

PERIODIC BOUNDARY CONDITIONS

Friday, 29 November 2019 09:08

BLOCH THEOREM

$$\psi(x + L) = \psi(x) e^{j k \cdot L}$$



1-neighbor $t_0 = -\frac{\hbar^2}{2ma^2}$

$$t_0 \psi_{i-1} + (E_{ci} - 2t_0) \psi_i + t_0 \psi_{i+1} = E \psi_i$$

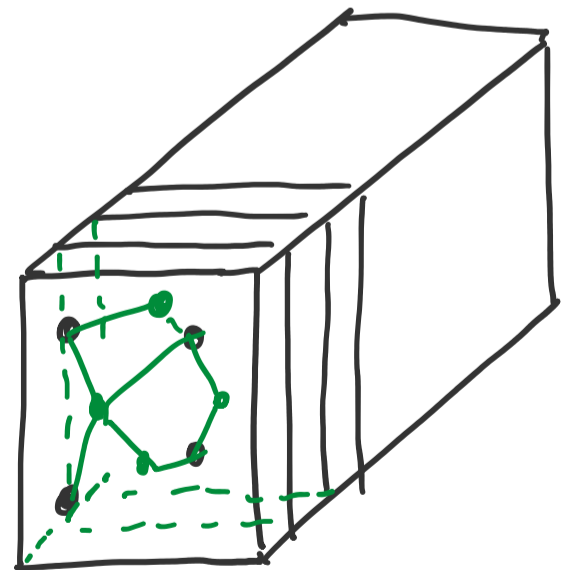
Point 1

$$t_0 \psi_0 + (E_{c1} - 2t_0) \psi_1 + t_0 \psi_2 = E \psi_1$$

$$\psi_0 = \psi_N e^{-j k x - L}$$

$$t_0 e^{-j k x - L} \psi_N + (E_{c1} - 2t_0) \psi_1 + t_0 \psi_2 = E \psi_1$$

$$H = \begin{bmatrix} E_{c1} - 2t_0 & t_0 & & & \\ & E_{c2} - 2t_0 & t_0 & & \\ & & \ddots & \ddots & \\ & & & E_{cN} - 2t_0 & t_0 \\ t_0 e^{j k x - L} & & & & \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix}$$



$s p_3 d_5 s^*$

$$H = \begin{bmatrix} H_{11} & H_{12} & H_{1N} e^{j k x - L} \\ H_{21} & H_{22} & H_{23} \\ & H_{32} & H_{33} & H_{3N} \\ & & & \ddots & \ddots \\ & & & & H_{N1} e^{j k x - L} \end{bmatrix}$$