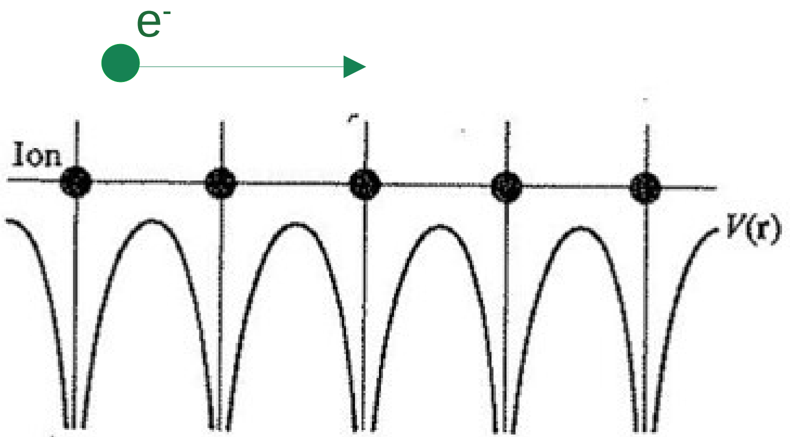
Bloch’s theorem

Recap of previous lectures

- Crystal lattices
- Reciprocal space and Brillouin zones
- Electrons in lattices and the independent electron approximation

Electrons in lattices

- Each electron experiences a potential $V(\boldsymbol{r})$ from the ions



$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- Potential has the same periodicity as the lattice

$$V(\mathbf{r}+\mathbf{a}) = V(\mathbf{r})$$

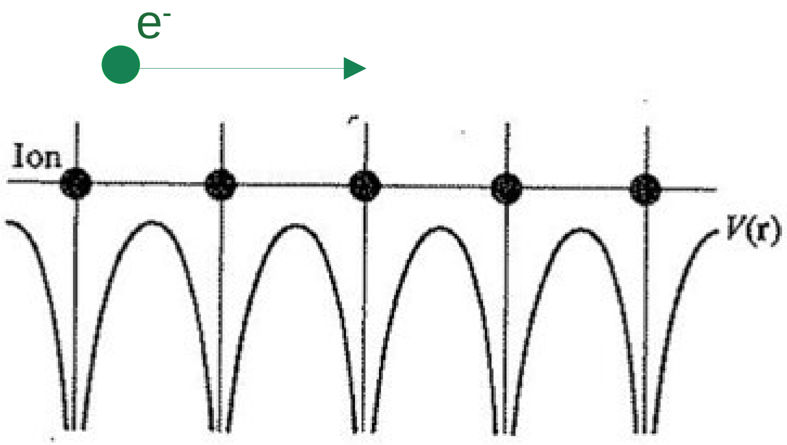
for primitive lattice vector $\mathbf{a}$

- **Bloch's theorem**: Special structure of eigenstates due to periodicity

One dimension

$$\left(\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right)\psi(x)=E\psi(x)$$

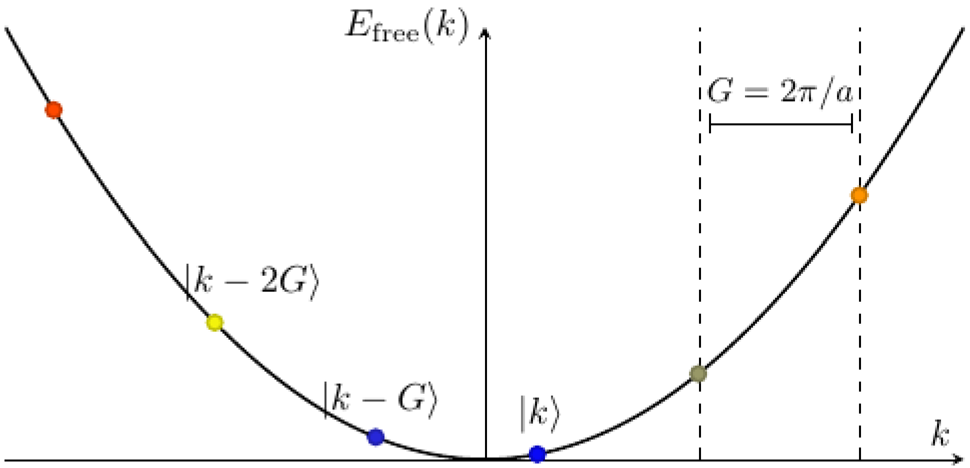
$$V(x+a)=V(x)$$



$$V(x)=\sum_{n=-\infty}^{\infty}V_n e^{\mathrm{i}nGx}$$

Coupling plane wave states

- A periodic lattice potential $V(x)$ only generates superpositions of plane wave states with wavevectors related by multiples of the reciprocal lattice constant $G = 2\pi/a$



$$\hat{V}\,|k\rangle = \sum_n V_n\,|k+nG\rangle$$

$$V(x+a) = V(x)$$

The structure of eigenstates

- A general form for eigenstates: $$\psi_q(x) = \sum_n b_n e^{\mathrm{i}(q+nG)x}$$

- **Bloch's theorem (1D)**

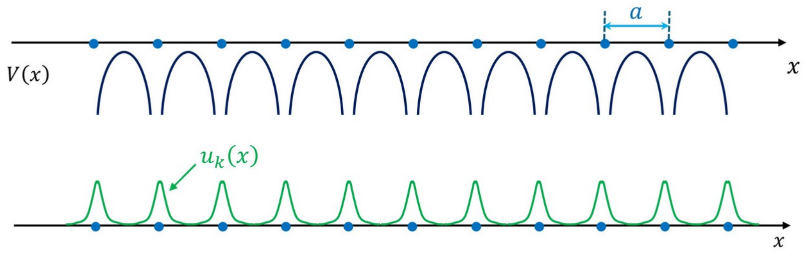
  Eigenstates of the Schrödinger equation with a periodic potential have the form

  $$\psi_q(x) = e^{\mathrm{i}qx} u_q(x)$$

  Where q is a wavevector in the first Brillouin zone $[-\pi, \pi]$ and $u_q(x)$ is a periodic function of x

The "Bloch wavefunction" (periodic)

$$u_q(x) = \sum_n b_n e^{\mathrm{i}nGx}$$



Three dimensions

- The same ideas all hold in three dimensions

$$V(x) = \sum_{n=-\infty}^{\infty} V_n e^{\mathrm{i}nGx}$$

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{\mathrm{i}\mathbf{G}\cdot\mathbf{r}}$$

$$\mathbf{G} \in \text{reciprocal lattice}$$

$$\downarrow$$

$$\psi_q(x) = e^{\mathrm{i}qx} \sum_n b_n e^{\mathrm{i}nGx}$$

$$\downarrow$$

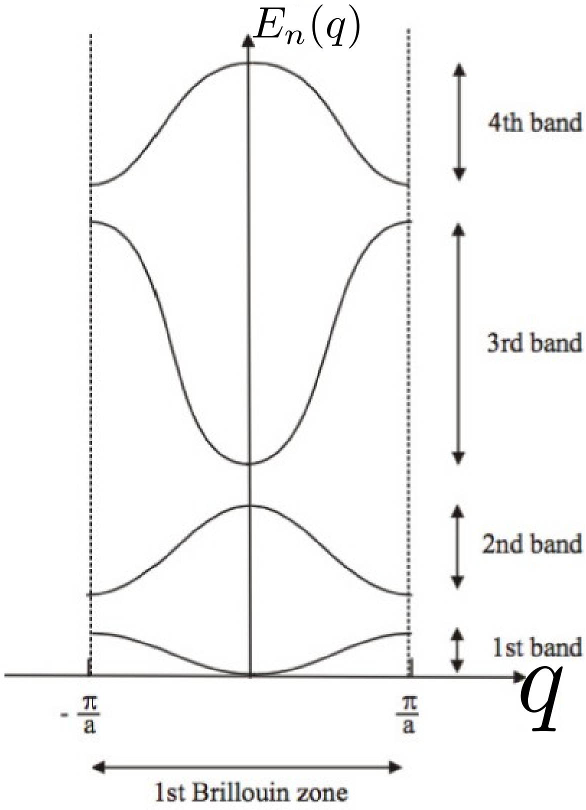
$$\psi_{\mathbf{q}}(\mathbf{r}) = e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{G}} b_{\mathbf{G}} e^{\mathrm{i}\mathbf{G}\cdot\mathbf{r}}$$
$$= e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} u_{\mathbf{q}}(\mathbf{r})$$

Band structure

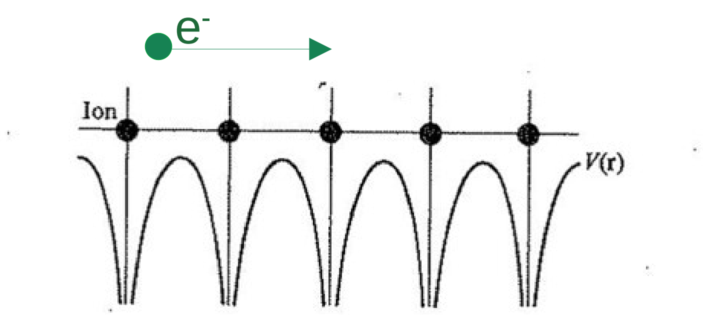
- For each wavevector $\boldsymbol{q}$ in the first Brillouin zone, there will be multiple eigenstates with different discrete energies

- Different "bands" $m = 1, 2,$...

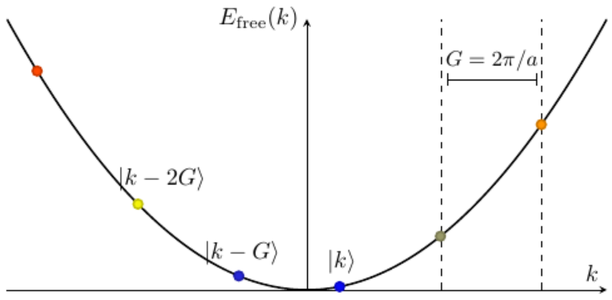
$$E_n(\mathbf{q}) \qquad u_{\mathbf{q},n}(\mathbf{r})$$



Summary



- Electrons in a periodic lattice potential
- Work in basis of plane waves
- Periodic potentials couple plane waves related by reciprocal lattice vectors



- Bloch's theorem: Wavefunctions are product of a periodic part $u_{\mathbf{q}}(\mathbf{r})$ (the "Bloch state") and a phase factor $e^{i\mathbf{q}\cdot\mathbf{r}}$

Further reading

- Section 7 of Kittel ‘Introduction to solid state physics’
- P. 134 of Ashcroft and Mermin ‘Solid state physics’: Alternative derivation based on symmetry operators and group theory
- My lecture notes: