Title: PSI Lecture - Condensed Matter - Lecture 9

Speakers: Aaron Szasz

Collection: PSI Lecture - Condensed Matter

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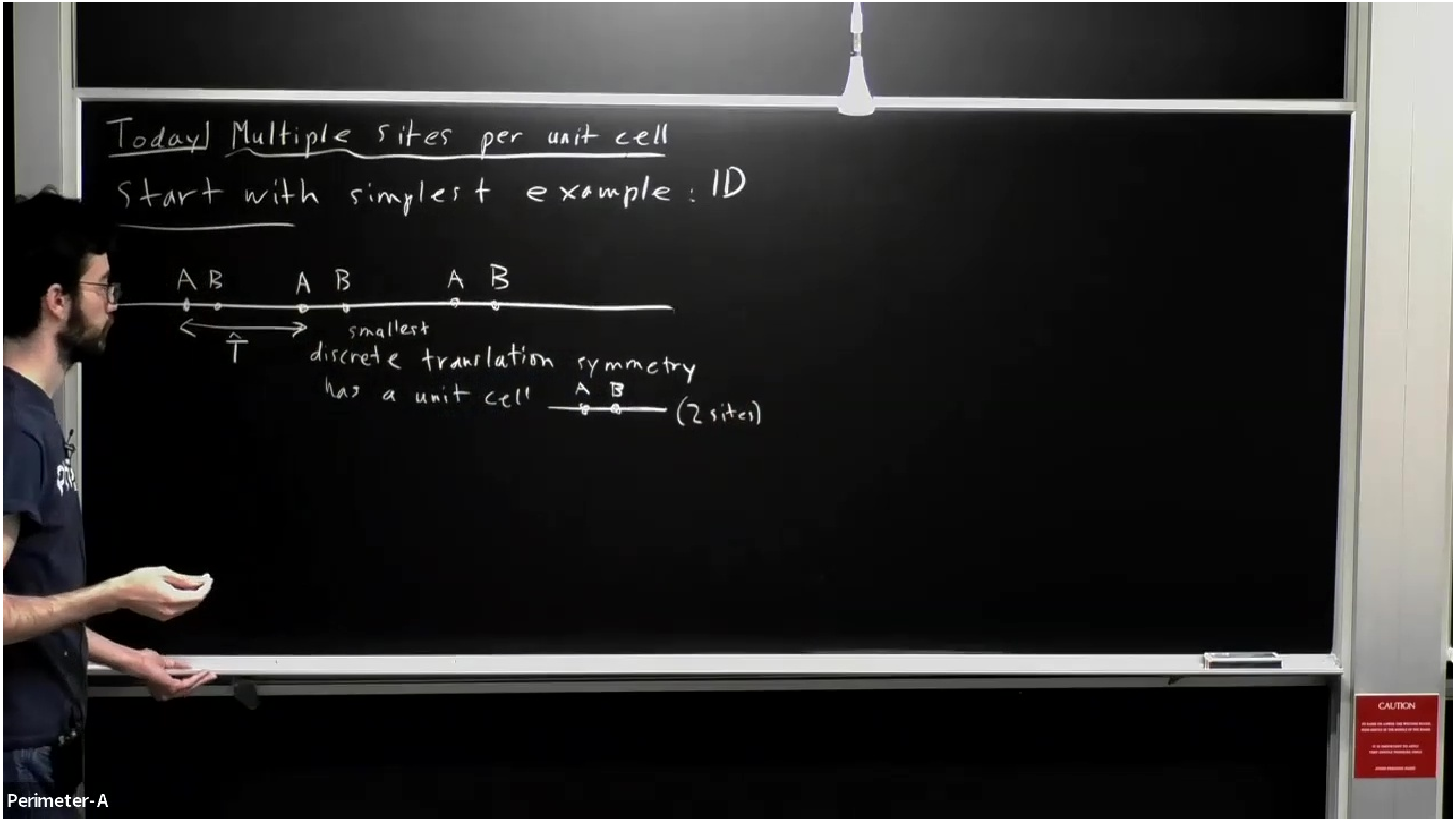

Today! Multiple sites per unit cell
Start with simplest example: 1D
A B A B A B
$\hat{T}$
smallest
discrete translation symmetry
has a unit cell A B (2 sites)
Perimeter-A

Perimeter-A

Today! Multiple sites per unit cell

Start with simplest example: 1D

A B A B A B

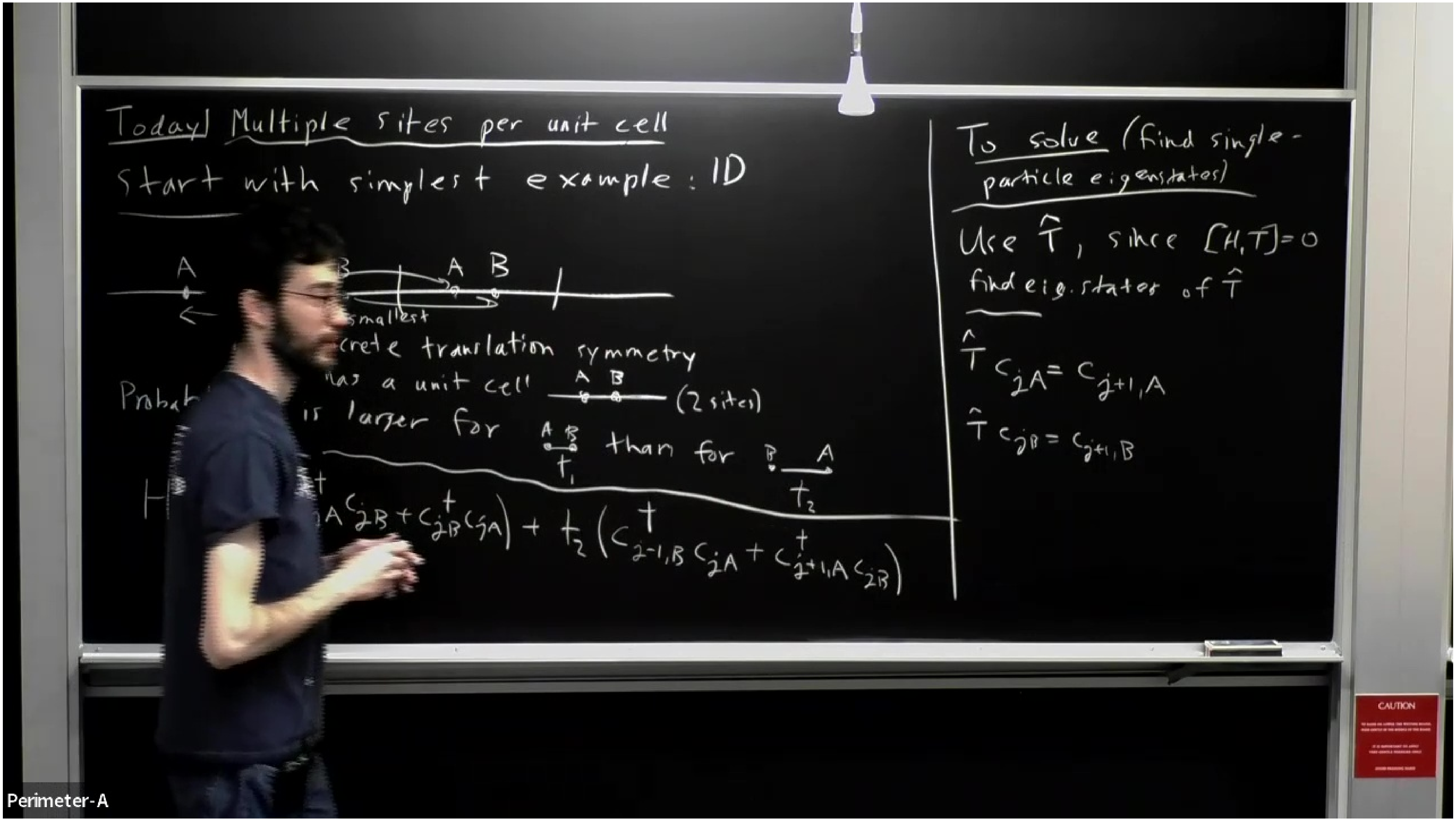
$\hat{T}$ smallest discrete translation symmetry has a unit cell A B (2 sites)

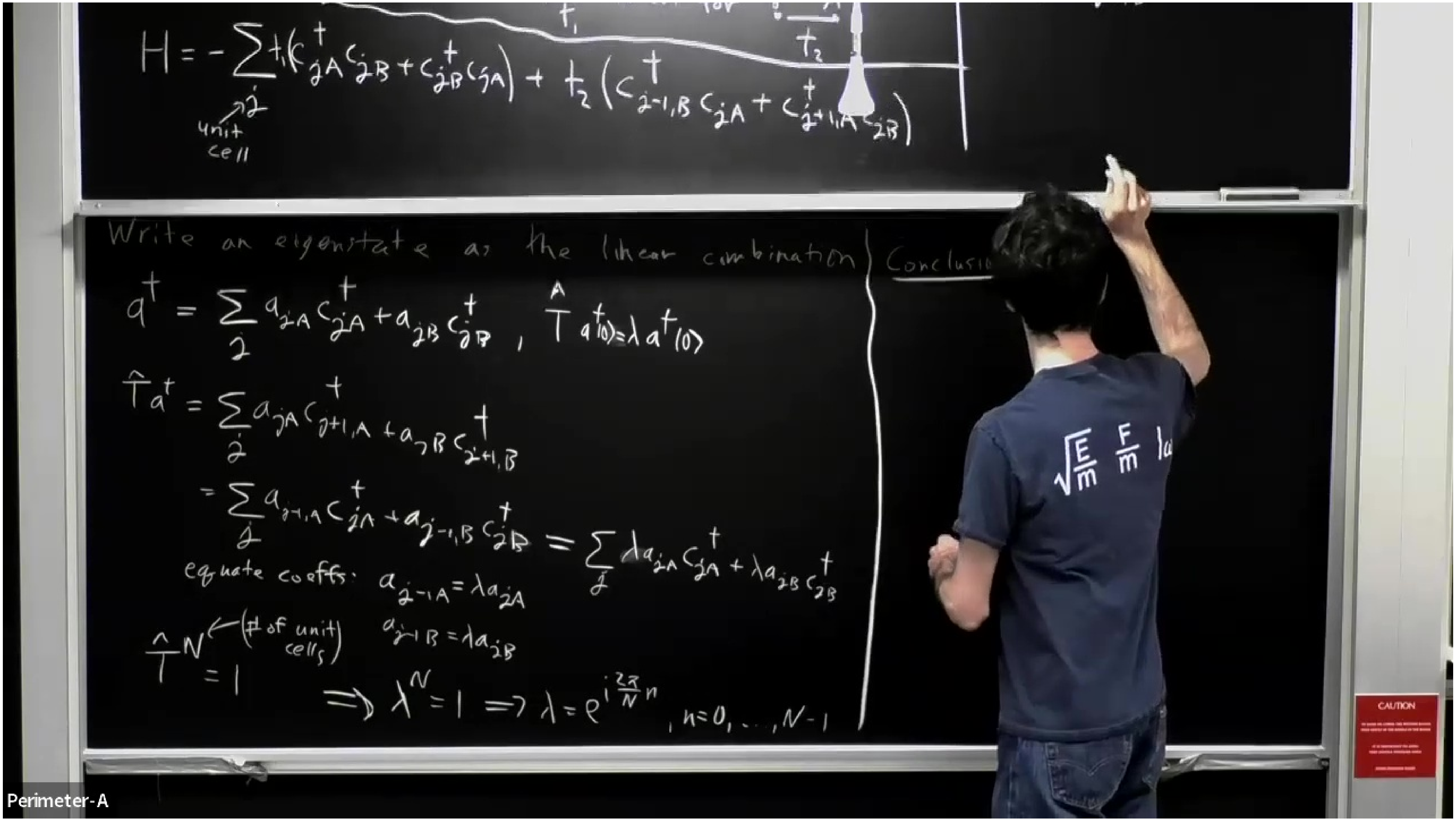
Probably "t" is larger for A B (t_1) than for B A (t_2)

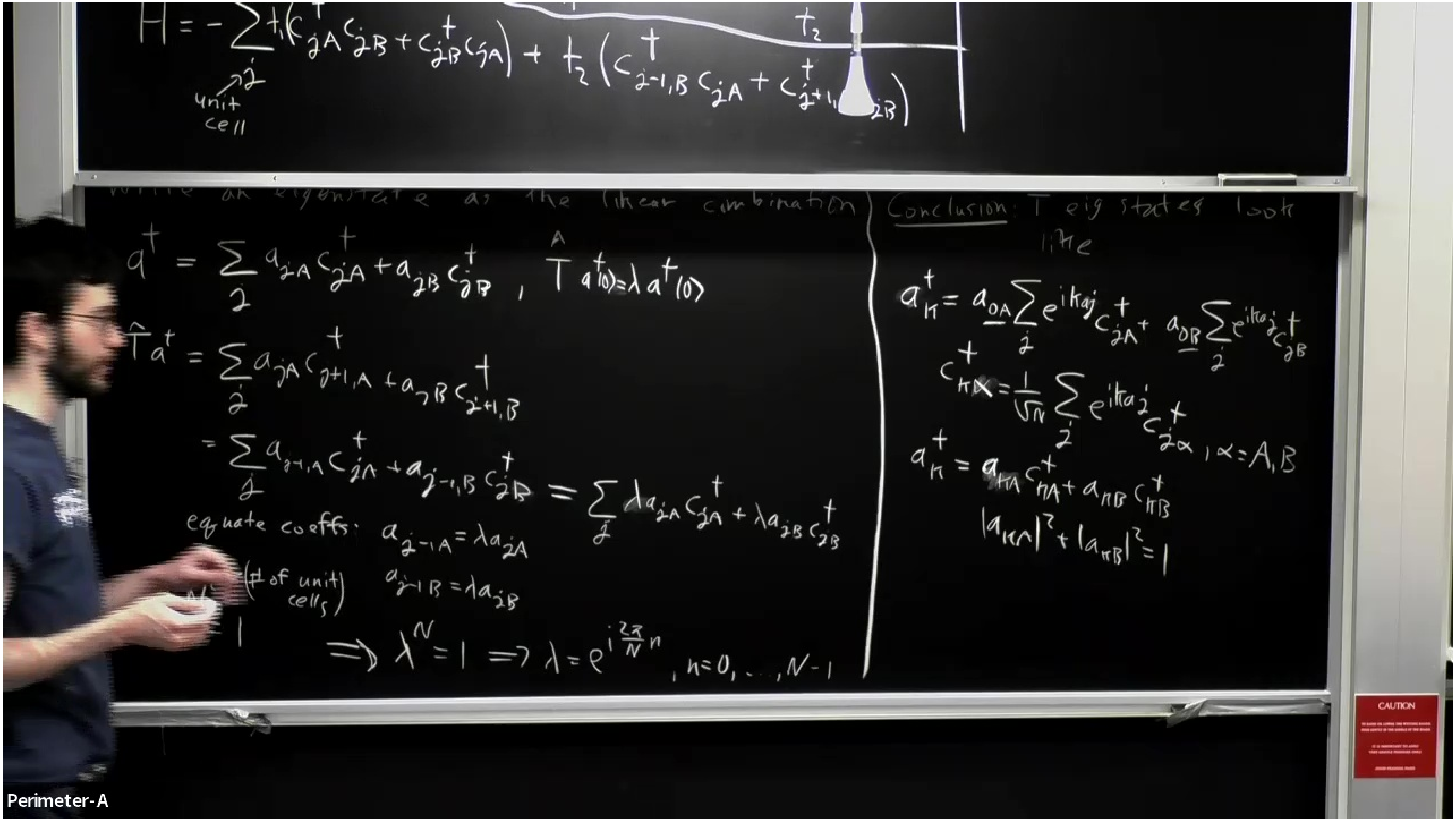
$$H = -\sum_{j} t_1 \left(c^\dagger_{jA} c_{jB} + c^\dagger_{jB} c_{jA}\right) + t_2 \left(c^\dagger_{j-1,B}\, c_{jA} + c^\dagger_{j+1,A}\, c_{jB}\right)$$

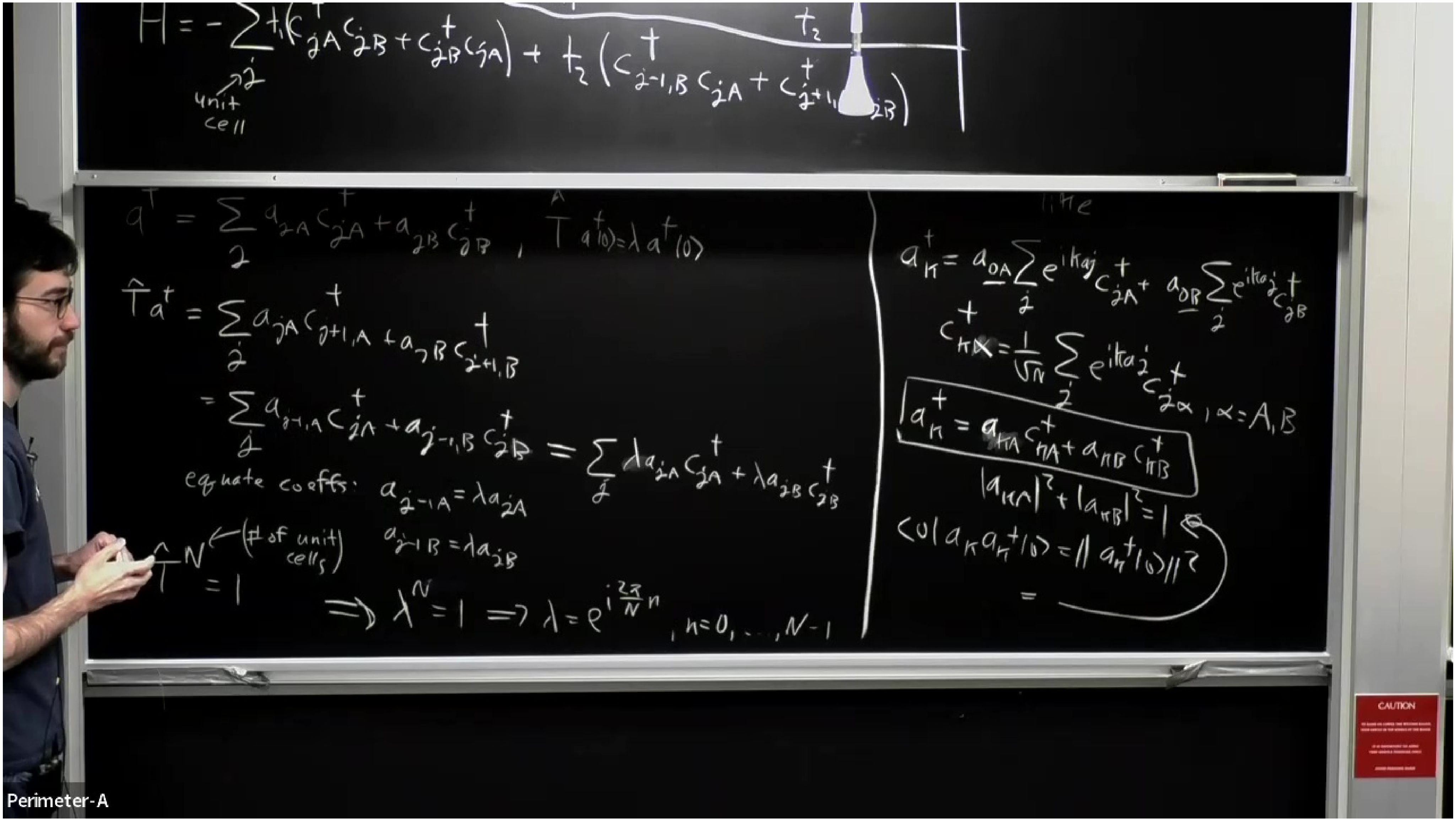
j: unit cell

To solve (find single-


Today! Multiple sites per unit cell
Start with simplest example: 1D
A
A B
smallest
crete translation symmetry
has a unit cell A B (2 sites)
is larger for A B than for B A
t1
t2
To solve (find single-particle eigenstates)
Use T̂, since [H, T] = 0
find eig. states of T̂
T̂ c_jA = c_j+1,A
T̂ c_jB = c_j+1,B
CAUTION
Perimeter-A


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


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


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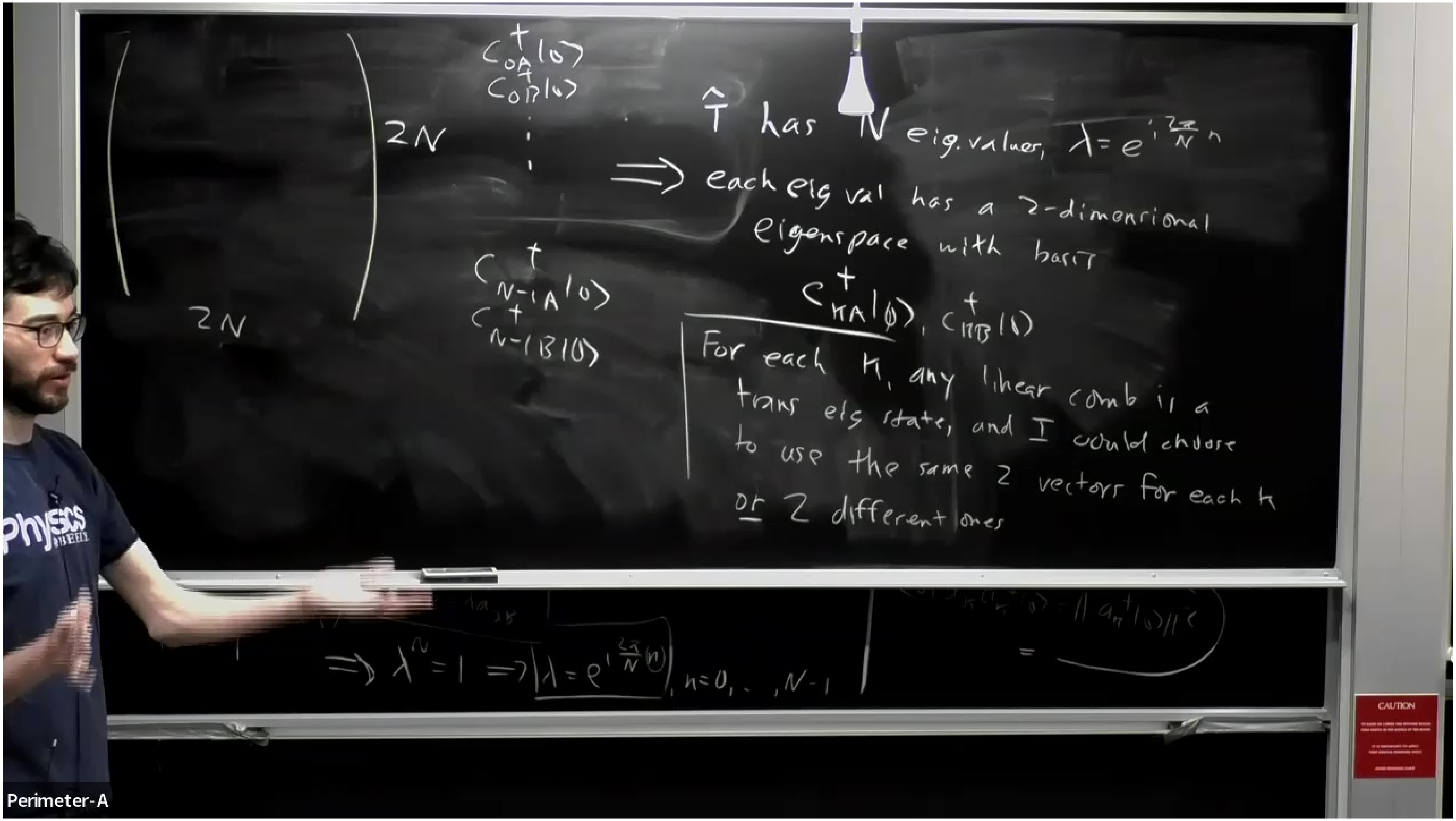
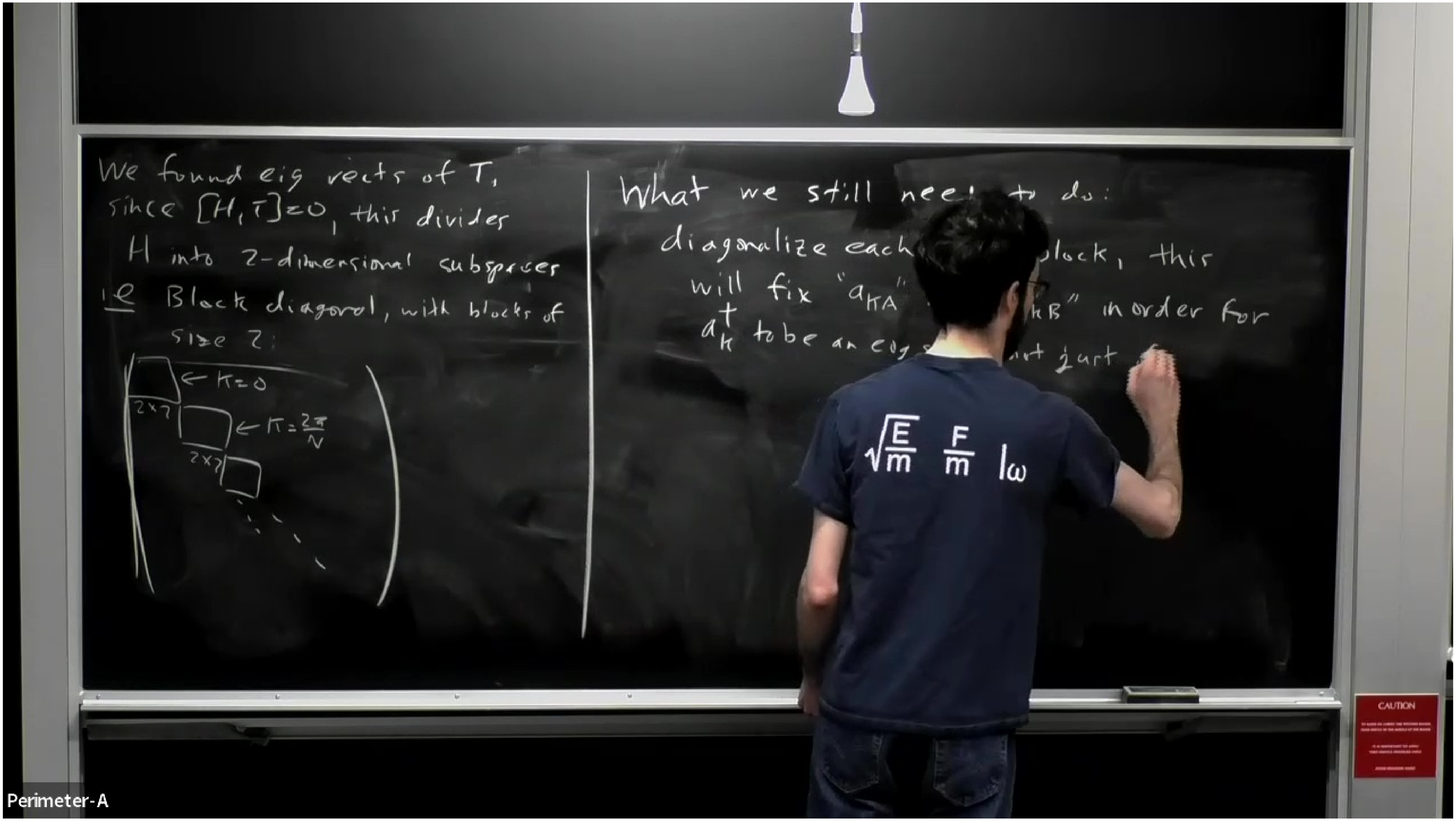
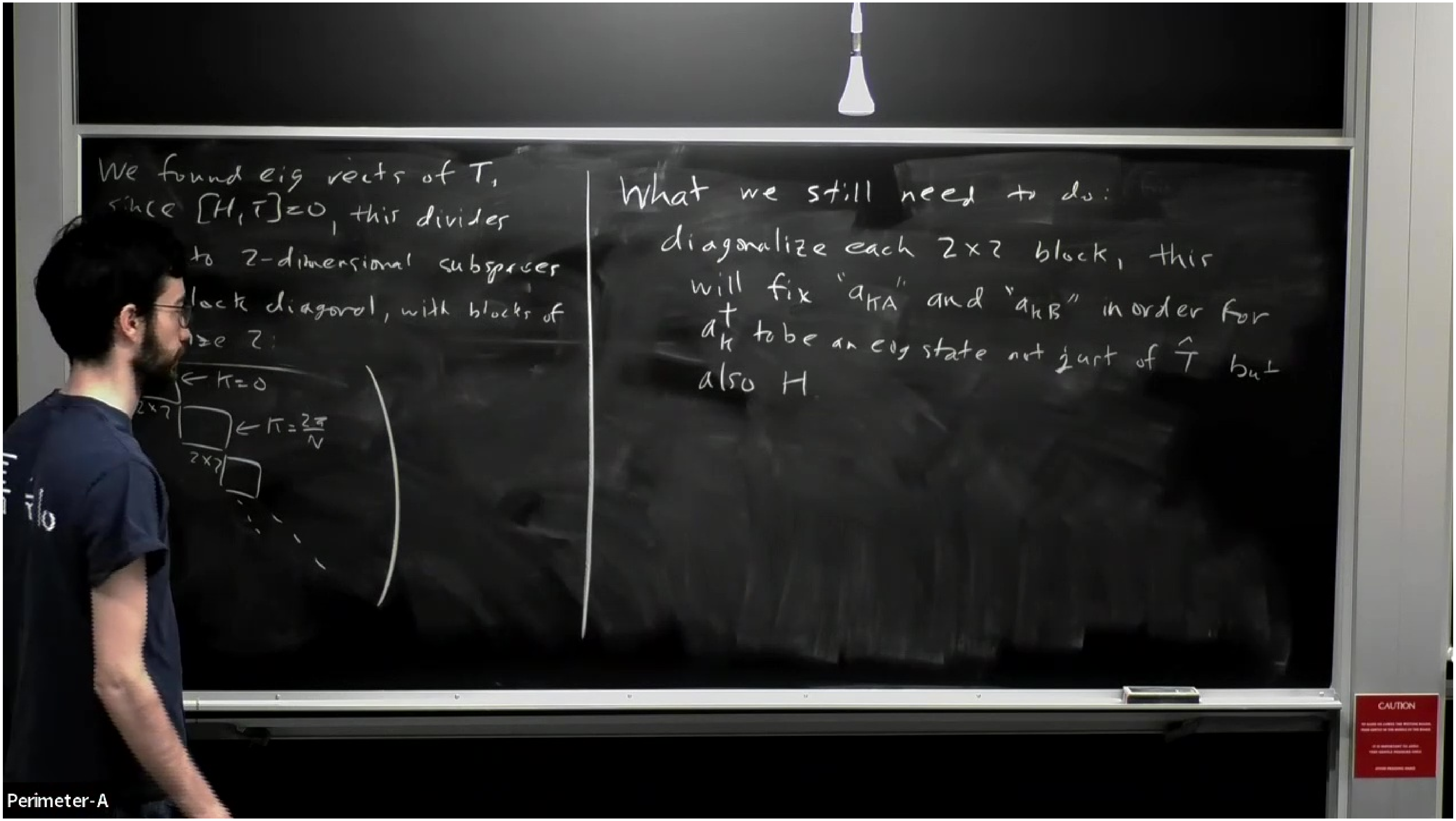
equate coeffs: $a_{j-1A} = \lambda a_{jA}$
$a_{j-1B} = \lambda a_{jB}$
$\hat{T}^N = 1$ (# of unit cells)
$\Rightarrow \lambda^N = 1 \Rightarrow \lambda = e^{i\frac{2\pi}{N}n}$, $n = 0, \dots, N-1$
like
$a^\dagger_k = a_{0A} \sum_j e^{ikaj} c^\dagger_{jA} + a_{0B} \sum_j e^{ikaj} c^\dagger_{jB}$
$c^\dagger_{k\alpha}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


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


We found eig vects of T,
since [H,T]=0, this divides
H into 2-dimensional subspaces
ie Block diagonal, with blocks of
size 2:
← k=0
2×2
← k=2π/N
2×2
2×2
What we still nee
to do:
diagonalize each
block, this
will fix "a_kA"
kB" in order for
a_k^† to be an eig
just
Perimeter-A
CAUTION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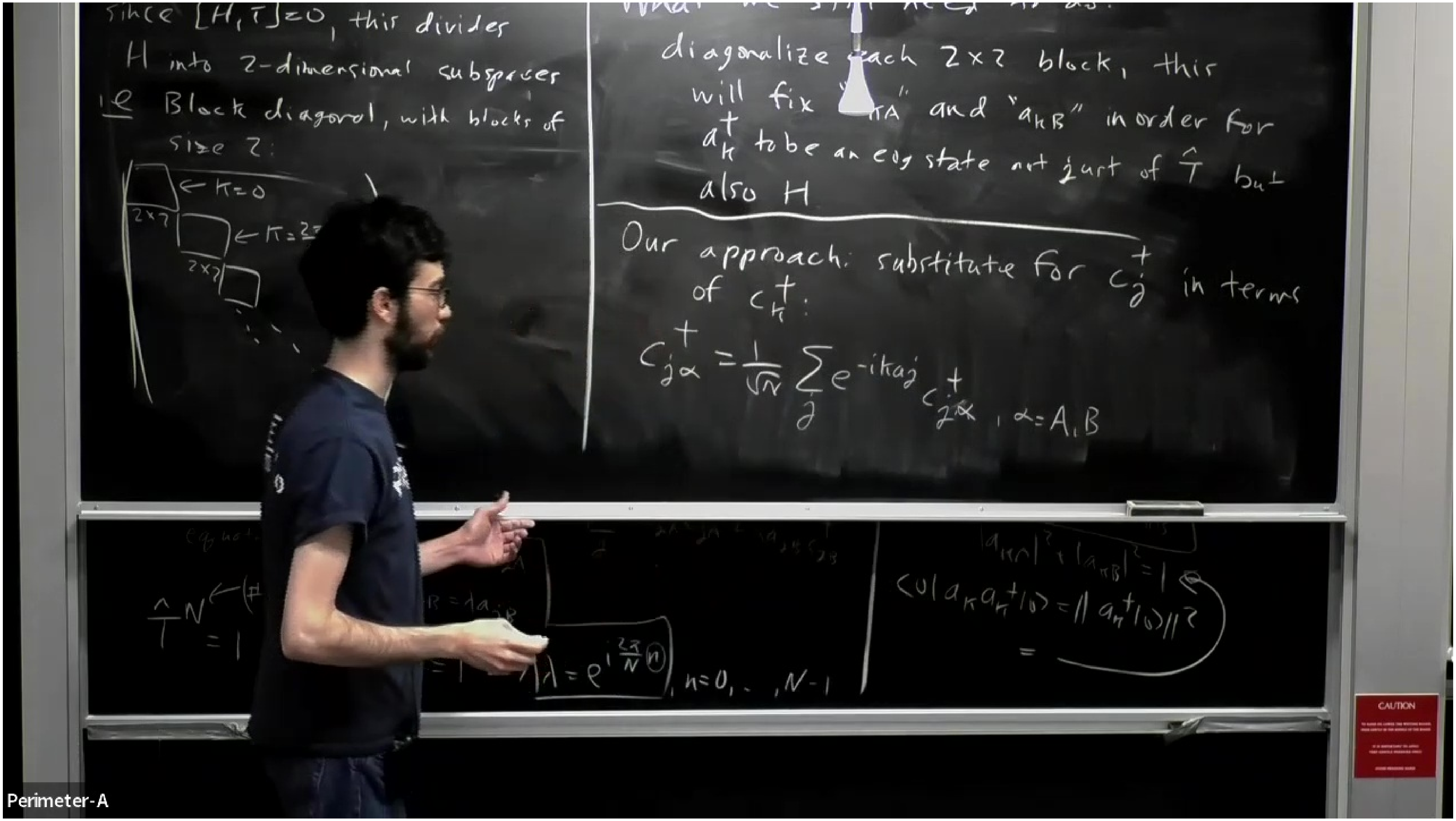
since [H, T] = 0, this divides
to 2-dimensional subspaces
lock diagonal, with blocks of
ize 2:
← k = 0
2×2
← k = 2π/N
2×2
What we still need to do:
diagonalize each 2×2 block, this
will fix "a_kA" and "a_kB" in order for
a_k^† to be an eig state not just of T̂ but
also H
Perimeter-A


since [H, T] = 0, this divides
H into 2-dimensional subspaces
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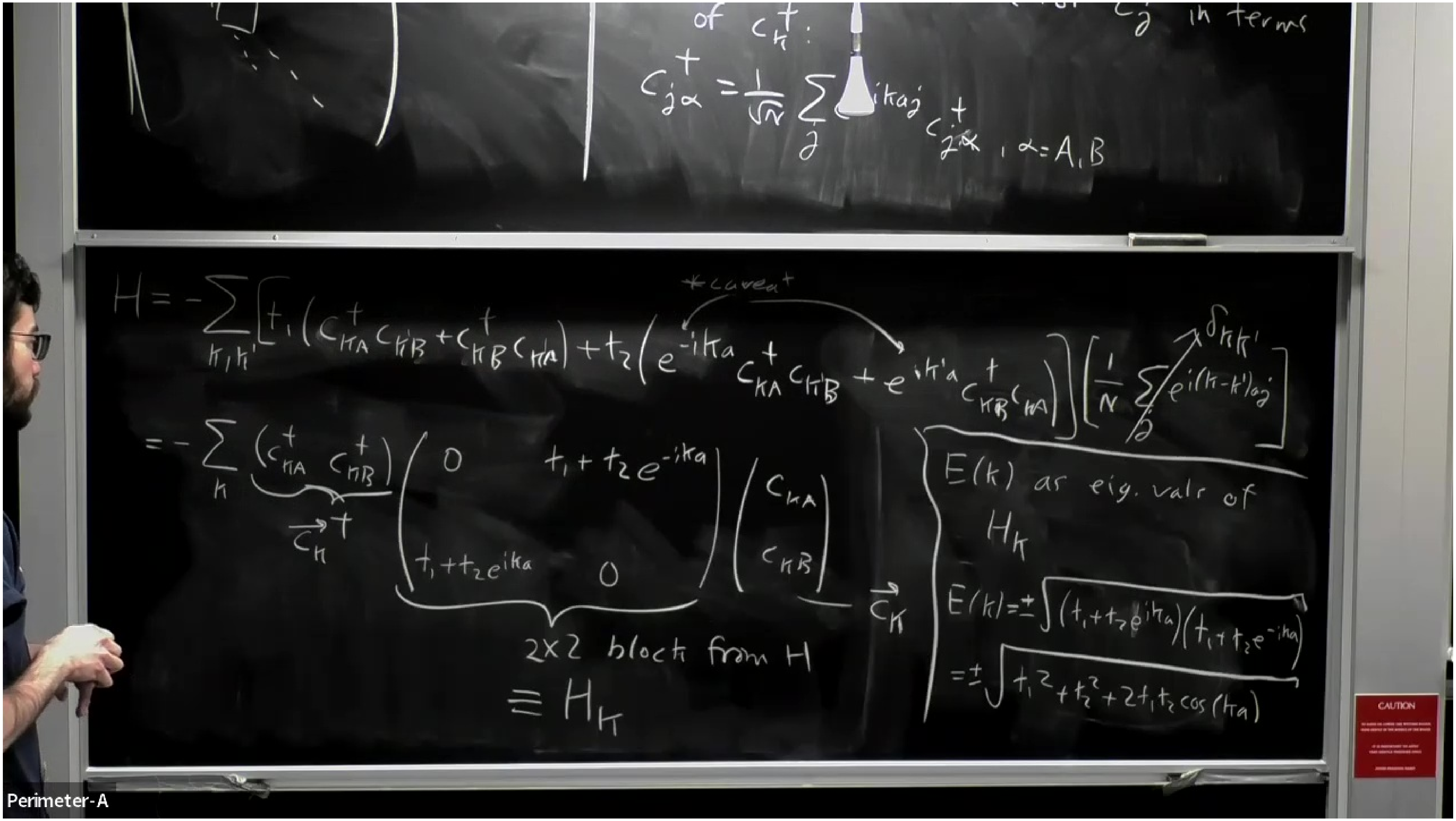
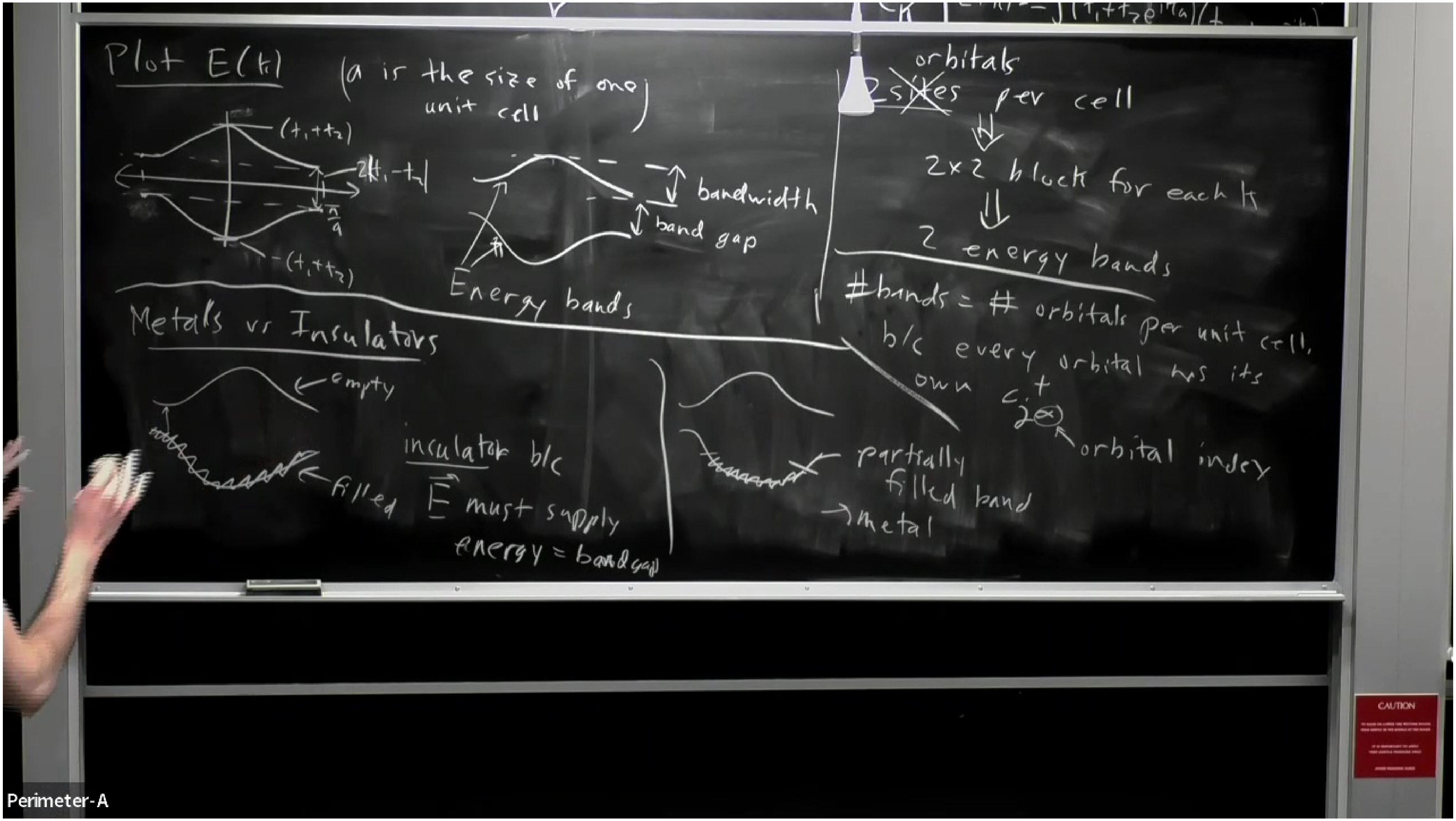
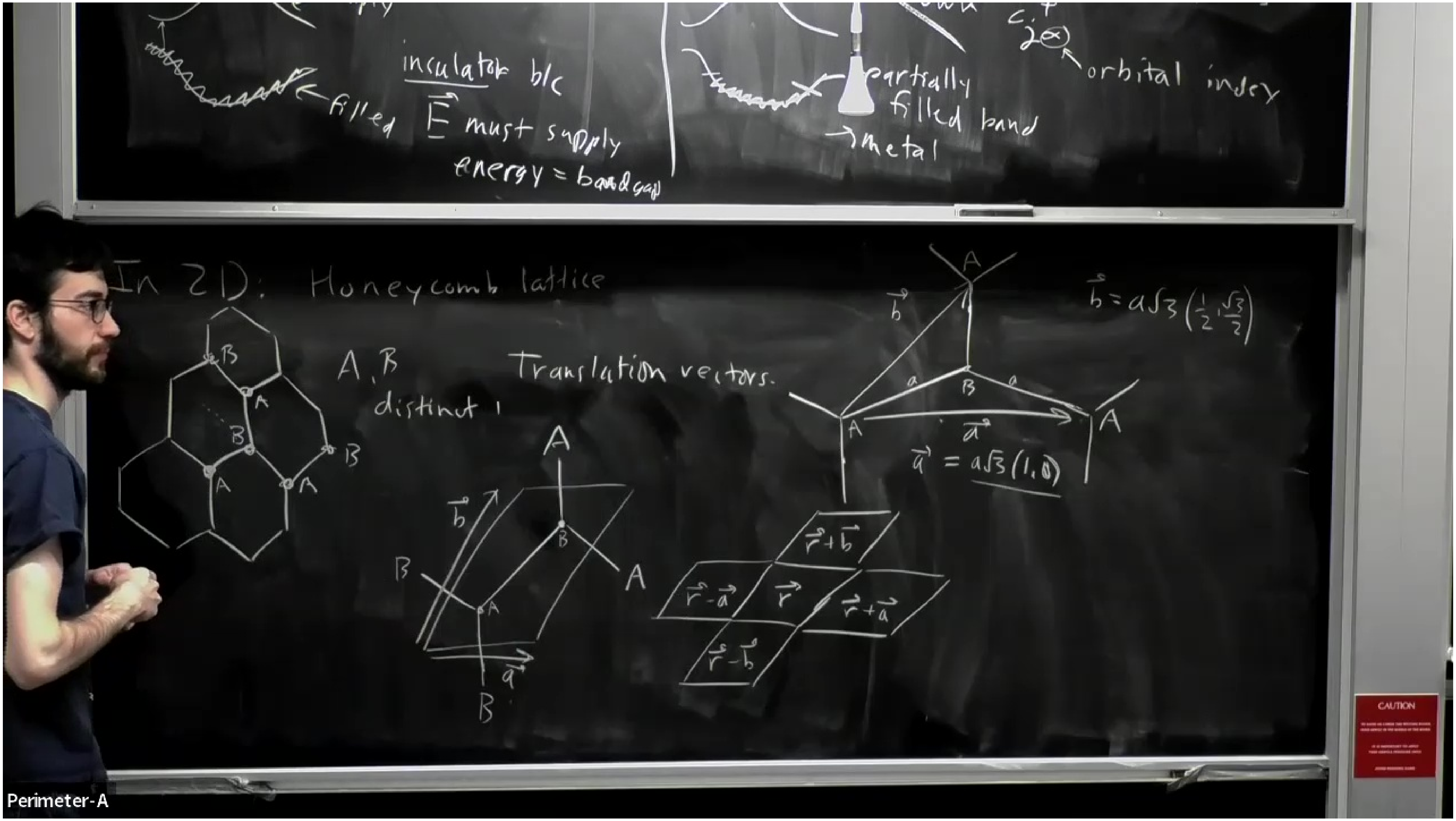
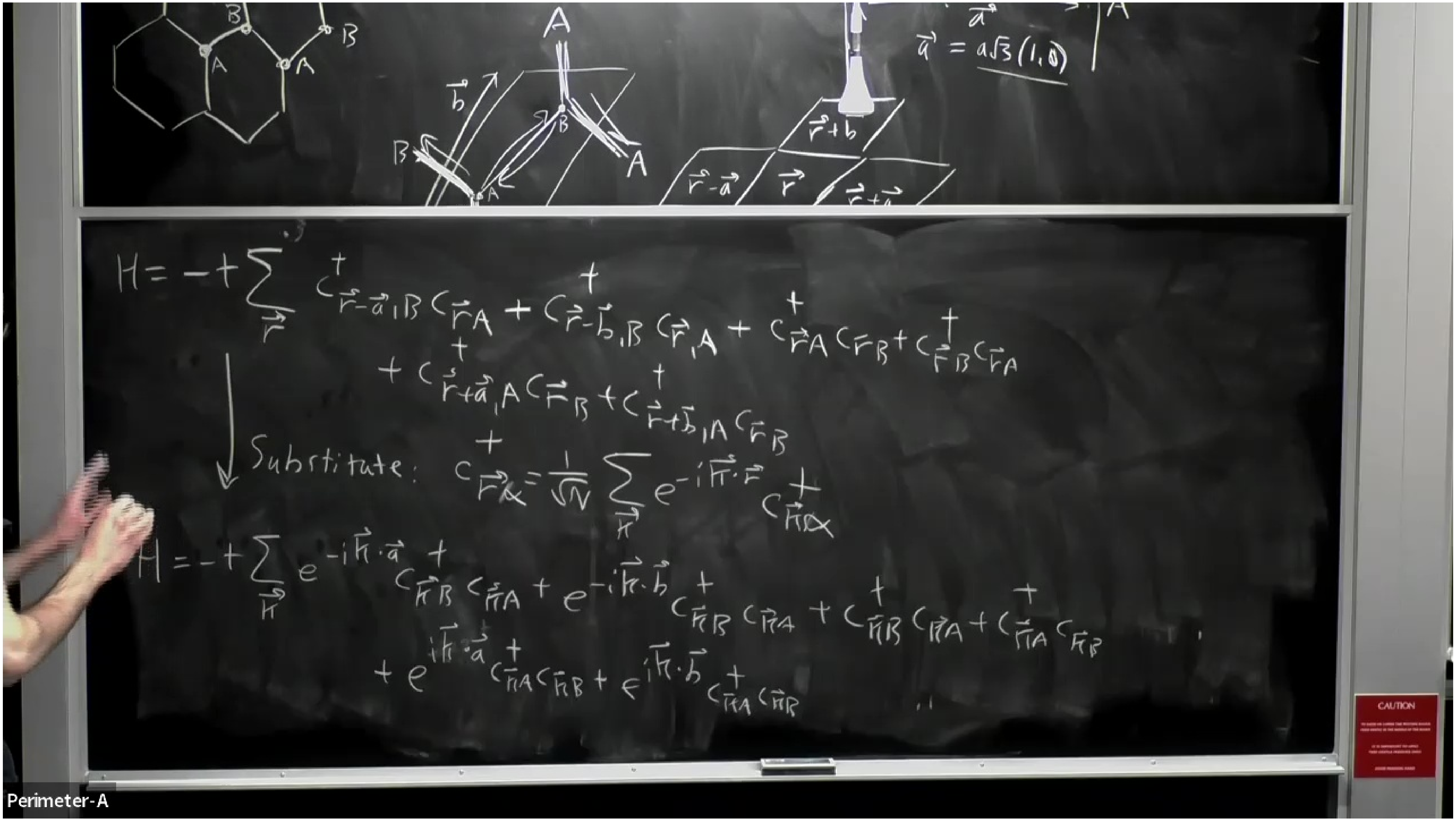
← k=0
2×2
2×2
diagonalize each 2×2 block, this
will fix "a_kA" and "a_kB" in order for
a_k^† to be an eig state not just of T̂ but
also H
Our approach: substitute for c_j^† in terms
of c_k^†:
c_jα^† = 1/√N Σ_j e^{-ikaj} c_jα^†, α = A, B
T̂^N = 1
λ = e^{i 2π/N n}, n = 0, .. , N-1
|a_kA|² + |a_kB|² = 1
⟨0| a_k a_k^† |0⟩ = ‖a_k^† |0⟩‖²
Perimeter-A
CAUTION



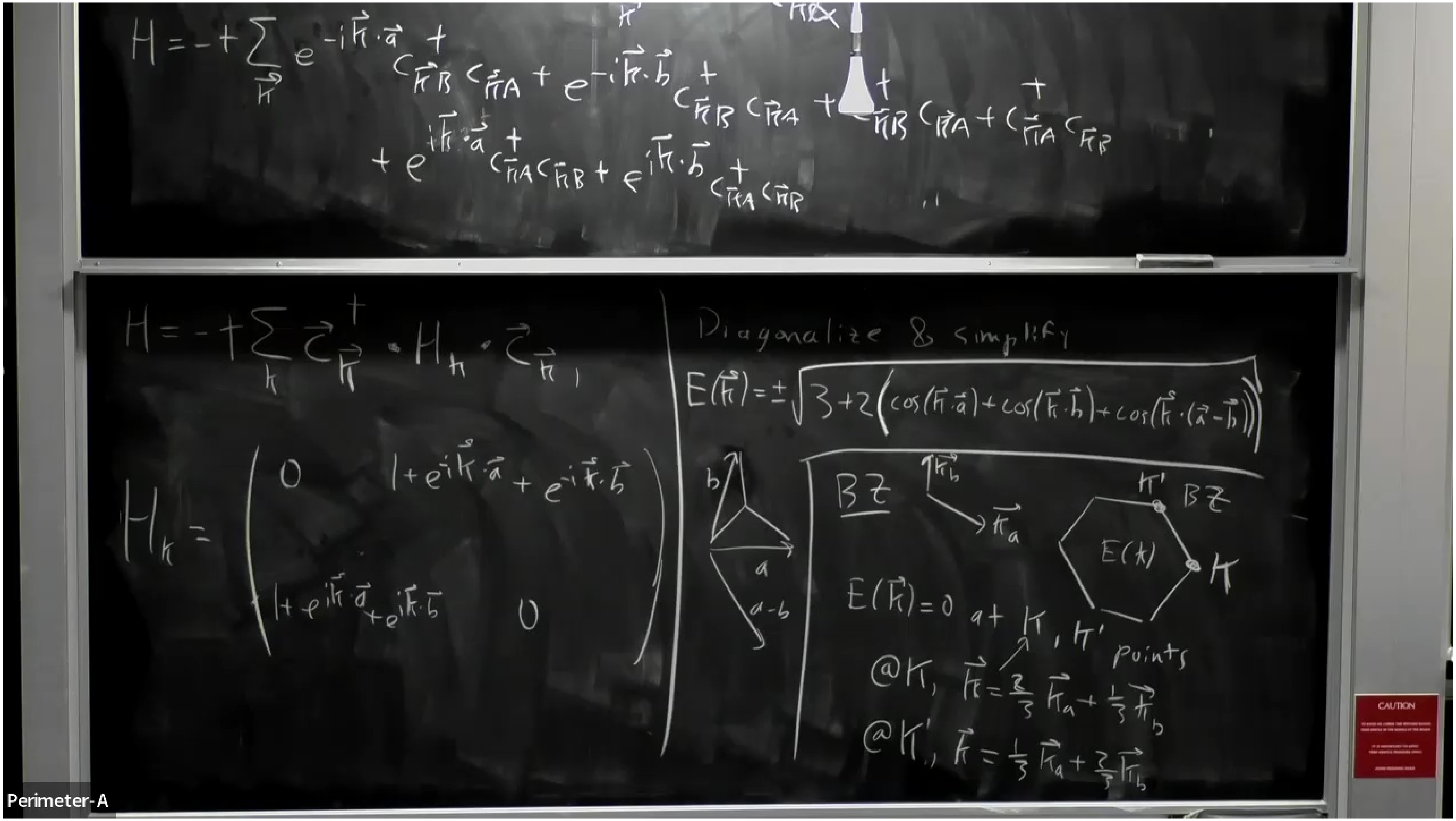
of $c_k^\dagger$: c_j in terms
$c_{j\alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikaj} c_{j\alpha}^\dagger$, $\alpha = A, B$
caveat
$H = -\sum_{k,k'} \left[t_1 \left(c_{kA}^\dagger c_{k'B} + c_{kB}^\dagger c_{k'A} \right) + t_2 \left(e^{-ika} c_{kA}^\dagger c_{k'B} + e^{ik'a} c_{kB}^\dagger c_{k'A}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

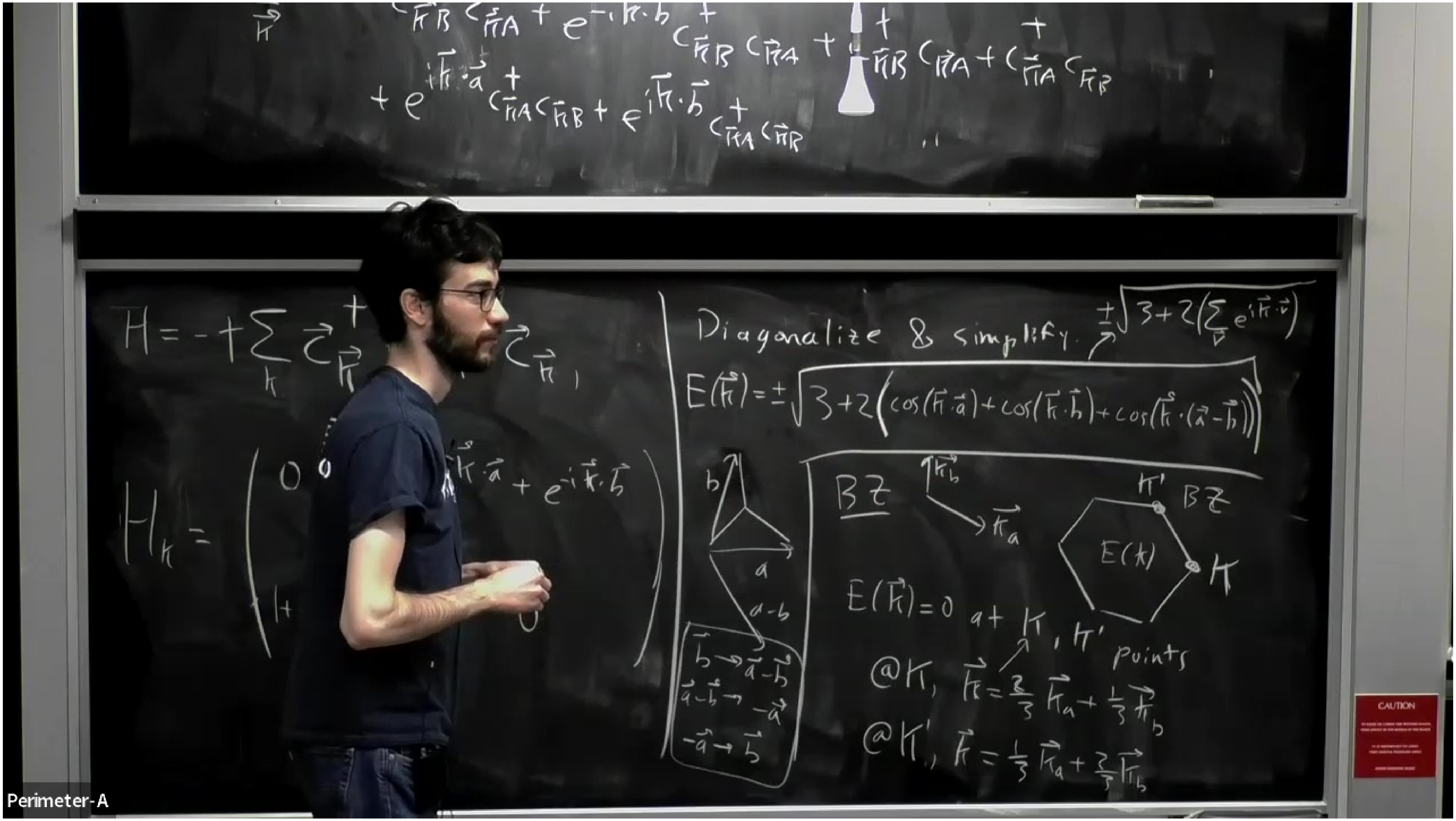

Plot E(k)
(a is the size of one unit cell)
(t_1+t_2)
$2|t_1-t_2|$
$\frac{\pi}{a}$
$-(t_1+t_2)$
bandwidth
band gap
Energy bands
Metals vs Insulators
empty
filled
insulator b/c $\vec{E}$ must supply energy = band gap
partially filled band
→ metal
orbitals
2 ~~sites~~ per cell
2×2 block for each k
2 energy bands
bands = # orbitals per unit cell,
b/c every orbital has its own $c_i^\dagger$
orbital index
Perimeter-A


insulator b/c
filled
E must supply
energy = band gap
partially
filled band
→ metal
orbital index
In 2D: Honeycomb lattice
A, B
distinct
Translation vectors.
b = a√3 (1/2, √3/2)
a = a√3 (1, 0)
r + b
r - a
r
r + a
r - b
Perimeter-A
CAUTION



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


$H = -t\sum_{\vec k} e^{-i\vec k\cdot\vec a} c^\dagger_{\vec k B} c_{\vec k A} + e^{-i\vec k\cdot\vec b} c^\dagger_{\vec k B} c_{\vec k A} + c^\dagger_{\vec k B} c_{\vec k A} + c^\dagger_{\vec k A} c_{\vec k B}$
$+ e^{i\vec k\cdot\vec a} c^\dagger_{\vec k A} c_{\vec k B} + e^{i\vec k\cdot\vec b} c^\dagger_{\vec k A} c_{\vec k B}$
$H = -t\sum_k \vec c^\dagger_{\vec k}\cdot H_k\cdot \vec c_{\vec k}$,
$H_k = \begin{pmatrix} 0 & 1+e^{-i\vec k\cdot\vec a}+e^{-i\vec k\cdot\vec b} \\ 1+e^{i\vec k\cdot\vec a}+e^{i\vec k\cdot\vec b} & 0\end{pmatrix}$
Diagonalize & simplify
$E(\vec k) = \pm\sqrt{3+2\left(\cos(\vec k\cdot\vec a)+\cos(\vec k\cdot\vec b)+\cos(\vec k\cdot(\vec a-\vec b))\right)}$
b
a
a-b
BZ
$\vec k_b$
$\vec k_a$
K'
BZ
E(k)
K
$E(\vec k)=0$ 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
CAUTION


Diagonalize & simplify.
$\pm\sqrt{3+2\left(\sum_{\vec{v}} e^{i\vec{k}\cdot\vec{v}}\right)}$
$E(\vec{k}) = \pm\sqrt{3+2\left(\cos(\vec{k}\cdot\vec{a})+\cos(\vec{k}\cdot\vec{b})+\cos(\vec{k}\cdot(\vec{a}-\vec{b}))\right)}$
BZ
$\vec{k}_b$
$\vec{k}_a$
K'
BZ
E(k)
K
$E(\vec{k}) = 0$ at K, K' points
@K, $\vec{k} = \frac{2}{3}\vec{k}_a + \frac{1}{3}\vec{k}_b$
@K', $\vec{k} = \frac{1}{3}\vec{k}_a + \frac{2}{3}\vec{k}_b$
b
a
a-b
$\vec{b} \to \vec{a}-\vec{b}$
$\vec{a}-\vec{b} \to -\vec{a}$
$-\vec{a} \to \vec{b}$
Perimeter-A