

Title: PSI Lecture - Condensed Matter - Lecture 7

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Collection: PSI Lecture - Condensed Matter

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Today | Tight-binding in 2D ; Brillouin zone (postpone 2 sites case to tomorrow)

Finish up some details from 1D:

- Add spin
- Add units

# Today | Tight-binding in 2D ; Brillouin zone ( postpone 2 sites case to tomorrow)

Finish up some details from 1D:

- Add spin
- Add units

Spin:  $H = -t \sum_j c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j$  spinless model  
 $c_j^\dagger |0\rangle = |\phi_j\rangle$

Define  $c_{js}^\dagger |0\rangle = |\phi_j\rangle |s\rangle$   $|s\rangle = |\uparrow\rangle$  or  $|\downarrow\rangle$

Recall + came from a matrix elt,  $\langle \phi_j | \overset{H}{\text{single-particle}} | \phi_{j+1} \rangle$   
 $\therefore H = -t \sum_{js} c_{js}^\dagger c_{j+1,s} + c_{j+1,s}^\dagger c_{js}$   $\Rightarrow$  matrix elt. diagonal in spin

2 copies of what we had before,  
 1 for spin  $\uparrow$ , one for  $\downarrow$   
 Solution is the same, but can fill each  $k$  orbital twice

Finish up some details from 1D:

- Add spin
- Add units

Units To solve, we found translation eigenstates

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikj} c_j^\dagger$$

$$c_k^\dagger |0\rangle$$

$$H = \sum_k -2t \cos(k) c_k^\dagger c_k$$

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

Spin:  $H = -t \sum_j c_{j+1}^\dagger c_j^\dagger + c_{j+1} c_j$  spinless model

$$c_j^\dagger = |\phi_j\rangle$$

Define  $c_{js}^\dagger |0\rangle = |\phi_j\rangle |s\rangle$   $|s\rangle = |\uparrow\rangle$  or  $|\downarrow\rangle$

Recall + came from a matrix elt,  $\langle \phi_j | \text{single-particle } H | \phi_{j+1} \rangle$

$$\therefore H = -t \sum_{j,s} c_{j+1,s}^\dagger c_{j,s}^\dagger + c_{j+1,s} c_{j,s}$$

$\Rightarrow$  matrix elt diagonal in spin

2 copies of what we had before,

1 for spin  $\uparrow$ , one for  $\downarrow$   
Solution is the same, but can fill each  $k$  orbital twice

$$H = \sum_k -2 + \cos(k) c_k^\dagger c_k$$

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

< copies of what we had before,  
 1 for  $\uparrow$ , one for  $\downarrow$   
 Solution is the same, but can fill each  $k$  orbital twice

Want to think of this as a Fourier transform.  
 - nice if  $j$  has units of length,  $k$  if  $\frac{1}{\text{length}}$ .  
 Put in the lattice spacing:

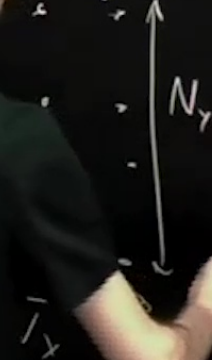
$\cdot \xleftrightarrow{a} \cdot \quad X = a \cdot j$

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_j \underbrace{e^{ikaj}}_{e^{ikx}} c_j^\dagger$$

$$H = \sum_k -2 + \cos(ka) c_k^\dagger c_k$$

In  
 ① Sim

2: Square lattice.



$$H = \sum_k -2t \cos(ka) c_k^\dagger c_k$$

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

< copies of what we had before,  
 1 for  $\uparrow$ , one for  $\downarrow$   
 Solution is the same, but can fill each  $k$  orbital twice

the lattice spacing

$$x = a \cdot j$$

$$k = \frac{2\pi}{Na} n$$

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikaj} c_k$$

$$e^{ikx}$$

$$H = \sum_k -2t \cos(ka) c_k^\dagger c_k$$

Simplest case: square lattice.

$c_{j,l}^\dagger |0\rangle = |0\rangle$   
 filled orbital at  $x=a_j$   
 $y=a_l$

$N_x$   $N_y$   $N = N_x \cdot N_y$   
 Periodic boundaries in  $x$  and  $y$

$$H = -t \sum_{j,l} \left( c_{j,l}^\dagger c_{j+1,l} + c_{j+1,l}^\dagger c_{j,l} + c_{j,l}^\dagger c_{j,l+1} + c_{j,l+1}^\dagger c_{j,l} \right)$$

Solve as in 1D

$$\hat{T}_x = \sum_{j \in \mathbb{Z}} c_{j+1, \uparrow}^\dagger c_{j, \uparrow}, \quad \hat{T}_y = \sum_{j \in \mathbb{Z}} c_{j, \uparrow}^\dagger c_{j+1, \downarrow}$$

↑ hops  $e^-$  left      ↑ hops  $e^-$  down

$$H = -t (\hat{T}_x + \hat{T}_x^\dagger + \hat{T}_y + \hat{T}_y^\dagger)$$

$$[T_x, T_x^\dagger] = 0, [T_x, T_y] = 0, \dots$$

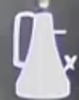
$\Rightarrow H, T_x, T_y$  can be simultaneously diagonalized.

look for eig states of  $T_x, T_y$

$$|c_{k_x, k_y} \rangle = \sum_{j \in \mathbb{Z}} a_{j \in \mathbb{Z}} c_{j \in \mathbb{Z}}^\dagger |0 \rangle$$

hops  $e^-$  left

hops  $e^-$  down



$$[T_x, T_x^\dagger] = 0, [T_x, T_y] = 0, \dots$$

$\Rightarrow H, T_x, T_y$  can be simultaneously diagonalized.

Look for eig states of  $T_x, T_y$

$$c_{k_x, k_y}^\dagger = \sum_{j \in \mathbb{Z}} a_{j \in \mathbb{Z}} c_{j \in \mathbb{Z}}^\dagger |0\rangle \quad \left\{ \begin{array}{l} T_x c_{k_x, k_y}^\dagger |0\rangle = \lambda \sum_{j \in \mathbb{Z}} a_{j \in \mathbb{Z}} c_{j \in \mathbb{Z}}^\dagger |0\rangle \\ = \sum_{j \in \mathbb{Z}} a_{j+1, \in \mathbb{Z}} c_{j \in \mathbb{Z}}^\dagger |0\rangle \Rightarrow a_{j+1, \in \mathbb{Z}} = \lambda a_{j \in \mathbb{Z}} \end{array} \right.$$

$$k_x = 2\pi \frac{n_x}{N_x a}, \quad T_x \text{ eig. val is } e^{ik_x a}$$

Can do the same for  $y$ :  $k_y = 2\pi \frac{n_y}{N_y a}$ , eig val  $e^{ik_y a}$

$$\lambda = e^{i \frac{2\pi}{N_x} n_x}$$

$$a_{0 \in \mathbb{Z}} - a_{N_x \in \mathbb{Z}} = \lambda_{N_x} a_{0 \in \mathbb{Z}} \Rightarrow \lambda_{N_x} = 1$$

$$n_x = 0, 1, \dots, N_x - 1$$

$$\begin{aligned}
 & \sum_{j,l} a_{j,l} c_{j,l} |0\rangle \} \quad |x\rangle_{k_x, k_y} = \lambda \sum_{j,l} a_{j,l} c_{j,l} |0\rangle \\
 & k_x = 2\pi \frac{n_x}{N_x a}, \quad T_x \text{ eig. val is } e^{ik_x a} = \sum_{j,l} a_{j+1,l} c_{j,l} |0\rangle \Rightarrow a_{j+1,l} = \lambda a_{j,l} \\
 & \text{Can do the same for } y: k_y = 2\pi \frac{n_y}{N_y a}, \text{ eig. val } e^{ik_y a} \quad \lambda = e^{i \frac{2\pi}{N_x} n_x} \quad a_{0l} - a_{N_x l} = \lambda_{N_x} a_{0l} \Rightarrow \boxed{\lambda_{N_x} = 1} \\
 & \quad n_x = 0, 1, \dots, N_x - 1
 \end{aligned}$$

Get state from  $a_{j+1,l} = \lambda_x a_{j,l}$ ,  $a_{j,l+1} = \lambda_y a_{j,l}$

$$\Rightarrow \boxed{c_{k_x, k_y}^+ = \frac{1}{\sqrt{N_x N_y}} \sum_{j,l} e^{i(k_x a j + k_y a l)} c_{j,l}^+}$$

To get this basis, substitute

$$c_{j,l}^+ \rightarrow \sum e^{-i(k_x a j + k_y a l)} c_{k_x, k_y}^+$$

$$c_{jl}^{\dagger} = \frac{1}{\sqrt{N_x N_y}} \sum_{k_x, k_y} e^{-i(k_x x_j + k_y y_l)} c_{k_x k_y}^{\dagger}$$

Perimeter-A

$$H = -t \sum_{j,l} \frac{1}{N_x N_y} \left( \sum_{k_x, k_y} e^{-i(k_x a(j+1) + k_y a l)} c_{k_x, k_y} \right) \left( \sum_{k'_x, k'_y} e^{i(k'_x a j + k'_y a l)} c_{k'_x, k'_y} \right) + [3 \text{ more}]$$

goal is to

we need

terms of  $k_x, k_y, k'_x, k'_y$ , so  
 $j, l$  dependence to the inside, get rid of it

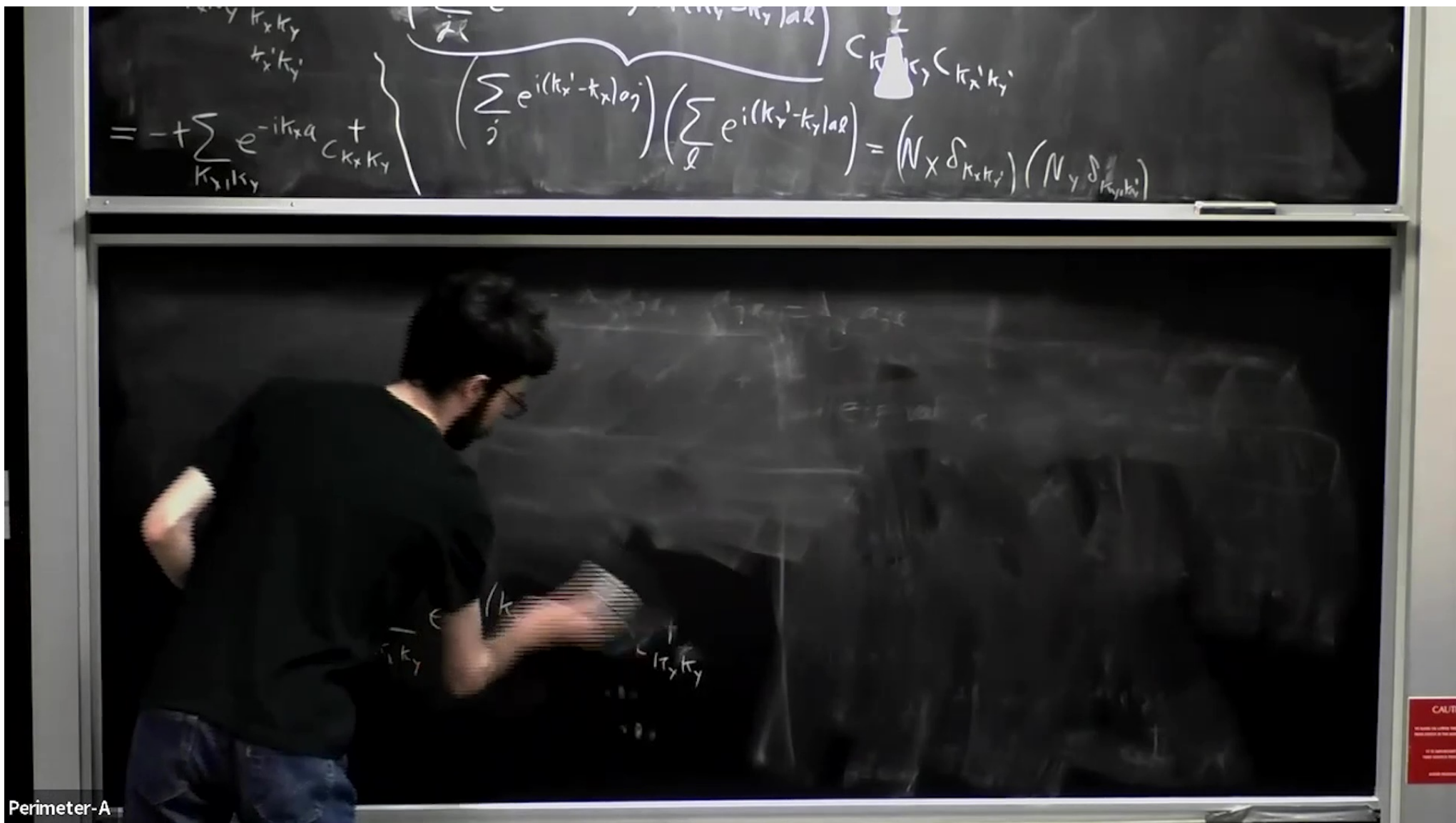
$$H = -t \frac{a}{N} \sum_{j,l}$$

$$j,l \left( \frac{1}{k_x k_y} \right) + \left( \sum_{k'_x, k'_y} e^{i(k'_x - k_x)a} \right) \left( \sum_{l} e^{i(k'_y - k_y)al} \right) c_{j,l} + [3 \text{ more}]$$

goal is to write in terms of  $k_x, k_y, k'_x, k'_y$ , so  
we move all  $j, l$  dependence to the inside, get rid of it

$$H = -\frac{t}{N_x N_y} \sum_{\substack{k_x, k_y \\ k'_x, k'_y}} e^{-ik_x a} \left( \sum_{j,l} e^{i(k'_x - k_x)a j + i(k'_y - k_y)al} \right) c_{j,l} + c_{k_x, k_y} c_{k'_x, k'_y}$$

$$\left( \sum_j e^{i(k'_x - k_x)a j} \right) \left( \sum_l e^{i(k'_y - k_y)al} \right) = (N_x \delta_{k_x, k'_x}) (N_y \delta_{k_y, k'_y})$$



$$= -t \sum_{k_x, k_y} e^{-ik_x a} + \left( \sum_j e^{i(k_x' - k_x) a j} \right) \left( \sum_l e^{i(k_y' - k_y) a l} \right) c_{k_x, k_y} c_{k_x', k_y'}$$

$$= (N_x \delta_{k_x, k_x'}) (N_y \delta_{k_y, k_y'})$$

Include all 4 terms:

To see

$$H = -t \sum_{k_x, k_y} \left( \underbrace{e^{-ik_x a} + e^{ik_x a}}_{2 \cos(k_x a)} + \underbrace{e^{-ik_y a} + e^{ik_y a}}_{2 \cos(k_y a)} \right) c_{k_x, k_y} c_{k_x, k_y}$$

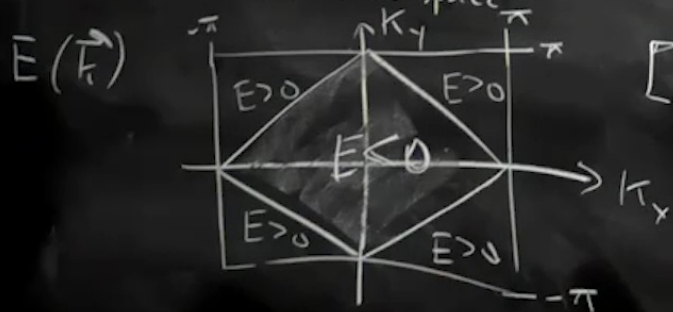
$$E(k_x, k_y) = -2 + (\cos(k_x a) + \cos(k_y a))$$

$$= -t \sum_{k_x, k_y} e^{-ik_x a} + \left( \sum_j e^{i(k'_x - k_x) a} \right) \left( \sum_l e^{i(k'_y - k_y) a} \right) c_{k_x, k_y} c_{k'_x, k'_y}$$

$$= (N_x \delta_{k_x, k'_x}) (N_y \delta_{k_y, k'_y})$$

Include all 4 terms.

To understand this, upgrade  $(k_x, k_y)$  to  $\vec{k}$ , i.e. introduce "momentum space"



$$H = -t \sum_{k_x, k_y} \left( e^{-ik_x a} + e^{ik_x a} + e^{-ik_y a} + e^{ik_y a} \right) c_{k_x, k_y} c_{k_x, k_y}$$

$$2 \cos(k_x a) \quad 2 \cos(k_y a)$$

$$E(k_x, k_y) = -2 + (\cos(k_x a) + \cos(k_y a))$$

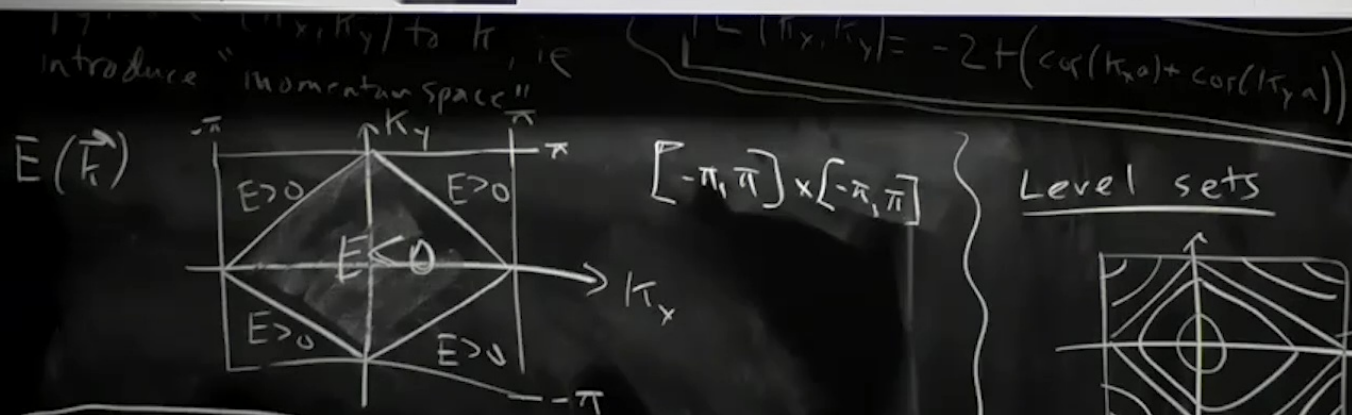
$$[-\pi, \pi] \times [-\pi, \pi]$$

Level sets



depending on # of  $e^-$ , many-body SS is filled up

$$= -t \sum_{\mathbf{k}_x, \mathbf{k}_y} e^{-i\mathbf{k}_x \mathbf{a}} + \dots \left( \sum_j e^{i(\mathbf{k}_x' - \mathbf{k}_x) a} \right) \left( \sum_l e^{i(\mathbf{k}_y' - \mathbf{k}_y) a} \right) = (N_x \delta_{\mathbf{k}_x \mathbf{k}_x'}) (N_y \delta_{\mathbf{k}_y \mathbf{k}_y'})$$

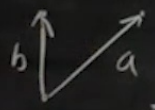


The energy separating filled & unfilled is the Fermi energy,  $E_F$ , and the level set is the Fermi surface

Depending on # of  $e^-$ , many-body GS is filled up to some level set

$$\begin{aligned} \vec{b} &= a(0,1) \\ \vec{a} &= a(1,0) \end{aligned}$$

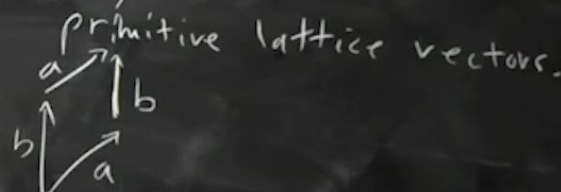
$$H = -t \left( \hat{T}_{\vec{a}} + \hat{T}_{\vec{a}}^\dagger + \hat{T}_{\vec{b}} + \hat{T}_{\vec{b}}^\dagger \right)$$



$T_b, T_{a-b}$

A choice of  $\vec{a}, \vec{b}$  defines a unit cell

Unit cell is

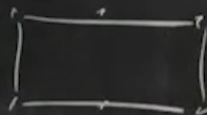


"primitive" if

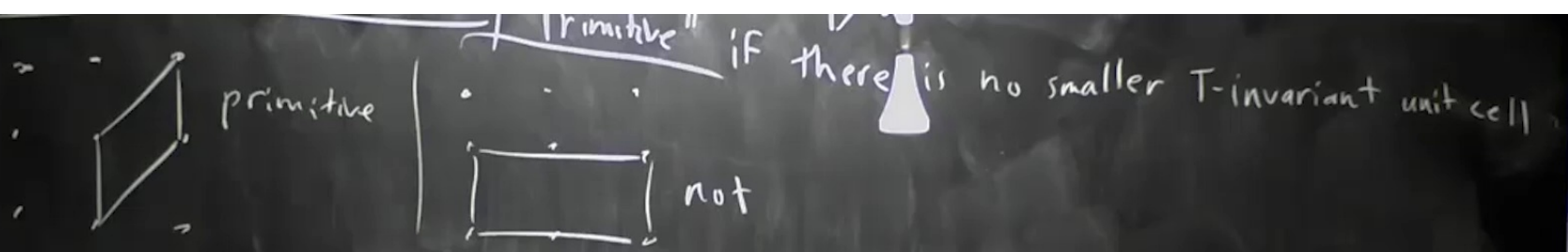
there is no smaller T-invariant unit cell



primitive



not

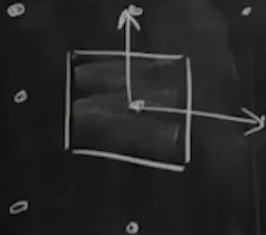


"Best" choice of primitive unit cell (& lattice vectors):

"Wigner-Seitz cell": all pts closer to a given lattice pt than to any other.

Nice because the unit cell has all symmetries of the lattice.

Ex



Lattice vectors are  $\perp$  to WS edges (faces in 3D)