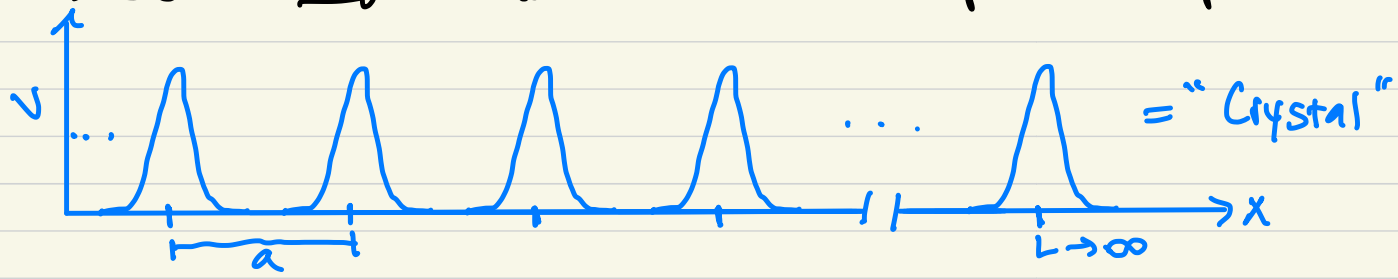
I. A: Electrons in 1D periodic potentials (G and P Ch.1)

- Simplest model of a solid
- Key feature: Periodicity
  - * Atoms of the same element are identical so tend to form ordered structures
- Consider single electron in a periodic potential (1D)



S.E.: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$

↳ $V(x) = V(x + \underbrace{m}_{\text{integer}} a)$ ← period

* Take Fourier transform of V:

$$V(x) = \sum_{n=-\infty}^{\infty} V_n \exp\left[i \underbrace{\frac{2\pi n}{a}}_{\text{wavenumber } h_n} x\right]$$

* What does periodicity mean for ψ and E?
  - Consider $V(x) = 0$ (trivially periodic)

    Wavefunctions are plane waves: $w_k(x) = \frac{1}{\sqrt{L}} e^{ikx}$ ← normalization, L = length of crystal

    Eigenvalues: $E = \frac{\hbar^2 k^2}{2m}$
  - w_k orthonormal, form complete set

- Now consider $V(x) \neq 0$. Apply H to ψ_k.

  Since $V(x)\psi_k(x) = \frac{1}{\sqrt{L}} \sum_n V_n e^{i(h_n + k)x}$,

$\langle x|H|\psi_k\rangle \in \{\psi_k(x), \psi_{k+h_1}(x), \psi_{k-h_1}(x), \psi_{k+h_2}(x), \psi_{k-h_2}(x) \cdots\}$

Subspace of plane waves w/ wavenumber $k + h_n$, S_k

Also, $H|\psi_{k+h_n}\rangle \in S_k$ (closed)

$\Rightarrow$ Only need to diagonalize H in subspaces S_k

$\Rightarrow$ eigenfuctions of H labeled as $\psi_k(x)$

$\Rightarrow S_k \neq S_{k'}$ iff $k \neq k' + 2\pi n/a$ for $n \in \mathbb{Z}$

$\Rightarrow$ All different k labels reside in $-\pi/a < k \leq \pi/a$

First Brillouin Zone

we can write: $\psi_k(x) = \sum_n C_n(k) \frac{1}{\sqrt{L}} e^{i(k+h_n)x}$

expansion coeffs.

$$\psi_k(x) = u_k(x) e^{ikx}$$

"Travelling plane wave"

where: $u_k(x) = \sum_n C_n(k) \frac{1}{\sqrt{L}} e^{ih_n x}$

Periodic function: $u_k(x+a) = u_k$

(recall, $h_n = \frac{2\pi n}{a}$ and $e^{in2\pi} = 1$)

Bloch's Theorem: Any (physical) solution of S.E. in periodic potential can be written in the form of travelling plane wave modulated by microscopically periodic function.

* Back to question: What does periodicity mean for ψ, E?
  - ψ's are "itinerant"
  - ψ's labelled by k in first BZ
  - $\psi_k(x) = u_k(x) e^{ikx}$
  - $\psi_k(x + t_n) = \psi_k(x) e^{ikt_n}$, $t_n = na$ $(n \in \mathbb{Z})$
  - At each k we have set of energies E_m ← eigenfunction label
  - Can plot $E_m(k)$ in first BZ → forms a "band"
    ↳ question: is k continuous in BZ?

* Lets consider "finite", "macroscopic" crystal:
  - $0 \le x \le L \equiv Na$ $N \in \mathbb{Z}$, N large but finite
  - If $a \sim \text{Å}$, $L \sim cm$, $N \sim 10^9$
  - $\psi(x + Na) \equiv \psi(x)$ → Born-Von Karman boundary conditions
    ↳ Only acceptable ks are: $e^{ikNa} = 1$

    so $k = \frac{2\pi}{Na} n$, $n \in \mathbb{Z}$

    ↳ answer: Discrete but dense!

Example: empty lattice

$V(x) = 0$