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EE-606: Solid State Devices
Lecture 5: Energy Bands

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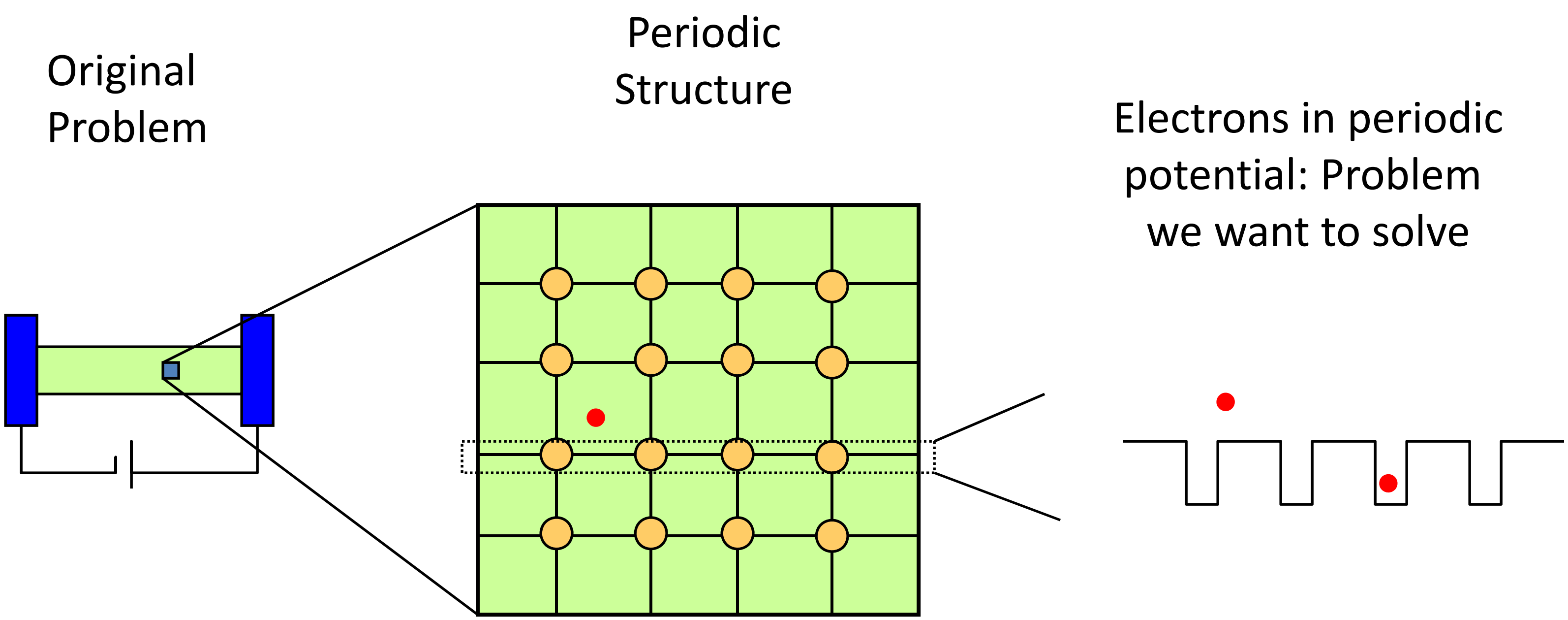
Outline

1) **Schrodinger equation in periodic U(x)**
2) Bloch theorem
3) Band structure
4) Properties of electronic bands
5) Conclusions

Reference: Vol. 6, Ch. 3 (pages 51-62)

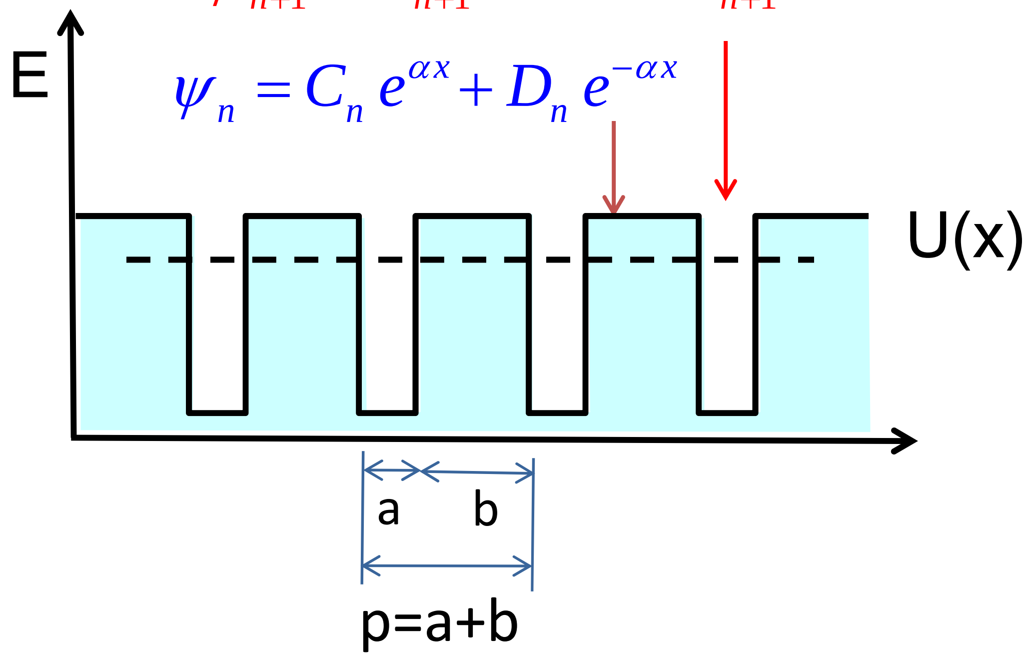
Getting Back to Crystals



Finally an (almost) Real Problem ...

$$\psi_{n+1} = A_{n+1}\sin kx + B_{n+1}\cos kx$$

$$\psi_n = C_n e^{\alpha x} + D_n e^{-\alpha x}$$



But N atoms have two 2N unknown constants to find ....
For large N, isn't there a better way ?

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2) **Bloch theorem**

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Four Steps of Finding Energy Levels in Crystals

1) $$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

2) $$\psi(x = -\infty) = 0$$
$$\psi(x = +\infty) = 0$$

3) $$\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$$
$$\frac{d\psi}{dx}\bigg|_{x=x_B^-} = \frac{d\psi}{dx}\bigg|_{x=x_B^+}$$

4) Det(coefficient matix)=0

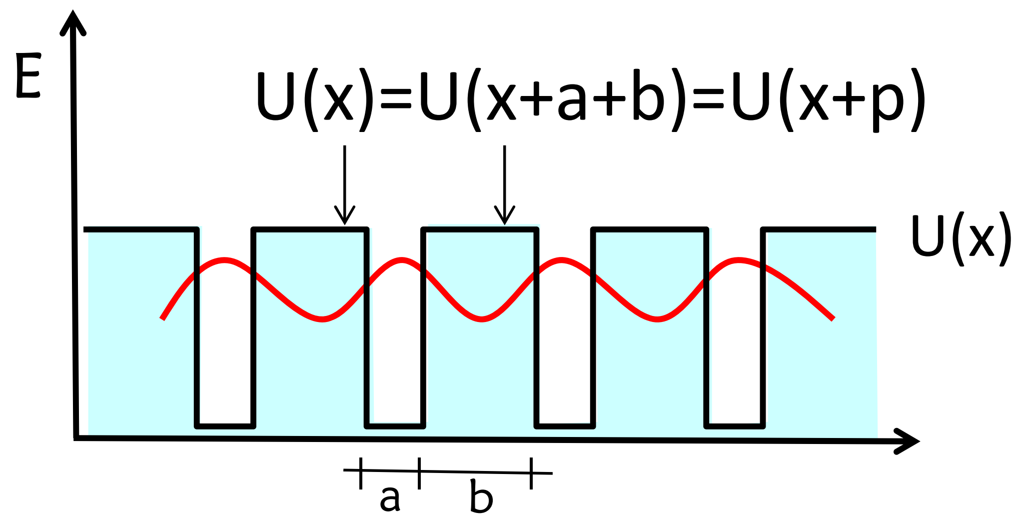
Set 2N-2 equations for 2N-2 unknowns

N is very large for crystal, but changing steps 2 and 3 a little bit we can still solve the problem in a few minutes!

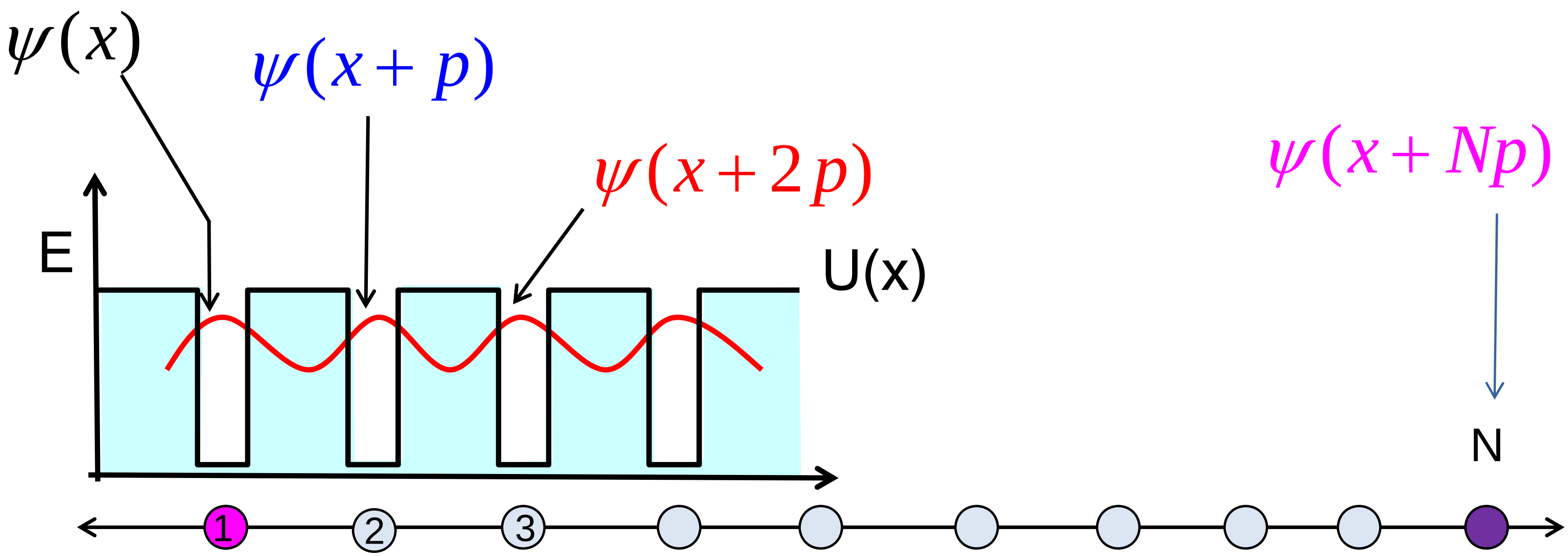
Periodic U(x) and Bloch's Theorem

not our old (k)

$$|\psi(x)|^2 = |\psi(x+p)|^2 \quad \Rightarrow \quad \psi(x+p) = \psi(x)\,e^{ikp}$$



Phase-factor for N-cells

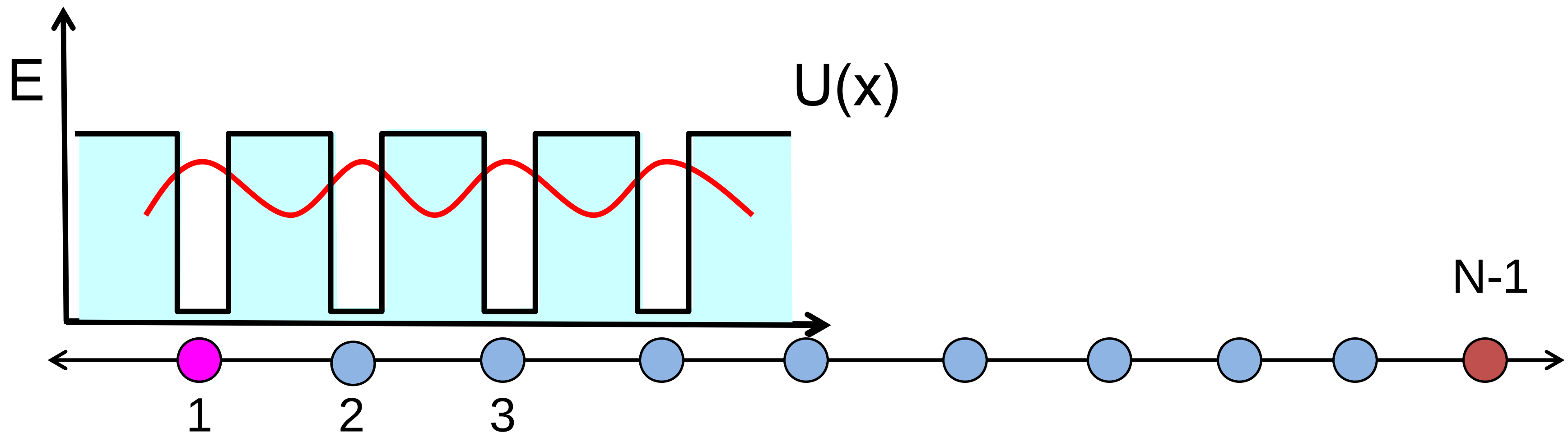


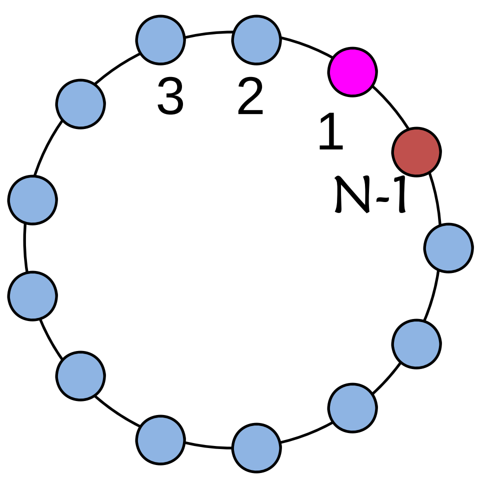
$$\psi[x+p] = \psi(x)e^{ikp}$$

$$\psi[x+2p] = \psi(x+p)e^{ikp}$$
$$= \psi(x)e^{ikp\times 2}$$

$$\psi[x+Np] = \psi(x)e^{ikpN}$$

Step 2: Periodic Boundary Condition





$$\psi[x+Np] = \psi(x)e^{ikpN}$$

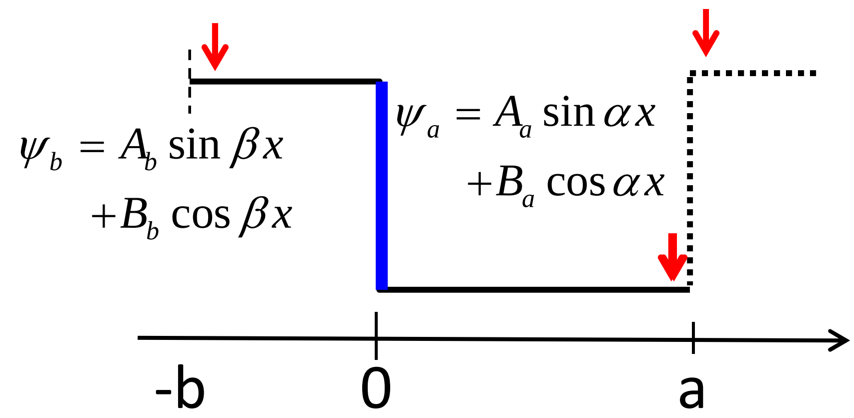
$$e^{ikpN} = 1 \equiv e^{\pm i2\pi n}$$

$$k = \pm\frac{2\pi n}{Np} \quad n = -\frac{N}{2}.....-1,0,1,....\frac{N}{2}$$

$$k_{\max} = \frac{\pi}{p}, \quad k_{\min} = -\frac{\pi}{p}$$

Step 3: Boundary Conditions

$$\alpha \equiv \sqrt{2mE/\hbar^2} \qquad \beta \equiv i\sqrt{2m(U_0 - E)/\hbar^2}$$



$$\psi\big|_{x=0^-} = \psi\big|_{x=0^+}$$

$$\left.\frac{d\psi}{dx}\right|_{x=0^-} = \left.\frac{d\psi}{dx}\right|_{x=0^+}$$

$$B_a = B_b$$

$$\alpha A_a = \beta A_b$$

$$\psi_a\big|_{x=a} = \psi_b\big|_{x=-b}\, e^{ikp}$$

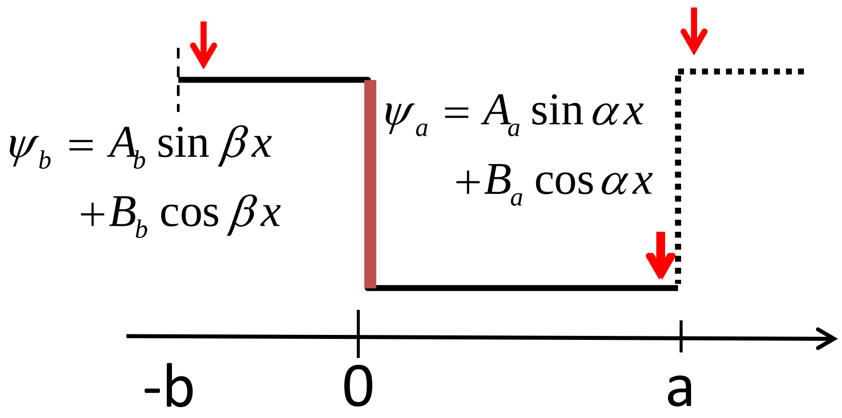
$$\left.\frac{d\psi_a}{dx}\right|_{x=a} = \left.\frac{d\psi_b}{dx}\right|_{x=-b} e^{ikp}$$

$$A_a \sin \alpha a + B_a \cos \alpha a = e^{ik(a+b)}[-A_b \sin \beta b + B_b \cos \beta b]$$

$$\alpha A_a \sin \alpha a - \alpha B_a \cos \alpha a = e^{ik(a+b)}[\beta A_b \sin \beta b + \beta B_b \cos \beta b]$$

Step 4: Det(matrix)=0 for Energy-levels

$$B_a = B_b$$
$$\alpha A_a = \beta A_b$$



$$A_a \sin \alpha a + B_a \cos \alpha a = e^{ik(a+b)}[-A_b \sin \beta b + B_b \cos \beta b]$$

$$\alpha A_a \sin \alpha a - \alpha B_a \cos \alpha a = e^{ik(a+b)}[\beta A_b \sin \beta b + \beta B_b \cos \beta b]$$

$\Rightarrow$

4)
$$\begin{pmatrix} 0 & 1 & 0 & -1 \\ \alpha & 0 & \beta & 0 \\ * & * & & \\ * & & & \end{pmatrix} \begin{bmatrix} A_a \\ B_a \\ A_b \\ B_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$\Downarrow$

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}} \times \ldots\ldots\ldots\ldots = \cos kp \qquad \xi \equiv \frac{E}{U_0} \qquad \alpha_0 \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$

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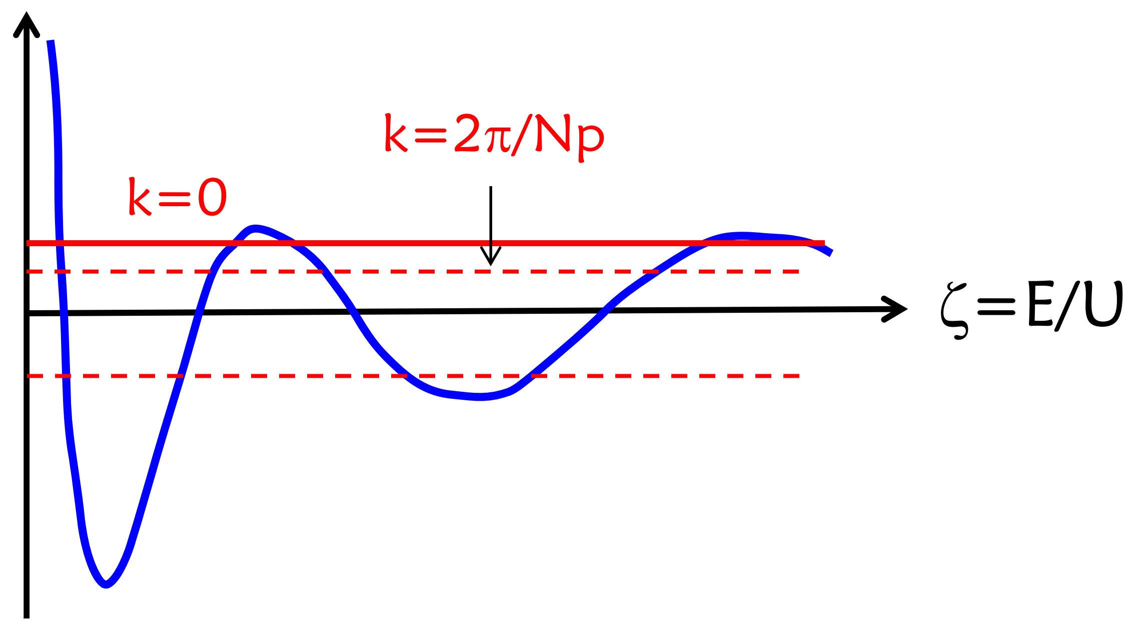
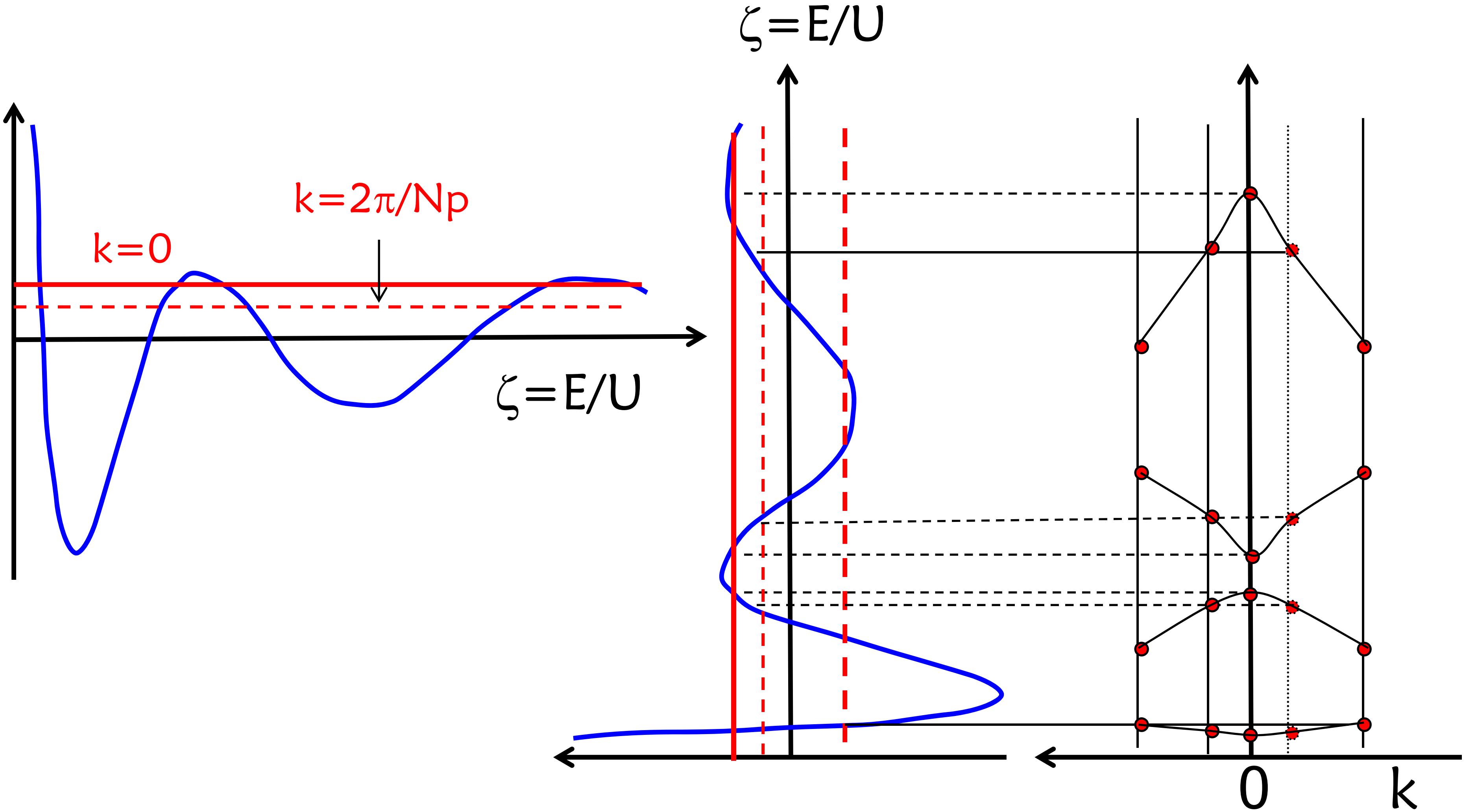
Graphical solution to Energy Levels

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}} \times \ldots\ldots\ldots\ldots = \cos kp$$

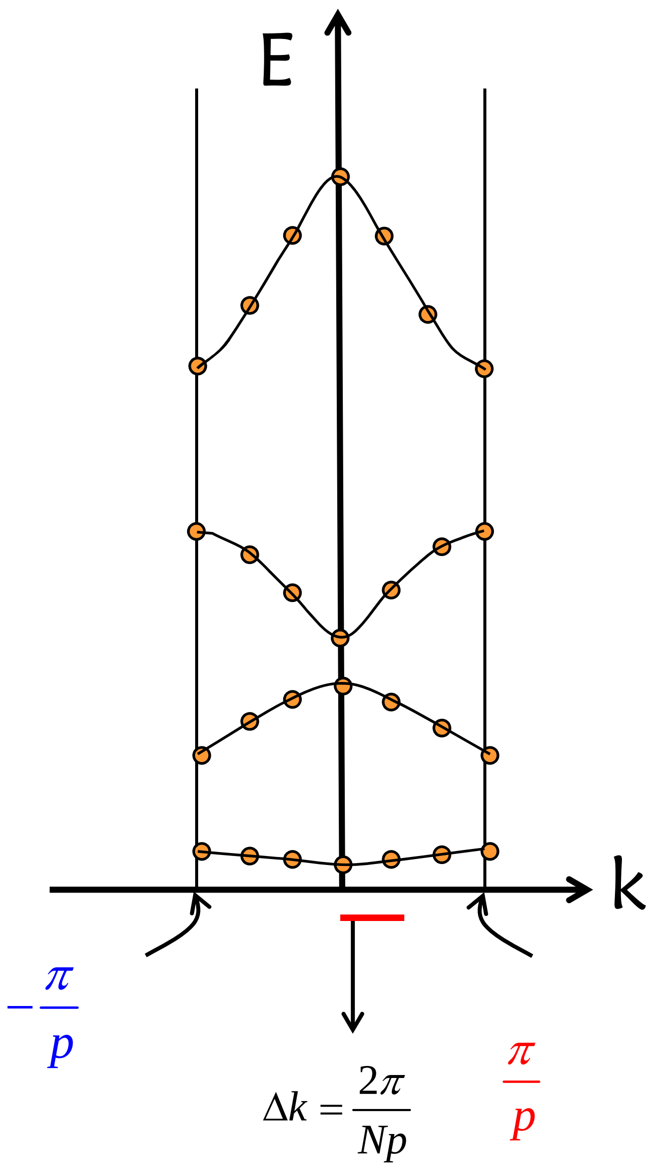
$$k = \pm\frac{2\pi n}{Np} \quad n = -\frac{N}{2}\ldots\ldots -1, 0, 1, \ldots\ldots \frac{N}{2}$$



Energy Band Diagram



Brillouin Zone and Number of States



$$k = \pm\frac{2\pi n}{Np} \qquad n = -\frac{N}{2} \ldots\ldots -1, 0, 1, \ldots\ldots \frac{N}{2}$$

$$\frac{States}{band} = \frac{k_{max} - k_{min}}{\Delta k} = \frac{2\pi/p}{2\pi/Np} = N$$

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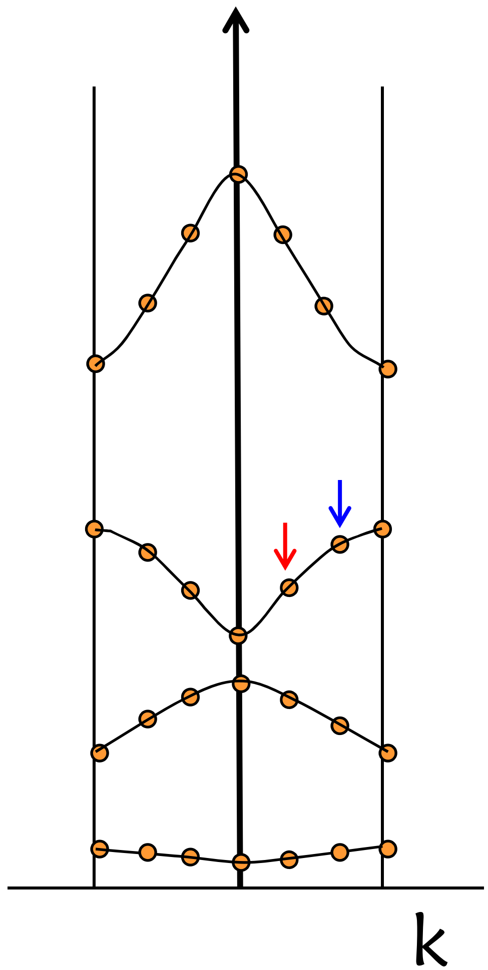
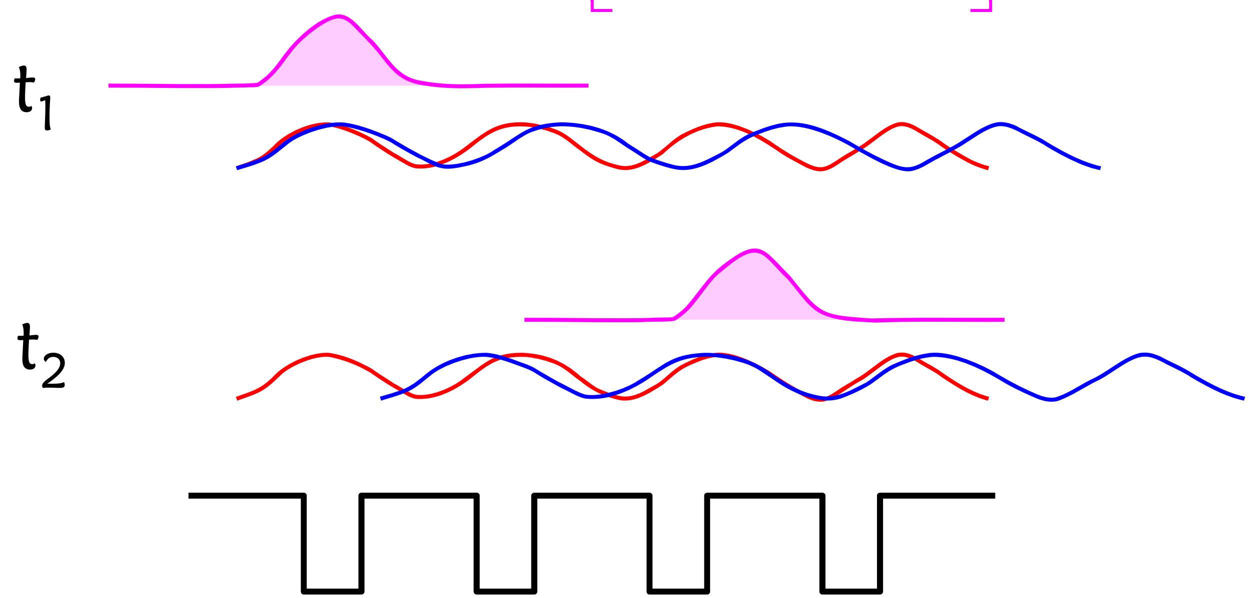
Wave Packet and Group Velocity



$$\psi(x,t) = Ae^{ikx - i\frac{E}{\hbar}t} + Ae^{i(k+\Delta k)x - i\left(\frac{E+\Delta E}{\hbar}\right)t}$$

$$= Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i(\Delta k)x - i\left(\frac{\Delta E}{\hbar}\right)t}\right]$$

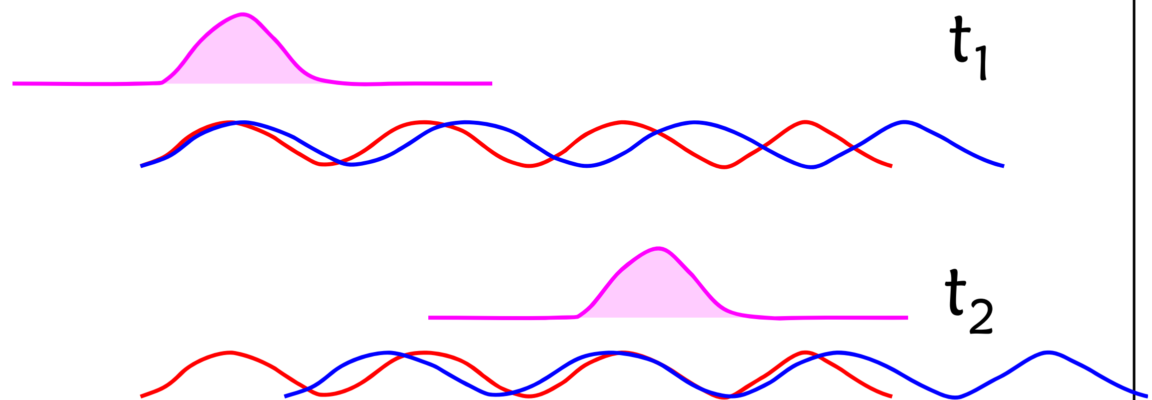


Group Velocity for a Given Band

$$\psi(x,t)$$

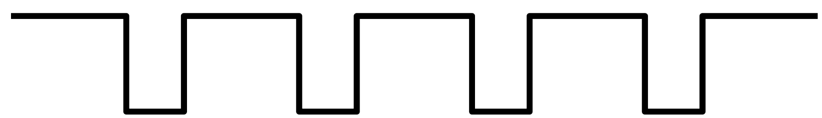
$$= Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i(\Delta k)x - i\left(\frac{\Delta E}{\hbar}\right)t}\right]$$

$$= Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i\times const.}\right]$$



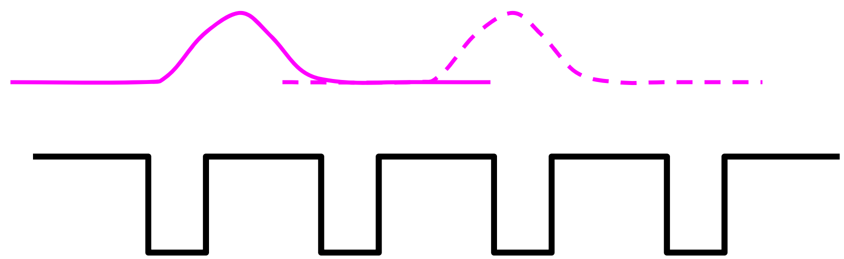
$$\upsilon = \frac{\Delta x}{\Delta t} = \frac{\Delta E}{\hbar \Delta k}$$

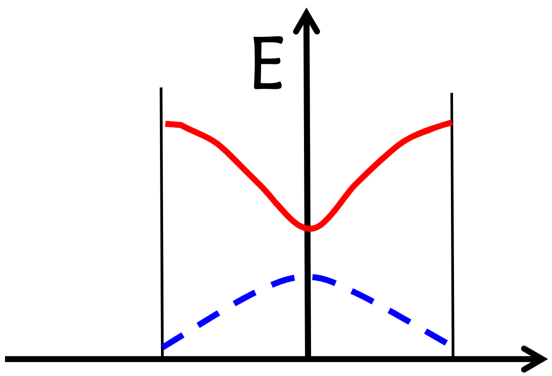
$$\because \quad \left[x\Delta k - t\frac{\Delta E}{\hbar}\right] = \text{constant.}$$

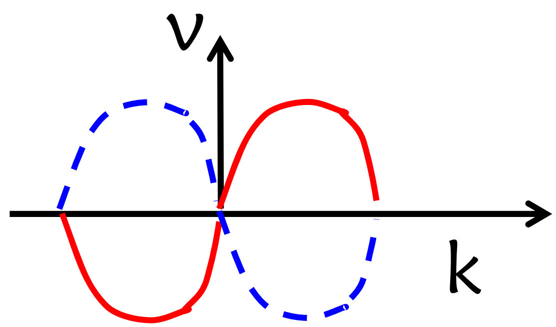


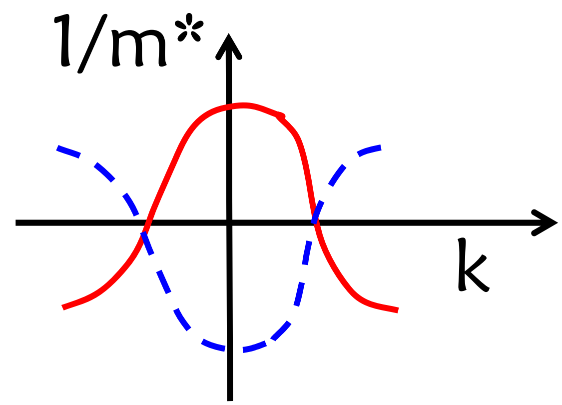
$$a = \frac{\Delta \upsilon}{\Delta t} = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{\Delta E}{\Delta k}\right] = \frac{1}{\hbar^2}\frac{d}{dk}\left[\frac{\Delta E}{\Delta k}\right]\frac{d(\hbar k)}{dt} = \frac{F}{m^*}$$

Effective Mass for a Given Band







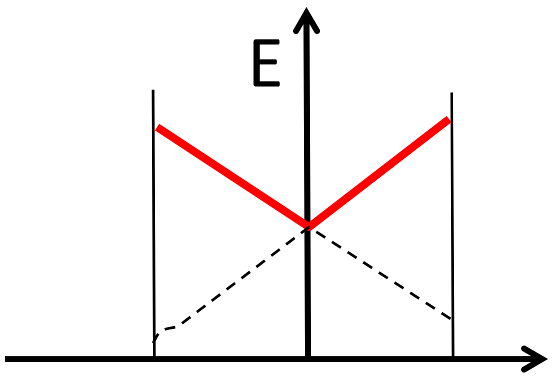


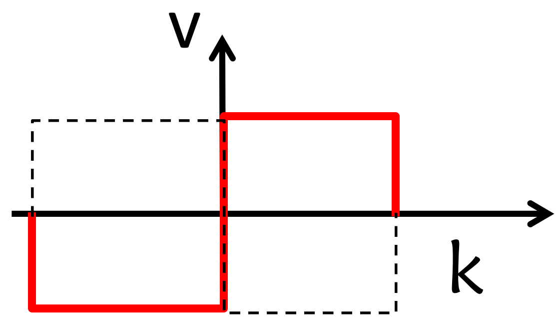
$$\upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k}$$

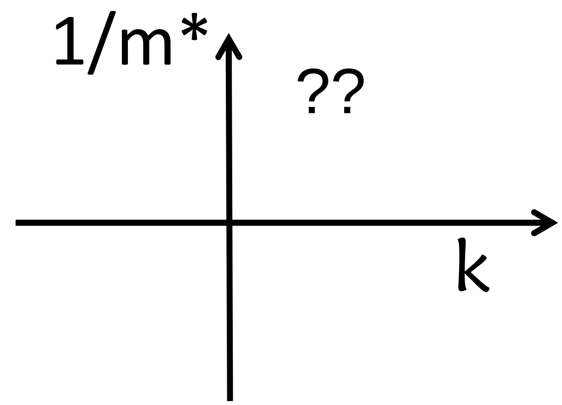
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

mass for each band

Effective Mass is not Essential …







$$F = \hbar \frac{\Delta k}{\Delta t}$$

$$\upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k}$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

$$k = k_0 + \int_0^t \frac{F}{\hbar} dt$$

$$x = x_0 + \int_0^t \upsilon dt$$

Conclusion

1) Solution of Schrodinger equation is relatively easy for systems with well-defined periodicity.

2) Electrons can only sit in-specific energy bands. Effective masses and band gaps summarize information about possible electronic states.

3) Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.

4) K-P model is analytically solvable. Real band-structures are solved on computer. Such solutions are relatively easy – we will do HW problems on nanohub.org on this topic.