Title: PSI Lecture - Condensed Matter - Lecture 3

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Collection: PSI Lecture - Condensed Matter

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Today: More second quantization

Last time: Introduced $c^\dagger, c$ using Slater determinants

Correction: Normalization factor should be $\frac{1}{\sqrt{N!}}$ (not $\frac{1}{\sqrt{N}}$)

Many-particle Hilbert space with basis

$$|0\rangle,\ |\phi_1\rangle, \ldots, |\phi_N\rangle,\ \frac{1}{\sqrt{2}}\begin{vmatrix} |\phi_1\rangle & |\phi_1\rangle \\ |\phi_2\rangle & |\phi_2\rangle \end{vmatrix}, \ldots$$

$$\{c_i^\dagger, c_j^\dagger\} = 0$$

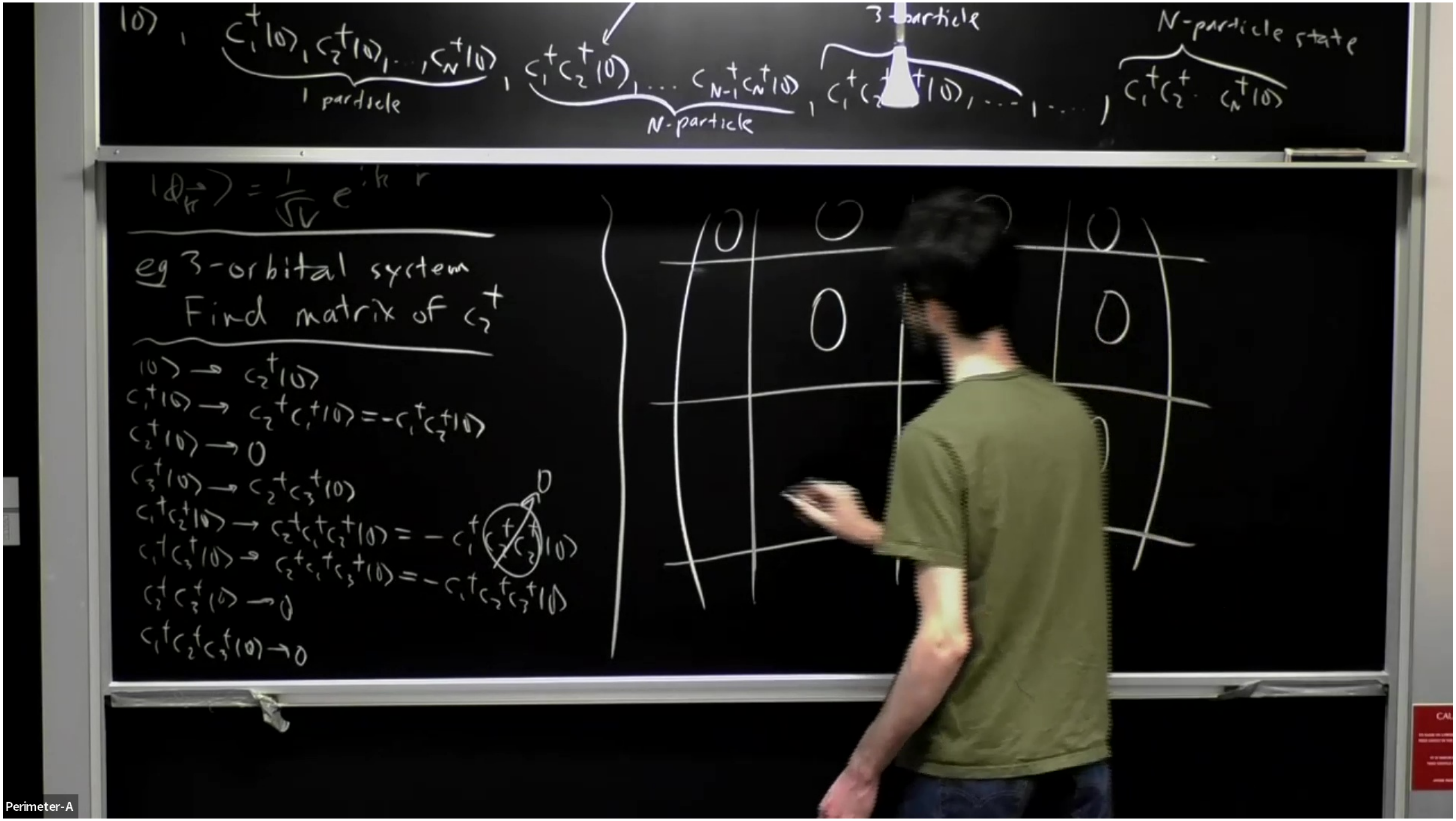
Write in terms of $c^\dagger$.

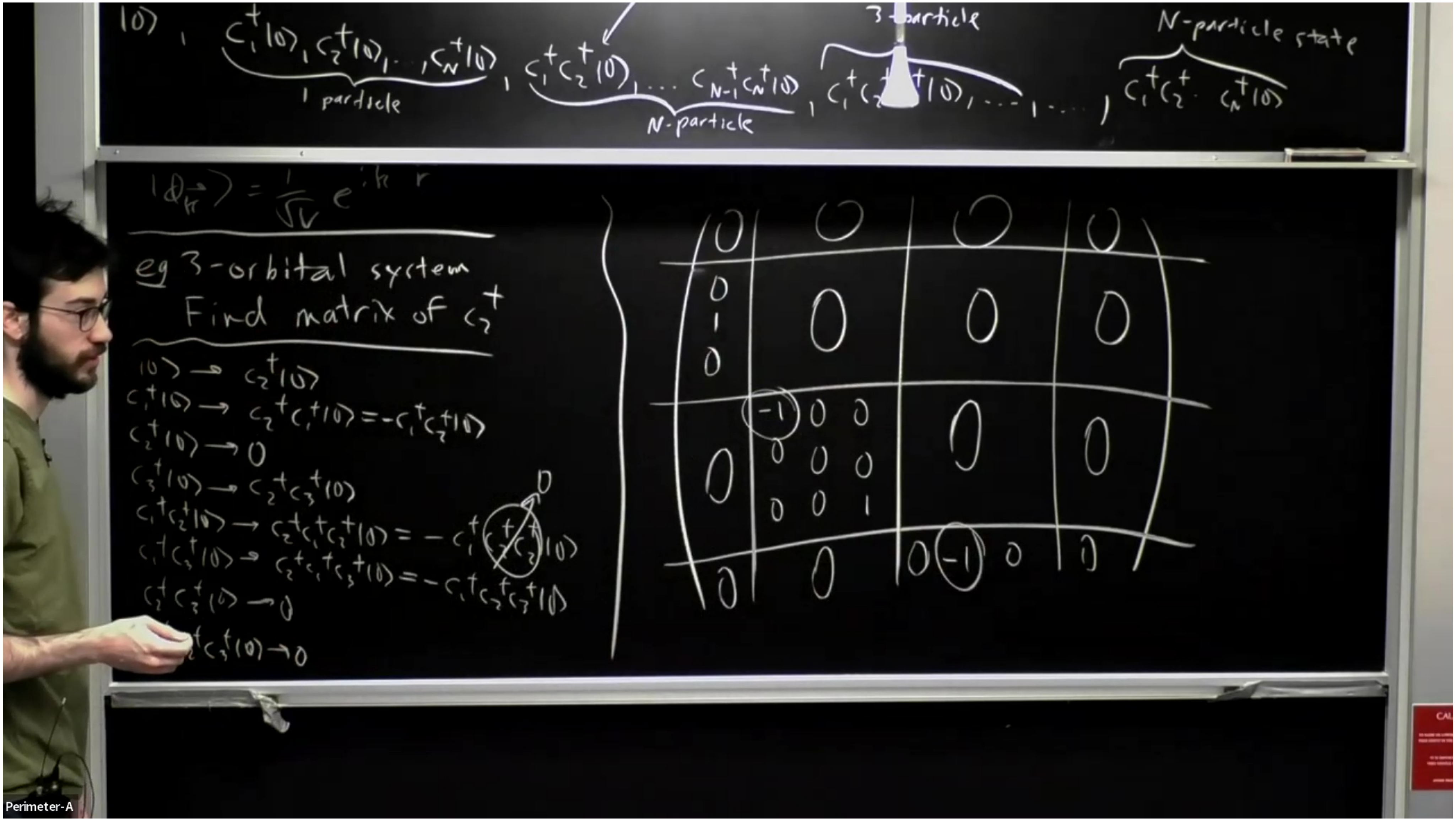
$$\underbrace{c_1^\dagger c_2^\dagger|0\rangle}_{} \to c_2^\dagger c_1^\dagger|0\rangle$$

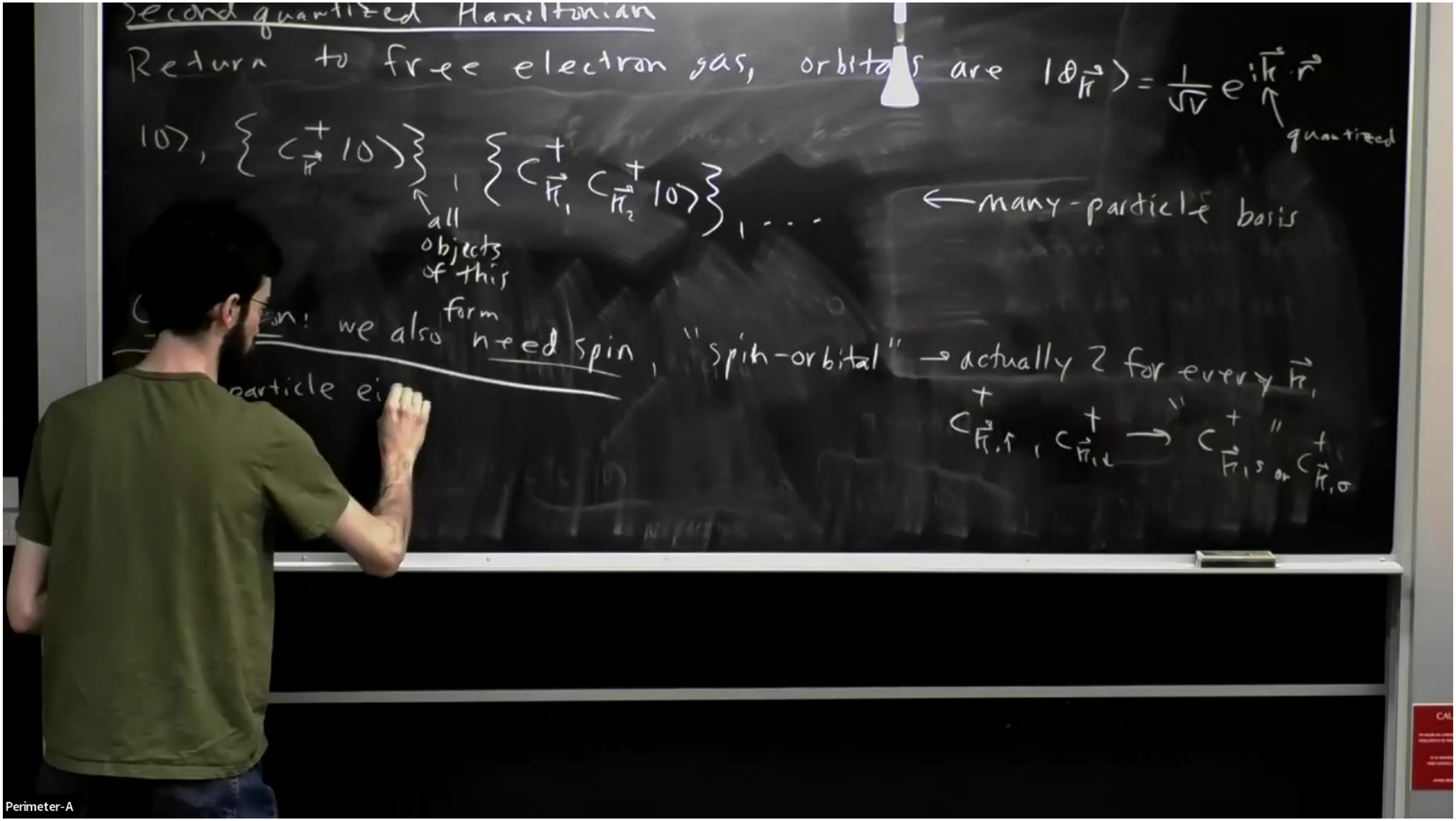
$\boxed{\text{Ok to define basis w/ } c^\dagger \text{ operators in any order. But must be consistent}}$

$$|0\rangle,\ \underbrace{c_1^\dagger|0\rangle, c_2^\dagger|0\rangle, \ldots, c_N^\dagger|0\rangle}_{1\text{ particle}},\ \underbrace{c_1^\dagger c_2^\dagger|0\rangle, \ldots, c_{N-1}^\dagger c_N^\dagger|0\rangle}_{N\text{-particle}},\ \overbrace{c_1^\dagger c_2^\dagger c_3^\dagger|0\rangle, \ldots}^{3\text{-particle}}, \ldots,\ \overbrace{c_1^\dagger c_2^\dagger \cdots c_N^\dagger|0\rangle}^{N\text{-particle state}}$$

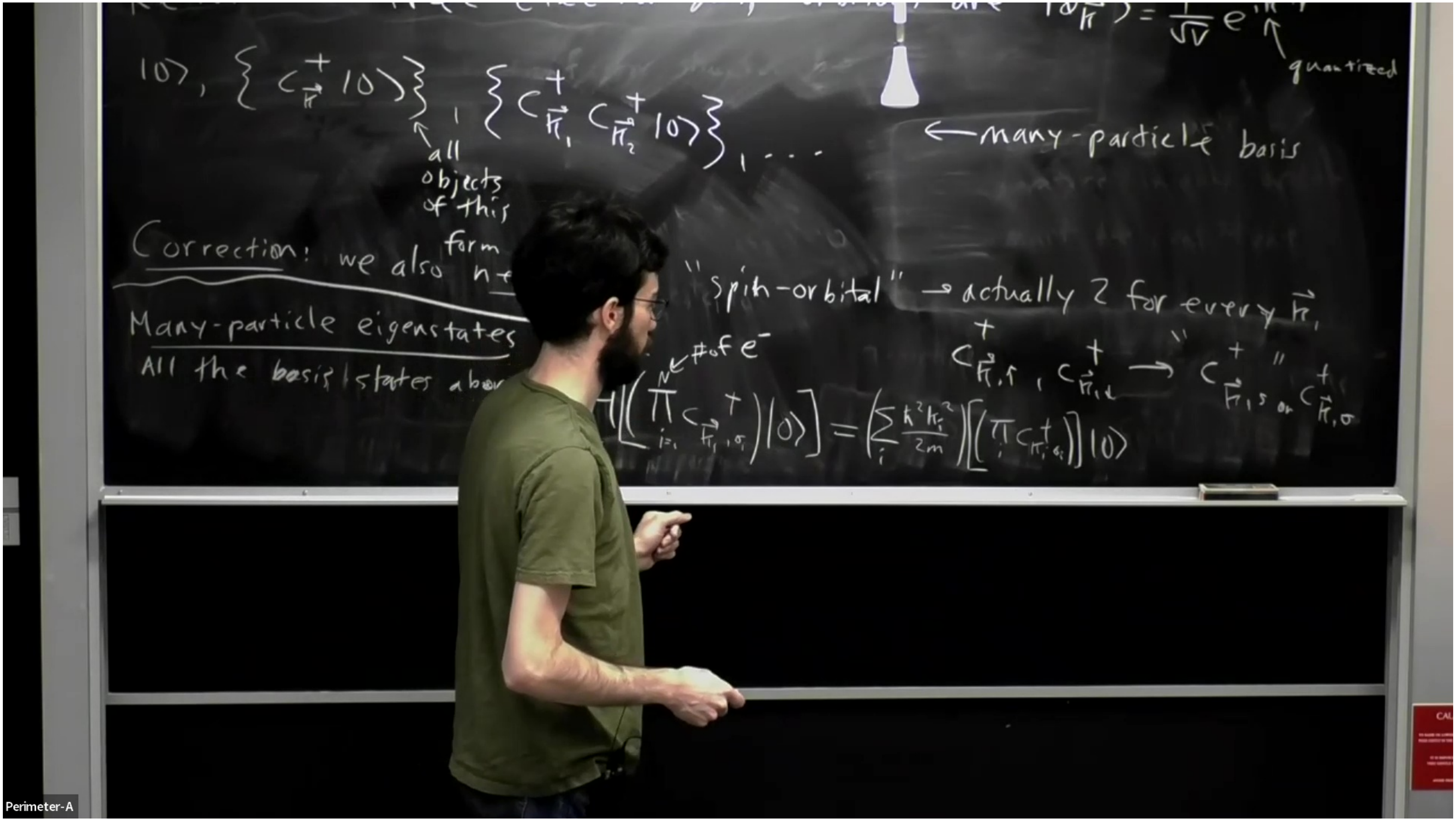
Perimeter-A

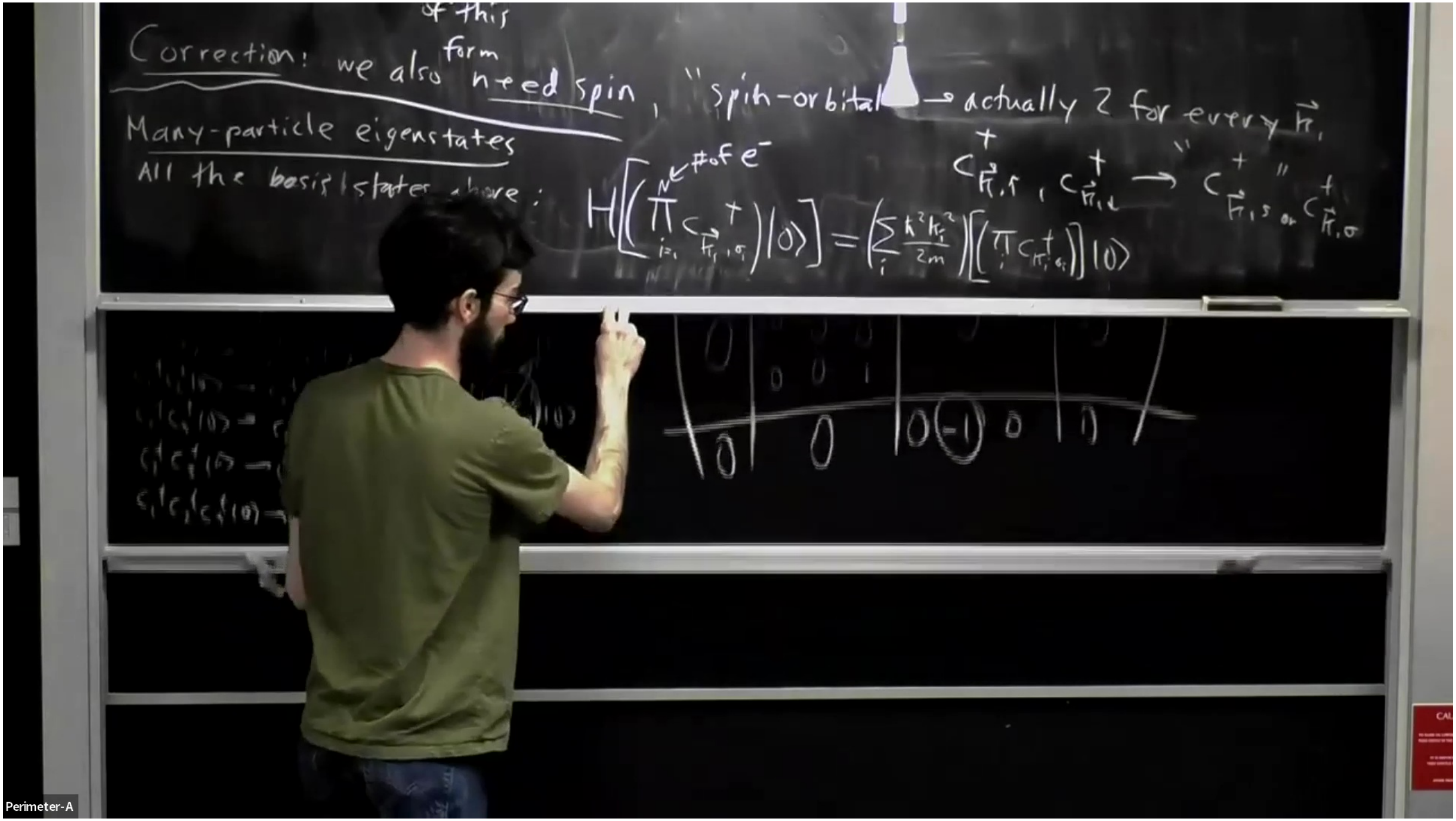

|0⟩, c1†|0⟩, c2†|0⟩, ..., cN†|0⟩, c1†c2†|0⟩, ... cN-1†cN†|0⟩, c1†c2†c3†|0⟩, ..., ..., c1†c2† ... cN†|0⟩
1 particle
N-particle
3-particle
N-particle state
eg 3-orbital system
Find matrix of c2†
|0⟩ → c2†|0⟩
c1†|0⟩ → c2†c1†|0⟩ = −c1†c2†|0⟩
c2†|0⟩ → 0
c3†|0⟩ → c2†c3†|0⟩
c1†c2†|0⟩ → c2†c1†c2†|0⟩ = −c1†c2†c2†|0⟩
c1†c3†|0⟩ → c2†c1†c3†|0⟩ = −c1†c2†c3†|0⟩
c2†c3†|0⟩ → 0
c1†c2†c3†|0⟩ → 0
Perimeter-A

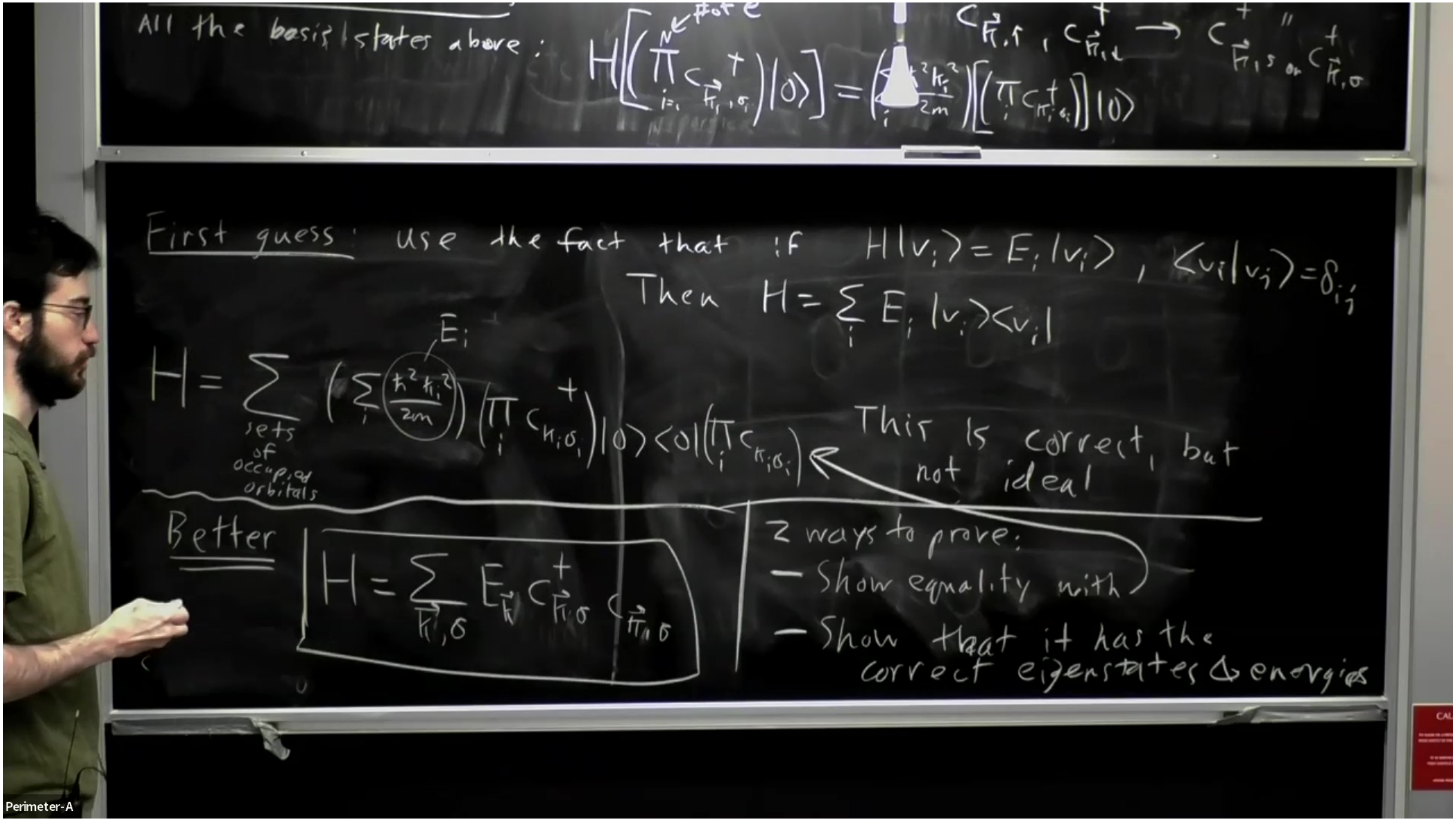

|0⟩ , c₁†|0⟩, c₂†|0⟩, ... , c_N†|0⟩ , c₁†c₂†|0⟩, ... c_{N-1}†c_N†|0⟩ , c₁†c₂†c₃†|0⟩, ... , ... , c₁†c₂† ... c_N†|0⟩
1 particle
N-particle
3-particle
N-particle state
eg 3-orbital system
Find matrix of c₂†
|0⟩ → c₂†|0⟩
c₁†|0⟩ → c₂†c₁†|0⟩ = −c₁†c₂†|0⟩
c₂†|0⟩ → 0
c₃†|0⟩ → c₂†c₃†|0⟩
c₁†c₂†|0⟩ → c₂†c₁†c₂†|0⟩ = −c₁†c₂†c₂†|0⟩
c₁†c₃†|0⟩ → c₂†c₁†c₃†|0⟩ = −c₁†c₂†c₃†|0⟩
c₂†c₃†|0⟩ → 0
Perimeter-A

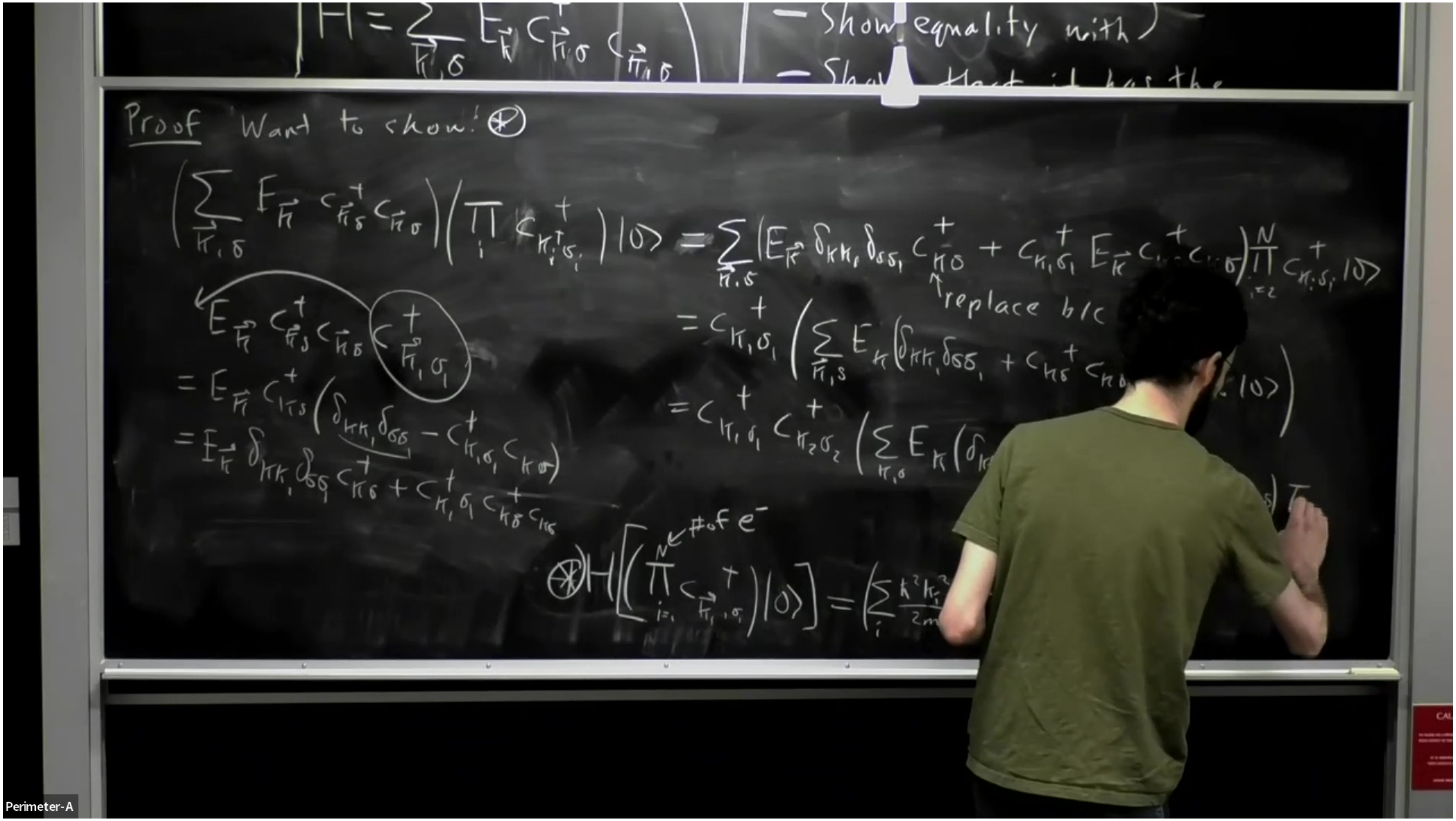


Second quantized Hamiltonian
Return to free electron gas, orbitals are $|\theta_{\vec{k}}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$
quantized
$|0\rangle$, $\{ c^\dagger_{\vec{k}} |0\rangle \}$, $\{ c^\dagger_{\vec{k}_1} c^\dagger_{\vec{k}_2} |0\rangle \}$, ...
all objects of this form
← many-particle basis
we also need spin, "spin-orbital" → actually 2 for every $\vec{k}$,
$c^\dagger_{\vec{k},\uparrow}$, $c^\dagger_{\vec{k},\downarrow}$ → "$c^\dagger_{\vec{k},s}$" or $c^\dagger_{\vec{k},\sigma}$
particle ei
Perimeter-A

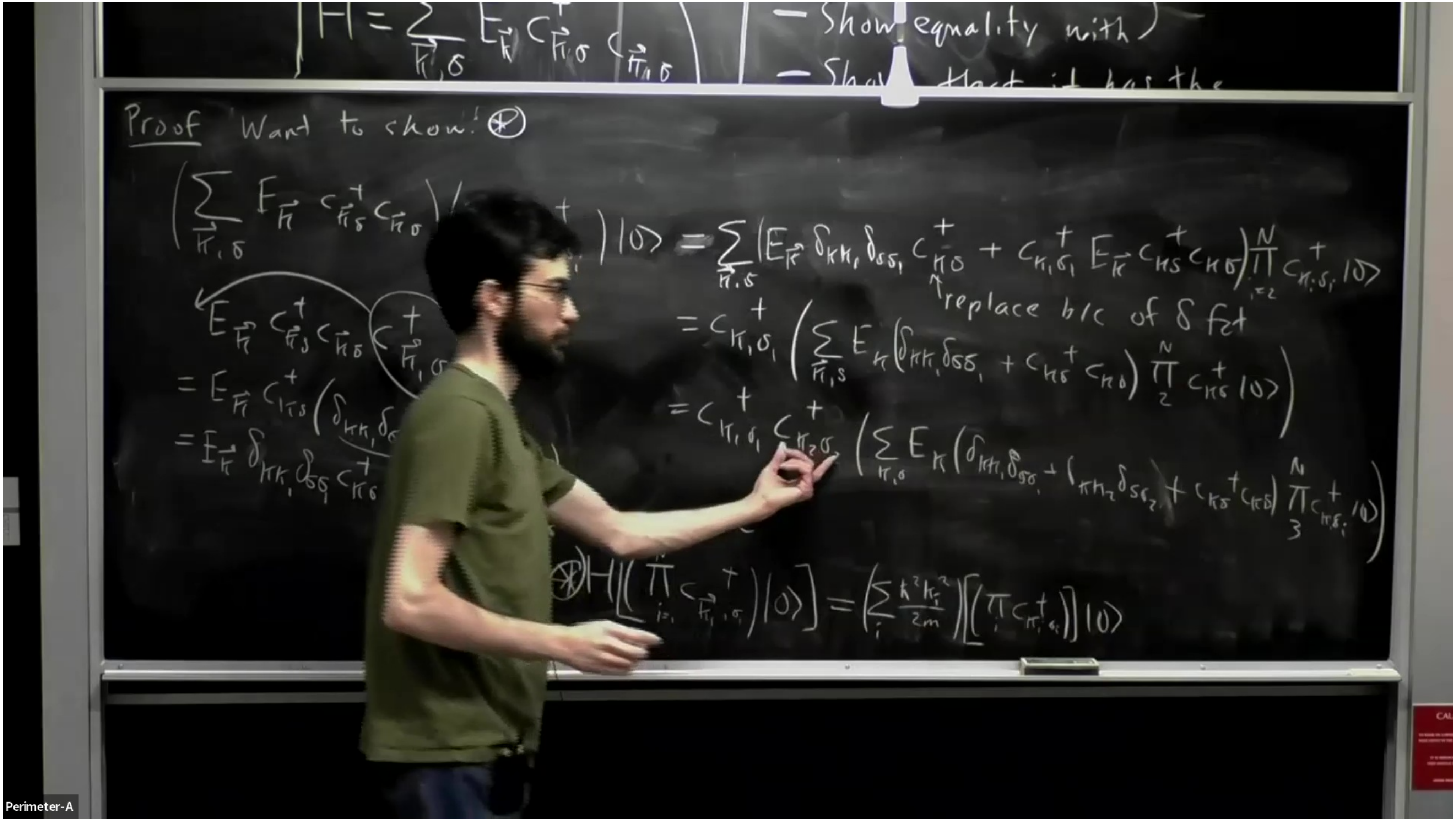

quantized
← many-particle basis
all objects of this form
Correction: we also
Many-particle eigenstates
All the basis states above
"spin-orbital" → actually 2 for every k
# of e⁻
Perimeter-A


of this form
Correction: we also need spin, "spin-orbital" → actually 2 for every k,
Many-particle eigenstates
All the basis states above:
Perimeter-A

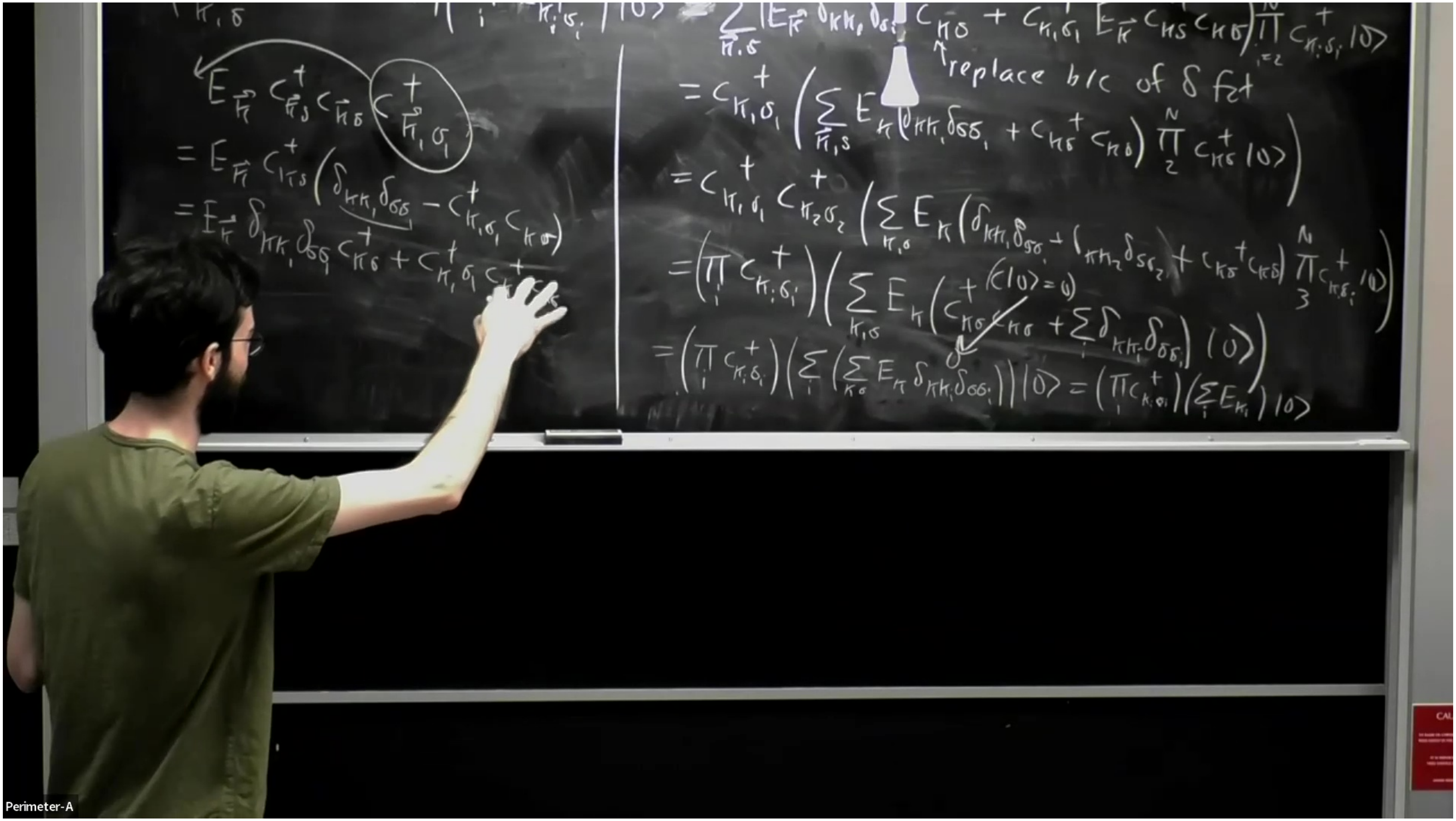

All the basis states above: $H\left[\left(\prod_{i=1}^{N \leftarrow \# \text{ of } e} c^\dagger_{\vec{k}_i,\sigma_i}\right)|0\rangle\right] = \left(\sum_i \frac{\hbar^2 k_i^2}{2m}\right)\left[\left(\prod_i c^\dagger_{\vec{k}_i,\sigma_i}\right)\right]|0\rangle$
$c^\dagger_{\vec{k},\uparrow}, c^\dagger_{\vec{k},\downarrow} \rightarrow c^\dagger_{\vec{k},s}$ " or $c^\dagger_{\vec{k},\sigma}$
First guess: use the fact that if $H|v_i\rangle = E_i|v_i\rangle$, $\langle v_i|v_j\rangle = \delta_{ij}$
Then $H = \sum_i E_i |v_i\rangle\langle v_i|$
$H = \sum_{\text{sets of occupied orbitals}} \left(\sum_i \frac{\hbar^2 k_i^2}{2m}\right)\left(\prod_i c^\dagger_{k_i\sigma_i}\right)|0\rangle\langle 0|\left(\prod_i c_{k_i\sigma_i}\right)$
E_i
This is correct, but not ideal
Better
$H = \sum_{\vec{k},\sigma} E_{\vec{k}}\, c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma}$
2 ways to prove:
— Show equality with
— Show that it has the correct eigenstates & energies
Perimeter-A

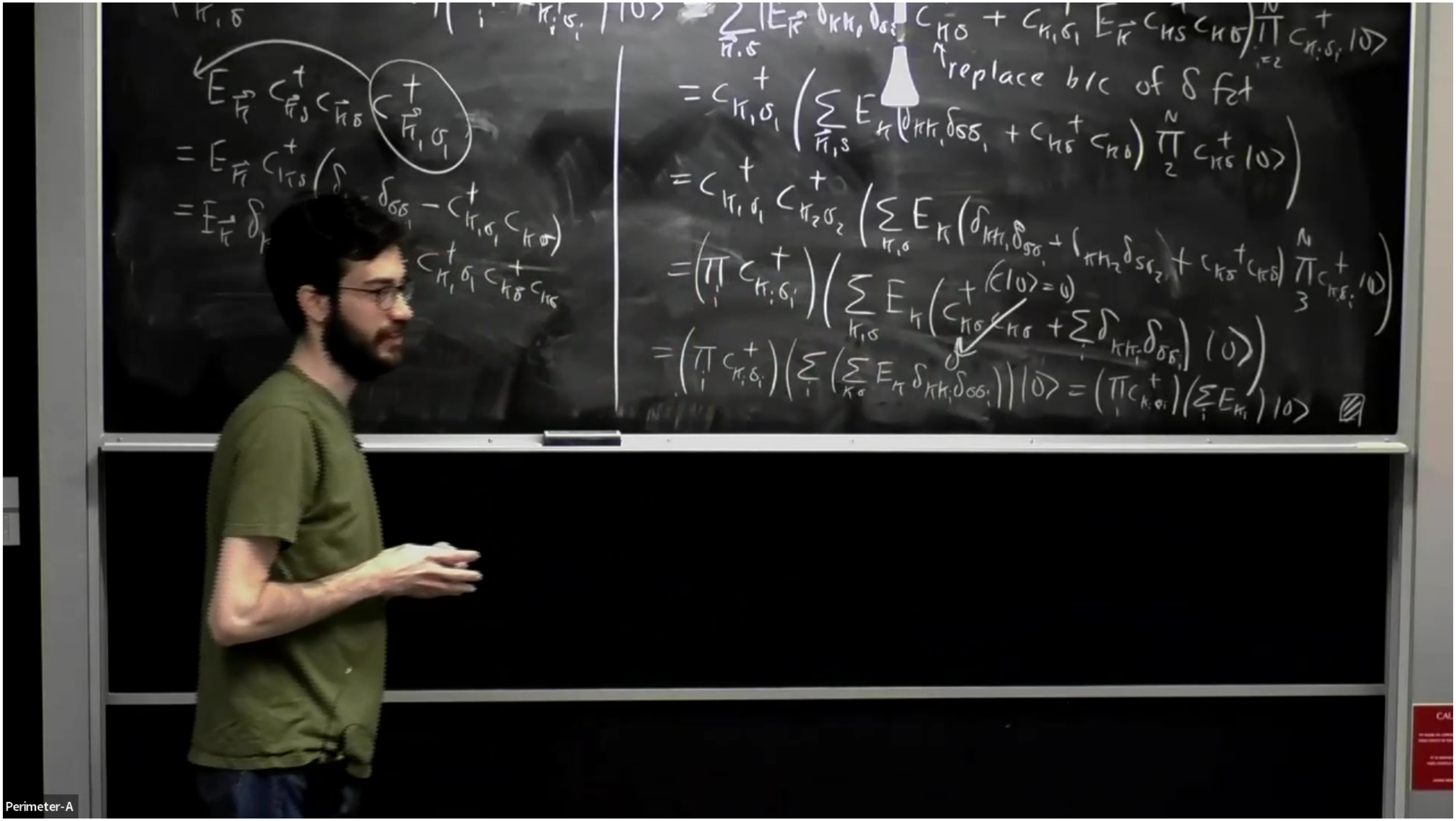


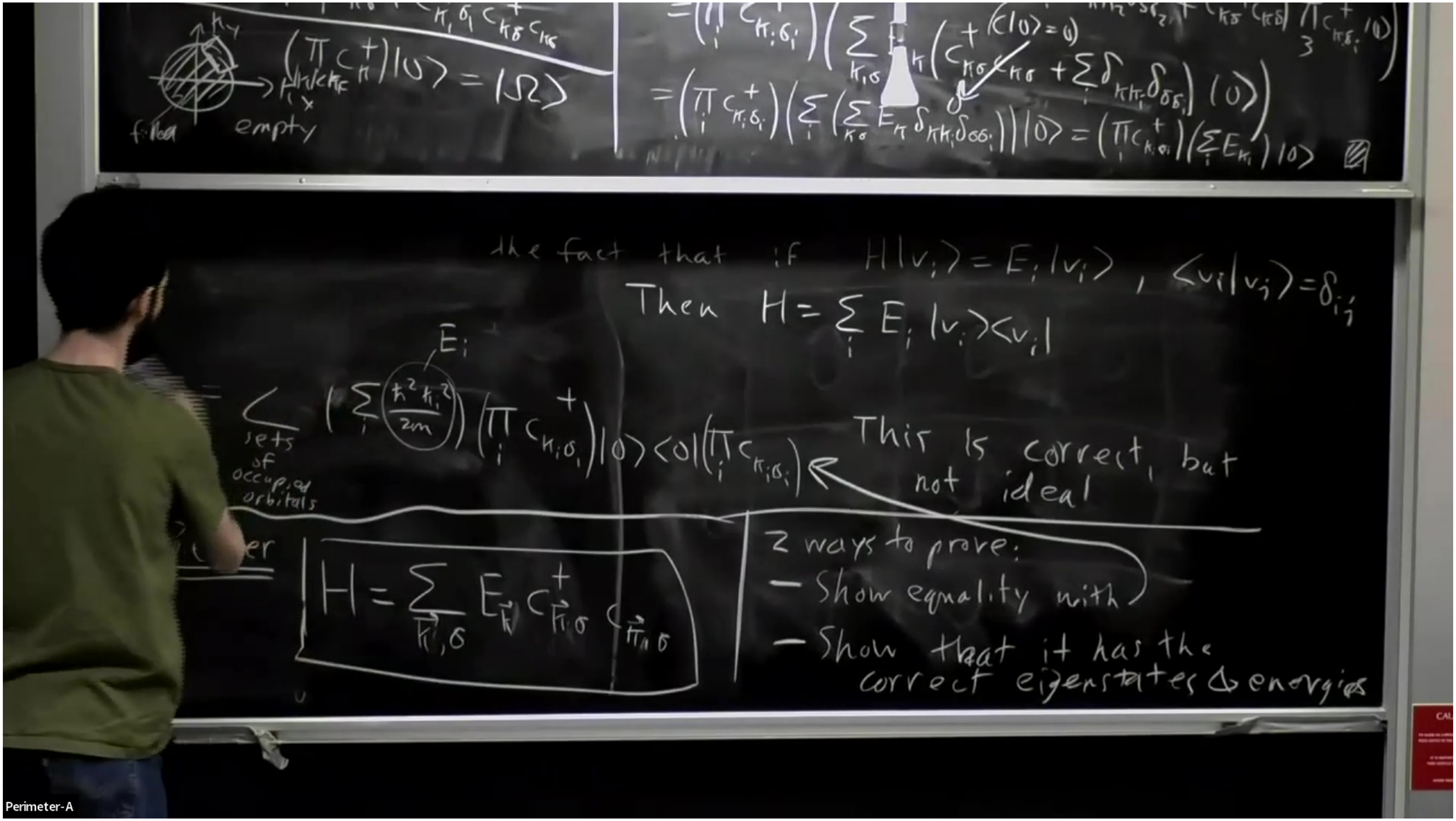
Show equality with
Proof Want to show:
replace b/c
# of e⁻
Perimeter-A



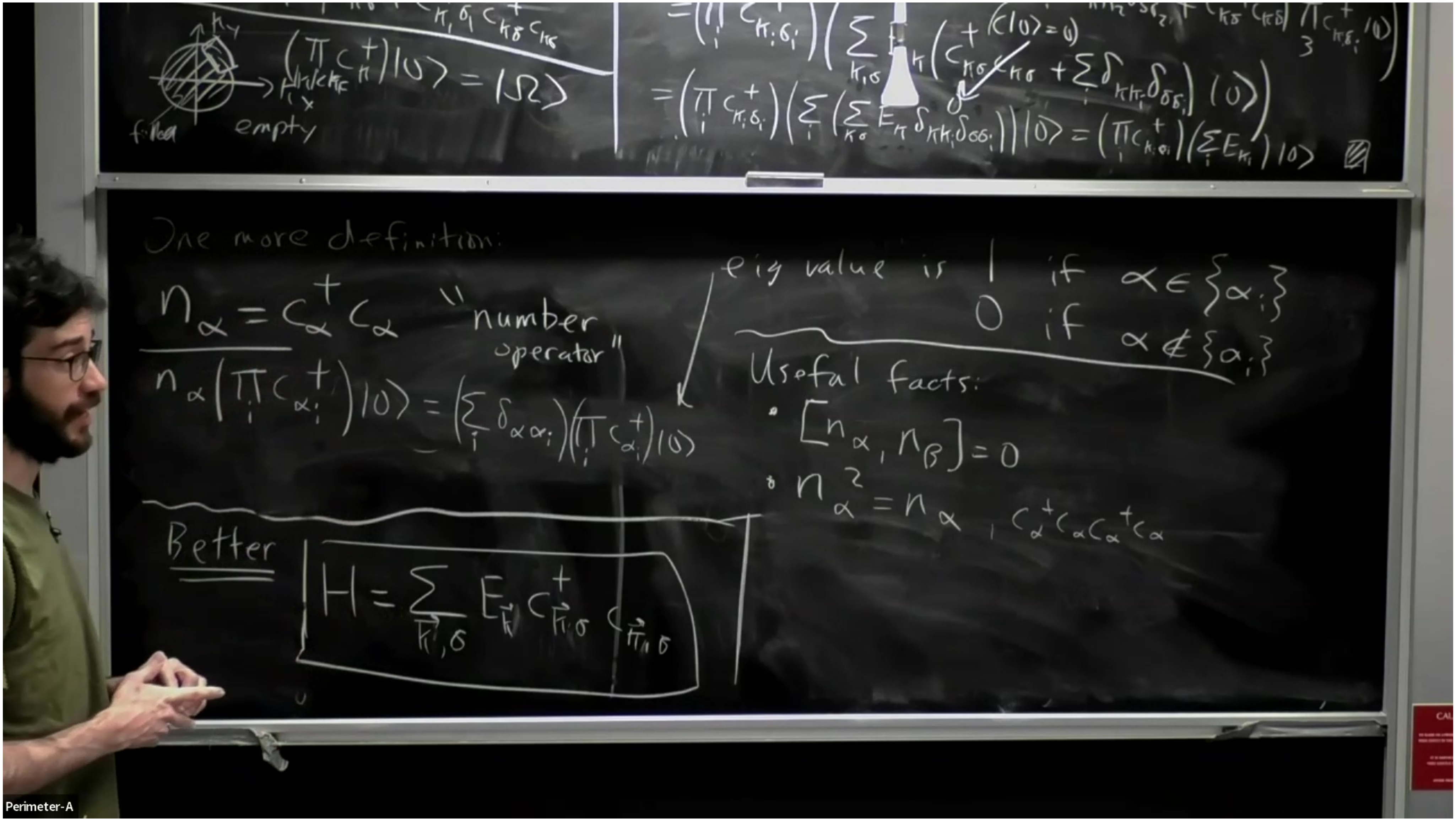
– Show equality with
Proof Want to show: ⊛
replace b/c of δ fct
Perimeter-A

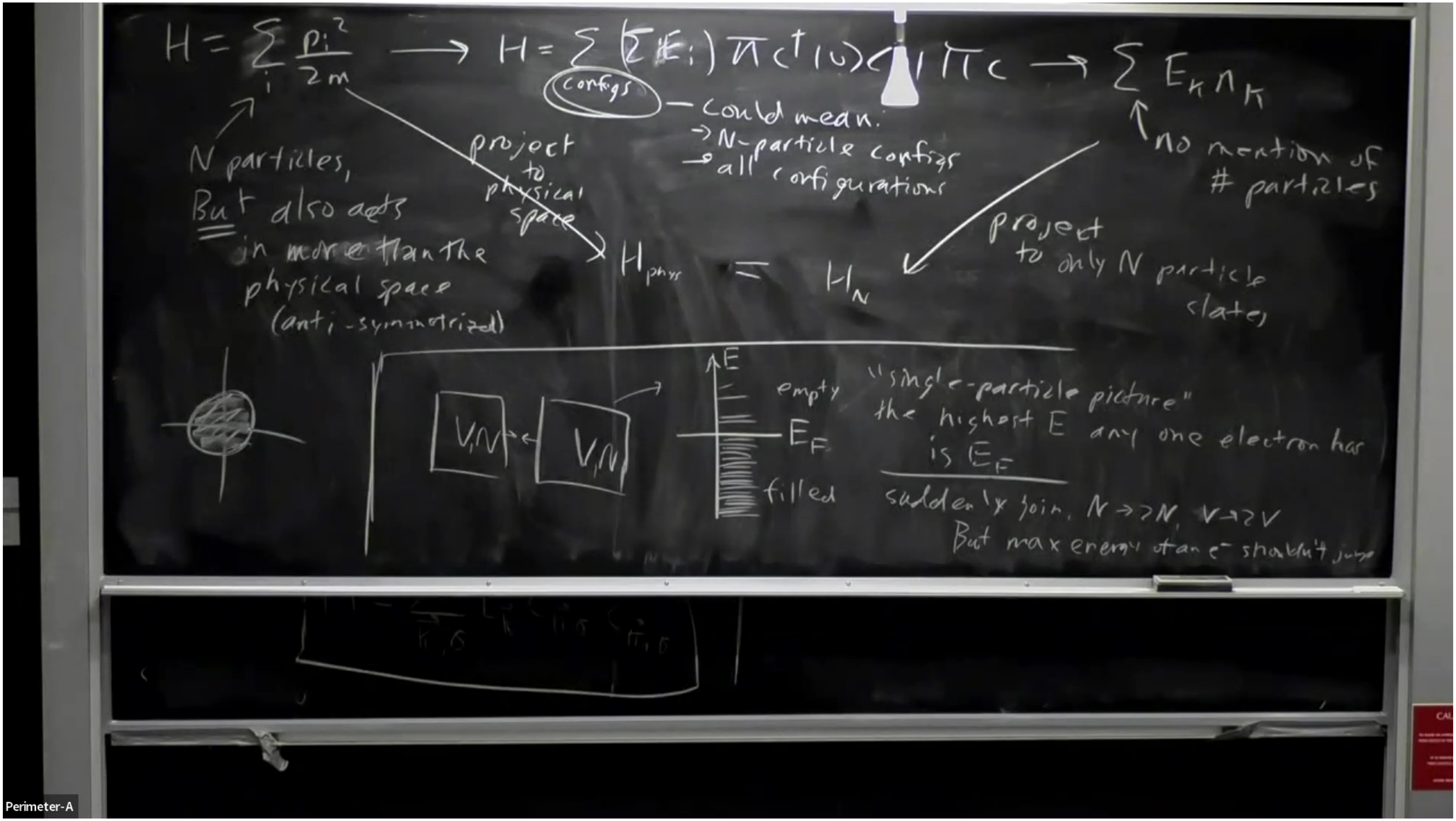

replace b/c of δ fct
Perimeter-A


replace b/c of δ fct
Perimeter-A



$(\prod c^{+}_{k})|0\rangle = |\Omega\rangle$
filled
empty
$= (\prod_i c^{+}_{k_i\sigma_i})(\sum_i (\sum_{k\sigma} E_k \delta_{kk_i}\delta_{\sigma\sigma_i}))|0\rangle = (\prod_i c^{+}_{k_i\sigma_i})(\sum_i E_{k_i})|0\rangle$
the fact that if $H|v_i\rangle = E_i|v_i\rangle$, $\langle v_i|v_j\rangle = \delta_{ij}$
Then $H = \sum_i E_i |v_i\rangle\langle v_i|$
E_i
$\sum (\sum_i \frac{k^2 k_i^2}{2m}) (\prod_i c^{+}_{k_i\sigma_i})|0\rangle\langle 0|(\prod_i c_{k_i\sigma_i})$
sets of occupied orbitals
This is correct, but not ideal
$H = \sum_{\vec{k},\sigma} E_{\vec{k}} c^{+}_{\vec{k},\sigma} c_{\vec{k},\sigma}$
2 ways to prove:
— Show equality with
— Show that it has the correct eigenstates & energies
Perimeter-A


One more definition:
n_α = c_α^† c_α "number operator"
n_α (Π_i c_{α_i}^†)|0⟩ = (Σ_i δ_{αα_i})(Π_i c_{α_i}^†)|0⟩
eig value is 1 if α ∈ {α_i}
0 if α ∉ {α_i}
Useful facts:
• [n_α, n_β] = 0
• n_α^2 = n_α , c_α^† c_α c_α^† c_α
Better
H = Σ_{k,σ} E_k c_{k,σ}^† c_{k,σ}
filled
empty
Perimeter-A



H = Σ p_i^2 / 2m → H = Σ (Σ E_i) Π c† |0⟩⟨0| Π c → Σ E_k n_k
configs
— could mean:
→ N-particle configs
→ all configurations
N particles,
But also acts in more than the physical space (anti-symmetrized)
project to physical space
no mention of # particles
project to only N particle states
H_phys = H_N
V, N
V, N
E
empty
E_F
filled
"single-particle picture"
the highest E any one electron has is E_F
suddenly join. N → 2N, V → 2V
But max energy of an e⁻ shouldn't jump
Perimeter-A