Title: PSI 2018/2019 - Condensed Matter - Lecture 4

Date: Nov 15, 2018 10:45 AM

URL: http://pirsa.org/18110022

Abstract:

Klein Gordon | (k) Kallen-Lehmann | SAM | 9) Causality

$$e^{i\bar{G}\cdot\bar{R}} = 1$$

$$f(r) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\bar{k}\cdot\bar{r}}\, f(\bar{k})$$

$e^{ik_x x}$ period $\frac{2\pi}{k_x}$

$e^{i\bar{G}\cdot\bar{r}}$ to have same periodicity as that of the Lattice

$$e^{i\bar{G}\cdot(\bar{r}+\bar{R})} = e^{i\bar{G}\cdot\bar{r}}$$

$$\Rightarrow \boxed{e^{iG\cdot R} = 1}$$

Tight binding Model

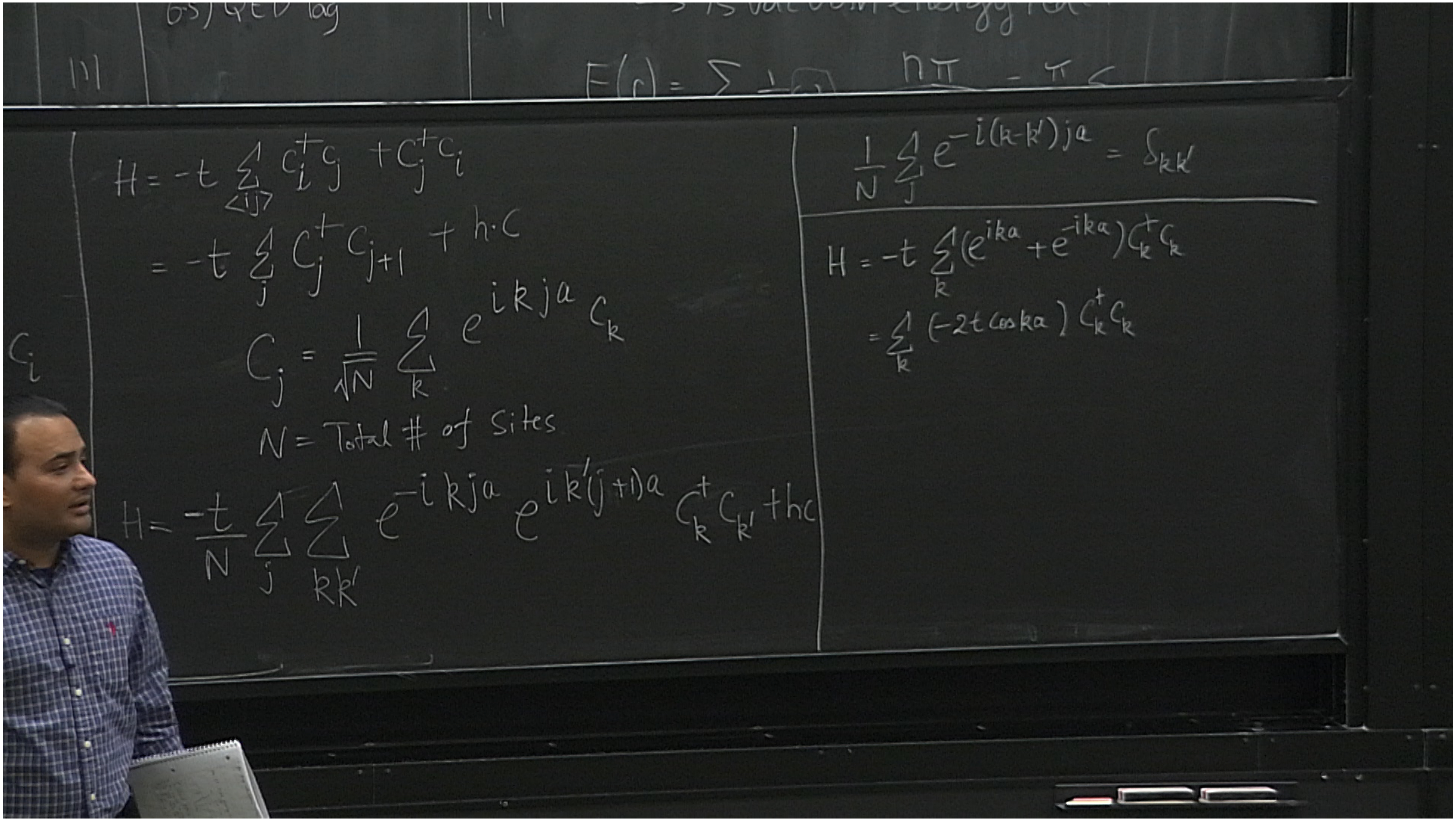
1D Lattice

$$H = -\sum_{ij}\left(t_{ij}\, c_i^\dagger c_j + t_{ji}\, c_j^\dagger c_i\right) + \sum_i V_i\, c_i^\dagger c_i$$

V_i = Constant

$H = H^\dagger \Rightarrow t_{ij} = t_{ji}^*$ & V_i = Constant = Real = V

$$\sum_i V_i c_i^\dagger c_i = V \sum_i c_i^\dagger c_i = V N_e$$


QED lag
$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + c_j^\dagger c_i$
$= -t \sum_j c_j^\dagger c_{j+1} + h.c$
$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikja} c_k$
N = Total # of Sites
$H = \frac{-t}{N} \sum_j \sum_{kk'} e^{-ikja} e^{ik'(j+1)a} c_k^\dagger c_{k'} + hc$
$\frac{1}{N} \sum_j e^{-i(k-k')ja} = \delta_{kk'}$
$H = -t \sum_k (e^{ika} + e^{-ika}) c_k^\dagger c_k$
$= \sum_k (-2t \cos ka) c_k^\dagger c_k$
c_i

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

$$= -t \sum_j c_j^\dagger c_{j+1} + h.c$$

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

N = Total # of Sites

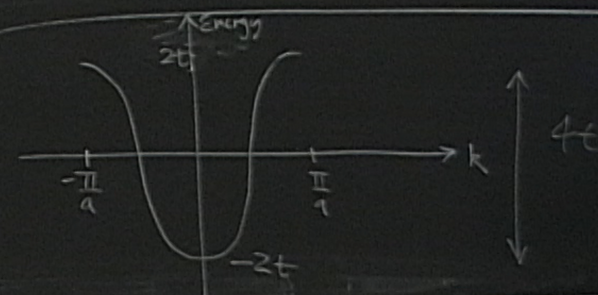
$$H = \frac{-t}{N} \sum_j \sum_{kk'} e^{-ikja} e^{ik'(j+1)a} c_k^\dagger c_{k'} + hc$$

$$\frac{1}{N} \sum_j e^{-i(k-k')ja} = \delta_{kk'}$$

$$H = -t \sum_k (e^{ika} + e^{-ika}) c_k^\dagger c_k$$

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

For free electrons $H = \sum_k \epsilon(k)\, c_k^\dagger c_k$, $\epsilon(k) = \frac{\hbar^2 k^2}{2m}$



$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{p,k}(x) + U(x)\,\psi_{p,k}(x) = E_p(k)\,\psi_{p,k}(x)$$

$k \equiv$ quasimomentum

$p \equiv$ Some additional quantum number

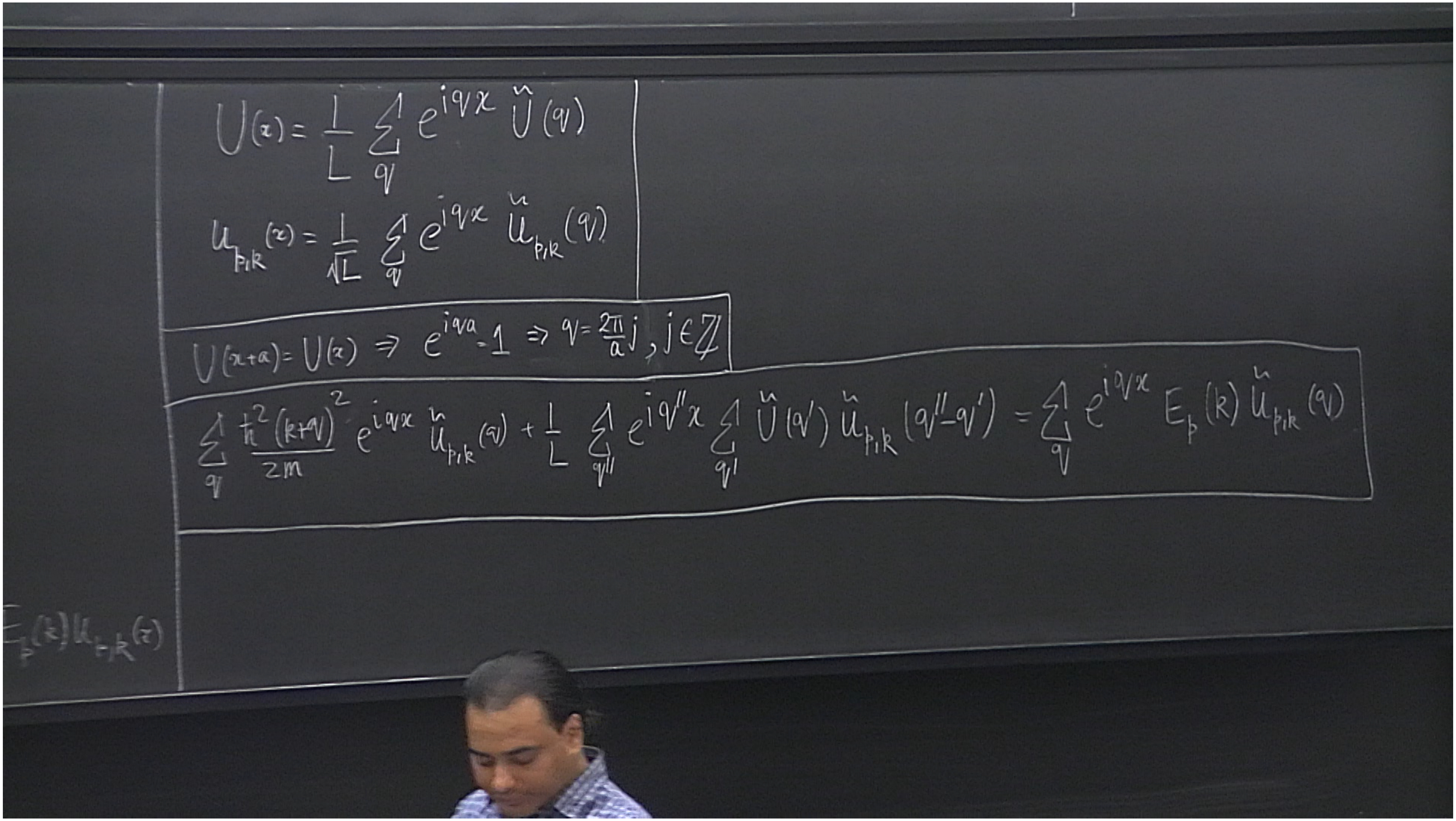
$$U(x+a) = U(x)$$

Bloch's theorem: $\psi_{p,k}(x) = e^{ikx}\,u_{p,k}(x)$

where $u_{p,k}(x) = u_{p,k}(x+a)$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(-k^2 u_{p,k}(x) + 2ik\,u'_{p,k}(x) + u''_{p,k}(x)\right) + U(x)\,u_{p,k}(x) = E_p(k)\,u_{p,k}(x)$$

$$U(x) = \frac{1}{L}\sum_q$$


$U(x) = \frac{1}{L}\sum_q e^{iqx}\hat{U}(q)$
$u_{p,k}(x) = \frac{1}{\sqrt{L}}\sum_q e^{iqx}\hat{u}_{p,k}(q)$
$U(x+a) = U(x) \Rightarrow e^{iqa} = 1 \Rightarrow q = \frac{2\pi}{a}j,\ j \in \mathbb{Z}$
$\sum_q \frac{\hbar^2(k+q)^2}{2m} e^{iqx}\hat{u}_{p,k}(q) + \frac{1}{L}\sum_{q''} e^{iq''x}\sum_{q'}\hat{U}(q')\hat{u}_{p,k}(q''-q') = \sum_q e^{iqx}E_p(k)\hat{u}_{p,k}(q)$
$E_p(k)u_{p,k}(x)$

$$U(x) = \frac{1}{L}\sum_q e^{iqx}\,\hat{U}(q)$$

$$u_{p,k}(x) = \frac{1}{\sqrt{L}}\sum_q e^{iqx}\,\hat{u}_{p,k}(q)$$

$$U(x+a) = U(x) \Rightarrow e^{iqa} = 1 \Rightarrow q = \frac{2\pi}{a}j,\ j \in \mathbb{Z}$$

$$\sum_q \frac{\hbar^2 (k+q)^2}{2m} e^{iqx}\,\hat{u}_{p,k}(q) + \frac{1}{L}\sum_{q''} e^{iq''x} \sum_{q'} \hat{U}(q')\,\hat{u}_{p,k}(q''-q') = \sum_q e^{iqx} E_p(k)\,\hat{u}_{p,k}(q)$$

$$E_p(k)\,u_{p,k}(x)$$

$$\sum_q \left[\frac{\hbar^2 (k+q)^2}{2m}\hat{u}_{p,k}(q) + \frac{1}{L}\sum_{q'} \hat{U}(q')\,\hat{u}_{p,k}(q-q') - E_p(k)\,\hat{u}_{p,k}(q)\right] = 0$$

Unperturbed Solutions, set $U(x)=0$

$$\left(\frac{\hbar^2(k+q)^2}{2m} - E_p^{(0)}(k)\right)\tilde{u}^{(0)}_{p,k}(q) = 0$$

$$\Rightarrow \quad E_p^{(0)}(k) = \frac{\hbar^2(k+q)^2}{2m}$$

Unperturbed Solutions, set $U(x)=0$

$$\left(\frac{\hbar^2(k+q)^2}{2m} - E_p^{(0)}(k)\right)\tilde{u}^{(0)}_{p,k}(q) = 0$$

$$\Rightarrow \quad E_p^{(0)}(k) = \frac{\hbar^2(k+q)^2}{2m}$$

Choose: $\tilde{u}^{(0)}_{p,k}(q) = \delta_{p,q}$

$$u^{(0)}_{p,k}(x) = \frac{1}{\sqrt{L}}\sum_q e^{iqx}\,\tilde{u}^{(0)}_{p,k}(q) = \frac{1}{\sqrt{L}}e^{ipx}$$

$$\Rightarrow \psi^{(0)}_{p,k}(x) = \frac{1}{\sqrt{L}}e^{i(k+p)x}$$

$$\psi^{(0)}_{p,k}(x+a) = e^{ika}\,\psi^{(0)}_{p,k}(x)$$

$$\Rightarrow \frac{1}{\sqrt{L}}e^{i(k+p)(x+a)} = \frac{1}{\sqrt{L}}e^{ika}\,e^{i(k+p)x}$$

$$\Rightarrow e^{ipa} = 1 \Rightarrow p = \frac{2\pi}{a}n \quad \text{where } n \in \mathbb{Z}$$

Unperturbed Solutions, set $U(x) = 0$

$$\left(\frac{\hbar^2 (k+q)^2}{2m} - E_p^{(0)}(k) \right) \tilde{u}_{p,k}^{(0)}(q) = 0$$

$$\Rightarrow \quad E_p^{(0)}(k) = \frac{\hbar^2 (k+q)^2}{2m}$$

Choose: $\tilde{u}_{p,k}^{(0)}(q) = \delta_{p,q}$

$$u_{p,k}^{(0)}(x) = \frac{1}{\sqrt{L}} \sum_q e^{iqx} \tilde{u}_{p,k}^{(0)}(q) = \frac{1}{\sqrt{L}} e^{ipx}$$

$$\Rightarrow \psi_{p,k}^{(0)}(x) = \frac{1}{\sqrt{L}} e^{i(k+p)x}$$

$$\psi_{p,k}^{(0)}(x+a) = e^{ika} \psi_{p,k}^{(0)}(x)$$

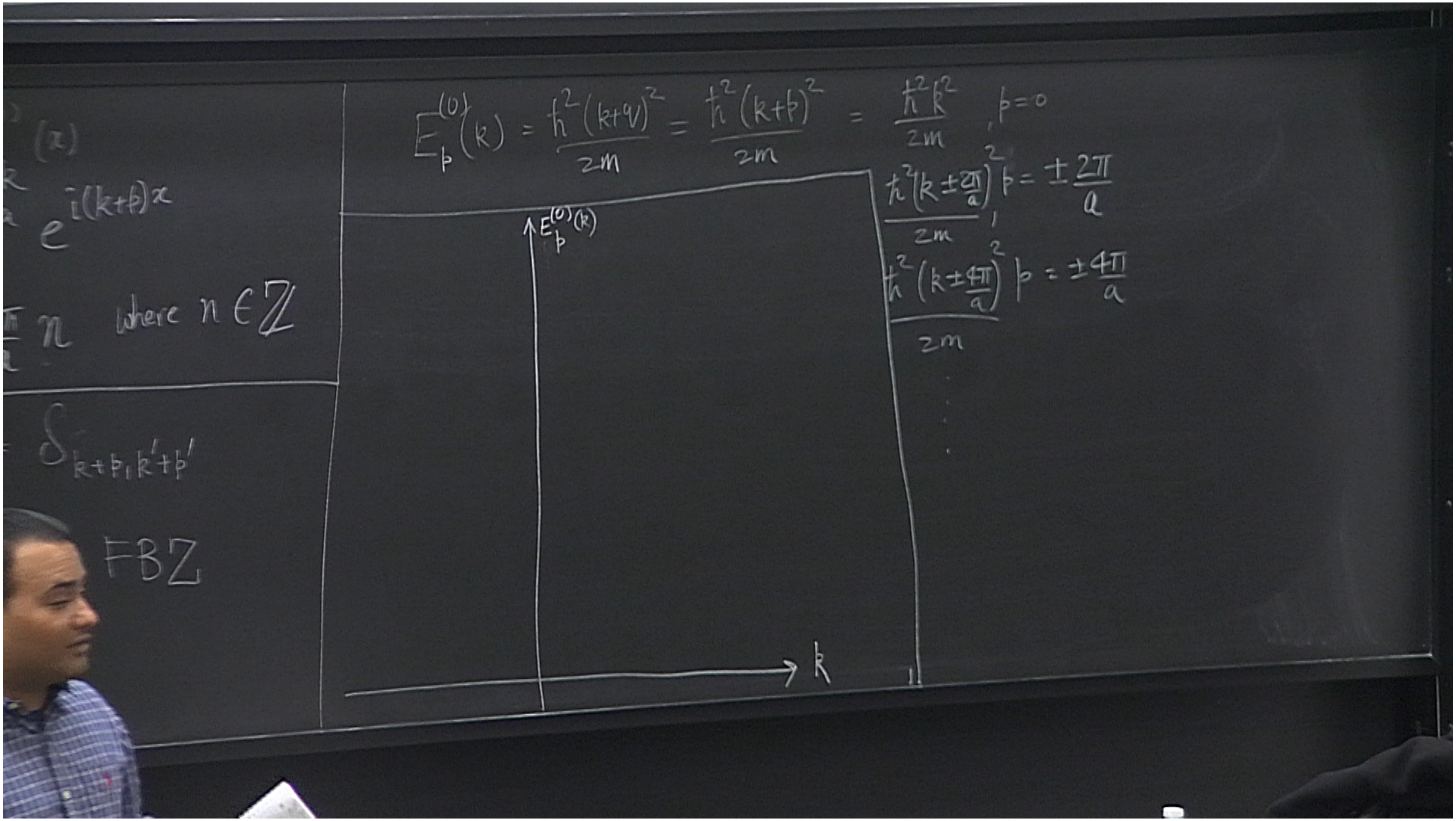
$$\Rightarrow \frac{1}{\sqrt{L}} e^{i(k+p)(x+a)} = \frac{1}{\sqrt{L}} e^{ika} e^{i(k+p)x}$$

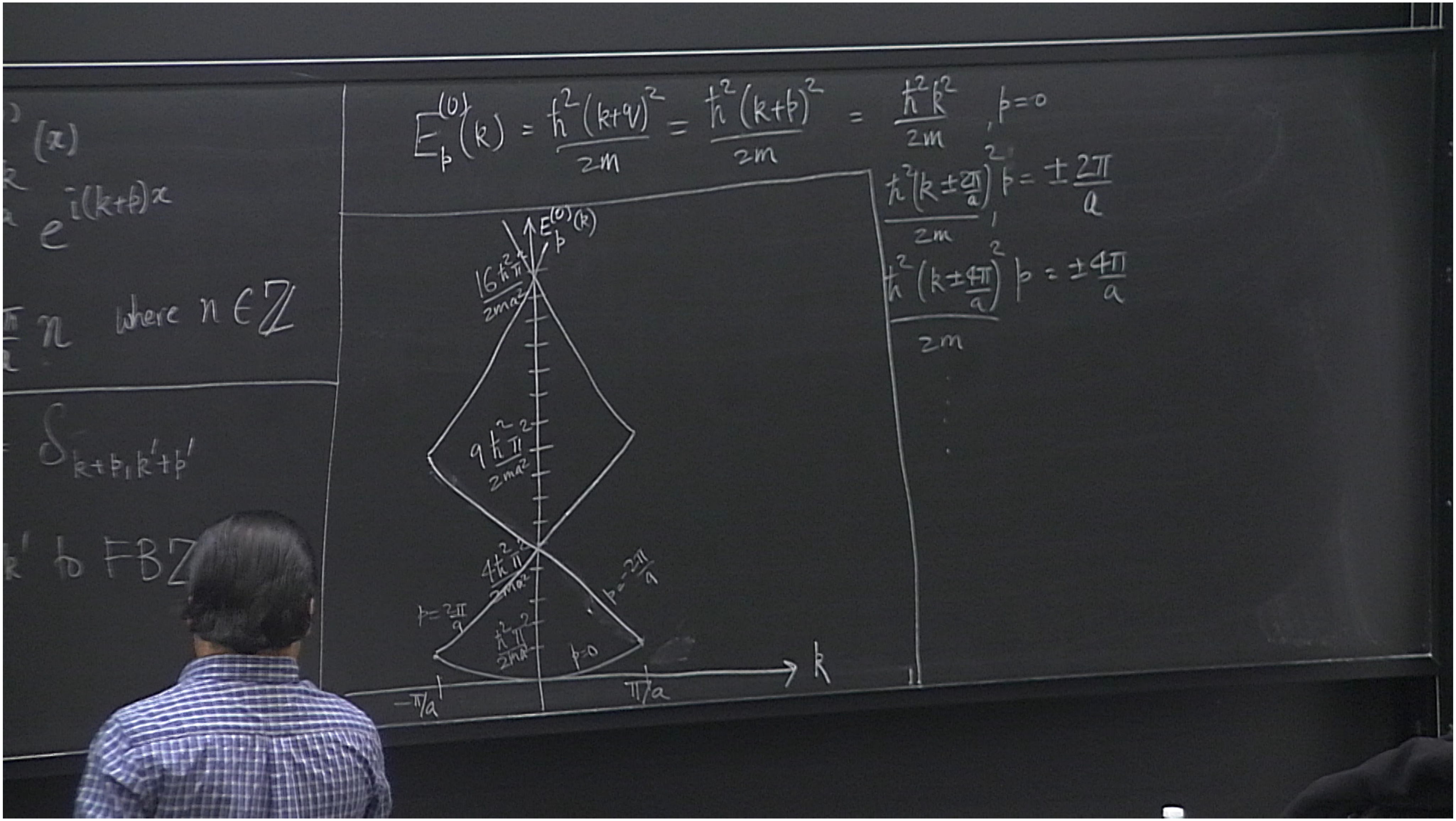
$$\Rightarrow e^{ipa} = 1 \Rightarrow p = \frac{2\pi}{a} n \quad \text{where } n \in \mathbb{Z}$$

$$\int dx\, \psi_{p,k}^{*(0)}(x)\, \psi_{p',k'}^{(0)}(x) = \delta_{k+p,\, k'+p'}$$

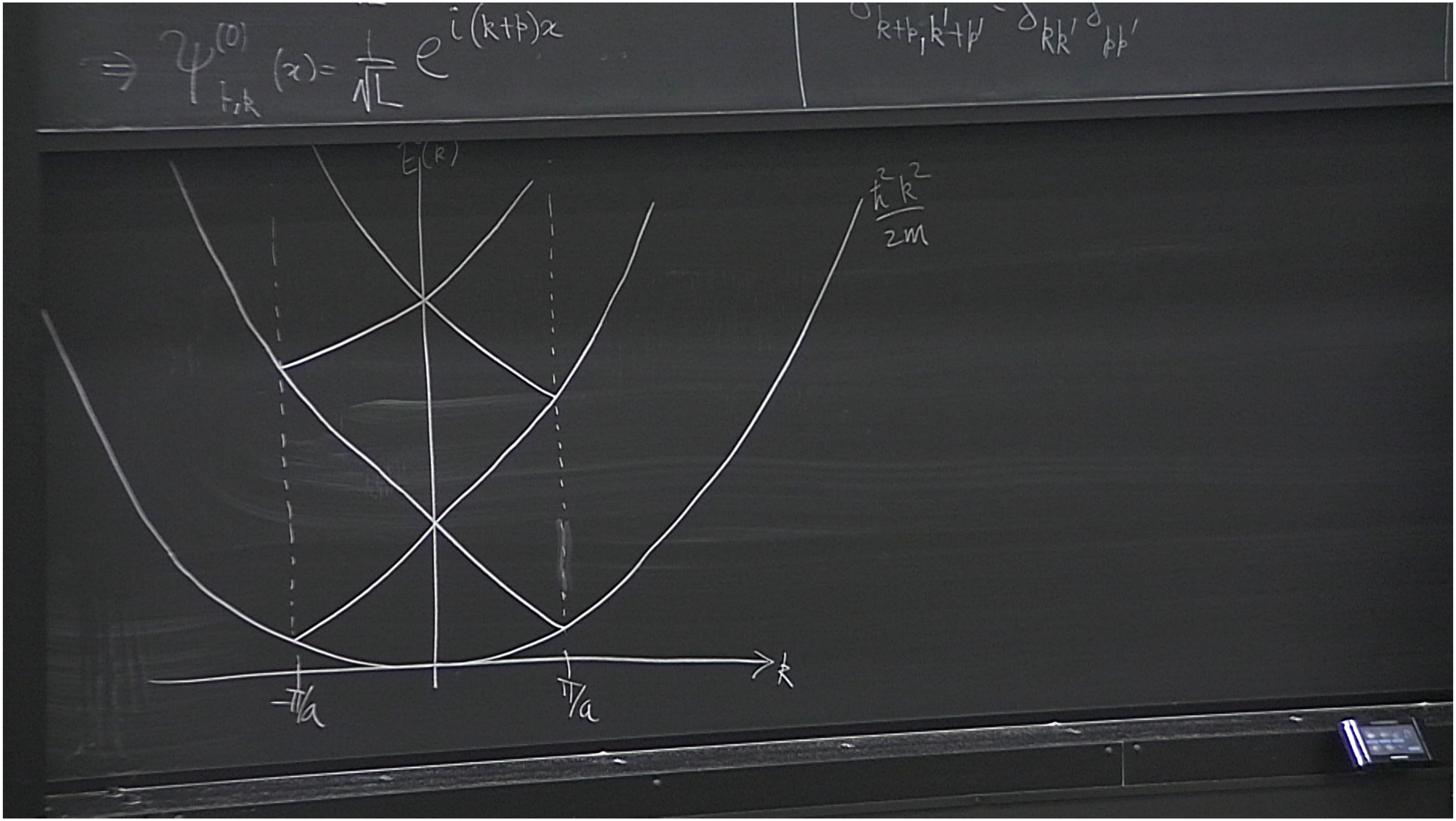
If we restrict k and k' to FBZ

$$\delta_{k+p,\, k'+p'} = \delta_{kk'} \delta_{pp'}$$


$E^{(0)}_p(k) = \frac{\hbar^2(k+q)^2}{2m} = \frac{\hbar^2(k+p)^2}{2m} = \frac{\hbar^2 k^2}{2m}, \; p=0$
$\frac{\hbar^2(k \pm \frac{2\pi}{a})^2}{2m}, \; p = \pm\frac{2\pi}{a}$
$\frac{\hbar^2(k \pm \frac{4\pi}{a})^2}{2m}, \; p = \pm\frac{4\pi}{a}$
$E^{(0)}_p(k)$
k
$e^{-i(k+p)x}$
where $n \in \mathbb{Z}$
$\delta_{k+p, k'+p'}$
FBZ



E_p^(0)(k) = ħ^2(k+q)^2 / 2m = ħ^2(k+p)^2 / 2m = ħ^2k^2 / 2m , p=0
ħ^2(k ± 2π/a)^2 / 2m , p = ± 2π/a
ħ^2(k ± 4π/a)^2 / 2m , p = ± 4π/a
where n ∈ Z
k' to FBZ
16ħ^2π^2 / 2ma^2
9ħ^2π^2 / 2ma^2
4ħ^2π^2 / 2ma^2
ħ^2π^2 / 2ma^2
p = 2π/a
p = -2π/a
p=0
-π/a
π/a
k


$\Rightarrow \psi^{(0)}_{p,k}(x) = \frac{1}{\sqrt{L}} e^{i(k+p)x}$
$\delta_{k+p,k'+p'} = \delta_{kk'}\delta_{pp'}$
$E(k)$
$\frac{\hbar^2 k^2}{2m}$
k
$-\pi/a$
π/a