(5).

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - aV_0\sum_n \delta(x-na)\psi = E\psi.$$

[This is called the Krönig-Penny model]

(a). NFE approx.

$\Rightarrow$ Band gap at ZB corr to $k = G/2$ $= 2V(G)$

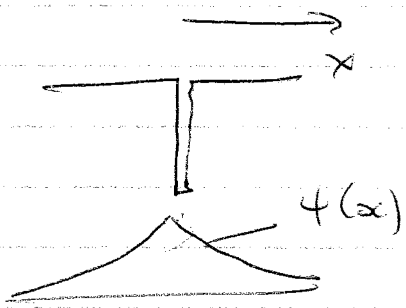
$$V(G) = \frac{1}{L}\int_{-L/2}^{L/2} dx\, e^{iGx} V(x)$$

$$= \frac{aV_0}{L}\sum_n \int_{-L/2}^{L/2} dx\, e^{iGx}\,\delta(x-na).$$

$$= \frac{aV_0}{L}\sum_{n=-\frac{N}{2}}^{N/2} \underbrace{e^{iGna}}_{\equiv 1} \qquad \text{where } N = aL.$$

$$= \frac{aV_0 N}{L} = V_0 \quad \forall G.$$

(b) Single δ-f^n potential.



$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - aV_0\delta(x)\right]\psi = E\psi.$$

Sol^n for $x \neq 0$ ~~is~~

— assume bound state of energy $= E_0 < 0$

Satisfies $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -E_0\psi \qquad E_0 > 0.$

$$\psi = e^{\pm x/q} \qquad q^2 = \frac{2mE_0}{\hbar^2}$$

Choose $e^{x/q}$ for $x > 0$ so sol^n well behaved

$e^{-x/q}$ for $x < 0$ as $|x| \to \infty$

Solve for E_0 by matching at $x=0$

Take $$\int_{-\varepsilon}^{\varepsilon} dx \left\{ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - aV_0\psi\,\delta(x) \right\} = -\underbrace{\int_{-\varepsilon}^{\varepsilon} dx\, E_0\psi}$$

In limit $\varepsilon \to 0$ $\quad$ RHS $\to 0$

$$\text{LHS} = -\frac{\hbar^2}{2m}\left[\left.\frac{d\psi}{dx}\right|_R - \left.\frac{d\psi}{dx}\right|_L\right] - aV_0\psi(0)$$

$$= \frac{\hbar^2}{2m}\cdot\frac{2}{\xi}\psi(0) - aV_0\psi(0) = 0$$

$$\therefore \xi = \frac{2mV_0a}{\hbar^2} = \frac{1}{\kappa}$$

Normalisation $\quad \psi(x) = \dfrac{1}{\sqrt{\xi}}\, e^{-|x|/\xi}$.

Tight binding in limit $a/\xi \gg 1$

$$t = \int_{-\infty}^{\infty} dx\, \psi(x)\psi(x-a)\cdot H$$

$$= \frac{aV_0}{\xi}\, e^{-a/\xi}$$

Bandwidth $W = 4t$

$$= \frac{4aV_0}{\xi}\, e^{-a/\xi}$$