

ECE 495N

**Fundamentals of
Nanoelectronics**

Fall 2008

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**Lecture: 19
Title: Bandstructure II
Date: October 15, 2008**

**Video Lectures posted at:
<https://www.nanohub.org/resources/5346/>**

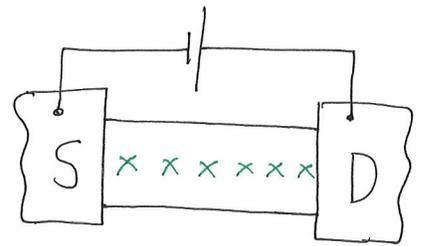
**Class notes taken by: Panagopoulos Georgios
Purdue University**



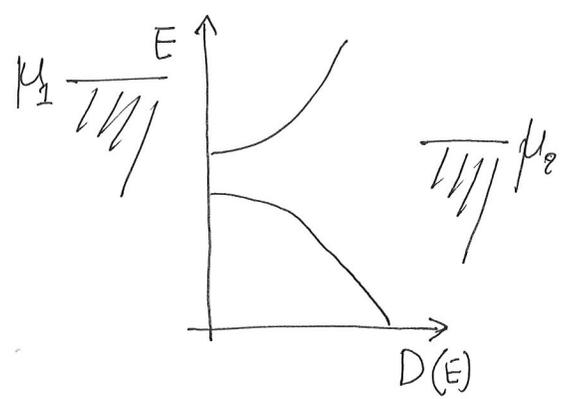
$$E \Phi(\vec{r}) = \left(-\frac{\hbar^2}{2m} \nabla^2 + U \right) \Phi(\vec{r})$$

$$\Phi(\vec{r}) = \sum_n \phi_n u_n(\vec{r})$$

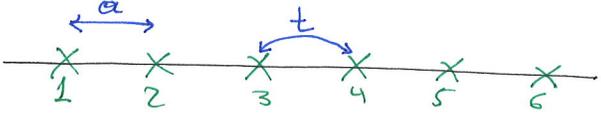
known set of functions



$$E[S] \{\phi\} = [H] \{\phi\}$$



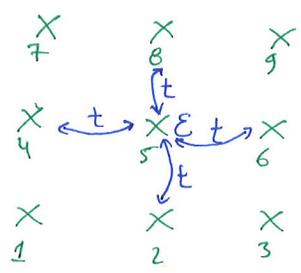
— 1-D lattice



$$E \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{Bmatrix} = \begin{bmatrix} \epsilon & t & t' & \dots & \\ t & \epsilon & t & t' & \\ t' & t & \epsilon & t & t' \\ & t' & t & \epsilon & t & t' \\ & & & & \ddots & \\ & & & & t' & t & \epsilon \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{Bmatrix}$$

$$\phi_n = \phi_0 e^{i n k a}$$

— 2-D lattice (square)



$$E \phi_n = \sum_m H_{nm} \phi_m \quad (I)$$

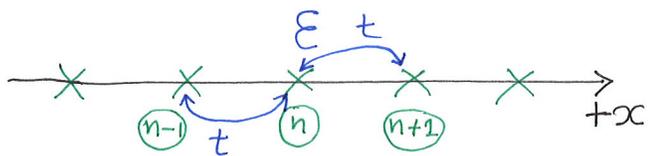
$$\phi_n = \phi_0 e^{i \vec{k} \cdot \vec{d}_n} \quad (II)$$

$$(I) \stackrel{(II)}{\Rightarrow} E \phi_0 e^{i \vec{k} \cdot \vec{d}_n} = \sum_m H_{nm} \phi_0 e^{i \vec{k} \cdot \vec{d}_m}$$

$$\Rightarrow E = \sum_m H_{nm} e^{i \vec{k} \cdot (\vec{d}_m - \vec{d}_n)} = E(\vec{k})$$

This is the general principle and it holds for all the cases, 1-D, 2-D, 3-D lattices

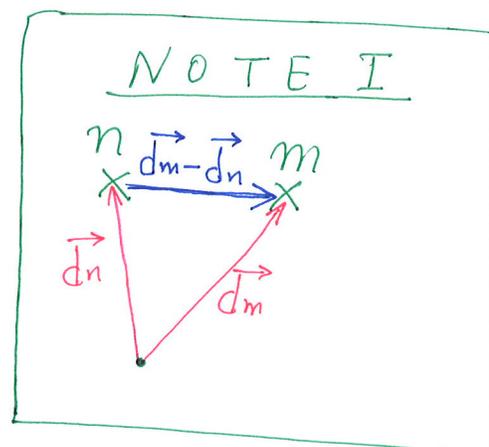
Example - Application 1



Nearest Neighbor model

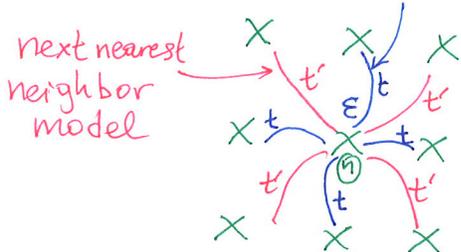
$$E(\vec{r}) = \epsilon + t e^{i k a} + t e^{-i k a}$$

$$= \epsilon + 2t \cos k a$$



Example - Application 2

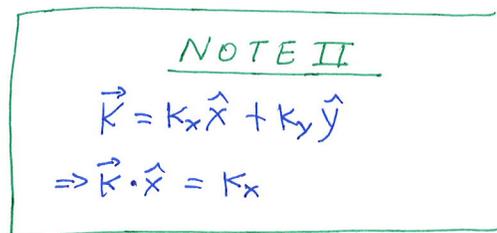
nearest neighbor model



The solid is periodic, hence from each point we see the same environment and we can stand everywhere we want and to take the summation

$$E(\vec{r}) = \epsilon + t \underbrace{e^{i \vec{k} \cdot a \hat{x}}}_{= e^{i k_x a}} + t \underbrace{e^{i \vec{k} \cdot a \hat{y}}}_{= e^{i k_y a}}$$

$$+ t e^{-i \vec{k} \cdot a \hat{x}} + t e^{-i \vec{k} \cdot a \hat{y}}$$



$$= \epsilon + t e^{i k_x a} + t e^{i k_y a} + t e^{-i k_x a} + t e^{-i k_y a}$$

$$= \epsilon + 2t \cos k_x a + 2t \cos k_y a$$

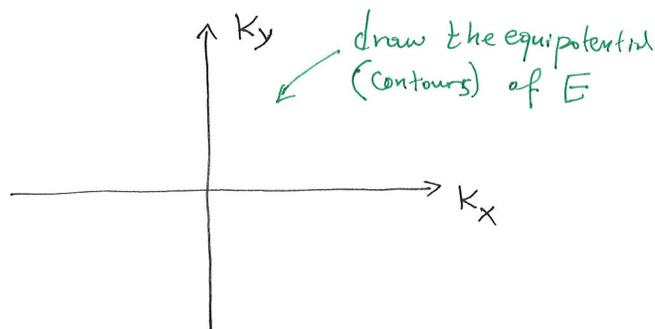
$$E'(\vec{r}) = E(\vec{r}) + t' e^{i \vec{k} \cdot (a \hat{x} - a \hat{y})}$$

$$+ t' e^{i \vec{k} \cdot (-a \hat{x} + a \hat{y})}$$

$$+ t' e^{i \vec{k} \cdot (-a \hat{x} - a \hat{y})}$$

$$+ t' e^{i \vec{k} \cdot (a \hat{x} + a \hat{y})}$$

$$= E(\vec{r}) + t' \left[(e^{i k_x a} + e^{-i k_x a}) (e^{i k_y a} + e^{-i k_y a}) \right]$$



$$\Rightarrow E'(\vec{r}) = E(\vec{r}) + 4t' \cos k_x a \cos k_y a$$

$$= E + 2t \cos k_x a + 2t \sin k_y a + 4t' \cos k_x a \cos k_y a$$