

Курс: [Електронна структура та властивості низькорозмірних систем](#)

Лектор: Олександр Кордюк

### Лекція 3: Електрони в періодичному потенціалі - зонна структура

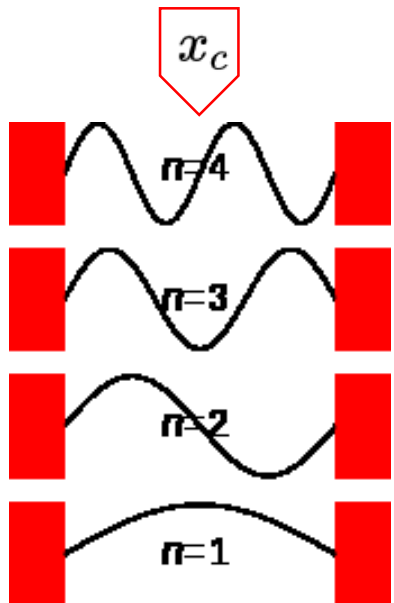
- Вільні електрони з граничними умовами
- Від хвиль пласких до блохівських. Зона Брілюєна
- Наближення слабкого потенціала – зонна щілина
- Метод сильного зв'язку – модель перескоків
- Зонні щілини та модель перескоків у 2D
- Кількість електронних станів: метал або ізолятор
- Приклади дискретизації станів у низькорозмірних системах
- *Задача додому:* побудувати  $\text{DOS}(\omega)$  у моделі перескоків до найближчих сусідів для 1D та 2D

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + \cancel{V(x)\psi(x, t)}$$

$$\psi(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}}$$

## Particle in a box

$$\psi_n(x, t) = \begin{cases} A \sin\left(k_n \left(x - x_c + \frac{L}{2}\right)\right) e^{-i\omega_n t} \\ 0 \end{cases}$$



$$k_n = \frac{n\pi}{L}, \quad E_n = \hbar\omega_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

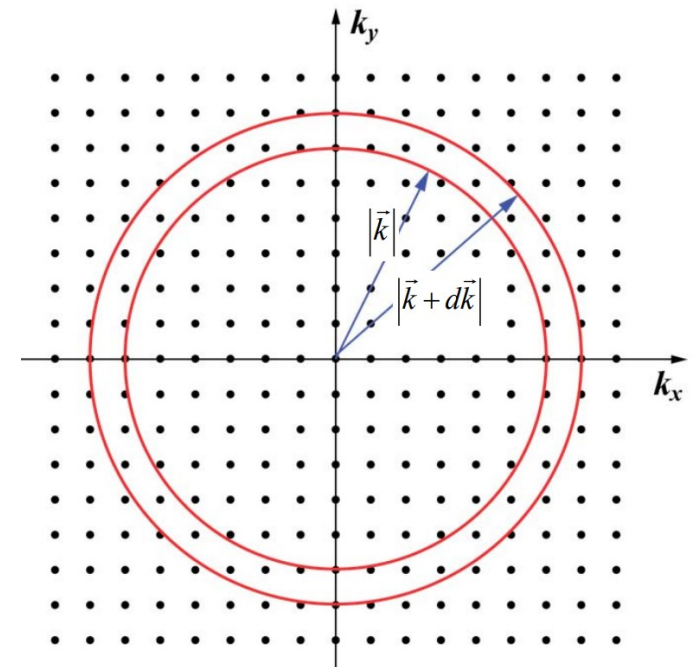
$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin(k_n x) & \text{for } n \text{ even} \\ \sqrt{\frac{2}{L}} \cos(k_n x) & \text{for } n \text{ odd.} \end{cases}$$

## Born-Von Karman boundary condition

$$\psi(x + L, t) = \psi(x, t)$$

$$k_{x,y,z} = \frac{2\pi n_{x,y,z}}{L}$$

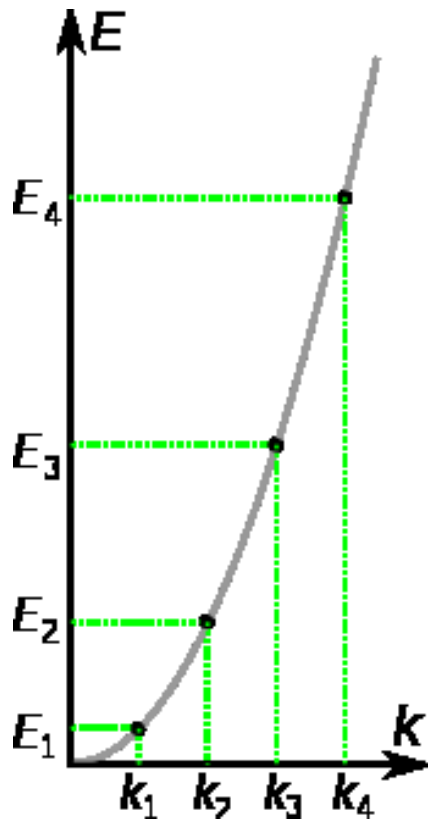
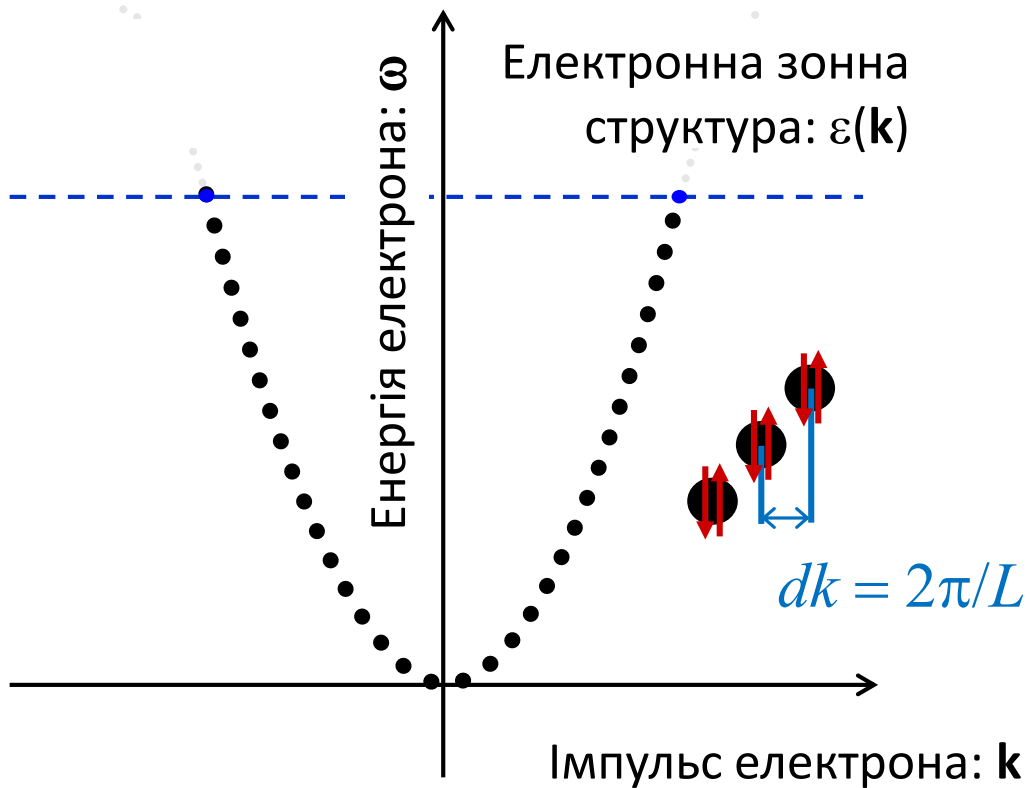
$$\varepsilon_k = \frac{\hbar^2 (2\pi)^2 (n_x^2 + n_y^2 + n_z^2)}{2mL^2}$$



# Born-Von Karman boundary condition



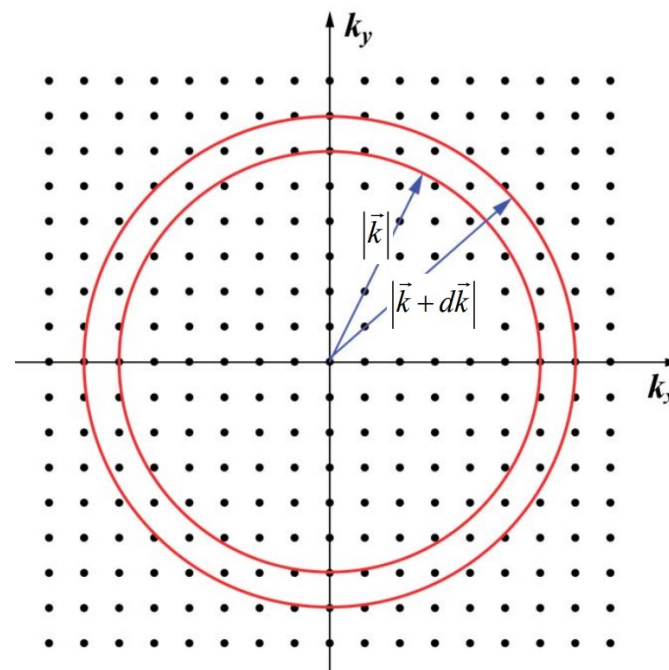
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$$



$$\psi(x + L, t) = \psi(x, t)$$

$$k_{x,y,z} = \frac{2\pi n_{x,y,z}}{L}$$

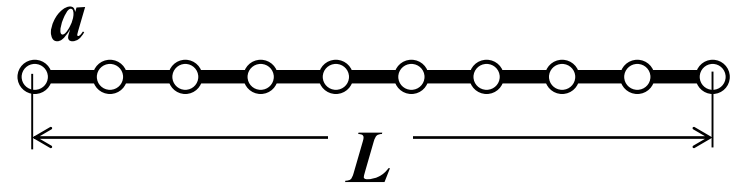
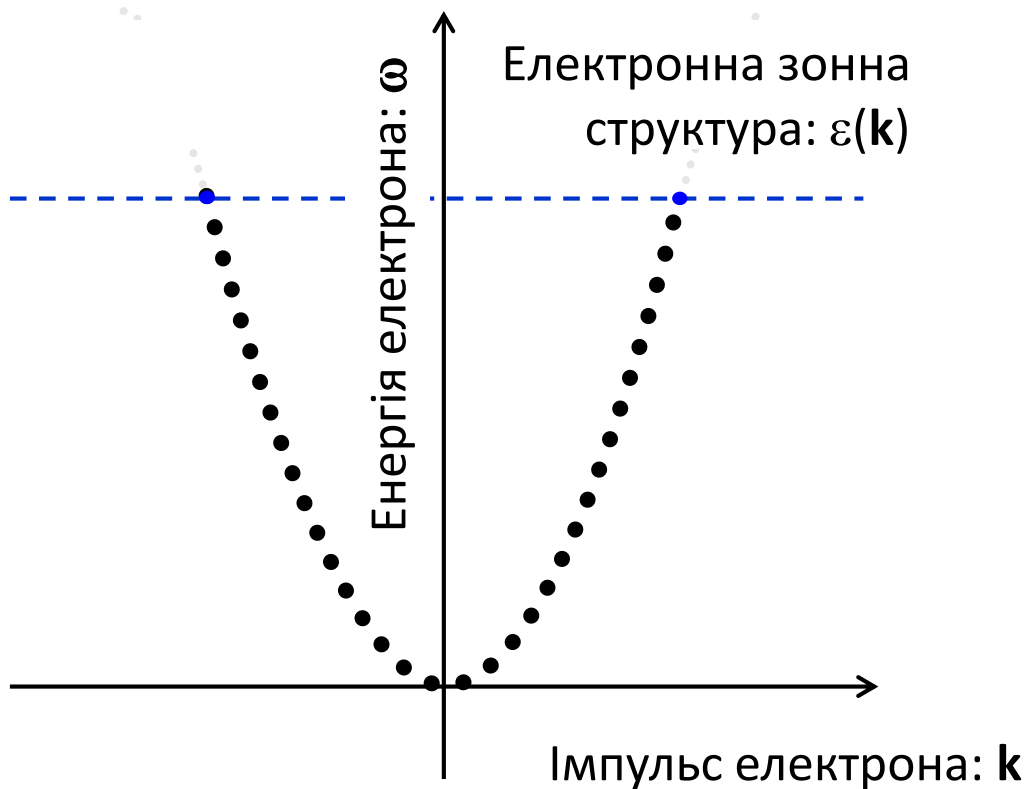
$$\varepsilon_k = \frac{\hbar^2 (2\pi)^2 (n_x^2 + n_y^2 + n_z^2)}{2mL^2}$$



# Від хвиль пласких до блохівських



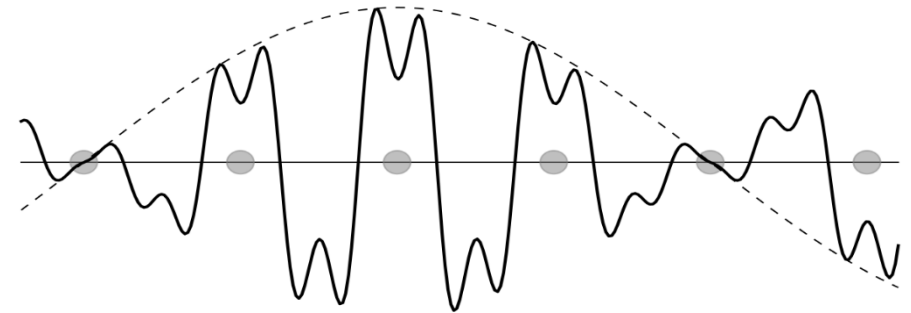
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$$



$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$

Теорема Блоха

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{n} \cdot \mathbf{a})$$

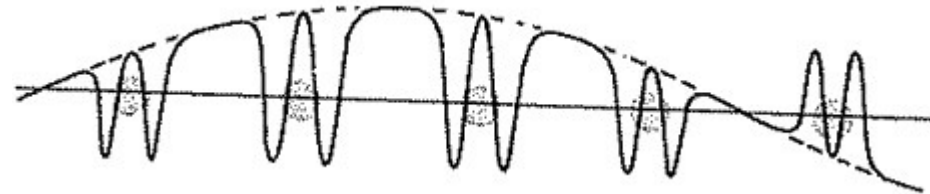


$$\psi_{n\mathbf{k}} = \psi_n(\mathbf{k} + \mathbf{K})$$

## Теорема Блоха

$$H\psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right) \psi = \mathcal{E}\psi \quad U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r})$$

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$

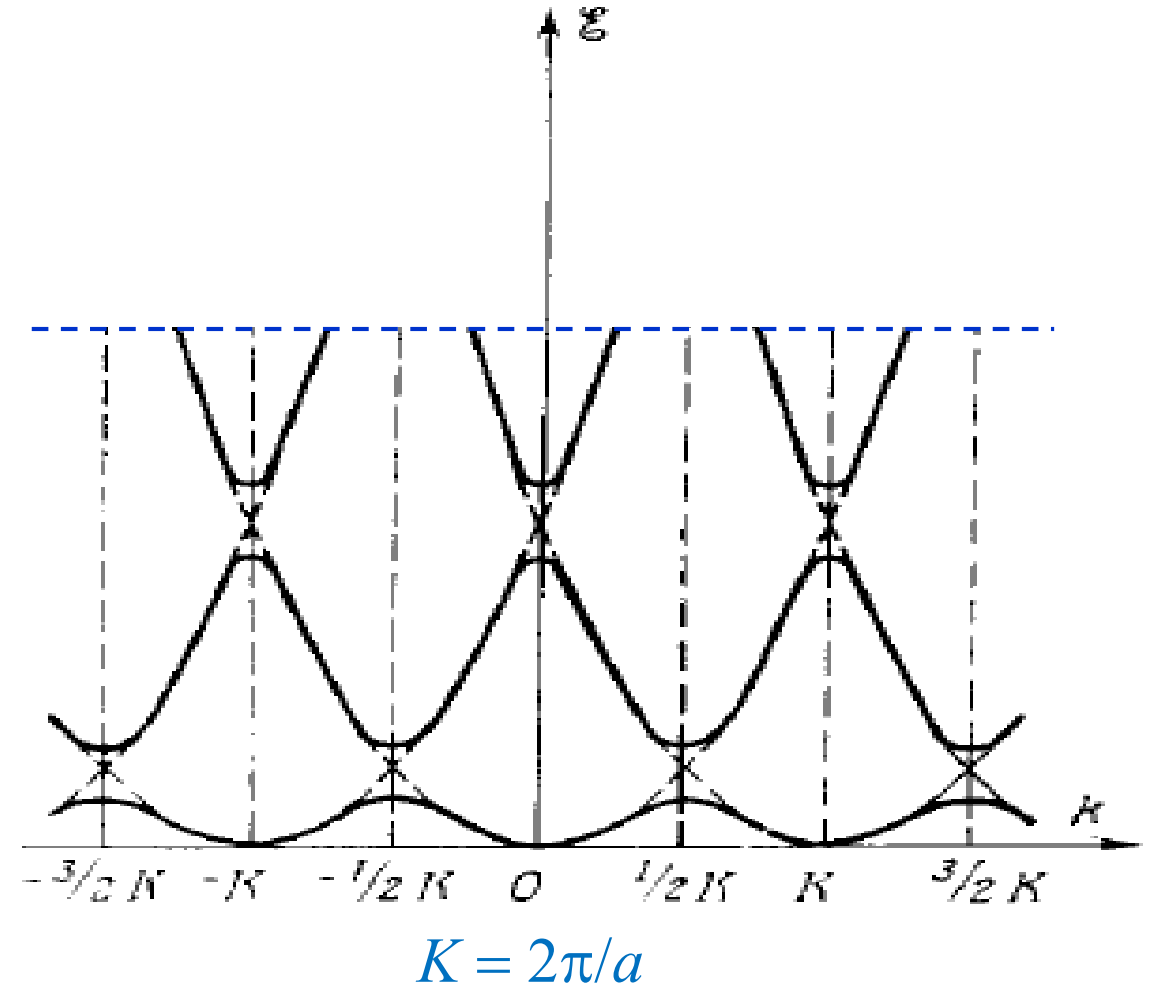
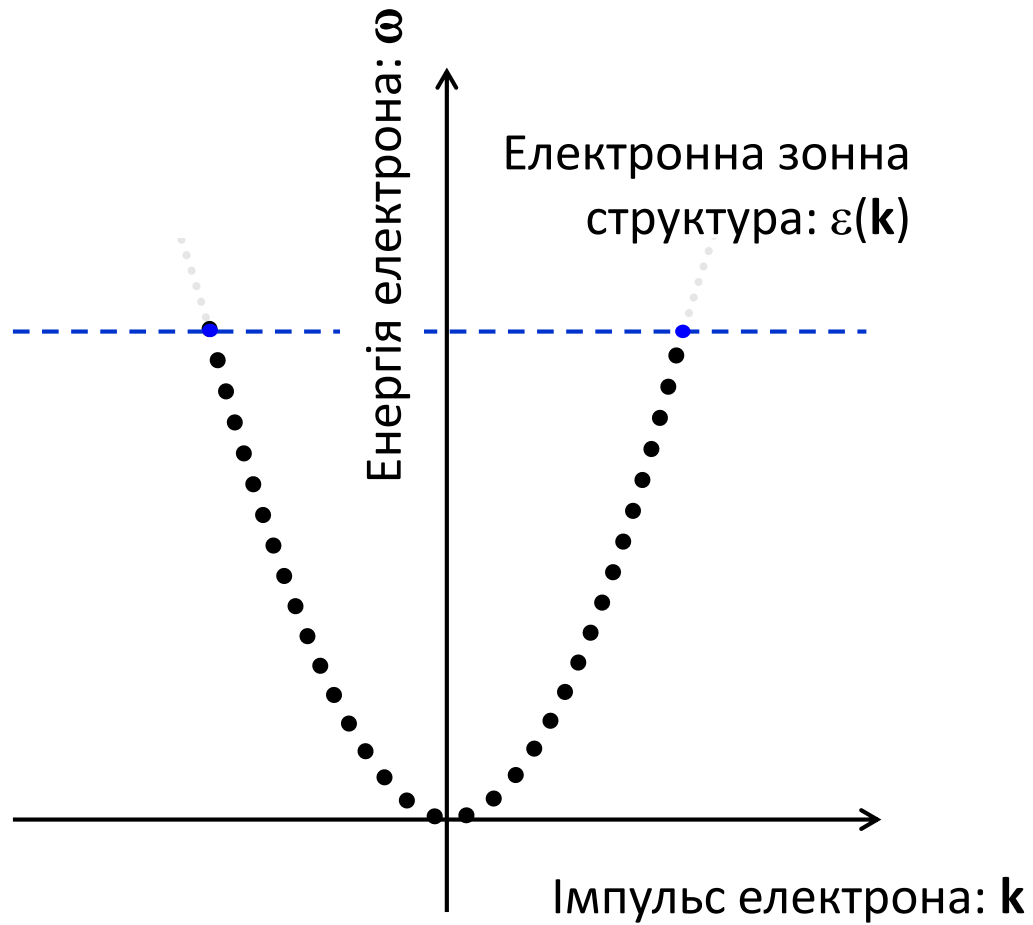
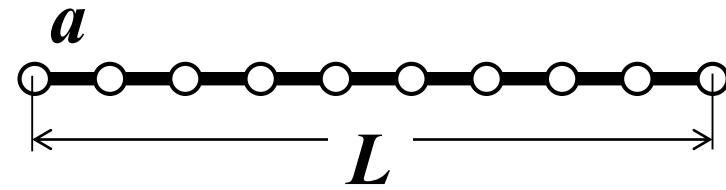


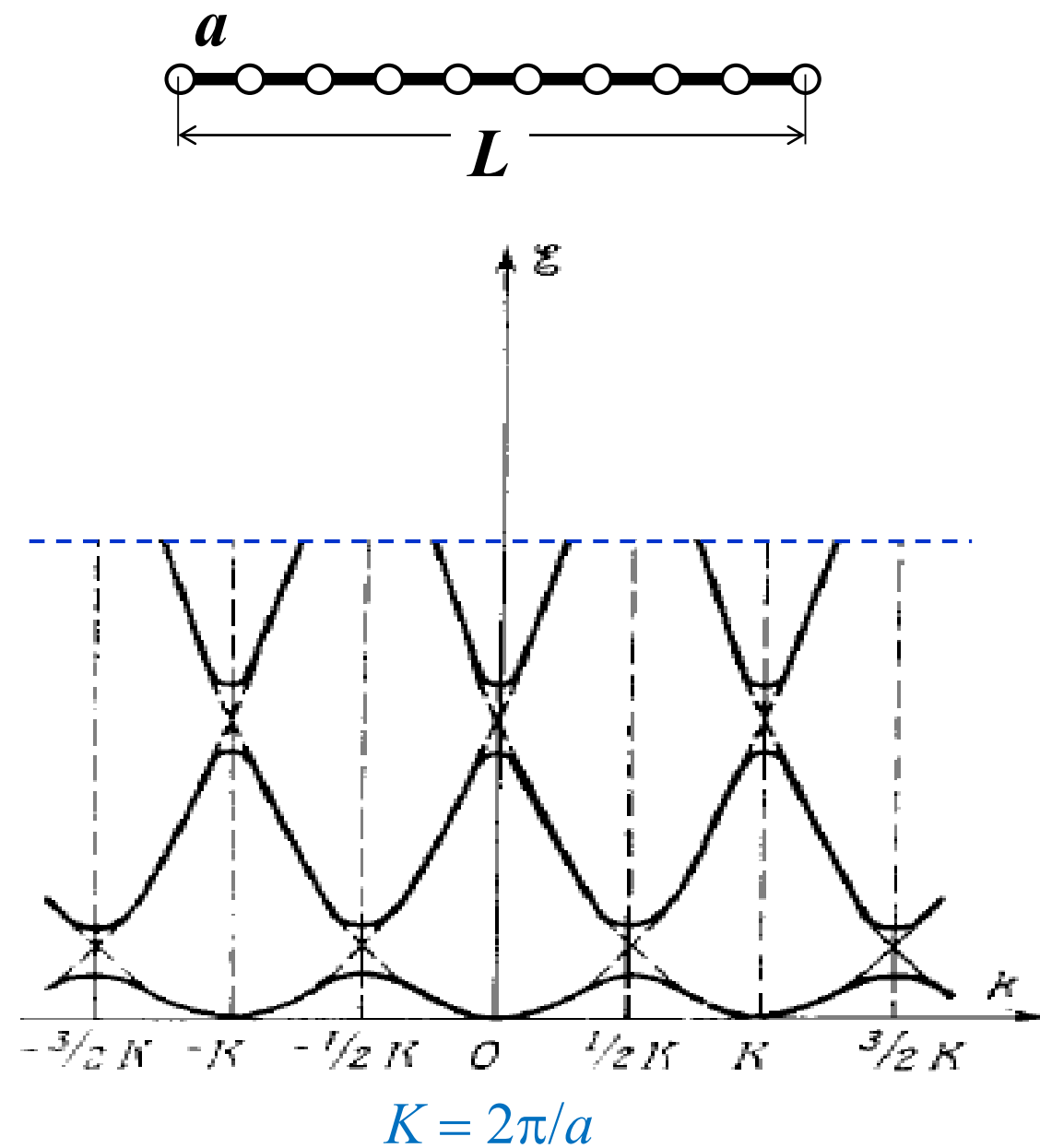
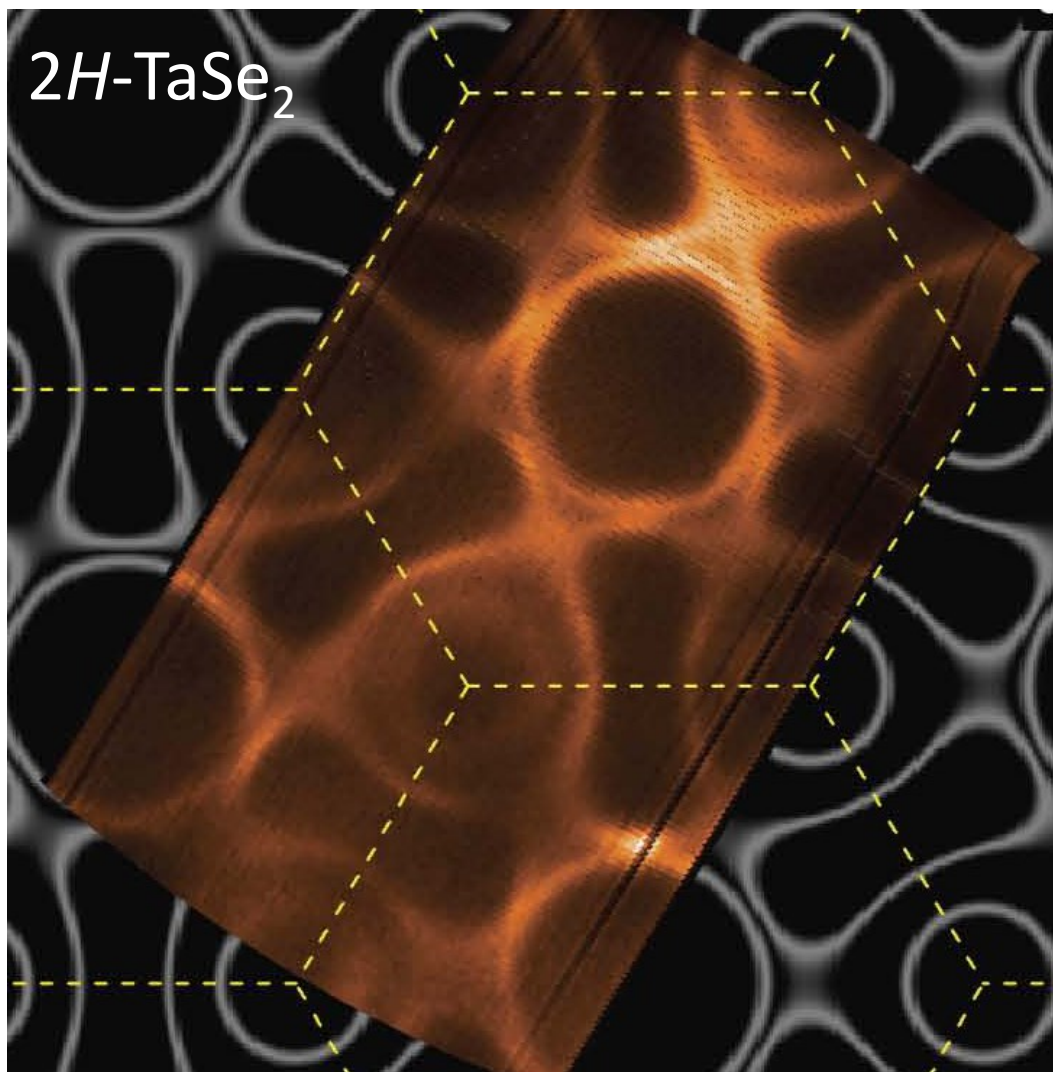
$$\psi_{n\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \text{ де } u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

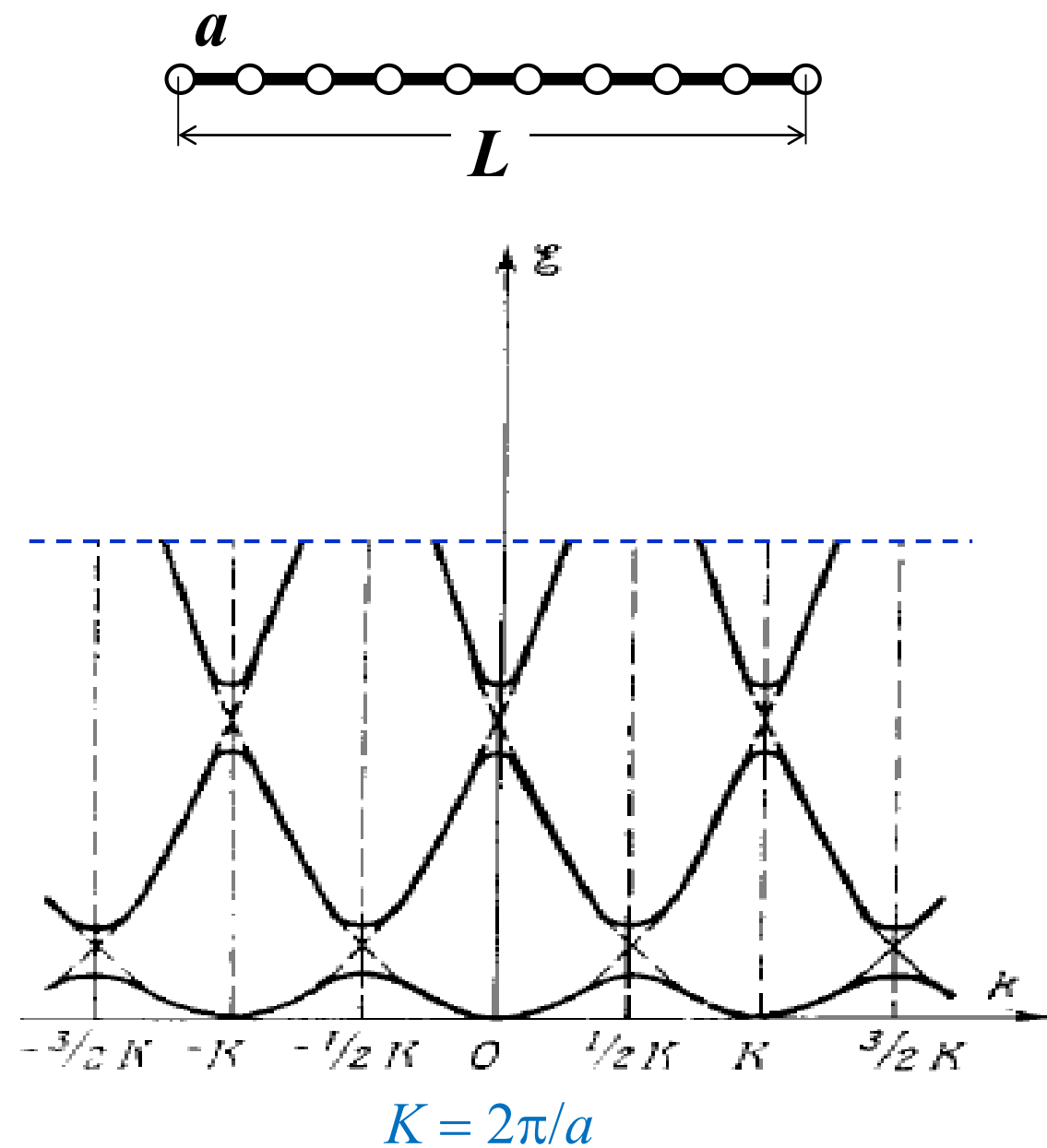
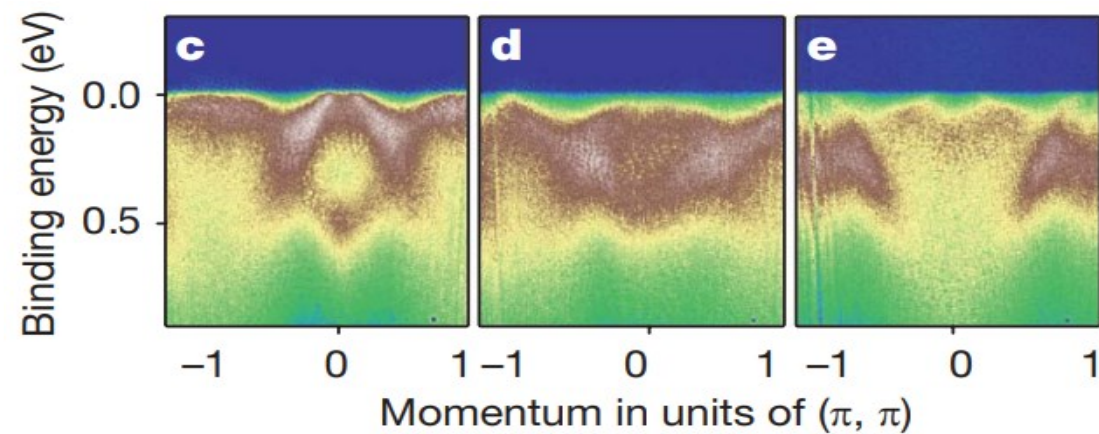
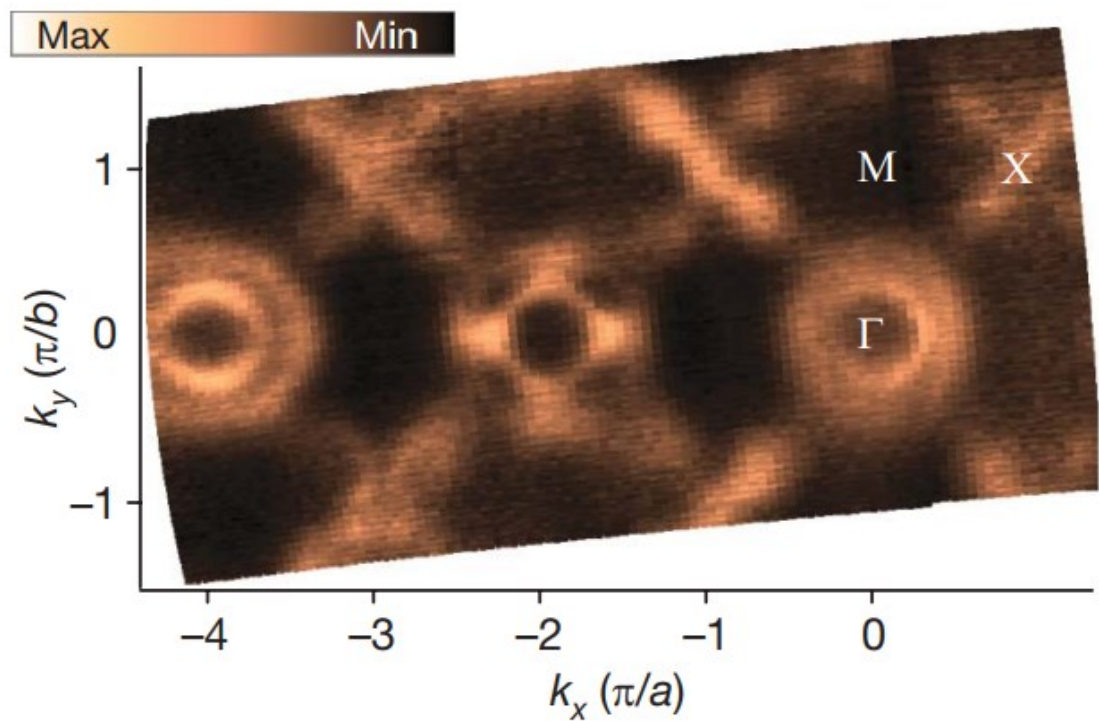
$$\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \psi(\mathbf{r})$$

$$\begin{aligned} \psi_{n, \mathbf{k} + \mathbf{K}}(\mathbf{r}) &= \psi_{n\mathbf{k}}(\mathbf{r}) \\ \mathcal{E}_{n, \mathbf{k} + \mathbf{K}} &= \mathcal{E}_{n\mathbf{k}} \end{aligned}$$

# Від хвиль пласких до блохівських

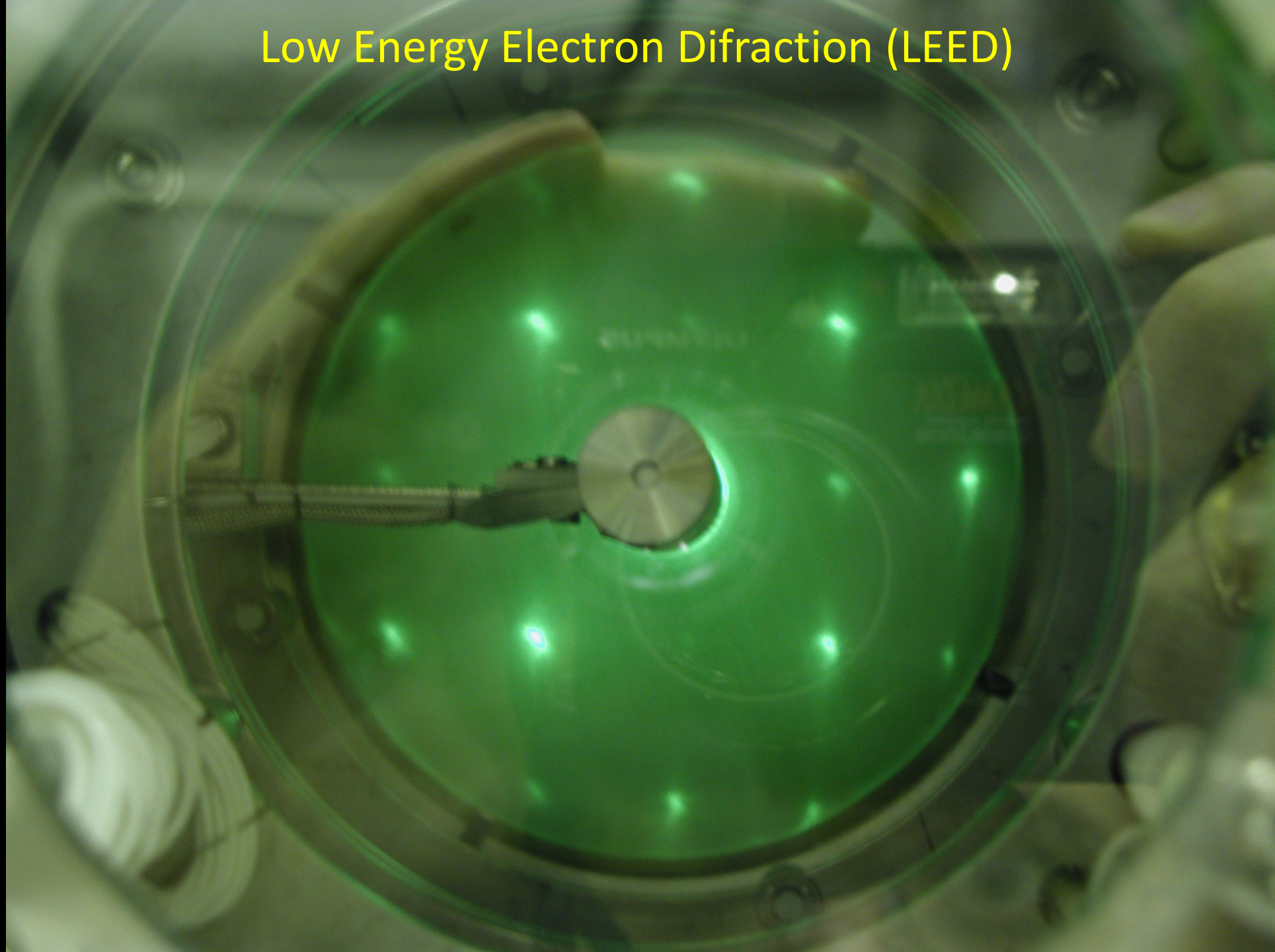




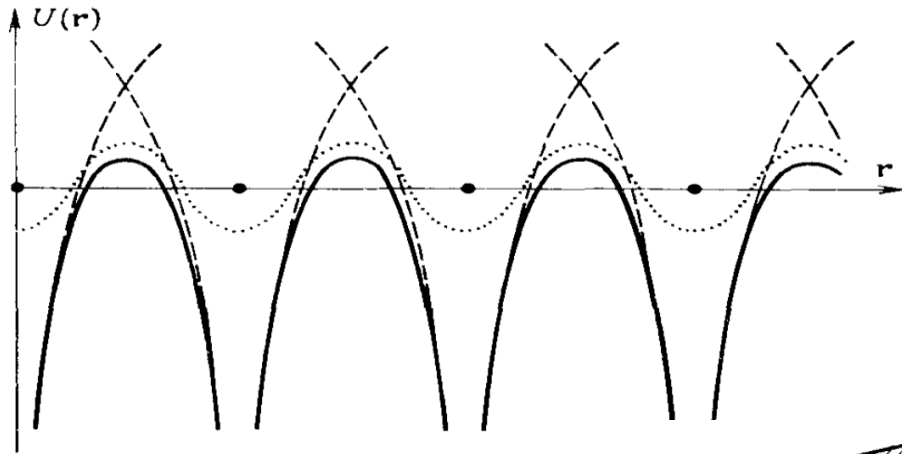
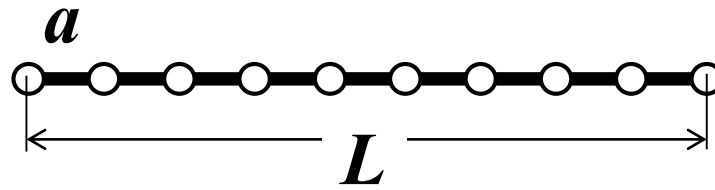




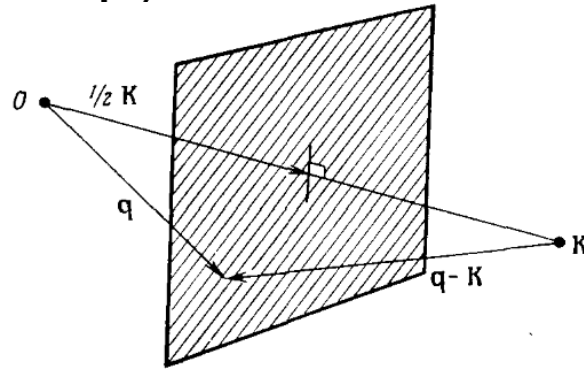
# Low Energy Electron Diffraction (LEED)



# Band gaps

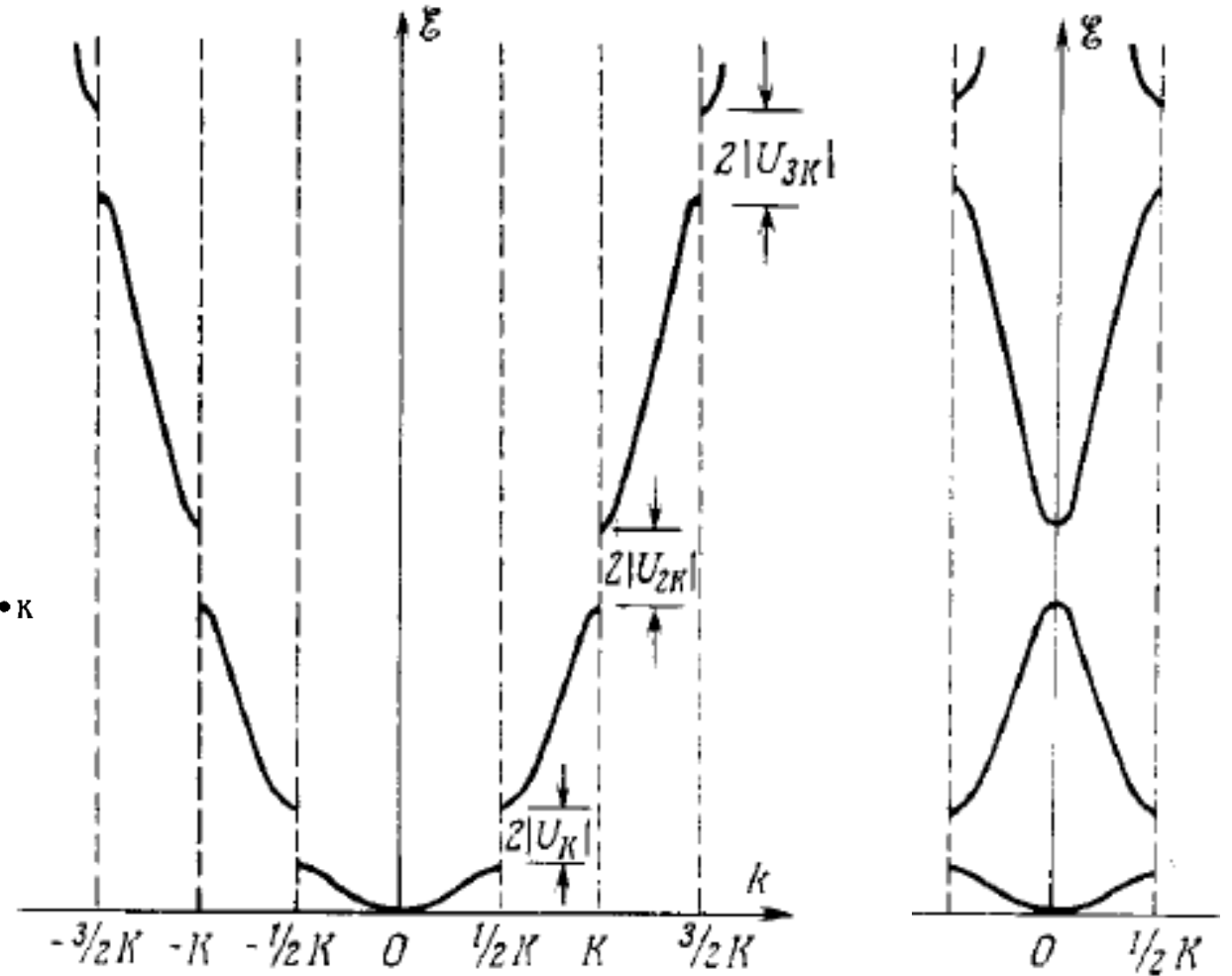


$$\begin{vmatrix} \mathcal{E} - \mathcal{E}_q^0 & -U_K \\ -U_K^* & \mathcal{E} - \mathcal{E}_{q-K}^0 \end{vmatrix} = 0$$



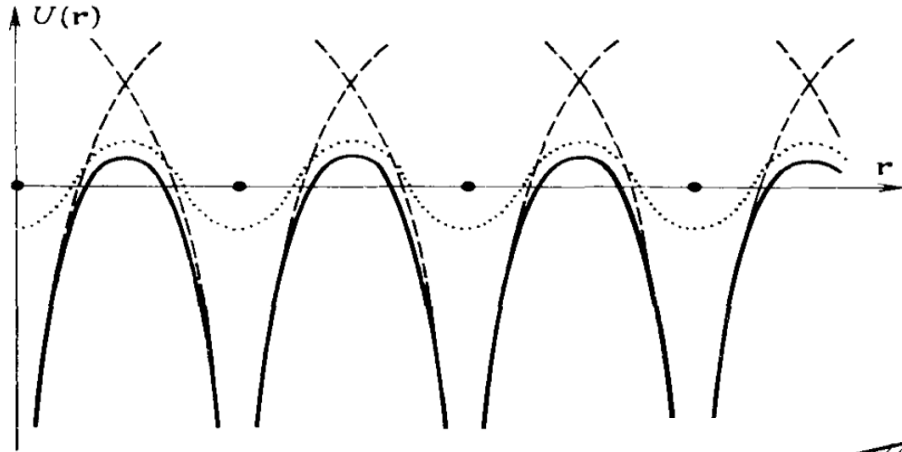
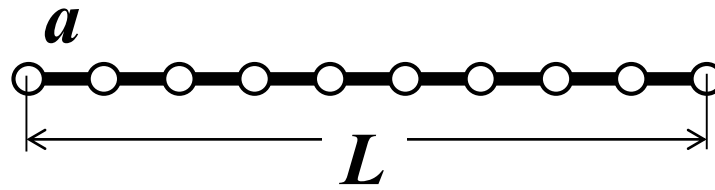
$$(\mathcal{E} - \mathcal{E}_q^0)(\mathcal{E} - \mathcal{E}_{q-K}^0) = |U_K|^2$$

$$\mathcal{E} = \frac{1}{2} (\mathcal{E}_q^0 + \mathcal{E}_{q-K}^0) \pm \left[ \left( \frac{\mathcal{E}_q^0 - \mathcal{E}_{q-K}^0}{2} \right)^2 + |U_K|^2 \right]^{1/2}$$

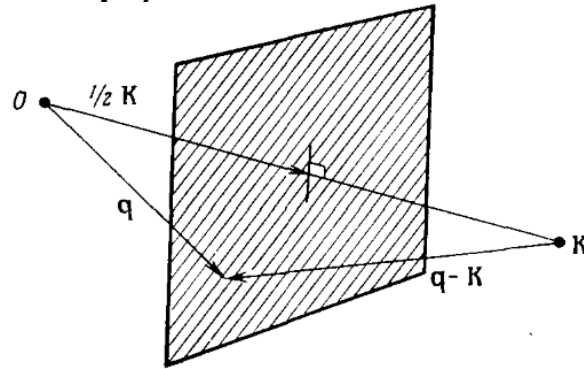


$$K = 2\pi/a$$

# Band gaps

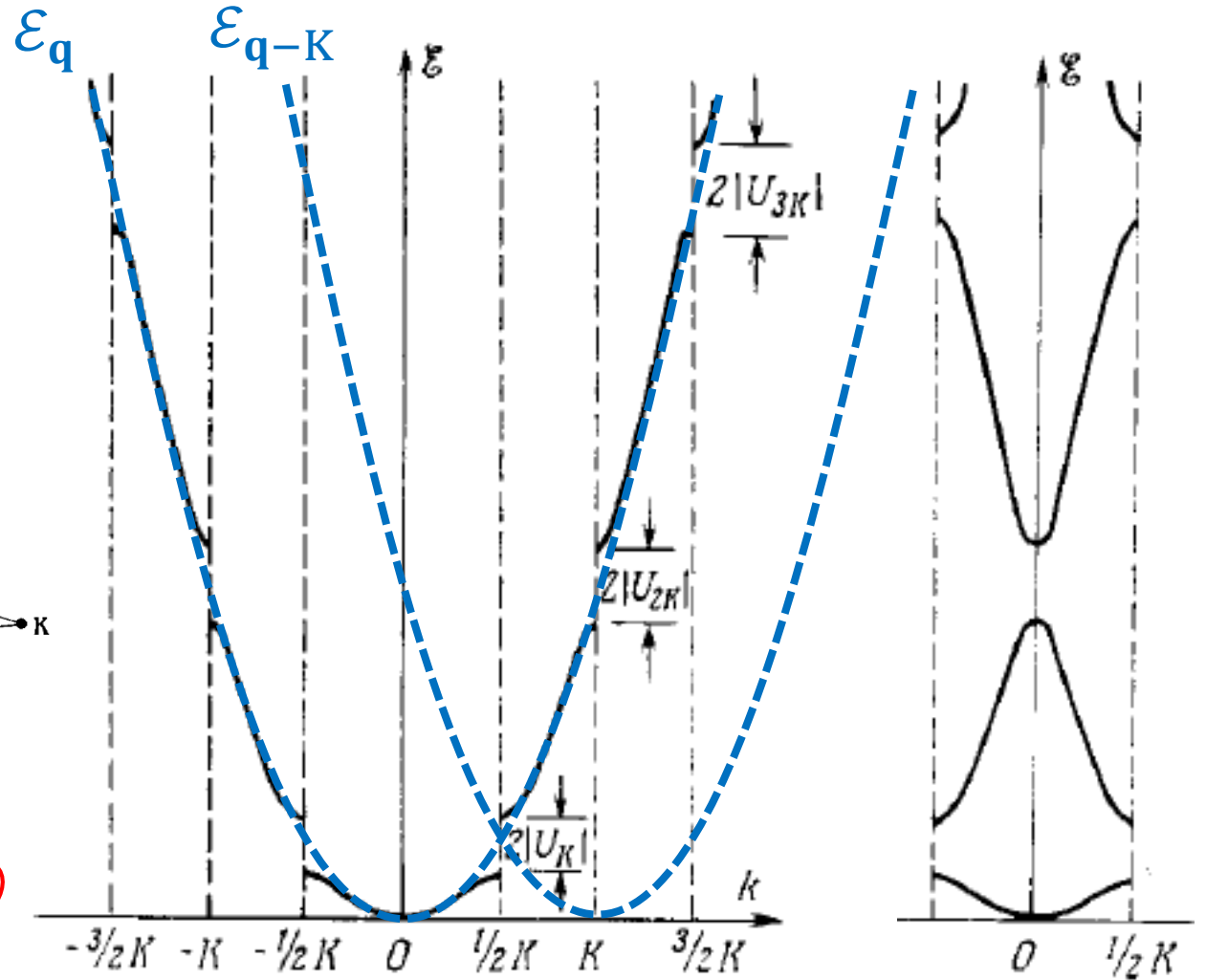


$$\begin{vmatrix} \mathcal{E} - \mathcal{E}_q^0 & -U_K \\ -U_K^* & \mathcal{E} - \mathcal{E}_{q-K}^0 \end{vmatrix} = 0$$



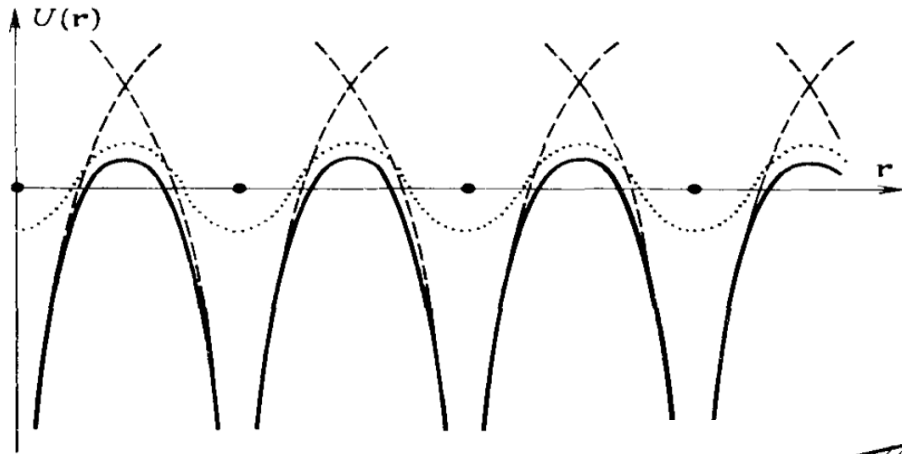
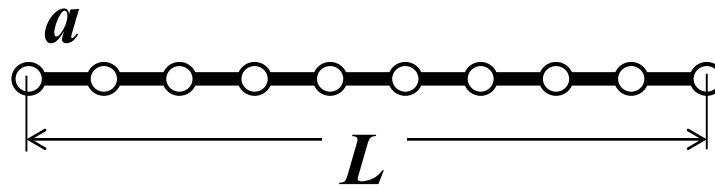
$$(\mathcal{E} - \mathcal{E}_q^0)(\mathcal{E} - \mathcal{E}_{q-K}^0) = |U_K|^2$$

$$\mathcal{E} = \frac{1}{2} (\mathcal{E}_q^0 + \mathcal{E}_{q-K}^0) \pm \left[ \left( \frac{\mathcal{E}_q^0 - \mathcal{E}_{q-K}^0}{2} \right)^2 + |U_K|^2 \right]^{1/2}$$

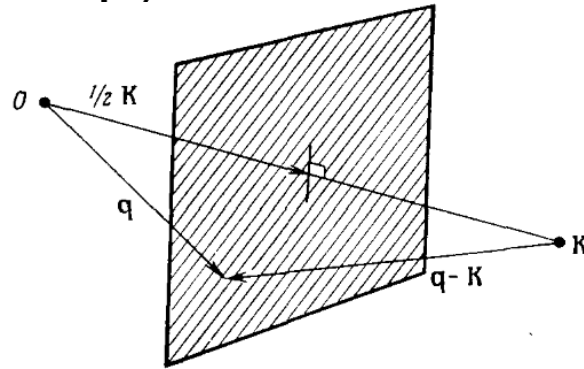


$$K = 2\pi/a$$

# Band gaps

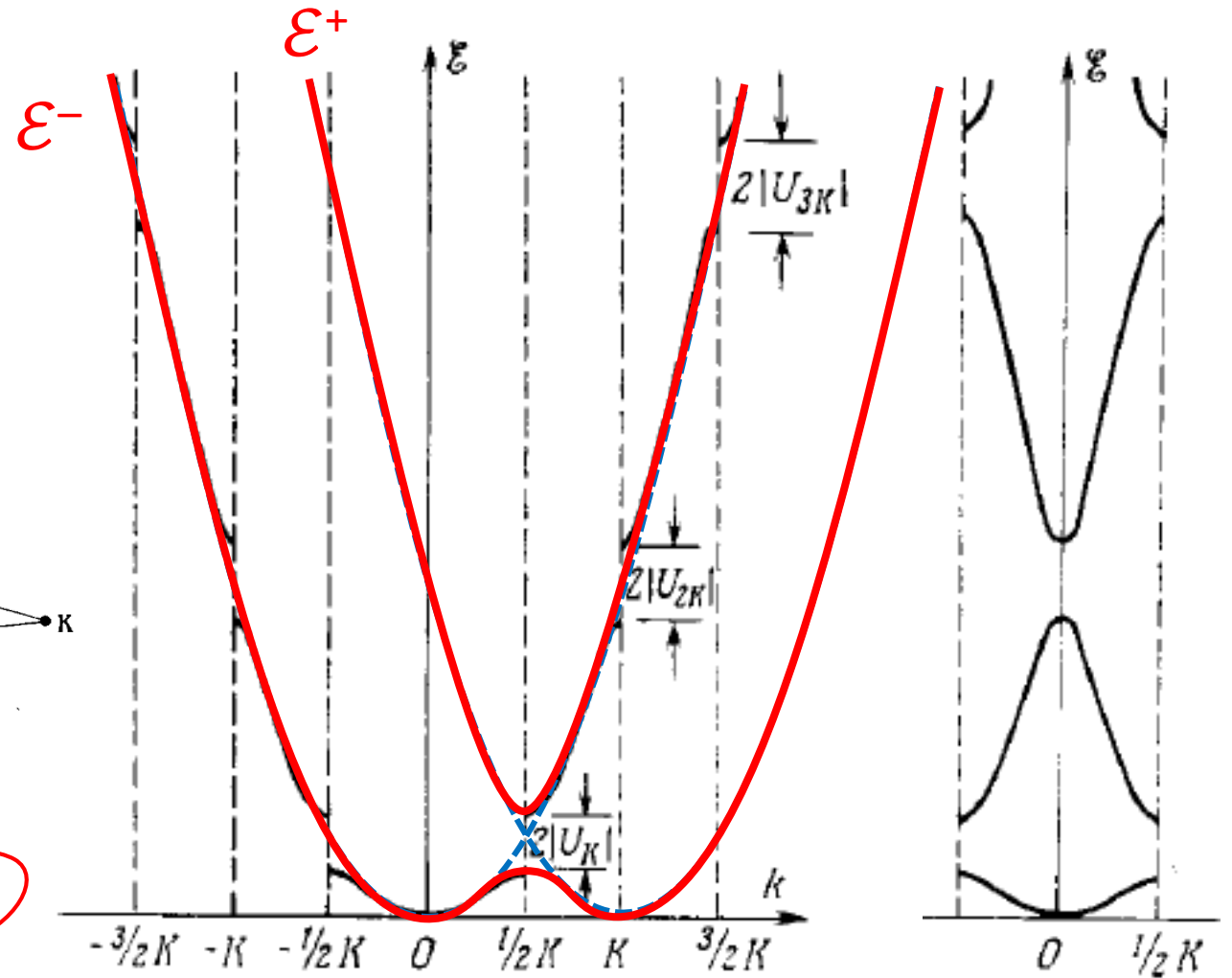


$$\begin{vmatrix} \mathcal{E} - \mathcal{E}_q^0 & -U_K \\ -U_K^* & \mathcal{E} - \mathcal{E}_{q-K}^0 \end{vmatrix} = 0$$

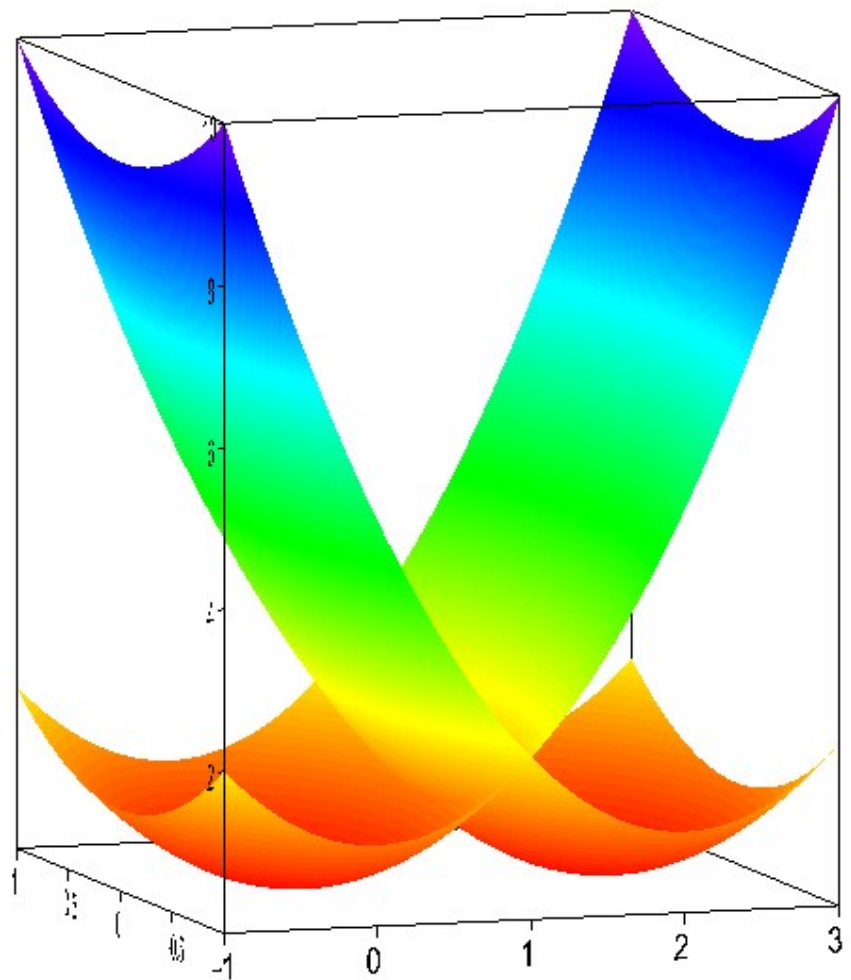


$$(\mathcal{E} - \mathcal{E}_q^0)(\mathcal{E} - \mathcal{E}_{q-K}^0) = |U_K|^2$$

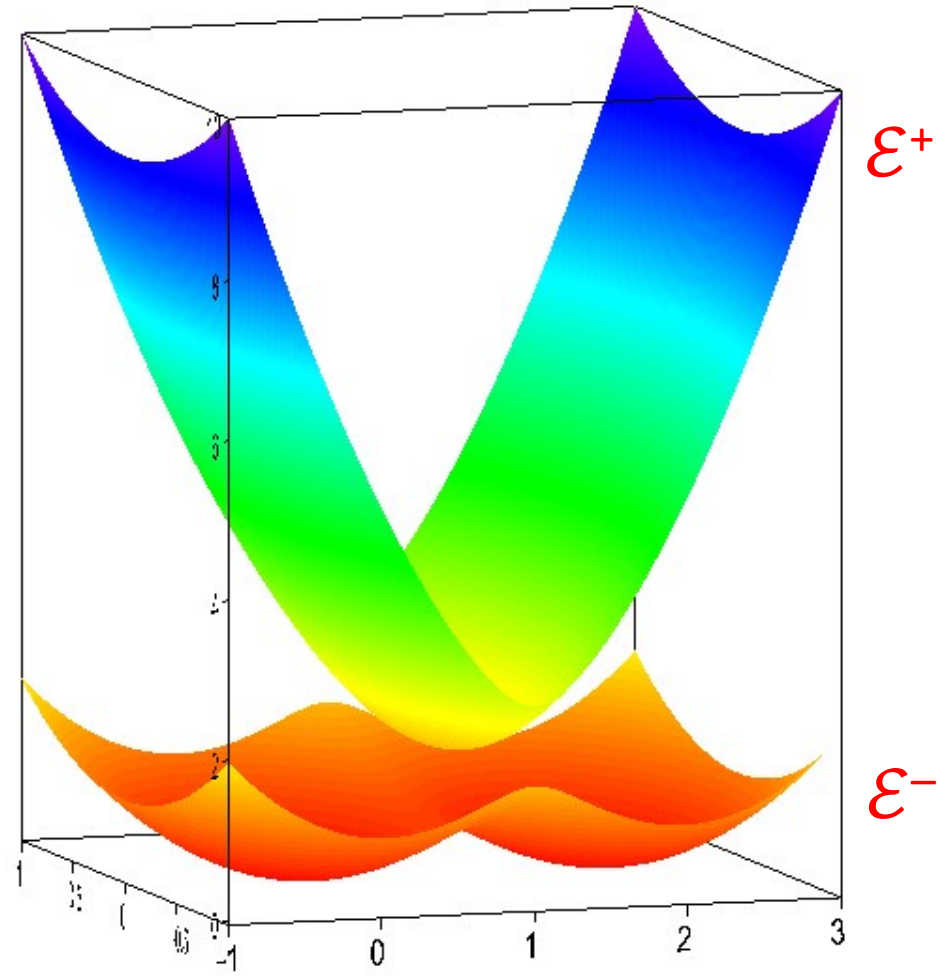
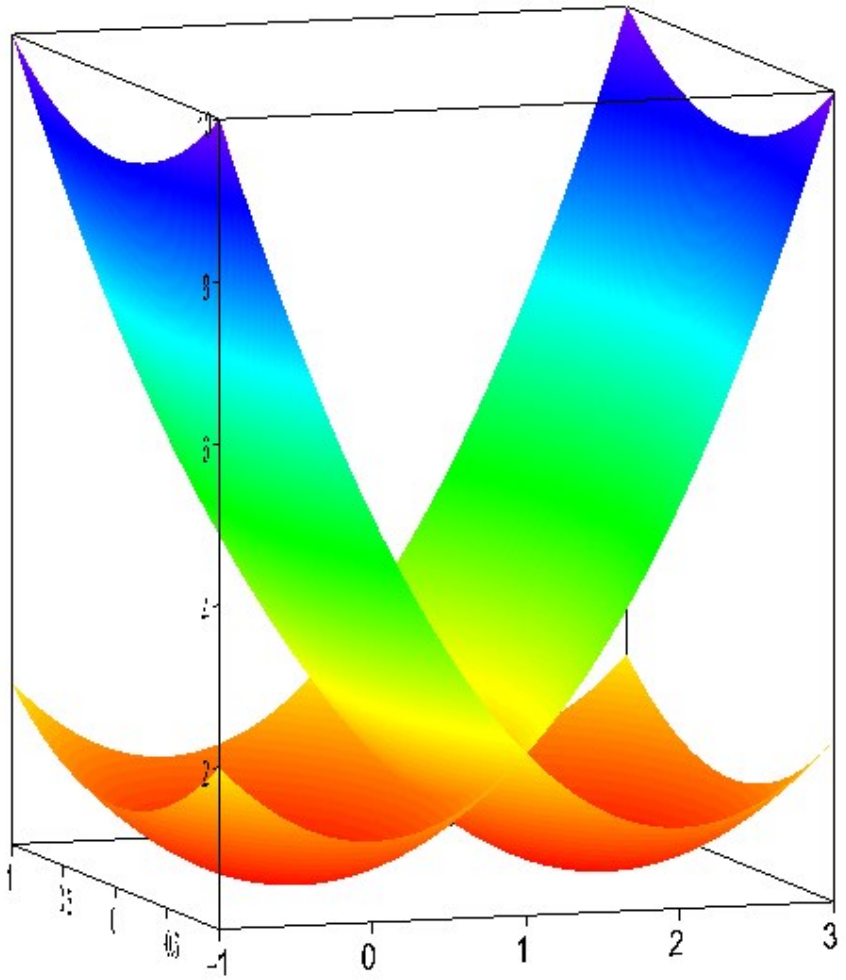
$$\mathcal{E}^{\pm} = \frac{1}{2} (\mathcal{E}_q^0 + \mathcal{E}_{q-K}^0) \pm \left[ \left( \frac{\mathcal{E}_q^0 - \mathcal{E}_{q-K}^0}{2} \right)^2 + |U_K|^2 \right]^{1/2}$$



$$K = 2\pi/a$$



$$\mathcal{E} = \frac{1}{2} (\mathcal{E}_{\mathbf{q}}^0 + \mathcal{E}_{\mathbf{q}-\mathbf{K}}^0) \pm \left[ \left( \frac{\mathcal{E}_{\mathbf{q}}^0 - \mathcal{E}_{\mathbf{q}-\mathbf{K}}^0}{2} \right)^2 + |U_{\mathbf{K}}|^2 \right]^{1/2}$$



$\text{Disp0} = (x)^2 + y^2$   
 $\text{Disp1} = (x-2)^2 + y^2$

$$\mathcal{E}^{\pm} = \frac{1}{2} (\mathcal{E}_q^0 + \mathcal{E}_{q-K}^0) \pm \left[ \left( \frac{\mathcal{E}_q^0 - \mathcal{E}_{q-K}^0}{2} \right)^2 + |U_K|^2 \right]^{1/2}$$

Variable Delta = 0.5

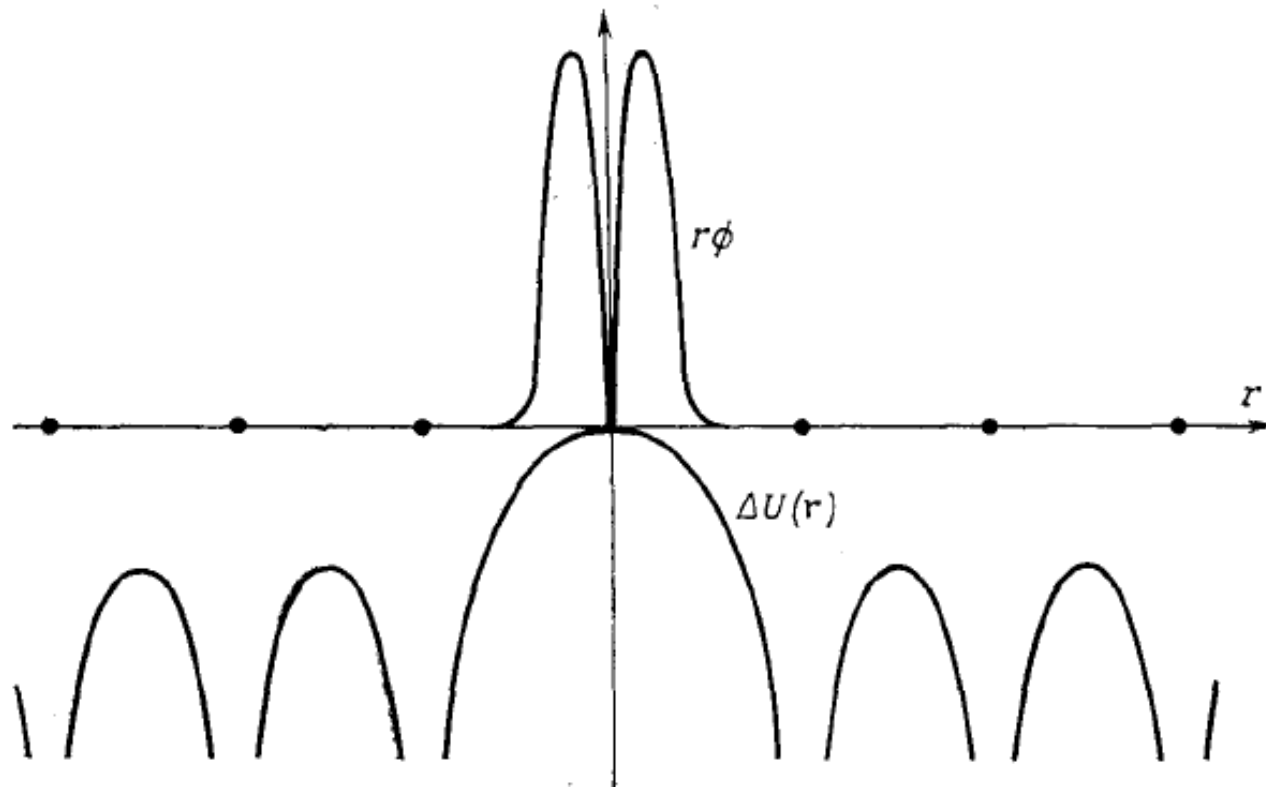
$$\text{Disp2} = (\text{Disp1}(x)(y) + \text{Disp0}(x)(y))/2 + \text{sqrt}(\left( (\text{Disp1}(x)(y) - \text{Disp0}(x)(y) )/2 \right)^2 + \text{Delta}^2)$$

$$\text{Disp3} = (\text{Disp1}(x)(y) + \text{Disp0}(x)(y))/2 - \text{sqrt}(\left( (\text{Disp1}(x)(y) - \text{Disp0}(x)(y) )/2 \right)^2 + \text{Delta}^2)$$

## Метод сильного зв'язку – Tight binding (TB) model

$$H_{\text{at}}\psi_n = E_n\psi_n$$

$$H = H_{\text{at}} + \Delta U(\mathbf{r})$$



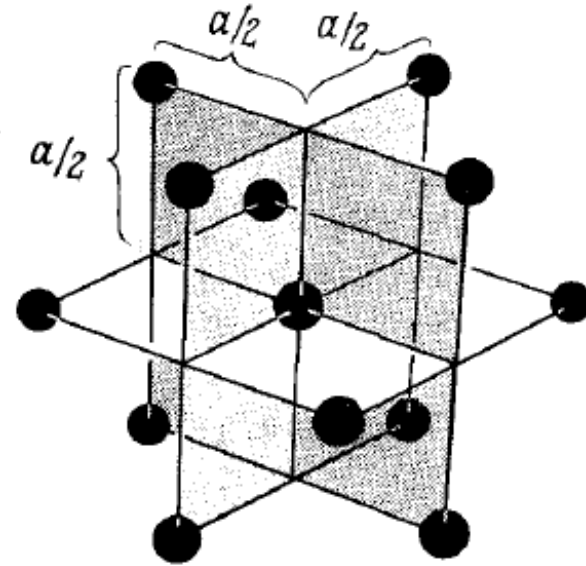
## Метод сильного зв'язку – Tight binding (TB) model

$$\xi(\mathbf{k}) = E_s - \frac{\beta + \sum \gamma(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}}{1 + \sum \alpha(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}}$$

$$\beta = - \int d\mathbf{r} \Delta U(\mathbf{r}) |\phi(\mathbf{r})|^2,$$

$$\alpha(\mathbf{R}) = \int d\mathbf{r} \phi^*(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R}),$$

$$\gamma(\mathbf{R}) = - \int d\mathbf{r} \phi^*(\mathbf{r}) \Delta U(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R}).$$



$$\xi(\mathbf{k}) = E_s - \beta - 4\gamma (\cos \frac{1}{2}k_x a \cos \frac{1}{2}k_y a + \cos \frac{1}{2}k_y a \cos \frac{1}{2}k_z a + \cos \frac{1}{2}k_z a \cos \frac{1}{2}k_x a)$$



# Модель перескоків

$$|\varphi\rangle = \sum_n |n\rangle \langle n | \varphi\rangle$$

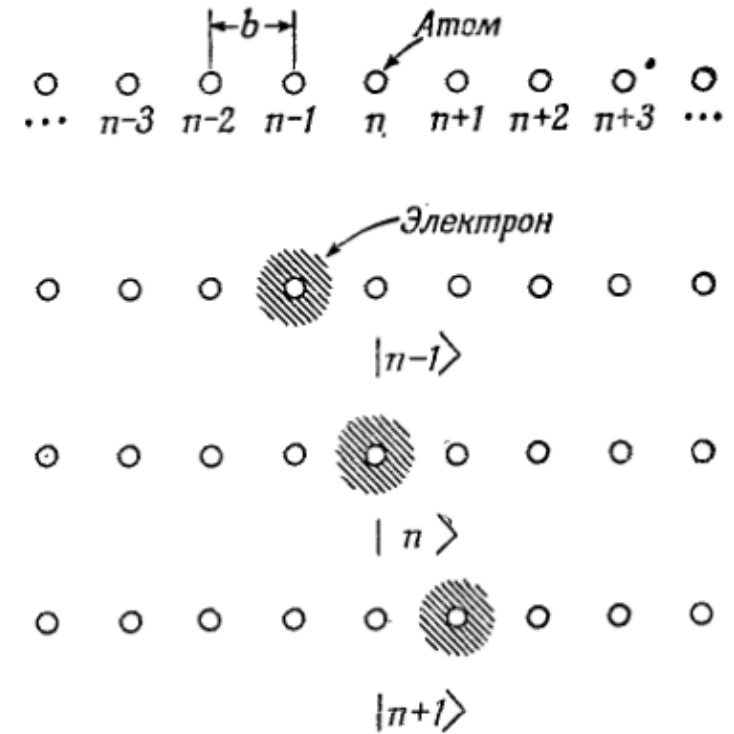
$$|\varphi\rangle = \sum_n |n\rangle C_n$$

$$\begin{aligned} & \vdots & & \vdots \\ i\hbar \frac{dC_{n-1}}{dt} &= E_0 C_{n-1} - AC_{n-2} - AC_n, \\ i\hbar \frac{dC_n}{dt} &= E_0 C_n - AC_{n-1} - AC_{n+1}, \\ i\hbar \frac{dC_{n+1}}{dt} &= E_0 C_{n+1} - AC_n - AC_{n+2}. \\ & \vdots & & \vdots \end{aligned}$$

$$i\hbar \frac{dC_n(t)}{dt} = E_0 C_n(t) - AC_{n+1}(t) - AC_{n-1}(t) \quad C_n = a(x_n) e^{-iEt/\hbar}$$

$$Ea(x_n) = E_0 a(x_n) - Aa(x_{n+1}) - Aa(x_{n-1})$$

Базисні стани електронів



$$Ea(x_n) = E_0 a(x_n) - Aa(x_{n+1}) - Aa(x_{n-1}) \quad x_{n+1} = x_n + b$$

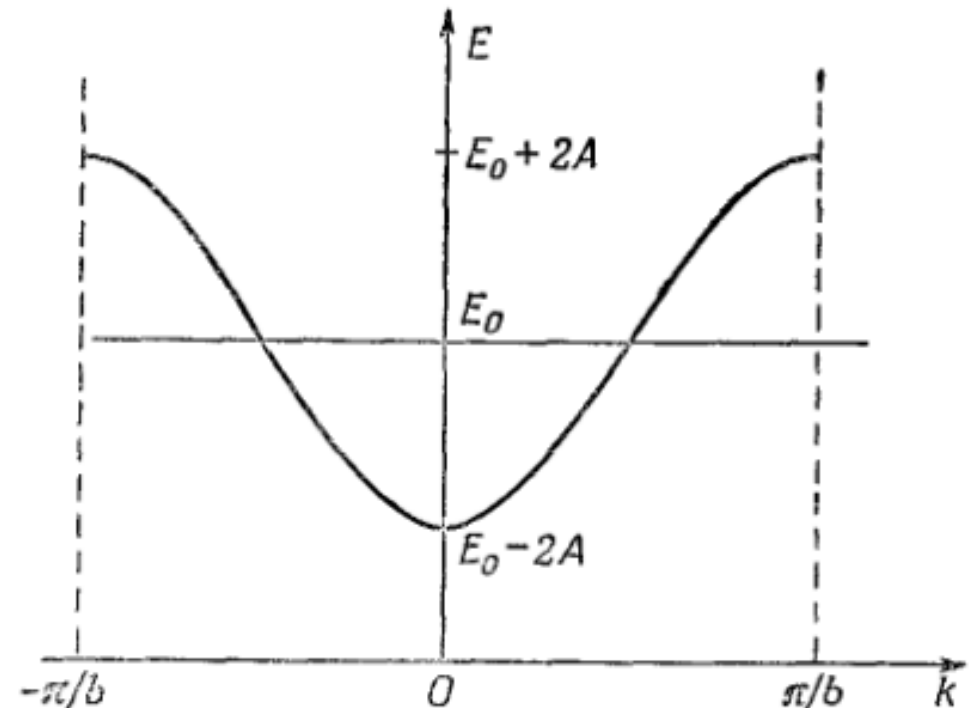
$$Ea(x_n) = E_0 a(x_n) - Aa(x_n + b) - Aa(x_n - b)$$

$$a(x_n) = e^{ikx_n} \quad Ee^{ikx_n} = E_0 e^{ikx_n} - Ae^{ik(x_n+b)} - Ae^{ik(x_n-b)}$$

$$E = E_0 - Ae^{ikb} - Ae^{-ikb}$$

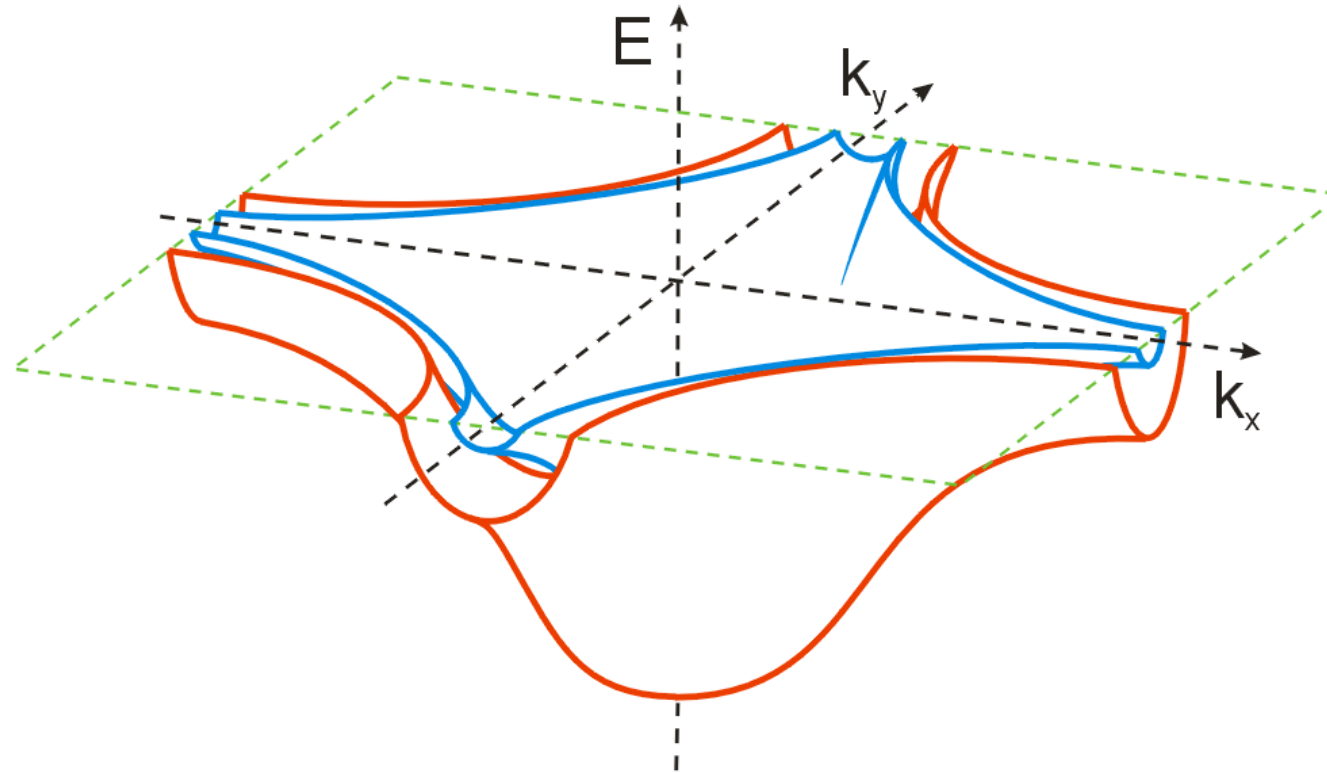
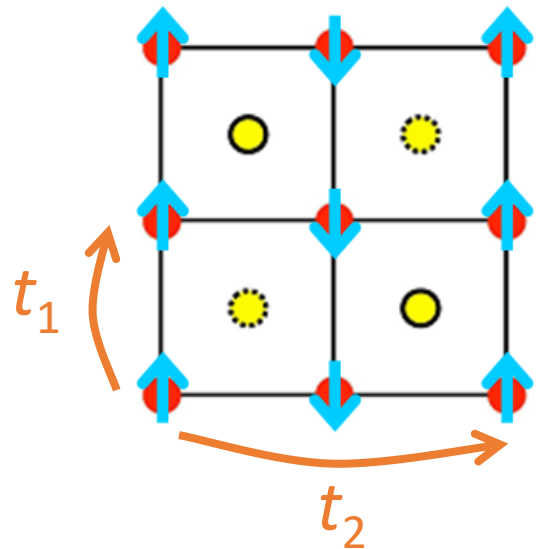
$$E = E_0 - 2A \cos kb$$

$$E = E_0 + t_1 \cos(ak) + t_2 \cos(2ak) + \dots$$



## Модель перескоків в 2D

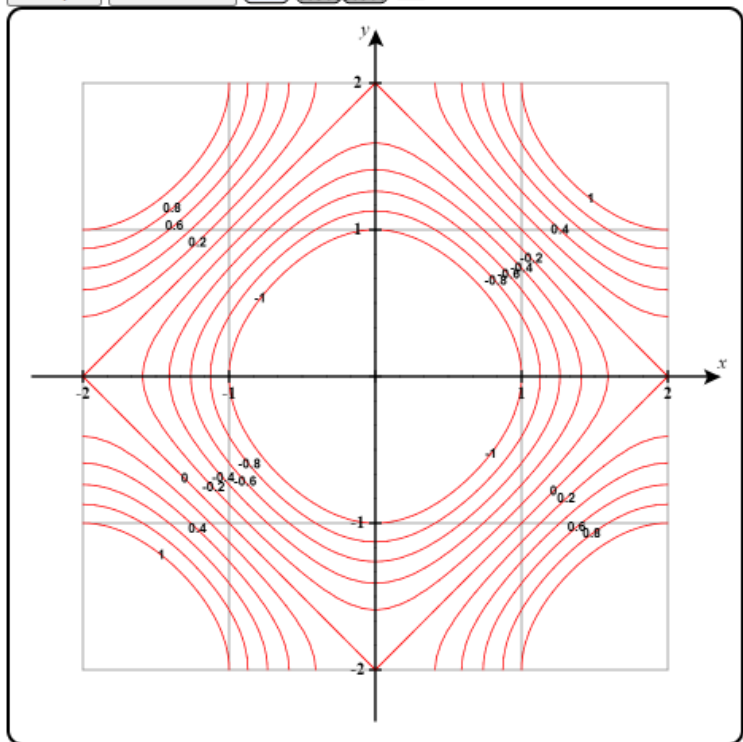
$$E = E_0 + t_1(\cos(ak_x) + \cos(ak_y)) + t_2(\cos(2ak_x) + \cos(2ak_y)) + \dots$$



$$\varepsilon(k) = \varepsilon_0 + t_1 \cos(ka) + t_2 \cos(2ka)$$



Graph 3D Mode



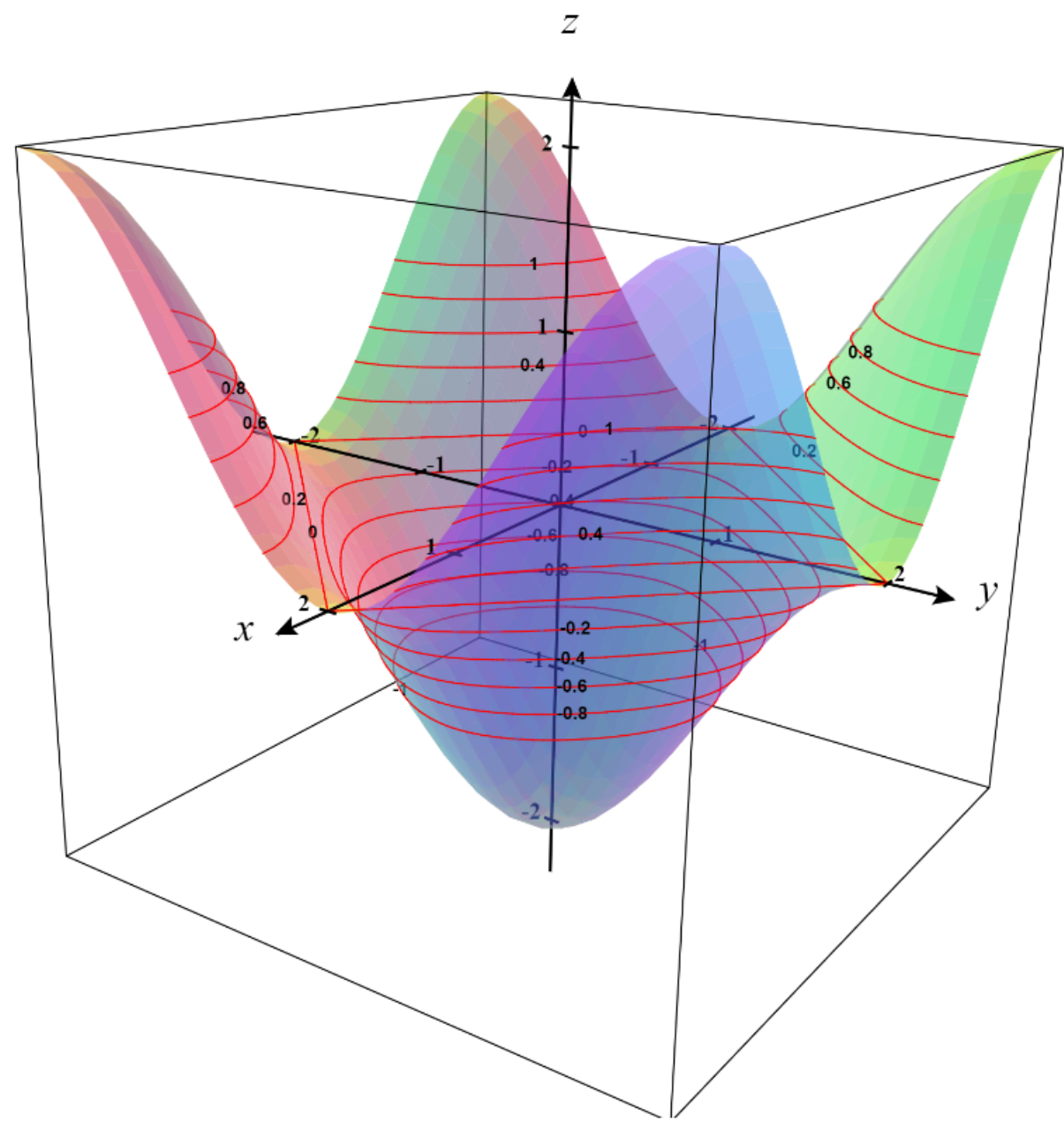
x =

y =

Add to graph:

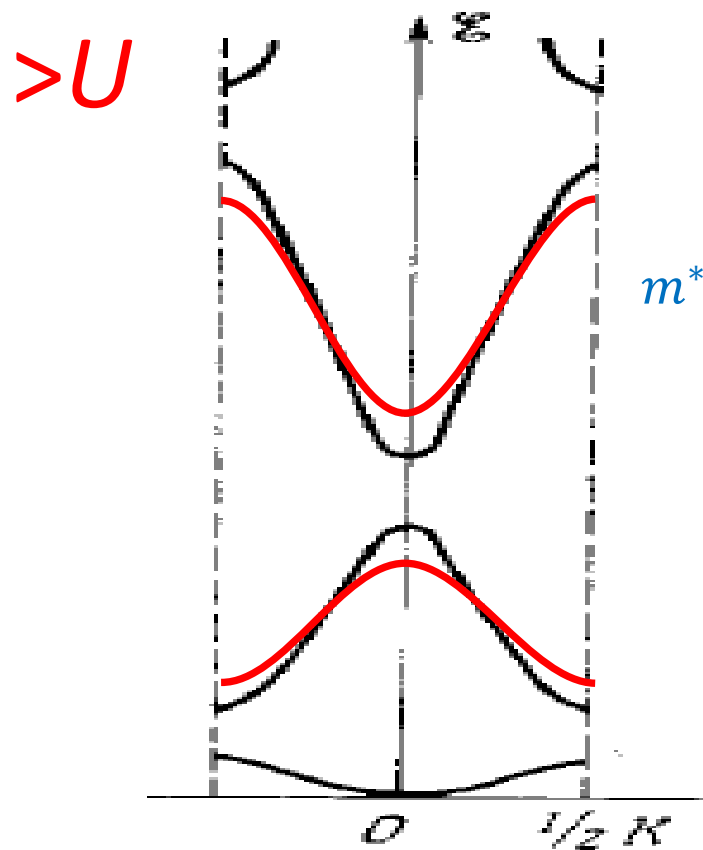
$z = -\cos(\pi x/2) - \cos(\pi y/2)$

Number of Gridlines



## Наближення слабого зв'язку

$$\mathcal{E} = \frac{1}{2} (\mathcal{E}_q^0 + \mathcal{E}_{q-K}^0) \pm \left[ \left( \frac{\mathcal{E}_q^0 - \mathcal{E}_{q-K}^0}{2} \right)^2 + |U_K|^2 \right]^{1/2}$$

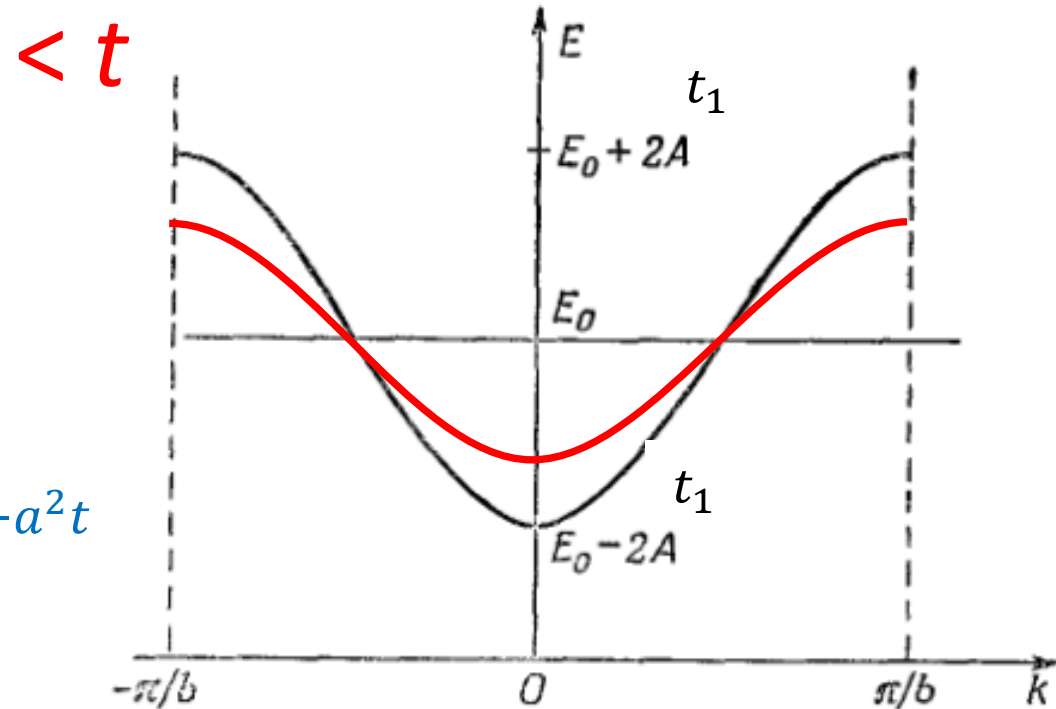


$$m^* = \pm \frac{a^2 m^2 |U_{nK}|}{(n\pi)^2}$$

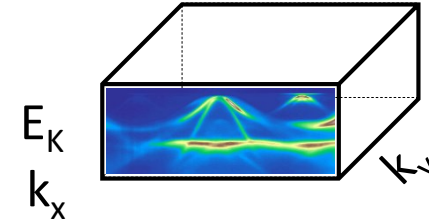
$$m^* = -a^2 t$$

## Модель перескоків

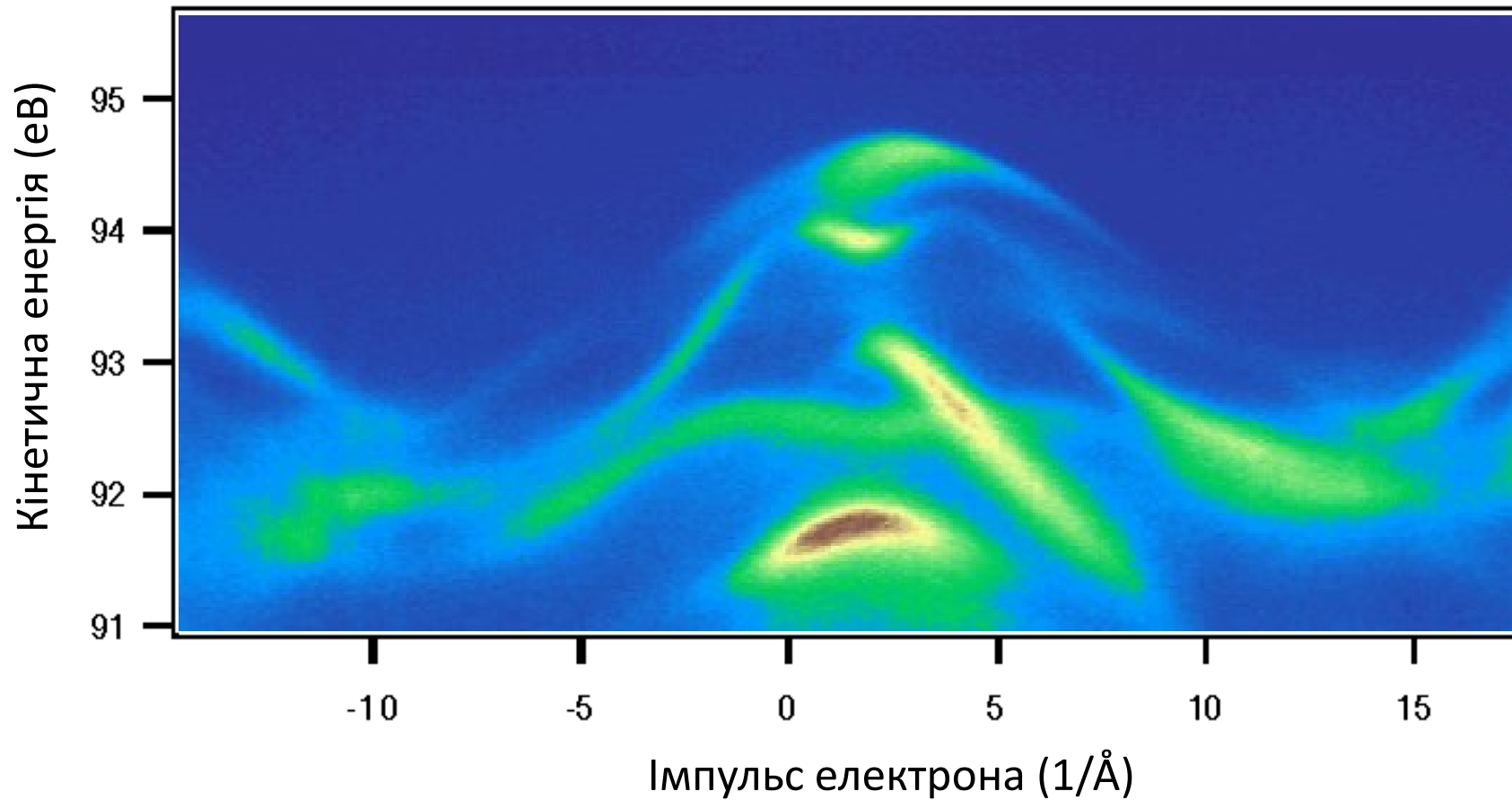
$$E = E_0 + t_1 \cos(ak) + t_2 \cos(2ak) + \dots$$



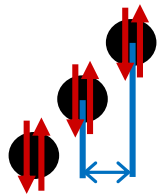
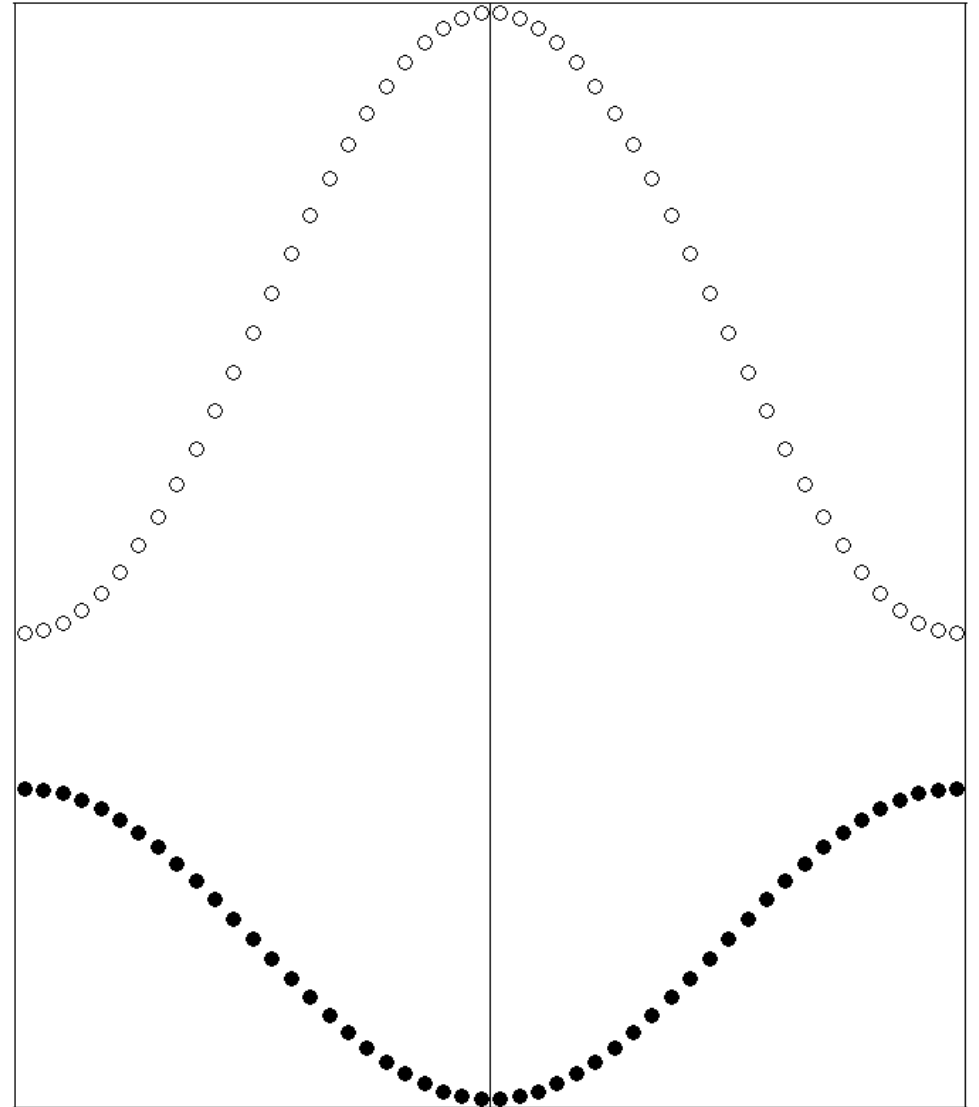
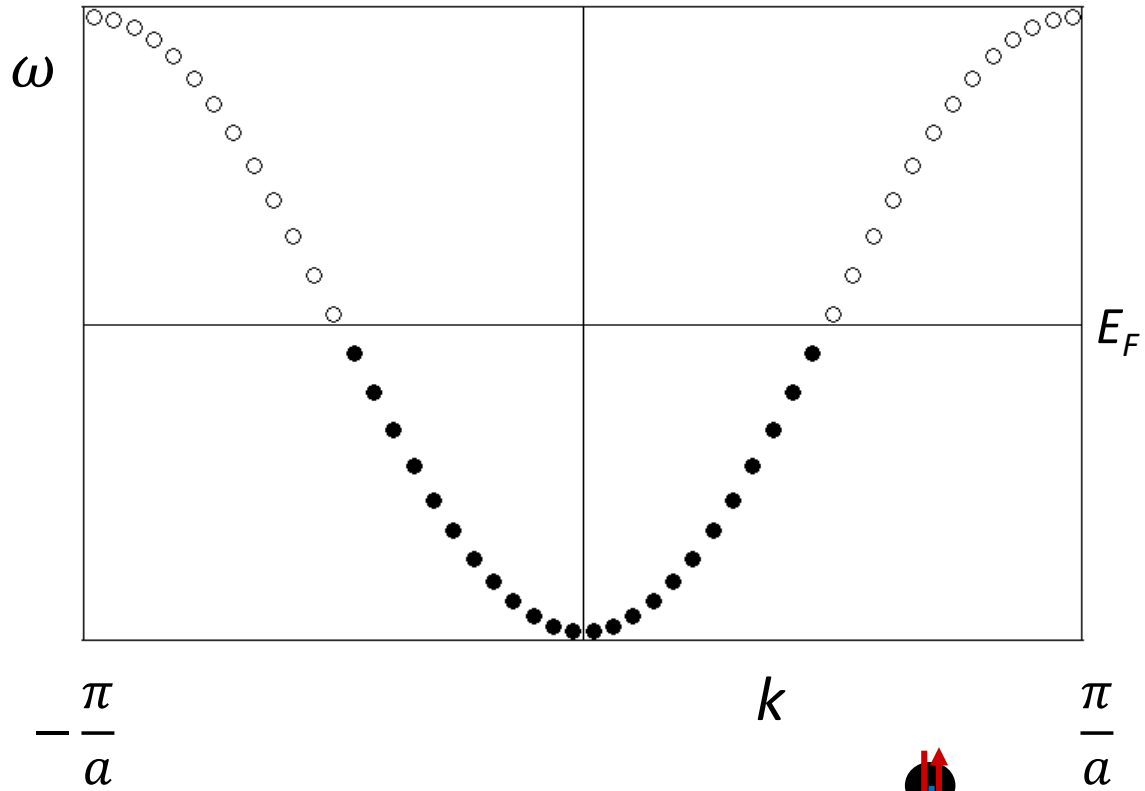
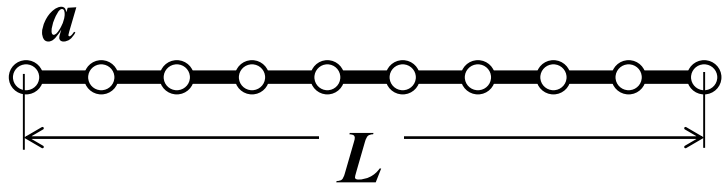
# Electronic spectrum in momentum-energy 3D space



TiSe<sub>2</sub> - «excitonic insulator»

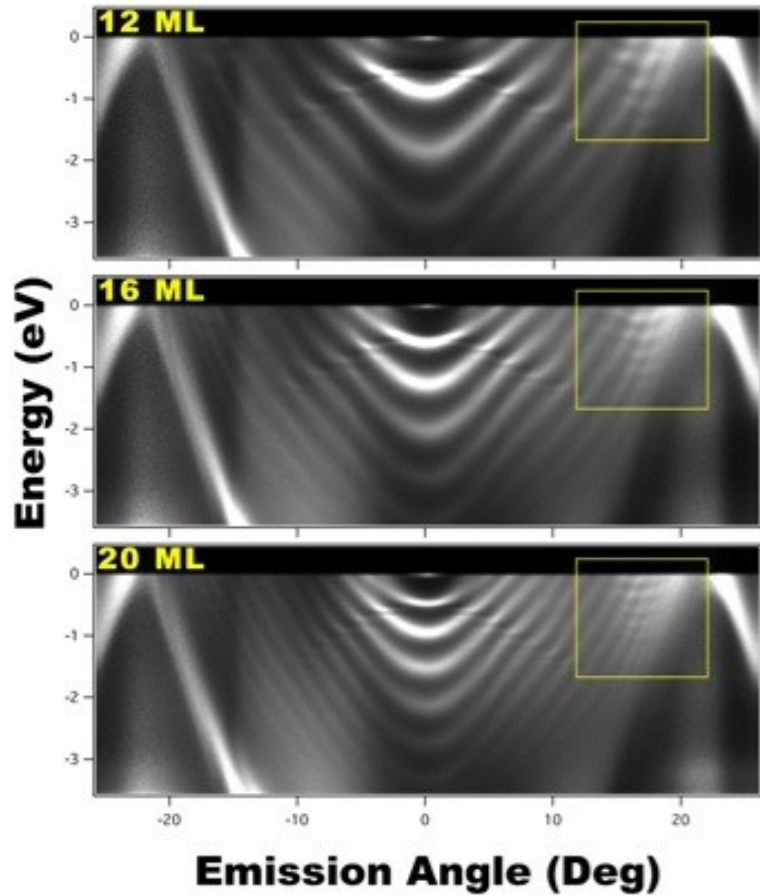


# Metal vs Insulator



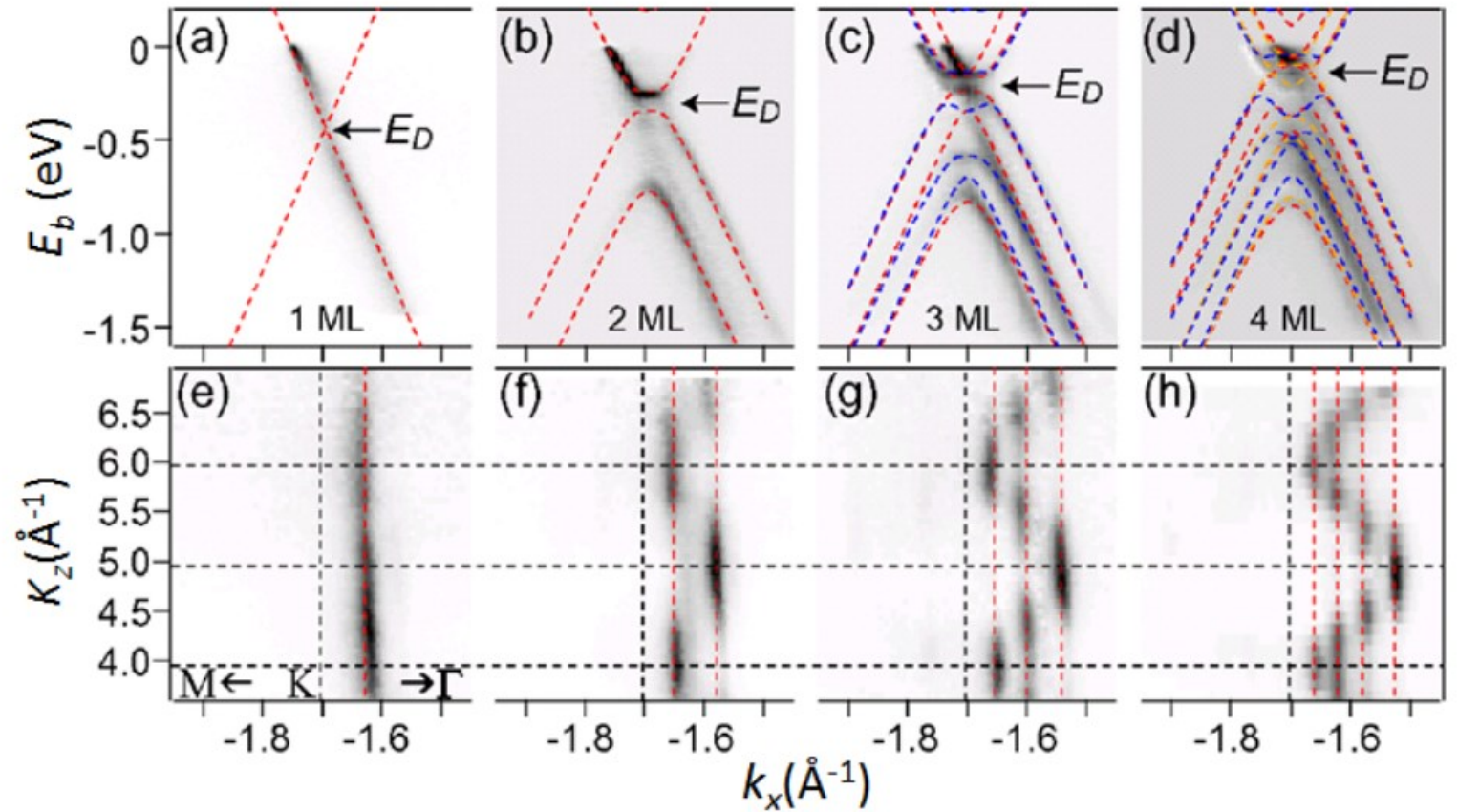
$$dk = 2\pi/L$$

## Quantum confinement



ARPES data for atomically-uniform Ag films of 12, 16 and 20 monolayers (ML) grown on Si(111)-(7x7) substrates

<http://groups.mrl.uiuc.edu/chiang/Speer/Nathan%20J%20Speer/Umklaup-Mediated%20Quantized%20States.html>



ARPES data on graphene multilayers

V. N. Strocov <https://arxiv.org/abs/1801.07505>