Title: PSI Lecture - Condensed Matter - Lecture 5

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Collection: PSI Lecture - Condensed Matter

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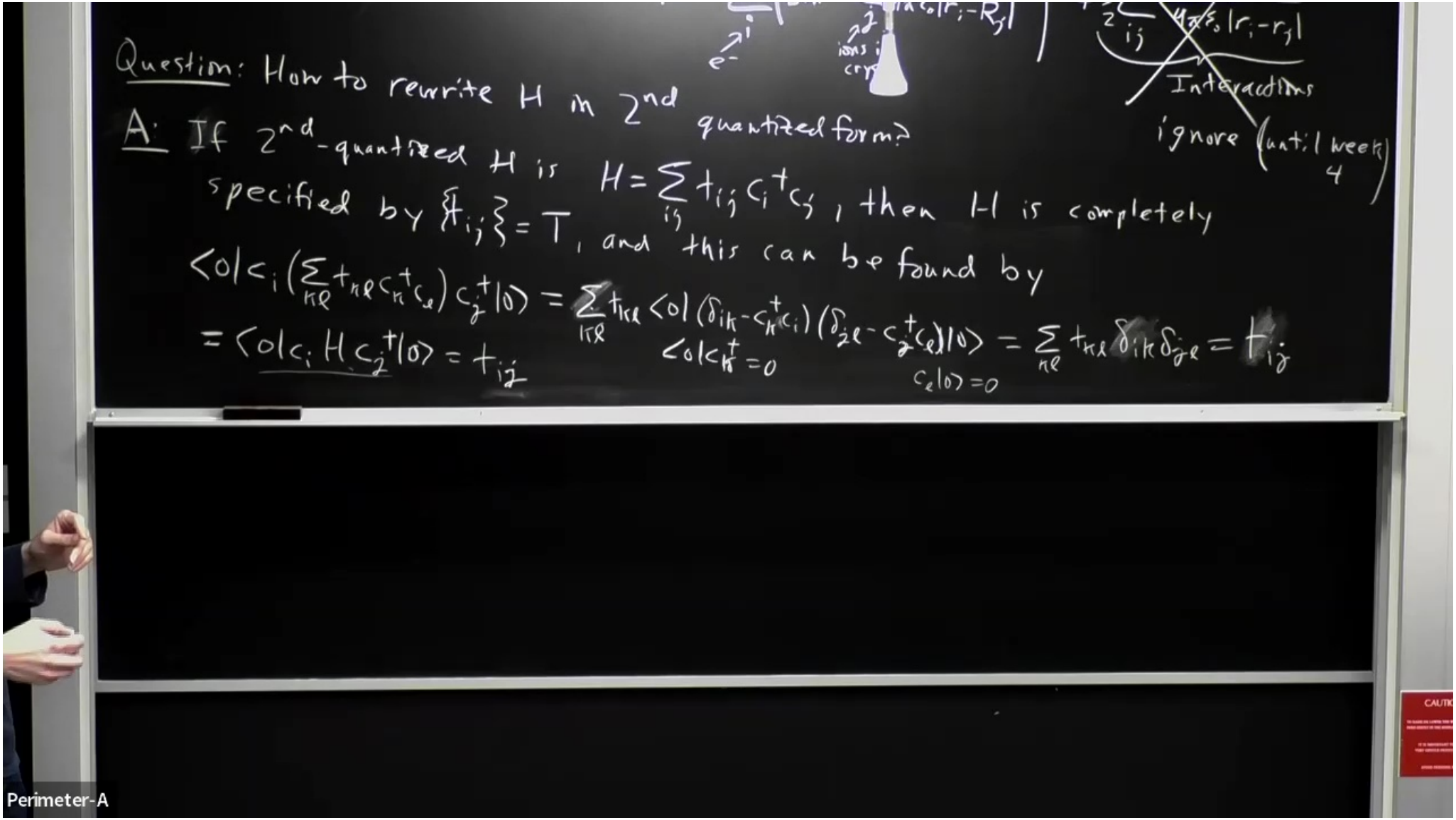
Today: Tight-binding models, e^- on a 1D lattice

System we want to study:

$$H = \sum_i^{e^-} \left(\frac{p_i^2}{2m} - \sum_j^{\text{ions in crystal}} \frac{Ze^2}{4\pi\varepsilon_0 |r_i - R_j|} \right) + \frac{1}{2} \sum_{ij} \frac{e^2}{4\pi\varepsilon_0 |r_i - r_j|}$$

Interactions

ignore (until 1 week 4)


Question: How to rewrite H in 2nd quantized form?
A: If 2nd-quantized H is $H=\sum_{ij} t_{ij} c_i^\dagger c_j$, then H is completely specified by $\{t_{ij}\}=T$, and this can be found by
$\langle 0|c_i\left(\sum_{k\ell} t_{k\ell} c_k^\dagger c_\ell\right) c_j^\dagger|0\rangle = \sum_{k\ell} t_{k\ell}\langle 0|(\delta_{ik}-c_k^\dagger c_i)(\delta_{j\ell}-c_j^\dagger c_\ell)|0\rangle = \sum_{k\ell} t_{k\ell}\delta_{ik}\delta_{j\ell} = t_{ij}$
$= \langle 0|c_i H c_j^\dagger|0\rangle = t_{ij}$
$\langle 0|c_k^\dagger = 0$
$c_\ell|0\rangle = 0$
Interactions
ignore (until week 4)
Perimeter-A

$\langle 0|c_i \left(\sum_{kl} t_{kl} c_k^\dagger c_l\right) c_j^\dagger|0\rangle = \sum_{kl} t_{kl} \langle 0|(\delta_{ik} - c_k^\dagger c_i)(\delta_{jl} - c_j^\dagger c_l)|0\rangle = \sum_{kl} t_{kl} \delta_{ik}\delta_{jl} = t_{ij}$

$= \langle 0|c_i H c_j^\dagger|0\rangle = t_{ij}$

$\langle 0|c_k^\dagger = 0$ $\quad c_l|0\rangle = 0$

and this can be found by

Note: The H in $\langle 0|c_i H c_j^\dagger|0\rangle$ can be single-particle because $T = P_1 H P_1$ for P_1 the projection to the 1-particle space

Use this to convert our H for e^- on a lattice.

Steps: ① Pick an ON basis of single-particle orbitals

②

$\langle 0 | c_i \left(\sum_{kl} t_{kl} c_k^\dagger c_l \right) c_j^\dagger | 0 \rangle = \sum_{kl} t_{kl} \langle 0 | (\delta_{ik} - c_k^\dagger c_i)(\delta_{jl} - c_j^\dagger c_l) | 0 \rangle = \sum_{kl} t_{kl} \delta_{ik} \delta_{jl} = t_{ij}$

$= \langle 0 | c_i H c_j^\dagger | 0 \rangle = t_{ij}$

$\langle 0 | c_k^\dagger = 0$ $\quad$ $c_l | 0 \rangle = 0$

and this can be found by

Because $I = P_1 H P_1$ for P_1 the projection to the 1-particle space

Use this to convert our H for e^- on a lattice.

Steps: ① Pick an ON basis of single-particle orbitals

② Find matrix elts.

extra step: many approximations

$\langle 0|c_i\left(\sum_{k\ell} t_{k\ell} c_k^\dagger c_\ell\right) c_j^\dagger|0\rangle = \sum_{k\ell} t_{k\ell} \langle 0|(\delta_{ik} - c_k^\dagger c_i)(\delta_{j\ell} - c_j^\dagger c_\ell)|0\rangle = \sum_{k\ell} t_{k\ell}\,\delta_{ik}\delta_{j\ell} = t_{ij}$

$= \langle 0|c_i H c_j^\dagger|0\rangle = t_{ij}$

$\langle 0|c_k^\dagger = 0$

$c_\ell|0\rangle = 0$

and this can be found by

projection to the 1-particle space

Use this to convert our H for e^- on a lattice.

Steps: ① Pick an ON basis of single-particle orbitals

② Find matrix elts.

extra step: many approximations

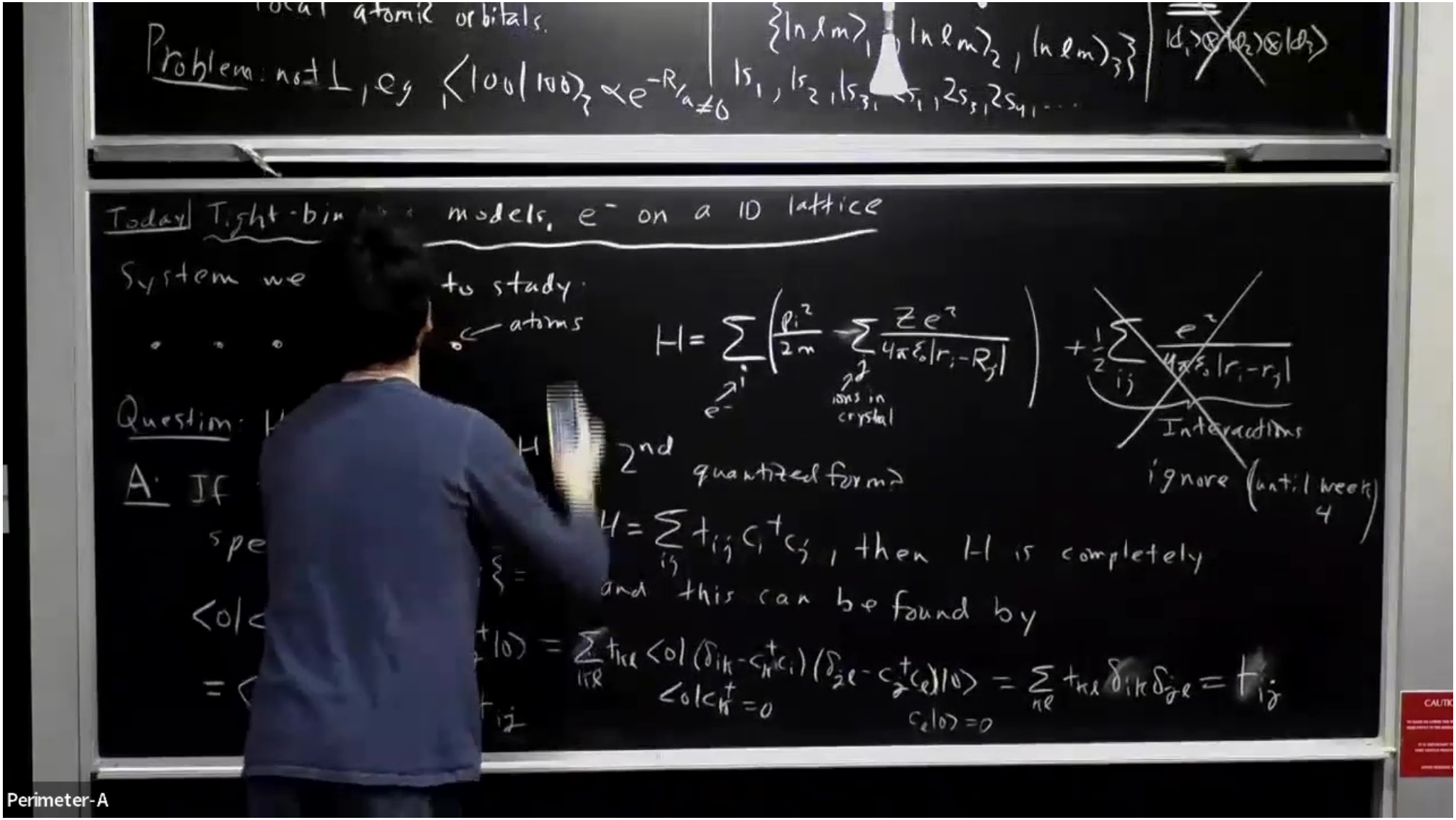
Claim: a natural choice of basis is local atomic orbitals.

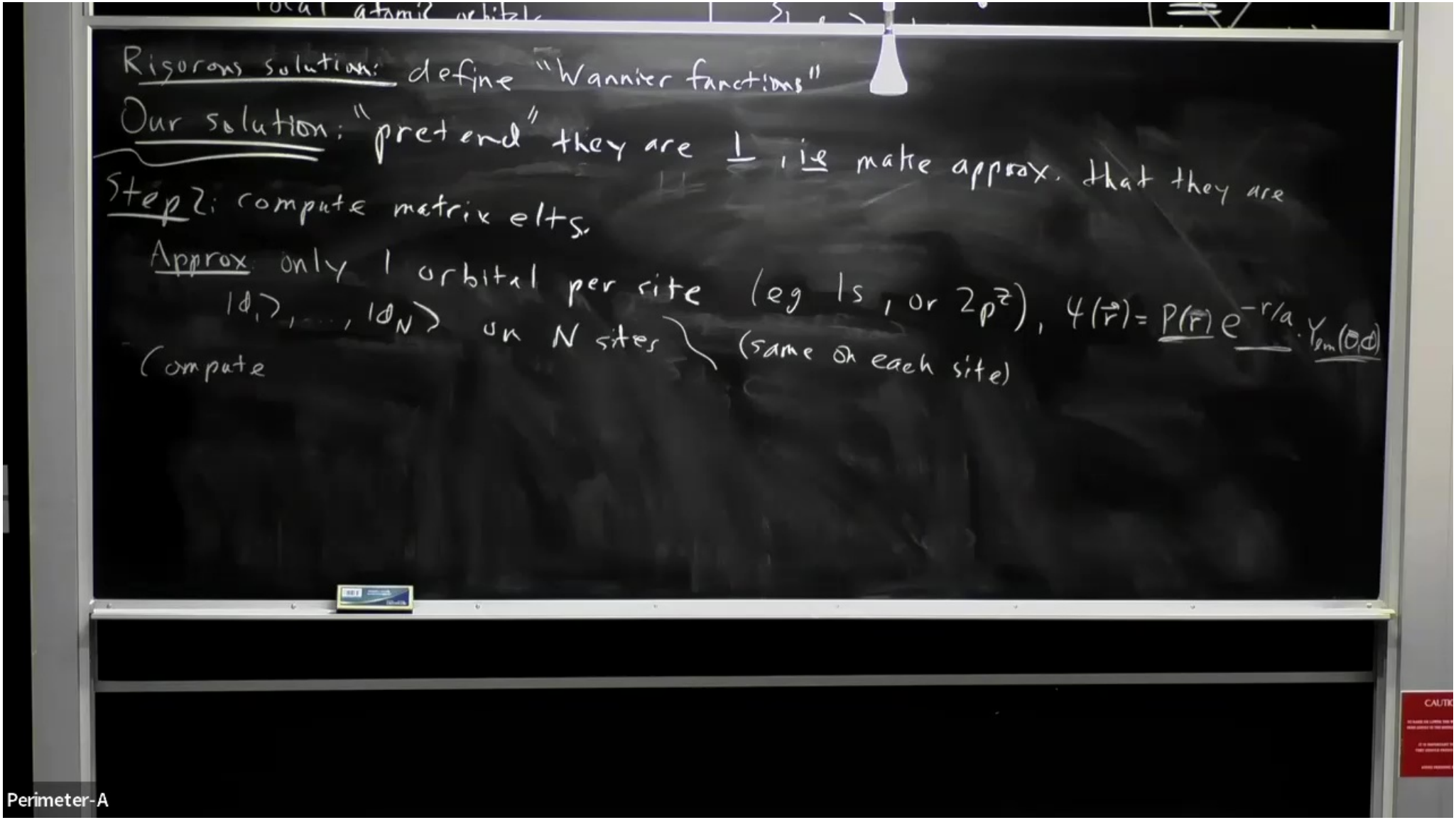
ex: 1 2 3

$\{|n\ell m\rangle_1, |n\ell m\rangle_2, |n\ell m\rangle_3\}$

$1s_1, 1s_2, 1s_3, 2s_1, 2s_3, 2s_4, \ldots$

~~NOT~~ ~~$|\phi_1\rangle \otimes |\phi_2\rangle \otimes |\phi_3\rangle$~~


atomic orbitals.
Problem: not ⊥, e.g. ⟨100|100⟩ ∝ e^{-R/a} ≠ 0
{|nlm⟩_1, |nlm⟩_2, |nlm⟩_3}
|1s_1⟩, |1s_2⟩, |1s_3⟩, |1s_4⟩, |2s_1⟩, |2s_2⟩, ...
Today: Tight-bin... models, e⁻ on a 1D lattice
System we ... to study:
atoms
H = Σ_i (p_i²/2m − Σ_j Ze²/(4πε₀|r_i − R_j|)) + ½ Σ_{ij} e²/(4πε₀|r_i − r_j|)
e⁻
ions in crystal
Interactions
ignore (until week 4)
Question: H
A: If
2nd quantized form
H = Σ_{ij} t_ij c_i† c_j, then H is completely
and this can be found by
⟨0|c ... = Σ_{ik} t_ik ⟨0|(δ_ik − c_i† c_i)(δ_jℓ − c_j† c_ℓ)|0⟩ = Σ_{nℓ} t_nℓ δ_in δ_jℓ = t_ij
⟨0|c_i† = 0
c_ℓ|0⟩ = 0


Rigorous solution: define "Wannier functions"
Our solution: "pretend" they are 1, i.e. make approx. that they are
Step 2: compute matrix elts.
Approx: only 1 orbital per site (eg 1s, or $2p^z$), $\psi(\vec{r}) = P(r)\, e^{-r/a} \cdot Y_{lm}(\theta\phi)$
$|\phi_1\rangle, \ldots, |\phi_N\rangle$ on N sites } (same on each site)
(compute
Perimeter-A

define "Wannier functions"

Our solution: "pretend" they are $\perp$, i.e. make approx. that they are

Step 2: compute matrix elts.

Approx: only 1 orbital per site (eg 1s, or $2p^z$), $\psi(\vec{r}) = R(r)\, e^{-r/a} \cdot Y_{lm}(\theta,\phi)$

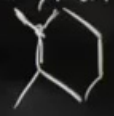
$|\phi_1\rangle, \ldots, |\phi_N\rangle$ on N sites } (same on each site)

Compute matrix elements

$1s, 2s, 2p_1 \ldots \quad |n\,l\,m\rangle$, $n = 1000$

Carbon

crystal of C



C has $1s^\uparrow, 1s^\downarrow$, has 4 valence e⁻: 3 form "σ" bonds, 1 leftover

Step 2: compute matrix elts.

Approx: only 1 orbital per site (eg 1s, or $2p^z$), $\psi(\vec{r}) = P(r)\, e^{-r/a} \cdot Y_{lm}(\theta,\phi)$

$|\phi_1\rangle, \ldots, |\phi_N\rangle$ on N sites (same on each site)

$1s, 2s, 2p, \ldots \quad |n\,l\,m\rangle$, $n = 1, 2, \ldots$

Compute matrix elements

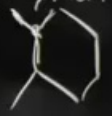
Diagonal $\langle \phi_i | \frac{p^2}{2m} + \sum_{j} \frac{ze^2}{4\pi\varepsilon_0 |x - jR|} | \phi_i \rangle$ (i at $\vec{R}$)

$= \underbrace{\langle \phi_i | \frac{p^2}{2m} - \frac{ze^2}{4\pi\varepsilon_0 |x - iR|} | \phi_i \rangle}_{E_n} - \frac{ze^2}{4\pi\varepsilon_0} \sum_{j \neq i} \langle \phi_i | \frac{1}{|x - jR|} | \phi_i \rangle$

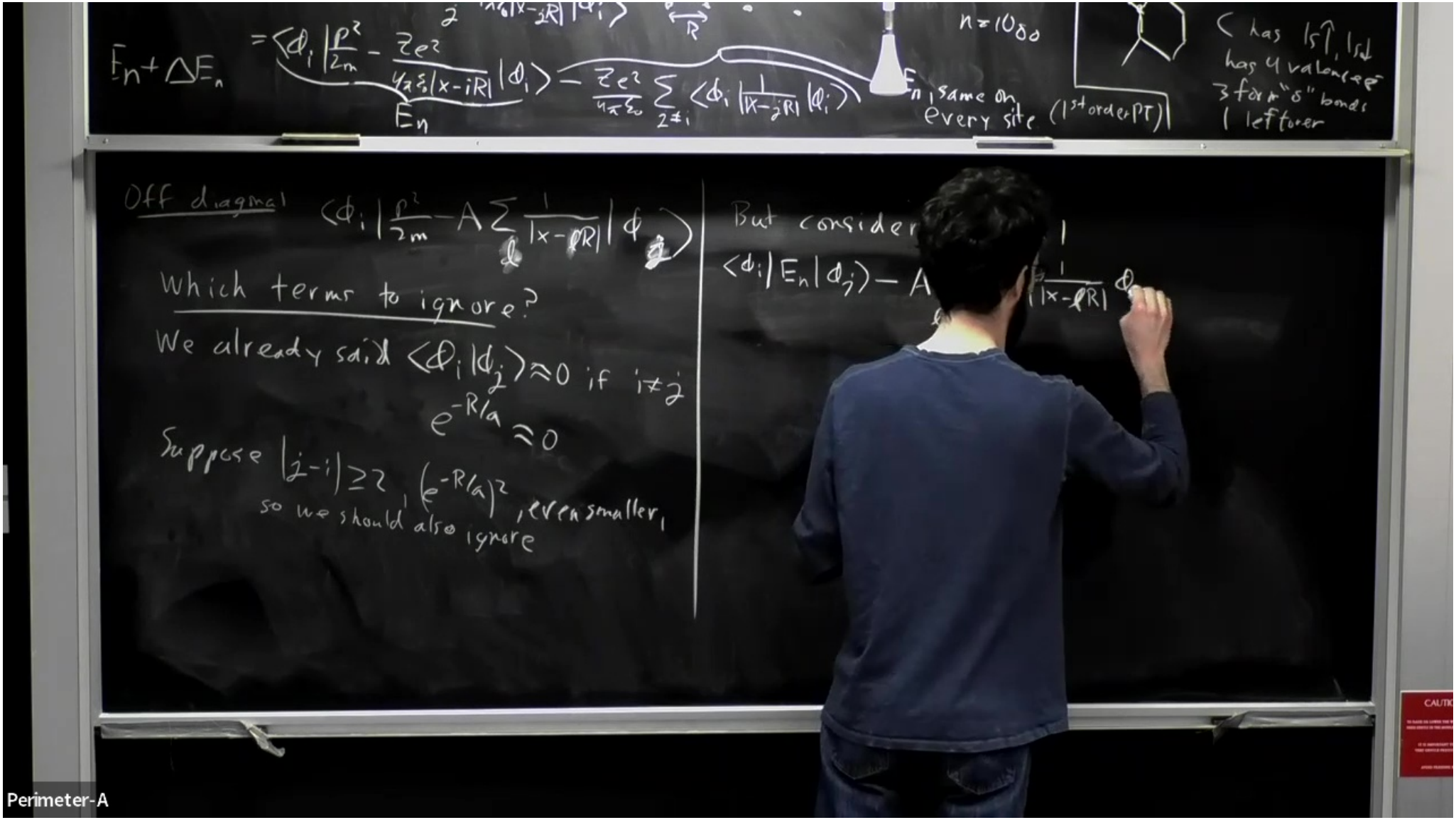
ΔE_n, same on every site (1st order PT)

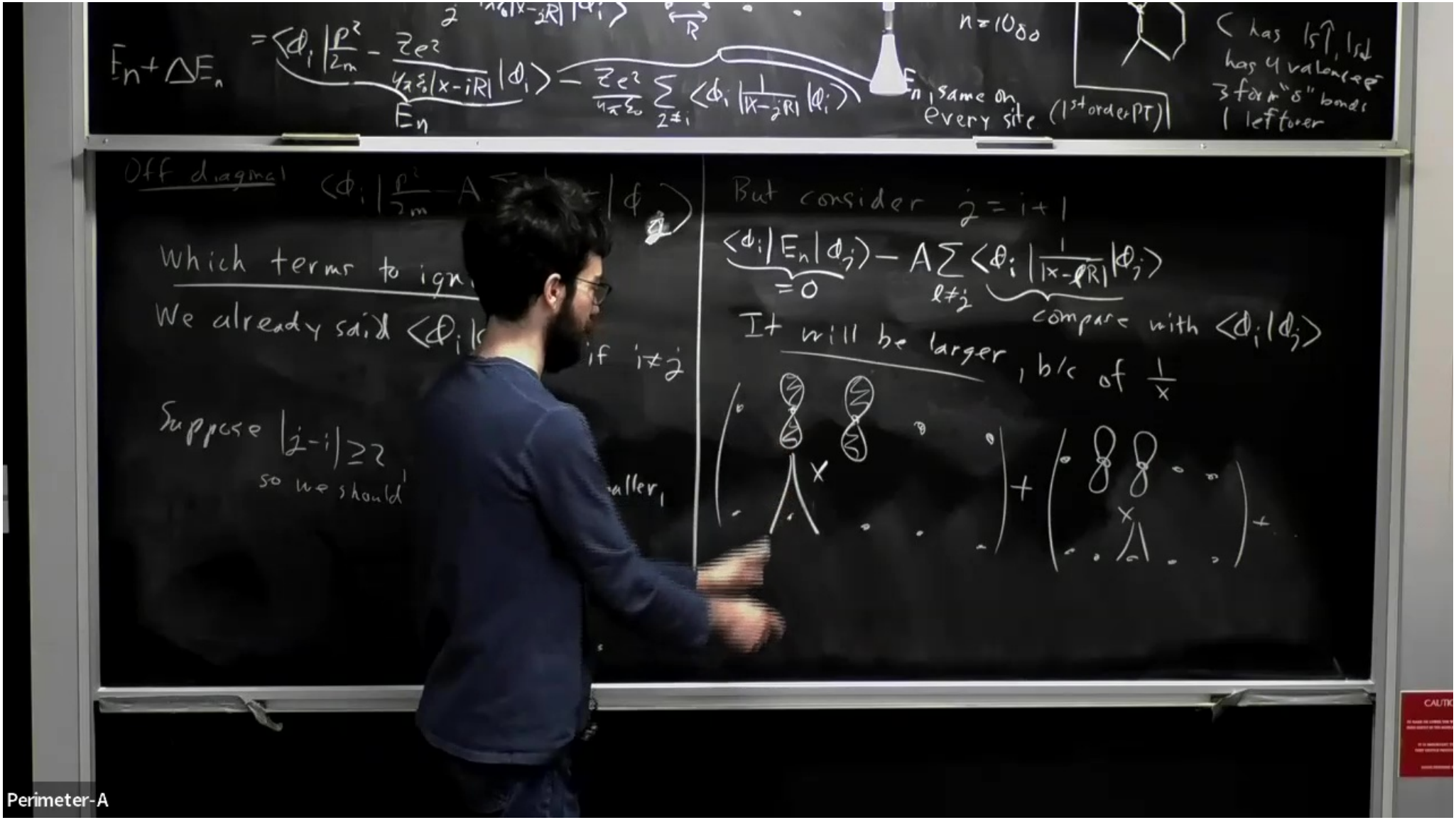
Carbon

crystal of C



(has $1s^\uparrow, 1s^\downarrow$ has 4 valence e^- 3 form "σ" bonds 1 leftover


$E_n + \Delta E_n = \langle \phi_i | \frac{p^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 |x - iR|} | \phi_i \rangle - \frac{Ze^2}{4\pi\epsilon_0} \sum_{j \neq i} \langle \phi_i | \frac{1}{|x - jR|} | \phi_i \rangle$
E_n
E_n, same on every site (1^{st} order PT)
$n \approx 10^{80}$
R
C has $1s^2$, $1s^2$ has 4 valence e^- 3 form "σ" bonds 1 leftover
Off diagonal $\langle \phi_i | \frac{p^2}{2m} - A \sum_{\ell} \frac{1}{|x - \ell R|} | \phi_j \rangle$
Which terms to ignore?
We already said $\langle \phi_i | \phi_j \rangle \approx 0$ if $i \neq j$
$e^{-R/a} \approx 0$
Suppose $|j - i| \geq 2$, $(e^{-R/a})^2$, even smaller, so we should also ignore
But consider
$\langle \phi_i | E_n | \phi_j \rangle - A$
$\frac{1}{|x - \ell R|} \phi$


$E_n + \Delta E_n = \langle \phi_i | \frac{p^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0 |x - iR|} | \phi_i \rangle - \frac{Ze^2}{4\pi\varepsilon_0} \sum_{j \neq i} \langle \phi_i | \frac{1}{|x - jR|} | \phi_i \rangle$
E_n
E_n, same on every site (1^{st} order PT)
$n = 10^{80}$
R
C has $1s^2$, $1s^2$ has 4 valence e⁻ 3 form "σ" bonds 1 left over
Off diagonal
Which terms to ign
We already said
if $i \neq j$
Suppose $|j - i| \geq 2$
so we should
But consider $j = i + 1$
$\langle \phi_i | E_n | \phi_j \rangle - A \sum_{l \neq j} \langle \phi_i | \frac{1}{|x - lR|} | \phi_j \rangle$
$= 0$
compare with $\langle \phi_i | \phi_j \rangle$
It will be larger, b/c of $\frac{1}{x}$

$E_n + \Delta E_n = \langle \phi_i | \frac{p^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0 |x - iR|} | \phi_i \rangle - \frac{Ze^2}{4\pi\varepsilon_0} \sum_{j \neq i} \langle \phi_i | \frac{1}{|x - jR|} | \phi_i \rangle$

E_n $\quad E_n$, same on every site (1st order PT)

$n = 10^{80}$

C has $1s^2 2s^2 2p^2$, Si has 4 valence e^- $\rightarrow$ form "δ" bonds + 1 leftover

Which terms to ignore?

We already said $\langle \phi_i | \phi_j \rangle \approx 0$ if $i \neq j$

$e^{-R/a} \approx 0$

Suppose $|j - i| \geq 2$, $(e^{-R/a})^2$, even smaller, so we should also ignore (or cancel out)

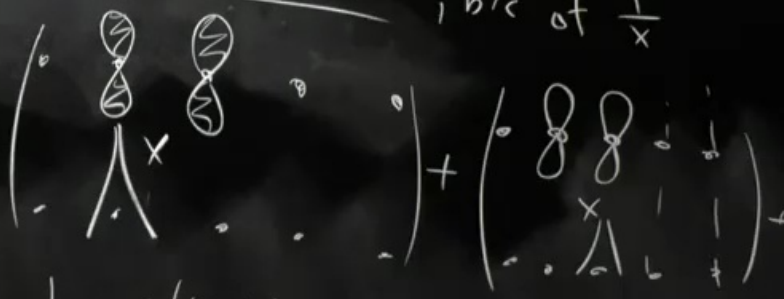
Thus it is a consistent approx. to set $\langle \phi_i | \phi_j \rangle = 0$

But $t \neq 0$

$\langle \phi_i | E_n | \phi_j \rangle - A \sum_{l \neq j} \langle \phi_i | \frac{1}{|x - lR|} | \phi_j \rangle$

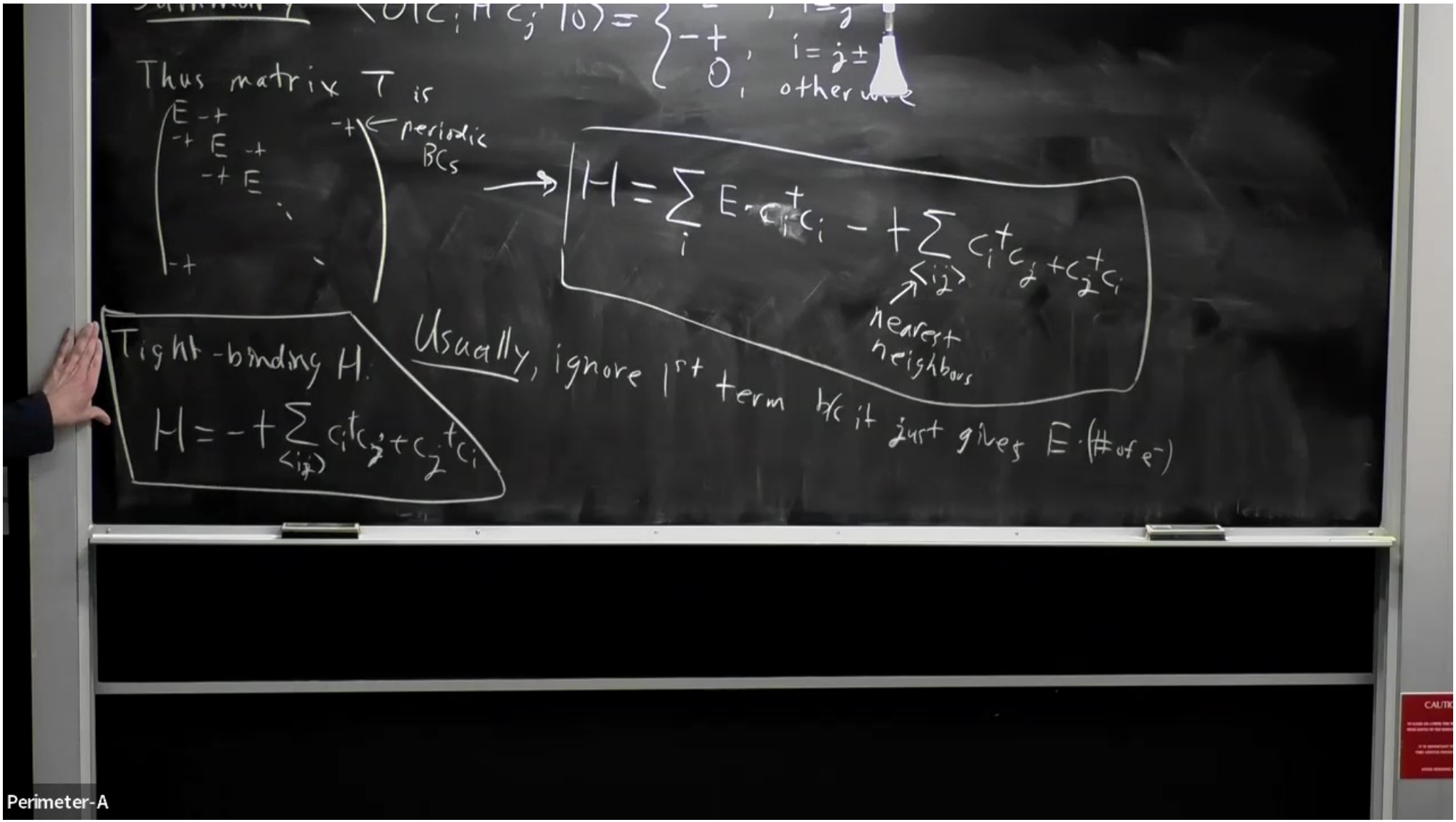
$= 0$ $\qquad$ compare with $\langle \phi_i | \phi_j \rangle$

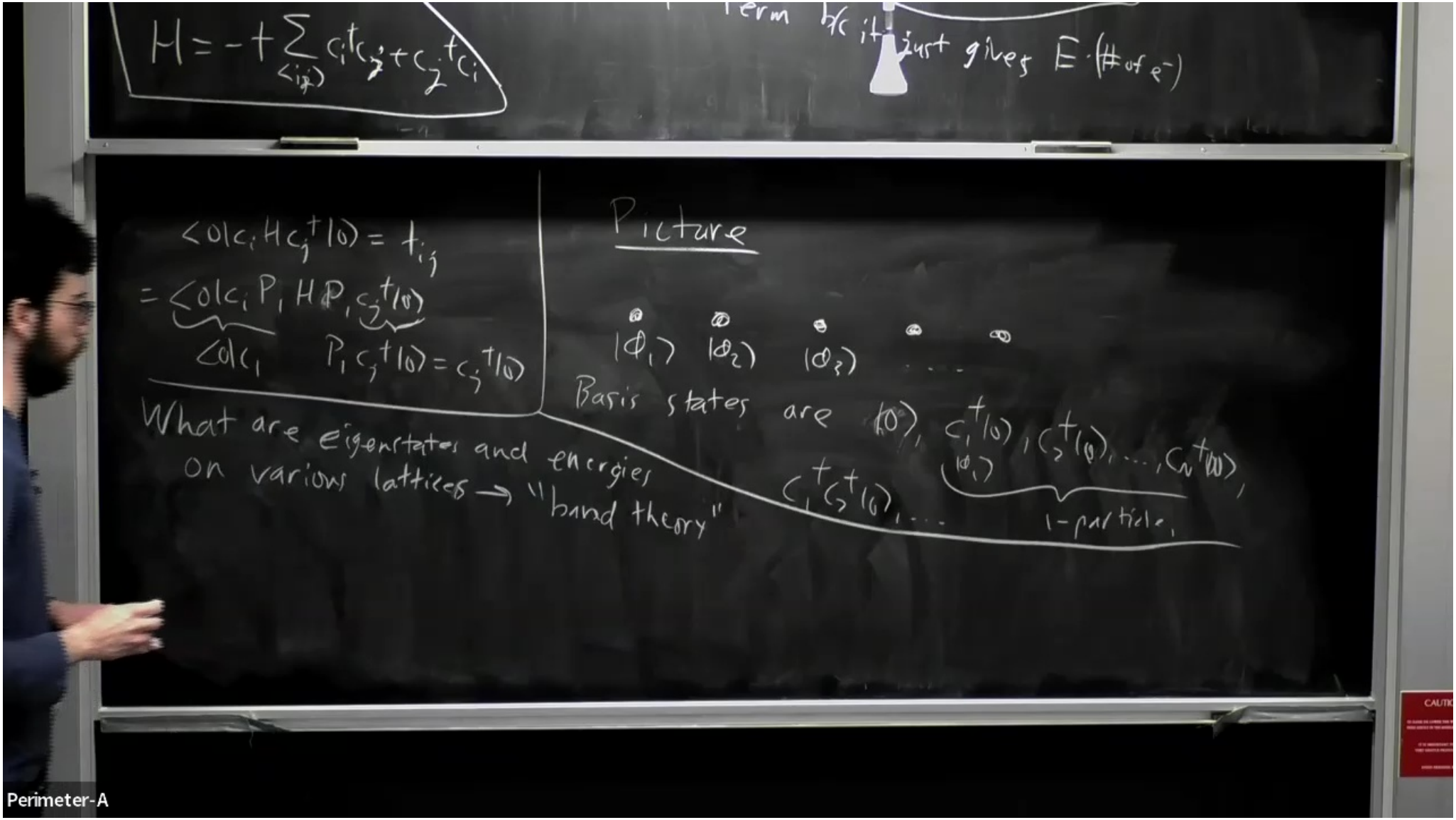
It will be larger, b/c of $\frac{1}{x}$



$t \equiv A\left(\langle \phi_i | \frac{1}{|x - iR|} | \phi_{i+1} \rangle + \langle \phi_i | \frac{1}{|x - (i+1)R|} | \phi_{i+1} \rangle \right)$

$\gg \langle \phi_i | \phi_{i+1} \rangle$


Thus matrix T is
periodic BCs
Tight-binding H:
Usually, ignore 1st term b/c it just gives E·(# of e⁻)
nearest neighbors


$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + c_j^\dagger c_i$
term
just gives $E \cdot (\#\text{ of } e^-)$
$\langle 0 | c_i H c_j^\dagger | 0 \rangle = t_{ij}$
$= \langle 0 | c_i P_1 H P_1 c_j^\dagger | 0 \rangle$
$\langle 0 | c_i \quad P_1 c_j^\dagger | 0 \rangle = c_j^\dagger | 0 \rangle$
Picture
$|\phi_1\rangle$ $|\phi_2\rangle$ $|\phi_3\rangle$ ...
Basis states are $|0\rangle$, $c_1^\dagger|0\rangle$, $c_2^\dagger|0\rangle$, ..., $c_N^\dagger|0\rangle$,
$|\phi_i\rangle$
1-particle
$c_1^\dagger c_2^\dagger |0\rangle$, ...
What are eigenstates and energies
on various lattices → "band theory"

$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + c_j^\dagger c_i$

term $\propto c_i^\dagger c_i$ just gives $E \cdot (\#\text{ of } e^-)$

$\langle 0 | c_i \quad P_i c_j^\dagger |0\rangle = c_j^\dagger |0\rangle$

$|\phi_1\rangle \quad |\phi_2\rangle \quad |\phi_3\rangle \quad \ldots$

Basis states are $|0\rangle$, $c_1^\dagger|0\rangle$, $c_2^\dagger|0\rangle, \ldots, c_N^\dagger|0\rangle$, $|\phi_i\rangle$ 1-particle,

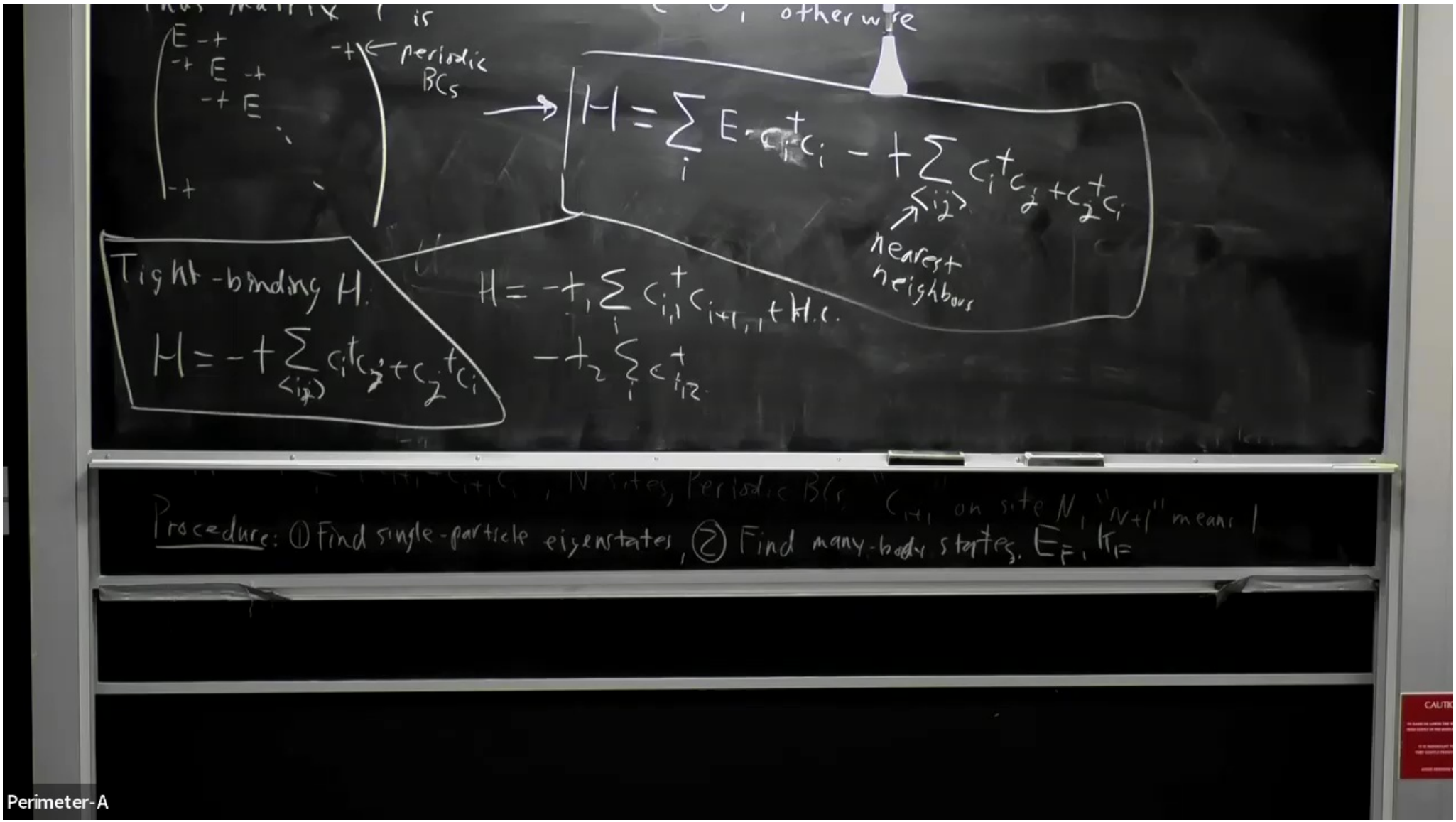
$c_1^\dagger c_2^\dagger |0\rangle, \ldots$

What are eigenstates and energies on various lattices → "band theory"

First example: 1D chain

$H = -t \sum_i c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i$, N sites, Periodic BCs; "c_{i+1}" on site N, "$N+1$" means 1

Procedure: ① Find single-particle eigenstates, ② Find many-body states. E_F, $T =$


periodic BCs
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Tight-binding H.
Procedure: ① Find single-particle eigenstates, ② Find many-body states.