

Title: PSI Lecture - Condensed Matter - Lecture 8

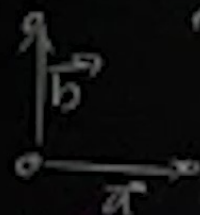
Speakers: Aaron Szasz

Collection: PSI Lecture - Condensed Matter

Date: January 25, 2022 - 11:30 AM

URL: <https://pirsa.org/22010019>

Re-write 2D square lattice



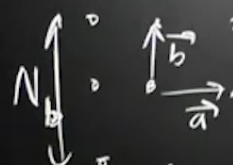
$$\vec{a} = a(1, 0)$$

$$\vec{b} = a(0, 1)$$

$$H = -t \sum_{\vec{r}} \left(C_{\vec{r}+\vec{a}}^\dagger C_{\vec{r}} + C_{\vec{r}}^\dagger C_{\vec{r}+\vec{a}} \right. \\ \left. + C_{\vec{r}+\vec{b}}^\dagger C_{\vec{r}} + C_{\vec{r}}^\dagger C_{\vec{r}+\vec{b}} \right)$$

$$+ C_{\vec{r}+\vec{a}}^\dagger C_{\vec{r}} + C_{\vec{r}}^\dagger C_{\vec{r}+\vec{a}} \\ + C_{\vec{r}+\vec{b}}^\dagger C_{\vec{r}} + C_{\vec{r}}^\dagger C_{\vec{r}+\vec{b}}$$

- HW Deadline: Mon, Jan 31
- Mid-course survey



$$\vec{a} = a(1, 0)$$

$$\vec{b} = a(0, 1)$$

$$c_{\vec{r}}^{\dagger} = \frac{1}{\sqrt{N_a N_b}} \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}} c_{\vec{r}}^{\dagger} \xrightarrow{N_1} c_{\vec{r}}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{k} \cdot \vec{r}} c_{\vec{r}}^{\dagger}$$

Substitute

$$H = -t \sum_{\vec{r}, \vec{r}'} (e^{-i\vec{k} \cdot \vec{a}} + e^{i\vec{k}' \cdot \vec{a}} + e^{-i\vec{k} \cdot \vec{b}} + e^{i\vec{k}' \cdot \vec{b}}) c_{\vec{r}}^{\dagger} c_{\vec{r}'} \left[\frac{1}{N} \sum_{\vec{r}} e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} \right]$$

$$H = -t \sum_{\vec{k}, \vec{k}'} \left(e^{i\vec{k} \cdot \vec{a}} + e^{i\vec{k} \cdot \vec{a}} + e^{-i\vec{k}' \cdot \vec{b}} + e^{i\vec{k}' \cdot \vec{b}} \right) c_{\vec{k}}^{\dagger} c_{\vec{k}'} \left[\frac{1}{N} \sum_{\vec{r}} e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} \right]$$

$$H = -t \sum_{\vec{k}} \left(\sum_{\vec{v}} e^{i\vec{k} \cdot \vec{v}} \right) c_{\vec{k}}^{\dagger} c_{\vec{k}} \quad \{\vec{v}\} \text{ is all primitive lattice vectors,}$$

Nice formulation: manifestly has the symmetry of the lattice. $\vec{a}_1, -\vec{a}_1, \vec{b}_1, -\vec{b}_1$ all vectors to nearest sites



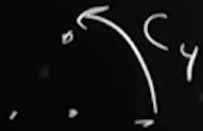
$$\vec{a} \rightarrow \vec{b} \rightarrow -\vec{a} \rightarrow -\vec{b} \rightarrow \vec{a}; \quad H \rightarrow H, \quad E(\vec{k}) \rightarrow E(\vec{\pi})$$

$$E(\vec{k}) = t \left(\cos(\vec{k} \cdot \vec{a}) + \cos(\vec{k} \cdot \vec{b}) \right)$$

$$H = -t \sum_{\vec{k}, \vec{k}'} \left(e^{i\vec{k} \cdot \vec{a}} + e^{i\vec{k} \cdot \vec{b}} + e^{-i\vec{k}' \cdot \vec{a}} + e^{i\vec{k}' \cdot \vec{b}} \right) c_{\vec{k}}^\dagger c_{\vec{k}'} \left[\frac{1}{N} \sum_{\vec{r}} e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} \right]$$

$$H = -t \sum_{\vec{k}} \left(\sum_{\vec{v}} e^{i\vec{k} \cdot \vec{v}} \right) c_{\vec{k}}^\dagger c_{\vec{k}} \quad \{\vec{v}\} \text{ is all primitive lattice vectors,}$$

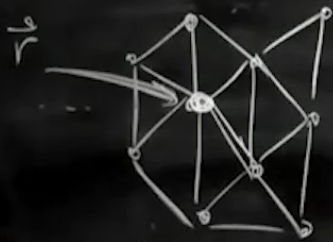
Nice formulation: manifestly has the symmetry of the lattice. $\vec{a}_1, -\vec{a}_1, \vec{b}_1, -\vec{b}_1$ all vectors to nearest sites



$$\vec{a} \rightarrow \vec{b} \rightarrow -\vec{a} \rightarrow -\vec{b} \rightarrow \vec{a}; \quad H \rightarrow H, \quad E(\vec{k}) \rightarrow E(\vec{k})$$

$$E(\vec{k}) = -2t + (t \cos(\vec{k} \cdot \vec{a}) + t \cos(\vec{k} \cdot \vec{b})) \\ = -2t + (t \cos(k_x a) + t \cos(k_y a))$$

Triangular lattice



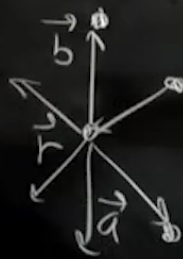
$$H = -t \sum_{\vec{r}} \left(c_{\vec{r}+\vec{a}}^\dagger c_{\vec{r}} + c_{\vec{r}+\vec{b}}^\dagger c_{\vec{r}} + c_{\vec{r}+(\vec{a}+\vec{b})}^\dagger c_{\vec{r}} \right. \\ \left. + c_{\vec{r}}^\dagger c_{\vec{r}+\vec{a}} + c_{\vec{r}}^\dagger c_{\vec{r}+\vec{b}} + c_{\vec{r}}^\dagger c_{\vec{r}+(\vec{a}+\vec{b})} \right)$$

$$= -t \sum_{\vec{r}} (\text{first three same})$$

all hopping

directions:

$\vec{a}, \vec{b}, \vec{a}+\vec{b},$
 $-\vec{a}, -\vec{b}, -\vec{a}-\vec{b}$



$$+ c_{\vec{r}-\vec{a}}^\dagger c_{\vec{r}} + c_{\vec{r}-\vec{b}}^\dagger c_{\vec{r}} + c_{\vec{r}-(\vec{a}+\vec{b})}^\dagger c_{\vec{r}} \\ = -t \sum_{\vec{r}} \sum_{\vec{v}} c_{\vec{r}+\vec{v}}^\dagger c_{\vec{r}}$$



all hopping
directions:
 $\vec{a}, \vec{b}, \vec{a}+\vec{b},$
 $-\vec{a}, -\vec{b}, -\vec{a}-\vec{b}$

$$= -t \sum_{\vec{r}} (\text{first} + \text{rec same})$$

$$+ c_{\vec{r}-\vec{a}}^\dagger (c_{\vec{r}} + c_{\vec{r}-\vec{b}}^\dagger c_{\vec{r}} + c_{\vec{r}-(\vec{a}+\vec{b})}^\dagger c_{\vec{r}})$$

$$= -t \sum_{\vec{r}} \sum_{\vec{v}} c_{\vec{r}+\vec{v}}^\dagger c_{\vec{r}}$$

Substitute:

$$H = -t \sum_{\vec{r}} \sum_{\vec{v}} (e^{i\vec{k} \cdot \vec{v}}) c_{\vec{r}+\vec{v}}^\dagger c_{\vec{r}}$$

$$E(\vec{k}) = -2t (\cos(\vec{k} \cdot \vec{a}) + \cos(\vec{k} \cdot \vec{b}) + \cos(\vec{k} \cdot (\vec{a}+\vec{b})))$$

"Draw" $E(\vec{k})$ in momentum space.
my space

"Draw" $E(\vec{k})$ in momentum space.

What is my space?

square lattice, we had $\vec{k} \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^2$

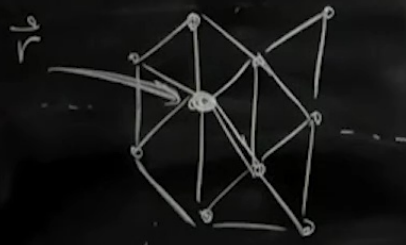
came from eig vals $e^{i\frac{2\pi}{N}n}$, $n=0, \dots, N-1$, $k = \frac{2\pi}{N}n$, $\therefore k \in [0, 2\pi] \sim [-\pi, \pi]$
 in eig vect $a_N = a_0 \lambda^N$ b/c $T^N = \mathbb{1}$

$$E(\vec{k}) = -2 + (\cos(\vec{k} \cdot \vec{a}) + \cos(\vec{k} \cdot \vec{b}) + \cos(\vec{k} \cdot (\vec{a} + \vec{b})))$$

$$\vec{a}, \vec{b}, \vec{a} + \vec{b}, \\ -\vec{a}, -\vec{b}, -\vec{a} - \vec{b}$$

$$e^{i\vec{k}\cdot\vec{r}_n}, n=0, \dots, N-1, \quad \vec{r}_n = \frac{2\vec{a}}{N}n, \quad \therefore \vec{k} \in [0, 2\pi] \sim [-\pi, \pi]$$

Triangular lattice



Trans invariance along $\vec{a}, \vec{b}, \vec{a}+\vec{b}$

Periodic BCs?

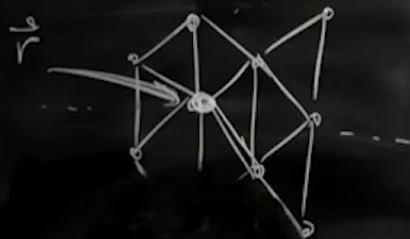
$$T_{\vec{a}}^N = \mathbb{1}$$

$$T_{\vec{b}}^N = \mathbb{1}$$

Action on eig state.

$$\psi = \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} c_{\vec{r}}$$

Triangular lattice



Trans invariance along $\vec{a}$, $\vec{b}$, $\vec{a} + \vec{b}$

Periodic BCs?

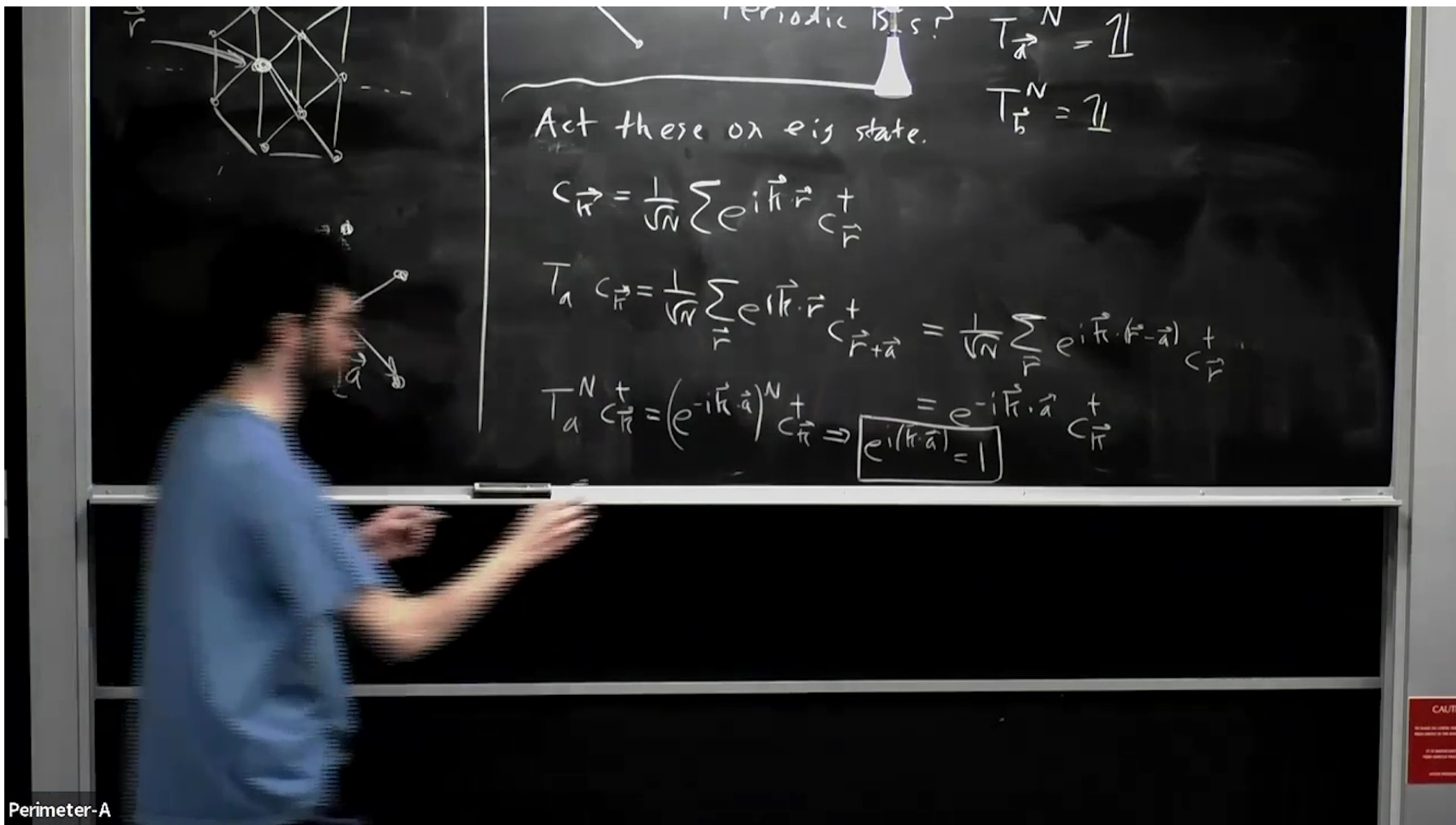
$$T_{\vec{a}}^N = \mathbb{1}$$

$$T_{\vec{b}}^N = \mathbb{1}$$

Act these on eig state.

$$c_{\vec{r}} = \frac{1}{\sqrt{N}} \sum e^{i\vec{k} \cdot \vec{r}} c_{\vec{r}}$$

$$T_{\vec{a}}^N c_{\vec{r}} =$$





$$T_a^+ C_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}} C_{\vec{r}} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{k} \cdot (\vec{r} - \vec{a})} C_{\vec{r}}^+ \\ T_a^+ C_{\vec{k}} = (e^{-i\vec{k} \cdot \vec{a}})^{N_a} C_{\vec{k}}^+ = e^{-i\vec{k} \cdot \vec{a}} C_{\vec{k}}^+ \\ \boxed{e^{i(\vec{k} \cdot \vec{a}) N_a} = 1}$$

Quantization condition: $\vec{k} \cdot \vec{a} = \frac{2\pi}{N_a} n_a, n_a = 0, 1, \dots, N_a - 1$

Find these $\vec{k}$?

$$\vec{k} \cdot \vec{b} = \frac{2\pi}{N_b} n_b, n_b = 0, \dots, N_b - 1$$

Easiest way is to define "reciprocal lattice vectors"

$$\vec{k}_a \cdot \vec{a} = 2\pi, \vec{k}_a \cdot \vec{b} = 0$$

$$\vec{k}_b \cdot \vec{b} = 2\pi, \vec{k}_b \cdot \vec{a} = 0$$

In that case, let $\vec{k} = \frac{n_a}{N_a} \vec{k}_a + \frac{n_b}{N_b} \vec{k}_b$,
and it will automatically
satisfy $\otimes$



$$\psi(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \psi_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k} \cdot (\vec{r} - \vec{a})} \psi_{\vec{k}}$$

$$T_a \psi_{\vec{k}} = (e^{-i\vec{k} \cdot \vec{a}})^{N_a} \psi_{\vec{k}} = e^{-i\vec{k} \cdot \vec{a}} \psi_{\vec{k}}$$

$$e^{i(\vec{k} \cdot \vec{a}) N_a} = 1$$

Quantization condition: $\vec{k} \cdot \vec{a} = \frac{2\pi}{N_a} n_a, n_a = 0, 1, \dots, N_a - 1$

Find these $\vec{k}$?

$$\vec{k} \cdot \vec{b} = \frac{2\pi}{N_b} n_b, n_b = 0, \dots, N_b - 1$$

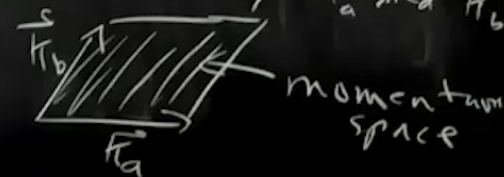
Easiest way is to define "reciprocal lattice vectors"

$$\vec{k}_a \cdot \vec{a} = 2\pi, \vec{k}_a \cdot \vec{b} = 0$$

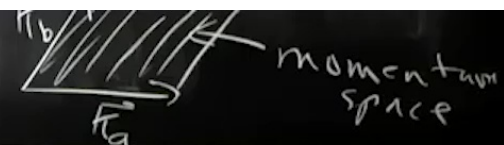
$$\vec{k}_b \cdot \vec{b} = 2\pi, \vec{k}_b \cdot \vec{a} = 0$$

In that case, let $\vec{k} = \frac{n_a}{N_a} \vec{k}_a + \frac{n_b}{N_b} \vec{k}_b$,
and it will automatically satisfy *

The space of allowed $\vec{k}$ is the //ogram bounded by $\vec{k}_a$ and $\vec{k}_b$



and it will automatically satisfy (*)



Triangular lattice

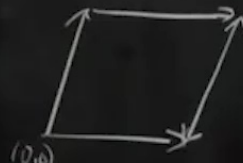


For triangular lattice:

$$\vec{a} = a \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right) \quad \vec{b} = a(0, 1)$$

$$\vec{k}_a = \frac{4\pi}{\sqrt{3}a} (1, 0), \quad \vec{k}_b = \frac{4\pi}{\sqrt{3}a} \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right)$$

→ Momentum space

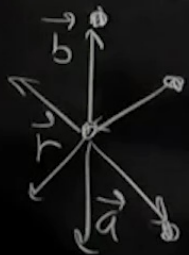
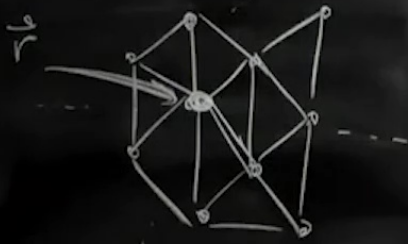


$$\leftarrow \text{area} \left(\frac{4\pi}{\sqrt{3}a} \right)^2 \sin\left(\frac{\pi}{3}\right)$$

$$\frac{16\pi^2}{3a^2} \cdot \frac{\sqrt{3}}{2} = \frac{8\pi^2}{\sqrt{3}a^2}$$

cf area of $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^2 = \frac{4\pi^2}{a^2}$
important: if we naively let $k_x \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ & $k_y \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ then we miss part of momentum space

Triangular lattice



For Hexagonal lattice:

$$\vec{a} = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \quad \vec{b} = a(0, 1)$$

$$\vec{k}_a = \frac{4\pi}{\sqrt{3}a}(1, 0), \quad \vec{k}_b = \frac{4\pi}{a}(0, 1)$$

→
Momentum space



$$\text{cf area of } \left[-\frac{\pi}{a}, \frac{\pi}{a}\right] \times \left[-\frac{\pi}{a}, \frac{\pi}{a}\right] = \frac{4\pi^2}{a^2}$$

important: if we naively let $k_x \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ & $k_y \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ then we miss part of momentum space

Problem: $E(\vec{k})$ has all lattice sym. but $\square$ does not

Solution?

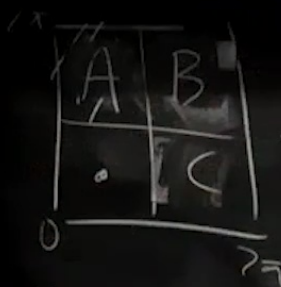
$$\sin\left(\frac{\pi}{3}\right)$$

$$\frac{\pi^2}{a^2}$$

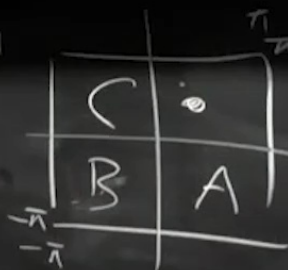


$$\frac{16\pi^2}{3a^2} \cdot \frac{\sqrt{3}}{2} = \frac{8\pi^2}{\sqrt{3}a^2}$$

Solution? Use square lattice as an analogy



Symmetrical

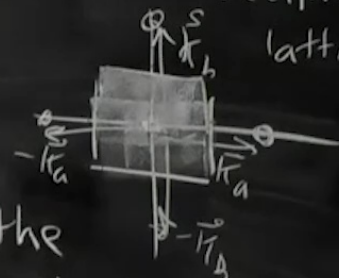


In our new language,

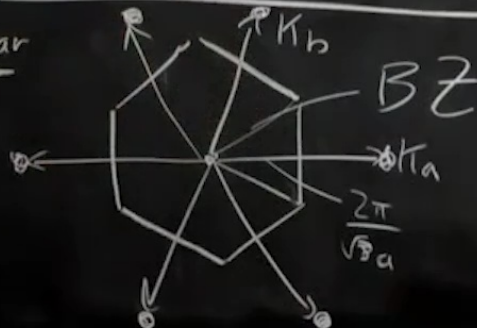
$$\vec{F}_a = \frac{2\pi}{a}(1,0)$$

$$\vec{F}_b = \frac{2\pi}{a}(0,1)$$

"reciprocal lattice"



Triangular



Claim

given 2π periodicity in

$\vec{K} \cdot \vec{a}$ and $\vec{K} \cdot \vec{b}$ equivalent to $1/\text{volume}$

"Brillouin zone" is the Wigner-Seitz cell of the recip. latt.

Quick check:

$$\frac{6 \cdot 4\pi^2}{3\sqrt{3}a^2} = \frac{8\pi^2}{\sqrt{3}a}$$

