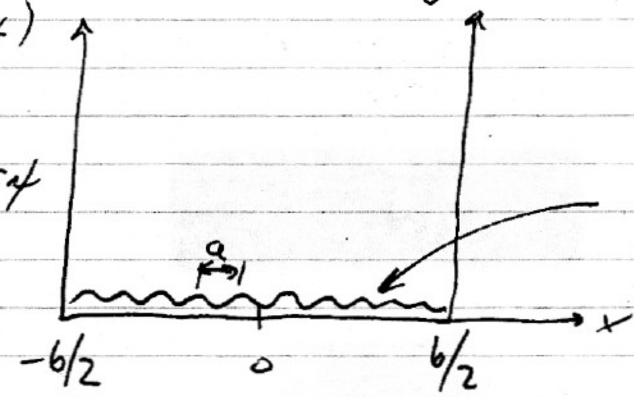
Solution to the Schröd Eq for a Periodic Potential

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

For example
$V(x) = \cos\left(\frac{2\pi x}{a}\right)$



periodic perturbation to the potential period a.

$\boxed{b = Na}$

We can write the perturbation as a Fourier series

$$V(x) = \sum_{s=-\infty}^{\infty} V_s\, e^{i2\pi s x/a}$$

Fourier Sum
V_s complex

$$V(x+a) = \sum_{s=-\infty}^{\infty} V_s\, e^{i2\pi s x/a}\, \cancel{e^{i2\pi s}}$$

1 for all s.

The unperturbed WF's are running waves

$$\psi_n^0(x) = e^{ik_n x} = e^{i2\pi n x/b} \qquad \psi_n^0(x+b) = \psi_n^0(x)$$

The 1^{st} order correction can be written in terms of the unperturbed WFs:

$$\psi_m^1(x) = \sum_{n=-\infty}^{\infty} a_{mn}\, \psi_n^0(x)$$

The coefficients become

$$a_{mn} = \frac{\int_{-\infty} \psi_n^{0*}\, V(x)\, \psi_m^0(x)\, dx}{E_m^0 - E_n^0}$$

(exactly what we derived before in class)

Where $\quad E_m^0 = \frac{\hbar^2 k_m^2}{2m} \qquad E_n^0 = \frac{\hbar^2 k_n^2}{2m}$

Putting all this in gives

$$a_{mn} = \frac{2m \int e^{-ik_n x}\left(\sum_{s=-\infty}^{\infty} V_s e^{i2\pi s x/a}\right) e^{ik_m x}\, dx}{\hbar^2 (k_m^2 - k_n^2)}$$

$$= \frac{2m}{\hbar^2 (k_m^2 - k_n^2)} \sum_{s=-\infty}^{\infty} V_s \int_{-b/2}^{b/2} e^{i\left(k_m - k_n + \frac{2\pi s}{a}\right)x}\, dx$$

$$\cancel{k_m - k_n = \frac{2\pi}{b}(m-n) \quad \text{and} \quad b = Na}$$

so $\cancel{k_m - k_n + \frac{2\pi s}{a} = \frac{2\pi}{Na}(m-n) + \frac{2\pi}{a} s}$

$$\cancel{= \frac{2\pi}{Na}(m - n + Ns)}$$

$$a_{mn} = \frac{2m}{\hbar^2 (k_m^2 - k_n^2)} \sum_{s=-\infty}^{\infty} V_s \frac{1}{i\left(k_m - k_n + \frac{2\pi s}{a}\right)} e^{i\left(k_m - k_n + \frac{2\pi s}{a}\right)x}\Bigg|_{-b/2}^{b/2}$$

$$\left(k_m - k_n + \frac{2\pi s}{a}\right) b/2 = \cancel{2}\pi(m - n + sN) \qquad \text{since } b = Na$$

$$= \cancel{2}\pi \times \text{integer}$$

So the integral is

$$e^{i\cancel{2}\pi\,\text{integer}} - e^{-i\cancel{2}\pi\,\text{integer}} = 0$$

UNLESS $\quad k_m + \frac{2\pi s}{a} - k_n = 0$

Thus a_{mn} is non-zero only when

$$k_n - k_m = \frac{2\pi s}{a} \quad \text{where } s \text{ is an integer.}$$

In other words, the perturbed wave function can be expanded in terms of other simple running waves with wavevectors

$$k_n = k_m, \; k_m \pm \frac{2\pi}{a}, \; k_m \pm \frac{4\pi}{a}, \; k_m \pm \frac{6\pi}{a}, \text{ etc.}$$

Reciprocal lattice vectors

Thus, in general $\quad e^{ik_n x} = e^{i(k_n - \frac{2\pi s}{a})x}$

$K = \frac{2\pi}{a} s$ are the set of all Reciprocal Lattice vectors

$$\psi_k(x) = \sum_{s=-\infty}^{\infty} a_s(k)\, e^{i(k + \frac{2\pi s}{a})x}$$

Sum over all the plane waves which differ in k by $2\pi s/a$.

Exact solution for running wave of wavevector k. (Formerly $\psi_n^0 = e^{ik_n x}$)

Factor out the e^{ikx}

$$\psi_k(x) = e^{ikx} \sum_{s=-\infty}^{\infty} a_s(k)\, e^{i2\pi s x/a}$$

$$\equiv e^{ikx}\, u_k(x)$$

Note that $u_k(x)$ is periodic in x with period a

$$u_k(x+a) = \sum_{s=-\infty}^{\infty} a_s(k)\, e^{i2\pi s x/a}\, \cancel{e^{i2\pi s}}^{\,1}$$

$$= u_k(x)$$

This is a special case of Floquet's Theorem called Bloch's Thm.

Bloch's Theorem.

$$\boxed{\begin{array}{l}\text{The eigenfunctions of the Schrödinger equation for a periodic potential are always of the form:}\\[1ex] \qquad \psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r}) \\[1ex] \text{where } u_k(\vec{r}) \text{ is periodic in } x, y, \text{ and } z, \text{ with the same period as the period of the potential in each coordinate}\end{array}}$$