Magnitude of the Energy gap

The WF at the borders of the Brillouin Zone ($k = \pm\pi/a$) are

$$\psi_+ = A\cos(x\pi/a) \qquad \psi_- = B\sin(\pi x/a)$$

A and B are obtained from the normalization

$$\int_0^a |\psi_+|^2 dx = \int_0^a |\psi_-|^2 dx = 1$$

$$\cos^2 x = [1 + \cos(2x)]/2$$
$$\sin^2 x = [1 - \cos(2x)]/2$$

we find that $A = B = \sqrt{\frac{2}{a}}$

$$\psi_+(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{\pi x}{a}\right) \qquad \psi_-(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$$

Let us suppose that the potential energy of the electrons in the crystal at point x in space

$$U(x) = U\cos\left(\frac{2\pi x}{a}\right)$$

$$E_g = \int_0^a U(x)\left[|\psi_+(x)|^2 - |\psi_-(x)|^2\right]dx$$

$$= U\left(\frac{2}{a}\right)\int_0^a \cos\left(\frac{2\pi x}{a}\right)\left[1 + \cos\left(\frac{2\pi x}{a}\right) - 1 + \cos\left(\frac{2\pi x}{a}\right)\right]\frac{1}{2}\,dx$$

$$= U\left(\frac{2}{a}\right)\int_0^a \cos^2\left(\frac{2\pi x}{a}\right)dx$$

$$= U$$

The gap is equal to the Fourier component of the potential of the crystal

Bloch function

Felix Bloch, swiss physicist, proved an important theorem, which states that solutions to Schrödinger equation for a periodic potential must be

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$$

where $u_{\vec{k}}(\vec{r})$ has the periodicity of the crystal $\Rightarrow u_{\vec{k}}(\vec{r}+\vec{T}) = u_{\vec{k}}(\vec{r})$ for $\vec{T}$ any translation vector of the lattice.

The eigenfunctions of the wave equation for a periodic potential are the product of a plane wave $e^{i\vec{k}\cdot\vec{r}}$ and a function $u_{\vec{k}}(\vec{r})$ with the periodicity of the crystal lattice.

Proof of Bloch theorem

Let's consider a crystal with N lattice points on a ring of lenght Na.

The potential is periodic with period a, so

$$U(x) = U(x+sa) \qquad s \in \mathbb{Z}$$

By the symmetry of the problem we know that the solution must have some periodicity

$$\psi(x+a) = e^{i\phi}\,\psi(x)$$

where ϕ is a phase $\left(|\psi(x+a)|^2 = |\psi(x)|^2\right)$.

Going around a full circle

$$\psi(x+Na) = e^{iN\phi}\,\psi(x)$$

It follows that $N\phi = 2\pi s \Rightarrow \phi = \frac{2\pi}{N}s$

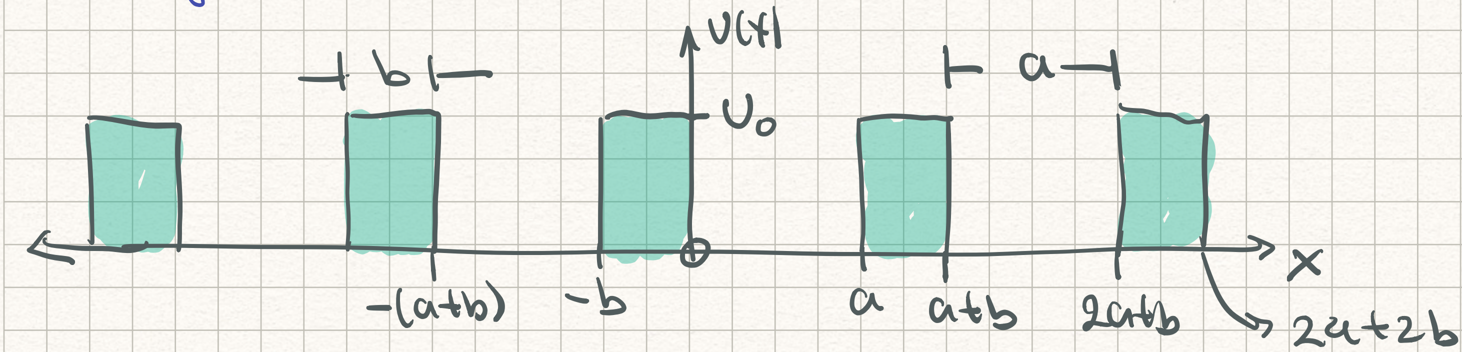
for $s = 0, 1, 2, \ldots, N-1$

the $\psi_k(x) = u_{\vec{k}}(x)\, e^{i\,2\pi s x/Na}$ satisfies

Schrödinger Eq, provided that $u_{\vec{k}}(x+a) = u_{\vec{k}}(x)$

Kronig-Penney model

we can obtain the solution to the WF in terms of elementary functions for a potential arraged as



Schrödinger Eq.

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$$

$V(x)$: potential $\qquad$ E: energy eingenvalue

(*) In the region $0 < x < a$: $V(x) = 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\,\psi(x)$$

which has solution

$$\psi(x) = A e^{iqx} + B e^{-iqx} \qquad \text{with} \quad E = \frac{\hbar^2 q^2}{2m}$$

describing plane waves travelling to the right and to the left.

⊗ $-b < x < 0$ the potential $U(x) = U_0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + U_0\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = (E - U_0)\psi(x)$$

the solutions ar

$$\psi(x) = C e^{Qx} + D e^{-Qx} \qquad \text{with} \quad U_0 - E = \frac{\hbar^2 Q^2}{2m}$$

Depending on whether $U_0 - E < 0$ (> 0) the solution describes exponential decay (travelling waves).

We can use Bloch theorem to relate the WF in the region $a < x < a+b$ with the WF in $-b < x < 0$:

$$\psi(a < x < a+b) = \psi(-b < x < 0)\, e^{ik(a+b)}$$

we can define the wavevector k as the index of the solution.

The constants A, B, C and D are chosen so that $\psi(x)$ and $d\psi/dx$ are continuous functions.

at $x=0$ and $x=a$

$$\frac{\partial}{\partial x}\left(Ae^{iqx}+Be^{-iqx}\right)=iq\left(Ae^{iqx}-Be^{-iqx}\right)$$

$$\frac{\partial}{\partial x}\left(Ce^{Qx}+De^{-Qx}\right)=Q\left(Ce^{Qx}-De^{-Qx}\right)$$

$\boxed{\text{At } x=0}$

$$A+B=C+D$$

$$iq(A-B)=Q(C-D)$$

At $x=a$ (here we use BT)

$$Ae^{iqa}+Be^{-iqa}=\left(Ce^{-Qb}+De^{Qb}\right)e^{ik(a+b)}$$

$$iq\left(Ae^{iqa}-Be^{-iqa}\right)=Q\left(Ce^{-Qb}-De^{Qb}\right)e^{ik(a+b)}$$

we condense these Eq. as a matricial Eq. $M\vec{v}=\vec{0}$

$$M=\begin{bmatrix} 1 & 1 & -1 & -1 \\ iq & -iq & -Q & Q \\ e^{iqa} & e^{iqa} & -e^{-bQ}e^{ik(a+b)} & -e^{bQ}e^{ik(a+b)} \\ iqe^{iqa} & -iqe^{iqa} & -Qe^{-bQ}e^{ik(a+b)} & Qe^{bQ}e^{ik(a+b)} \end{bmatrix}$$

$\vec{v}=(A,B,C,D)^T$

we have nontrivial solutions given $\det(M)=0$

$$\cos[k(a+b)]=\cos(qa)\cosh(bQ)+\left(\frac{Q^2-q^2}{2qQ}\right)\sin(qa)\sinh(bQ)$$

This result can be simplified if we represent the potential as a periodic delta function

⇒ we take the limit $b \to 0$ and $U_0 \to \infty$
in such a way that $P = \frac{Q^2 ab}{2}$ is finite

$\sinh(bQ) \approx bQ$ $\qquad \frac{2P}{Qa} = Qb$

$\cosh(bQ) \approx 1$

$$\cos(ka) = \cos(qa) + \frac{Q^2 - q^2}{2qQ} \sin(qa)\, bQ$$

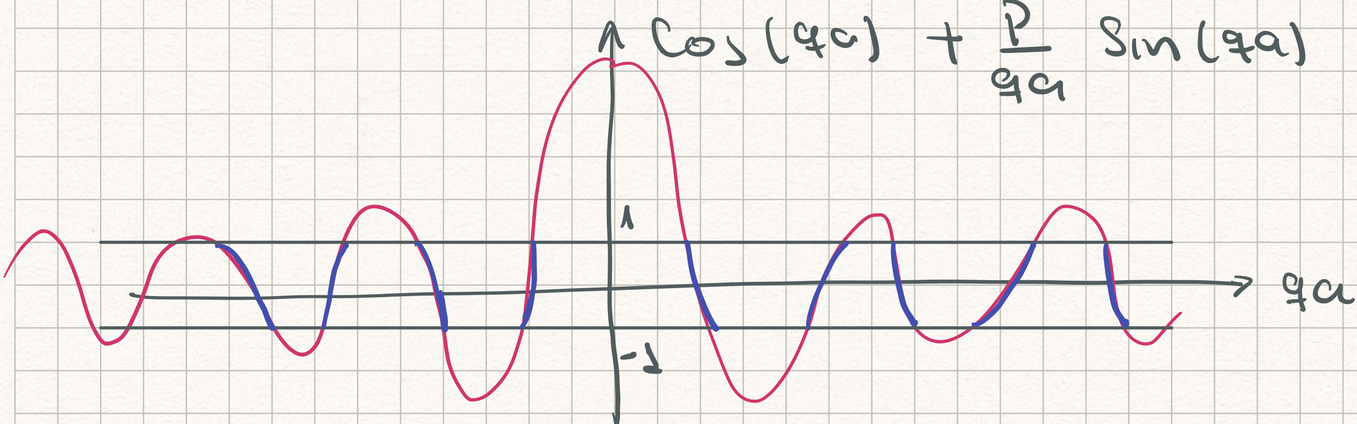
$$= \cos(qa) + \frac{Q^2 - q^2}{2q} b \sin(qa)$$

Also note that $Q^2 \gg q^2$ ⇒ the exponential decay is very large ⇒ due to the δ-potential

$$\cos(ka) = \cos(qa) + \frac{Q^2 b}{2q} \sin(qa)$$

$$= \cos(qa) + \frac{Q^2 ba}{2qa} \sin(qa)$$

$$= \cos(qa) + \frac{P}{qa} \sin(qa)$$



The allowed values of the energy are those ranges of $qa = \left(\frac{2mE}{\hbar^2}\right)^{1/2} a$ for which the function lies between -1 and 1. For other values of the energy there are nontravelling

wave or Bloch-type solution to the wf $\Rightarrow$
there are forbidden gaps in the energy spectrum

Note that the gaps are given by the values of the index k rather than by q (which associated to the energy)