

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

Date: Nov 15, 2018 10:45 AM

URL: <http://pirsa.org/18110022>

Abstract:

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

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

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

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

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

$$\Rightarrow \boxed{e^{i\vec{G}\cdot\vec{R}} = 1}$$

Tight binding Model

1D Lattice

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

$$V_i = \text{Constant}$$

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

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

65) QED lag

$$E(\omega) = \sum_{-\pi}^{\pi} \frac{1}{\omega} \dots$$

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

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

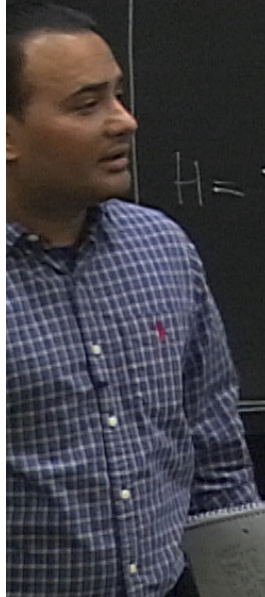
$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikja} c_k$$

N = Total # of sites

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

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

$$H = -t \sum_k (e^{ika} + e^{-ika}) c_k^\dagger c_k = \sum_k (-2t \cos ka) c_k^\dagger c_k$$



65) QED lag

$$E(k) = \sum_{n \in \mathbb{Z}} \frac{1}{|n|} e^{in\pi} - \pi <$$

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

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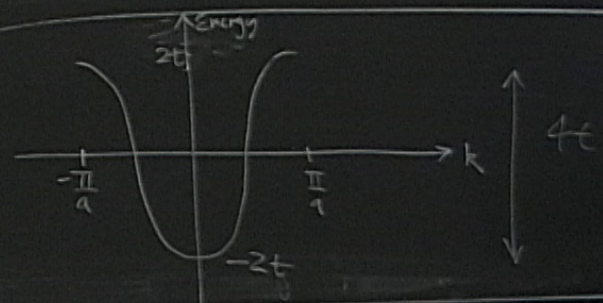
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For free electrons $H = \sum_k E(k) c_k^\dagger c_k$, $E(k) = \frac{\hbar^2 k^2}{2m}$



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

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

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

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

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

$$u_{pik}(x) = \frac{1}{\sqrt{L}} \sum_q e^{iqx} \tilde{u}_{pik}(q)$$

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

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

$$E_p(k) u_{pik}(x)$$



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

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

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

z_m $u_{p,k}$ $u_{p,k}^{(0)}$ $u_{p,k}^{(1)}$ $u_{p,k}^{(2)}$ $u_{p,k}^{(3)}$ $u_{p,k}^{(4)}$ $u_{p,k}^{(5)}$ $u_{p,k}^{(6)}$ $u_{p,k}^{(7)}$ $u_{p,k}^{(8)}$ $u_{p,k}^{(9)}$ $u_{p,k}^{(10)}$ $u_{p,k}^{(11)}$ $u_{p,k}^{(12)}$ $u_{p,k}^{(13)}$ $u_{p,k}^{(14)}$ $u_{p,k}^{(15)}$ $u_{p,k}^{(16)}$ $u_{p,k}^{(17)}$ $u_{p,k}^{(18)}$ $u_{p,k}^{(19)}$ $u_{p,k}^{(20)}$ $u_{p,k}^{(21)}$ $u_{p,k}^{(22)}$ $u_{p,k}^{(23)}$ $u_{p,k}^{(24)}$ $u_{p,k}^{(25)}$ $u_{p,k}^{(26)}$ $u_{p,k}^{(27)}$ $u_{p,k}^{(28)}$ $u_{p,k}^{(29)}$ $u_{p,k}^{(30)}$ $u_{p,k}^{(31)}$ $u_{p,k}^{(32)}$ $u_{p,k}^{(33)}$ $u_{p,k}^{(34)}$ $u_{p,k}^{(35)}$ $u_{p,k}^{(36)}$ $u_{p,k}^{(37)}$ $u_{p,k}^{(38)}$ $u_{p,k}^{(39)}$ $u_{p,k}^{(40)}$ $u_{p,k}^{(41)}$ $u_{p,k}^{(42)}$ $u_{p,k}^{(43)}$ $u_{p,k}^{(44)}$ $u_{p,k}^{(45)}$ $u_{p,k}^{(46)}$ $u_{p,k}^{(47)}$ $u_{p,k}^{(48)}$ $u_{p,k}^{(49)}$ $u_{p,k}^{(50)}$ $u_{p,k}^{(51)}$ $u_{p,k}^{(52)}$ $u_{p,k}^{(53)}$ $u_{p,k}^{(54)}$ $u_{p,k}^{(55)}$ $u_{p,k}^{(56)}$ $u_{p,k}^{(57)}$ $u_{p,k}^{(58)}$ $u_{p,k}^{(59)}$ $u_{p,k}^{(60)}$ $u_{p,k}^{(61)}$ $u_{p,k}^{(62)}$ $u_{p,k}^{(63)}$ $u_{p,k}^{(64)}$ $u_{p,k}^{(65)}$ $u_{p,k}^{(66)}$ $u_{p,k}^{(67)}$ $u_{p,k}^{(68)}$ $u_{p,k}^{(69)}$ $u_{p,k}^{(70)}$ $u_{p,k}^{(71)}$ $u_{p,k}^{(72)}$ $u_{p,k}^{(73)}$ $u_{p,k}^{(74)}$ $u_{p,k}^{(75)}$ $u_{p,k}^{(76)}$ $u_{p,k}^{(77)}$ $u_{p,k}^{(78)}$ $u_{p,k}^{(79)}$ $u_{p,k}^{(80)}$ $u_{p,k}^{(81)}$ $u_{p,k}^{(82)}$ $u_{p,k}^{(83)}$ $u_{p,k}^{(84)}$ $u_{p,k}^{(85)}$ $u_{p,k}^{(86)}$ $u_{p,k}^{(87)}$ $u_{p,k}^{(88)}$ $u_{p,k}^{(89)}$ $u_{p,k}^{(90)}$ $u_{p,k}^{(91)}$ $u_{p,k}^{(92)}$ $u_{p,k}^{(93)}$ $u_{p,k}^{(94)}$ $u_{p,k}^{(95)}$ $u_{p,k}^{(96)}$ $u_{p,k}^{(97)}$ $u_{p,k}^{(98)}$ $u_{p,k}^{(99)}$ $u_{p,k}^{(100)}$

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

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

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

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

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

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

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

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

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

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

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

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

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

If we restrict k and k' to FBZ

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

(x)

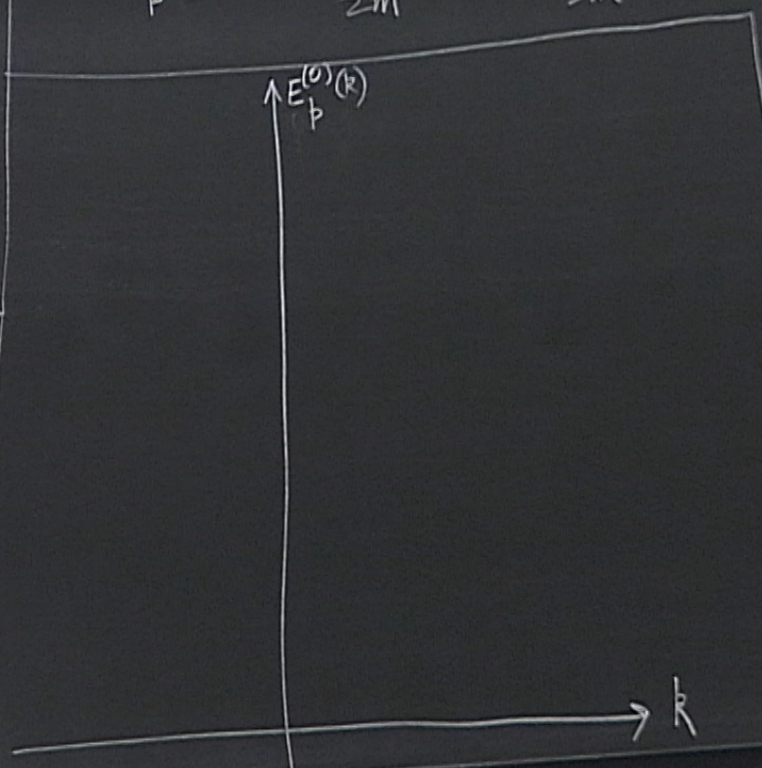
$$e^{i(k+b)x}$$

where $n \in \mathbb{Z}$

$$\delta_{k+b, k'+b'}$$

FBZ

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



$$\frac{\hbar^2 (k \pm \frac{2\pi}{a})^2}{2m}, \quad b = \pm \frac{2\pi}{a}$$

$$\frac{\hbar^2 (k \pm \frac{4\pi}{a})^2}{2m}, \quad b = \pm \frac{4\pi}{a}$$

(x)

$$e^{i(k+b)x}$$

n where $n \in \mathbb{Z}$

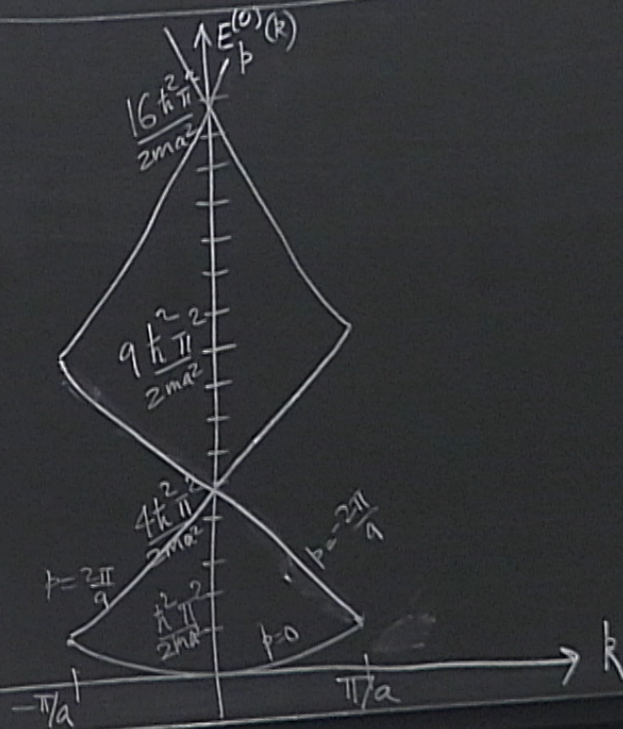
$$\delta_{k+b, k'+b'}$$

k' to FBZ

$$E_b^{(0)}(k) = \frac{\hbar^2 (k+b)^2}{2m} = \frac{\hbar^2 (k+b)^2}{2m} = \frac{\hbar^2 k^2}{2m}, \quad b=0$$

$$\frac{\hbar^2 (k \pm \frac{2\pi}{a})^2}{2m}, \quad b = \pm \frac{2\pi}{a}$$

$$\frac{\hbar^2 (k \pm \frac{4\pi}{a})^2}{2m}, \quad b = \pm \frac{4\pi}{a}$$



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

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

