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 ..

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May 2015

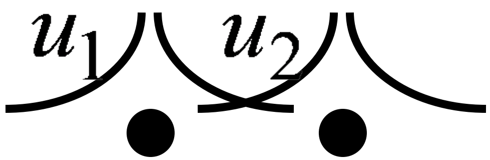
http://nanohub.org/groups/lnebook

1.4a Dispersion Relation

$$\boxed{E[S]\{\psi\} = [H]\{\psi\}}$$

$$E\begin{bmatrix} 1 & s \\ s & 1 \end{bmatrix}\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \varepsilon' & t' \\ t' & \varepsilon' \end{bmatrix}\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

Hydrogen Molecule

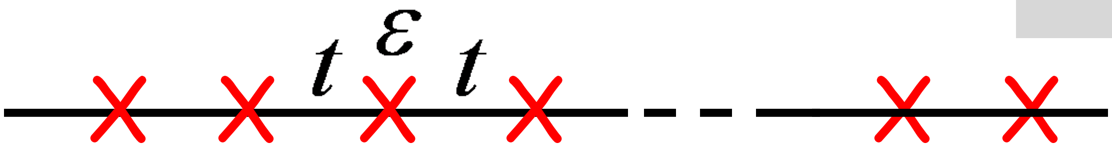


$$E\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \frac{1}{1-s^2}\begin{bmatrix} \varepsilon' - t's & t' - \varepsilon's \\ t' - \varepsilon's & \varepsilon' - t's \end{bmatrix}\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

$$E\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

$$\boxed{E\{\psi\} = [H]\{\psi\}}$$

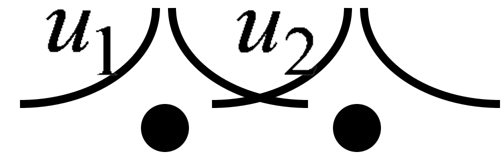
1.4b Dispersion Relation



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

$$H_{mn}=\int dV\, u_m^*(\vec{r})\, H_{op}\, u_n(\vec{r})$$

Hydrogen Molecule

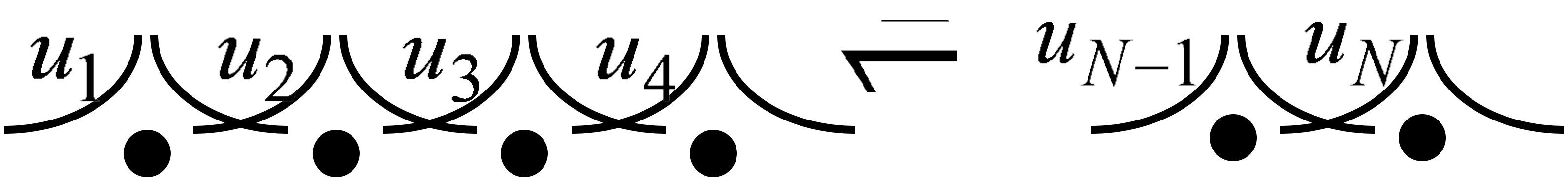


$$E\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}=\begin{bmatrix}\varepsilon & t\\ t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

$\varepsilon - t$

$\varepsilon + t$

“Hydrogen Solid”



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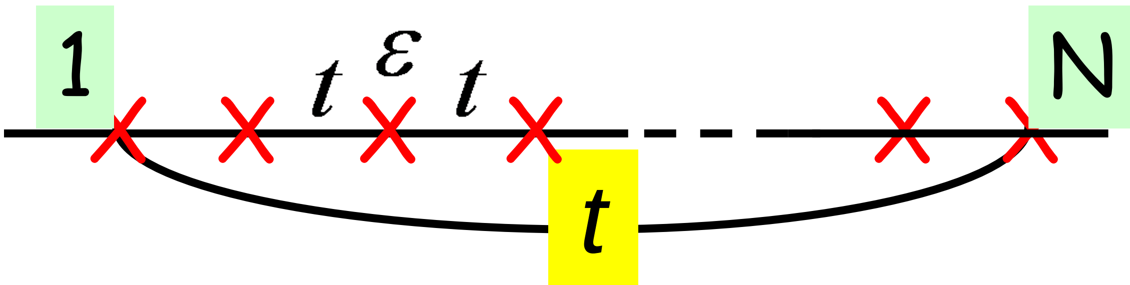
1.4c Dispersion Relation

$$E = t\,e^{-ika} + \varepsilon + t\,e^{+ika}$$



$a:$ *Lattice spacing*

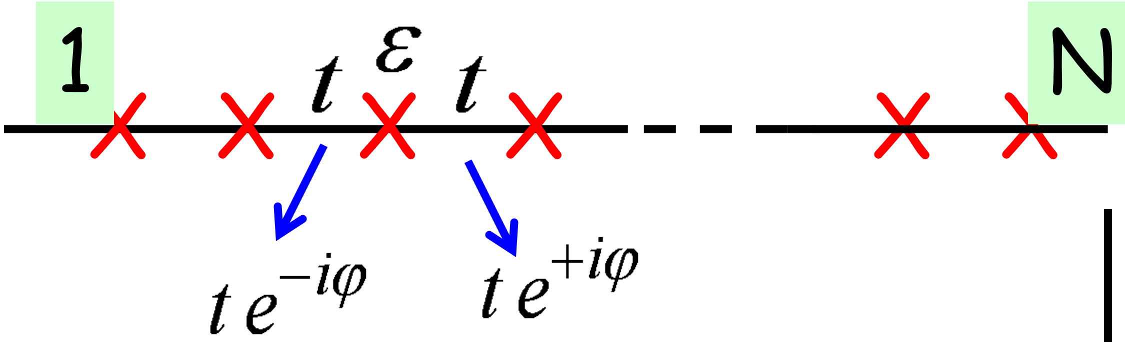
$$E\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix} = \begin{bmatrix}\varepsilon & t & 0 & \cdots & t\\ t & \varepsilon & t & 0 & \cdots\\ 0 & t & \varepsilon & t & 0 & \cdots\\ \vdots & \vdots & \vdots & & \\ t & \cdots & 0 & t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\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

$$E\psi_n = +t\,\psi_{n-1} + \varepsilon\,\psi_n + t\,\psi_{n+1}$$

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

$$\frac{\psi_{n-1}}{\psi_n} = \frac{e^{+i(n-1)ka}}{e^{+inka}} = e^{-ika}$$

$$E = t\frac{\psi_{n-1}}{\psi_n} + \varepsilon + t\frac{\psi_{n+1}}{\psi_n} = +t\,e^{-ika} + \varepsilon + t\,e^{+ika}$$



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

$$H_{mn} = \int dV\, u_m^*(\vec{r})\, H_{op}\, u_n(\vec{r})$$

$$E = t\,e^{-ika} + \varepsilon + t\,e^{+ika}$$

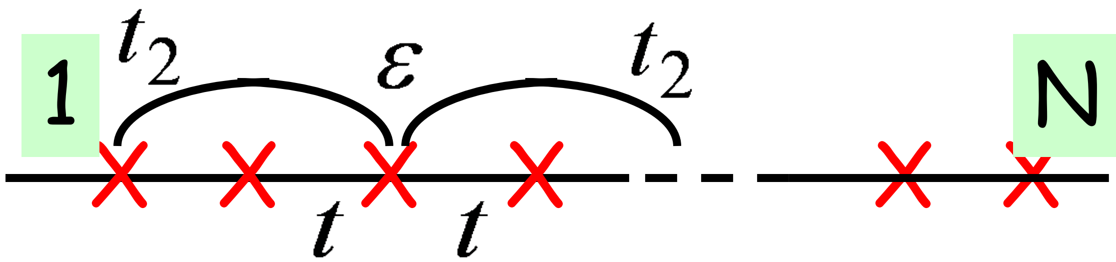
$$= \varepsilon + 2t\,\cos ka$$

$$E = te^{-i\varphi}e^{-ika} + \varepsilon$$

$$+\,t\,e^{+i\varphi}e^{+ika}$$

$$= \varepsilon + 2t\,\cos(ka+\varphi)$$

1.4e Dispersion Relation



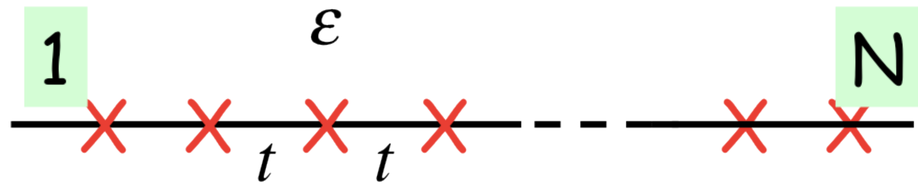
$$E = t_2\, e^{-i2ka} + t\, e^{-ika} + \varepsilon + t\, e^{+ika} + t_2\, e^{+i2ka}$$

$$= \varepsilon + 2t\cos ka + 2t_2\cos 2ka$$

1.4f Dispersion Relation

$$E_c = \varepsilon + 2t \quad \rightarrow \quad \varepsilon = E_c - 2t$$

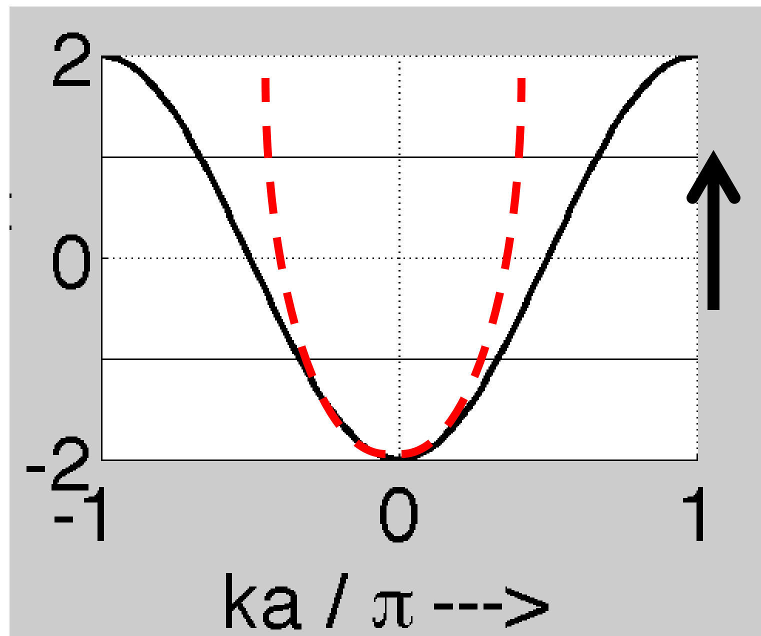
$$t = -\frac{\hbar^2}{2ma^2}$$



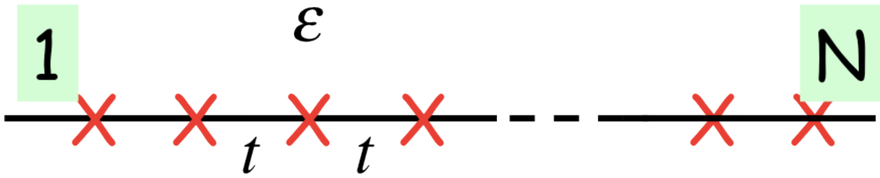
$$E = \varepsilon + 2t\cos ka$$

$$\varepsilon + 2t\left(1 - \frac{k^2a^2}{2} + \cdots\right)$$

$$E = E_c + \frac{\hbar^2k^2}{2m}$$



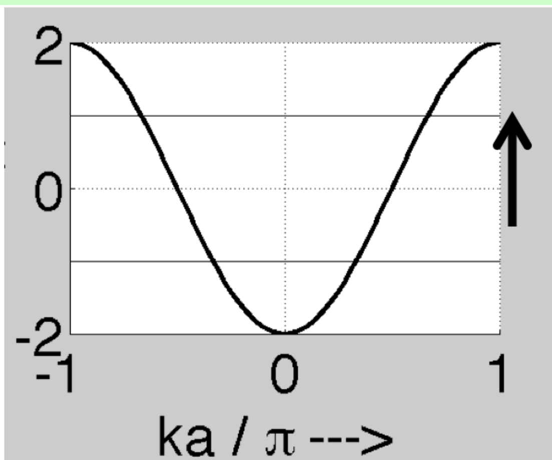
$$\frac{E - \varepsilon}{|t|}$$



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

N x N matrix has N eigenvalues

Allowed energies look continuous !!



$$\frac{E-\varepsilon}{|t|}$$

Coming up next ..

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