$
$v(1,2)v(3,4) - v(1,3)v(2,4)$
$+ v(1,4)v(2,3) = 0$
CAUTION


1-RDM
· Purity of (ρ1) = ⟨v| ψq† ψp |v⟩ : ω1 = tr[ρ1 − ρ1²] = 0
ℓ×ℓ
· Plücker relations: Ω = Σ ψr ⊗ ψr†
Ω|v⟩ ⊗ |v⟩ = 0 ;
ℓ=4, n=2
|Ω|v⟩ ⊗ |v⟩|² = ω1
CAUTION


Plücker relations:
acts on
Ω|v⟩ ⊗ |v⟩ = 0 ;
l = 4, n = 2
v(1,2) v(3,4) − v(1,3) v(2,4)
+ v(1,4) v(2,3) = 0
|Ω|v⟩ ⊗ |v⟩|² = ω₁ = Σ_{p,q} ⟨v|ψ_q^† ψ_p|v⟩⟨v|ψ_q ψ_p^†|v⟩
ω₁ =
CAUTION


Plücker relations: Ω = Σ ψ_r ⊗ ψ_r^+
acts on
Ω|v⟩ ⊗ |v⟩ = 0 ;
l = 4, n = 2
v(1,2) v(3,4) − v(1,3) v(2,4) + v(1,4) v(2,3) = 0
|Ω|v⟩ ⊗ |v⟩|^2 = ω_1 = Σ_{p,q} ⟨v|ψ_q^+ ψ_p|v⟩⟨v|ψ_q ψ_p^+|v⟩ = tr[ρ_1 ρ_{1,c}]
ρ_1^{qp}
ρ_{1,c} = δ − ρ_1
CAUTION

$$\omega_1 = \mathrm{tr}[\rho_1 \rho_{1,c}] = 0$$

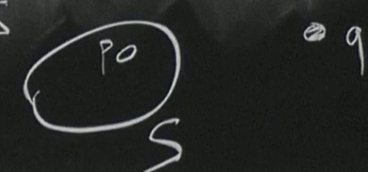
$$\Updownarrow$$

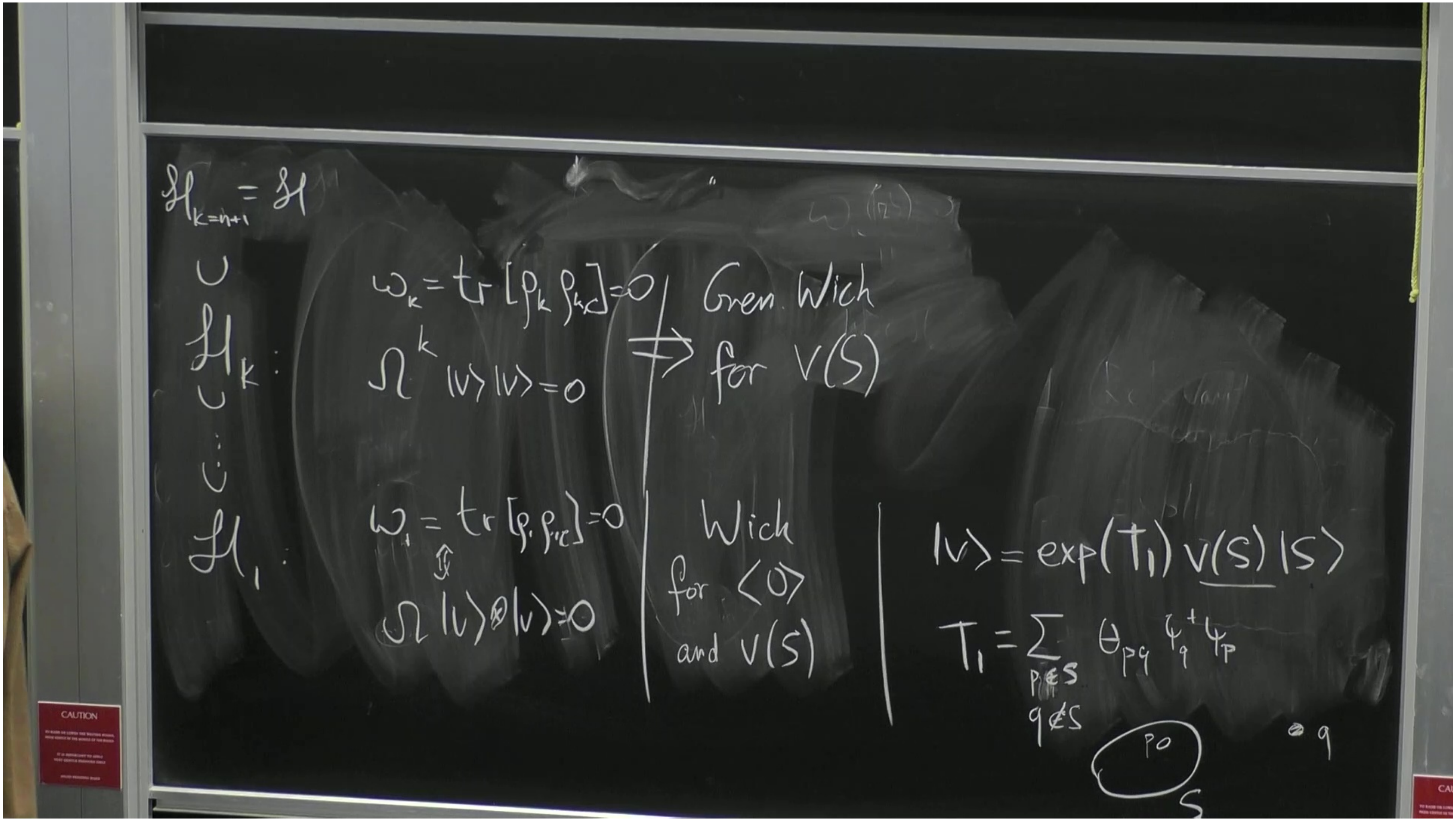
$$\Omega\, |v\rangle \otimes |v\rangle = 0$$

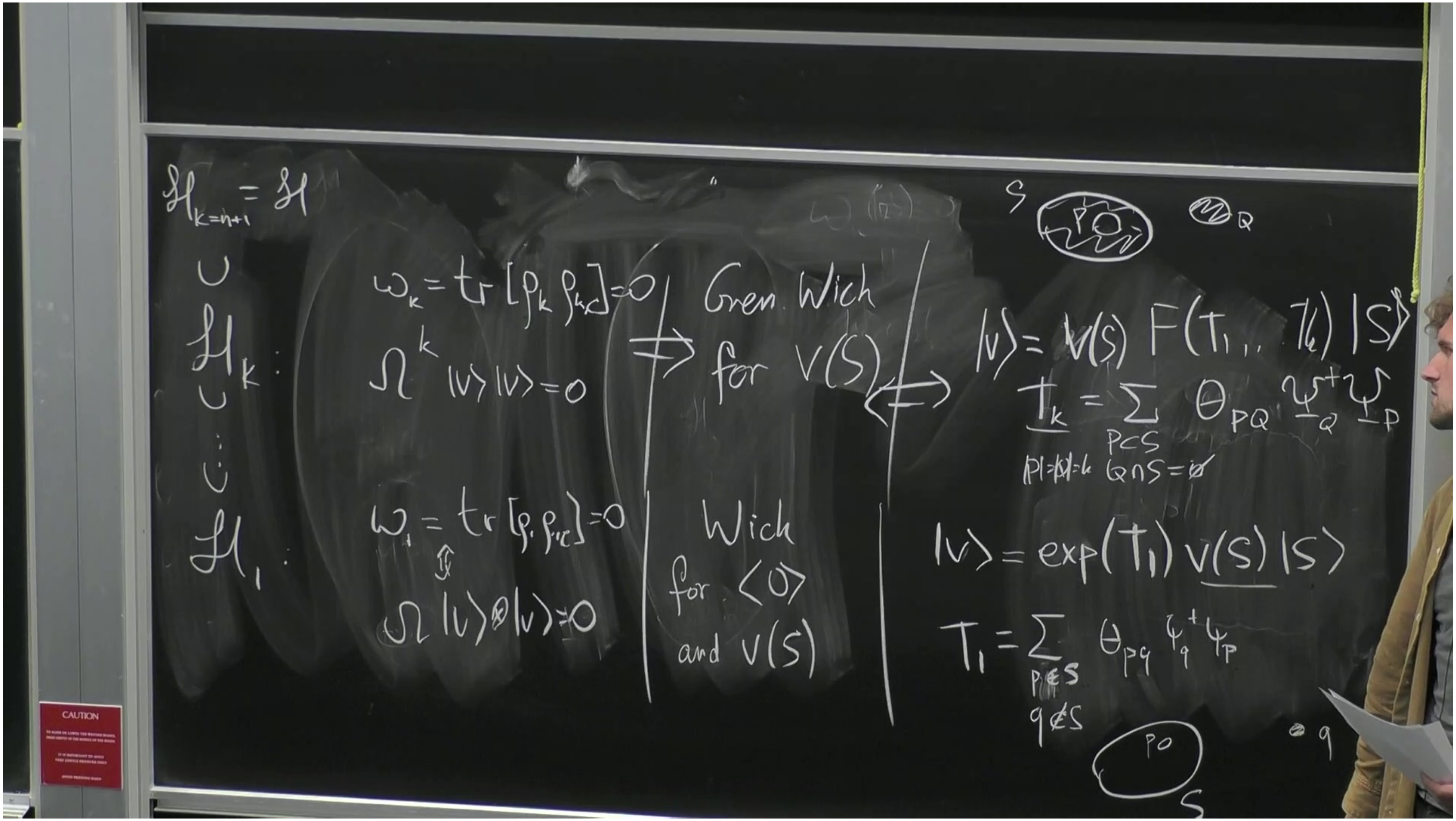
Wick
for $\langle O \rangle$
and $V(S)$

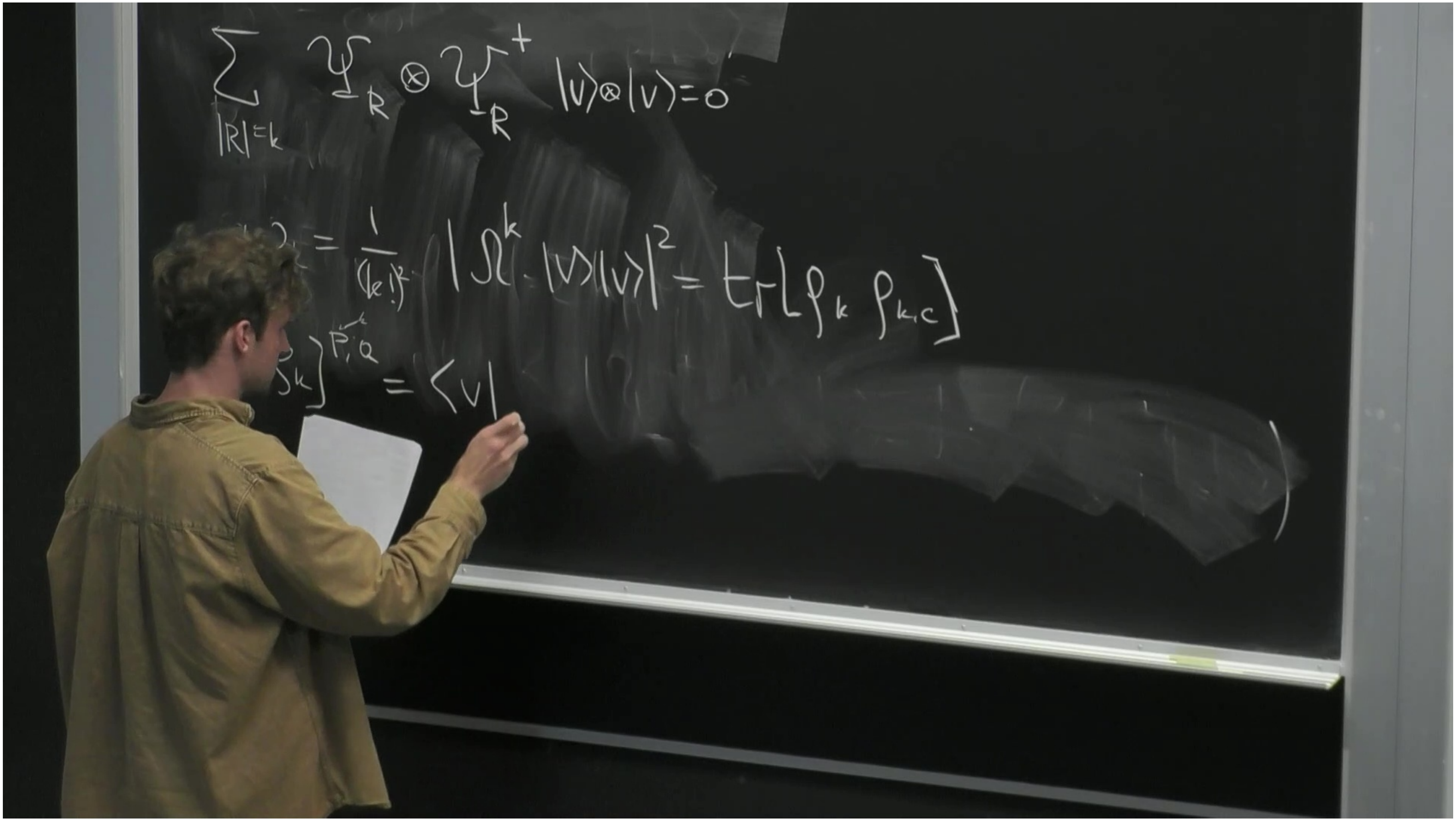
$$|v\rangle = \exp(T_1)\, V(S)\, |S\rangle$$

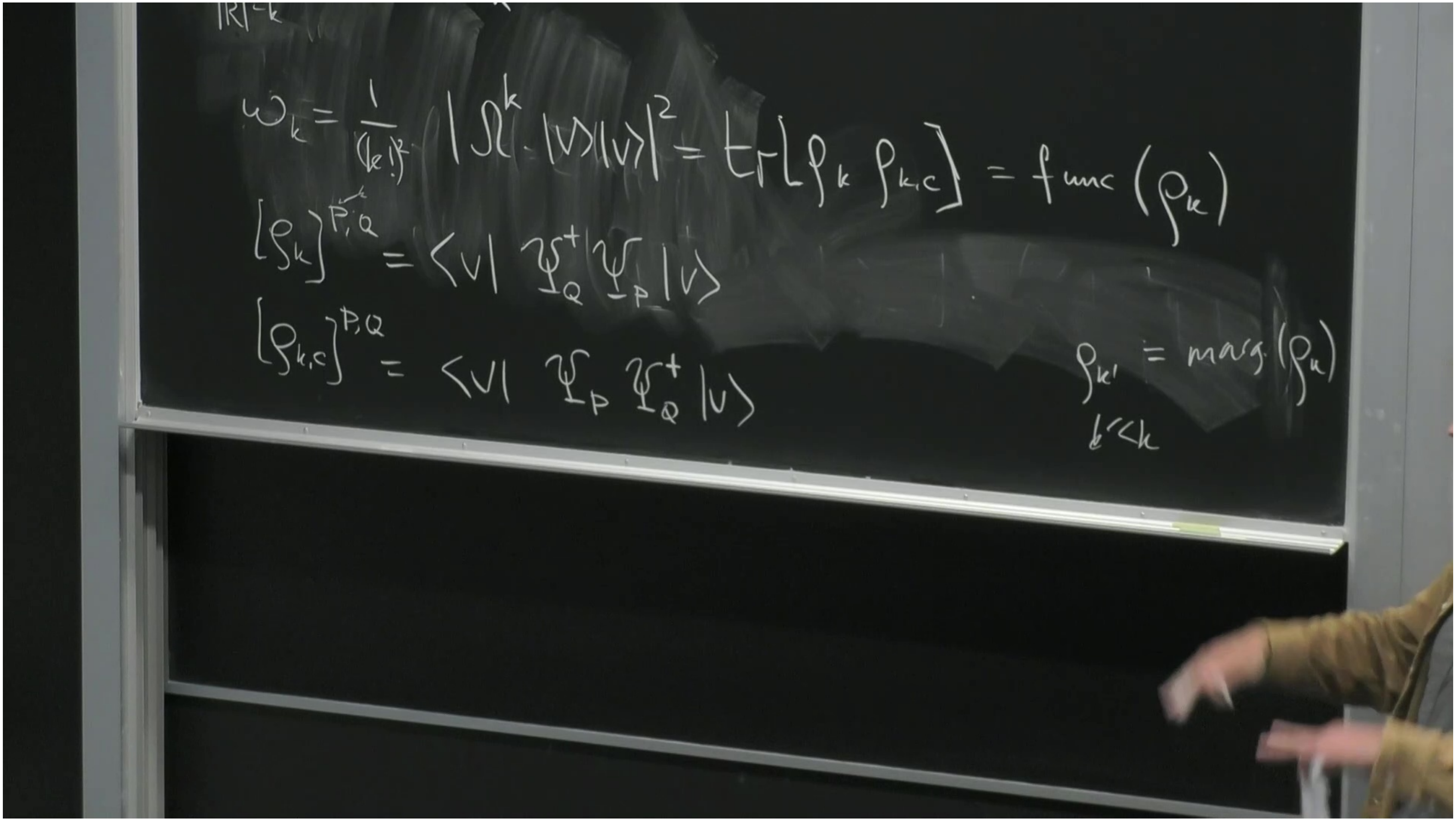
$$T_1 = \sum_{\substack{p \in S \\ q \notin S}} \theta_{pq}\, \psi_q^\dagger \psi_p$$

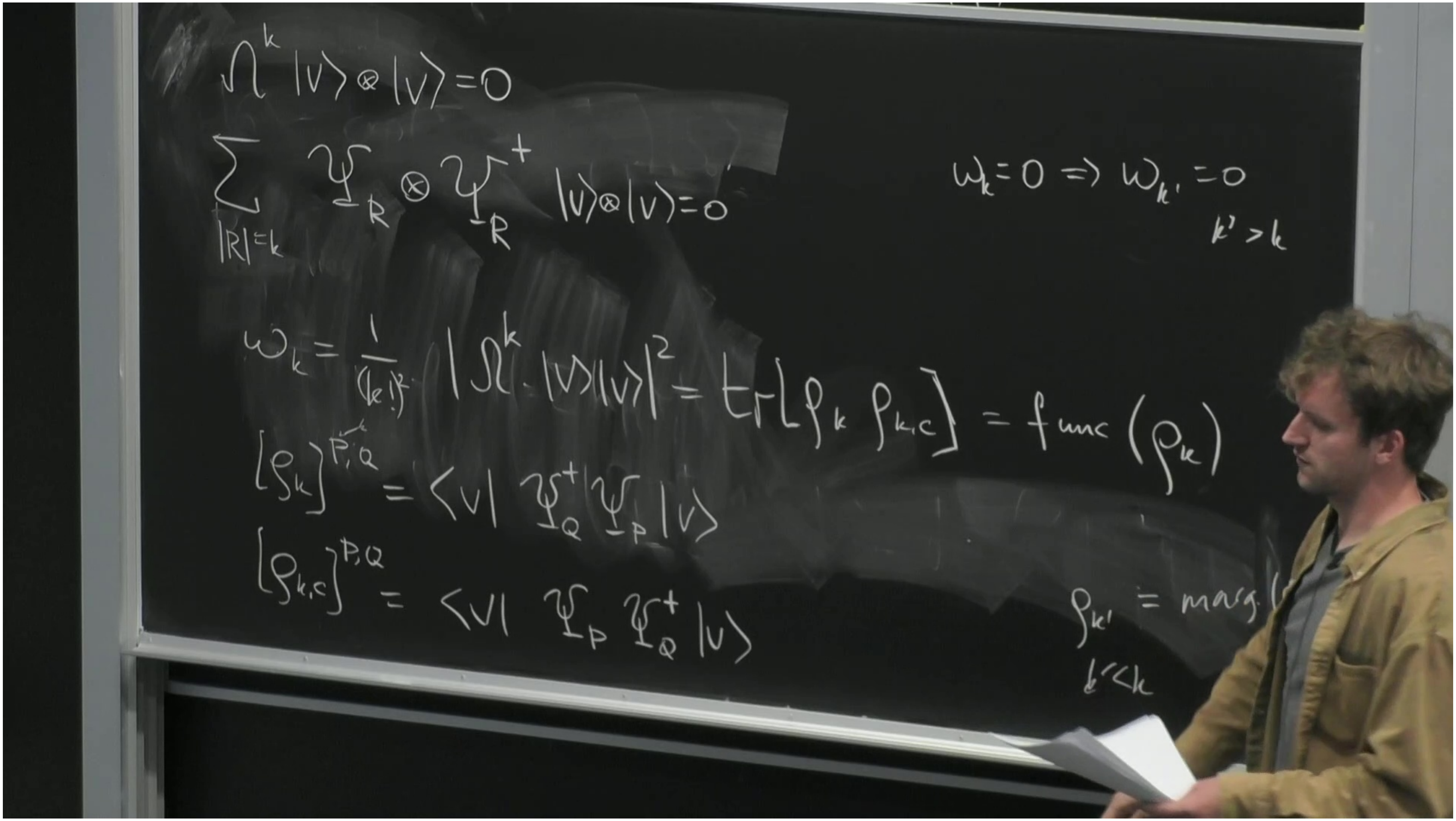


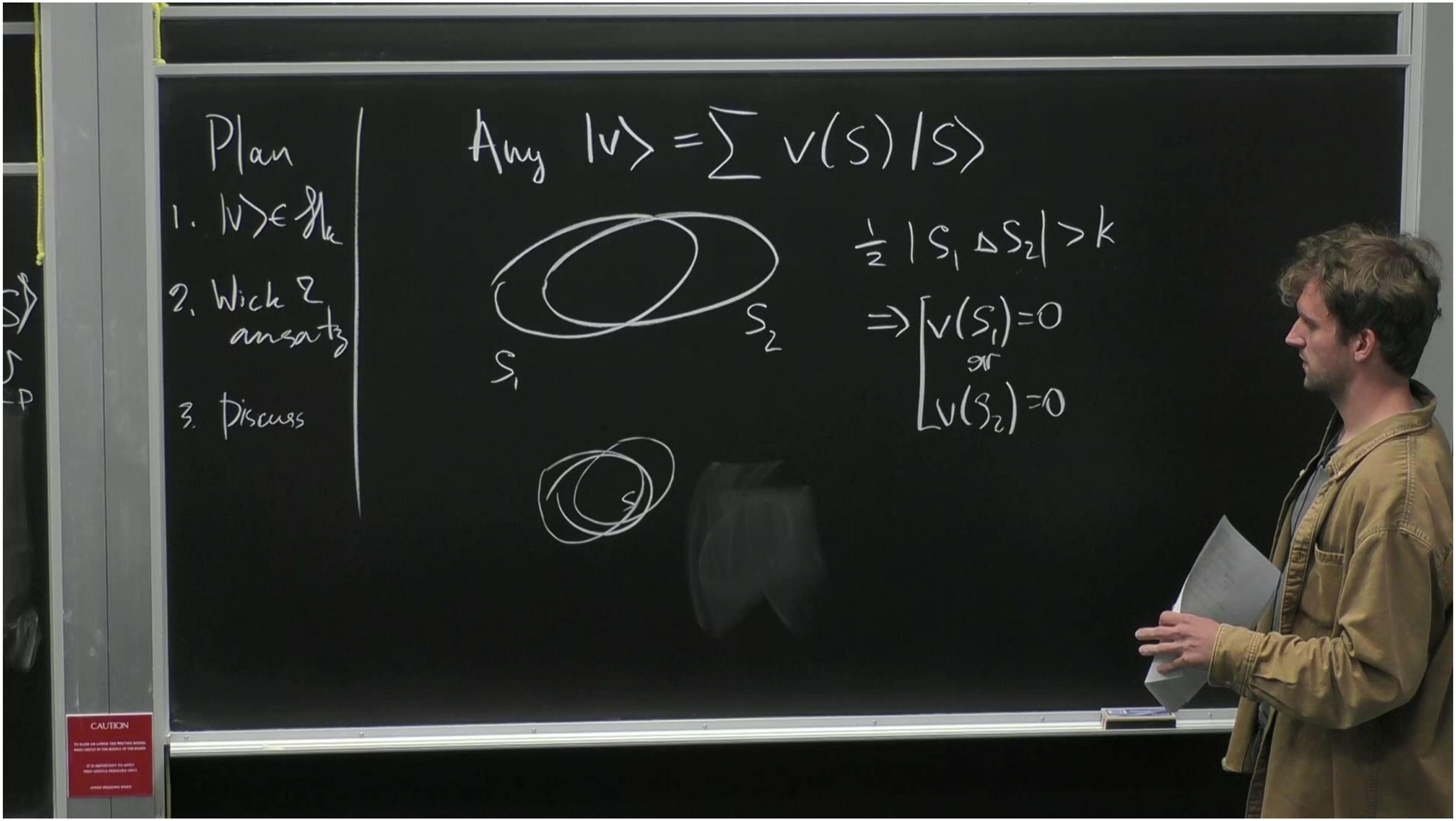

H_{k=n+1} = H
∪
H_k : ω_k = tr [ρ_k ρ_{k,c}] = 0
Ω^k |v⟩|v⟩ = 0
⇏ Gen. Wick for V(S)
∪
H_1 : ω_1 = tr [ρ_1 ρ_{1,c}] = 0
⇕
Ω |v⟩⊗|v⟩ = 0
Wick for ⟨O⟩ and V(S)
|v⟩ = exp(T_1) V(S) |S⟩
T_1 = Σ_{p∈S, q∉S} θ_{pq} ψ_q^† ψ_p
p
q
S
CAUTION

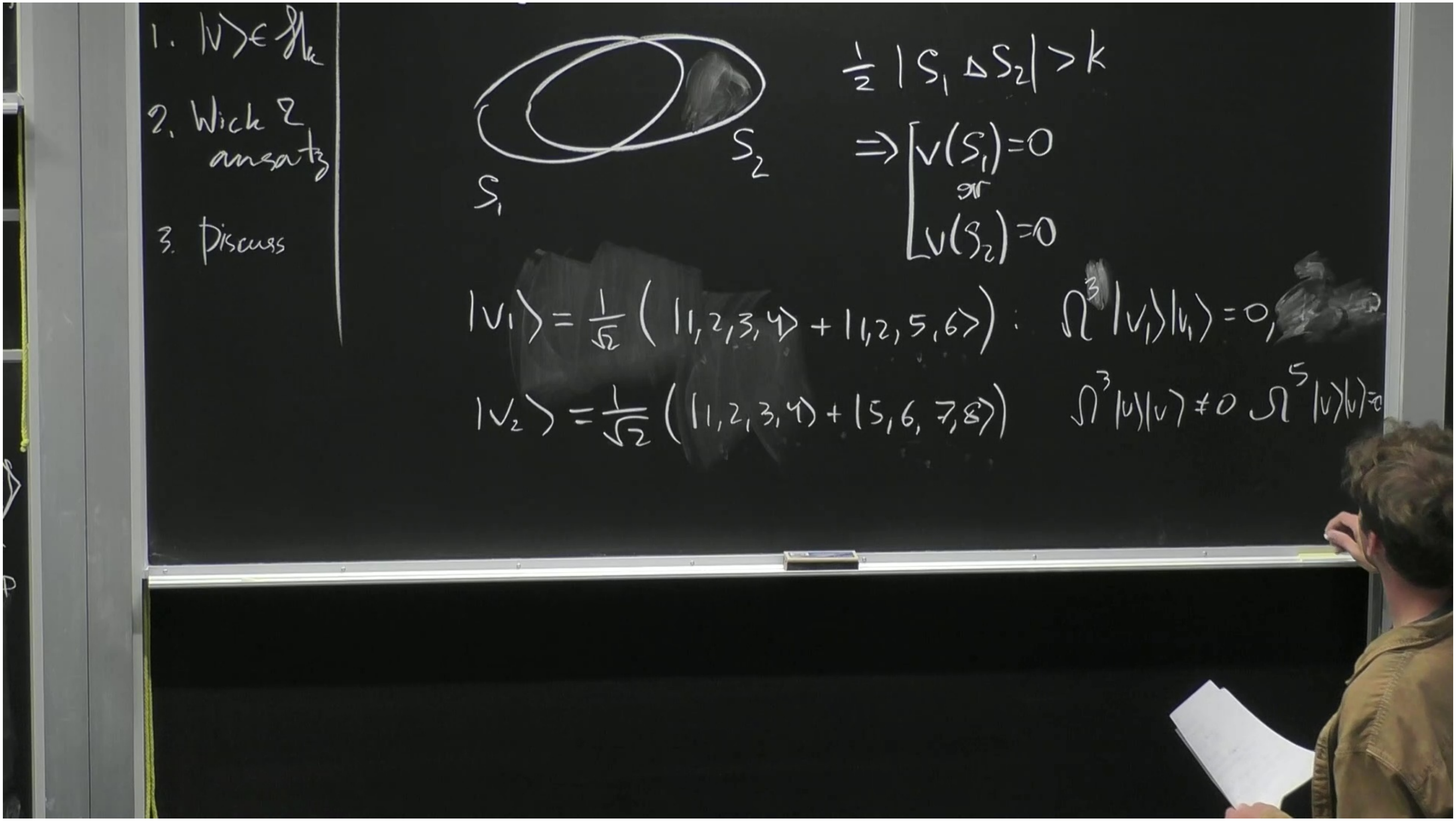

Gen. Wick
for V(S)
Wick
for ⟨O⟩
and V(S)
|v⟩ = V(S) F(T_1, .., T_k) |S⟩
|v⟩ = exp(T_1) V(S) |S⟩
ω_k = tr [ρ_k ρ_{k,c}] = 0
ω_1 = tr [ρ_1 ρ_{1,c}] = 0
p ∈ S
q ∉ S

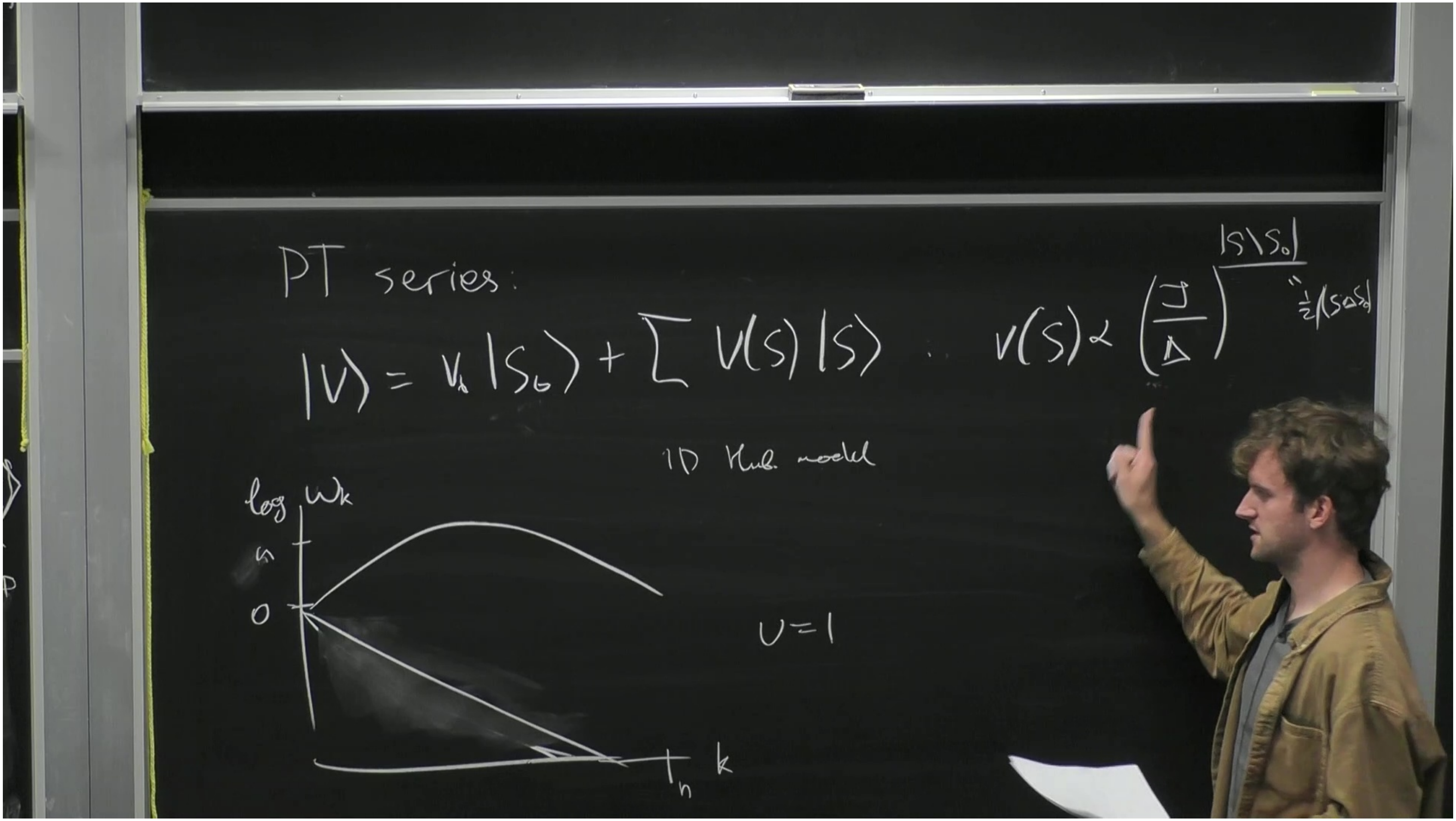


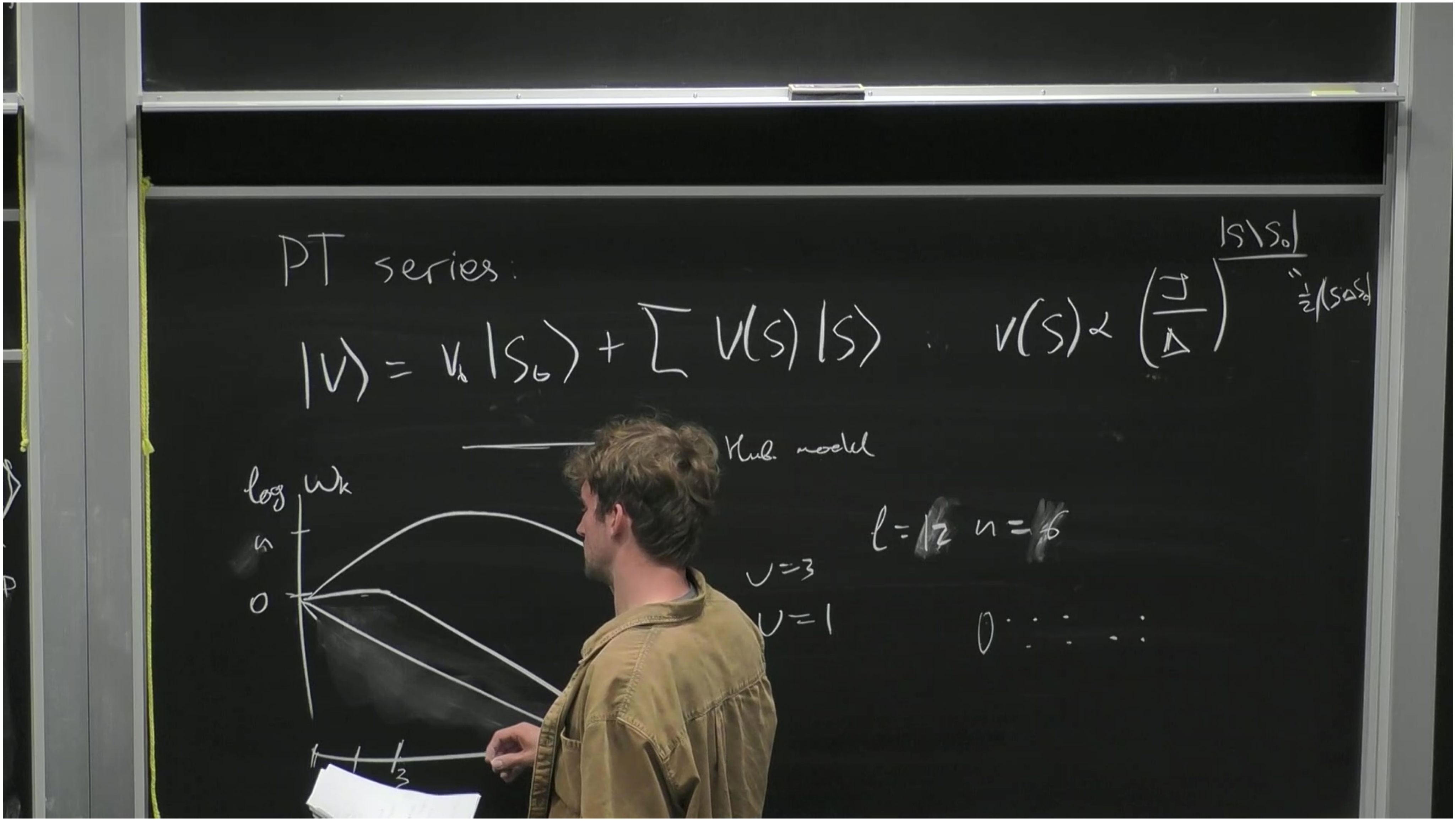

$\omega_k = \frac{1}{(k!)^2} | \Omega^k \cdot |v\rangle |v\rangle |^2 = tr[\rho_k \rho_{k,c}] = func(\rho_k)$
$[\rho_k]^{P,Q} = \langle v| \Psi_Q^+ \Psi_P |v\rangle$
$[\rho_{k,c}]^{P,Q} = \langle v| \Psi_P \Psi_Q^+ |v\rangle$
$\rho_{k'} = marg(\rho_k)$
$k' < k$

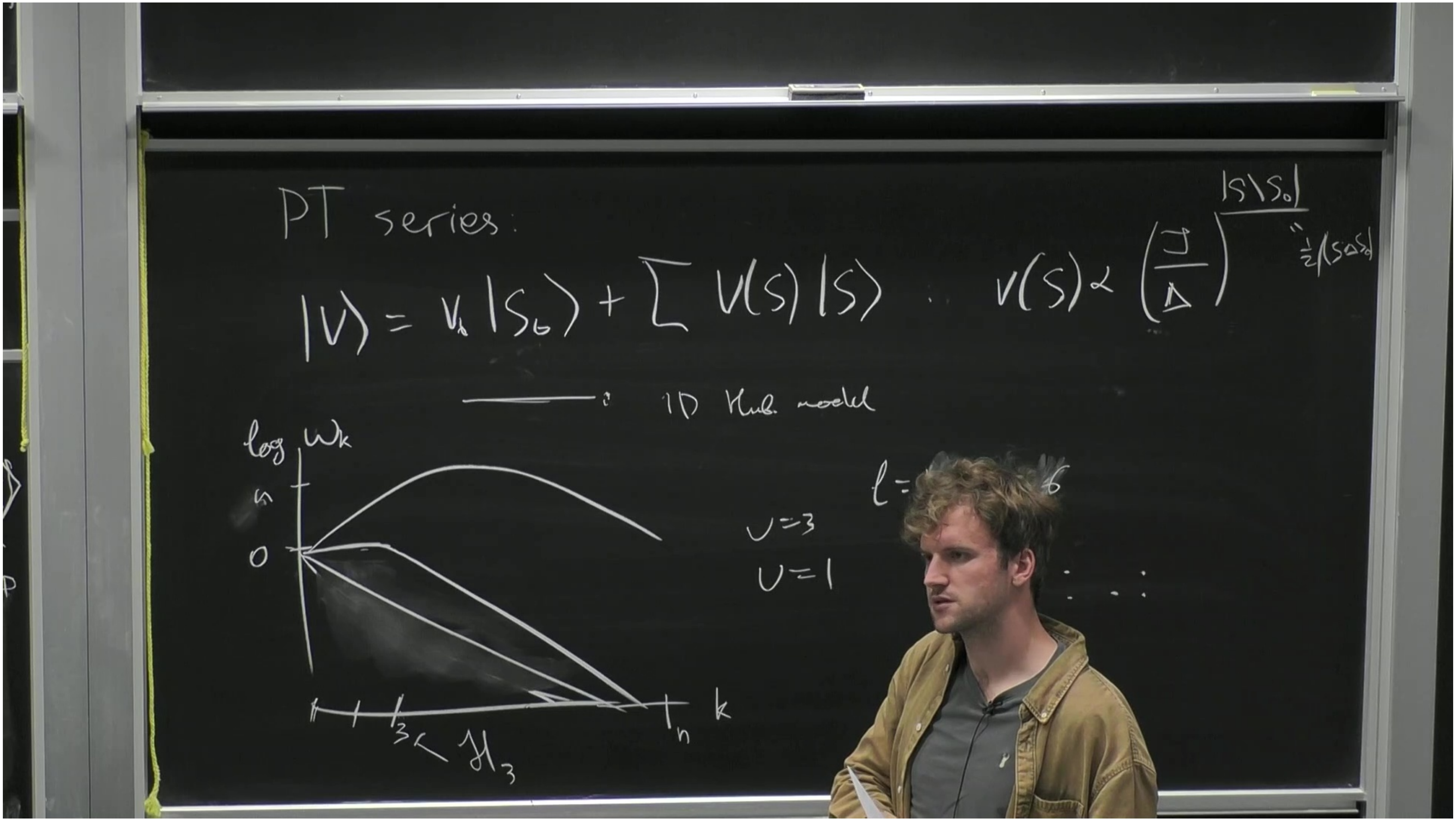

$\Omega^k |v\rangle \otimes |v\rangle = 0$
$\sum_{|R|=k} \Psi_R \otimes \Psi_R^\dagger |v\rangle \otimes |v\rangle = 0$
$\omega_k = 0 \Rightarrow \omega_{k'} = 0$
$k' > k$
$\omega_k = \frac{1}{(k!)^2} |\Omega^k \cdot |v\rangle|v\rangle|^2 = tr[\rho_k \rho_{k,c}] = func(\rho_k)$
$[\rho_k]^{P,Q} = \langle v| \Psi_Q^\dagger \Psi_P |v\rangle$
$[\rho_{k,c}]^{P,Q} = \langle v| \Psi_P \Psi_Q^\dagger |v\rangle$
$\rho_{k'} = marg.($
$k' < k$


Plan
1. |v⟩ ∈ $\mathcal{H}_k$
2. Wick & ansatz
3. Discuss
Any |v⟩ = Σ v(S) |S⟩
S₁
S₂
½ |S₁ Δ S₂| > k
⇒ v(S₁) = 0 or v(S₂) = 0
CAUTION

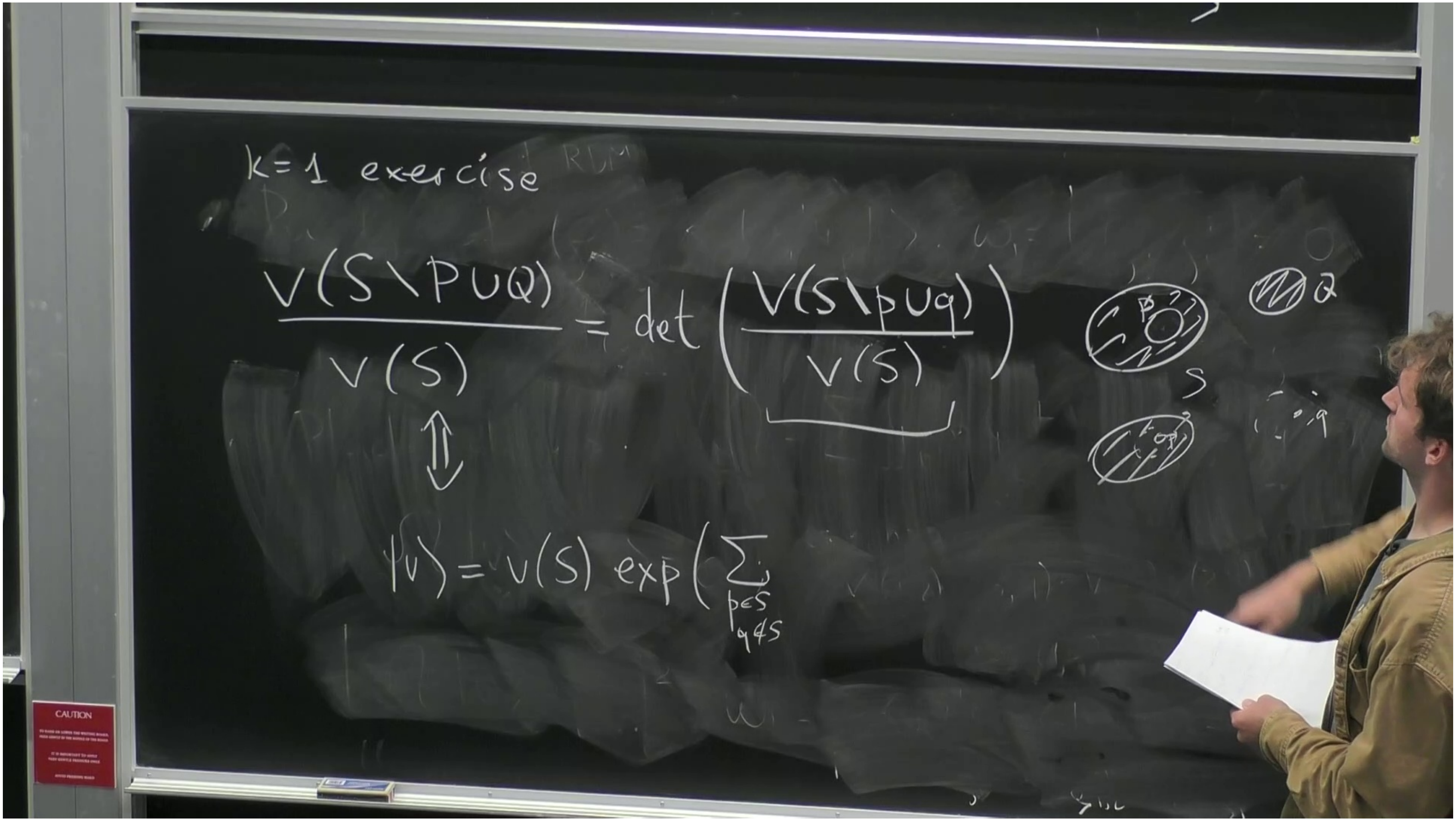

1. |v⟩ ∈ ℋk
2. Wick & ansatz
3. Discuss
S1
S2
½ |S1 Δ S2| > k
⇒ v(S1) = 0
or
v(S2) = 0
|v1⟩ = 1/√2 (|1,2,3,4⟩ + |1,2,5,6⟩) : Ω3 |v1⟩|v1⟩ = 0,
|v2⟩ = 1/√2 (|1,2,3,4⟩ + |5,6,7,8⟩) Ω3 |v⟩|v⟩ ≠ 0 Ω5 |v⟩|v⟩ = 0

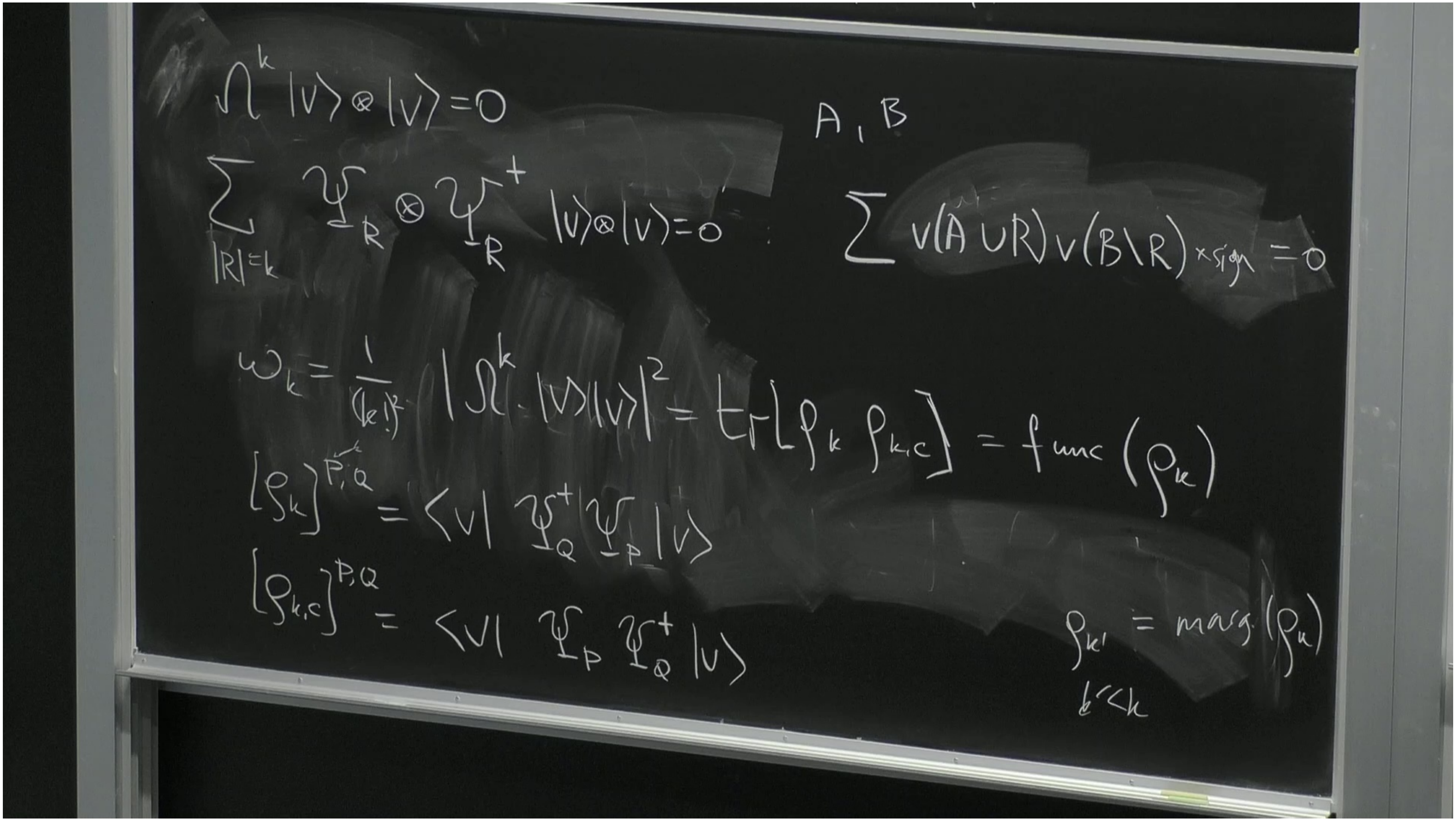

PT series:
|ψ⟩ = ψ₀ |S₀⟩ + Σ ψ(S) |S⟩
ψ(S) ∝ (J/Δ)^{|S\S₀|}
1D Hub. model
log w_k
0
U=1
k
n


PT series:
Hub. model
log Wk

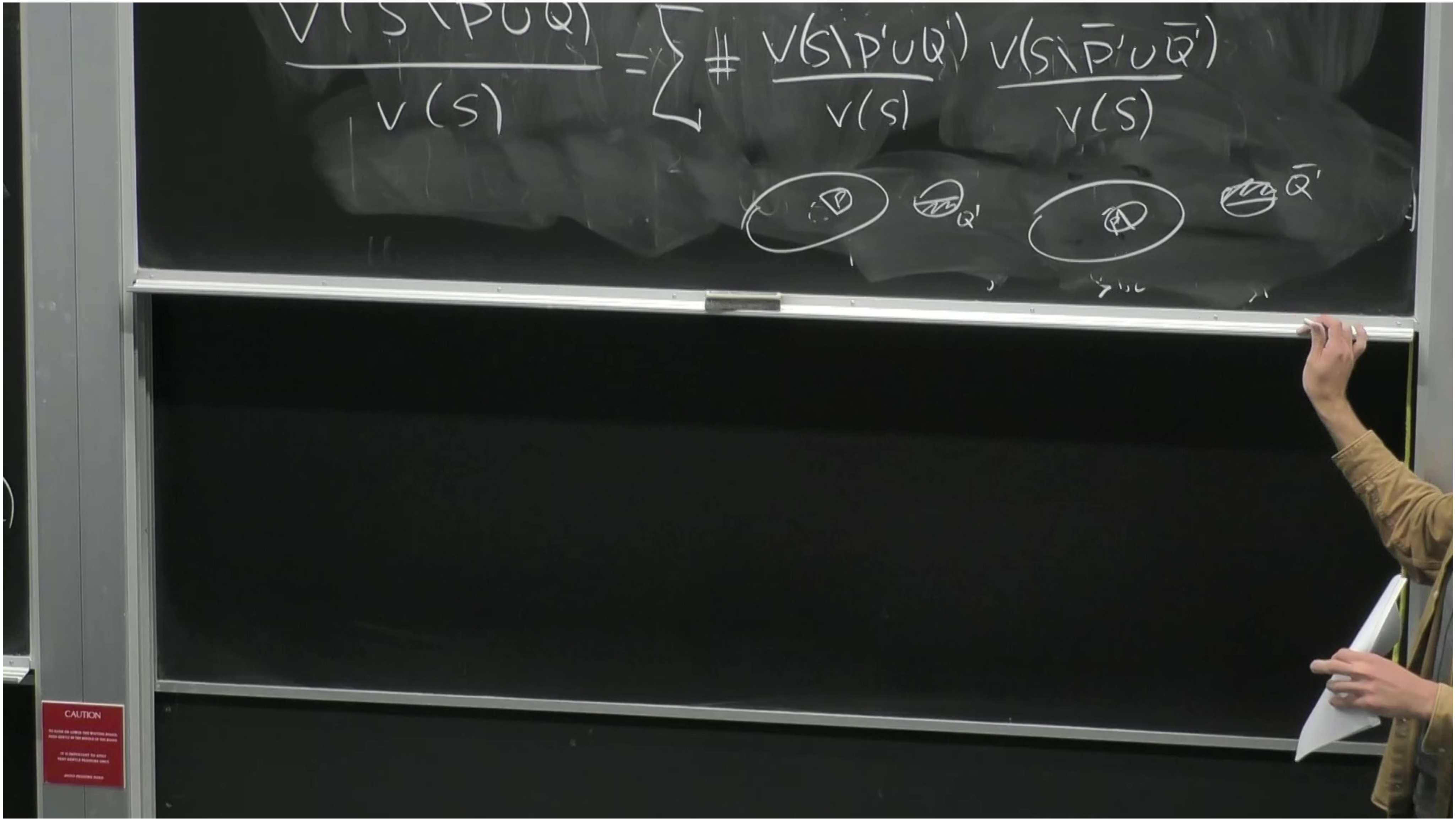


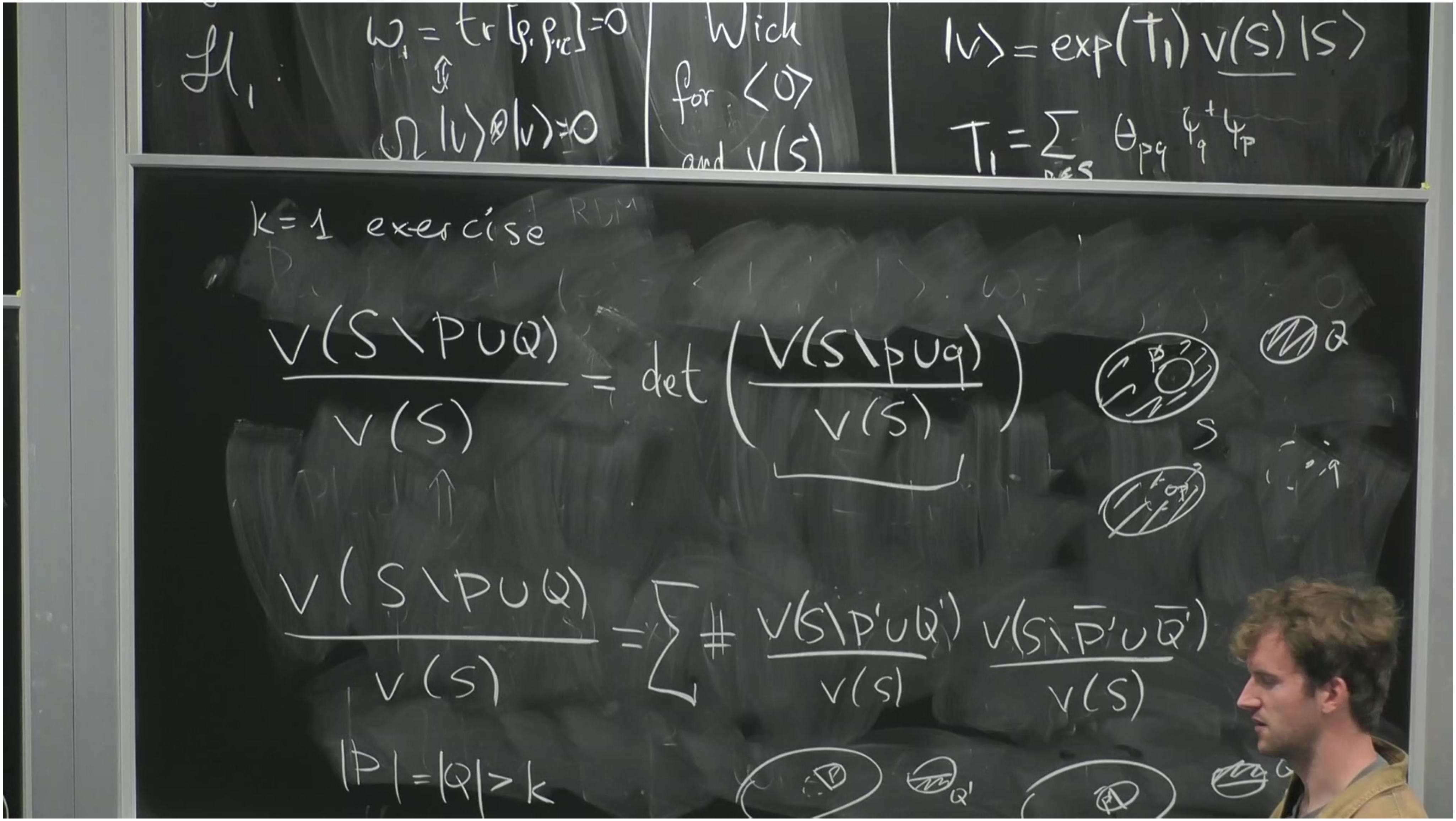
PT series:
$|V\rangle = V_0 |S_0\rangle + \sum V(S) |S\rangle$
$V(S) \propto \left(\frac{J}{\Delta}\right)^{|S \setminus S_0|}$
1D Hub. model
log w_k
$U=3$
$U=1$
k

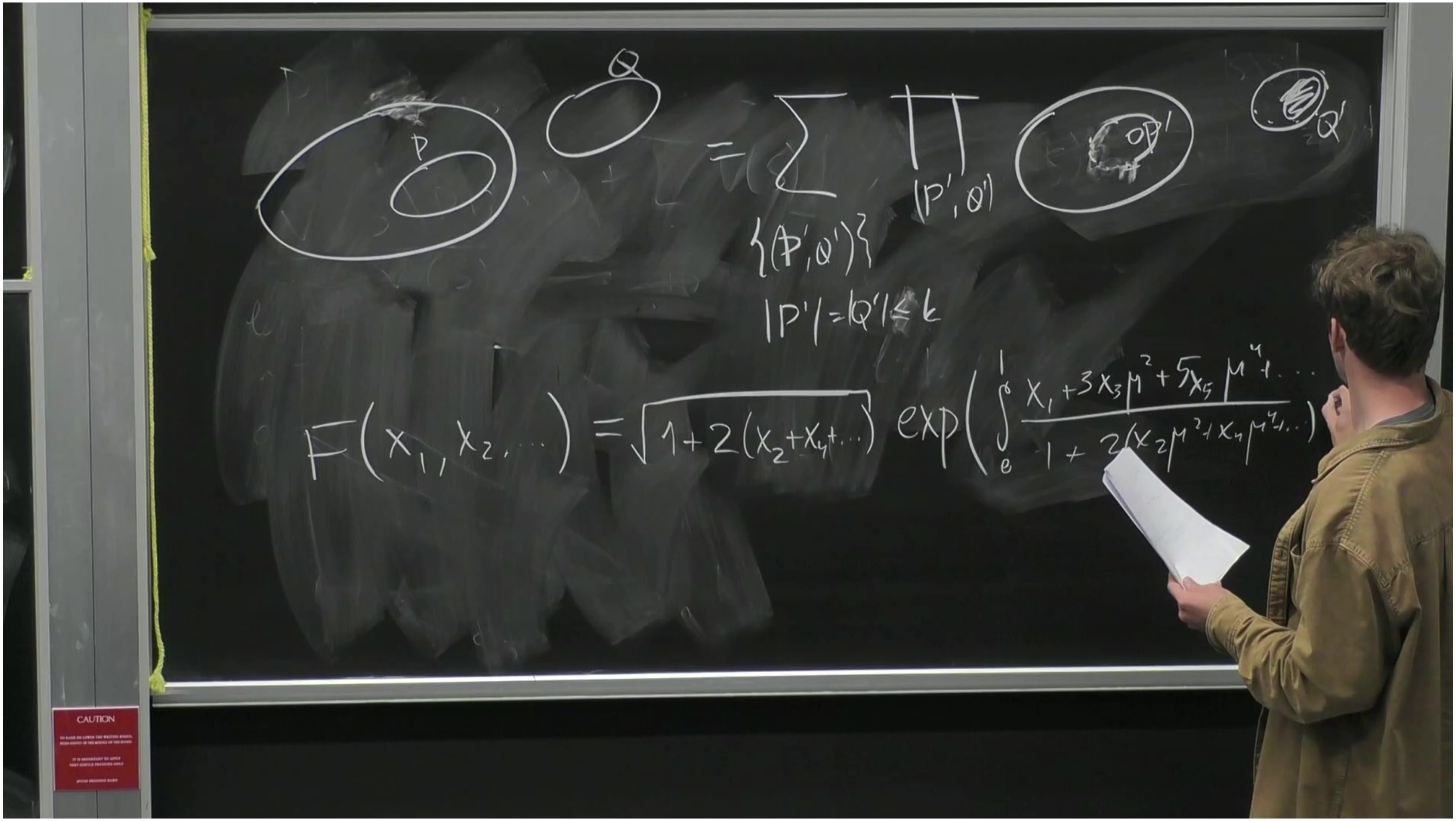

k=1 exercise
V(S\PUQ) / V(S) = det(V(S\pUq) / V(S))
⇕
|v⟩ = v(S) exp(Σ
p∈S
q∉S
Q
S

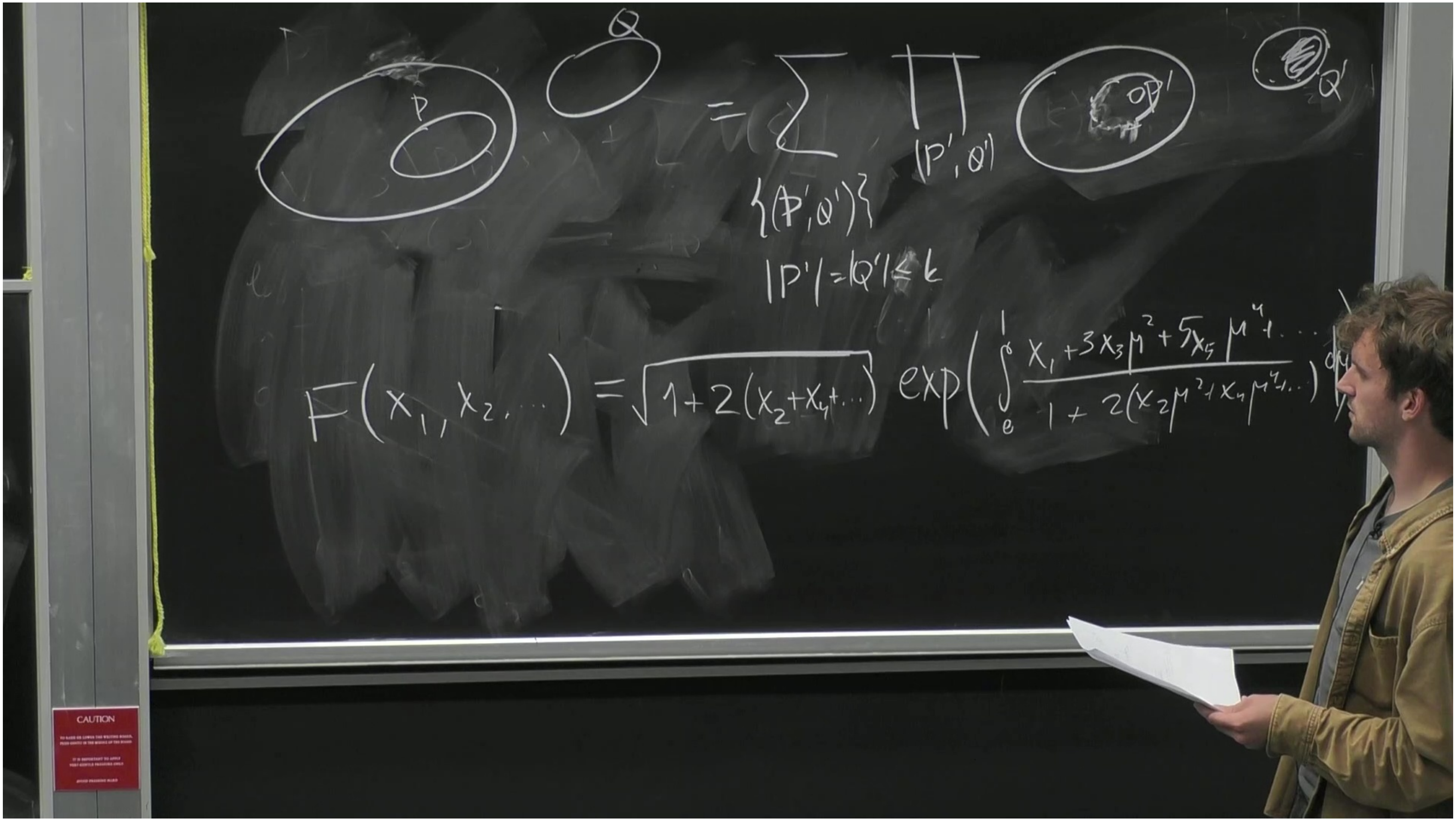


$\Omega^k |v\rangle \otimes |v\rangle = 0$
$\sum_{|R|=k} \Psi_R \otimes \Psi_R^{+} |v\rangle \otimes |v\rangle = 0$
A, B
$\sum v(A \cup R)\, v(B \setminus R) \times \text{sign} = 0$
$\omega_k = \frac{1}{(k!)^2} |\Omega^k |v\rangle|v\rangle|^2 = \mathrm{tr}[\rho_k \rho_{k,c}] = \mathrm{func}(\rho_k)$
$[\rho_k]^{P,Q} = \langle v| \Psi_Q^{+} \Psi_P |v\rangle$
$[\rho_{k,c}]^{P,Q} = \langle v| \Psi_P \Psi_Q^{+} |v\rangle$
$\rho_{k'} = \mathrm{marg.}(\rho_k)$
$k' < k$


CAUTION


ω₁ = tr[ρ₁ ρ₁,c] = 0
Ω |ν⟩ ⊗ |ν⟩ = 0
Wick
for ⟨O⟩
and ν(S)
|ν⟩ = exp(T₁) ν(S) |S⟩
T₁ = Σ θ_pq ψ_q† ψ_p
k = 1 exercise
ν(S \ P ∪ Q) / ν(S) = det (ν(S \ p ∪ q) / ν(S))
ν(S \ P ∪ Q) / ν(S) = Σ # ν(S \ P' ∪ Q') / ν(S) · ν(S \ P̄' ∪ Q̄') / ν(S)
|P| = |Q| > k


Q
P
= ∑ ∏
{(P',Q')} (P',Q')
|P'|=|Q'|≤k
OP'
Q'
F(x1, x2, ...) = √(1+2(x2+x4+...)) exp(∫ε^1 (x1+3x3μ^2+5x5μ^4+...)/(1+2(x2μ^2+x4μ^4+...))
CAUTION


P
Q
= Σ Π
{(P', Q')}
|P'| = |Q'| ≤ k
(P', Q')
F(x1, x2, ...) = √(1 + 2(x2 + x4 + ...)) exp(∫ x1 + 3x3μ² + 5x5μ⁴ + ... / 1 + 2(x2μ² + x4μ⁴ + ...) dμ)
CAUTION

$$\Omega^k |v\rangle \otimes |v\rangle = 0$$

$$\sum_{|R|=k} \Psi_R \otimes \Psi_R^\dagger \, |v\rangle \otimes |v\rangle = 0$$

A, B

$$Z(\beta) = \sum \omega_k \beta^{2k}$$

$$\sum_{|R|=k} v(A \cup R)\, v(B \setminus R) \times \text{sign} = 0$$

$$\omega_k = \frac{1}{(k!)^2} \left| \Omega^k \cdot |v\rangle|v\rangle \right|^2 = \mathrm{tr}[\rho_k \, \rho_{k,c}] = \text{func}(\rho_k)$$

$$[\rho_k]^{P,Q} = \langle v| \Psi_Q^\dagger \Psi_P |v\rangle$$

$$[\rho_{k,c}]^{P,Q} = \langle v| \Psi_P \Psi_Q^\dagger |v\rangle$$

$$\rho_{k'} = \text{marg.}(\rho_k)$$

$k' < k$