FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

1. Schrodinger Equation

2. Contact-ing Schrodinger

3. Advanced Examples

4. Spin Transport

1.1. Introduction

1.2. Wave Equation

1.3. Differential to Matrix Equation

1.4. Dispersion Relation

1.5. Counting States

1.6. Beyond 1-D

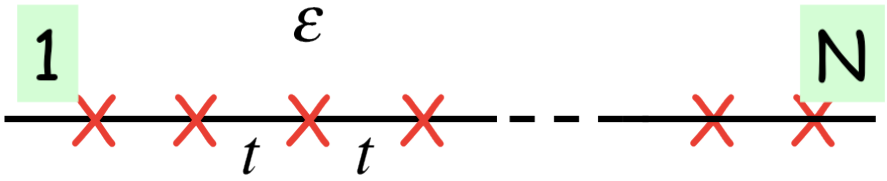
1.7. Lattice with a Basis

1.8. Graphene

1.9. Reciprocal Lattice / Valleys

1.10. Summing up ..

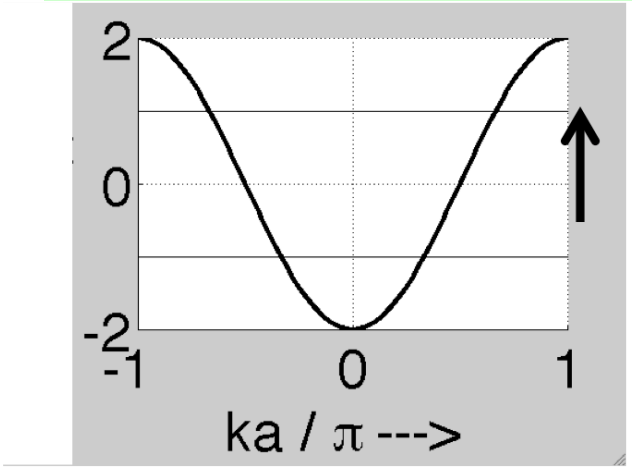
1.5a Counting States



N x N matrix has
N eigenvalues

$$E\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix}=\begin{bmatrix}\varepsilon & t & 0 & \cdots & t\\ t & \varepsilon & t & 0 & \cdots\\ 0 & t & \varepsilon & t & 0 & \cdots\\ \vdots & \vdots & \vdots & & & \\ t & \cdots & 0 & t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix}$$

Allowed energies look continuous !!



a : *Lattice spacing*

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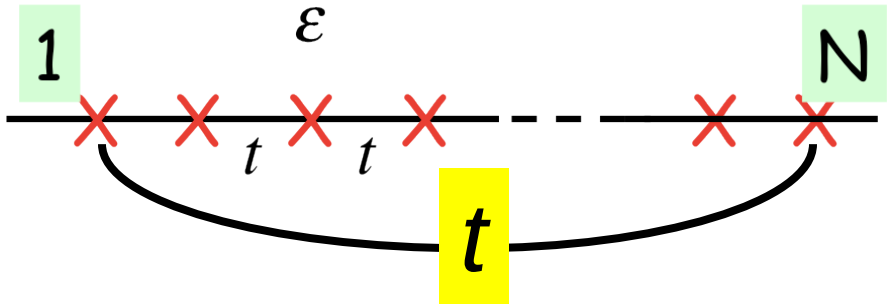


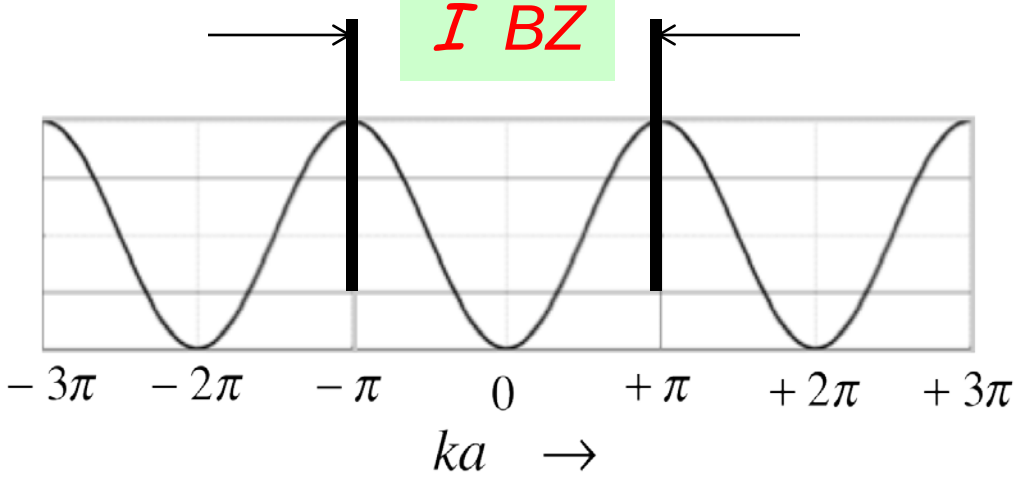
$$\psi_n = \psi_0 e^{+inka}$$

$$k'a \rightarrow ka + 2\pi$$

$$\psi_n' = \psi_0 e^{+inka} e^{+in2\pi}$$

$$= \psi_n$$

I BZ

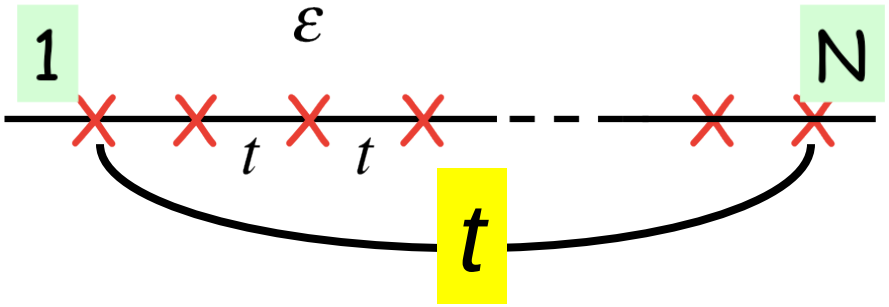


$$E = \varepsilon + 2t \cos ka$$

Can consider k's only in first Brillouin Zone

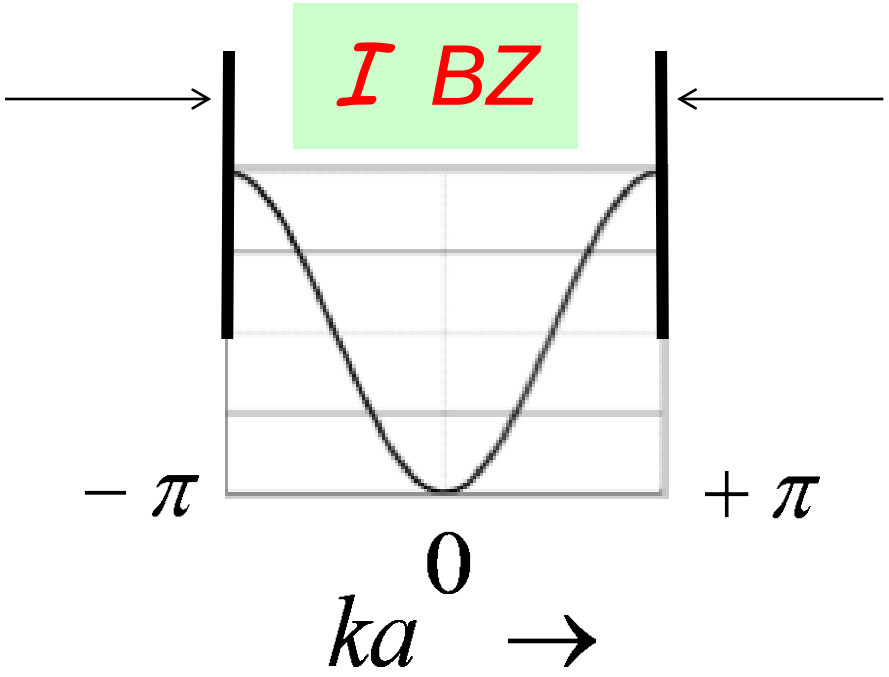
because lattice is discrete

a : *Lattice spacing*



$$\psi_0 = \psi_N = \psi_0 e^{+iNka}$$

$$Nka = 2\pi\nu$$

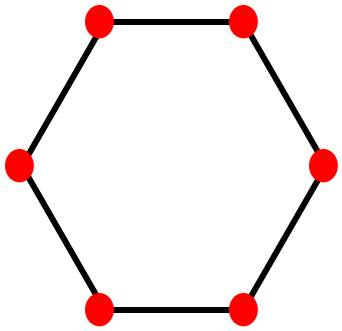


$$ka = \frac{2\pi}{N}\nu$$

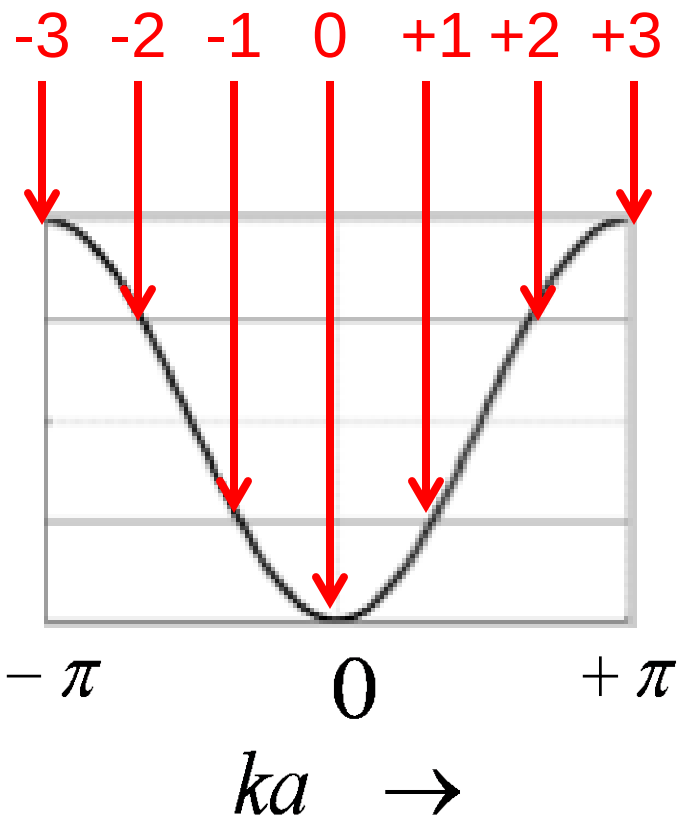
$$\rightarrow \quad k = \frac{2\pi}{Na}\nu$$

$$E = \varepsilon + 2t\cos ka$$

$$Benzene \rightarrow N = 6$$



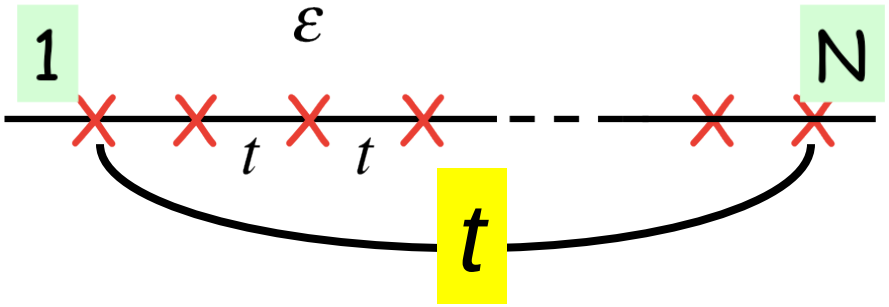
$$ka = \frac{2\pi}{6}\nu \rightarrow \nu =$$



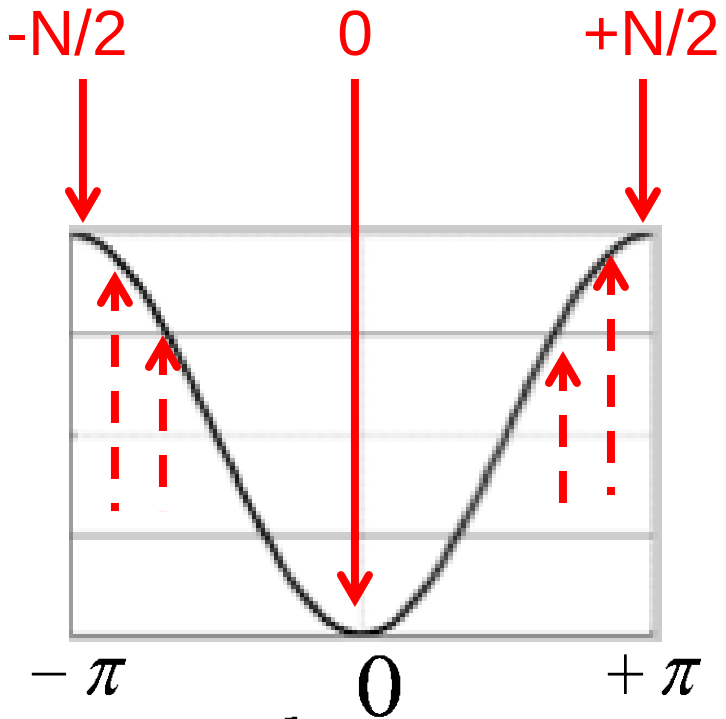
$$H = \begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & t \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & 0 & 0 \\ 0 & 0 & t & \varepsilon & t & 0 \\ 0 & 0 & 0 & t & \varepsilon & t \\ t & 0 & 0 & 0 & t & \varepsilon \end{bmatrix}$$

$$E = \varepsilon + 2t\cos ka$$

a : Lattice spacing



$$ka = \frac{2\pi}{N}\nu \quad \downarrow \quad \nu =$$



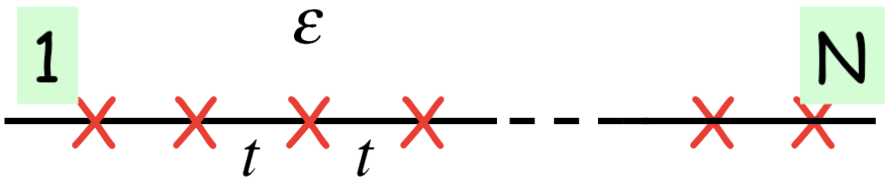
$$Range\ in\ z \rightarrow Sampling\ in\ k$$

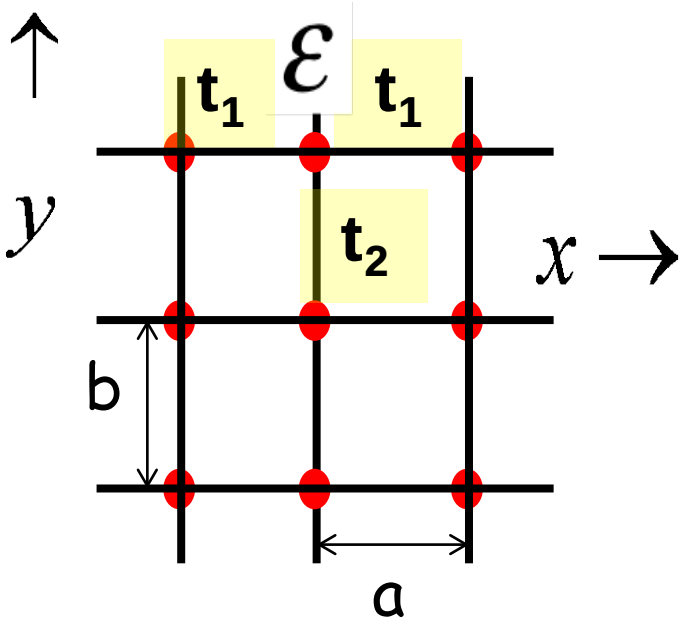
$$Sampling\ in\ z \rightarrow Range\ in\ k$$

Like
Discrete Fourier Transforms !

$$E = \varepsilon + 2t\cos ka$$

Coming up next ..





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