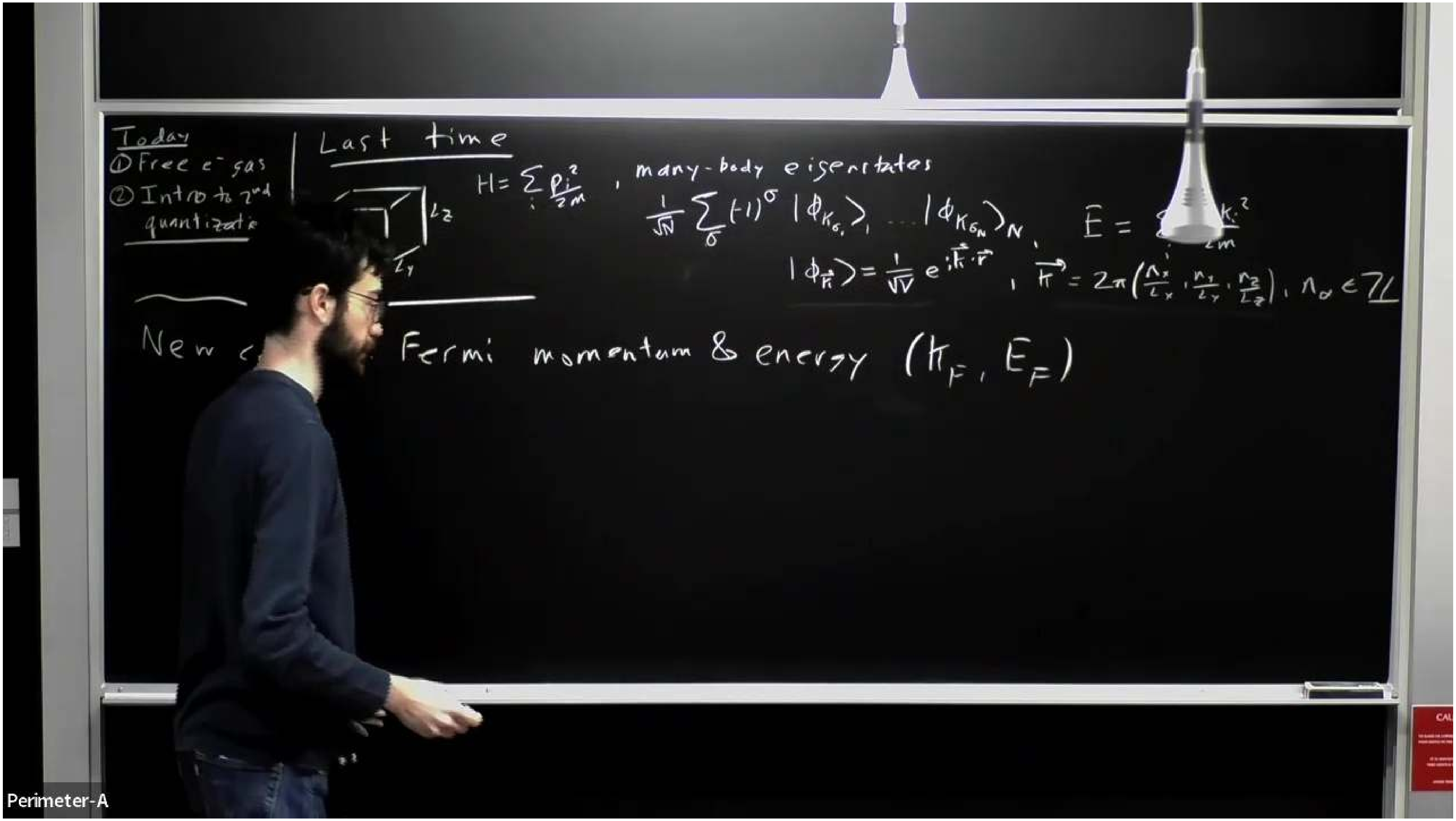
Title: PSI Lecture - Condensed Matter - Lecture 2

Speakers: Aaron Szasz

Collection: PSI Lecture - Condensed Matter

Date: January 11, 2022 - 11:30 AM

URL: https://pirsa.org/22010013



Today
① Free e^- gas
② Intro to 2nd quantizatio

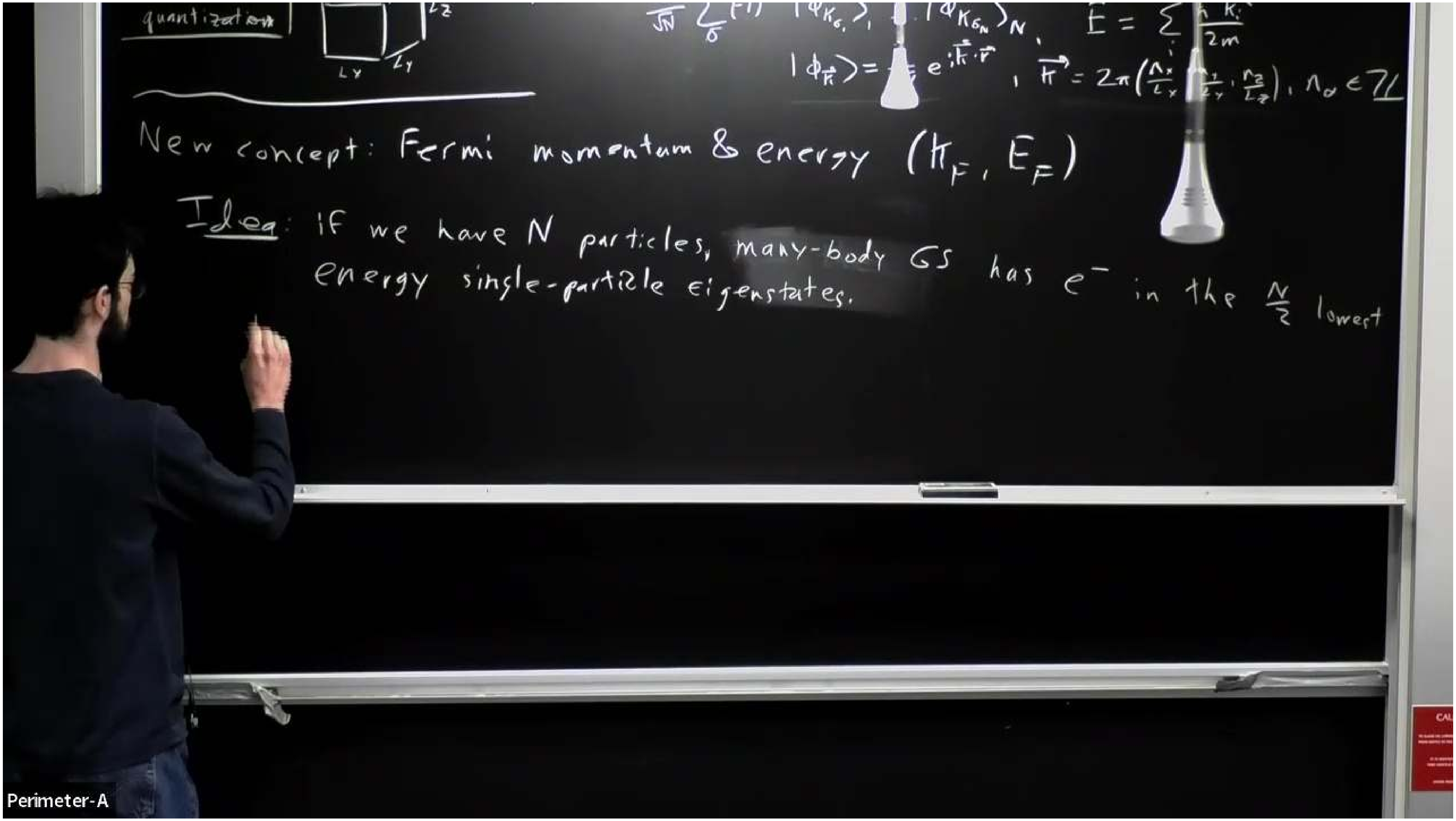
Last time

$H = \sum_i \frac{p_i^2}{2m}$, many-body eigenstates

$\frac{1}{\sqrt{N}} \sum_\sigma (-1)^\sigma |\phi_{k_{\sigma_1}}\rangle_1 \dots |\phi_{k_{\sigma_N}}\rangle_N$, $E = \sum_i \frac{k_i^2}{2m}$

$|\phi_{\vec{k}}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$, $\vec{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right)$, $n_\alpha \in \mathbb{Z}$

New c Fermi momentum & energy (k_F, E_F)



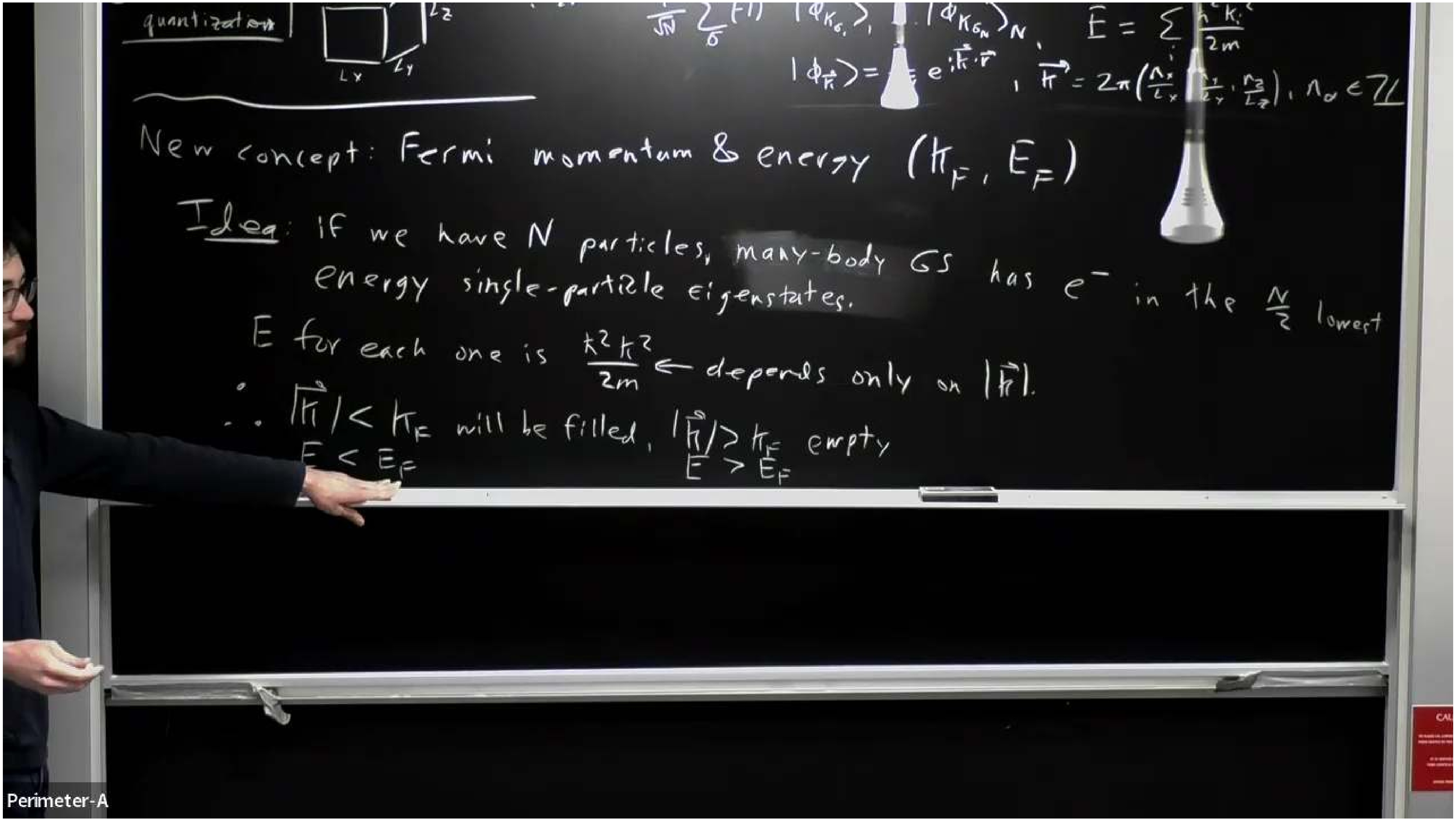
quantization

$\frac{1}{\sqrt{N}}\sum_{\sigma}(-1)^{\sigma}|\phi_{k_{\sigma_1}}\rangle_1 \cdots |\phi_{k_{\sigma_N}}\rangle_N$, $E = \sum_i \frac{\hbar^2 k_i^2}{2m}$

$|\phi_{\vec{k}}\rangle = \ e^{i\vec{k}\cdot\vec{r}}$, $\vec{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right)$, $n_\alpha \in \mathbb{Z}$

New concept: Fermi momentum & energy (k_F, E_F)

Idea: if we have N particles, many-body GS has e^- in the $\frac{N}{2}$ lowest energy single-particle eigenstates.



quantization

L_x L_y L_z

$\frac{1}{\sqrt{N}} \sum_{\sigma} (-1) \; |\phi_{k_{\sigma_1}}\rangle_1 \cdots |\phi_{k_{\sigma_N}}\rangle_N$, $E = \sum_i \frac{\hbar^2 k_i^2}{2m}$

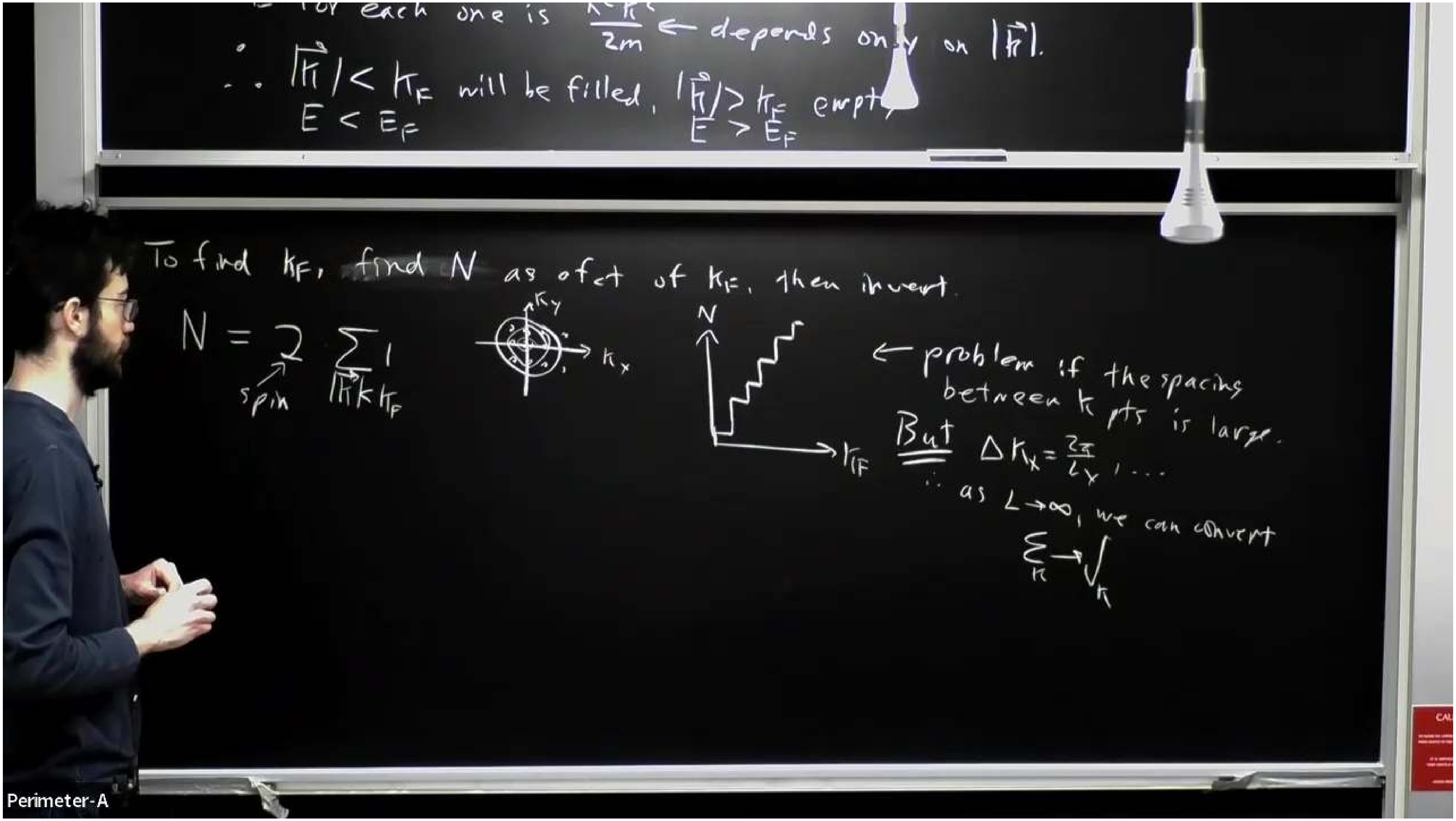
$|\phi_{\vec{k}}\rangle = \; e^{i\vec{k}\cdot\vec{r}}$, $\vec{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right)$, $n_\alpha \in \mathbb{Z}$

New concept: Fermi momentum & energy (k_F, E_F)

Idea: If we have N particles, many-body GS has e^- in the $\frac{N}{2}$ lowest energy single-particle eigenstates.

E for each one is $\frac{\hbar^2 k^2}{2m} \leftarrow$ depends only on $|\vec{k}|$.

$\therefore$ $|\vec{k}| < k_F$ will be filled, $|\vec{k}| > k_F$ empty
$E < E_F$ $\qquad E > E_F$



for each one is $\frac{\hbar^2 k^2}{2m}$ ← depends only on $|\vec{k}|$.

$\therefore$ $|\vec{k}| < k_F$ will be filled, $|\vec{k}| > k_F$ empty
$E < E_F$ $\qquad$ $E > E_F$

To find k_F, find N as of fct of k_F, then invert.

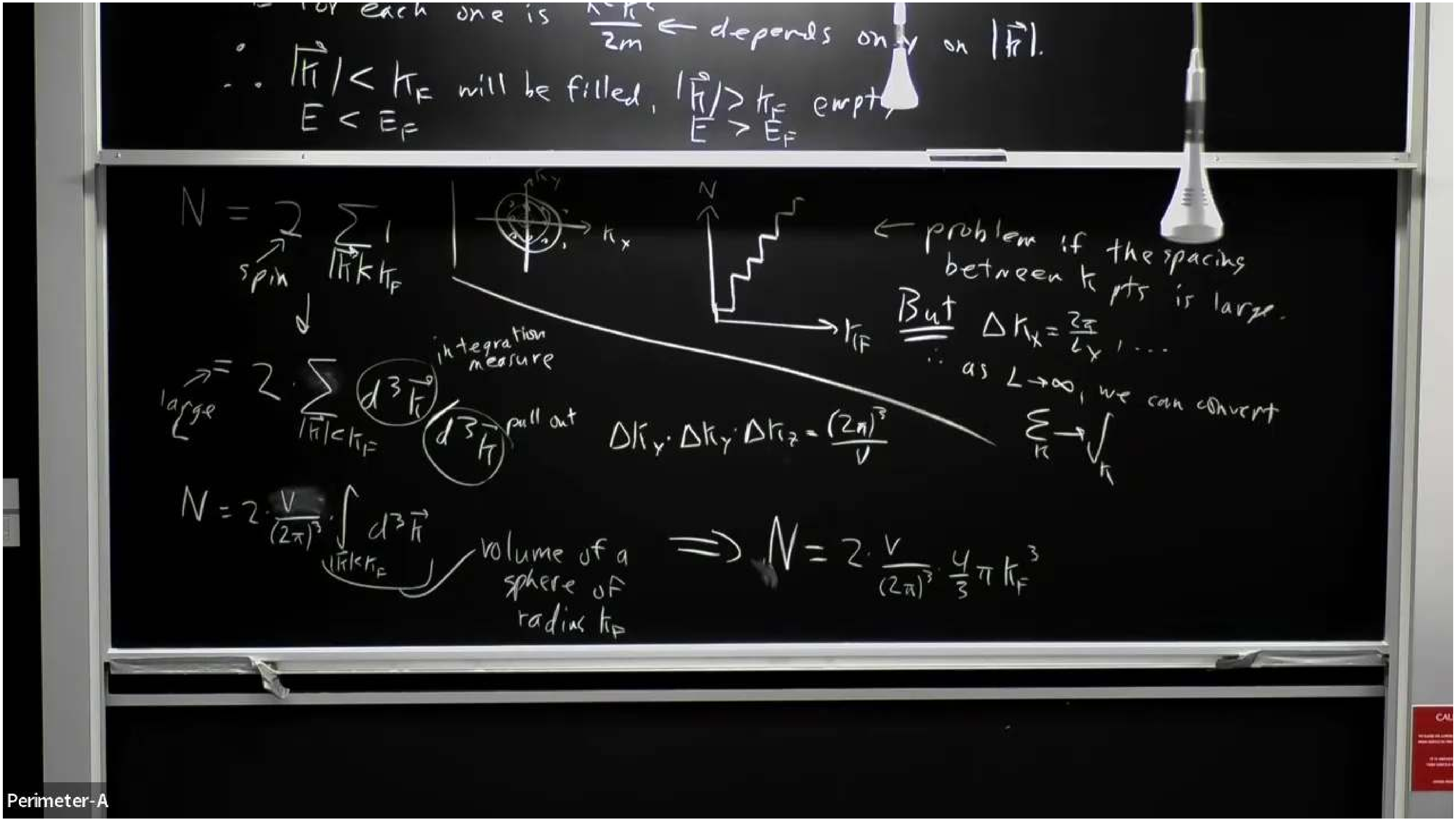
$$N = \underset{\substack{\nearrow \\ \text{spin}}}{2} \sum_{|\vec{k}| < k_F} 1$$

← problem if the spacing between k pts is large.

But $\Delta k_x = \frac{2\pi}{L_x}, \ldots$

$\therefore$ as $L \to \infty$, we can convert

$$\sum_k \to \int_k$$



for each one is $\frac{\hbar^2 k^2}{2m}$ ← depends only on $|\vec{k}|$.

$\therefore$ $|\vec{k}| < k_F$ will be filled, $|\vec{k}| > k_F$ empty,
$E < E_F$ $\qquad$ $E > E_F$

$$N = 2 \sum_{|\vec{k}| < k_F} 1$$

spin

$$= 2 \cdot \sum_{|\vec{k}|<k_F} \boxed{d^3\vec{k}}$$

large

integration measure

$d^3\vec{k}$ pull out

← problem if the spacing between k pts is large.

But $\Delta k_x = \frac{2\pi}{L_x}, \ldots$

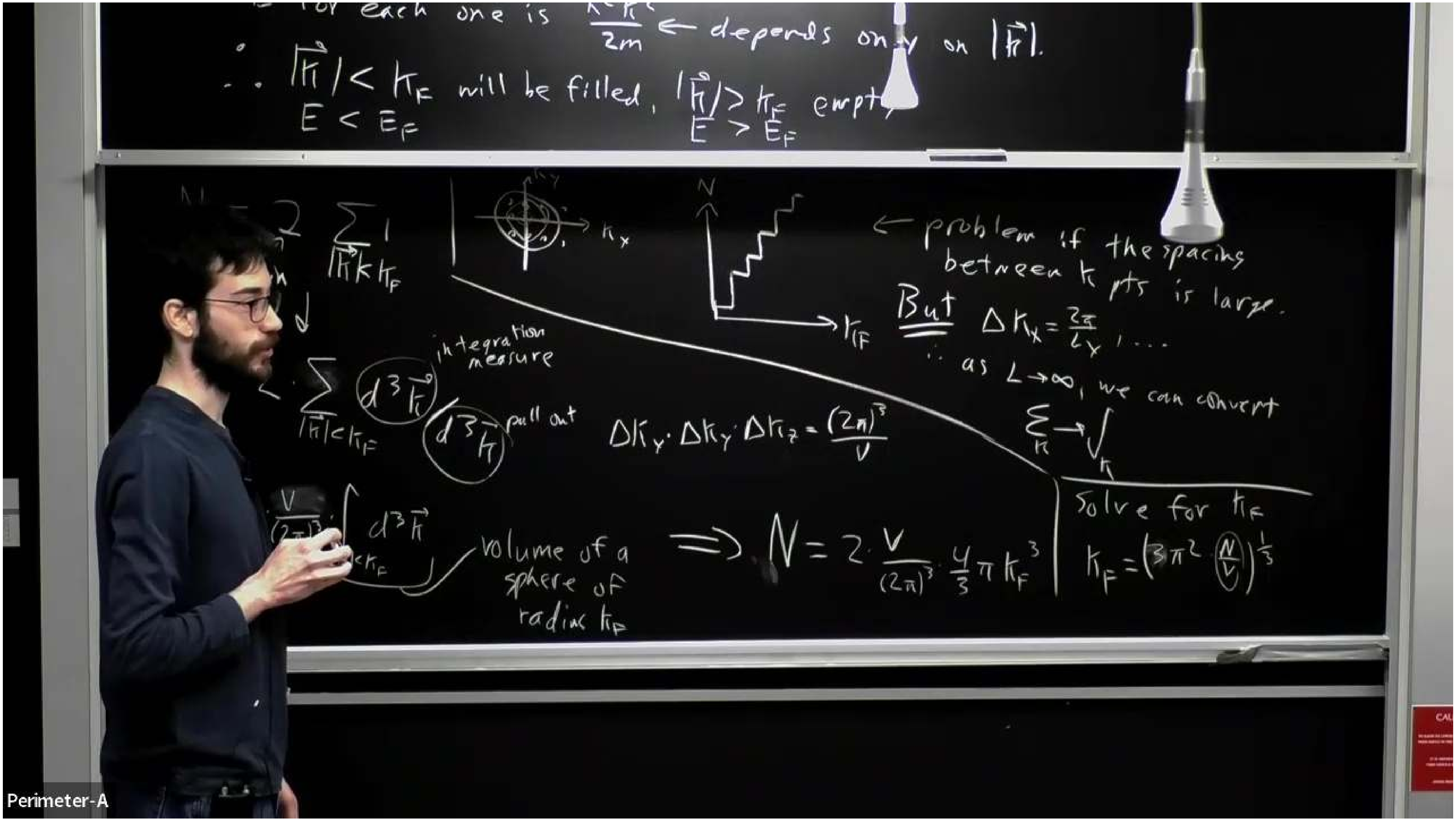
$\therefore$ as $L \to \infty$, we can convert $\sum_k \to \int_k$

$$\Delta k_x \cdot \Delta k_y \cdot \Delta k_z = \frac{(2\pi)^3}{V}$$

$$N = 2 \cdot \frac{V}{(2\pi)^3} \cdot \underbrace{\int_{|\vec{k}|<k_F} d^3\vec{k}}$$

volume of a sphere of radius k_F

$$\Longrightarrow N = 2 \cdot \frac{V}{(2\pi)^3} \cdot \frac{4}{3}\pi k_F^3$$



for each one is $\frac{\hbar^2 k^2}{2m}$ ← depends only on $|\vec{k}|$.

$\therefore$ $|\vec{k}| < k_F$ will be filled, $|\vec{k}| > k_F$ empty
$E < E_F$ $E > E_F$

$$N = 2 \sum_{|\vec{k}| < k_F} 1$$

$$\downarrow$$

$$\sum_{|\vec{k}| < k_F} \boxed{d^3\vec{k}} \quad \text{integration measure}$$

$$\boxed{d^3\vec{k}} \text{ pull out}$$

$$\Delta k_x \cdot \Delta k_y \cdot \Delta k_z = \frac{(2\pi)^3}{V}$$

$$\frac{V}{(2\pi)^3} \underbrace{\int_{|\vec{k}| < k_F} d^3\vec{k}}_{\text{volume of a sphere of radius } k_F}$$

$$\Longrightarrow N = 2 \cdot \frac{V}{(2\pi)^3} \cdot \frac{4}{3}\pi k_F^3$$

← problem if the spacing between k pts is large.

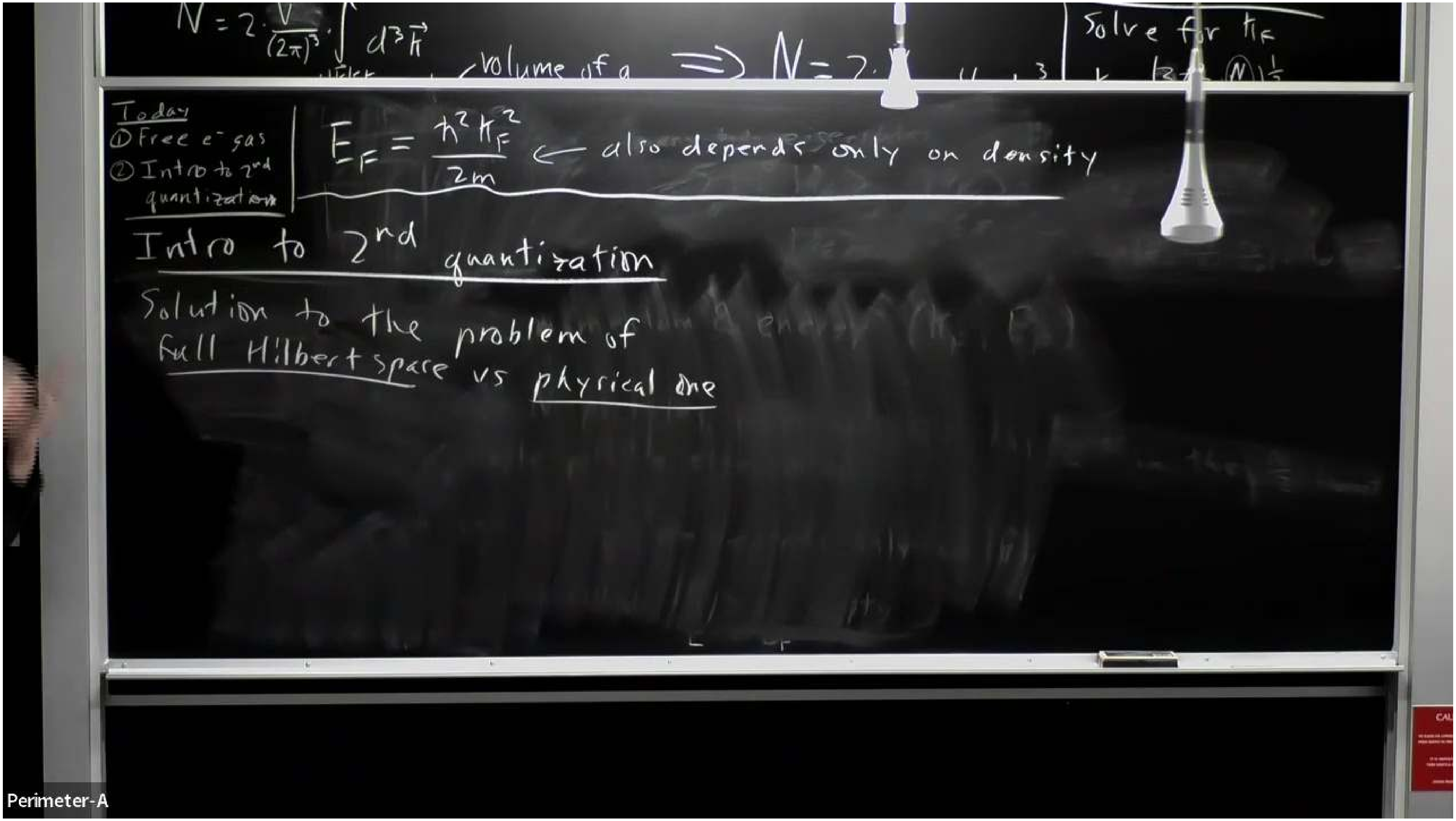
But $\Delta k_x = \frac{2\pi}{L_x}, \ldots$

$\therefore$ as $L \to \infty$, we can convert

$$\sum_{k} \to \int_{k}$$

Solve for k_F

$$k_F = \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}}$$



$N = 2 \cdot \frac{V}{(2\pi)^3} \int d^3\vec{k}$ ← volume of a $\Longrightarrow N = 2 \cdot$

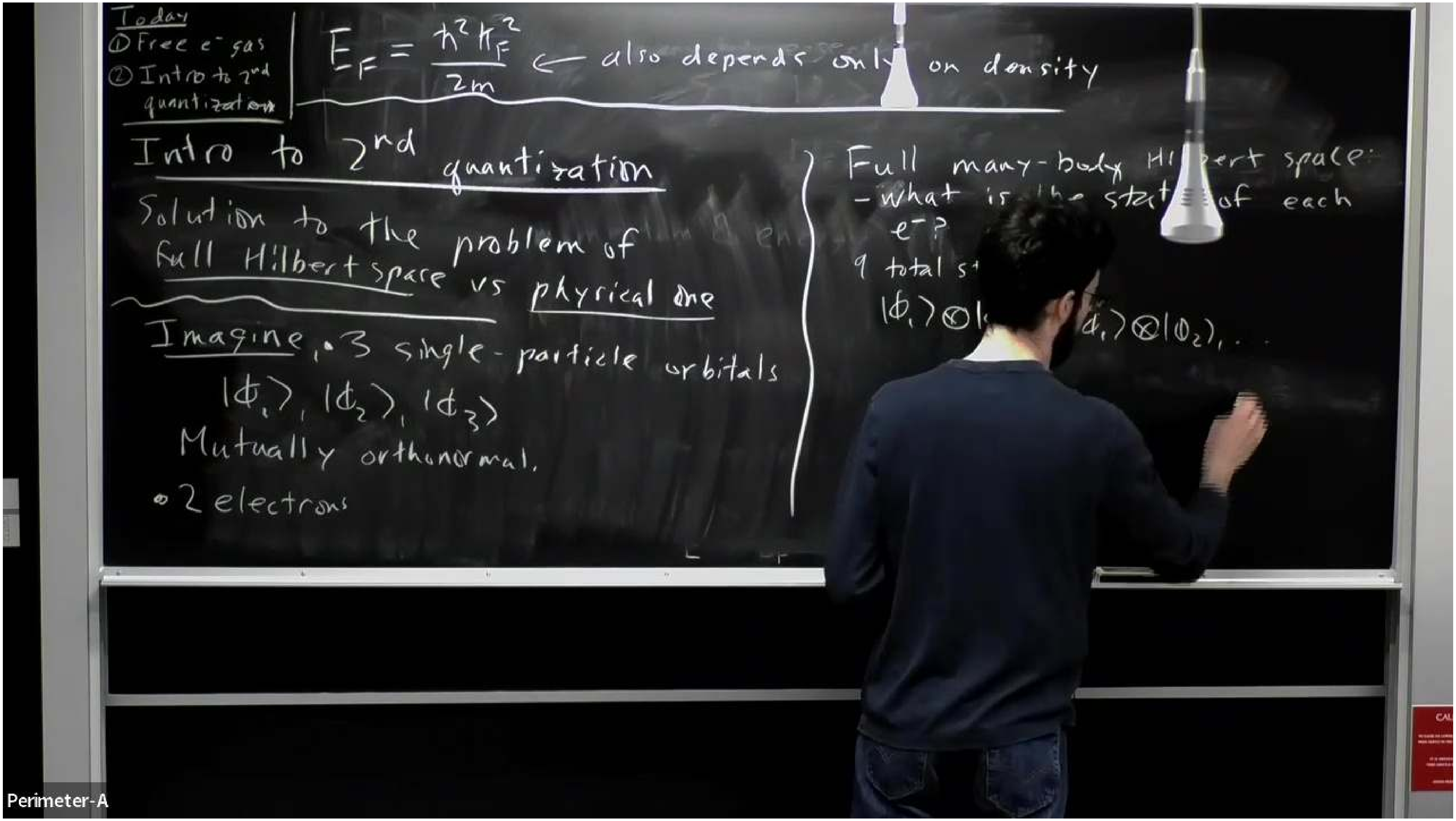
Solve for k_F

Today
① Free e^- gas
② Intro to 2nd quantization

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$ ← also depends only on density

Intro to 2nd quantization

Solution to the problem of full Hilbert space vs physical one



Today
① Free e⁻ gas
② Intro to 2nd quantization

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$ ← also depends only on density

Intro to 2nd quantization

Solution to the problem of full Hilbert space vs physical one

Imagine, • 3 single-particle orbitals

$|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$

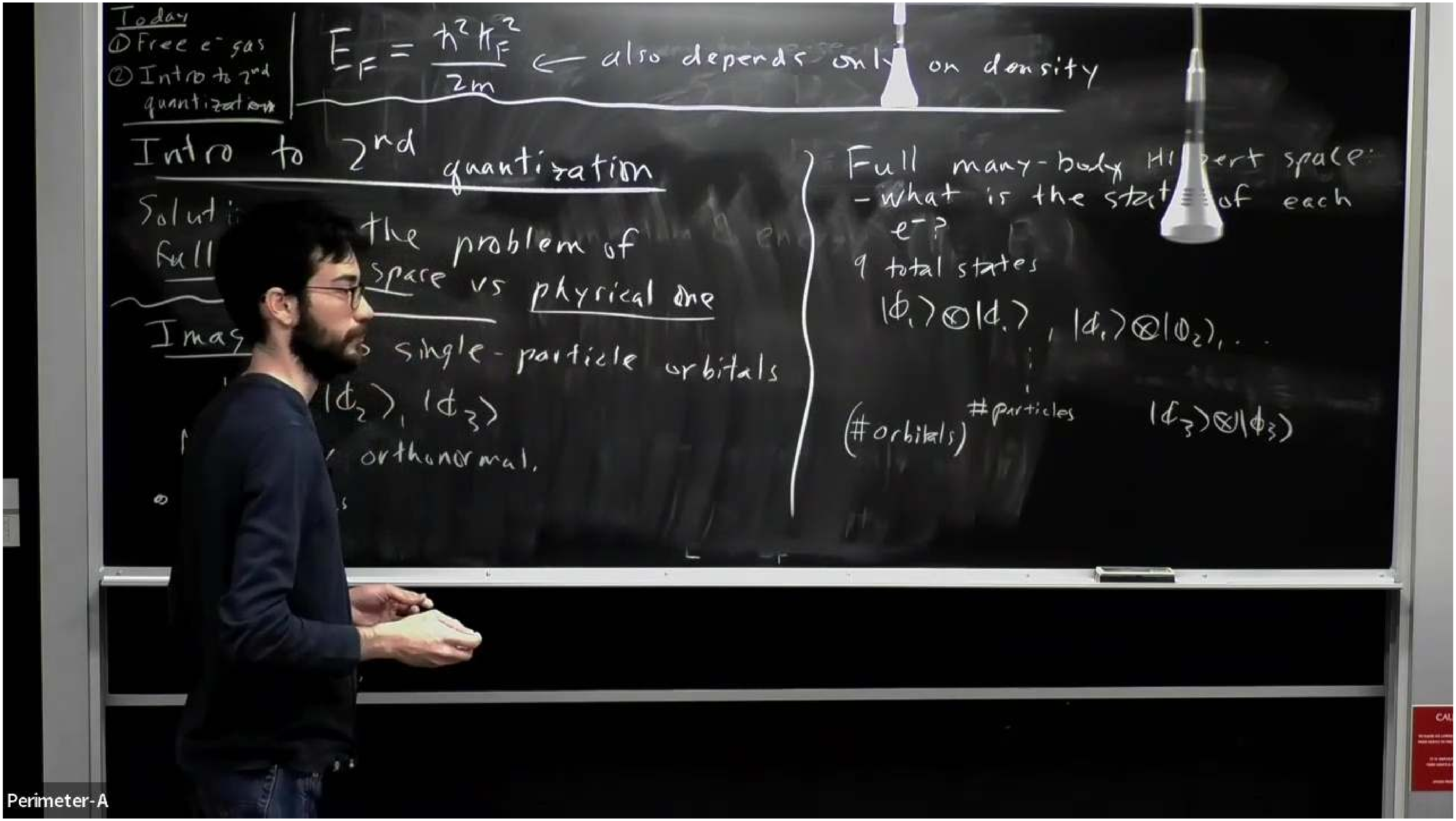
Mutually orthonormal.

• 2 electrons

Full many-body Hilbert space:
- what is the state of each e⁻?

9 total st

$|\phi_1\rangle \otimes |$ $\phi_1\rangle \otimes |\phi_2\rangle, \ldots$



Today
① Free e⁻ gas
② Intro to 2nd quantization

$$E_F = \frac{\hbar^2 k_F^2}{2m} \leftarrow \text{also depends only on density}$$

Intro to 2nd quantization

Solut the problem of
Full space vs physical one

Imag single-particle orbitals

$|\phi_2\rangle, |\phi_3\rangle$

orthonormal.

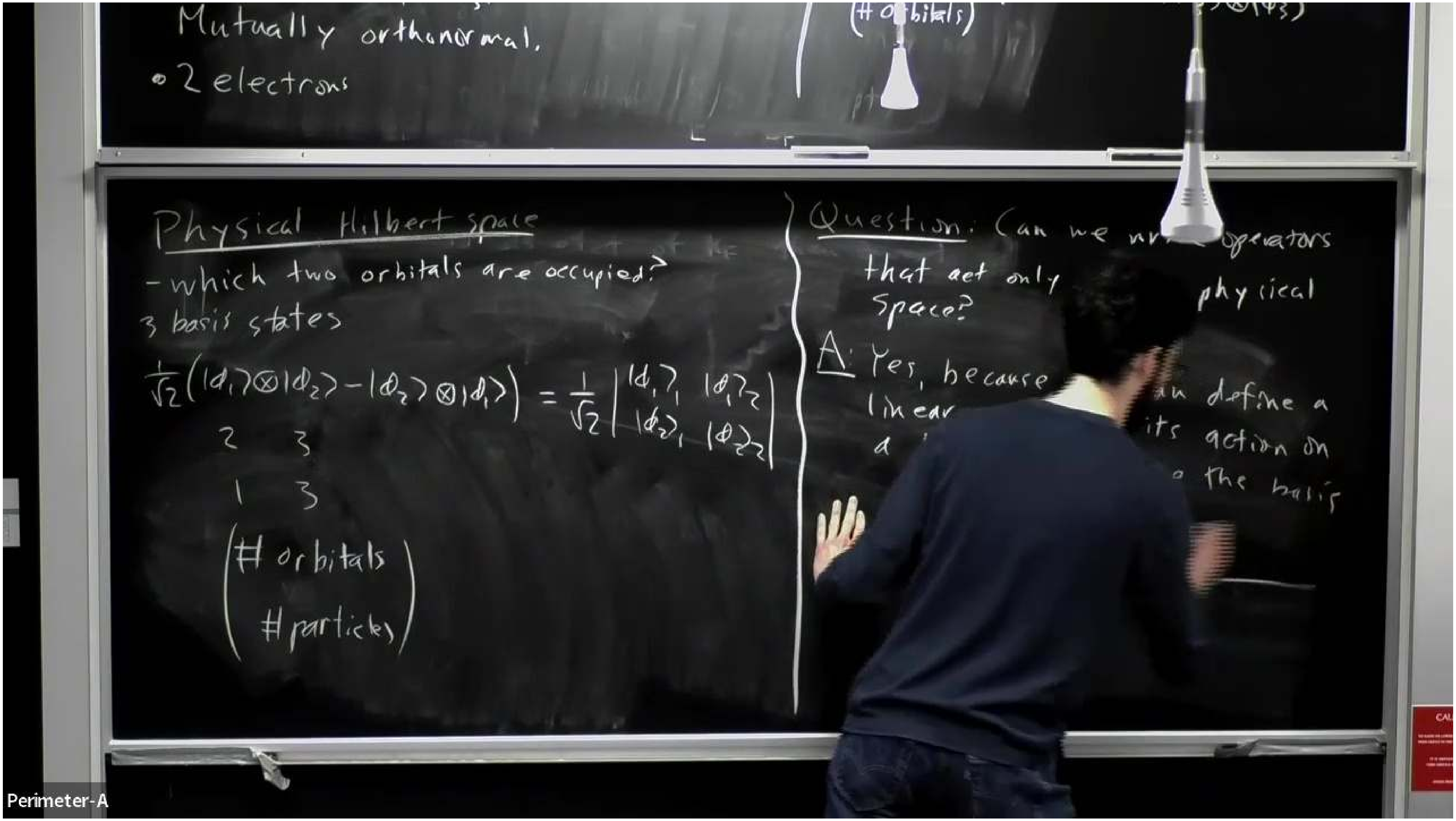
Full many-body Hilbert space:
- what is the state of each e⁻?

9 total states

$|\phi_1\rangle \otimes |\phi_1\rangle, \; |\phi_1\rangle \otimes |\phi_2\rangle, \ldots$

$\vdots$

$(\#\text{orbitals})^{\#\text{particles}}$ $\quad |\phi_3\rangle \otimes |\phi_3\rangle$



Mutually orthonormal.

- 2 electrons

(# orbitals)

$\otimes|\phi_3\rangle$

Physical Hilbert space

- which two orbitals are occupied?

3 basis states

$$\frac{1}{\sqrt{2}}\left(|\phi_1\rangle\otimes|\phi_2\rangle-|\phi_2\rangle\otimes|\phi_1\rangle\right)=\frac{1}{\sqrt{2}}\begin{vmatrix}|\phi_1\rangle_1 & |\phi_1\rangle_2\\ |\phi_2\rangle_1 & |\phi_2\rangle_2\end{vmatrix}$$

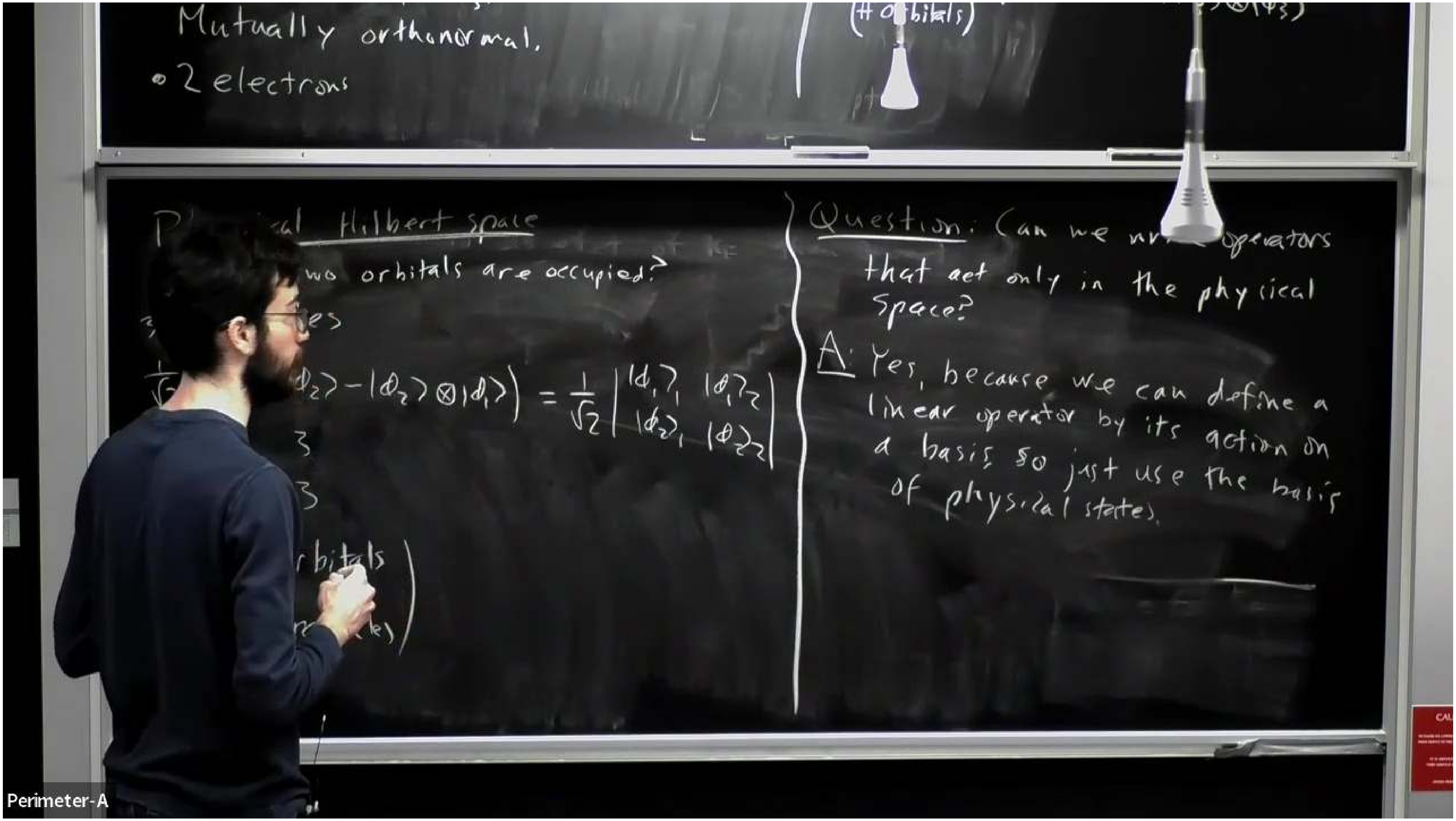
2 3

1 3

$$\binom{\#\text{orbitals}}{\#\text{particles}}$$

Question: Can we wr operators that act only phy sical space?

A: Yes, because an define a linear its action on a the basis



Mutually orthonormal.

- 2 electrons

(# orbitals)

$\otimes|\phi_3\rangle$

Ph...al Hilbert space

...wo orbitals are occupied?

...es

$\frac{1}{\sqrt{2}}(\ldots\phi_2\rangle - |\phi_2\rangle\otimes|\phi_1\rangle) = \frac{1}{\sqrt{2}}\begin{vmatrix} |\phi_1\rangle_1 & |\phi_1\rangle_2 \\ |\phi_2\rangle_1 & |\phi_2\rangle_2 \end{vmatrix}$

...3

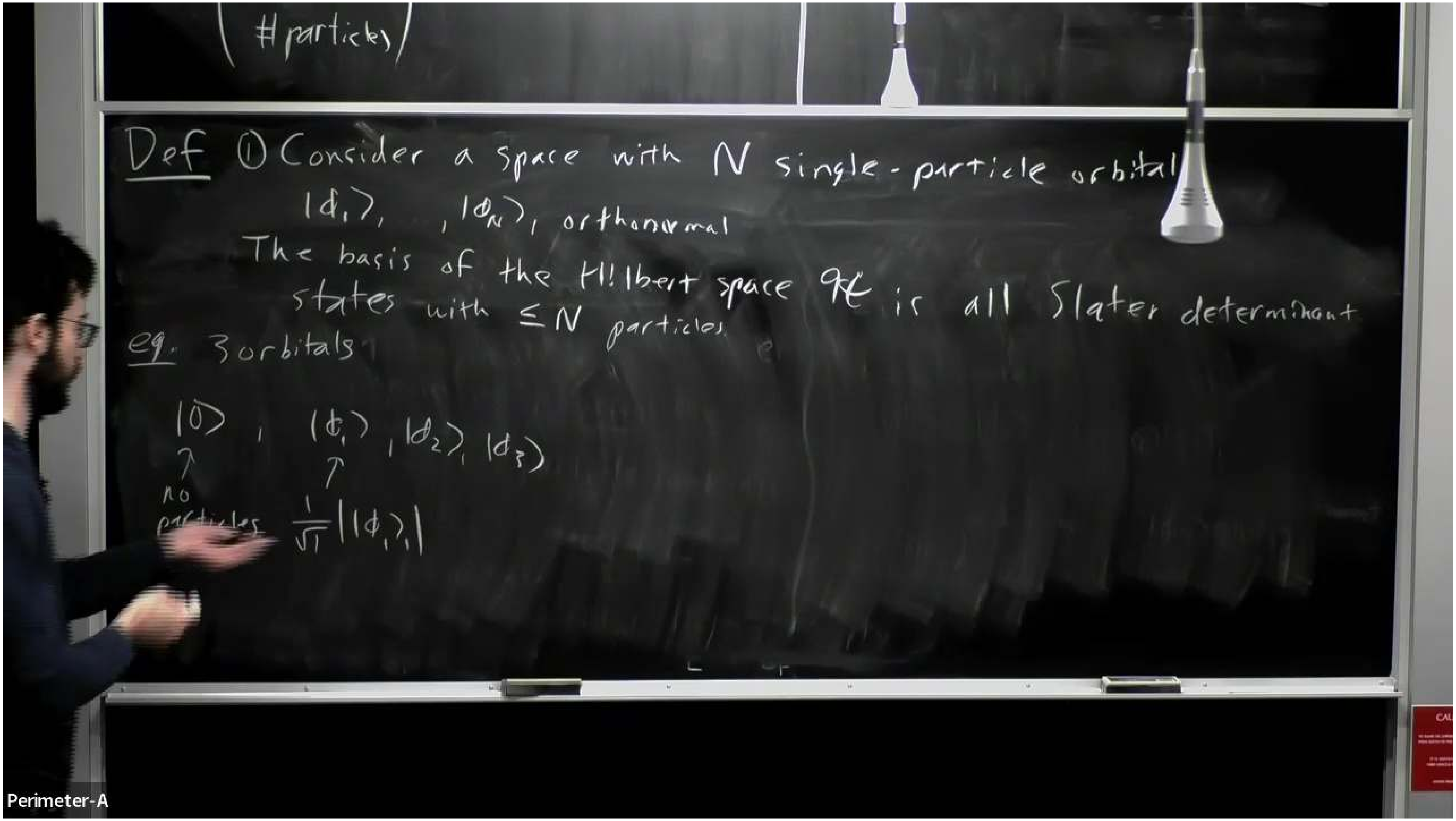
...3

...rbitals

...les)

Question: Can we wr... operators that act only in the physical space?

A: Yes, because we can define a linear operator by its action on a basis so just use the basis of physical states.



$\left(\# \text{particles} \right)$

<u>Def</u> ① Consider a space with N single-particle orbital

$|\phi_1\rangle, \quad , |\phi_N\rangle$, orthonormal

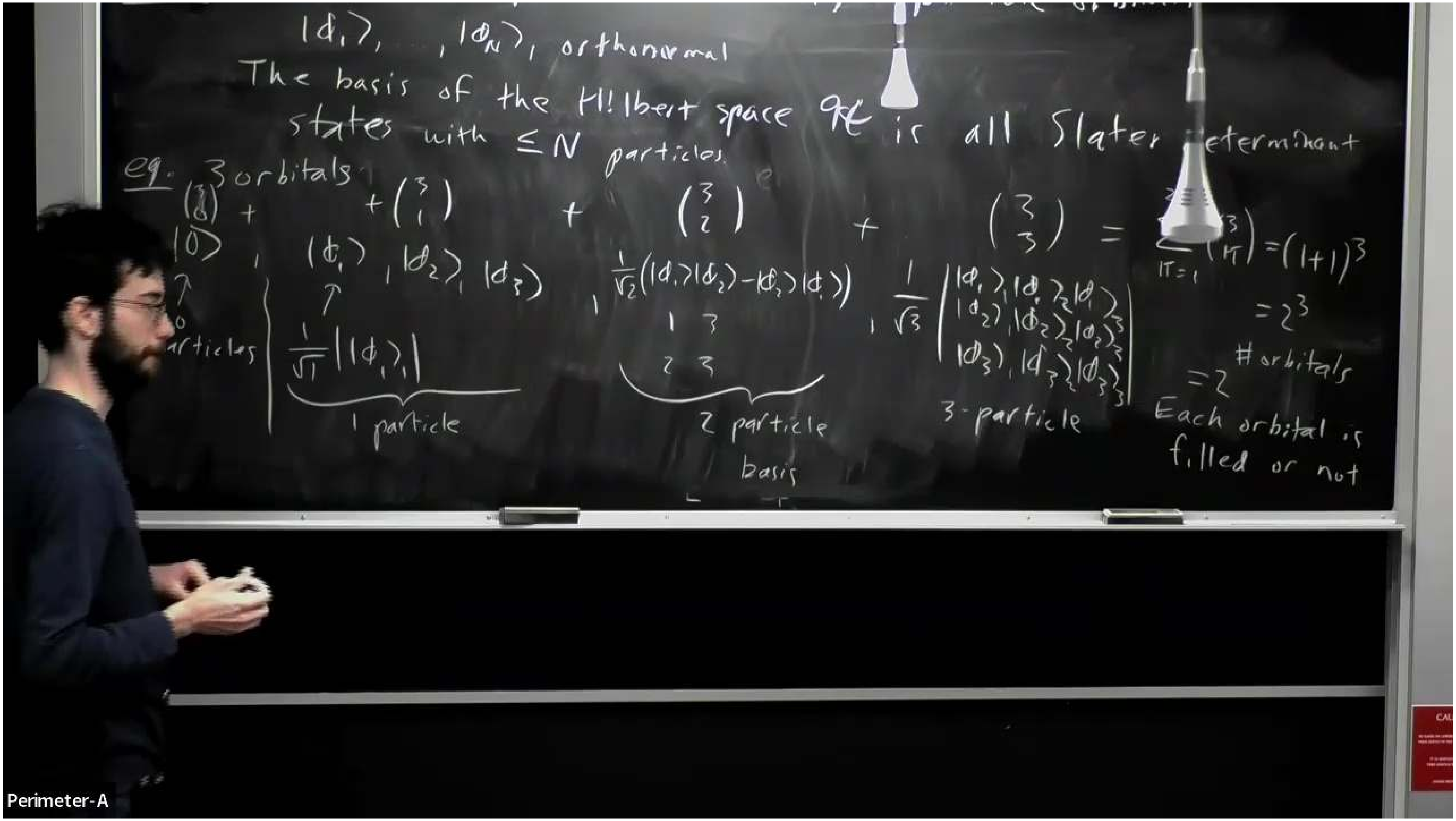
The basis of the Hilbert space $\mathcal{H}$ is all Slater determinant states with $\leq N$ particles

<u>eg.</u> 3 orbitals

$$|0\rangle \;,\; |\phi_1\rangle \;,\; |\phi_2\rangle ,\; |\phi_3\rangle$$

$\uparrow$ no particles

$\uparrow$ $\frac{1}{\sqrt{1}} \left| |\phi_1\rangle \right|$



$|\phi_1\rangle, \ldots, |\phi_N\rangle$, orthonormal

The basis of the Hilbert space $\mathcal{H}$ is all Slater determinant states with $\leq N$ particles.

eg. 3 orbitals

$$\binom{3}{0} + \binom{3}{1} + \binom{3}{2} + \binom{3}{3} = \sum_{n=1}^{3}\binom{3}{n} = (1+1)^3$$

$$= 2^3$$

$$= 2^{\#\,\text{orbitals}}$$

$|0\rangle$, $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$, $\frac{1}{\sqrt{2}}(|\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle)$, $\frac{1}{\sqrt{3}}\begin{vmatrix} |\phi_1\rangle_1 & |\phi_1\rangle_2 & |\phi_1\rangle_3 \\ |\phi_2\rangle_1 & |\phi_2\rangle_2 & |\phi_2\rangle_3 \\ |\phi_3\rangle_1 & |\phi_3\rangle_2 & |\phi_3\rangle_3 \end{vmatrix}$

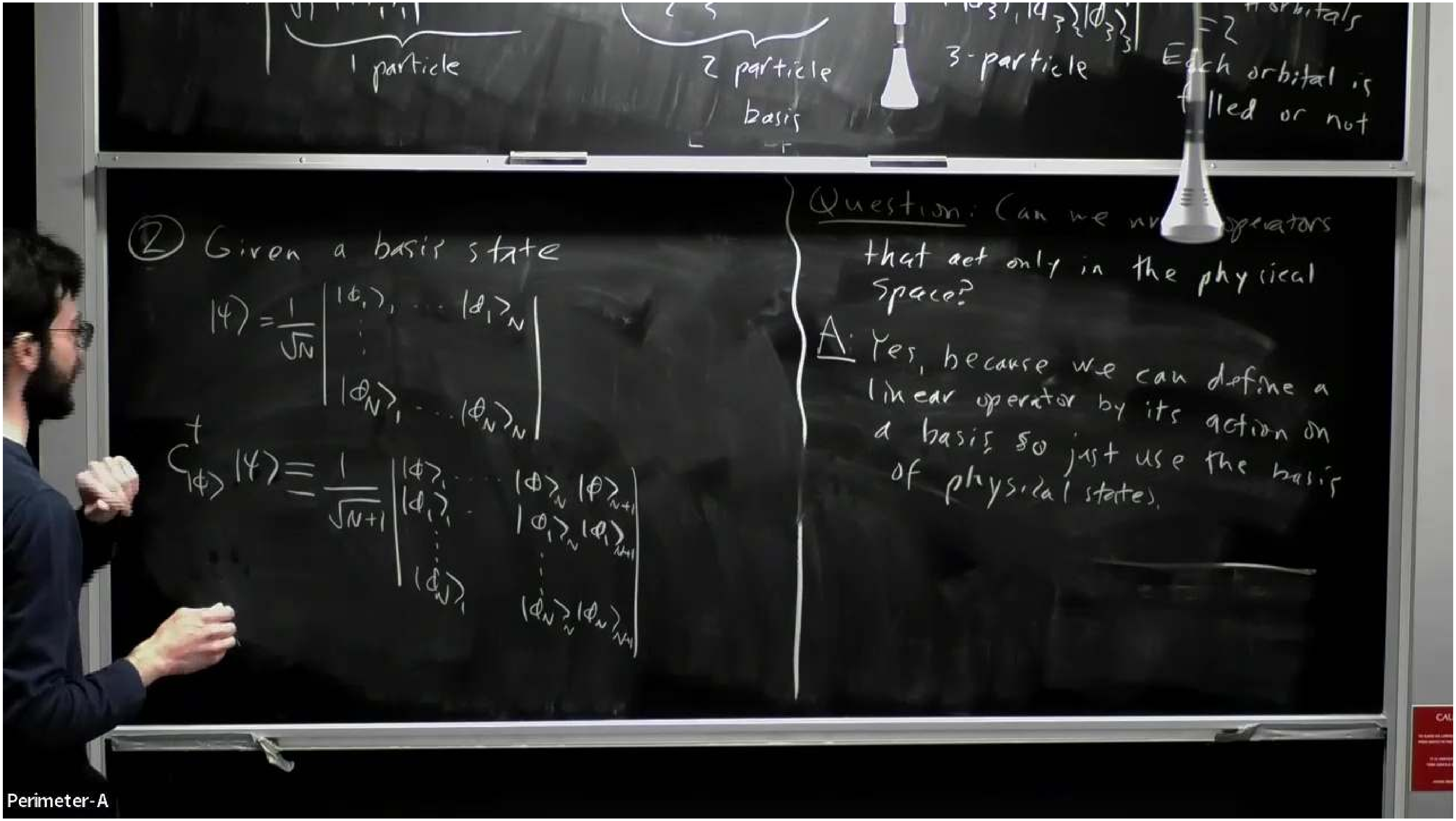
$\uparrow$ 0 particles

$\uparrow$ $\underbrace{\frac{1}{\sqrt{1}}\big|\,|\phi_1\rangle_1\big|}_{\text{1 particle}}$

$\underbrace{\begin{matrix}1 & 3\\ 2 & 3\end{matrix}}_{\text{2 particle basis}}$

3-particle

Each orbital is filled or not



$|\phi_3\rangle_1, |\phi_3\rangle_2 |\phi_3\rangle_3|$

1 particle

2 particle basis

3-particle

orbitals = 2

E ch orbital is
 lled or not

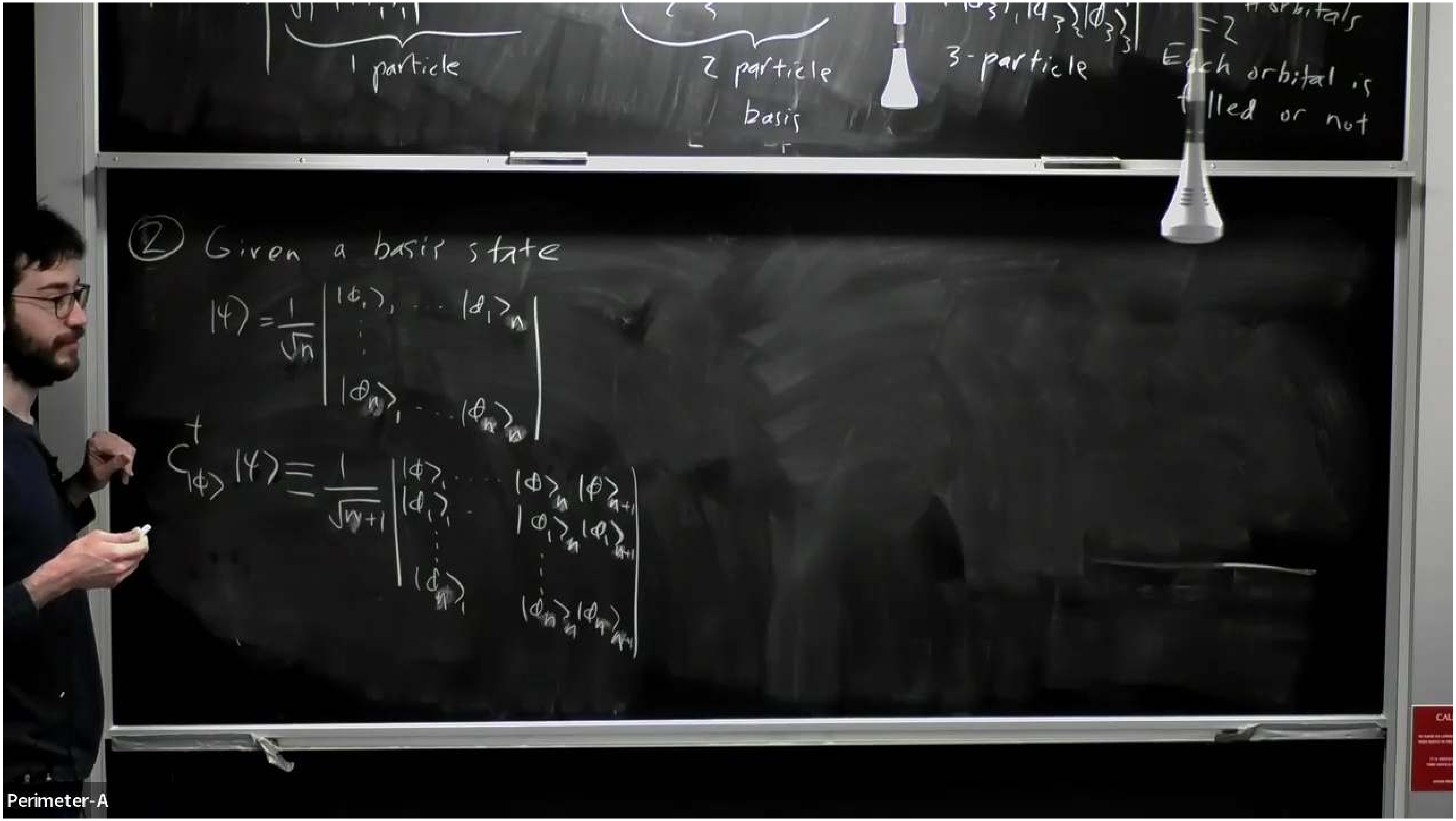
② Given a basis state

$$|\psi\rangle = \frac{1}{\sqrt{N}} \begin{vmatrix} |\phi_1\rangle_1 & \cdots & |\phi_1\rangle_N \\ \vdots & & \\ |\phi_N\rangle_1 & \cdots & |\phi_N\rangle_N \end{vmatrix}$$

$$c^\dagger_{|\phi\rangle} |\psi\rangle \equiv \frac{1}{\sqrt{N+1}} \begin{vmatrix} |\phi\rangle_1 & \cdots & |\phi\rangle_N & |\phi\rangle_{N+1} \\ |\phi_1\rangle_1 & \cdot & |\phi_1\rangle_N & |\phi_1\rangle_{N+1} \\ \vdots & & \vdots & \\ |\phi_N\rangle_1 & & |\phi_N\rangle_N & |\phi_N\rangle_{N+1} \end{vmatrix}$$

Question: Can we wr perators that act only in the physical space?

A: Yes, because we can define a linear operator by its action on a basis so just use the basis of physical states.



1 particle

2 particle basis

3-particle

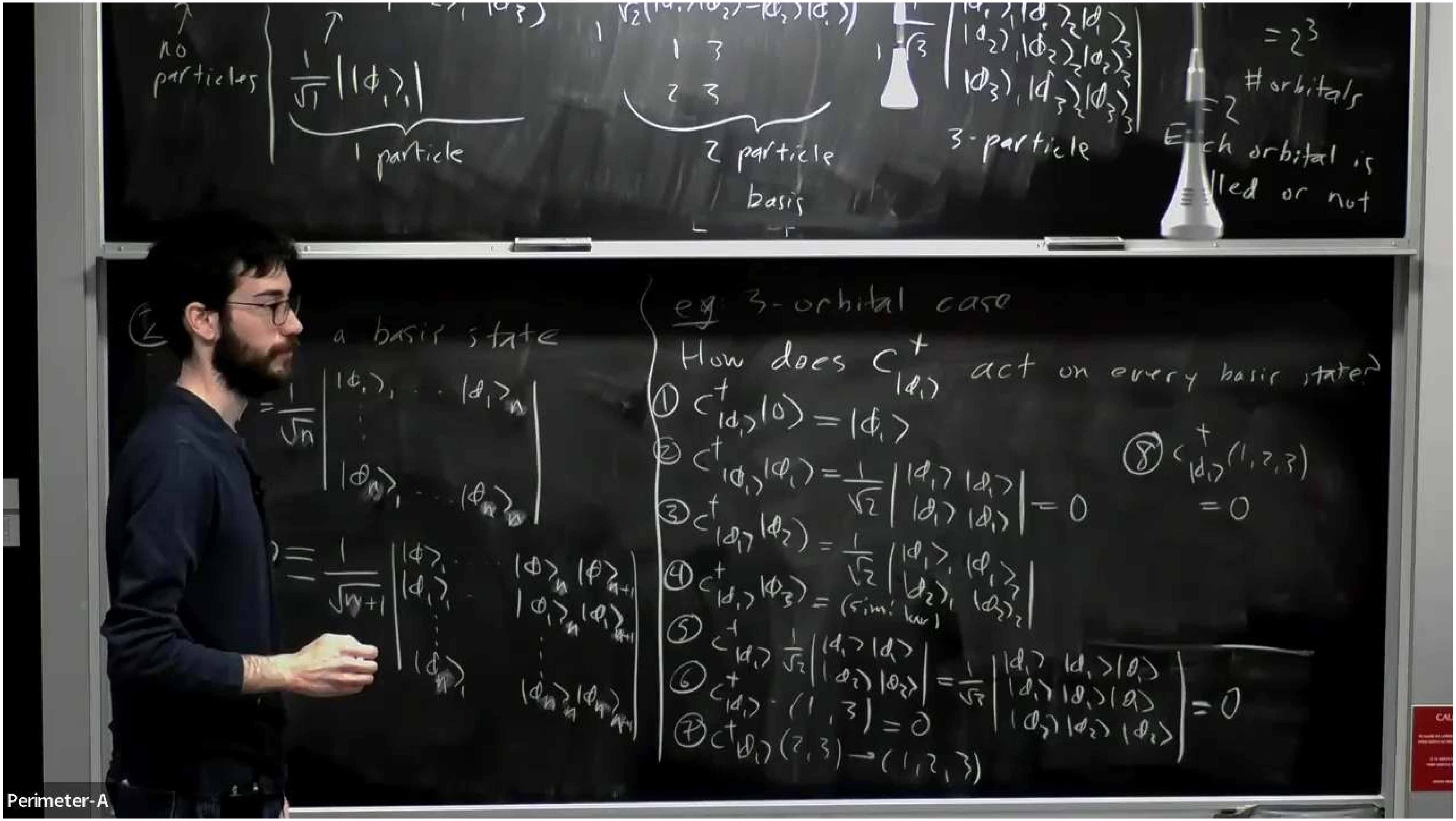
$= 2$

Each orbital is filled or not

② Given a basis state

$$|\psi\rangle = \frac{1}{\sqrt{n}} \begin{vmatrix} |\phi_1\rangle_1 & \cdots & |\phi_1\rangle_n \\ \vdots & & \\ |\phi_n\rangle_1 & \cdots & |\phi_n\rangle_n \end{vmatrix}$$

$$c^{\dagger}_{|\phi\rangle}|\psi\rangle \equiv \frac{1}{\sqrt{n+1}} \begin{vmatrix} |\phi\rangle_1 & \cdots & |\phi\rangle_n & |\phi\rangle_{n+1} \\ |\phi_1\rangle_1 & \cdot & |\phi_1\rangle_n & |\phi_1\rangle_{n+1} \\ \vdots & & \vdots & \\ |\phi_n\rangle_1 & & |\phi_n\rangle_n & |\phi_n\rangle_{n+1} \end{vmatrix}$$



no particles

$\frac{1}{\sqrt{1}}\big||\phi_1\rangle_1\big|$

1 particle

1 3

2 3

2 particle basis

3-particle

$= 2^3$

$= 2^{\#\text{orbitals}}$

E ch orbital is

lled or not

a basis state

$$= \frac{1}{\sqrt{n}}\begin{vmatrix} |\phi_1\rangle_1 & \cdots & |\phi_1\rangle_n \\ \vdots & & \\ |\phi_n\rangle_1 & \cdots & |\phi_n\rangle_n \end{vmatrix}$$

$$= \frac{1}{\sqrt{n+1}}\begin{vmatrix} |\phi\rangle_1 & \cdots & |\phi\rangle_n & |\phi\rangle_{n+1} \\ |\phi_1\rangle_1 & \cdots & |\phi_1\rangle_n & |\phi_1\rangle_{n+1} \\ \vdots & & \vdots & \\ |\phi_n\rangle_1 & & |\phi_n\rangle_n & |\phi_n\rangle_{n+1} \end{vmatrix}$$

e.g. 3-orbital case

How does $c^\dagger_{|\phi_1\rangle}$ act on every basis state?

① $c^\dagger_{|\phi_1\rangle}|0\rangle = |\phi_1\rangle$

② $c^\dagger_{|\phi_1\rangle}|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{vmatrix} |\phi_1\rangle & |\phi_1\rangle \\ |\phi_1\rangle & |\phi_1\rangle \end{vmatrix} = 0$

③ $c^\dagger_{|\phi_1\rangle}|\phi_2\rangle = \frac{1}{\sqrt{2}}\begin{vmatrix} |\phi_1\rangle_1 & |\phi_1\rangle_2 \\ |\phi_2\rangle_1 & |\phi_2\rangle_2 \end{vmatrix}$

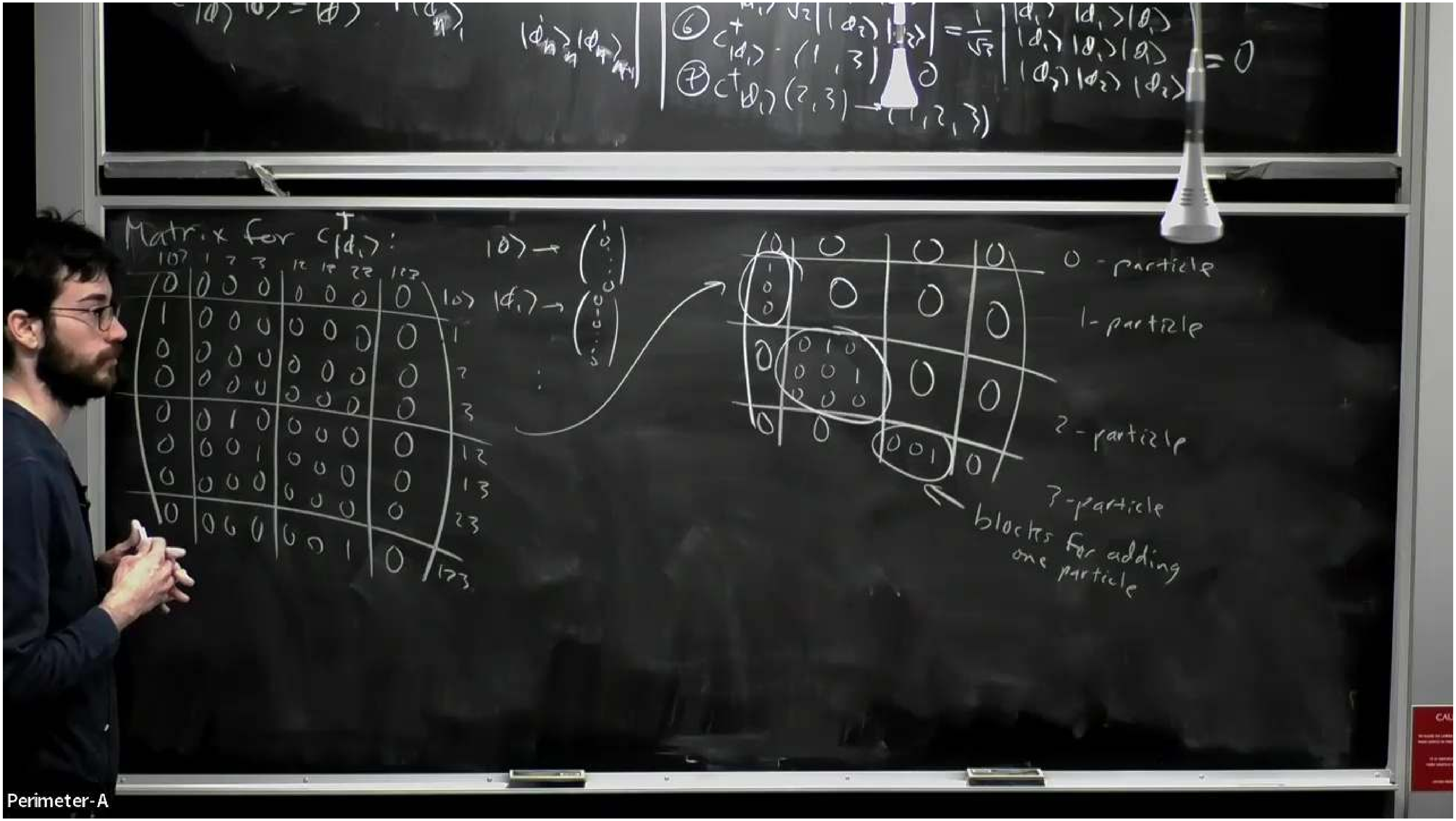
④ $c^\dagger_{|\phi_1\rangle}|\phi_3\rangle =$ (similar)

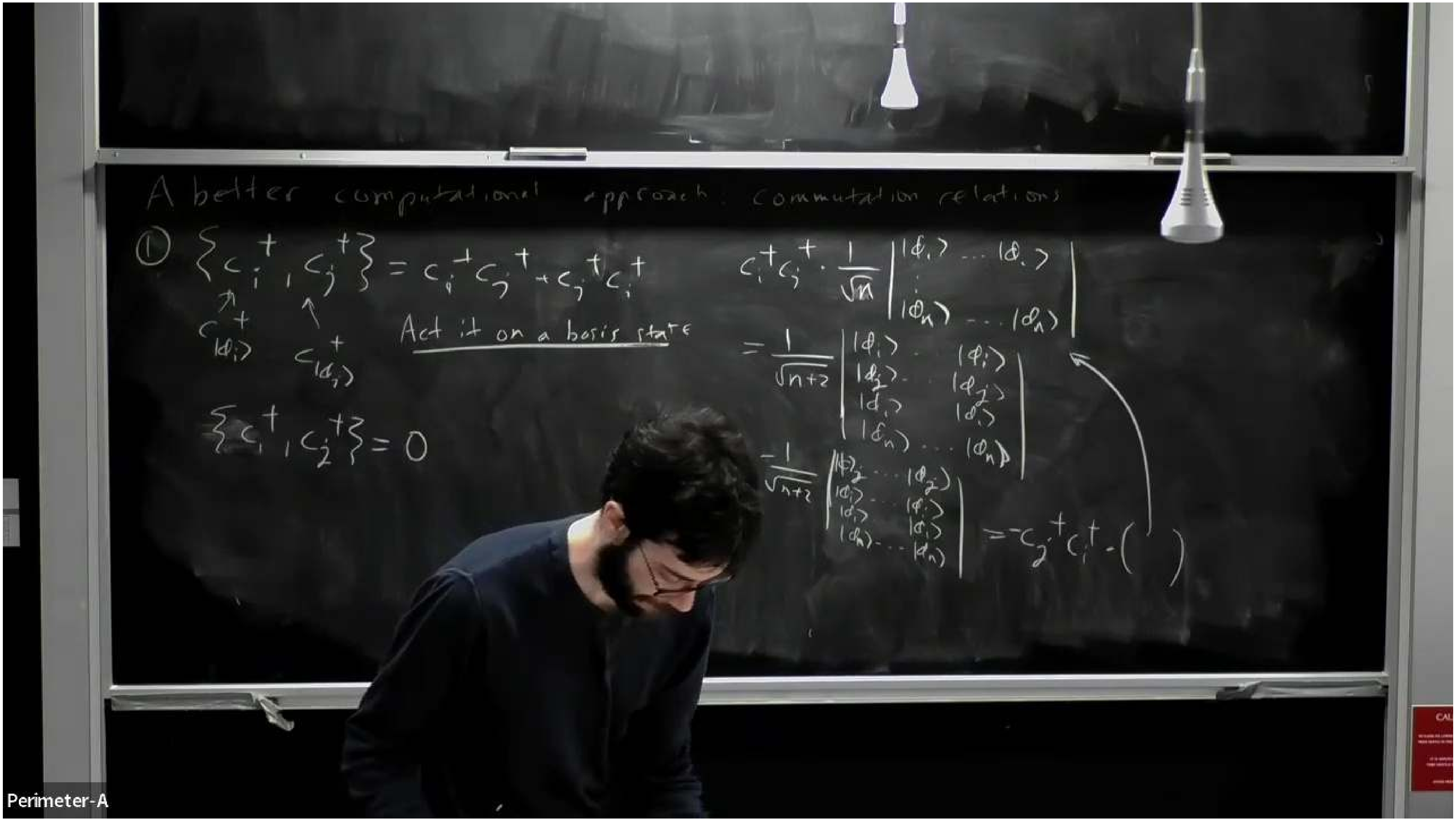
⑤ $c^\dagger_{|\phi_1\rangle}\frac{1}{\sqrt{2}}\begin{vmatrix} |\phi_1\rangle & |\phi_1\rangle \\ |\phi_2\rangle & |\phi_2\rangle \end{vmatrix} = \frac{1}{\sqrt{3}}\begin{vmatrix} |\phi_1\rangle & |\phi_1\rangle & |\phi_1\rangle \\ |\phi_1\rangle & |\phi_1\rangle & |\phi_1\rangle \\ |\phi_2\rangle & |\phi_2\rangle & |\phi_2\rangle \end{vmatrix} = 0$

⑥ $c^\dagger_{|\phi_1\rangle}(1,3) = 0$

⑦ $c^\dagger_{|\phi_1\rangle}(2,3) \rightarrow (1,2,3)$

⑧ $c^\dagger_{|\phi_1\rangle}(1,2,3) = 0$


Matrix for $c^\dagger_{|\phi_1\rangle}$:
$|0\rangle \rightarrow$
$|\phi_1\rangle \rightarrow$
0 - particle
1 - particle
2 - particle
3 - particle
blocks for adding one particle
Perimeter-A



A better computational approach: commutation relations

① $\{c_i^\dagger, c_j^\dagger\} = c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger$

$c^\dagger_{|\phi_i\rangle}$ $\quad c^\dagger_{|\phi_j\rangle}$

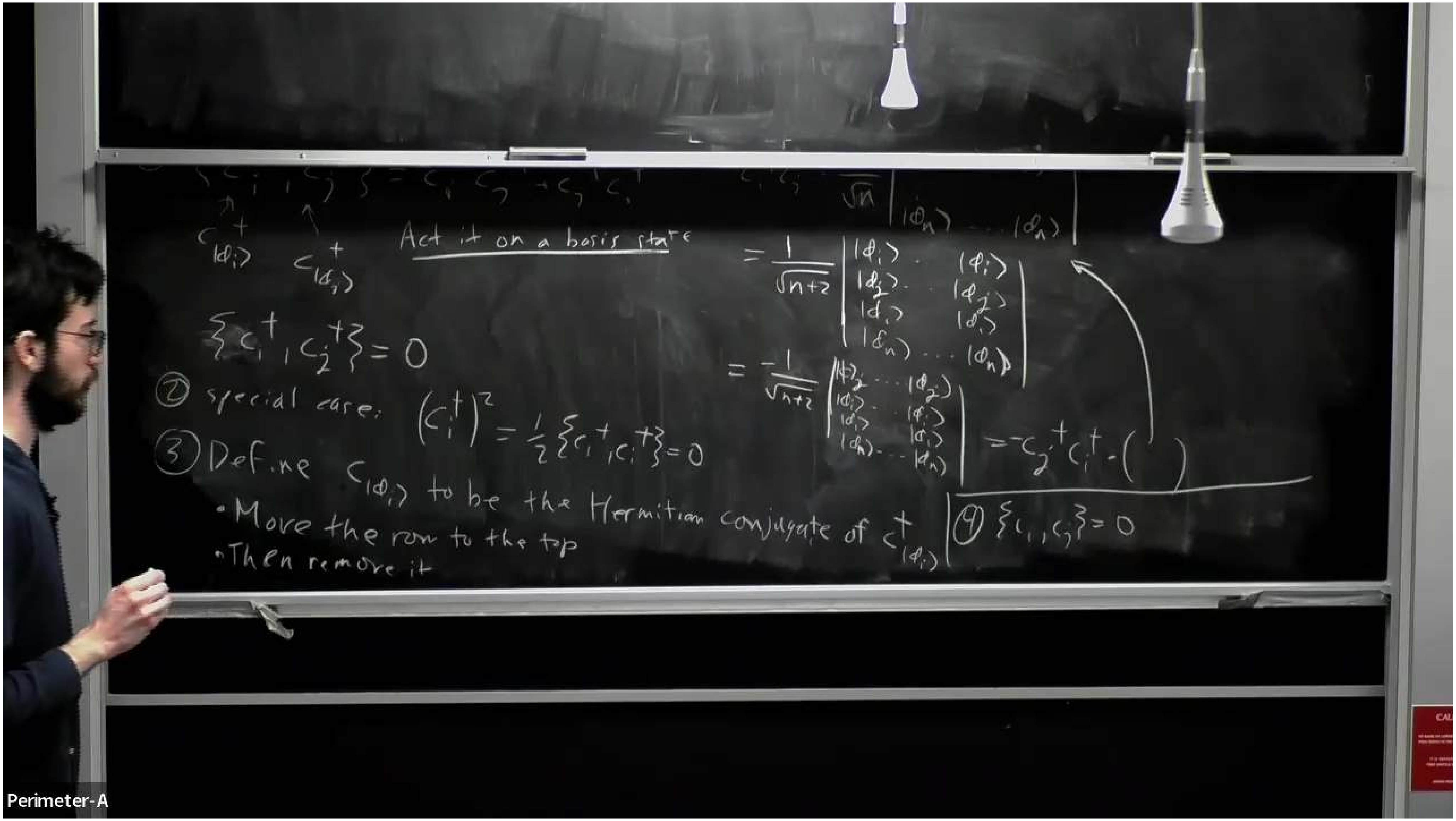
Act it on a basis state

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

$$c_i^\dagger c_j^\dagger \cdot \frac{1}{\sqrt{n}} \begin{vmatrix} |\phi_1\rangle & \dots & |\phi_1\rangle \\ \vdots & & \\ |\phi_n\rangle & \dots & |\phi_n\rangle \end{vmatrix}$$

$$= \frac{1}{\sqrt{n+2}} \begin{vmatrix} |\phi_i\rangle & \dots & |\phi_i\rangle \\ |\phi_j\rangle & \dots & |\phi_j\rangle \\ |\phi_1\rangle & & |\phi_1\rangle \\ |\phi_n\rangle & \dots & |\phi_n\rangle \end{vmatrix}$$

$$-\frac{1}{\sqrt{n+2}} \begin{vmatrix} |\phi_j\rangle & \dots & |\phi_j\rangle \\ |\phi_i\rangle & \dots & |\phi_i\rangle \\ |\phi_1\rangle & & |\phi_1\rangle \\ |\phi_n\rangle & \dots & |\phi_n\rangle \end{vmatrix} = -c_j^\dagger c_i^\dagger \cdot (\quad)$$



$\{c_i , c_j\} = c_i c_j + c_j c_i$

$c^{\dagger}_{|\phi_i\rangle}$ $c^{\dagger}_{|\phi_j\rangle}$

Act it on a basis state

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

② special case: $(c_i^{\dagger})^2 = \frac{1}{2}\{c_i^{\dagger}, c_i^{\dagger}\} = 0$

③ Define $c_{|\phi_i\rangle}$ to be the Hermitian conjugate of $c^{\dagger}_{|\phi_i\rangle}$

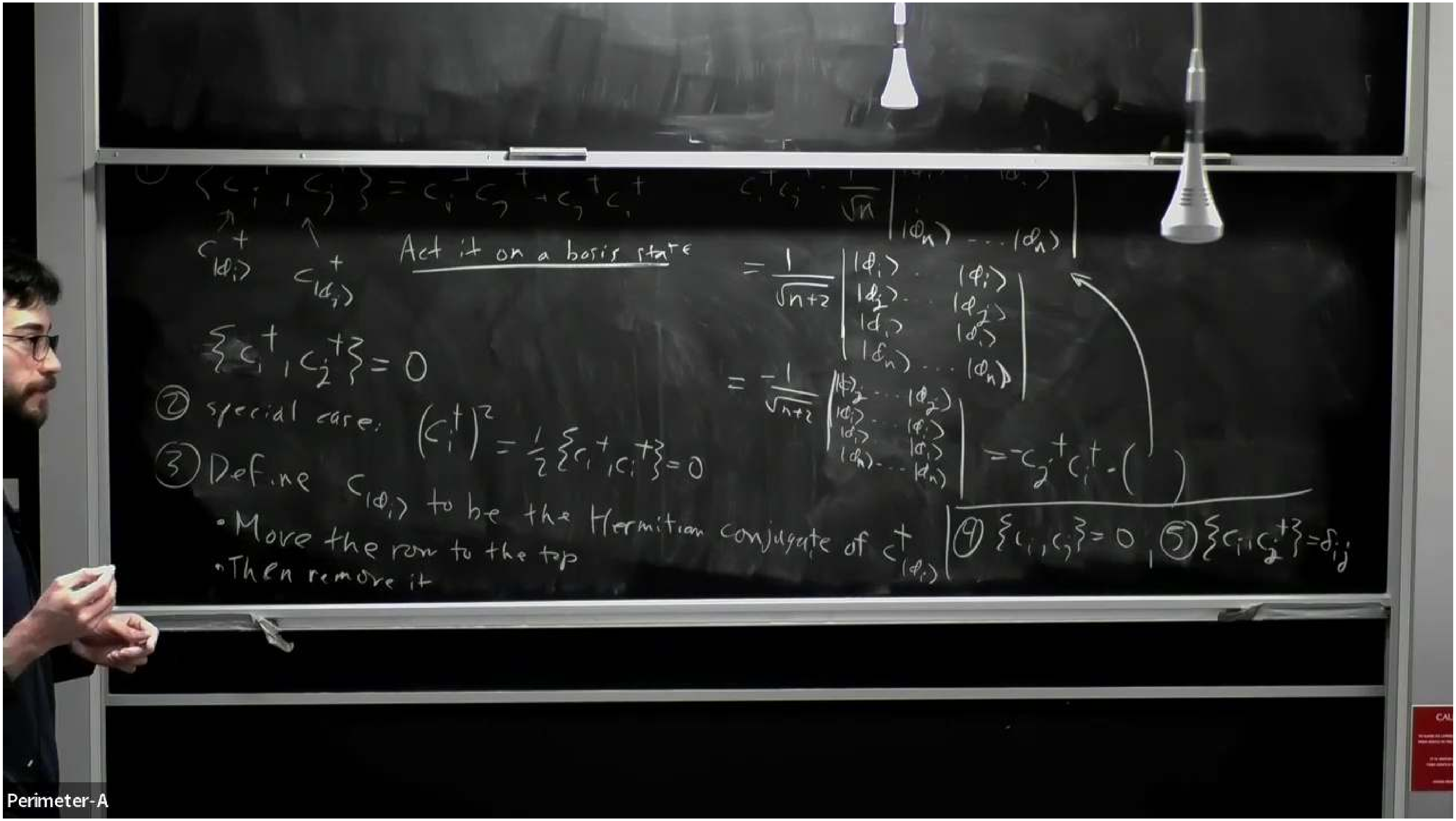
- Move the row to the top
- Then remove it

$$\frac{1}{\sqrt{n}}\begin{vmatrix} |\phi_n\rangle & \cdots & |\phi_n\rangle \end{vmatrix}$$

$$= \frac{1}{\sqrt{n+2}}\begin{vmatrix} |\phi_i\rangle & \cdots & |\phi_i\rangle \\ |\phi_j\rangle & \cdots & |\phi_j\rangle \\ |\phi_1\rangle & & |\phi_1\rangle \\ |\phi_n\rangle & \cdots & |\phi_n\rangle \end{vmatrix}$$

$$= -\frac{1}{\sqrt{n+2}}\begin{vmatrix} |\phi_j\rangle & \cdots & |\phi_j\rangle \\ |\phi_i\rangle & \cdots & |\phi_i\rangle \\ |\phi_1\rangle & & |\phi_1\rangle \\ |\phi_n\rangle & \cdots & |\phi_n\rangle \end{vmatrix} = -c_j^{\dagger} c_i^{\dagger} \cdot (\quad)$$

④ $\{c_i , c_j\} = 0$



① $\{c_i^\dagger, c_j^\dagger\} = c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger$

$c^\dagger_{|\phi_i\rangle}$ $c^\dagger_{|\phi_j\rangle}$

Act it on a basis state

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

② special case: $(c_i^\dagger)^2 = \frac{1}{2}\{c_i^\dagger, c_i^\dagger\} = 0$

③ Define $c_{|\phi_i\rangle}$ to be the Hermitian conjugate of $c^\dagger_{|\phi_i\rangle}$

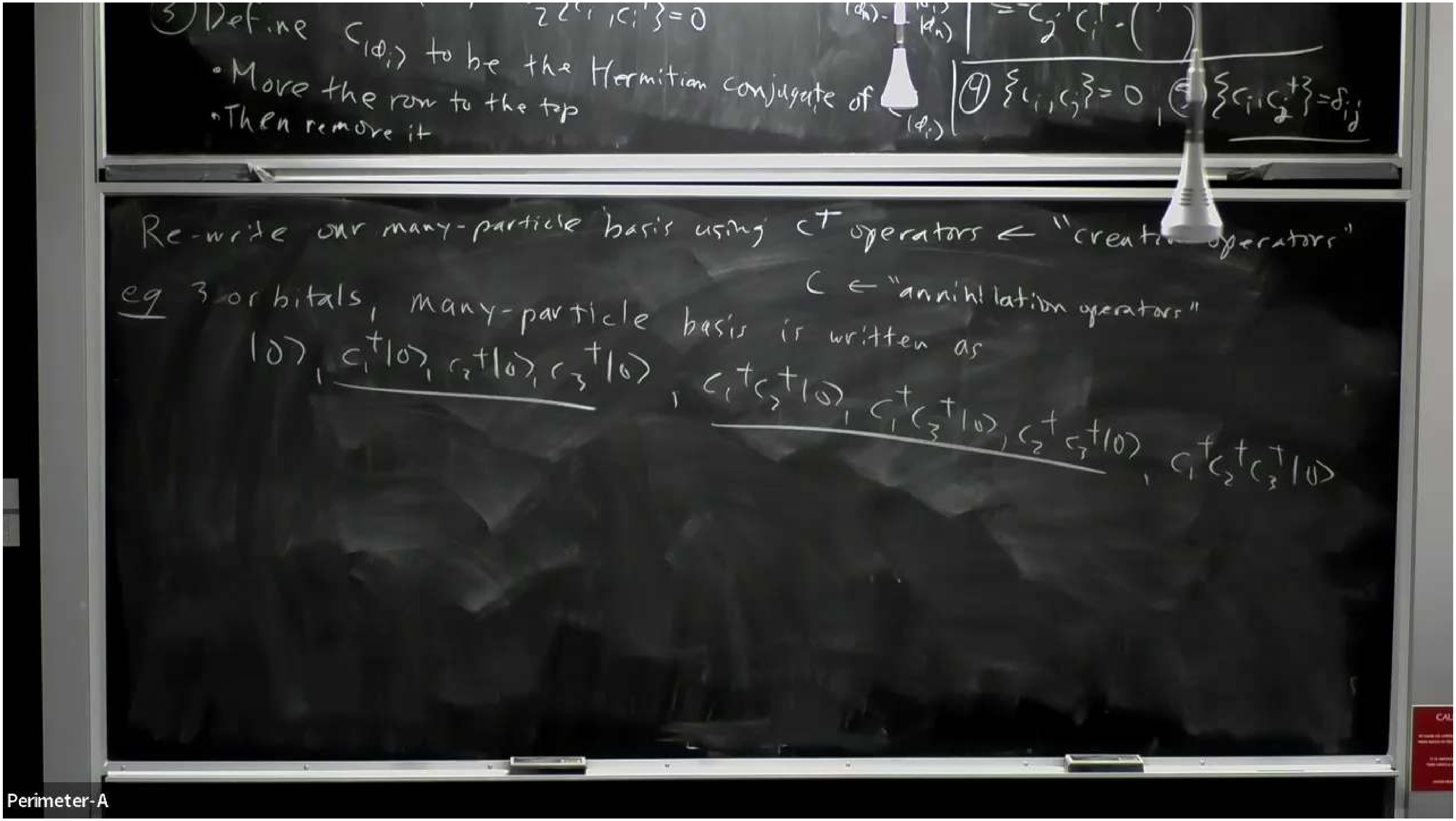
- Move the row to the top
- Then remove it

$$c_i^\dagger c_j^\dagger \cdot \frac{1}{\sqrt{n}} \begin{vmatrix} \vdots & & \vdots \\ |\phi_n\rangle & \cdots & |\phi_n\rangle \end{vmatrix}$$

$$= \frac{1}{\sqrt{n+2}} \begin{vmatrix} |\phi_i\rangle & \cdots & |\phi_i\rangle \\ |\phi_j\rangle & \cdots & |\phi_j\rangle \\ |\phi_1\rangle & & |\phi_1\rangle \\ |\phi_n\rangle & \cdots & |\phi_n\rangle \end{vmatrix}$$

$$= -\frac{1}{\sqrt{n+2}} \begin{vmatrix} |\phi_j\rangle & \cdots & |\phi_j\rangle \\ |\phi_i\rangle & \cdots & |\phi_i\rangle \\ |\phi_1\rangle & & |\phi_1\rangle \\ |\phi_n\rangle & \cdots & |\phi_n\rangle \end{vmatrix} = -c_j^\dagger c_i^\dagger \cdot (\quad)$$

④ $\{c_i, c_j\} = 0$, ⑤ $\{c_i, c_j^\dagger\} = \delta_{ij}$



$\{c_i, c_i\} = 0$

$= -c_j^\dagger c_i^\dagger - ($

③ Define $c_{|\phi_i\rangle}$ to be the Hermitian conjugate of $c_{|\phi_i\rangle}$

- More the row to the top
- Then remove it

④ $\{c_i, c_j\} = 0$, ⑤ $\{c_i, c_j^\dagger\} = \delta_{ij}$

Re-write our many-particle basis using $c^\dagger$ operators ← "creation operators"

c ← "annihilation operators"

eg 3 orbitals, many-particle basis is written as

$|0\rangle, \underline{c_1^\dagger|0\rangle, c_2^\dagger|0\rangle, c_3^\dagger|0\rangle}, \underline{c_1^\dagger c_2^\dagger|0\rangle, c_1^\dagger c_3^\dagger|0\rangle, c_2^\dagger c_3^\dagger|0\rangle}, c_1^\dagger c_2^\dagger c_3^\dagger|0\rangle$