Title: PSI Lecture - Condensed Matter - Lecture 6

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Collection: PSI Lecture - Condensed Matter

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Today Band theory, part I

Last time: derived tight-binding model, $H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + c_j^\dagger c_i$

Today: solve in 1D, start 2D

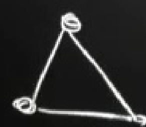
Perimeter-A

Today, solve in 1D, start 2D

Solve: – Find single-particle eigenstates & energies

– ∴ many-body states/energies

On the tutorial:



$$-t\left(c_0^\dagger c_1 + c_1^\dagger c_2 + c_2^\dagger c_0\right) + H.c.$$

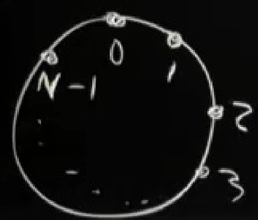
"Hermitian conjugate"

Found single-particle eigenstates.

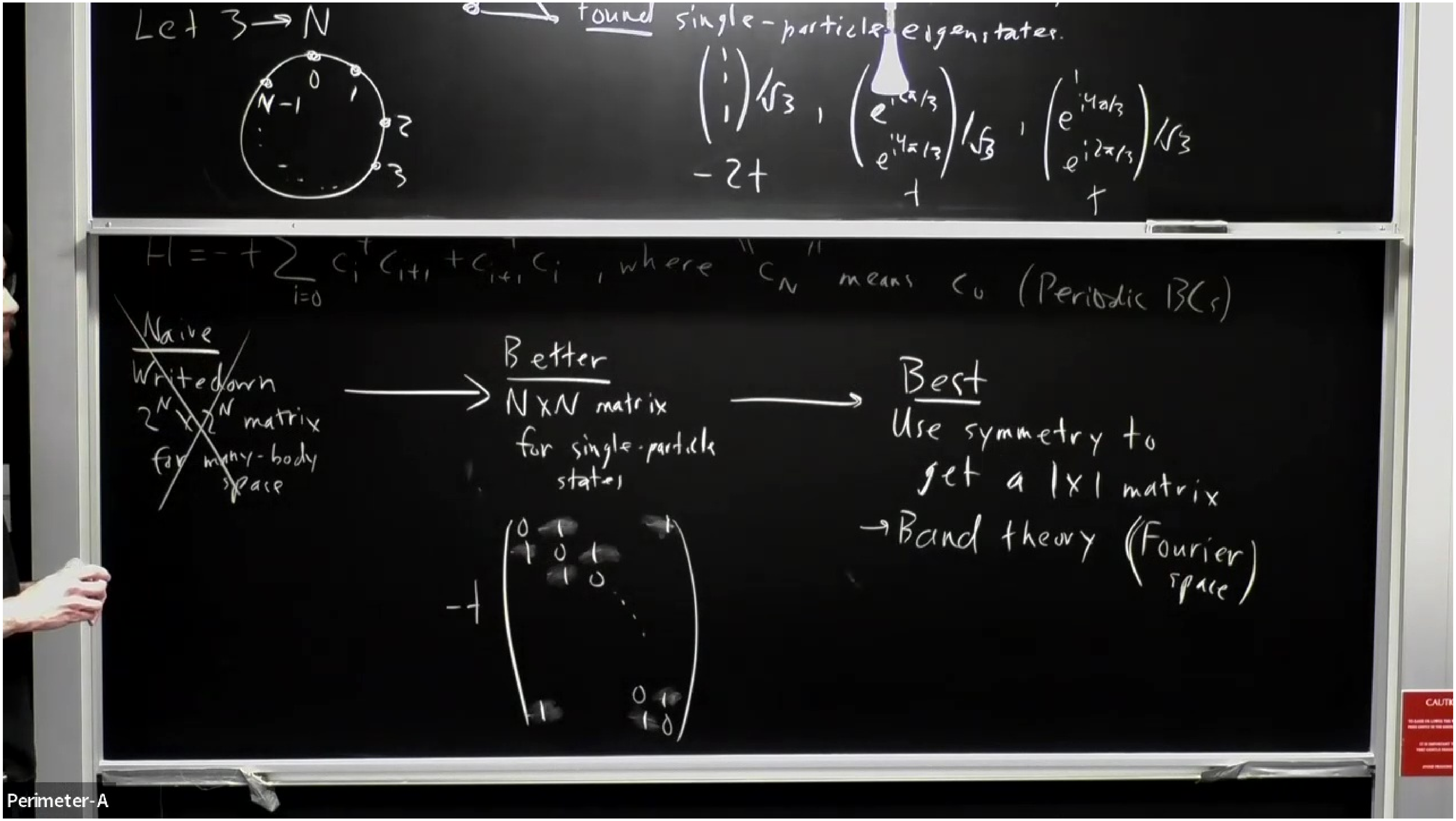
$$\begin{pmatrix}1\\1\\1\end{pmatrix}/\sqrt{3}, \quad \begin{pmatrix}1\\e^{i2\pi/3}\\e^{i4\pi/3}\end{pmatrix}/\sqrt{3}, \quad \begin{pmatrix}1\\e^{i4\pi/3}\\e^{i2\pi/3}\end{pmatrix}/\sqrt{3}$$

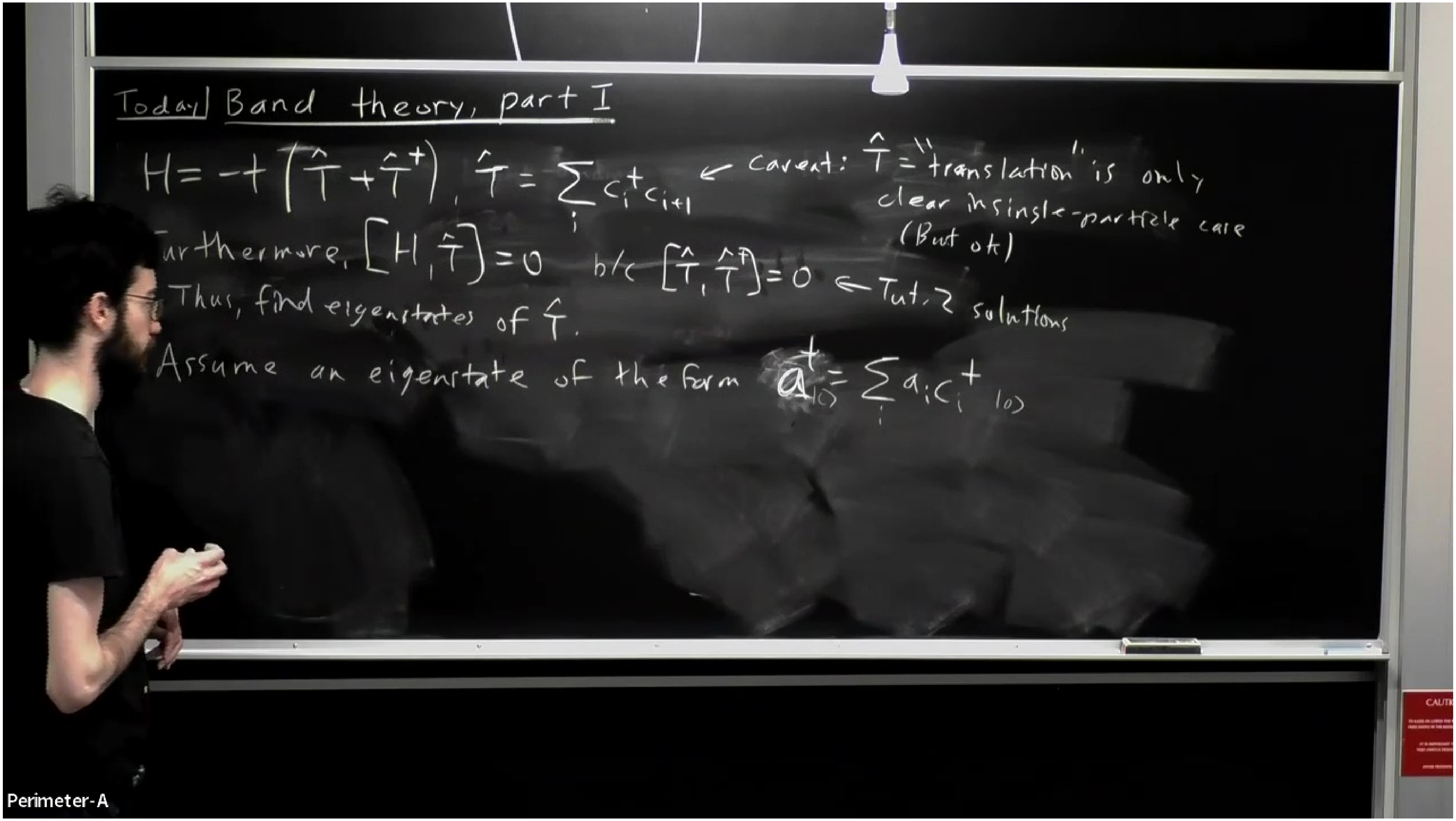
$$-2t \qquad\qquad t \qquad\qquad t$$

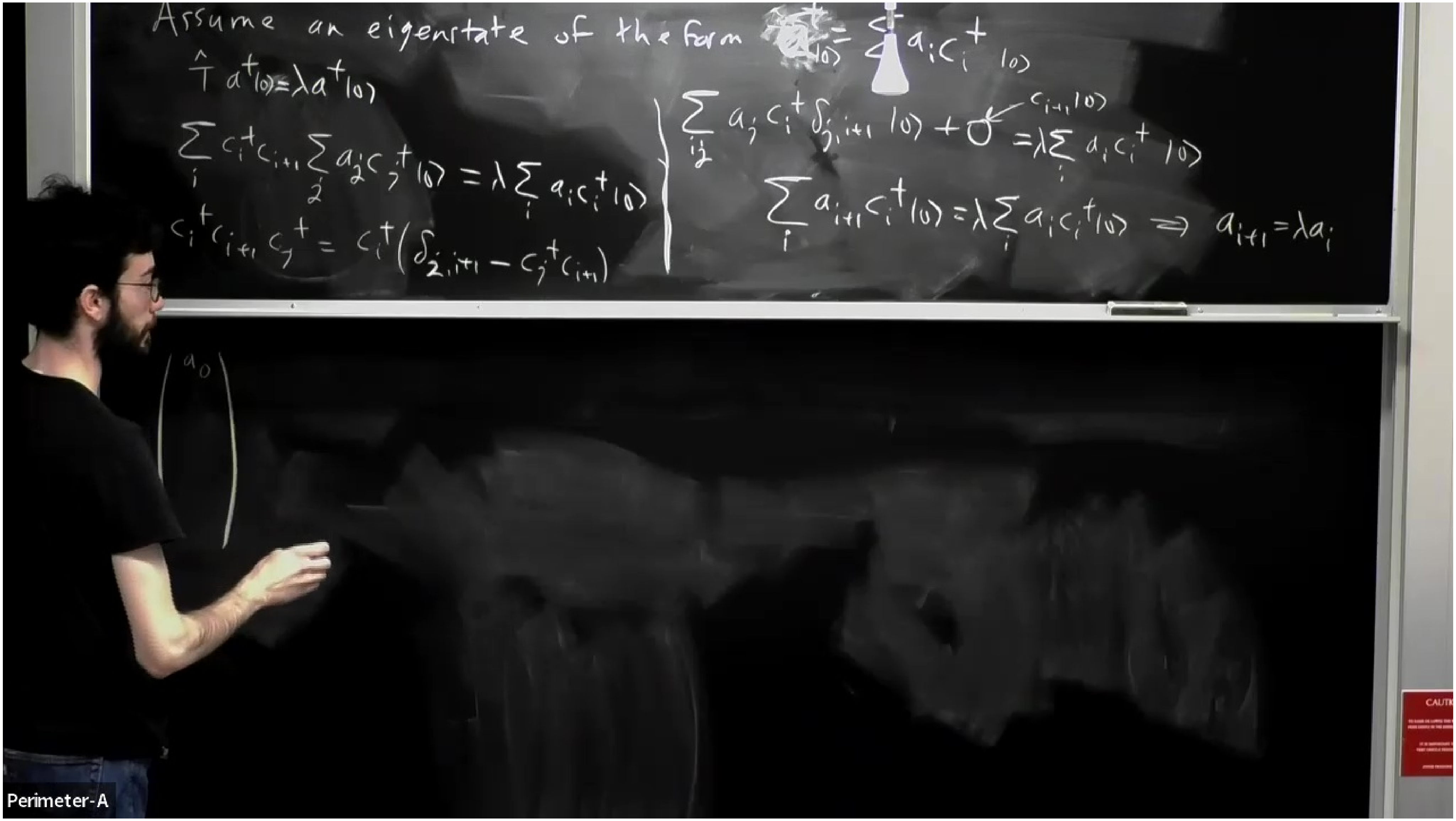
Let $3 \to N$

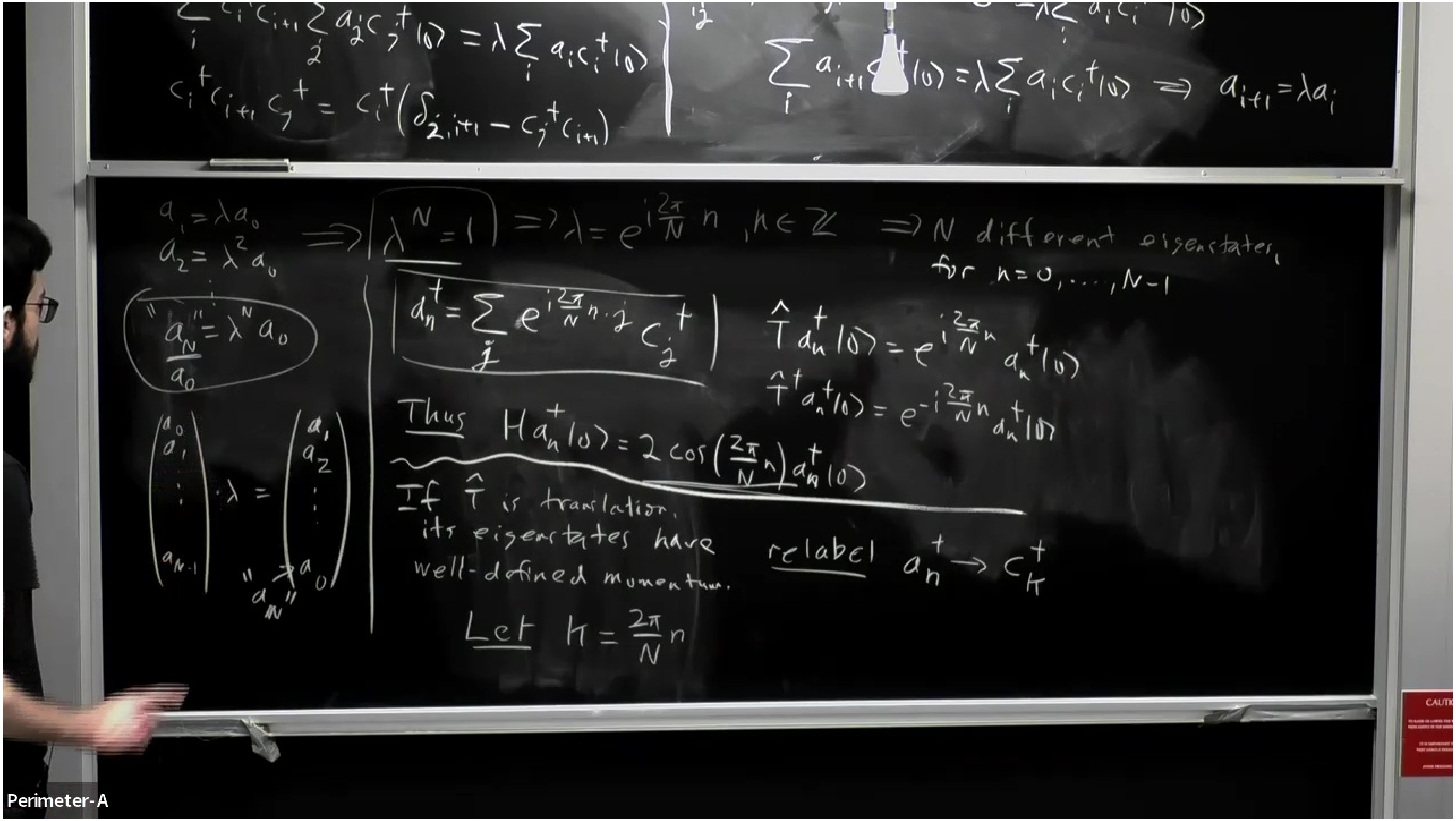


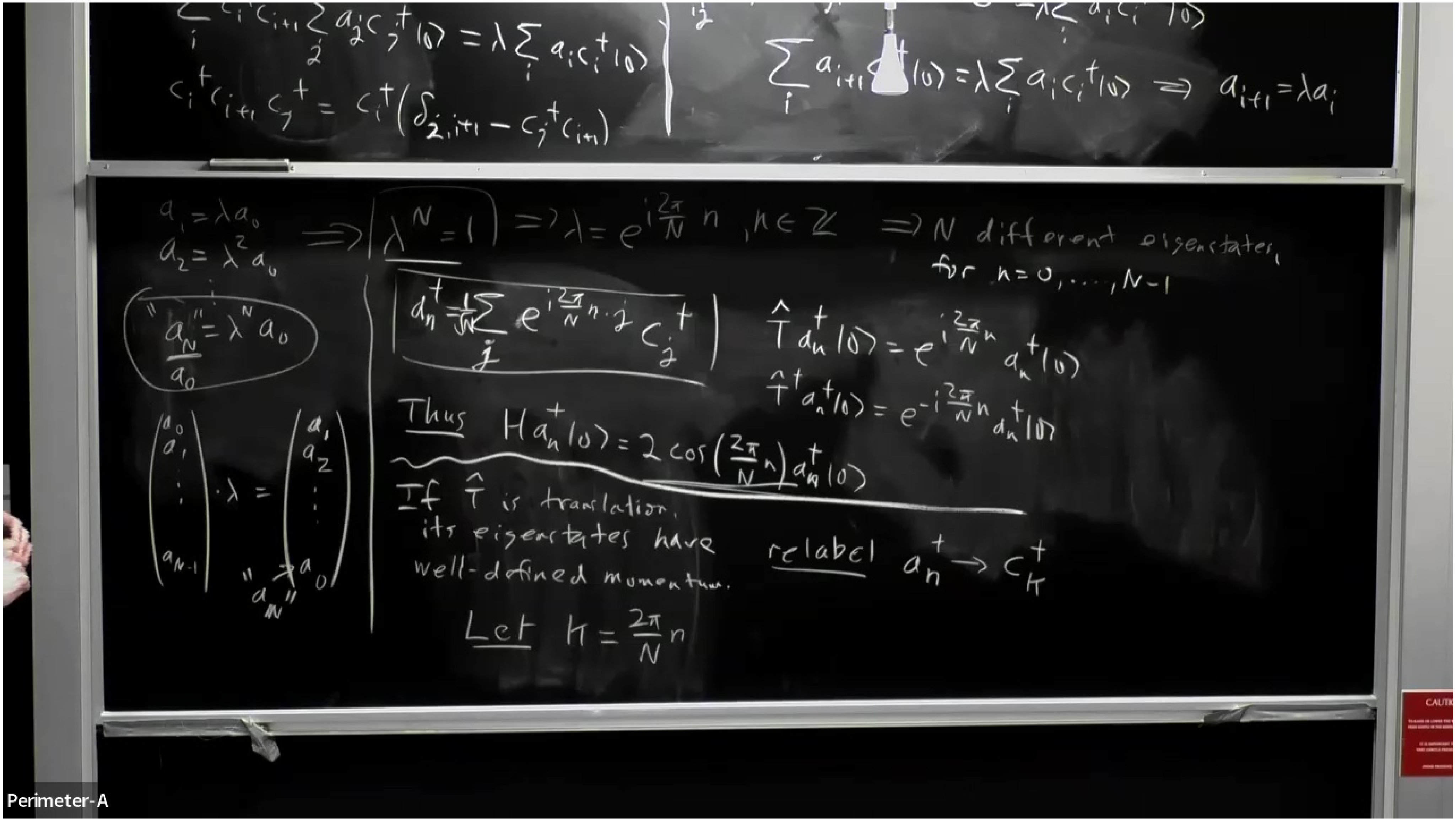
Perimeter-A

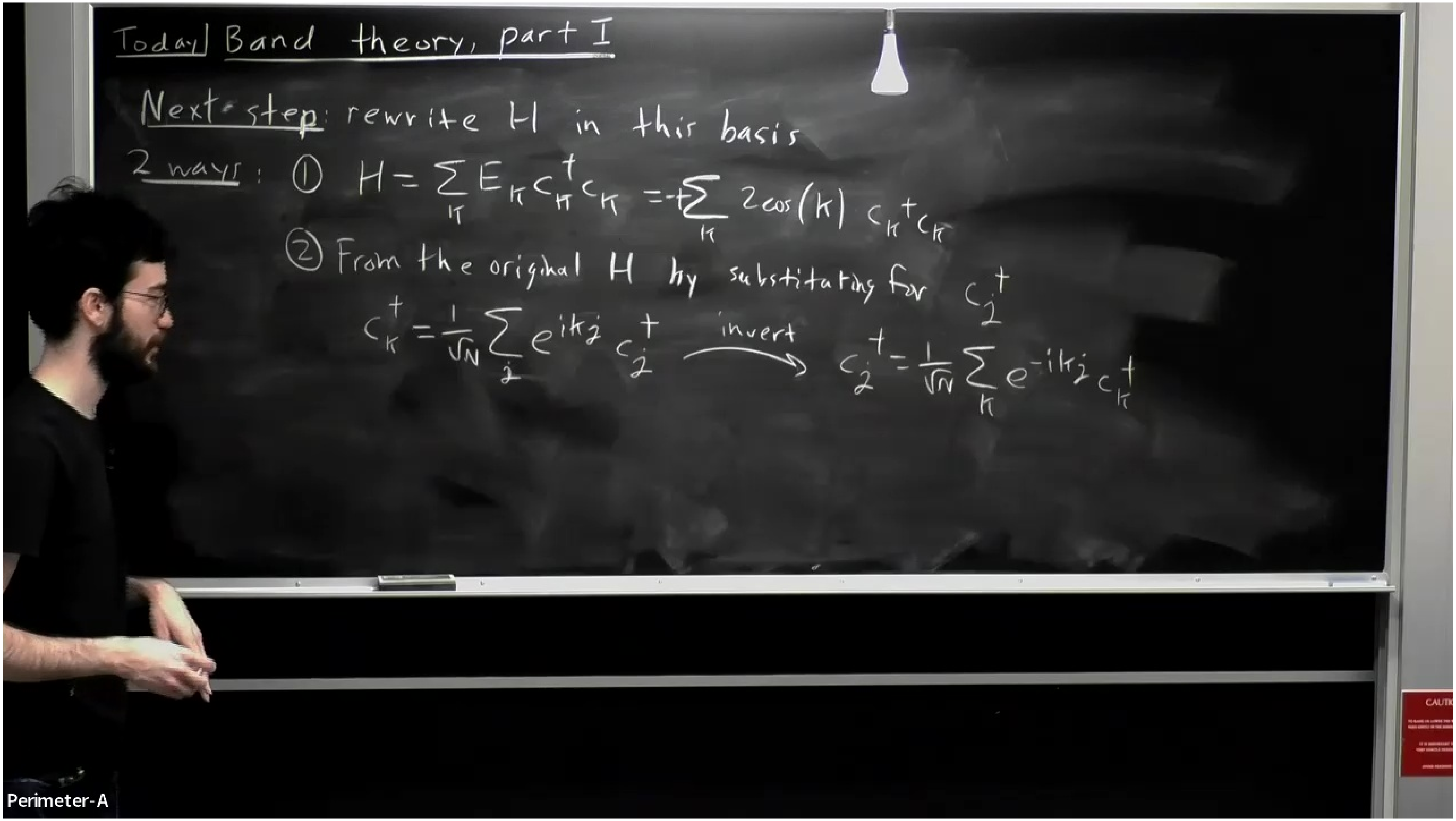

Let 3 → N
N-1 0 1 2 3
found single-particle eigenstates.
-2t
H = -t ∑ c_i^† c_{i+1} + c_{i+1}^† c_i , where "c_N" means c_0 (Periodic BCs)
i=0
Naive
Write down 2^N x 2^N matrix for many-body space
Better
N x N matrix for single-particle states
Best
Use symmetry to get a 1x1 matrix
→ Band theory (Fourier space)
Perimeter-A

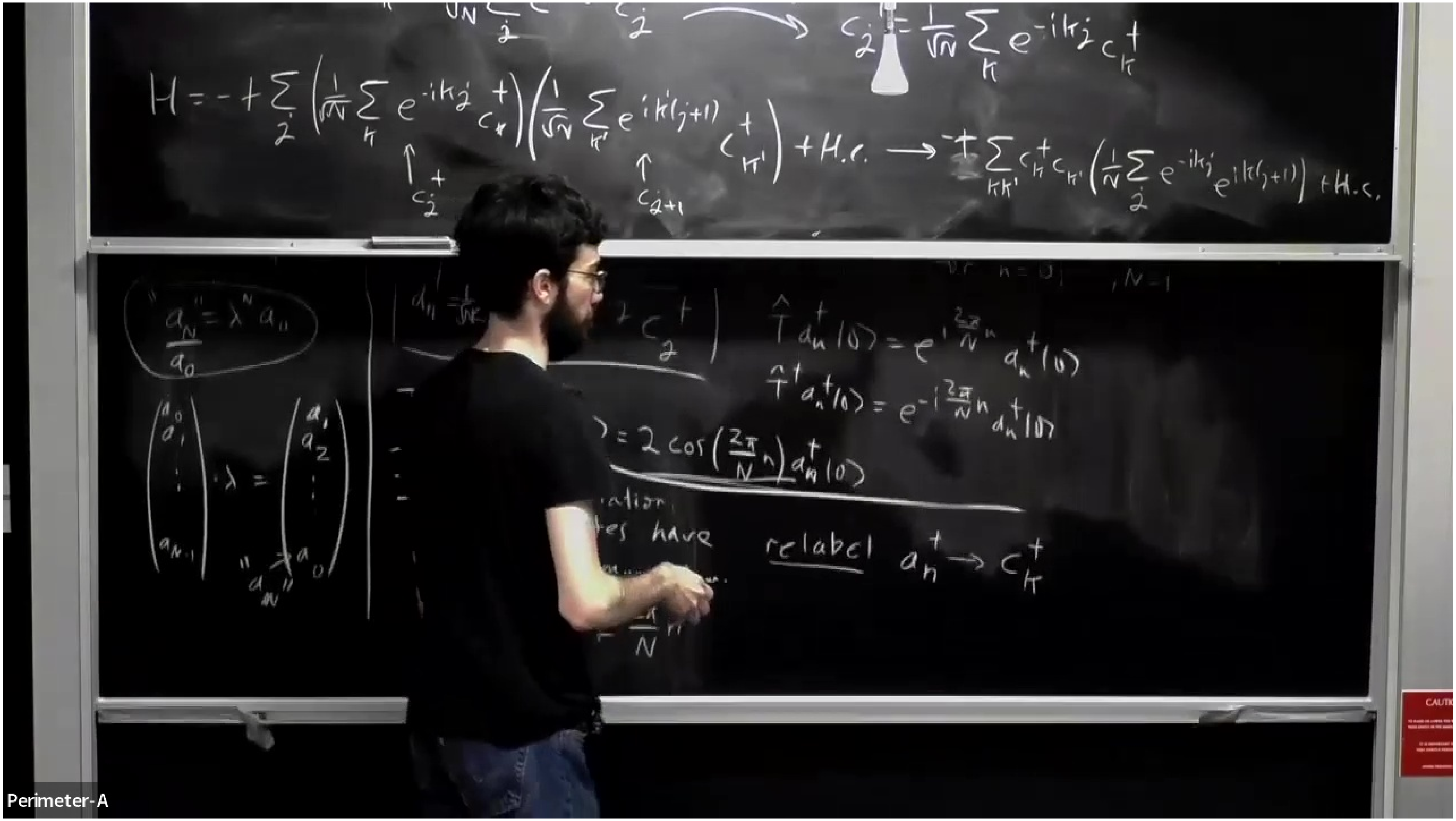

Today | Band theory, part I
$H = -t(\hat{T} + \hat{T}^\dagger)$, $\hat{T} = \sum_i c_i^\dagger c_{i+1}$ ← caveat: $\hat{T}$ = "translation" is only clear in single-particle case (But ok)
Furthermore, $[H, \hat{T}] = 0$ b/c $[\hat{T}, \hat{T}^\dagger] = 0$ ← Tut. 2 solutions
Thus, find eigenstates of $\hat{T}$.
Assume an eigenstate of the form $a^\dagger|0\rangle = \sum_i a_i c_i^\dagger |0\rangle$
Perimeter-A

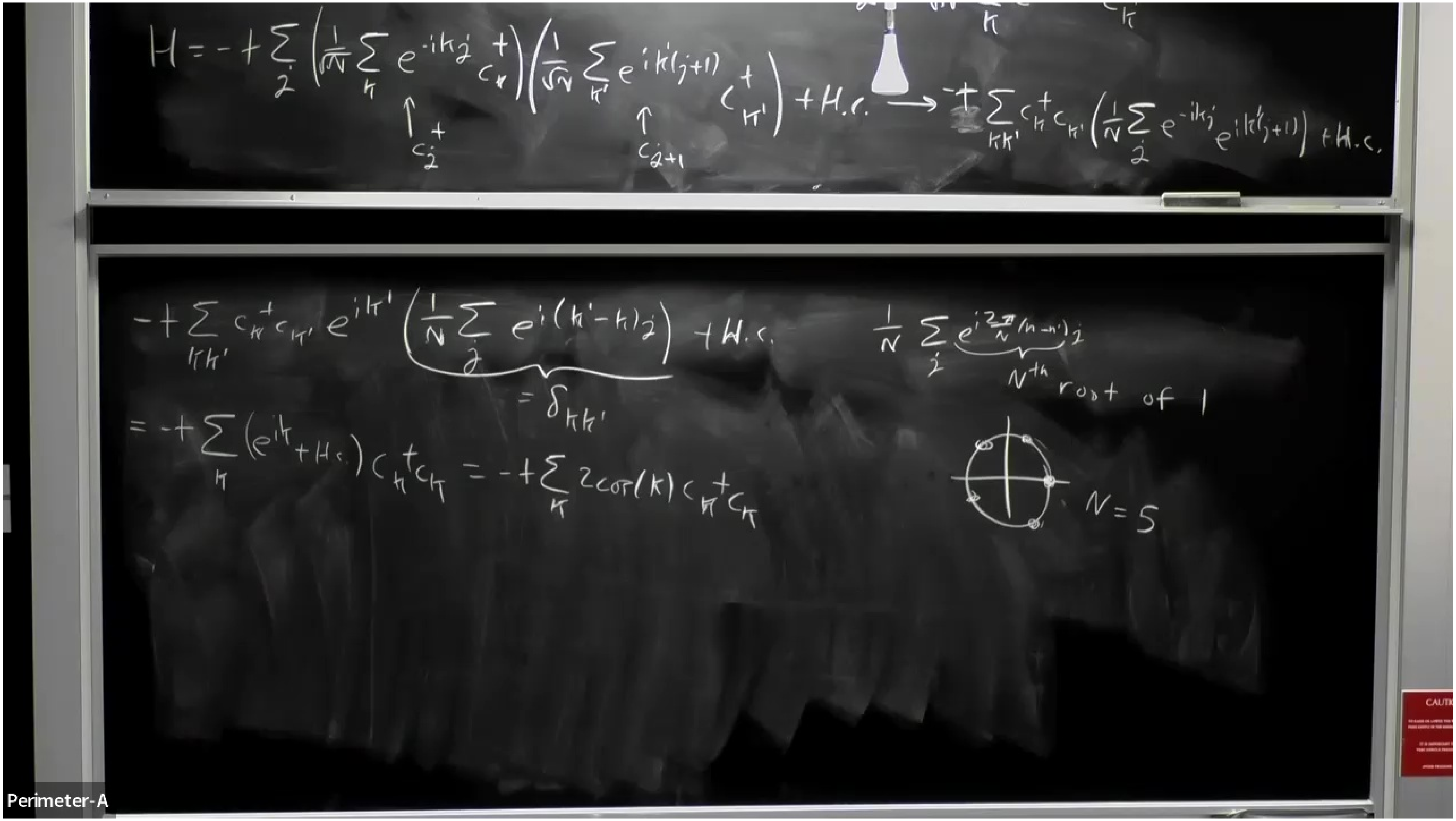

Assume an eigenstate of the form $a^\dagger|0\rangle = \sum a_i c_i^\dagger |0\rangle$
$\hat{T} a^\dagger|0\rangle = \lambda a^\dagger|0\rangle$
$\sum_i c_i^\dagger c_{i+1} \sum_j a_j c_j^\dagger |0\rangle = \lambda \sum_i a_i c_i^\dagger |0\rangle$
$c_i^\dagger c_{i+1} c_j^\dagger = c_i^\dagger(\delta_{j,i+1} - c_j^\dagger c_{i+1})$
$\sum_{ij} a_j c_i^\dagger \delta_{j,i+1}|0\rangle + 0 = \lambda\sum_i a_i c_i^\dagger|0\rangle$
$c_{i+1}|0\rangle$
$\sum_i a_{i+1} c_i^\dagger|0\rangle = \lambda \sum_i a_i c_i^\dagger |0\rangle \Rightarrow a_{i+1} = \lambda a_i$
a_0
Perimeter-A


$\sum_i c_i^\dagger c_{i+1} \sum_j a_j c_j^\dagger |0\rangle = \lambda \sum_i a_i c_i^\dagger |0\rangle$
$c_i^\dagger c_{i+1} c_j^\dagger = c_i^\dagger (\delta_{j,i+1} - c_j^\dagger c_{i+1})$
$\sum_i a_{i+1} c_i^\dagger |0\rangle = \lambda \sum_i a_i c_i^\dagger |0\rangle \Rightarrow a_{i+1} = \lambda a_i$
$a_1 = \lambda a_0$
$a_2 = \lambda^2 a_0$
$\boxed{\lambda^N = 1} \Rightarrow \lambda = e^{i \frac{2\pi}{N} n}, n \in \mathbb{Z} \Rightarrow N$ different eigenstates, for $n = 0, \dots, N-1$
"a_N" $= \lambda^N a_0$
$\boxed{a_n^\dagger = \sum_j e^{i \frac{2\pi}{N} n \cdot j} c_j^\dagger}$
$\hat{T} a_n^\dagger |0\rangle = e^{i \frac{2\pi}{N} n} a_n^\dagger |0\rangle$
$\hat{T}^\dagger a_n^\dagger |0\rangle = e^{-i \frac{2\pi}{N} n} a_n^\dagger |0\rangle$
Thus $H a_n^\dagger |0\rangle = 2 \cos\left(\frac{2\pi}{N} n\right) a_n^\dagger |0\rangle$
If $\hat{T}$ is translation, its eigenstates have well-defined momentum.
relabel $a_n^\dagger \to c_k^\dagger$
Let $k = \frac{2\pi}{N} n$
Perimeter-A


$\sum_i c_i^\dagger c_{i+1} \sum_j a_j c_j^\dagger |0\rangle = \lambda \sum_i a_i c_i^\dagger |0\rangle$
$c_i^\dagger c_{i+1} c_j^\dagger = c_i^\dagger (\delta_{j,i+1} - c_j^\dagger c_{i+1})$
$\sum_i a_{i+1} c_i^\dagger |0\rangle = \lambda \sum_i a_i c_i^\dagger |0\rangle \Rightarrow a_{i+1} = \lambda a_i$
$a_1 = \lambda a_0$
$a_2 = \lambda^2 a_0$
$\Rightarrow \lambda^N = 1 \Rightarrow \lambda = e^{i \frac{2\pi}{N} n}, n \in \mathbb{Z} \Rightarrow N$ different eigenstates,
for $n = 0, \ldots, N-1$
$"a_N" = \lambda^N a_0$
$\frac{a_N}{a_0}$
$a_n^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{i \frac{2\pi}{N} n \cdot j} c_j^\dagger$
$\hat{T} a_n^\dagger |0\rangle = e^{i \frac{2\pi}{N} n} a_n^\dagger |0\rangle$
$\hat{T}^\dagger a_n^\dagger |0\rangle = e^{-i \frac{2\pi}{N} n} a_n^\dagger |0\rangle$
$\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{N-1} \end{pmatrix} \cdot \lambda = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ "a_N" \to a_0 \end{pmatrix}$
Thus $H (a_n^\dagger |0\rangle) = 2 \cos\left(\frac{2\pi}{N} n\right) a_n^\dagger |0\rangle$
If $\hat{T}$ is translation,
its eigenstates have
well-defined momentum.
relabel $a_n^\dagger \to c_k^\dagger$
Let $k = \frac{2\pi}{N} n$
Perimeter-A


Today| Band theory, part I
Next step: rewrite H in this basis
2 ways: ① $H = \sum_k E_k c_k^\dagger c_k = -t \sum_k 2\cos(k)\, c_k^\dagger c_k$
② From the original H by substituting for $c_j^\dagger$
$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikj} c_j^\dagger \xrightarrow{\text{invert}} c_j^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k^\dagger$
Perimeter-A


$c_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k^\dagger$
$H = -t \sum_j \left(\frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k^\dagger \right) \left(\frac{1}{\sqrt{N}} \sum_{k'} e^{ik'(j+1)} c_{k'}^\dagger \right) + H.c. \longrightarrow -t \sum_{kk'} c_k^\dagger c_{k'} \left(\frac{1}{N} \sum_j e^{-ikj} e^{ik(j+1)} \right) + H.c.$
$c_j^\dagger$
c_{j+1}
"a_N" $= \lambda^N a_0$
$\hat{T}^\dagger a_n^\dagger |0\rangle = e^{i \frac{2\pi}{N} n} a_n^\dagger |0\rangle$
$\hat{T}^\dagger a_n^\dagger |0\rangle = e^{-i \frac{2\pi}{N} n} a_n^\dagger |0\rangle$
$= 2 \cos\left(\frac{2\pi}{N} n \right) a_n^\dagger |0\rangle$
relabel $a_n^\dagger \to c_k^\dagger$
Perimeter-A


$H = -t \sum_j \left(\frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k^\dagger\right)\left(\frac{1}{\sqrt{N}} \sum_{k'} e^{ik'(j+1)} c_{k'}\right) + H.c. \longrightarrow -t \sum_{kk'} c_k^\dagger c_{k'} \left(\frac{1}{N}\sum_j e^{-ikj} e^{ik'(j+1)}\right) + H.c.$
$c_j^\dagger$
c_{j+1}
$-t \sum_{kk'} c_k^\dagger c_{k'} e^{ik'} \underbrace{\left(\frac{1}{N}\sum_j e^{i(k'-k)j}\right)}_{=\delta_{kk'}} + H.c.$
$= -t \sum_k (e^{ik} + H.c.) c_k^\dagger c_k = -t \sum_k 2\cos(k) c_k^\dagger c_k$
$\frac{1}{N} \sum_j \underbrace{e^{i\frac{2\pi}{N}(n-n')j}}_{N^{th} \text{ root of } 1}$
$N = 5$
Perimeter-A

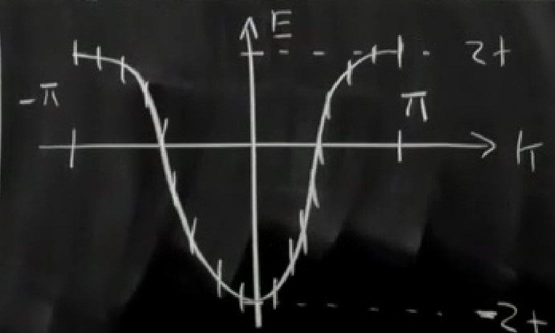
$$H = -t\sum_j \Big(\frac{1}{\sqrt N}\sum_k \underbrace{e^{-ikj} c_k^{+}}_{c_j^{+}}\Big)\Big(\frac{1}{\sqrt N}\sum_{k'} \underbrace{e^{ik'(j+1)} c_{k'}}_{c_{j+1}}\Big) + H.c. \longrightarrow -t\sum_{kk'} c_k^{+} c_{k'} \Big(\frac{1}{N}\sum_j e^{-ikj} e^{ik'(j+1)}\Big) + H.c.$$

$$-t\sum_{kk'} c_k^{+} c_{k'} e^{ik'} \underbrace{\Big(\frac{1}{N}\sum_j e^{i(k'-k)j}\Big)}_{=\delta_{kk'}} + H.c. \qquad \frac{1}{N}\sum_j \underbrace{e^{i\frac{2\pi}{N}(n-n')}}_{N^{th}\text{ root of } 1}{}^{j}$$

$$= -t\sum_k \left(e^{ik} + H.c.\right) c_k^{+} c_k = -t\sum_k 2\cos(k)\, c_k^{+} c_k$$

Know single-particle eigenstates, energies

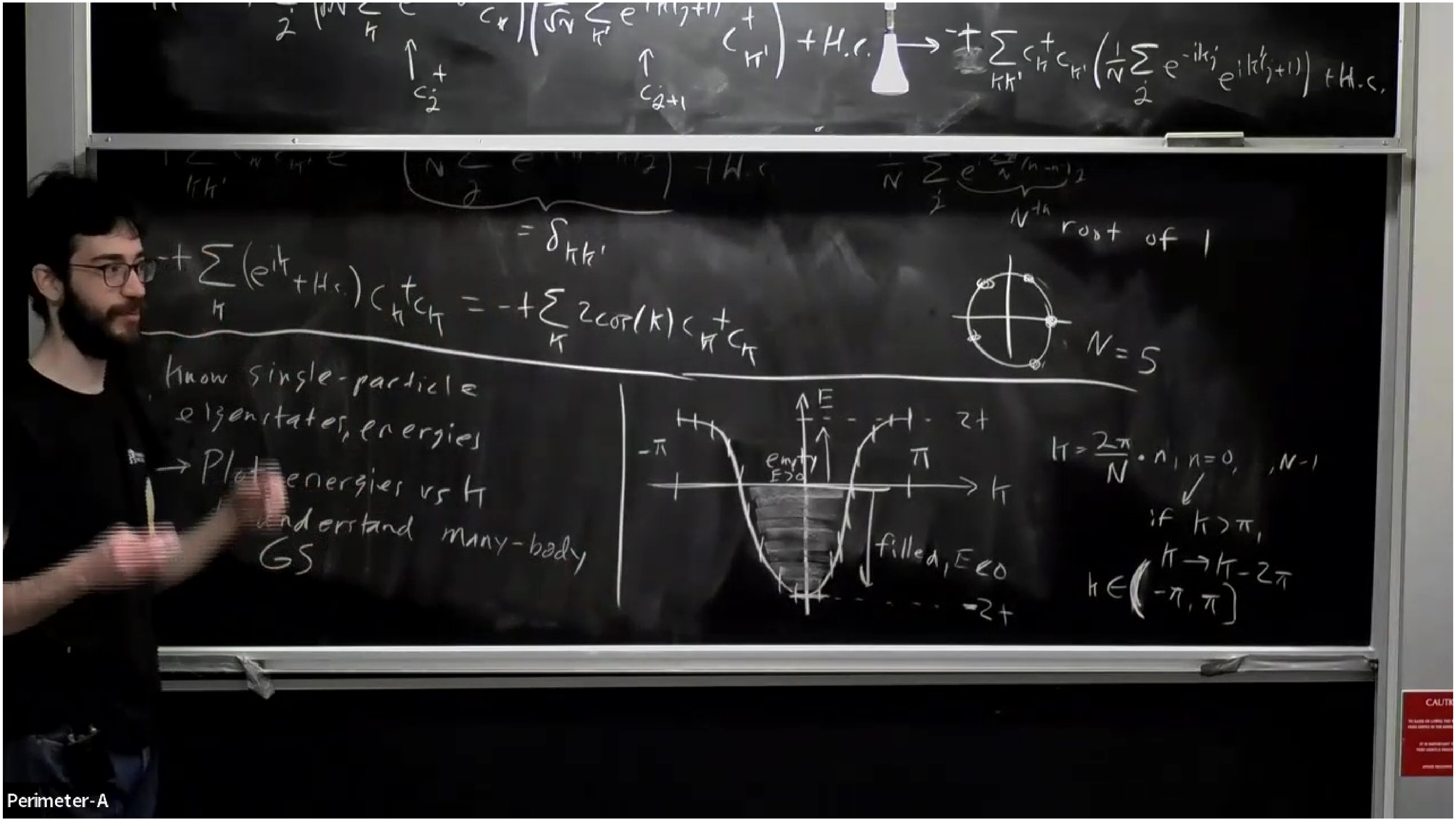
→ Plot energies vs k to understand many-body GS

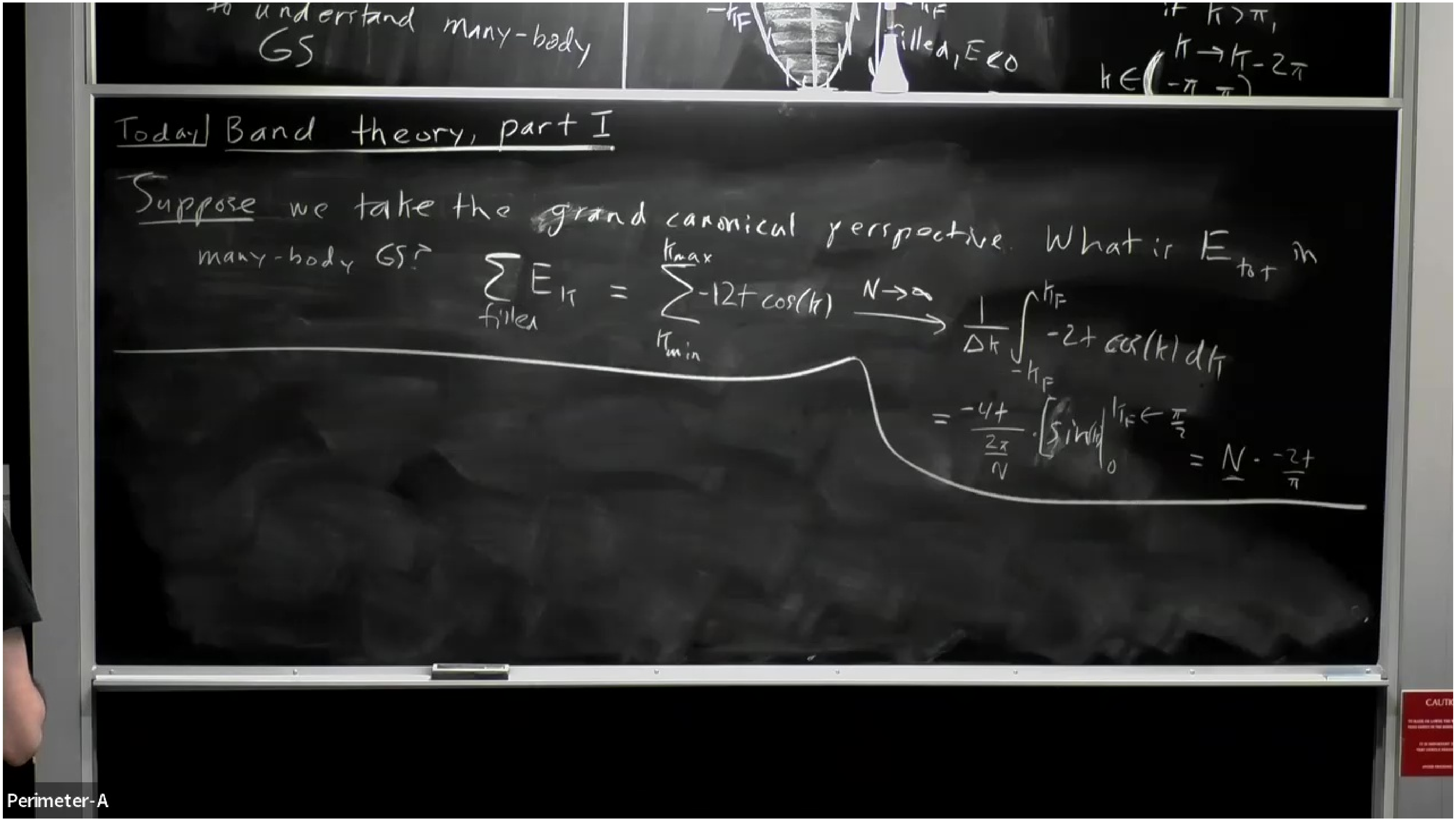


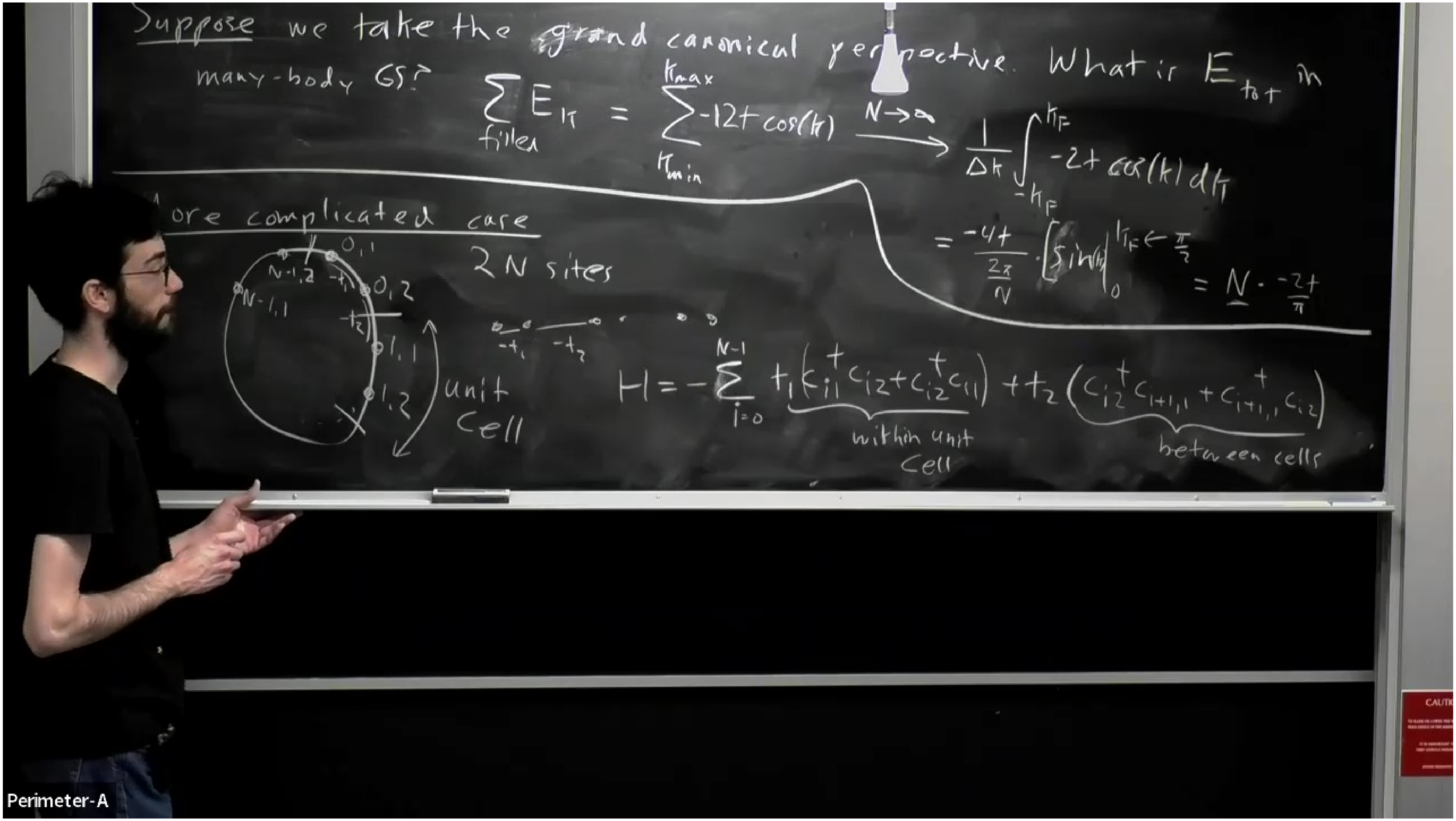
$k = \frac{2\pi}{N}\cdot n,\ n = 0, \ldots, N-1$

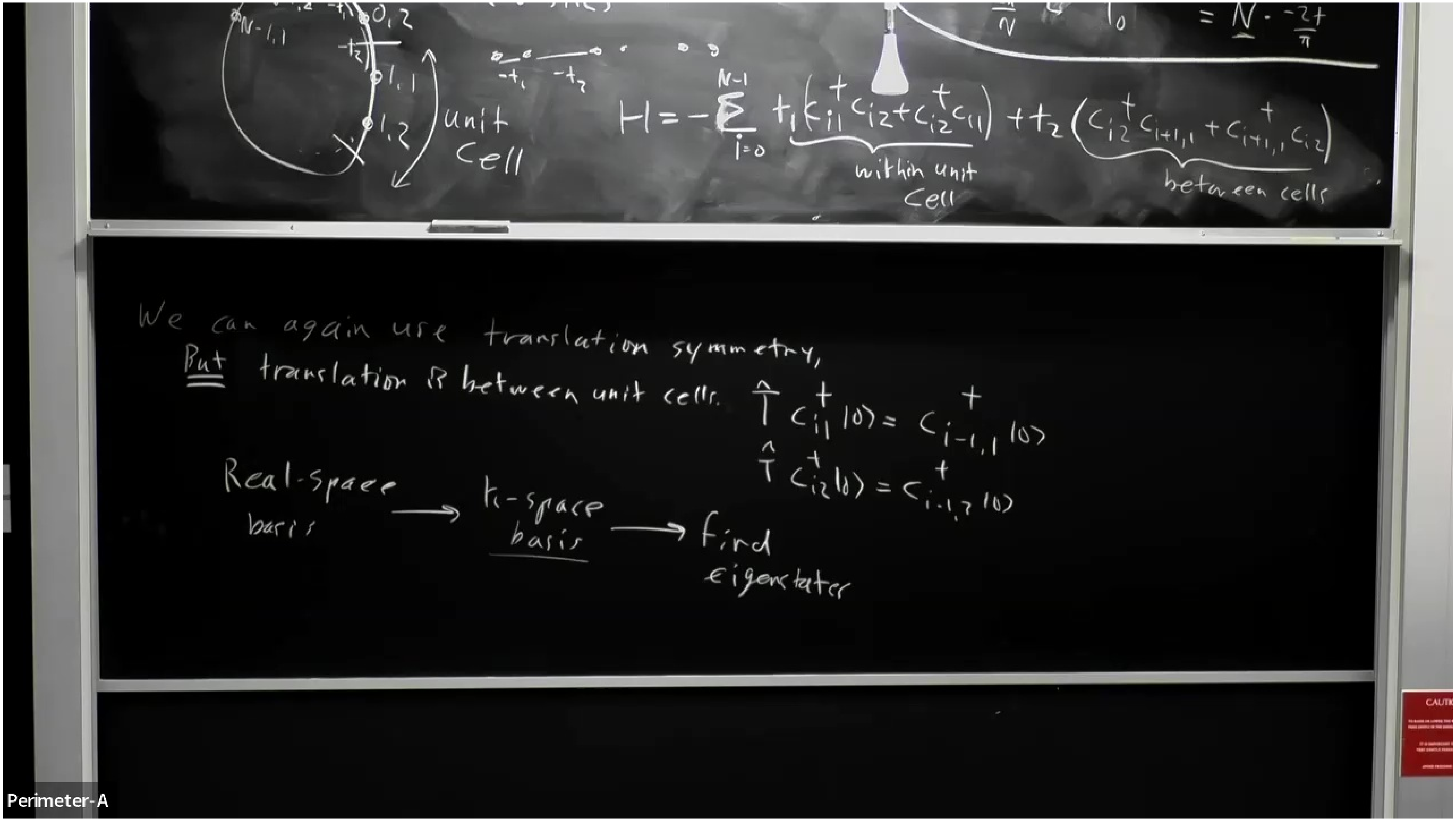
if $k > \pi$, $k \to k - 2\pi$

$k \in (-\pi, \pi]$


+H.c.
c_j^+
c_{j+1}
-t Σ_{kk'} c_k^+ c_{k'} (1/N Σ_j e^{-ikj} e^{ik'(j+1)}) +H.c.
= δ_{kk'}
N^{th} root of 1
-t Σ_k (e^{ik} + H.c.) c_k^+ c_k = -t Σ_k 2cos(k) c_k^+ c_k
N = 5
know single-particle eigenstates, energies
→ Plot energies vs k
understand many-body GS
E
2t
-π
π
empty E>0
k
filled, E<0
-2t
k = 2π/N · n, n = 0, ..., N-1
if k > π,
k → k - 2π
k ∈ (-π, π]
Perimeter-A


to understand many-body GS
filled, E<0
if k > π,
k → k - 2π
k ∈ (-π, π)
Today: Band theory, part I
Suppose we take the grand canonical perspective. What is E_tot in many-body GS?
Σ_filled E_k = Σ_{k_min}^{k_max} -2t cos(k) →(N→∞) 1/Δk ∫_{-k_F}^{k_F} -2t cos(k) dk
= -4t/(2π/N) · [sin(k)]_0^{k_F ← π/2} = N · -2t/π
Perimeter-A


Suppose we take the grand canonical perspective. What is E tot in many-body GS?
∑ E k = ∑ -12t cos(k) N→∞ 1/Δk ∫ -2t cos(k) dk
filled kmin kmax -kF kF
= -4t / (2π/N) · [sin(k)] kF ← π/2 0 = N · -2t/π
More complicated case
2N sites
0,1 0,2 N-1,2 N-1,1 1,1 1,2 -t1 -t2
unit cell
H = - ∑ t1 (ci1† ci2 + ci2† ci1) + t2 (ci2† ci+1,1 + ci+1,1† ci2)
i=0 N-1
within unit cell
between cells
Perimeter-A


unit cell
$H = -\sum_{i=0}^{N-1} t_1 \underbrace{(c_{i1}^\dagger c_{i2} + c_{i2}^\dagger c_{i1})}_{\text{within unit cell}} + t_2 \underbrace{(c_{i2}^\dagger c_{i+1,1} + c_{i+1,1}^\dagger c_{i2})}_{\text{between cells}}$
We can again use translation symmetry,
But translation is between unit cells.
$\hat{T} c_{i1}^\dagger |0\rangle = c_{i-1,1}^\dagger |0\rangle$
$\hat{T} c_{i2}^\dagger |0\rangle = c_{i-1,2}^\dagger |0\rangle$
Real-space basis → k-space basis → find eigenstates
Perimeter-A