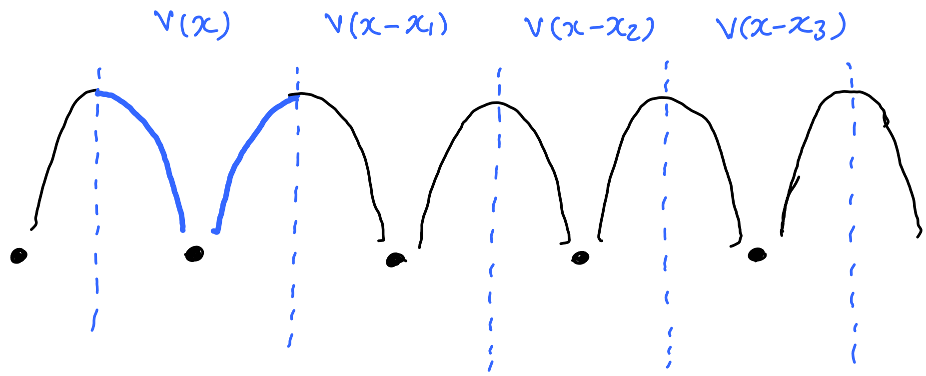
Note Title 2/15/2008

The tight bonding approximation

Consider the atoms in a solid:

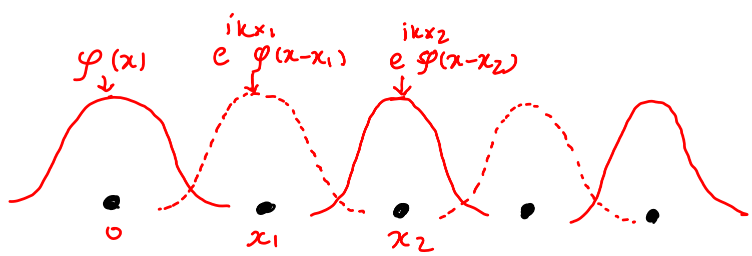


So we can write the Hamiltonian as:

$$\hat{H}\psi(x) = \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \sum_n V(x-x_n)\right]\psi(x) = E\psi(x)$$

Bloch theorem: $\psi(x+L) = e^{ikL}\psi(x)$

Consider electrons in s-orbital of each atom. So the wavefunction peaks around each atom.



So we can write for the ψ:

$$\psi = \sum_n e^{ikx_n}\varphi(x-x_n)$$

Let's calcute the energy:

The expectation value of the energy is:

$$E = \int_{-\infty}^{\infty}\psi^*\hat{H}\psi\,dx$$

$$= \int_{-\infty}^{\infty} \sum_m e^{-ikx_m} \varphi^*(x-x_m)\, \hat{H} \sum_n e^{-ikx_n} \varphi^*(x-x_n)\, dx$$

$$= \sum_n \sum_m \int_{-\infty}^{\infty} e^{ik(x_n - x_m)} \varphi^*(x-x_m)\, \hat{H}\, \varphi(x-x_n)\, dx$$

Now look at the figure for φ's. If φ's are localized around each atom, φ for two neighboring atoms may overlap, but for further atoms they don't overlap and;

$$\varphi^*(x-x_n)\, \varphi(x-x_m) = 0 \quad \text{if } |m-n| \geq 2$$

So we only need to keep three integrals:

$\underline{n=m}$:

$$\Rightarrow \sum_{x_n} \int_{-\infty}^{\infty} e^{ik(x_n-x_n)} \varphi^*(x-x_n)\, \hat{H}\, \varphi(x-x_n)$$

$$= \underset{\text{number of atoms}}{N} \int_{-\infty}^{\infty} \varphi^*(x)\, \hat{H}\, \varphi(x)\, dx \quad \text{let's call this } -E_0$$

$\underline{n-m=1}$: $\rightarrow x_n - x_m = L$ (two neighbors)

$$\sum_{x_n} \sum_{x_m} \int_{-\infty}^{\infty} e^{ik(x_n-x_m)} \varphi^*(x-x_m)\, \hat{H}\, \varphi(x-x_n)\, dx$$

$$= e^{ikL}\, \underbrace{N \int_{-\infty}^{\infty} \varphi^*(x-x_n)\, \hat{H}\, \varphi(x-x_n-L)\, dx}_{\equiv -t}$$

$$= -e^{ikL}\, t$$

$n-m=-1 \rightarrow x_n - x_m = -L$ (two neighbors)

$$\sum_{x_m}\sum_{x_n}\int_{-\infty}^{\infty} e^{ik(x_n-x_m)}\, \varphi^*(x-x_m)\,\hat{H}\,\varphi(x-x_n)\,dx$$

$$= e^{-ikL}\, N \underbrace{\int_{-\infty}^{\infty}\varphi^*(x-x_n)\,\hat{H}\,\varphi(x-x_n+L)\,dx}_{=-t}$$

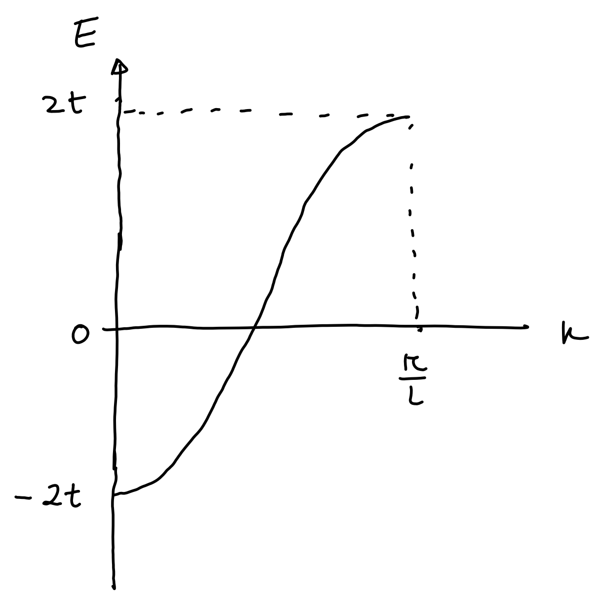
$$=-e^{-ikL}\,t$$

So the total energy is:

$$E=-E_0 - t e^{ikL} - t e^{-ikL} = -E_0 - t\left(e^{ikL}+e^{-ikL}\right)$$

$$=-E_0-2t\cos kL$$

Let shift the energy so $E_0=0 \Rightarrow \boxed{E=-2t\cos kL}$



Band width $= 4t$

In 3D, we will have:

$$E=-2t\cos k_xL - 2t\cos k_yL - 2t\cos k_zL$$

and the bandwidth will be: $(4t)(3)=12t$