Title: PSI Lecture - Condensed Matter - Lecture 9

Speakers: Aaron Szasz

Collection: PSI Lecture - Condensed Matter

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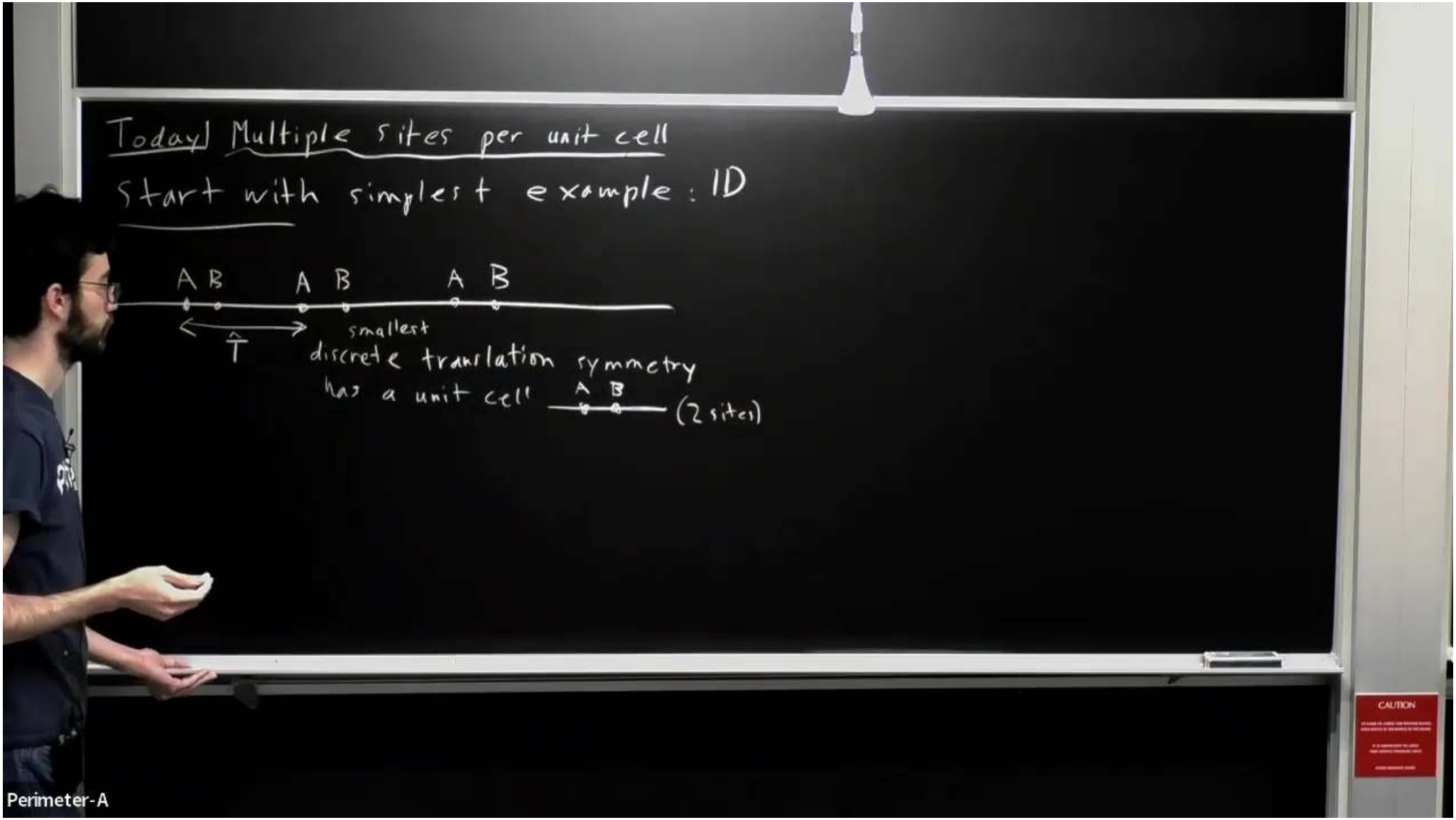
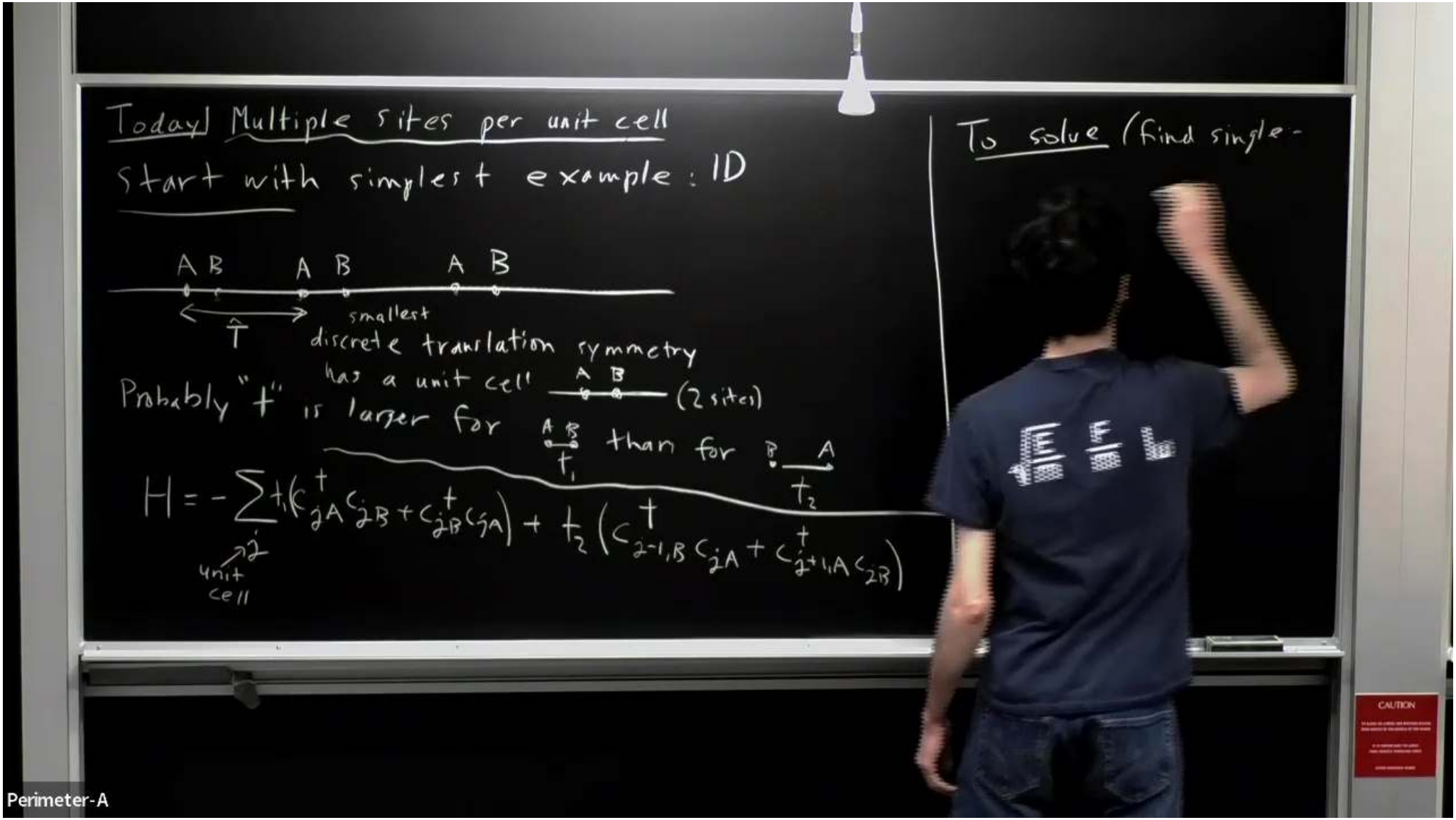
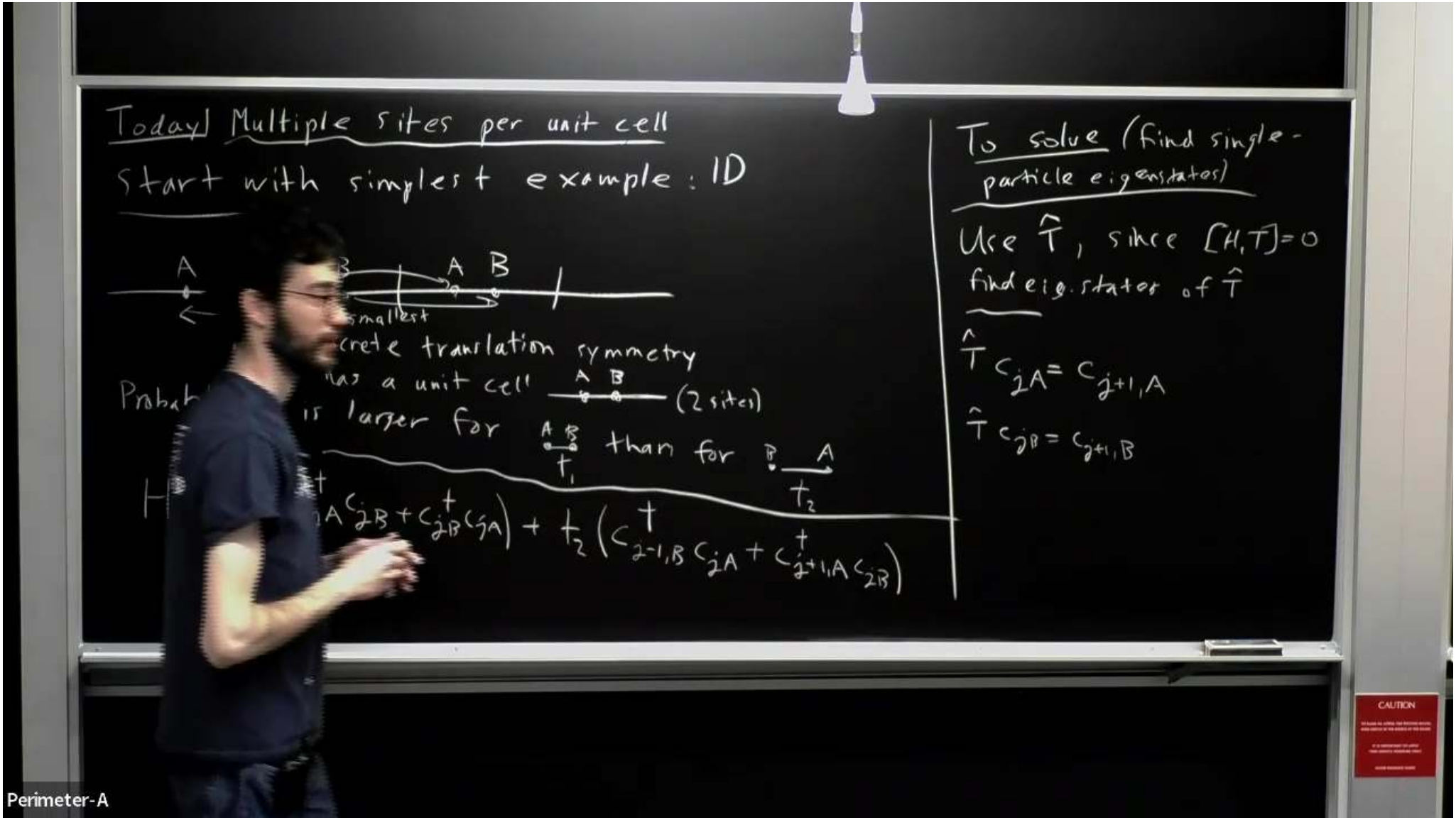
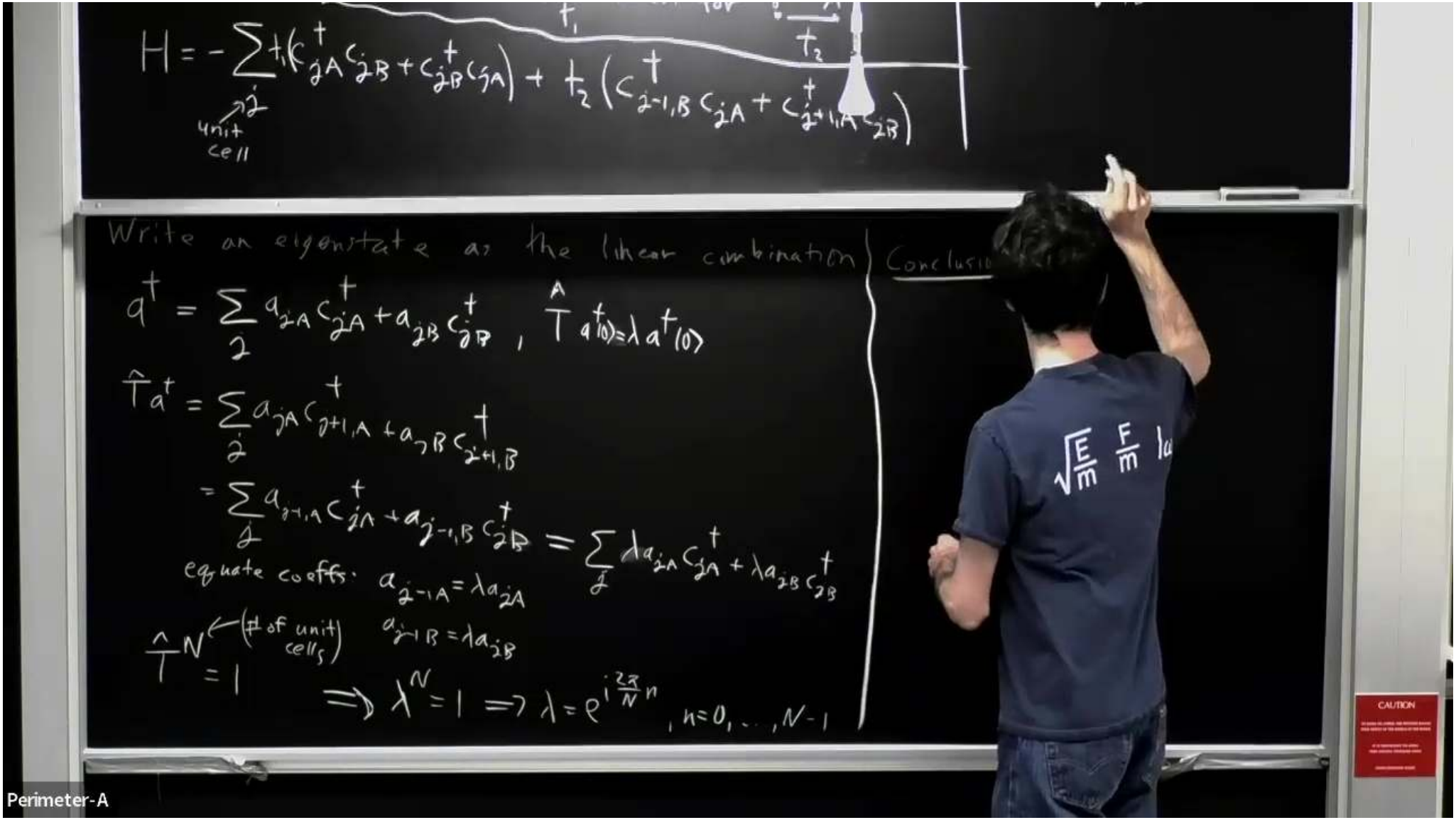
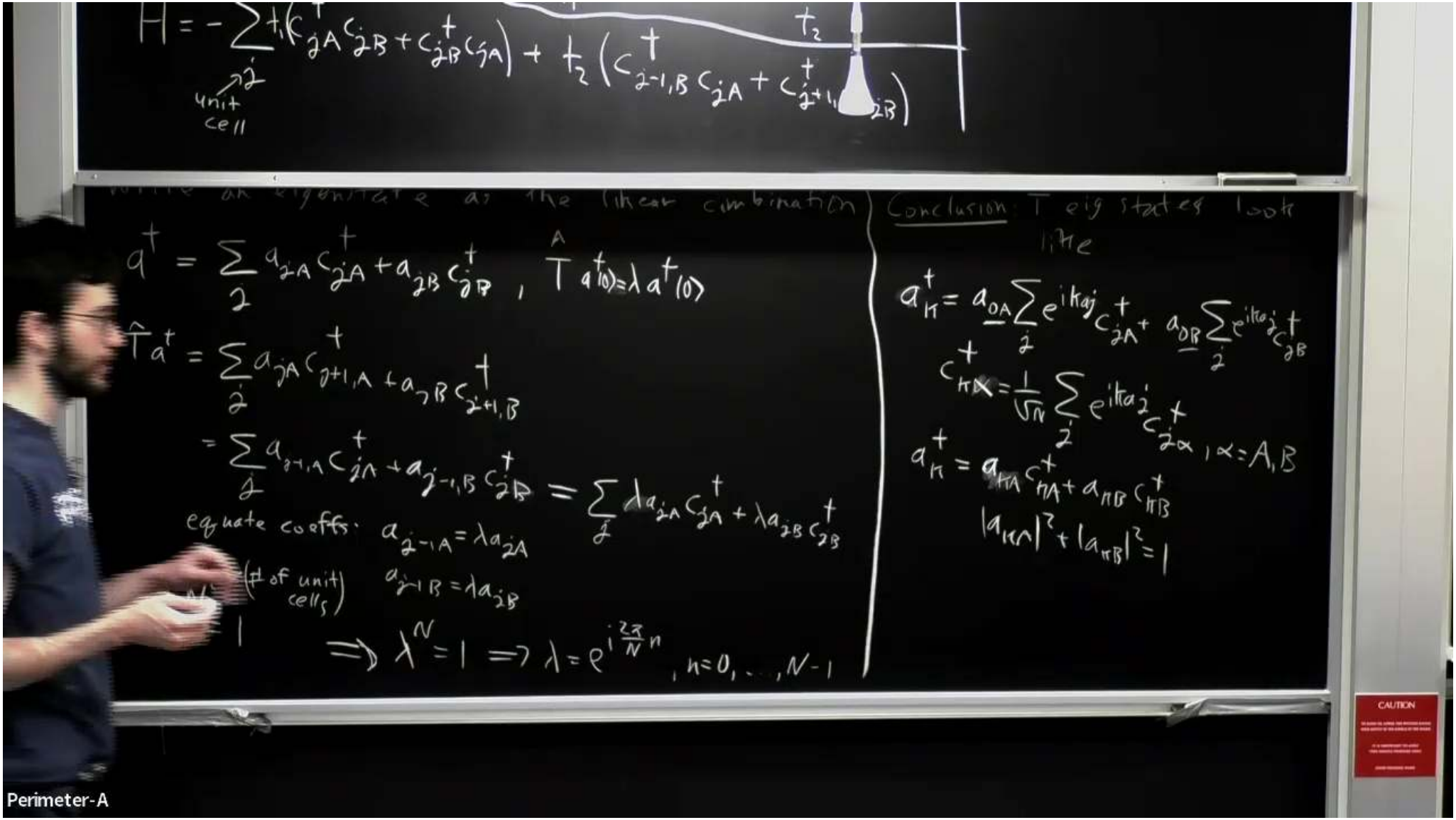
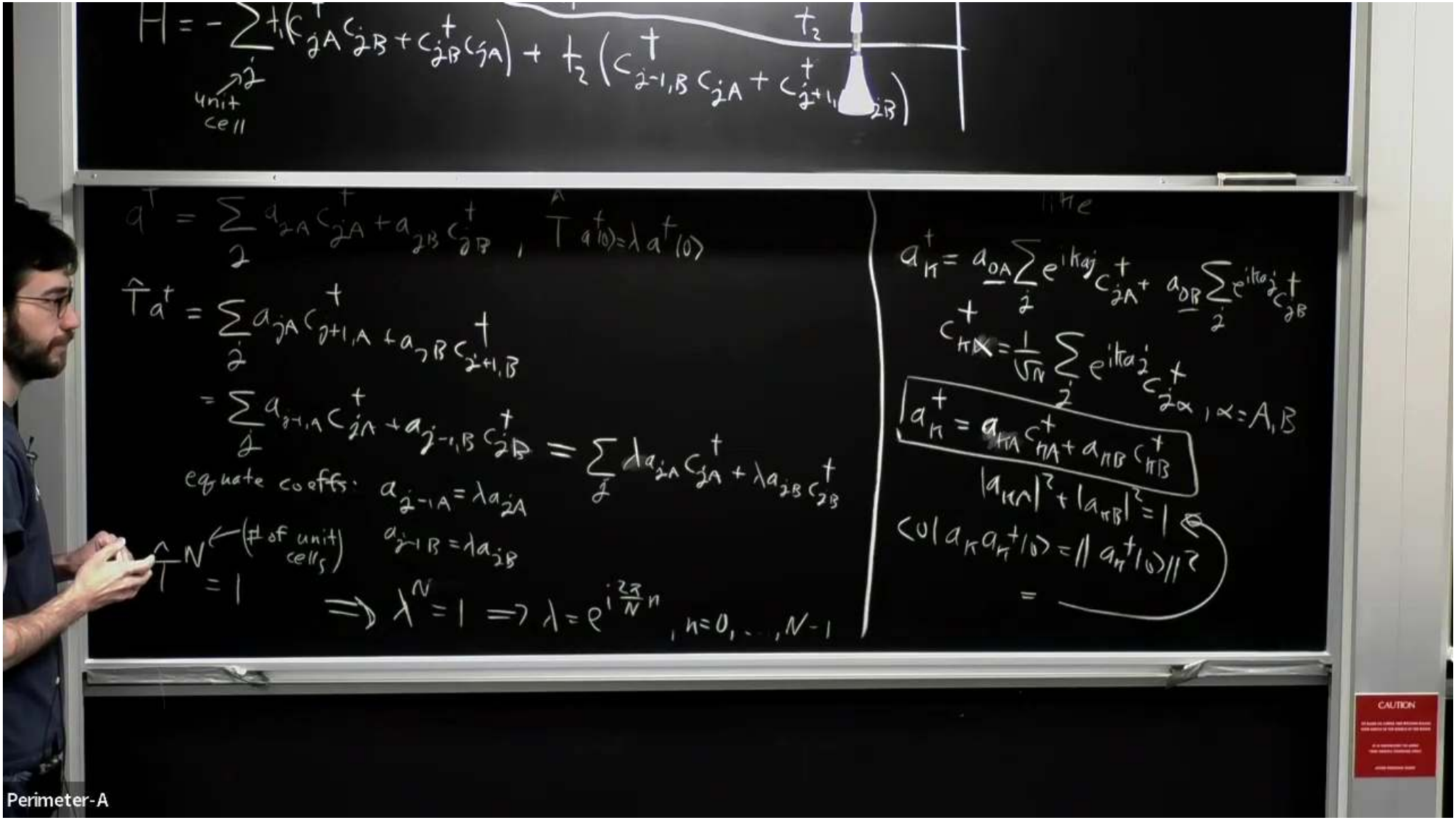

Today! Multiple sites per unit cell
start with simplest example: 1D
A B A B A B
smallest
$\hat{T}$
discrete translation symmetry
has a unit cell A B (2 sites)
CAUTION
Perimeter-A

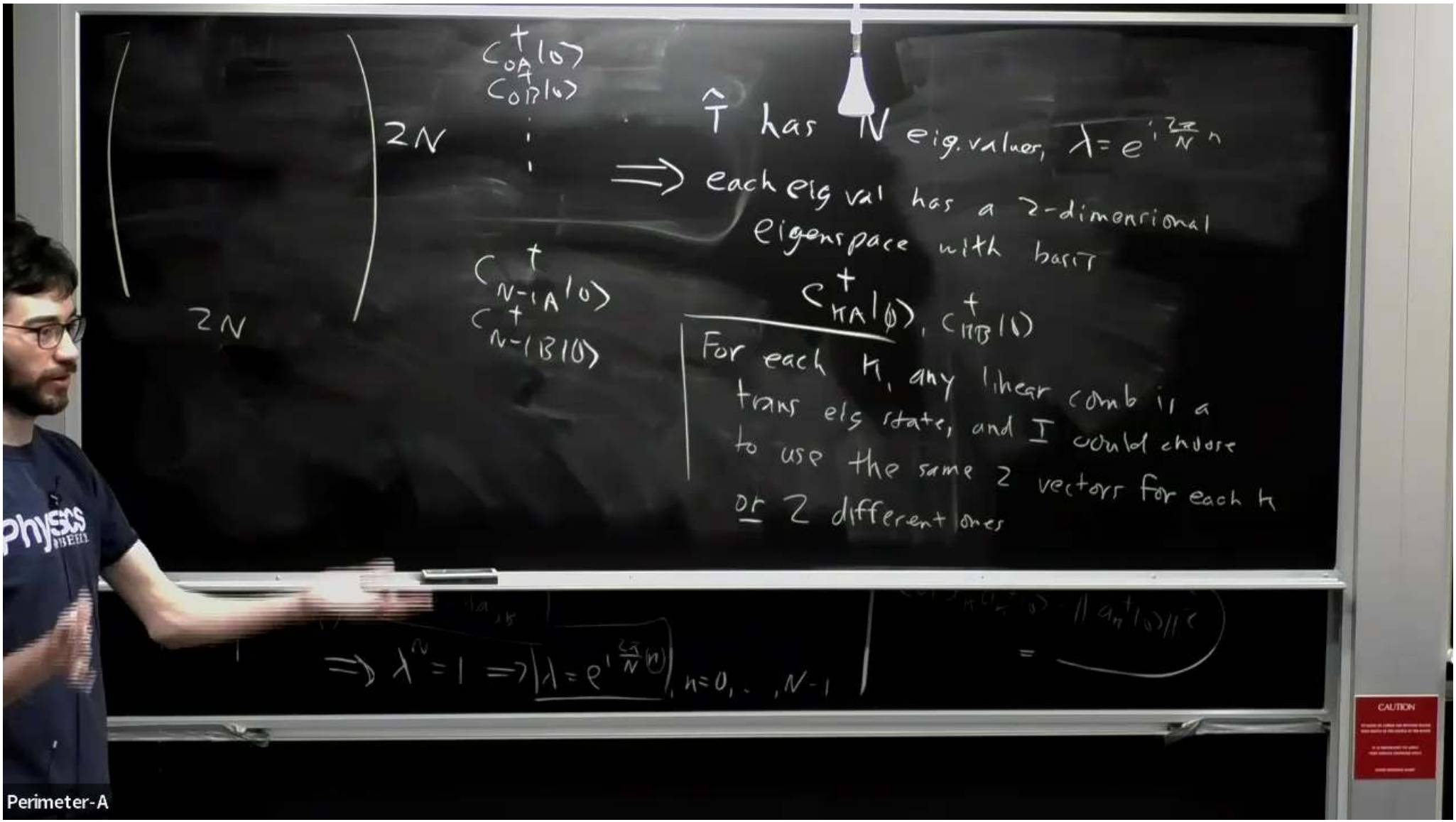

Today! Multiple sites per unit cell
start with simplest example: 1D
A B A B A B
smallest
discrete translation symmetry
has a unit cell
(2 sites)
Probably "t" is larger for
than for
$H = -\sum_j t_1 (c^\dagger_{jA} c_{jB} + c^\dagger_{jB} c_{jA}) + t_2 (c^\dagger_{j-1,B} c_{jA} + c^\dagger_{j+1,A} c_{jB})$
unit cell
To solve (find single-
CAUTION
Perimeter-A


Today: Multiple sites per unit cell
start with simplest example: 1D
A
A B
smallest
crete translation symmetry
as a unit cell
A B
(2 sites)
is larger for
than for
t_1
t_2
$+ t_2 \left(c^\dagger_{j-1,B} c_{jA} + c^\dagger_{j+1,A} c_{jB} \right)$
To solve (find single-particle eigenstates)
Use $\hat{T}$, since $[H, \hat{T}] = 0$
find eig. states of $\hat{T}$
$\hat{T} c_{jA} = c_{j+1,A}$
$\hat{T} c_{jB} = c_{j+1,B}$
CAUTION


$H = -\sum_j t_1 (c^\dagger_{jA} c_{jB} + c^\dagger_{jB} c_{jA}) + t_2 (c^\dagger_{j-1,B} c_{jA} + c^\dagger_{j+1,A} c_{jB})$
unit cell
t_1
t_2
Write an eigenstate as the linear combination
$q^\dagger = \sum_j a_{jA} c^\dagger_{jA} + a_{jB} c^\dagger_{jB}$, $\hat{T}\, q^\dagger|0\rangle = \lambda\, q^\dagger|0\rangle$
$\hat{T} a^\dagger = \sum_j a_{jA} c^\dagger_{j+1,A} + a_{jB} c^\dagger_{j+1,B}$
$= \sum_j a_{j-1,A} c^\dagger_{jA} + a_{j-1,B} c^\dagger_{jB} = \sum_j \lambda a_{jA} c^\dagger_{jA} + \lambda a_{jB} c^\dagger_{jB}$
equate coeffs: $a_{j-1,A} = \lambda a_{jA}$
$a_{j-1,B} = \lambda a_{jB}$
$\hat{T}^N = 1$ ← (# of unit cells)
$\Rightarrow \lambda^N = 1 \Rightarrow \lambda = e^{i\frac{2\pi}{N}n}$, $n = 0, \ldots, N-1$
Conclusio
CAUTION

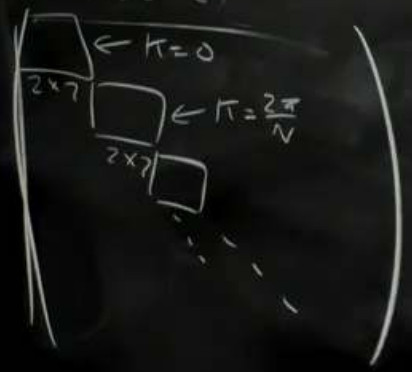

$H = -\sum_j t_1 (c^\dagger_{jA} c_{jB} + c^\dagger_{jB} c_{jA}) + t_2 (c^\dagger_{j-1,B} c_{jA} + c^\dagger_{j+1,A} c_{jB})$
unit cell
t_2
$q^\dagger = \sum_j a_{jA} c^\dagger_{jA} + a_{jB} c^\dagger_{jB}$, $\hat{T} a^\dagger |0\rangle = \lambda a^\dagger |0\rangle$
$\hat{T} a^\dagger = \sum_j a_{jA} c^\dagger_{j+1,A} + a_{jB} c^\dagger_{j+1,B}$
$= \sum_j a_{j+1,A} c^\dagger_{jA} + a_{j-1,B} c^\dagger_{jB} = \sum_j \lambda a_{jA} c^\dagger_{jA} + \lambda a_{jB} c^\dagger_{jB}$
equate coeffs. $a_{j-1,A} = \lambda a_{jA}$
(# of unit cells) $a_{j-1,B} = \lambda a_{jB}$
$\Rightarrow \lambda^N = 1 \Rightarrow \lambda = e^{i \frac{2\pi}{N} n}$, $n = 0, \ldots, N-1$
Conclusion: T eig states look like
$a^\dagger_{k} = a_{0A} \sum_j e^{ikaj} c^\dagger_{jA} + a_{0B} \sum_j e^{ikaj} c^\dagger_{jB}$
$c^\dagger_{k\alpha} = \frac{1}{\sqrt{N}} \sum_j e^{ikaj} c^\dagger_{j\alpha}$, $\alpha = A, B$
$a^\dagger_{k} = a_{kA} c^\dagger_{kA} + a_{kB} c^\dagger_{kB}$
$|a_{kA}|^2 + |a_{kB}|^2 = 1$
CAUTION


unit cell
equate coeffs:
CAUTION


$2N$
$2N$
$c_{0A}^\dagger|0\rangle$
$c_{0B}^\dagger|0\rangle$
$c_{N-1A}^\dagger|0\rangle$
$c_{N-1B}^\dagger|0\rangle$
$\hat{T}$ has N eig. values, $\lambda = e^{i\frac{2\pi}{N}n}$
$\Rightarrow$ each eig val has a 2-dimensional eigenspace with basis
$c_{nA}^\dagger|0\rangle$, $c_{nB}^\dagger|0\rangle$
For each n, any linear comb is a trans eig state, and I could choose to use the same 2 vectors for each n or 2 different ones
$\Rightarrow \lambda^N = 1 \Rightarrow \lambda = e^{i\frac{2\pi}{N}(n)}$, $n = 0, \ldots, N-1$
CAUTION

We found eig vects of T, since $[H,T]=0$, this divides H into 2-dimensional subspaces

i.e. Block diagonal, with blocks of size 2:



What we still need to do:

diagonalize each block, this will fix "a_{kA}" "a_{kB}" in order for $a_k^\dagger$ to be an eig[illegible] just [illegible]

$\sqrt{\frac{E}{m}}\ \frac{F}{m}\ l\omega$

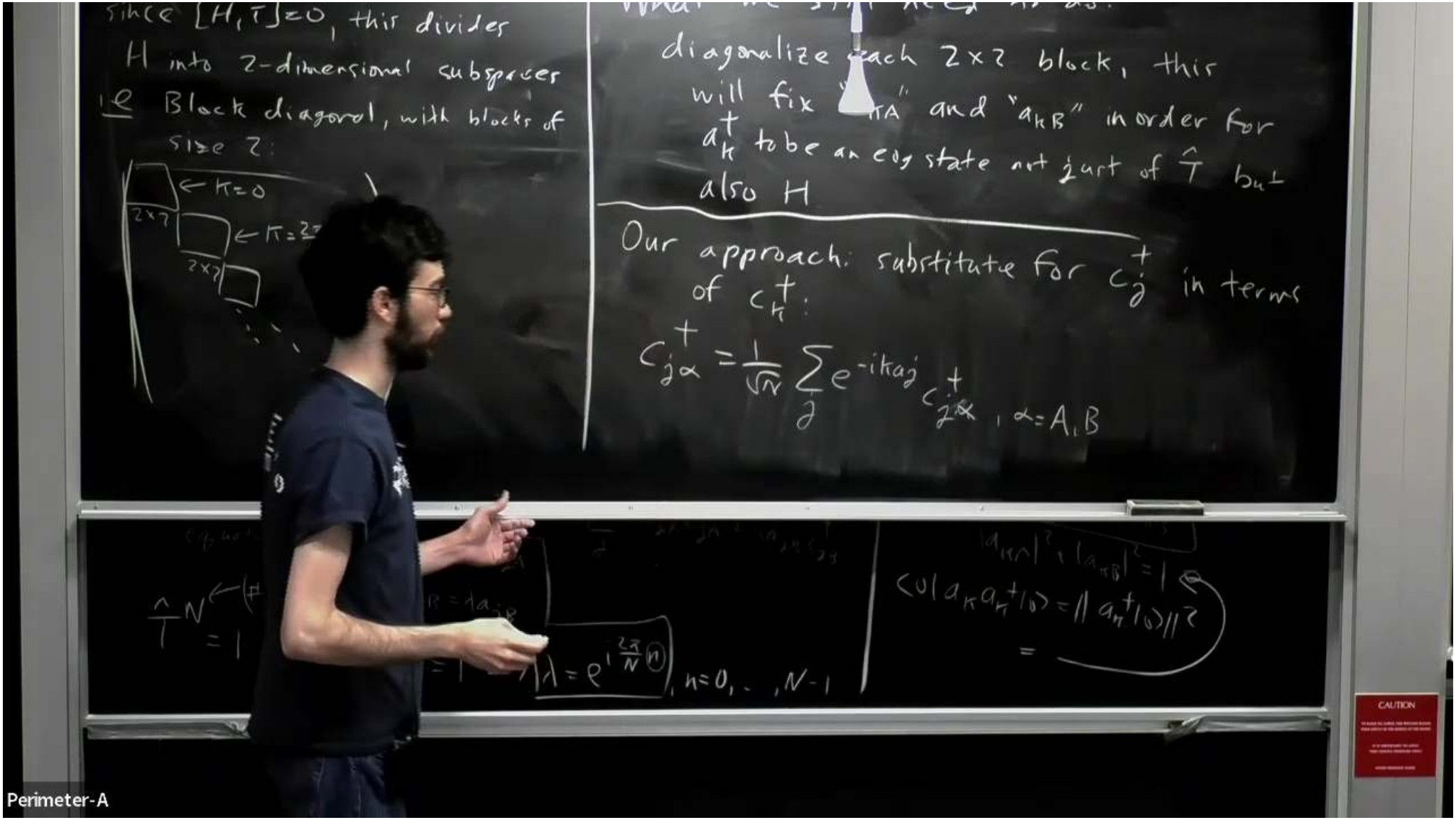
Perimeter-A

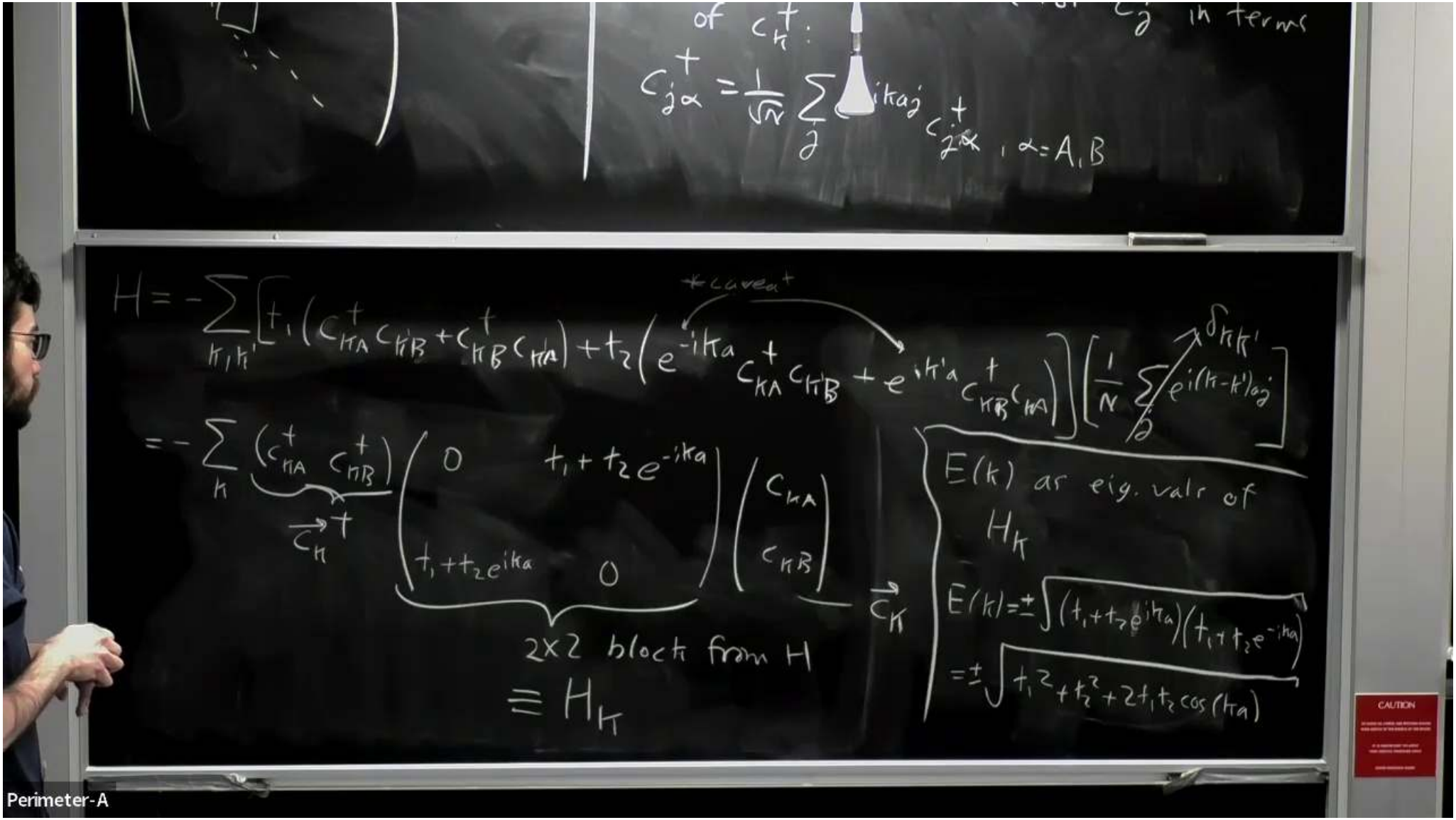
We found eig vects of T, since $[H,T]=0$, this divides to 2-dimensional subspaces lock diagonal, with blocks of ize 2:

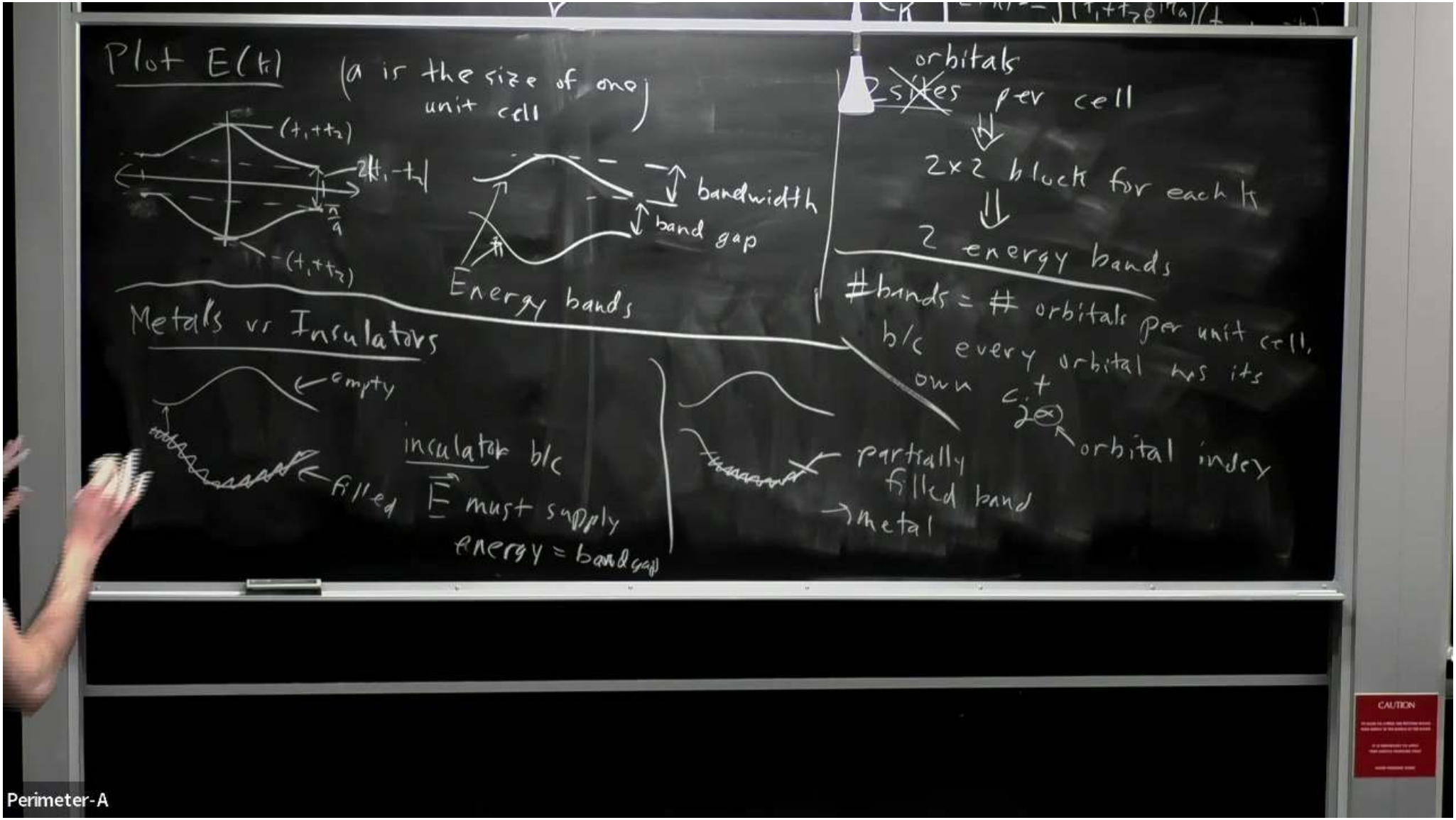
What we still need to do:

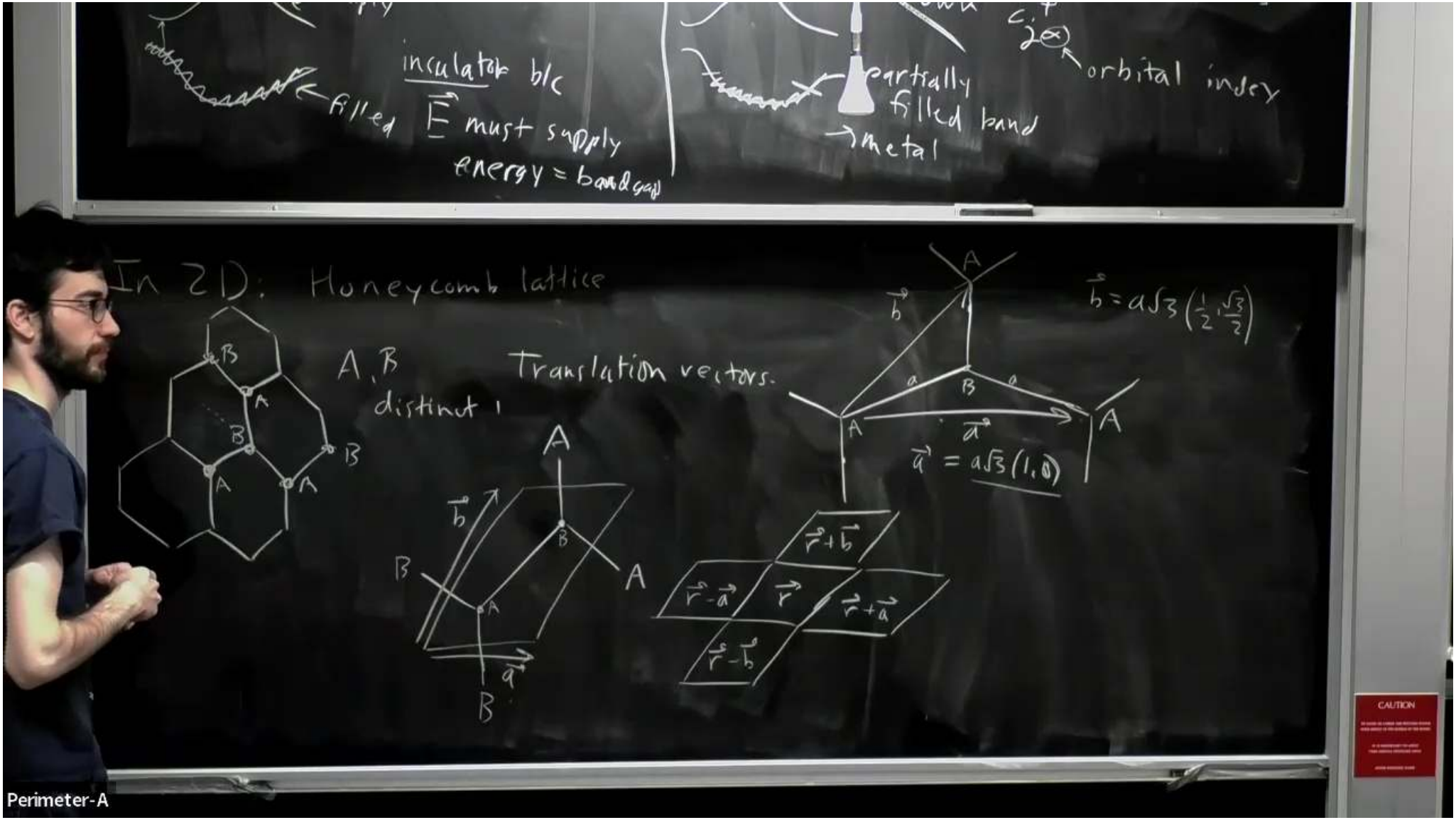
diagonalize each 2x2 block, this will fix "$a_{\pi A}$" and "$a_{\pi B}$" in order for $a_k^\dagger$ to be an eig state not just of $\hat{T}$ but also H

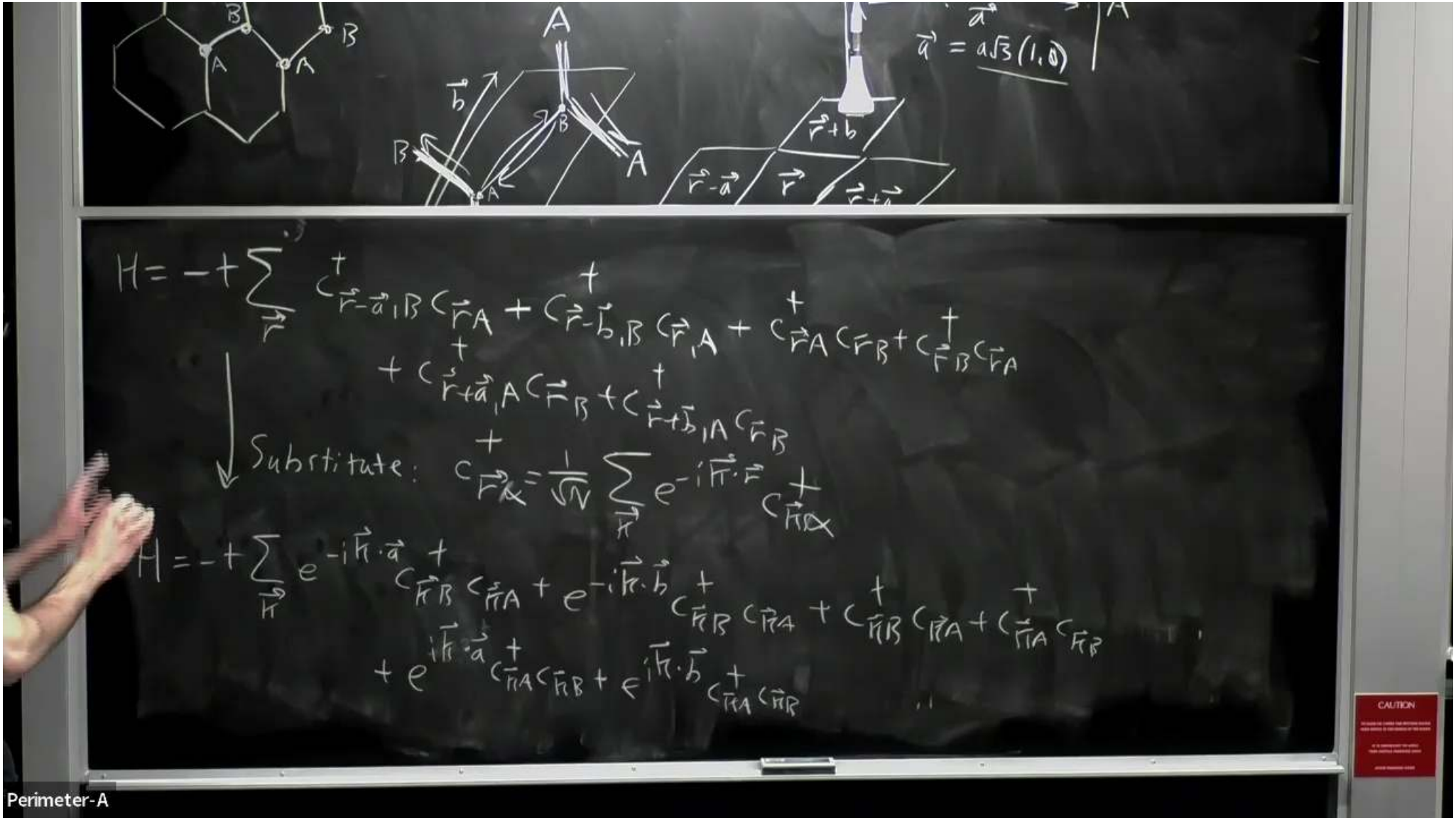
Perimeter-A


since $[H,\hat{T}]=0$, this divides
H into 2-dimensional subspaces
ie Block diagonal, with blocks of
size 2:
$k=0$
$k=\frac{2\pi}{N}$
2x2
2x2
diagonalize each 2x2 block, this
will fix "a_{kA}" and "a_{kB}" in order for
$a_k^\dagger$ to be an eig state not just of $\hat{T}$ but
also H
Our approach: substitute for $c_j^\dagger$ in terms
of $c_k^\dagger$:
$c_{j\alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikaj} c_{k\alpha}^\dagger$, $\alpha = A, B$
$\lambda = e^{i\frac{2\pi}{N}n}$, $n=0,\ldots,N-1$
$|a_{kA}|^2 + |a_{kB}|^2 = 1$
$\langle 0 | a_k a_k^\dagger | 0 \rangle = \| a_k^\dagger |0\rangle \|^2$
=
CAUTION


of $c_k^\dagger$:
$c_{j\alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikaj} c_{k\alpha}^\dagger$, $\alpha = A, B$
$H = -\sum_{k,k'} \left[t_1 \left(c_{kA}^\dagger c_{k'B} + c_{kB}^\dagger c_{k'A} \right) + t_2 \left(e^{-ik'a} c_{kA}^\dagger c_{k'B} + e^{ik'a} c_{kB}^\dagger c_{k'A} \right) \right] \left[\frac{1}{N} \sum_j e^{i(k-k')aj} \right]$
$\delta_{kk'}$
$= -\sum_k \begin{pmatrix} c_{kA}^\dagger & c_{kB}^\dagger \end{pmatrix} \begin{pmatrix} 0 & t_1 + t_2 e^{-ika} \\ t_1 + t_2 e^{ika} & 0 \end{pmatrix} \begin{pmatrix} c_{kA} \\ c_{kB} \end{pmatrix}$
$\vec{c}_k^\dagger$
$\vec{c}_k$
2x2 block from H
$\equiv H_k$
E(k) as eig. valr of H_k
$E(k) = \pm \sqrt{(t_1 + t_2 e^{ika})(t_1 + t_2 e^{-ika})}$
$= \pm \sqrt{t_1^2 + t_2^2 + 2 t_1 t_2 \cos(ka)}$
CAUTION


Plot E(t1)
(a is the size of one unit cell)
(t1+t2)
2t1-t2
π/a
-(t1+t2)
bandwidth
band gap
Energy bands
orbitals
2 sites per cell
2x2 block for each k
2 energy bands
#bands = # orbitals per unit cell, b/c every orbital has its own c,k
orbital index
Metals vs Insulators
empty
filled
insulator b/c E must supply energy = band gap
partially filled band
→ metal


insulator b/c
filled
$\vec{E}$ must supply
energy = band gap
partially
filled band
metal
orbital index
In 2D: Honeycomb lattice
A, B
distinct
Translation vectors.
$\vec{b} = a\sqrt{3}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$
$\vec{a} = a\sqrt{3}(1, 0)$
$\vec{r}+\vec{b}$
$\vec{r}-\vec{a}$
$\vec{r}$
$\vec{r}+\vec{a}$
$\vec{r}-\vec{b}$
CAUTION
Perimeter-A


A
B
$\vec{a} = a\sqrt{3}(1,0)$
$\vec{b}$
$\vec{r}+\vec{b}$
$\vec{r}-\vec{a}$
$\vec{r}$
$H = -t \sum_{\vec{r}} c^{\dagger}_{\vec{r}-\vec{a},B} c_{\vec{r},A} + c^{\dagger}_{\vec{r}-\vec{b},B} c_{\vec{r},A} + c^{\dagger}_{\vec{r},A} c_{\vec{r},B} + c^{\dagger}_{\vec{r},B} c_{\vec{r},A}$
$+ c^{\dagger}_{\vec{r}+\vec{a},A} c_{\vec{r},B} + c^{\dagger}_{\vec{r}+\vec{b},A} c_{\vec{r},B}$
Substitute: $c_{\vec{r},\alpha} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} c^{\dagger}_{\vec{k},\alpha}$
$H = -t \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{a}} c^{\dagger}_{\vec{k},B} c_{\vec{k},A} + e^{-i\vec{k}\cdot\vec{b}} c^{\dagger}_{\vec{k},B} c_{\vec{k},A} + c^{\dagger}_{\vec{k},B} c_{\vec{k},A} + c^{\dagger}_{\vec{k},A} c_{\vec{k},B}$
$+ e^{i\vec{k}\cdot\vec{a}} c^{\dagger}_{\vec{k},A} c_{\vec{k},B} + e^{i\vec{k}\cdot\vec{b}} c^{\dagger}_{\vec{k},A} c_{\vec{k},B}$
CAUTION

$$H = -t \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{a}} + c^{\dagger}_{\vec{k}B} c_{\vec{k}A} + e^{-i\vec{k}\cdot\vec{b}} + c^{\dagger}_{\vec{k}B} c_{\vec{k}A} + c^{\dagger}_{\vec{k}B} c_{\vec{k}A} + c^{\dagger}_{\vec{k}A} c_{\vec{k}B}$$

$$+ e^{i\vec{k}\cdot\vec{a}} c^{\dagger}_{\vec{k}A} c_{\vec{k}B} + e^{i\vec{k}\cdot\vec{b}} c^{\dagger}_{\vec{k}A} c_{\vec{k}B}$$

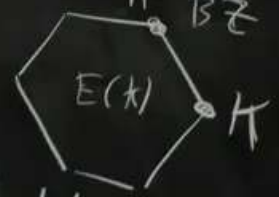
$$H = -t \sum_{\vec{k}} \vec{c}^{\dagger}_{\vec{k}} \cdot H_{\vec{k}} \cdot \vec{c}_{\vec{k}}$$

$$H_{\vec{k}} = \begin{pmatrix} 0 & 1 + e^{i\vec{k}\cdot\vec{a}} + e^{i\vec{k}\cdot\vec{b}} \\ 1 + e^{-i\vec{k}\cdot\vec{a}} + e^{-i\vec{k}\cdot\vec{b}} & 0 \end{pmatrix}$$

Diagonalize & simplify

$$E(\vec{k}) = \pm\sqrt{3 + 2\left(\cos(\vec{k}\cdot\vec{a}) + \cos(\vec{k}\cdot\vec{b}) + \cos(\vec{k}\cdot(\vec{a}-\vec{b}))\right)}$$

BZ

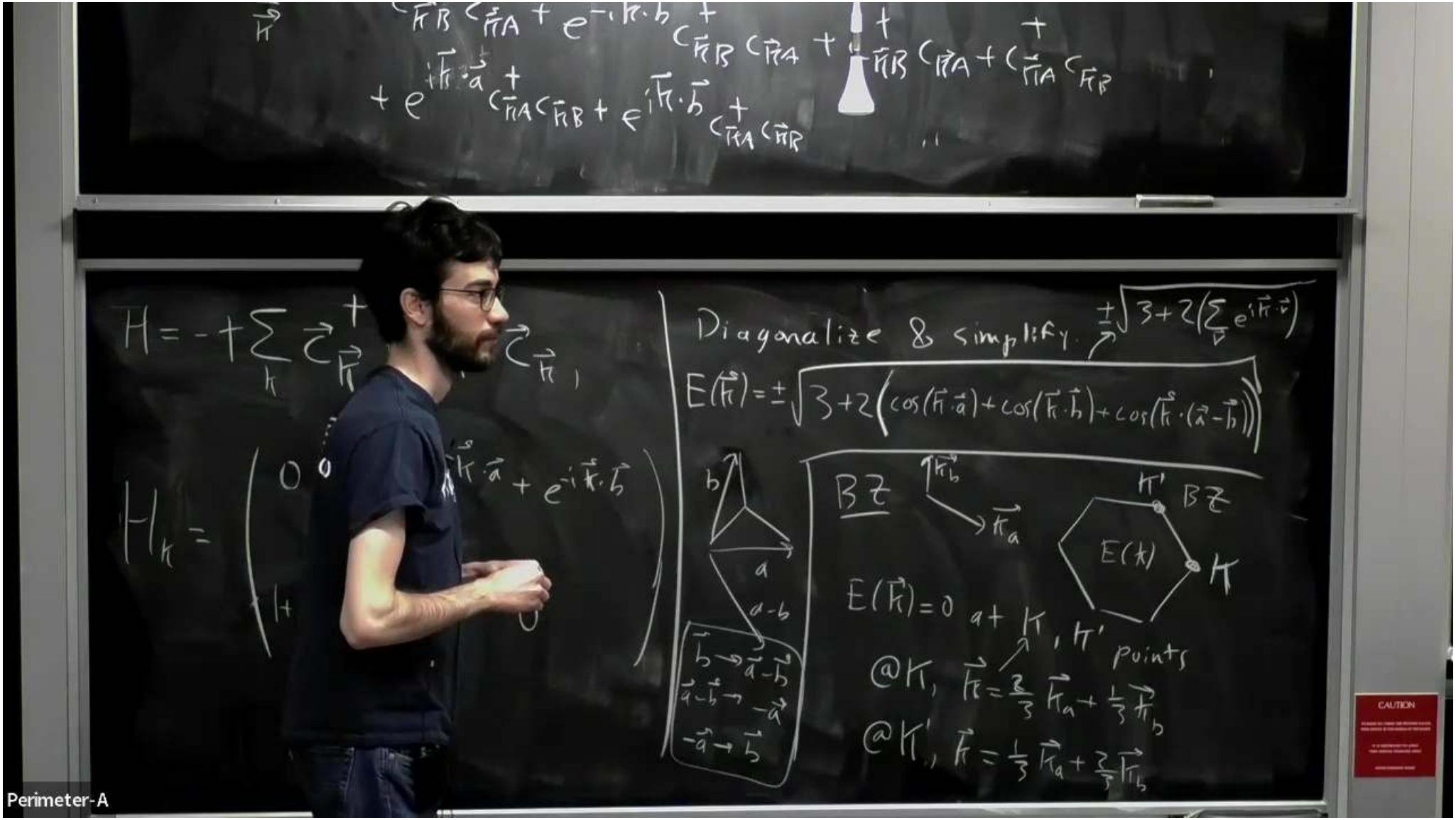


$E(\vec{k}) = 0$ at K, K' points

@K, $\vec{k} = \frac{2}{3}\vec{k}_a + \frac{1}{3}\vec{k}_b$

@K', $\vec{k} = \frac{1}{3}\vec{k}_a + \frac{2}{3}\vec{k}_b$

Perimeter-A


Diagonalize & simplify
BZ
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Perimeter-A