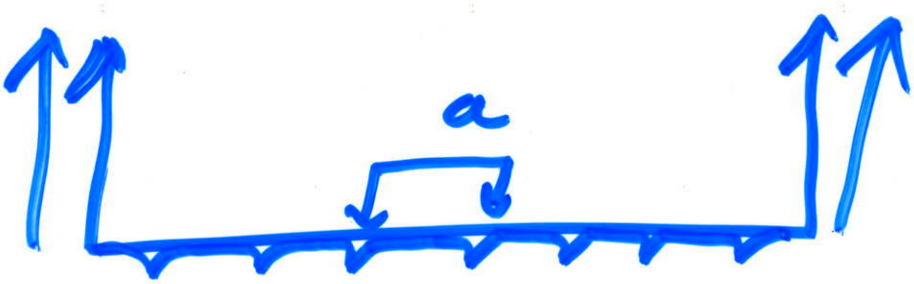
Bloch Waves

Use the free electron model as the unperturbed state.

Treat the small interaction with the lattice (periodic) as a perturbation. $U_{int} \ll E_F$



1-dim: $\psi_{free}(x) \propto e^{ikx}$

$$k = \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \pm \frac{6\pi}{L} \dots \pm k_F$$

3-dim: $\psi_{free}(\vec{r}) \propto e^{i\vec{k}\cdot\vec{r}} =$

$$= e^{ik_x x} \cdot e^{ik_y y} \cdot e^{ik_z z} = \psi_{free}(x)\,\psi_{free}(y)\,\psi_{free}(z)$$

Wavefunction $\psi_{(x)}$ is not measurable but $|\psi_{(x)}|^2 = \psi^*_{(x)} \cdot \psi_{(x)}$ is measurable.

$$|\psi(x+sa)|^2 = |\psi_{(x)}|^2$$

$\psi(x+a) = c\,\psi_{(x)}$ where c is a phase $c = e^{i\alpha} \Rightarrow |c|^2 = 1$

$$\psi(x+2a) = c\,\psi(x+a) = c^2\,\psi_{(x)}$$

$$\underline{\psi(x+sa) = c^s\,\psi_{(x)}}$$

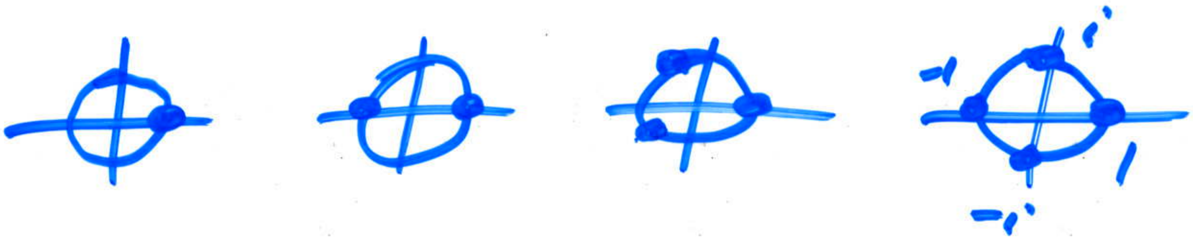
1-dim crystal, length L, N atoms, lattice spacing $\underline{a}$: $L = Na$

Impose periodic boundary conditions.

$$\psi(x+L) = \psi(x)$$

$$\psi(x+Na) = C^N \psi(x) = 1\ \psi(x)$$

$$C = \sqrt[N]{1} = N^{th} \text{ root of unity}$$



$$(1)^4 = (-1)^4 = (i)^4 = (-i)^4 = 1$$

$$C = e^{\frac{2\pi i}{N}}, e^{\frac{2\cdot 2\pi i}{N}}, e^{\frac{3\cdot 2\pi i}{N}} \ldots$$ N of those

$$C = e^{\frac{2\pi i m}{N}}$$

$$\psi(x+a) = e^{\frac{2\pi i m}{N}} \psi(x)$$ Bloch condition

Try $\psi_{(x)} = e^{ikx} u(x)$

where $u(x+a) = u(x)$ periodicity $= a$

$$\psi(x+a) = e^{ik(x+a)} u(x+a)$$

$$= e^{ika} \cdot \left[e^{ikx} u(x) \right] = e^{ika} \psi_{(x)}$$

$$ka = \frac{2\pi m}{N} \Rightarrow k = \frac{2\pi}{Na} m \quad \checkmark$$

these <u>are</u> the allowed wavevectors

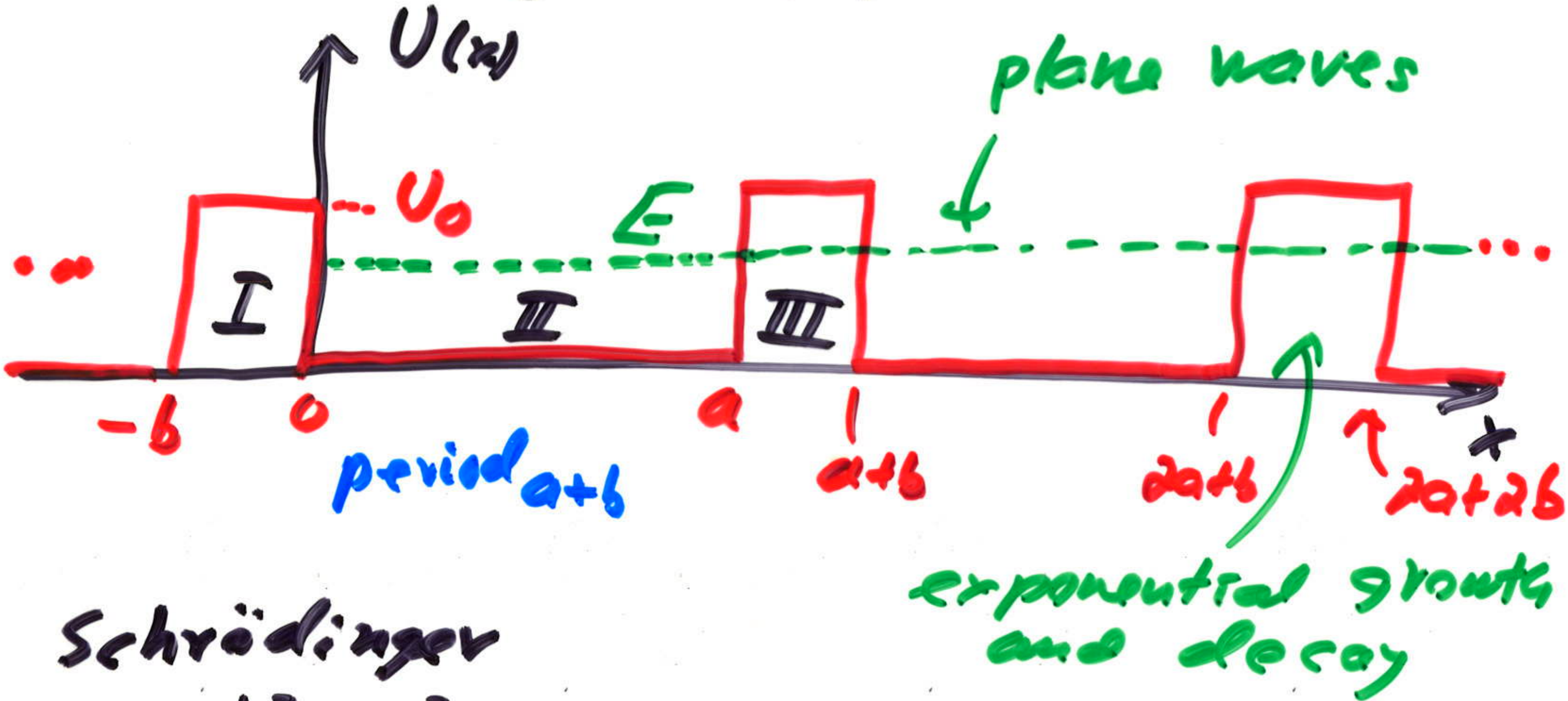
3-dim $\quad u(\vec{r}) = u(\vec{r} + \vec{T})$

$\vec{T}$ is a translation vector

$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

Bloch condition $\quad \psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u(\vec{r})$

1-dim Kronig-Penney model



Schrödinger

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\,\psi(x)$$

$\underline{0<x<a}$, $U(x) = 0$

$$\psi_{II}(x) = A e^{+iKx} + B e^{-iKx}$$

energy $E = \dfrac{\hbar^2 K^2}{2m}$

Inside the barrier, $-b < x < 0$, $U(x) = U_0$

tunneling solutions

$$\psi_I(x) = C e^{+Qx} + D e^{-Qx}$$

& III

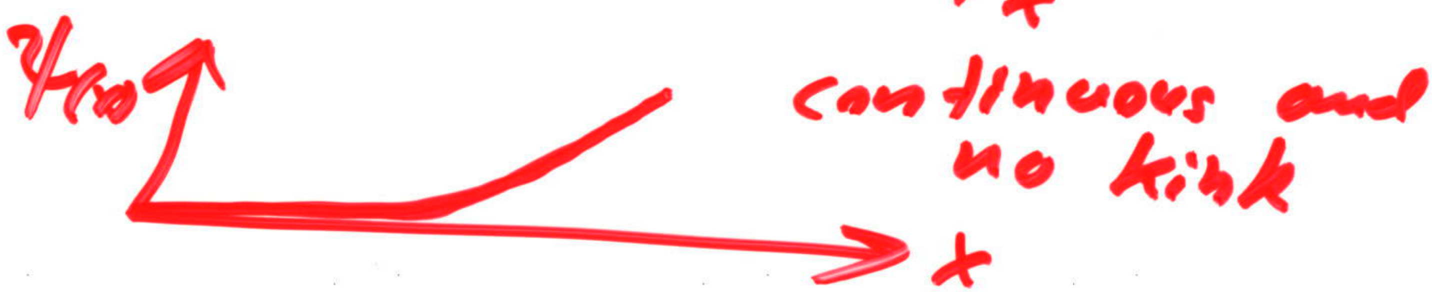
$$U_0 - E = \frac{\hbar^2 Q^2}{2m}$$

Impose Bloch condition

$$\psi_{I}(x) = \psi_{III}(x)\, e^{ik(a+b)}$$

$\psi(x)$ and $\frac{d\psi}{dx} = \psi'(x)$ are both continuous at both $x=0$, and $x=a$.

Aside: If $U(x)$ is discontinuous (like here) then $\psi'(x)$ is continuous but has a kink (change in slope)



at $x=0$

$$\psi_I(0) = \psi_{II}(0) \Rightarrow C + D = A + B$$

$$\Rightarrow A + B - C - D = 0$$

$$\psi_I'(0) = \psi_{II}'(0) \Rightarrow Q(C-D) = iR(A-B)$$

$$\Rightarrow iRA - iRB - QC + QD = 0$$

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at $x=a$

$$\psi_{II}(a) = \psi_{III}(a) = \psi_I(-b)\, e^{ik(a+b)}$$

$$A e^{iRa} + B e^{-iRa} = \left[C e^{-Qb} + D e^{+Qb}\right] e^{ik(a+b)}$$

$$\psi_{II}'(a) = \psi_{III}'(a) = \psi_I'(-b)\, e^{ik(a+b)}$$

$$iR\left[A e^{iRa} - B e^{-iRa}\right] = Q\left[C e^{-Qb} - D e^{+Qb}\right] e^{ik(a+b)}$$

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4 equations, 4 unknowns

$$\underline{\underline{M}} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

If $\underline{\underline{M}}$ has an inverse, then

$$\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \underline{\underline{M}}^{-1}\underline{\underline{M}}\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \underline{\underline{M}}^{-1}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

trivial solution

$\Rightarrow$ $\underline{\underline{M}}$ can not have an inverse

$\Rightarrow$ $\det(\underline{\underline{M}}) = 0$

$$\frac{Q^2 - R^2}{2QR} \sinh(Qb)\sin(Ra) + \cosh(Qb)\cos(Ra) = \cos\left[k(a+b)\right]$$

Simpler equation if Limit $b \to 0$

$U_0 \to \infty$ such that $\frac{Q^2 a b}{2} \equiv P$ finite

$$Q = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

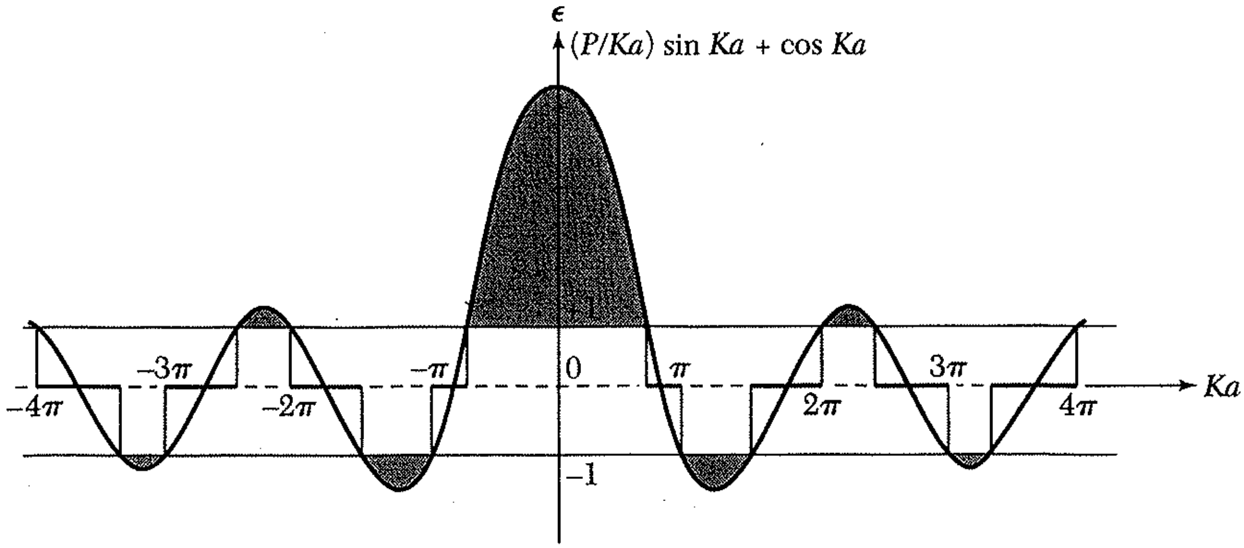

Figure 5 Plot of the function $(P/Ka)\sin Ka + \cos Ka$, for $P = 3\pi/2$. The allowed values of the energy ϵ are given by those ranges of $Ka = (2m\epsilon/\hbar^2)^{1/2}a$ for which the function lies between ± 1. For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.

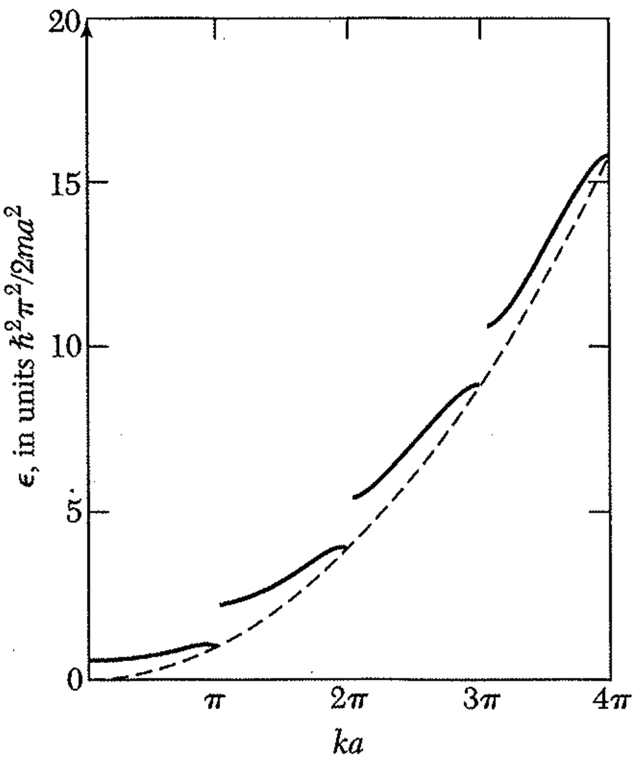

Figure 6 Plot of energy vs. wavenumber for the Kronig-Penney potential, with $P = 3\pi/2$. Notice the energy gaps at $ka = \pi, 2\pi, 3\pi \ldots$.