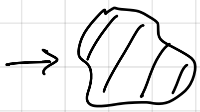
Applications of Quantum Mechanics

1. Scattering

1.1 Scattering in 1D.

Object $\longrightarrow$ learn about it by throwing stuff.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \underbrace{V(x)}_{\text{object}}\psi(x) = E\underbrace{\psi(x)}_{\text{"stuff"}}.$$



Assumptions on the potential : Localised in space

- $V(x) \longrightarrow 0$ as $x \to \pm\infty$
- $V(x) = 0$ for $|x| > L$.

This assumption means, as $|x| \to \infty$, we have $\psi(x) \sim \psi_0(x)$, where

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_0 = E\psi_0.$$

We will have two types of sol^{n}s.

(i) Bound states $(E<0)$: localised in a region of space.

$$\psi(x) \xrightarrow[|x|\to\infty]{} e^{-\lambda|x|}$$

$$\Rightarrow \quad E = -\frac{\hbar^2\lambda^2}{2m}$$

Properties :

- normalisable $\int_{-\infty}^{\infty}|\psi|^2dx < \infty$
- λ has discrete values.

(ii) Scattering states $(E>0)$:

$$\psi(x) \sim e^{\pm ikx}, \quad k\in\mathbb{R}, \quad k>0.$$

$$E = \frac{\hbar^2k^2}{2m}.$$

Rightmoving : $\psi(x) \sim e^{ikx}$ $\rightsquigarrow$

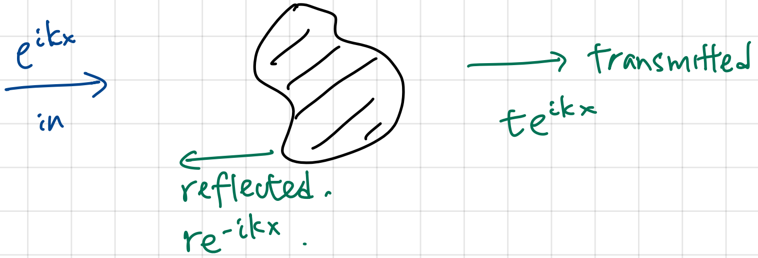
Leftmoving : $\psi(x) \sim e^{-ikx}$ $\leftsquigarrow$

Properties :

- non-normalisable $\int_{-\infty}^{\infty} |\psi|^2 dx = \infty$
- $k \in \mathbb{R}$. (continuous)

Reflection and Transmission amplitude

(a) Scattering from left



In equations,

$$\psi_R(x) \sim \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to \infty \end{cases}$$

rightmoving

Here, $r \in \mathbb{C}$ is the reflection amplitude / coeff.

$t \in \mathbb{C}$ transmission amplitude / coeff.

What can we say about r and t ?

consider

$$J(x) = -\frac{i\hbar}{2m}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right).$$

obeys

$$\frac{dJ}{dx} = 0$$

if ψ satisfies Schr eqn.

At $x \to -\infty$,

$$J(x) = \frac{\hbar}{2m} \cdot 2k(1-|r|^2)$$

At $x \to +\infty$,

$$J(x) = \frac{\hbar}{2m} \cdot 2k\,|t|^2.$$

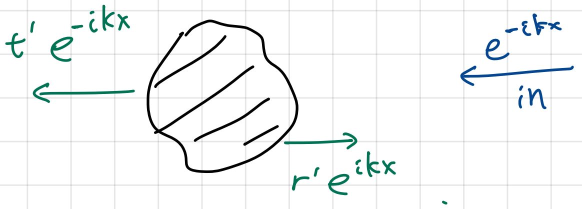
Then $J(x \to -\infty) = J(x \to \infty) \Rightarrow 1-|r|^2 = |t|^2$

$$\Rightarrow |r|^2 + |t|^2 = 1.$$

Then $R := |r|^2$ is prob. of reflection

$T := |t|^2$ transmission

(b) Scattering from the right



In equations,

$$\psi_L \sim \begin{cases} t' e^{-ikx} & x \to -\infty \\ e^{-ikx} + r' e^{ikx} & x \to \infty \end{cases}$$

By using $\frac{dJ}{dx} = 0$, we find

$$|t'|^2 + |r'|^2 = 1.$$

Schr. eqn only has 2 LI sol^n, so let's relate ψ_R and ψ_L.

Consider

$$\frac{1}{t^*}(\psi_R^* - r^* \psi_R) \sim \begin{cases} \frac{1}{t^*}\left(e^{-ikx} + r^* e^{ikx} - r^*(e^{ikx} + r e^{-ikx})\right) & x \to -\infty \\ \frac{1}{t^*}\left(t^* e^{-ikx} - r^* t e^{ikx}\right) & x \to \infty \end{cases}$$

$$= \begin{cases} e^{ikx}(1 - |r|^2)/t^* & x \to -\infty \\ e^{-ikx} - \frac{r^* t}{t^*} e^{ikx} & x \to \infty. \end{cases}$$

Then $t' = \frac{1 - |r|^2}{t^*} = \frac{|t|^2}{t^*} = t$,

$$r' = -\frac{r^*}{t^*} t$$

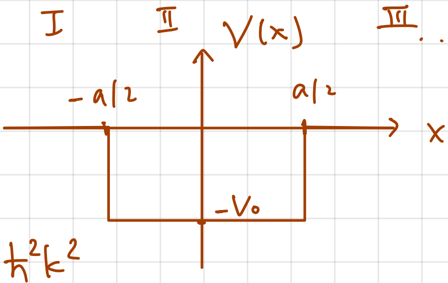
So transmission amplitude are same, reflection differs by a phase.

$$\Rightarrow R = |r|^2 = |r'|^2, \quad T = |t|^2 = |t'|^2.$$

Example

$$V(x) = \begin{cases} -V_0 & -a/2 < x < a/2 \\ 0 & o/w \end{cases} \quad , \quad V_0 > 0 \ \text{const.}$$

Task: evaluate r, t.



In regions I, III, $V(x) = 0$, then the basis of sol^n are

$$\psi(x) \sim e^{\pm ikx} , \quad E = \frac{\hbar^2 k^2}{2m}$$

In region II, $V(x) = -V_0$, then

$$\psi(x) \sim e^{\pm iqx} . \quad E = \frac{\hbar^2}{2m} q^2 - V_0$$

$$\Rightarrow q^2 = \frac{2mV_0}{\hbar^2} + k^2 .$$

Left scattering

$$\psi_R(x) = \begin{cases} e^{ikx} + re^{-ikx} \equiv \psi_I & x < -a/2 \\ Ae^{iqx} + Be^{-iqx} \equiv \psi_{II} & |x| < a/2 \\ te^{ikx} \equiv \psi_{III} & x > a/2 \end{cases}$$

Unknown: A, B, r, t. Solve by cty of f^n and derivative.

$$\psi_I(x = -a/2) = \psi_{II}(x = -a/2)$$

$$\psi_{II}(x = a/2) = \psi_{III}(x = a/2)$$

$$\psi_I'(x = -a/2) = \psi_{II}'(x = -a/2)$$

$$\psi_{II}'(x = a/2) = \psi_{III}'(x = a/2)$$

Resulting two expressions for r, t:

$$r = \frac{(k^2 - q^2)\sin(qa)e^{-ika}}{(q^2 + k^2)\sin(qa) + 2ikq\cos(qa)}$$

$$t = \frac{2iqke^{-ika}}{(q^2 + k^2)\sin(qa) + 2ikq\cos(qa)}$$

Comments: (1) soft throw: $k \to 0 \Rightarrow r \to -1, \ t \to 0$

(2) hard / fast throw: $k \to \infty \Rightarrow r \to 0, \ t \to 1$.

S-matrix

S: scattering

Defn

$$\text{Ingoing}: \begin{cases} \text{right} & I_R = e^{ikx} & x \to -\infty \\ \text{left} & I_L = e^{-ikx} & x \to +\infty \end{cases}$$

$$\text{Outgoing}: \begin{cases} \text{right} & O_R = e^{ikx} & x \to +\infty \\ \text{left} & O_L = e^{-ikx} & x \to -\infty \end{cases}$$

Write

$$\Psi_R = \underbrace{I_R + rO_L}_{x \to -\infty} + \underbrace{tO_R}_{x \to \infty}$$

$$\Psi_L = \underbrace{I_L + r'O_R}_{x \to \infty} + \underbrace{t'O_L}_{x \to -\infty}$$

and $\begin{pmatrix} \Psi_R \\ \Psi_L \end{pmatrix} = \begin{pmatrix} I_R \\ I_L \end{pmatrix} + S \begin{pmatrix} O_R \\ O_L \end{pmatrix}$, where $S = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix}$ is S-matrix.

Claim: $SS^\dagger = \mathbb{1}$

Pf:

$$\begin{pmatrix} t & r \\ r' & t' \end{pmatrix}\begin{pmatrix} t^* & r'^* \\ r^* & t'^* \end{pmatrix} = \begin{pmatrix} |t|^2 + |r|^2 & t'r^* + rt'^* \\ t'r^* + r't^* & |r'|^2 + |t'|^2 \end{pmatrix} = \mathbb{1}. \qquad \square$$

Claim: $S^*(k) = S(-k)$

Pf: For Ψ_R, Ψ_L, it is true that

$$\Psi(x;k) = \Psi^*(x;-k)$$

So

$$\underset{\begin{pmatrix} \Psi_R \\ \Psi_L \end{pmatrix}}{\underset{\|}{\begin{pmatrix} \Psi_R^*(x,-k) \\ \Psi_L^*(x,-k) \end{pmatrix}}} = \begin{pmatrix} I_R^*(-k) \\ I_L^*(-k) \end{pmatrix} + S^*(-k) \begin{pmatrix} O_R^*(-k) \\ O_L^*(-k) \end{pmatrix}.$$

$\square$

Parity Basis

Defn Parity operator P:

$$Pf(x) = f(-x).$$

We will see the consequences on S-matrix when

$$V(x) = V(-x)$$

invariant under P (symmetric).

Properties:

(i) If $V(x)$ symmetric, then $[P, H] = 0$.

$\Rightarrow$ use eigenstate of P to organise spectrum / sol^{n}s.

(ii) $P = P^\dagger$ Hermitian $\Rightarrow$ eval $\lambda \in \mathbb{R}$.

$$P^2 f(x) = f(x) \Rightarrow \lambda^2 = 1 \Rightarrow \lambda = \pm 1.$$

(iii) When V symmetric,

$$\psi_R(x) = \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to \infty \end{cases}$$

$$\Rightarrow \underset{\displaystyle \psi_L(x).}{\underset{\shortparallel}{\psi_R(-x)}} = \begin{cases} te^{-ikx} & x \to -\infty \\ e^{-ikx} - re^{ikx} & x \to \infty \end{cases}$$

$$\Rightarrow r = r', \quad t = t'$$

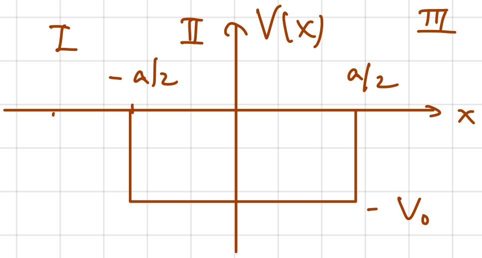
With these properties, define

$$\psi_+ \equiv \psi_R(x) + \psi_L(x) = \psi_R(x) + \psi_R(-x) \qquad \text{even}$$

$$\psi_- \equiv -\psi_R(x) + \psi_L(x) = -\psi_R(x) + \psi_R(-x) \qquad \text{odd}$$

and $P\psi_\pm = \pm\psi_\pm$ estates of P.

Example Even parity



$$\psi_+ = \psi_R + \psi_L = \begin{cases} e^{ikx} + (r+t')e^{-ikx} & \text{I} \\ \tilde{A}(e^{iqx} + e^{-iqx}) & \text{II} \\ (t+r')e^{ikx} + e^{-ikx} & \text{III}. \end{cases}$$

and
$$\left.\begin{aligned} \psi_+^{I}(x=-a/2) &= \psi_+^{II}(x=-a/2), \\ \psi_+^{\prime I}(x=-a/2) &= \psi_+^{\prime II}(x=-a/2) \end{aligned}\right\} \text{ Solve for } \tilde{A}, (r+t)$$

Odd parity

$$\psi_- = -\psi_R + \psi_L = \begin{cases} -e^{ikx} + (r+t')\,e^{-ikx} & \mathrm{I} \\ \tilde{B}\,(e^{iqx} - e^{-iqx}) & \mathrm{II} \\ (-t+r)\,e^{ikx} - e^{-ikx} & \mathrm{III} \end{cases}$$

$$\Rightarrow \left. \begin{aligned} \psi_-^{\mathrm{II}}(x=a/2) &= \psi_-^{\mathrm{III}}(x=a/2) \\ \psi_-^{\prime\mathrm{II}}(x=a/2) &= \psi_-^{\prime\mathrm{III}}(x=a/2) \end{aligned} \right| \quad \tilde{B}\,,\ (r-t)$$

Sol^n:

$$t + r = -e^{-ika}\left(\frac{q\tan\left(\frac{qa}{2}\right) - ik}{q\tan\left(\frac{qa}{2}\right) + ik}\right)$$

$$r - t = e^{ika}\left(\frac{q + ik\tan\left(\frac{qa}{2}\right)}{q - ik\tan\left(\frac{qa}{2}\right)}\right)$$

S-matrix in partity basis:

$$\text{Ingoing}\ \begin{cases} \text{parity even} & I_+ \sim e^{-ik|x|} \\ \text{parity odd} & I_- \sim \operatorname{sgn}(x)\, e^{ik|x|}. \end{cases}$$

$$\text{Outgoing}\ \begin{cases} \text{even} & O_+ \sim e^{ik|x|} \\ \text{odd} & O_- \sim -\operatorname{sgn}(x)\, e^{-ik|x|}. \end{cases}$$

$$\begin{pmatrix} I_+ \\ I_- \end{pmatrix} = \mathcal{M}\begin{pmatrix} I_R \\ I_L \end{pmatrix}, \quad \begin{pmatrix} O_+ \\ O_- \end{pmatrix} = \mathcal{M}\begin{pmatrix} O_R \\ O_L \end{pmatrix}$$

where $\mathcal{M} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$, and

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} I_+ \\ I_- \end{pmatrix} + S^P \begin{pmatrix} O_+ \\ O_- \end{pmatrix}$$

with

$$S^P = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} = \mathcal{M} S \mathcal{M}^{-1} = \begin{pmatrix} t + (r+r')/2 & (r-r')/2 \\ (r'-r)/2 & t - (r+r')/2 \end{pmatrix}.$$

$$\Rightarrow S_{+-} = S_{-+} = 0, \quad S_{++} = t + r, \quad S_{--} = t - r.$$

Recall $r' = -r^* t/t^* = r \Rightarrow \mathrm{Re}(rt^*) = 0$

$$\Rightarrow |r+t|^2 = 1, \quad |r-t|^2 = 1$$

So $S_{++} = t + r = e^{2i\delta_+}$, $S_{--} = t - r = e^{2i\delta_-}$, where $\delta_\pm$ are phase shifts.

Bound States $(E<0)$

Key: extend $k \in \mathbb{C}$ (before, we had $k>0$)

Assume now $V(x) = V(-x)$. With this, consider the even parity sol^n

$$\psi_+(x) = I_+ + S_{++} O_+ = \begin{cases} e^{ikx} + S_{++} e^{-ikx} & x \to -\infty \\ e^{-ikx} + S_{++} e^{ikx} & x \to \infty \end{cases}$$

Set $k = i\lambda$, $\lambda > 0$.

$$\psi_+ \sim \begin{cases} e^{-\lambda x} + S_{++} e^{\lambda x} & x \to -\infty \\ \underbrace{e^{\lambda x}}_{\text{diverge}} + S_{++} \underbrace{e^{-\lambda x}}_{\text{decay}} & x \to \infty \end{cases}$$

$$\frac{1}{S_{++}} \psi_+ \sim \begin{cases} \frac{1}{S_{++}} e^{-\lambda x} + e^{\lambda x} & x \to -\infty \\ \underbrace{\frac{1}{S_{++}} e^{\lambda x}}_{\text{remove}} + \underbrace{e^{-\lambda x}}_{\text{kills}} & x \to \infty \end{cases}$$

$\Rightarrow$ Punchline: in order to have a normalisable sol^n at $x \to \pm\infty$, find situations where $S_{++}(k) \to \infty \Rightarrow$ looking for poles in k.

We see with this,

$$E = \frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2 \lambda^2}{2m} < 0.$$

Notes: (1) Repeat argument for S_{--} (odd parity)

(2) Set $k = -i\lambda$, $\lambda > 0$, then look for zeros for S_{++}.

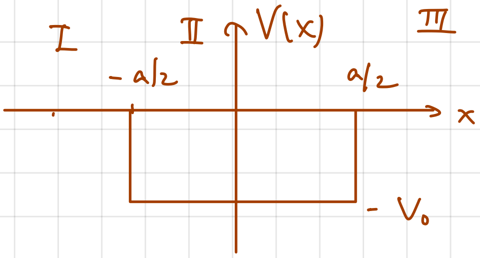
However, S_{++} is a phase. If $S_{++} \sim \frac{1}{k - i\lambda_*}$, we also have

$|S_{++}|^2 = 1$ ($|r \pm t|^2 = 1$). Then

$$S_{++} \sim \frac{k + i\lambda_*}{k - i\lambda_*} .$$

Example $S_{++} = r + t$

$$= -e^{-ika}\,\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik},$$

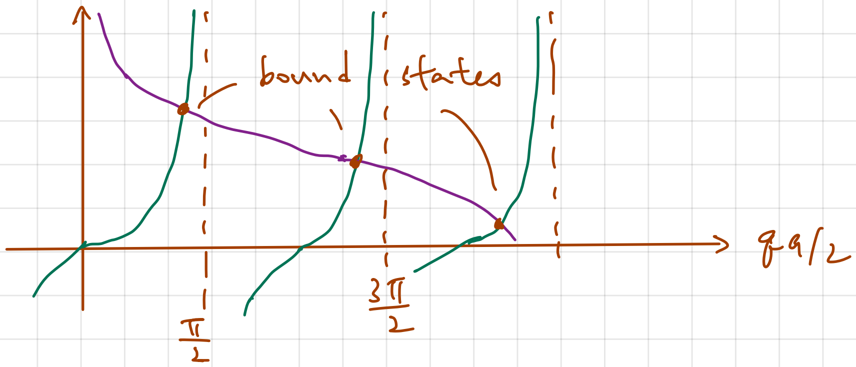


$$q^2 = k^2 + \frac{2mV_0}{\hbar^2} = k^2 + q_0^2 .$$

Find bound states: $k = i\lambda$, then poles are located at

$$\lambda = q(\lambda)\,\tan\left(\frac{q(\lambda)\,a}{2}\right)$$

$$\Rightarrow \sqrt{\frac{q_0^2}{q^2} - 1} = \tan\left(\frac{qa}{2}\right)$$



Comments:

(1) Key that $V_0 > 0$

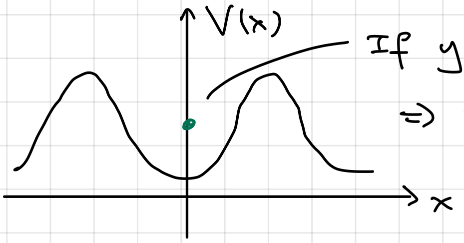
(2) Repeat for S_{--}.

(3) Discrete sol^n to $k = i\lambda$.

Resonances

Is there any other info hidden in S-matrix ?

Consider, e.g.



If you 'live' for a while
⇒ resonance
unstable / metastable state

This occurs when

$$k = k_0 - i\gamma \quad , \; k_0 , \gamma > 0 .$$

In this situation.

$$E = \frac{\hbar^2 k^2}{2m} = E_0 - i\Gamma/2 .$$

$$E_0 = \frac{\hbar^2}{2m}\left(k_0^2 - \gamma^2\right) \quad , \quad \Gamma = \frac{2\hbar^2}{m}\gamma k_0$$

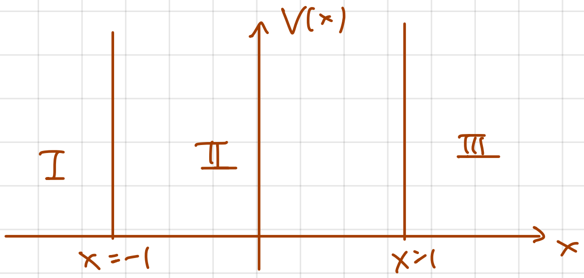
Interpretation :

$$\psi(x,t) \sim \underbrace{(\quad \cdot \quad)}_{\text{spatial}} e^{-iEt/\hbar}$$

$$e^{-iEt/\hbar} = e^{-iE_0 t/\hbar} \underbrace{e^{-\Gamma t/2\hbar}}_{\text{decay characteristics of unstable states}}$$

Nomenclature :

- Γ is the width of the state
- $\tau = \hbar/\Gamma$ is the half-life of the state.



Example $V(x) = V_0\left(\delta(x-1) + \delta(x+1)\right)$

Outside $x = \pm 1$,

$$\psi(x) \sim e^{\pm ikx}$$

Use parity (even)

I : $\psi_I^+ = e^{ikx} + S_{++}(k)\, e^{-ikx}$ $\quad x < -1$

II : $\psi_I^+ = A\cos(kx)$ $\quad |x| < 1$

III : $\psi_I^+ = e^{-ikx} + S_{++}(k)\, e^{ikx}$ $\quad x > 1$

Impose B.C.

(i) Cty at $x = \pm 1$

(ii) derivative at $x = \pm 1$.

$$\lim_{\varepsilon\to 0}\left(\frac{\partial\psi}{\partial x}\Big|_{1+\varepsilon} - \frac{\partial\psi}{\partial x}\Big|_{1-\varepsilon}\right)$$

$$= \frac{2m}{\hbar}\lim_{\varepsilon\to 0}\int_{1-\varepsilon}^{1+\varepsilon} V(x)\,\psi(x)\,dx = U_0\,\psi(1), \qquad U_0 = \frac{2mV_0}{\hbar^2}.$$

Can find

$$S_{++} = e^{-2ik}\left(\frac{(2k-iU_0)\,e^{ik} - iU_0\,e^{-ik}}{(2k+iU_0)\,e^{-ik} + iU_0\,e^{ik}}\right)$$

Location of poles

$$\Rightarrow e^{2ik} = -\left(1 - \frac{2ik}{U_0}\right) \qquad (*)$$

Take limits :

- $U_0 \to \infty$, then sol^n to $(*)$

$$k_n = (n+\tfrac{1}{2})\pi, \quad n \in \mathbb{Z}$$

- $U_0 \gg 1$

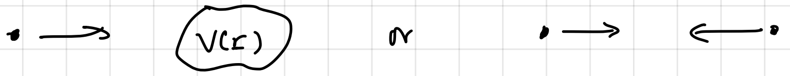
$$k = k_n + \frac{\delta k^{(1)}}{U_0} + \frac{\delta k^{(2)}}{U_0^2} + \dots = k_n + \sum_{i=1}\frac{\delta k^{(i)}}{U_0^i}.$$

Sol^n $(n=0)$:

$$k = \underbrace{\frac{\pi}{2} + \left(-\frac{2\pi}{U_0} + \frac{\pi}{2U_0^2} + \dots\right)}_{k_0} - \underbrace{i\left(\frac{\pi^2}{4U_0^2}\right.}_{+i\Gamma}\left. + \dots\right)$$

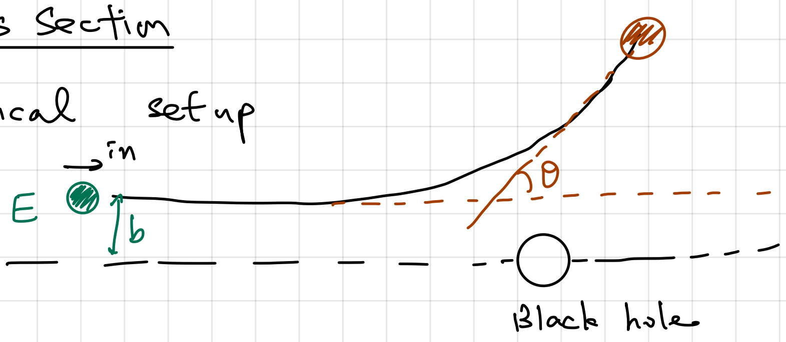
1.2 Scattering in 3D

Scattering $\quad H = \frac{p^2}{2m} + V(r).$



Cross Section

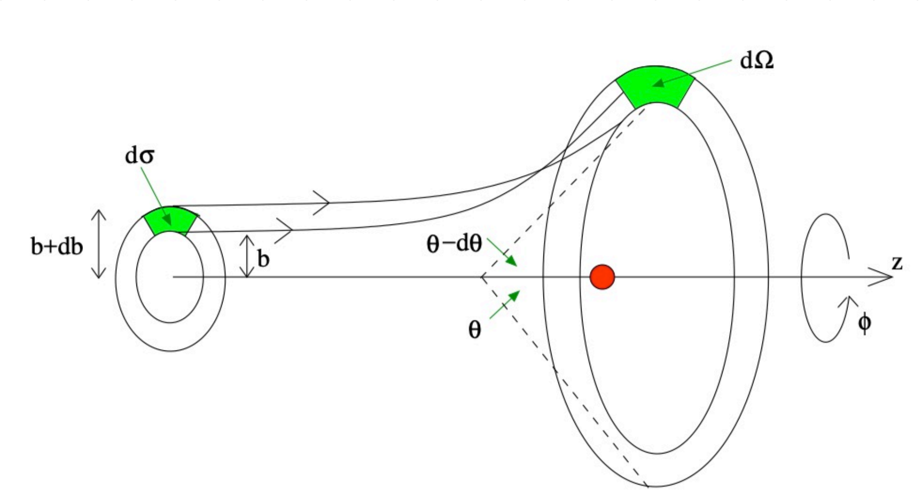
Classical setup



E : energy,

b : impact parameter

θ : scattering angle.



$d\sigma = b\,db\,d\phi$: cross-sectional area

$d\Omega = \sin\theta\,d\theta\,d\phi$: solid angle sphere.

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$: differential cross section.

Another point of view:

$\mathcal{L}$ = # incident particles per unit area . per unit time (luminosity)

No. of particles entering $d\sigma$:

$$dN = \mathcal{L}\,d\sigma$$: event rate

$$\frac{d\sigma}{d\Omega} = \frac{1}{\mathcal{L}}\frac{dN}{d\Omega} = \frac{\#\text{ particles scattered into } d\Omega}{\#\text{ particles incident}}$$

$$= \frac{\text{scattered flux}}{\text{incident flux}}$$

We can also define

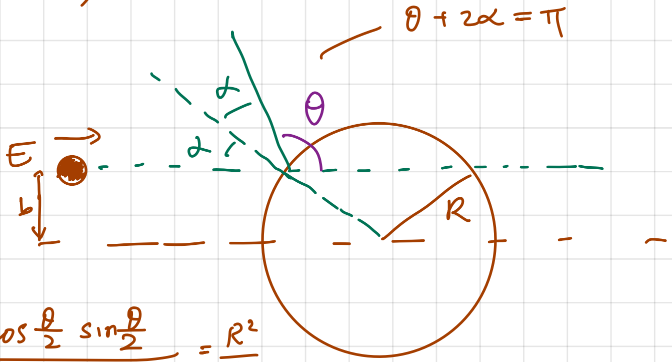
$$\sigma_T = \int d\Omega\,\frac{d\sigma}{d\Omega}$$: total cross section.

Units: $\frac{d\sigma}{d\Omega}$, σ_T are measured in units of area.

Common unit: 1 barn = $10^{-28}\,m^2$ (size of uranium nucleus)

Example (Hard sphere, elastic bounce)

$$V(r) = \begin{cases} \infty & r<R \\ 0 & r>R \end{cases}$$



We have $b = R\sin\alpha = R\cos\frac{\theta}{2}$,

Then $$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{R^2}{2}\,\frac{\cos\frac{\theta}{2}\sin\frac{\theta}{2}}{\sin\theta} = \frac{R^2}{4}.$$

$$\sigma_T = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\, R^2/4 = \pi R^2 = \text{Area of sphere.}$$

Example (Rutherford scattering)

In IA D&R,

$$V(r) = \frac{A}{r}, \quad A = \frac{q_1 q_2}{4\pi\varepsilon_0} > 0$$

$$\Rightarrow 2bE = A\cot(\theta/2)$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \left(\frac{A}{4E}\right)^2 \frac{1}{\sin^4\theta/2}.$$

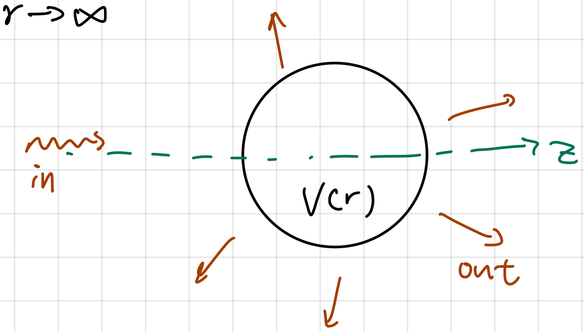
Note: $\sigma_T \to \infty$ because divergence $\theta \to 0$, because $V(r)$ does not vanish rapidly enough as $r \to \infty$ $\Rightarrow$ effective infinite area of influence.

1.2.2 Scattering Amplitude (Quantum)

Assume
- $V(\underline{r}) = V(r)$: central / sph. sym potential,
- $V(r\to\infty) = 0$

Asymptotic form of sol^n

$$\psi(\underline{r}) = \underbrace{e^{ikz}}_{\text{incident}} + \underbrace{f(\theta,\phi)\frac{e^{ikr}}{r}}_{\text{scattered}} + \dots \quad r\to\infty$$

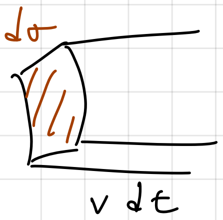


$\boxed{\text{Goal: determine } f(\theta,\phi)}$ Why? Relate it to $\frac{d\sigma}{d\Omega}$.

$\psi_{incident} = e^{ikz}$ $\qquad\qquad$ $\psi_{scattered} = \frac{1}{r} f(\theta,\phi)\, e^{ikr}$

Incident probability

$$dP = |\psi_{inc}|^2\, dV = v\, dt\, d\sigma$$



Scattered probability

$$dP = |\psi_{scattered}|^2\, dV = \frac{|f|^2}{r^2} V dt \underbrace{dA}_{=r^2 d\Omega}$$

$$= |f|^2\, v\, dt\, d\Omega$$

Probability is conserved, so

$$\boxed{\frac{d\sigma}{d\Omega} = |f|^2}$$

Note: Can also deduce from prob. current $\underline{J}$.

Partial Waves

Quantify and organise solⁿ to Schr. based on boundary conditions.

Schr. eqn:

$$\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{2m}{\hbar^2}\left(V(r) - E\right)\right)\psi(\underline{r}) = 0$$

assuming $\psi(r,\theta,\phi) = \psi(r,\theta)$
since $V(\underline{r}) = V(r)$.

Write $\qquad \psi(r,\theta) = \sum_{l=0} R_l(r)\, P_l(\cos\theta)$.

Legendre poly.

Ang: $\qquad \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) P_l(\cos\theta) = -l(l+1)\, P_l(\cos\theta)$.

Radial: $\qquad \left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{r^2} - U(r) + k^2\right) R_l(r) = 0.$

$U(r) = \frac{2m}{\hbar^2} V(r)$ $\qquad\qquad$ $E = \frac{\hbar^2}{2m}k^2$

(a) $U(r) = 0,\ l = 0$:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r} + k^2\right) R_0(r) = 0$$

$$\Rightarrow R_0(r) = A\,\frac{e^{-ikr}}{r} + B\,\frac{e^{ikr}}{r}$$

($rR_l(r)$ obeys 1D Schr. eqn).

(b) $U(r) = 0$, plane waves

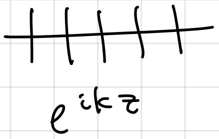
$$\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2 \Rightarrow \psi \sim e^{\pm ikz}$$

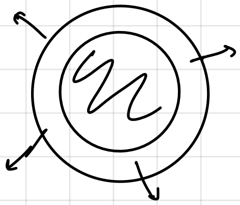
$$\psi_{\text{incident}} = e^{ikz}$$

How to relate incident (cartesian) with scattered (sph. polar)?

$$\psi_{\text{inc}} = e^{i\rho\cos\theta},$$

where $z = r\cos\theta$, $\rho = kr$.





$$\psi_{\text{inc}} = \sum_{l=0}^{\infty} (2l+1)\, u_l(\rho)\, P_l(\cos\theta).$$

↖ coeff. to be determined

To determine $u_l(\rho)$, use

$$\int_{-1}^{1} d(\cos\theta)\, P_l(\cos\theta)\, P_m(\cos\theta) = \frac{2}{2l+1}\,\delta_{lm}.$$

Integrate both sides,

$$\int_{-1}^{1} d(\cos\theta)\, P_m(\cos\theta)\, e^{i\rho\cos\theta} = \sum_l (2l+1)\int_{-1}^{1} d(\cos\theta)\, P_l(\cos\theta)\, P_m(\cos\theta)\ u_l(\rho)$$

$$\Rightarrow u_l(\rho) = \frac{1}{2}\int_{-1}^{1} d(\cos\theta)\, P_l(\cos\theta)\, e^{i\rho\cos\theta}$$

$$= \frac{1}{2}\int_{-1}^{1} dw\, P_l(w)\, e^{i\rho w} \qquad (w = \cos\theta).$$

$$= \frac{1}{2}\int_{-1}^{1} dw\, P_l(w)\,\frac{1}{i\rho}\,\frac{d}{dw}\left(e^{i\rho w}\right).$$

$P_l(1) = 1$

$P_l(-1) = (-1)^l$

$$= \frac{1}{2i\rho}\left[P_l(w)\, e^{i\rho w}\right]_{-1}^{1} - \frac{1}{2i\rho}\int_{-1}^{1} dw\, e^{i\rho w}\,\frac{d}{dw}P_l(w).$$

$$= \frac{1}{2i\rho}\left(e^{i\rho} - (-1)^l e^{-i\rho}\right) - \frac{1}{2(i\rho)^2}\int_{-1}^{1} dw\, \frac{d}{dw}P_l(w)\,\frac{d}{dw}\left(e^{i\rho w}\right).$$

So

$$\psi_{\text{inc}} = \sum_{\ell\geq 0} \frac{2\ell+1}{2i\rho}\left(\underset{\text{outgoing}}{\underset{\swarrow}{e^{i\rho}}} - (-1)^{\ell}\underset{\text{ingoing}}{\underset{\searrow}{e^{-i\rho}}}\right) P_\ell(\cos\theta) + O\left(\tfrac{1}{\rho^2}\right). \qquad (1)$$

sph. waves

Combine,

$$\psi(\underline{r}) = \underbrace{e^{ikz}}_{\psi_{\text{inc}}} + \underbrace{f(\theta)\frac{e^{ikr}}{r}}_{\psi_{\text{scattered}}} + \dots \qquad r\to\infty$$

Define $$f(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{k} f_\ell(k)\, P_\ell(\cos\theta). \qquad (2).$$

Then replace (1), (2).

$$\psi(\underline{r}) = \sum_{\ell=0} \frac{2\ell+1}{2ik}\left((-1)^{\ell+1}\frac{e^{-ikr}}{r} + (1+2if_\ell)\frac{e^{ikr}}{r}\right) P_\ell(\cos\theta) + \dots$$

From here, we define S-matrix.

$$S_\ell := 1+2if_\ell$$

Can show using conservation of prob. or 1D analogy

$$S_\ell = e^{2i\delta_\ell}, \qquad \delta_\ell : \text{phase shift}$$

$$\Rightarrow \quad f_\ell = e^{i\delta_\ell}\sin\delta_\ell.$$

Optical Theorem

We had

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

$$= \frac{1}{k^2}\sum_{\ell,\ell'} (2\ell+1)(2\ell'+1) f_\ell f_{\ell'}^{*} P_\ell(\cos\theta) P_{\ell'}(\cos\theta)$$

$$\Rightarrow \quad \sigma_T = 2\pi\int_{-1}^{1} d(\cos\theta)\,\frac{d\sigma}{d\Omega}$$

$$= \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\,|f_\ell^2| = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell. \qquad (3)$$

Note $$f(\theta) = \frac{1}{k}\sum_\ell (2\ell+1) f_\ell P_\ell(\cos\theta).$$

$$f(0) = \frac{1}{k}\sum_{l}(2l+1)\, e^{i\delta_l}\sin\delta_l \, P_l(1)$$

$$= \frac{1}{k}\sum_{l}(2l+1)(\cos\delta_l + i\sin\delta_l)\sin(\delta_l)$$

$$\Rightarrow \mathrm{Im}(f(0)) = \frac{1}{k}\sum_{l}(2l+1)\sin^2\delta_l .$$

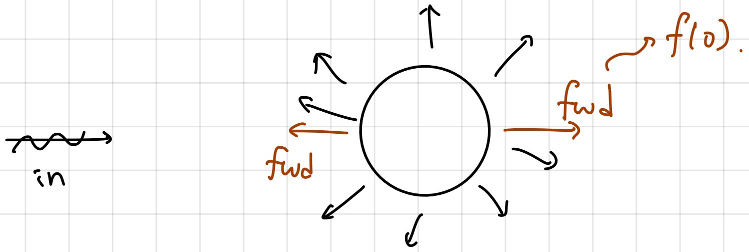
Then (3) reads

$$\boxed{\sigma_T = \frac{4\pi}{k}\,\mathrm{Im}(f(0))}$$

Comments :

(1) Opt. thm. is a consequence of conservation of prob. (means it applies for any $V(r)$)

(2) Intuition :



Opt. thm. $\Rightarrow$ σ_T is given by forward direction.

Example (Hard sphere)

$$V(r) = \begin{cases} \infty & r<a \\ 0 & r>a . \end{cases}$$

Quantum version of the classical example.

For $r>a$, sol^n to Schr. eqn is

$$\psi(r,\theta) = \sum_{l=0}^{\infty} R_l(r)\, P_l(\cos\theta)$$

with

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right)(r R_l(r)) = 0$$

For any l, sol^{n}s $j_l(kr)$, $n_l(kr)$ (spherical Bessel f^n).

Note About $j_\ell(kr)$, $n_\ell(kr)$

- $\ell = 0$: $j_0(\rho) = \frac{\sin\rho}{\rho}$, $n_0(\rho) = -\frac{\cos\rho}{\rho}$ $(\sim e^{\pm ikr}/r)$.

- $\ell > 0$: $j_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\sin\rho}{\rho}$.

$$n_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(-\frac{\cos\rho}{\rho}\right)$$

- As $\rho \to \infty$, $(r \to \infty)$ $j_\ell(\rho) \to \frac{\sin(\rho - \ell\pi/2)}{\rho}$, $n_\ell(\rho) \to \frac{\cos(\rho - \ell\pi/2)}{\rho}$.

- As $\rho \to 0$, $j_\ell(\rho) \to \frac{\rho^\ell}{(2\ell-1)!!}$, $n_\ell(\rho) \to -(2\ell-1)!!\,\rho^{-(\ell+1)}$

For us. general sol^n

$$R_\ell(r) = A_\ell\left(\cos\alpha_\ell\, j_\ell(\rho) - \sin\alpha_\ell\, n_\ell(\rho)\right) , \rho = kr.$$

- BC : $\psi(r=a) = 0$.

- Inspect behaviour as $r \to \infty$ to read off $S_\ell(f_\ell, \delta_\ell) \Rightarrow \sigma_T$.

Impose BC : at $r = a$, $R_\ell(a) = 0$

$$\Rightarrow \cos\alpha_\ell\, j_\ell(ka) - \sin\alpha_\ell\, n_\ell(ka) = 0$$

$$\Rightarrow \boxed{\tan\alpha_\ell = j_\ell(ka) / n_\ell(ka).} \qquad (1)$$

Asymptotic behaviour.

$$R_\ell(r) \sim \frac{A_\ell}{\rho}\sin\left(\rho - \frac{\ell\pi}{2} + \alpha_\ell + \dots\right) \qquad (2)$$

Compare

$$R_\ell(\rho) \sim (-1)^{\ell+1}\frac{e^{-ikr}}{kr} + S_\ell\frac{e^{ikr}}{kr} + \dots \quad S_\ell = e^{2i\delta_\ell} .$$

Rewrite (2) in basis of exp.

$$R_\ell(\rho) \sim -A_\ell\, e^{-i\pi\ell/2}\, e^{-i\alpha_\ell}\left((-1)^{\ell+1}\frac{e^{-ikr}}{kr} + e^{2i\alpha_\ell}\frac{e^{ikr}}{kr}\right) + \dots$$

$$\Rightarrow \alpha_\ell = \delta_\ell . \quad S_\ell = e^{2i\alpha_\ell} .$$

Then

$$\sigma_T = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\alpha_\ell .$$

where α_ℓ is sol^n to (1).

Analyse σ_T, for that we need to solve (1).

For $l=0$,

$$\tan\delta_0 = \frac{j_0(ka)}{n_0(ka)} = -\tan(ka)$$

$$\Rightarrow \delta_0 = -ka.$$

For $l>0$, $ka \ll 1$, $\delta_l \ll 1$.

$$\tan\delta_l = \frac{j_l(ka)}{n_l(ka)} \xrightarrow[ka\ll 1]{} -\frac{(ka)^{2l+1}}{(2l+1)!!\,(2l-1)!!}$$

$$\Rightarrow \delta_l \approx -\frac{(ka)^{2l+1}}{(2l+1)!!\,(2l-1)!!}$$

Note: potential barrier $-\frac{l(l+1)}{r^2}$ surpress higher l in α_l.

The cross section as $ka \ll 1$.

$$\sigma_T = \frac{4\pi}{k^2}\sin^2\alpha_0 + \dots = \frac{4\pi}{k^2}\sin^2(ka) + \dots \overset{k\to 0}{=} 4\pi a^2.$$

Recall classical: $\sigma_T^c = \pi a^2$.

Def^n (Scattering length) Low k (momenta) behaviour is 'generic'

$$\delta_l \sim (ka_s)^{2l+1}$$

and a_s is the scattering length (relavant scale/size of the problem).

$$\Rightarrow \sigma_T \underset{k\to 0}{=} 4\pi a_s^2.$$

Bound States

Brave: $k = i\lambda$

$$\psi(\underline{r}) \sim \sum_l \left((-1)^l \frac{e^{-ikr}}{kr} + S_l \frac{e^{ikr}}{kr} \right) P_l(\cos\theta).$$

$$\downarrow \qquad\qquad \downarrow 0 \qquad\qquad \downarrow$$

$$\frac{e^{kr}}{r} \qquad\qquad\qquad \frac{e^{-kr}}{r}.$$

Bound states are poles in $S_l(k=i\lambda)$.

Example Consider

$$V(r) = \begin{cases} -V_0 \equiv -\frac{\hbar^2\gamma^2}{2m} & r<a \\ 0 & r>a \end{cases}$$

Focus on $l=0$ (s-wave) for simplicity.

(I) $r>a$: $\left(\frac{d^2}{dr^2} + k^2\right)(r\psi_I) = 0 \Rightarrow \psi_I = A\,\frac{\sin(kr+\delta_0)}{r}$

(II) $r<a$: $\left(\frac{d^2}{dr^2} + k^2 + \gamma^2\right)(r\psi_{II}) = 0$

$$\Rightarrow \psi_{II} = B\,\frac{\sin\left(\sqrt{k^2+\gamma^2}\,r\right)}{r} + C\,\frac{\cos\left(\sqrt{k^2+\gamma^2}\,r\right)}{r}$$

$C=0$ by regularity at $r=0$

BC: $\psi_I(r=a) = \psi_{II}(r=a)$, $\psi_I'(r=a) = \psi_{II}'(r=a)$

$$\Rightarrow \frac{\tan(ka+\delta_0)}{ka} = \frac{\tan\left(\sqrt{k^2+\gamma^2}\,a\right)}{\sqrt{k^2+\gamma^2}\,a}.$$

Limits: (i) $k \gg \delta \Rightarrow \delta_0 \to 0$, particle doesn't see potential

(ii) $k^2 \ll \gamma^2$, $ka \ll 1$.

$$\delta_0 \sim ka\left(\frac{\tan\gamma a}{\gamma a} - 1\right) \equiv -(k a_s).$$

$$\Rightarrow a_s = a\left(1 - \frac{\tan\gamma a}{\gamma a}\right)$$

Attractive

$$\overset{\gamma \ll 1}{=} a - \left(a + \frac{a^3\gamma^3}{3} + \dots\right) = -\frac{a^3\gamma^3}{3} + \dots < 0.$$

Bound states: look for poles. Define

$$f(k) = \frac{\tan(ka+\delta_0)}{ka}$$

$$S_0 = e^{i2\delta_0} = e^{-2ika}\,\frac{1+if(a)}{1-if(a)}$$

$$f(k) = -i \Rightarrow \tan\left(\sqrt{k^2+\gamma^2}\,a\right) = \frac{\sqrt{k^2+\gamma^2}}{ik}.$$

No real solⁿ for $k \in \mathbb{R}$. Look at solⁿ for $k = i\lambda$.

When $\lambda \to 0$ $(E \to 0)$, eqn for B.S.

$$\tan \gamma a = -\frac{\gamma}{\lambda} \to \infty$$

occurs when

$$\gamma^* = \frac{\pi}{a}\left(n+\frac{1}{2}\right), \qquad n \in \mathbb{Z}.$$

Recall

$$a_s = a\left(1 - \frac{\tan \gamma a}{\gamma a}\right) \xrightarrow[\gamma = \gamma^*]{} \text{diverges} \Rightarrow \sigma_T \to \infty.$$

B.S. at threshold.

Summary: (1) Bound states $\doteq$ poles in S-matrix

(2) Bound state threshold $\equiv$ divergent scattering length / σ_T.

Resonances

What happens for $k = k_0 - i\gamma$, $E = E_0 - i\Gamma/2$, with

$E_0 = \frac{\hbar^2}{2m}(k_0^2 - \gamma^2)$, $\Gamma = \frac{2\hbar^2}{m}\gamma k_0$?

In 3D this happens often

$$\left(\frac{d^2}{dr^2} \underbrace{-\frac{\ell(\ell+1)}{r^2}}_{\text{repulsive}} \underbrace{-U(r)}_{\text{adjust s.t. attractive potentials will create dips.}} + k^2\right)(r R_\ell(r)] = 0.$$

What happens to the S-matrix ?

$$S_\ell(E) = e^{2i\delta_\ell} \sim \frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}$$ near resonance.

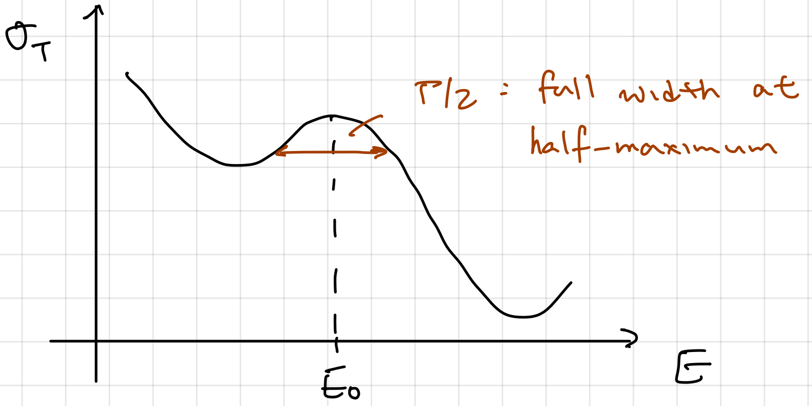
What happens to σ_T ?

$$\sigma_T \sim \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell.$$

Note $\sin^2\delta_\ell = \frac{1}{2}(1 - \cos 2\delta_\ell)$. then, near resonance,

$$\cos 2\delta_\ell = \frac{(E-E_0)^2 - \Gamma^2/4}{(E-E_0)^2 + \Gamma^2/4}. \Rightarrow \sin^2\delta_\ell = \frac{\Gamma^2}{4(E-E_0)^2 + \Gamma^2}$$

$$\Rightarrow \sigma_T \sim \frac{4\pi}{k^2}(2\ell+1)\frac{\Gamma^2}{4(E-E_0)^2 + \Gamma^2}$$



Lippmanns – Schwinger equation

How do we say something when we cannot solve eqn exactly?

Schr eqn:
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r})\right)\psi(\underline{r}) = E\psi(\underline{r}).$$

$$\Rightarrow \left(\frac{\hbar^2}{2m}\nabla^2 + E\right)\psi(\underline{r}) = V(\underline{r})\,\psi(\underline{r}).$$

A formal sol^n

$$\boxed{\psi(\underline{r}) = \phi(\underline{r}) + \int G(\underline{r}-\underline{r}')\,V(\underline{r}')\,\psi(\underline{r}')\,d^3\underline{r}'.} \qquad (1)$$

where $(\nabla^2+k^2)\,\phi(\underline{r}) = 0$, $E = \frac{\hbar^2}{2m}k^2$, and

$$(\nabla^2+k^2)\,\underbrace{G(\underline{r}-\underline{r}')}_{\text{Green's } f^n.} = \frac{2m}{\hbar^2}\,\delta^3(\underline{r}-\underline{r}'). \qquad (2)$$

Outline: 1) Construct G

2) See how to obtain approx sol^n via (1)

1) Construct $G(\underline{r}-\underline{r}')$, and solve (2) using Fourier transform

$$G(\underline{r}-\underline{r}') = \int \frac{d^3q}{(2\pi)^3}\,G(\underline{q})\,e^{i\underline{q}\cdot(\underline{r}-\underline{r}')}$$

$$\delta^3(\underline{r}-\underline{r}') = \int \frac{d^3q}{(2\pi)^3}\,e^{i\underline{q}\cdot(\underline{r}-\underline{r}')}$$

Then (2) $\Rightarrow$

$$(-q^2+k^2)\,G(\underline{q}) = \frac{2m}{\hbar}$$

$$\Rightarrow \quad G(\underline{q}) = -\frac{2m}{\hbar^2}\cdot\frac{1}{q^2-k^2}.$$

$$\Rightarrow G(\underline{r}-\underline{r}') = -\frac{2m}{\hbar^2}\int \frac{d^3\underline{q}}{(2\pi)^3}\,\frac{e^{i\underline{q}\cdot(\underline{r}-\underline{r}')}}{q^2-k^2}$$

$\underline{x} = \underline{r}-\underline{r}'; \quad x = |\underline{x}|$

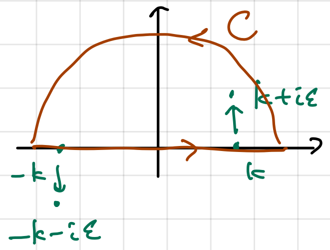
$$= -\frac{2m}{\hbar^2}\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\int_0^\infty dq\, q^2\,\frac{e^{iqx\cos\theta}}{q^2-k^2}\cdot\frac{1}{(2\pi)^3}$$

$$= -\frac{2m}{\hbar^2}\cdot\frac{1}{(2\pi)^2}\int_0^\infty dq\,\frac{q}{ix}\,\frac{e^{iqx}-e^{-iqx}}{q^2-k^2}$$

$$= -\frac{2m}{\hbar^2}\cdot\frac{1}{(2\pi)^2 ix}\int_{-\infty}^{\infty} dq\,\frac{q\,e^{iqx}}{q^2-k^2}$$

In integrand,

$$\frac{q}{q^2-k^2} = \frac{1}{2}\left(\frac{1}{q+k}+\frac{1}{q-k}\right)$$



$$\Rightarrow \underset{\underset{2\pi i\,\mathrm{Res}}{\parallel}}{\oint} = \int_{-\infty}^{\infty} + \underbrace{\int_C}_{\to 0}$$

So

$$G^+(\underline{r}-\underline{r}') = \lim_{\varepsilon\to 0}\left(-\frac{2m}{\hbar^2}\,\frac{1}{(2\pi)^2 ix}\int_{-\infty}^{\infty} dq\,\frac{e^{iqx}}{2}\left(\frac{1}{q-(k+\varepsilon)}+\frac{1}{q+(k+\varepsilon)}\right)\right)$$

$$= -\frac{2m}{\hbar^2}\cdot\frac{1}{4\pi}\cdot\frac{e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}$$

Then, formal solⁿ is (with b.c. for scattering).

$$\psi(\underline{r}) = e^{i\underline{k}\cdot\underline{r}} \underbrace{-\frac{2m}{\hbar^2}\int d^3\underline{r}'\,\frac{e^{ik|\underline{r}-\underline{r}'|}}{4\pi|\underline{r}-\underline{r}'|}\,V(\underline{r}')\,\psi(\underline{r}')}$$

where choose $\phi(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}$ (incident wavefⁿ)

because G^+ is the scattered part of wavefⁿ (outgoing)

Look at the asymp. behaviour as $\underline{r} \gg \underline{r}'$.

assuming $V(\underline{r}')$ localised

$$|\underline{r}-\underline{r}'| = \sqrt{\underline{r}^2 - 2\underline{r}\cdot\underline{r}' + \underline{r}'^2} \approx r - \frac{\underline{r}\cdot\underline{r}'}{r}.$$

Note We are assuming $V(\underline{r}')$ has compact support

$$\psi(k,\underline{r}) = e^{i\underline{k}\cdot\underline{r}} - \frac{2m}{\hbar^2}\left(\int d^3\underline{r}'\, e^{-ik\left(\frac{\underline{r}\cdot\underline{r}'}{r}\right)}\,V(\underline{r}')\,\psi(k,\underline{r}')\right)e^{\frac{ikr}{4\pi r}} + \ldots$$

Write $\underline{k} = k\hat{z}$, then

$$\psi(k,\underline{r}) = e^{ikz} \underbrace{- \frac{2m}{\hbar^2}\cdot\frac{1}{4\pi}\int d^3\underline{r}' \, e^{-ik\underline{r}\cdot\underline{r}'/r} \, V(r')\,\psi(\underline{k},\underline{r}')}_{=f(\theta,\phi)}$$

Born approx. and expansion (series)

$$\psi(k,\underline{r}) = \phi_0(k,\underline{r}) + \int d^3\underline{r}' \; G^+(k,\underline{r}-\underline{r}')\, V(\underline{r}')\,\psi(k,\underline{r}') \tag{1}$$

Assume $V(r)$ has a small param : $V \sim \varepsilon$, then we can find part sol^n

$$\psi = \phi_0 + \varepsilon\psi_1 + \mathcal{O}(\varepsilon^2).$$

Replacing (1),

$$\cancel{\phi_0} + \varepsilon = \cancel{\phi_0} + \int d^3\underline{r}' \; G\, V(\phi_0 + \varepsilon\psi_1).$$

To order ε,

$$\varepsilon\psi_1 = \int d^3\underline{r}' \; G^+(k,\underline{r}-\underline{r}')\, V(\underline{r}')\,\phi_0(\underline{k},\underline{r}')$$

In this approximation, $\hat{\underline{r}} = \underline{r}/r$.

$$f(\theta,\phi) = -\frac{2m}{\hbar^2}\cdot\frac{1}{4\pi}\int d^3\underline{r}' \; e^{-ik\hat{\underline{r}}\cdot\underline{r}'}\, V(\underline{r}')\, e^{i\underline{k}\cdot\underline{r}'} + \mathcal{O}(\varepsilon^2)$$

$$\textcircled{=} -\frac{2m}{\hbar^2}\cdot\frac{1}{4\pi}\int d^3\underline{r}' \; e^{i\underline{q}\cdot\underline{r}}\, V(\underline{r}') + \dots$$

where $\underline{q} = \underline{k} - k\hat{\underline{r}} \equiv \underline{k} - \underline{k}'$, $\underline{k}' = k\hat{\underline{r}}$.

$$\textcircled{=} -\frac{2m}{\hbar^2}\cdot\frac{1}{4\pi}\hat{V}(\underline{q}).$$ ← Fourier transform

Then, finally the differential cross-section

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 |\hat{V}(\underline{q})|^2 + \dots}$$

This is Born-Approximation.

How do we go beyond leading order in ε?

We have (1)

$$\psi(k,\underline{r}') = \phi_0(\underline{r}') + \int d^3\underline{r}'' \; G^+(\underline{r}'-\underline{r}'')\, V(\underline{r}'')\,\psi(k,\underline{r}'')$$

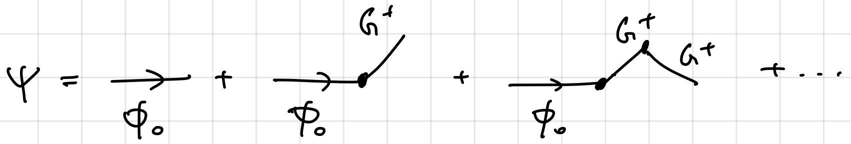
$$\Rightarrow \psi(k,\underline{r}) = \phi_0(\underline{r}) + \int d^3\underline{r}'\, G^+ V \phi_0$$

$$+ \int d^3\underline{r}' \int d^3\underline{r}''\, G^+(\underline{r}-\underline{r}')\, V(\underline{r}')\, G^+(\underline{r}'-\underline{r}'')\, V(\underline{r}'')\, \psi(\underline{r}'').$$

$$= \phi_0 + \int G^+ V \phi_0 + \iint G^+ V G^+ V \phi_0 + \iiint G^+ V G^+ V G^+ V \phi_0 + \dots$$

This is Born Series.

Diagramatic now:



Example (Yukawa theory)

$$V(\underline{r}) = A\,\frac{e^{-\mu r}}{r} \quad (\text{Coulomb } \mu = 0).$$

Task: evaluate $d\sigma/d\Omega$ in the Born-approx.

We need $\hat{V}(\underline{q})$.

$$\hat{V}(\underline{q}) = \int d^3\underline{r}\; e^{i\underline{q}\cdot\underline{r}}\, A\,\frac{e^{-\mu r}}{r}$$

$$= \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^\infty dr\; r^2\, e^{iqr\cos\theta}\, A\,\frac{e^{-\mu r}}{r}$$

$$= 2\pi \int_0^\infty dr \cdot \frac{1}{iq}\left(e^{iqr} - e^{-iqr}\right) e^{-\mu r} \cdot A$$

$\underline{q} = \underline{k} - k\hat{\underline{r}}$, $\quad q^2 = 2k^2 - 2\underline{k}\cdot\underline{k}' = 2k^2(1-\cos\theta) = 4k^2\sin^2\frac{\theta}{2}.$

Then

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right) |\hat{V}(q)|^2 + \dots$$

$$= \left(2mA \cdot \frac{1}{\hbar^2\mu + 8mE\sin^2\theta/2}\right)^2 + \dots$$

with $k^2 = 2mE/\hbar^2$.

Note when $\mu \to 0$, $\quad \frac{d\sigma}{d\Omega} = \left(\frac{A}{4E}\right)^2 \cdot \frac{1}{\sin^4\theta/2} + \dots$

(1) Curiosity that classical = QM in Born-approx.

(2) What we did ($\mu = 0$) is wrong! Because $V(r)$ does not goes to 0 rapidly enough. For Coulomb,

long-range force

$$R_\ell(r) \sim e^{\pm i(kr - \gamma(a)\log(kr))}$$

2. Variational Method

Solve Schr. eqn.

- Put bound on spectrum Hamiltonian
- Method when perturbation thm. fails.

Main idea. Consider Hamiltonian

$$H|n\rangle = E_n|n\rangle, \quad n = 1, 2, \dots, \quad E_n \le E_{n+1}.$$

We want to say something about E_n.

Strategy: guess.

Outline :

(1) Ground state energy

(2) ∃ of bound states

(3) Excited states

(4) Helium atom.

2.1 Ground state energy

We want an estimate for E_0 g.s. energy

Thm For any state $|\psi\rangle$. the expected energy

$$\langle E\rangle = \langle\psi|H|\psi\rangle, \quad \langle\psi|\psi\rangle = 1 \ \text{(for simplicity)}$$

then $\langle E\rangle \geq E_0$.

Pf : $|\psi\rangle = \sum_{n=0}^{\infty} a_n |n\rangle$. , where $\sum |a_n|^2 = 1$, then

$$\langle E\rangle = \sum_{n,m} a_m^* a_n \langle m|H|n\rangle .$$

$$= \sum_{n,m} a_m^* a_n E_n \delta_{mn}$$

$$= \sum_{n=0}^{\infty} |a_n|^2 E_n = E_0 + \sum_n |a_n|^2 (E_n - E_0) \geq E_0 \qquad \square$$

Now we can implement strategy (guess)

Consider $|\Psi(\alpha_i)\rangle$ either normalised or not.

$$E = \frac{\langle \psi(\alpha_i)|H|\psi(\alpha_i)\rangle}{\langle \psi(\alpha_i)|\psi(\alpha_i)\rangle}$$

Still be true $E \geq E_0$.

Var method: minimise w.r.t. α_i to find an upper bound for E_0.

Most stringant bound $\left.\frac{\partial E}{\partial \alpha_i}\right|_{\alpha_i = \alpha_*} = 0$, then $E(\alpha_*) \geq E_0$.

Example $H = -\frac{d^2}{dx^2} + x^4$

What is ground state energy? We approx/estimate.

Guess : propose $|\psi(\alpha)\rangle$. normalisation $\int_{-\infty}^{\infty} dx\, |\psi|^2 = 1$

$$\psi_T(x,\alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

$$E(\alpha) = \langle\psi|H|\psi\rangle = \int_{-\infty}^{\infty} dx \;\; \psi(H\psi)$$

$$= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} dx \;\; e^{-\alpha x^2}\left(\alpha - \alpha^2 x^2 + x^4\right)$$

$$= \frac{\alpha}{2} + \frac{3}{4}\alpha^{-2}$$

$$\Rightarrow \frac{dE}{d\alpha} = \frac{1}{2} - \frac{3}{2}\alpha_*^{-3} = 0 \quad \Rightarrow \alpha_*^3 = 3 .$$

$$\Rightarrow E(\alpha_*) = 3^{1/3} \cdot \frac{3}{4} \simeq 1.081 .$$

Compare to numerical value of ground state $E_0 \simeq 1.06$. $E(\alpha_*) > E_0$.

Comments : (1) Rayleigh-Ritz method

(2) Seems pretty accurate, but we don't have any way to estimate the error.

(3) If $V(x)$ more complicated, then guesses are more inaccurate.

2.2 Bound States

For a given $V(r)$, if $|\psi(\alpha_i)\rangle$ gives $E(\alpha_i) < 0 \Rightarrow \exists$ bound states.

In 1D, can say more.

Thm Consider a potential $V(x)$ s.t. $V(x) = 0$ for $|x| > L$ for some L, a bound state exists if $\int_{-\infty}^{\infty} V(x)\, dx < 0$.

Pf : We have $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$. Use trial f^n

$$\psi_T(x,\alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

$$\Rightarrow E(\alpha) = \frac{\hbar^2}{4m}\alpha + \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} dx \;\; V(x)\, e^{-\alpha x^2/2}$$

$$\Rightarrow \frac{E(\alpha)}{\sqrt{\alpha}} = \frac{\hbar^2}{4m}\sqrt{\alpha} + \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx\; V(x)\; e^{-\alpha x^2/2}$$

$$\lim_{\alpha \to 0} \frac{E(\alpha)}{\sqrt{\alpha}} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx\; V(x).$$

If $\int_{-\infty}^{\infty} dx\; V(x) < 0 \Rightarrow E(\alpha) < 0 \Rightarrow \exists$ bound state. □

2.3 Excited States

Estimating E_n for $n \neq 0$ is difficult. Still, say to estimate E_1.

To do this, consider

$$\langle \psi(\alpha) | 0 \rangle = 0$$

where $|0\rangle$ is the true ground state.

This means

$$|\psi\rangle = \sum_{n\geq 1} a_n |n\rangle .$$

Then

$$E = \langle\psi|H|\psi\rangle = E_1 + \sum_n |a_n|^2 (E_n - E_1) \geq E_1$$

Example $H = -\frac{d^2}{dx^2} + x^4$. Estimate E_1.

What can we infer about $|0\rangle$? Use symmetry:

parity $P: x \longleftrightarrow -x$. Clearly $[H, P] = 0$. this has $V(x) = V(-x)$.

For any parity invariant H, the ground state is also parity invariant.

$$\psi_0(x) = \psi_0(-x).$$

Any odd f^n ($\psi(x) = -\psi(-x)$) will be orthogonal to ψ_0. Try

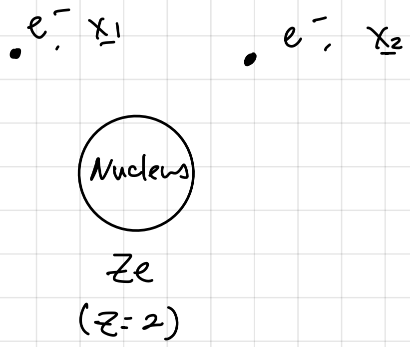
$$\psi_T(x, \alpha) = \left(\frac{4\alpha^3}{\pi}\right)^{1/2} x e^{-\alpha x^2/2} .$$

Ex. sheet $\Rightarrow E(\alpha_*) \approx 3.85$.

Numerical answer: $E_1 \approx 3.80$.

2.4 Helium Atom

$$H = \frac{p_1^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0} \cdot \frac{1}{r_1} + \frac{p_2^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0} \cdot \frac{1}{r_2} + \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\underline{x}_1 - \underline{x}_2|}$$



If we ignore interaction,

$$\psi(\underline{x}_1, \underline{x}_2) = \underbrace{\psi_{n_1, l_1, m_1}(\underline{x}_1)}_{\text{Hydrogen}} \psi_{n_2, l_2, m_2}(\underline{x}_2)$$

In this case,

$$E = -Z^2 \left(\frac{1}{n_1^2} + \frac{1}{n_2^2}\right) R_y , \quad R_y = \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \sim 13.6\, eV .$$

Test: $Z = 2$, $n_1 = n_2 = 1 \Rightarrow E = -8 R_y \sim -109\, eV$ Terrible!!

We need interaction, try to solve it approx.

- Perturbation theory
- Variational method ✓.

Guess / trial $\psi_T(x,\alpha) = \sqrt{\frac{\alpha^3}{\pi a_0^3}}\, e^{-r\alpha/a_0}$, $a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2}$

Note: $\alpha = 1$, we have g.s. of Hydrogen.

$$\psi_T(x_1, x_2, \alpha) = \psi_T(x_1,\alpha)\, \psi_T(x_2,\alpha).$$

Write

$$H = \frac{p_1^2}{2m} - \frac{\alpha e^2}{4\pi\varepsilon_0}\frac{1}{r_1} + \frac{p_2^2}{2m} - \frac{\alpha e^2}{4\pi\varepsilon_0}\cdot\frac{1}{r_2} + \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{|\underline{x}_1 - \underline{x}_2|} + (\alpha - Z)\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\right)$$

The energy of trial wavef^{n}

$$E(\alpha) = \int d^3x_1 \int d^3x_2\ \psi_T(x_1,\alpha)\,\psi_T(x_2,\alpha)\, H\, \psi_T(x_1,\alpha)\,\psi_T(x_2,\alpha)$$

$$= -2\alpha^2 R_y + \frac{e^2}{4\pi\varepsilon_0}\left(2(\alpha - Z)\int d^3x\, \frac{|\psi_T(x)|^2}{r} + \int d^3x_1 \int d^3x_2\, \frac{|\psi_T(\underline{x}_1)|^2\,|\psi_T(\underline{x}_2)|^2}{|\underline{x}_1 - \underline{x}_2|}\right)$$

then

$$\int d^3x\, \frac{|\psi_T(x)|^2}{r} = \frac{\alpha}{a_0}$$

$$\int d^3x_1 \int d^3x_2\, \frac{|\psi_T(\underline{x}_1)|^2\,|\psi_T(\underline{x}_2)|^2}{|\underline{x}_1 - \underline{x}_2|} = \frac{5\alpha}{8a_0}$$

$$\Rightarrow E(\alpha) = R_y\left(-2\alpha^2 + 4(\alpha - Z)\alpha + \frac{5\alpha}{4}\right). \quad R_y = \frac{e^2}{8\pi\varepsilon_0}\cdot\frac{1}{a_0}$$

Minimise

$$\left.\frac{\partial E}{\partial \alpha}\right|_{\alpha = \alpha_*} = 0 \Rightarrow \alpha_* = Z - \frac{5}{16}$$

$$E(\alpha_*) = -2\left(Z - \frac{5}{16}\right)^2 R_y \sim -77.5\ \text{eV} \quad (Z = 2)$$

Experimental: $E_0 \sim -79.0$ eV

Comments:

(1) Pretty good estimate, given simplicity of trial wave f^n

(2) Compare to perturbation $E_{pert} = E_{2H} + \Delta E \sim -74.8$ eV

(3) $\alpha_* = Z - \frac{5}{16}$

screening charge.

3. Solid State Physics

In many solids, atoms organise themselves in a crystal. ⇒ pattern.

Goal: pattern ⟷ periodicity

$$H = p^2/2m + \underbrace{V(x)}_{\text{periodic potentials}}.$$

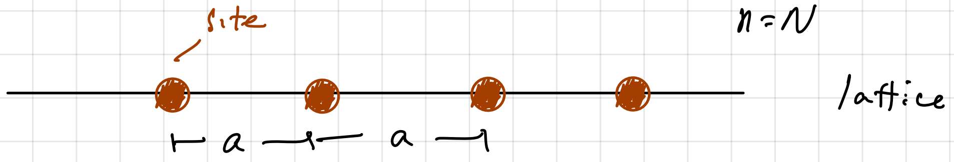
Two main stages:

- First, we will consider single e^- under influence of periodic V.
- Second, many e^-. —— atoms fixed generating $V(x)$.

(- Third, dynamics of atoms ⇒ phonons)

3.1 1D Band Structure

3.1.1 Tight-Binding Model



Idea:

(1) An electron sits at one site only. Possible states of e^- $|n\rangle$.

$$\Rightarrow \langle n|m\rangle = \delta_{mn}$$

(2) Add the lawyer of jumping between sites

Consider

$$H = \underbrace{E_0 \sum_{n=1}^{N} |n\rangle\langle n|}_{\text{e}^- \text{ stays on } |n\rangle} - \underbrace{t \sum_{n=1}^{N} \left(|n\rangle\langle n+1| + |n+1\rangle\langle n| \right)}_{\text{Introducing some movement for e}^- \text{ jump / hop}}$$

with t : hopping parameter (not time)

Since we have N sites, we need to specify boundary conditions at the edges. Simply choose

$$|N+1\rangle = |1\rangle$$

Find evals + estates.

$$|\psi\rangle = \sum_m \psi_m |m\rangle$$

where

$$H|\psi\rangle = E|\psi\rangle.$$

Find E and ψ_m.

$$\Rightarrow E_0 \sum_m \psi_m |m\rangle - t \sum_m \left(\psi_m |m\rangle + \psi_m |m+1\rangle \right) = \sum_m E \psi_m |m\rangle$$

$$\Rightarrow \quad E_0 \psi_n - t(\psi_{n+1} + \psi_{n-1}) = E\psi_n$$

Tridiagonal system, with sol^n

$$\psi_n = \frac{e^{ikna}}{\sqrt{N}} \quad \text{— choice of normalisation}$$

where

$$\boxed{E(k) = E_0 - 2t\cos(ka)}$$

Estate:

$$\boxed{|\psi\rangle = \sum_n \frac{e^{ikna}}{\sqrt{N}} |n\rangle}$$

with eval $E(k)$.

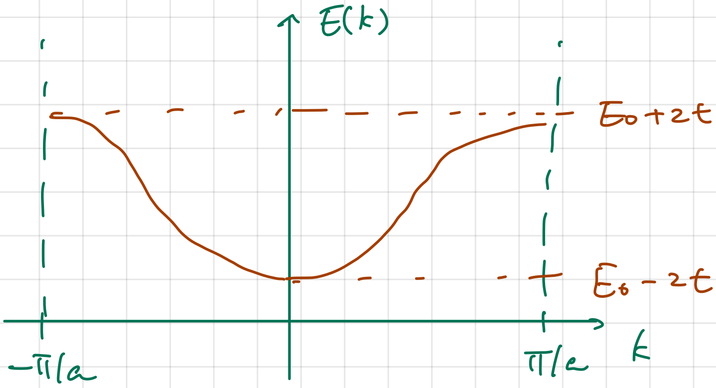
Comments :

(1) The sol^n remains unchanged if $k \mapsto k + 2\pi/a$.

$\Rightarrow k \in [-\pi/a, \pi/a)$. Brillouin zone

(2) Sol^n delocalises : $|\psi\rangle$ is a sum over sites and looks like a plane wave.

(3)



Band structure,

band width = 4t

(4) Impose periodic BC

$$\psi_{N+1} = \psi_1 \Rightarrow e^{ikNa} = 1.$$

$$\Rightarrow k = \frac{2\pi}{aN} i \qquad i=1,\dots,N$$

i.e. k quantised. So inside Brillouin zone, exactly N states

(5) For small k, i.e. $k \ll \pi/a$,

$$E(k) \simeq E_0 - 2t + ta^2k^2 + \dots$$

$$= E_0 - 2t + \frac{\hbar^2}{2m_{eff}} k^2 + \dots \quad , \quad m_{eff} \equiv \frac{\hbar^2}{2ta^2}$$

k is referred to as momentum (looks like KE).

3.1.2 Nearly free electrons

Upgrade: $H = \frac{p^2}{2m} + V(x)$, $V(x) = V(x+a)$.

Toy model:

- treat V perturbatively.
- We will place the system on an interval of length L, s.t.

$$L/a = N \in \mathbb{Z}$$

When $V(x)=0$, estates are plane waves

$$\psi_k(x) = \langle x|k\rangle = \frac{1}{\sqrt{L}} e^{ikx}$$

with k quantised multiple of $2\pi/L$.

States are orthonormal.

$$\langle k | k' \rangle = \frac{1}{L} \int_0^L dx \; e^{i(k-k')x} = \delta_{k,k'}.$$

and have energy

$$E_0(k) = \frac{\hbar^2 k^2}{2m}.$$

Add $V(x)$ perturbatively use pert. thy.

Do we use degenerate or non-degenerate formulas?

To see what case it is, inspect $V(x)$.

$$V(x) = V(x+a) = \sum_{n \in \mathbb{Z}} V_n \, e^{2\pi i n x/a} .$$

where $V_n = V_{-n}^*$ since potential is real.

$$V_n = \frac{1}{a} \int_0^a dx \; V(x) e^{-2\pi i n x/a}.$$

In non-deg case,

$$E(k) = E_0(k) + \langle k | V | k \rangle + \sum_{k' \neq k} \frac{|\langle k | V | k' \rangle|^2}{E_0(k) - E_0(k')} + \dots \qquad (*).$$

Inspect $\langle k | V | k' \rangle$

$$\Rightarrow \langle k | V | k' \rangle = \frac{1}{L} \int dx \sum_{n \in \mathbb{Z}} V_n \, e^{2\pi i n x/a} \, e^{i(k-k')x}$$

$$= \sum_{n \in \mathbb{Z}} V_n \, \delta_{k-k', \, 2\pi n/a}$$

Then we only have an overlap if

$$\boxed{k = k' + \frac{2\pi n}{a}} \qquad (1)$$

and the spectrum will be degenerate when

$$\boxed{E_0(k) = E_0(k') \Rightarrow k' = -k} \qquad (2)$$

Combining (1), (2), be careful at

$$k = \frac{\pi n}{a}, \qquad k' = -\frac{kn}{a}. \rightarrow$$ case that you need to use the degenerate formula

With this, divide the analysis in 3 parts:

(1) Low momentum $k \ll \pi/a$ (non-degenerate).

(2) At the edge : $k = n\pi/a$

(3) Near the edge : $k = n\pi/a + \delta$.

(1) Low momentum.

We can use (*) safely

$$E(k) = \underbrace{\frac{\hbar^2 k^2}{2m}}_{E_0} + \underbrace{V_0}_{\langle k|V|k\rangle} + \sum_{k' \neq k} \frac{\overbrace{|\langle k|V|k'\rangle|^2}^{(1)}}{\underbrace{E_0(k) - E_0(k')}_{\text{big when (1) applies}}} + \cdots$$

$$= V_0 + \frac{\hbar^2 k^2}{2m} + \dots$$

(2) At the edge : $k = n\pi/a$, $k' = -n\pi/a$.

We have $|k\rangle, |k'\rangle$. We want to construct the corrected estates

$$\alpha|k\rangle + \beta|k'\rangle.$$

$$\begin{pmatrix} \langle k|H|k\rangle & \langle k|H|k'\rangle \\ \langle k'|H|k\rangle & \langle k'|H|k'\rangle \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} E_0(k) + V_0 & V_n \\ \underbrace{V_{-n}}_{V_n^*} & E_0(k') + V_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Evals : $(E_0(k) + V_0 - E)^2 - |V_n|^2 = 0$

$$\boxed{\begin{aligned} E &= \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n| \\ \Delta E &= 2|V_n| \end{aligned}} \qquad E_0(k) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

(3) Close to edge : $k = \frac{n\pi}{a} + \delta$

$$|k\rangle = \left|\frac{n\pi}{a} + \delta\right\rangle , \qquad |k'\rangle = \left|-\frac{n\pi}{a} + \delta\right\rangle .$$

They will mix $k = k' + 2\pi n/a$. Again write 2x2 matrix.

$$\begin{pmatrix} E_0(k) + V_0 & V_n \\ V_n^* & E_0(k') + V_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Evals :

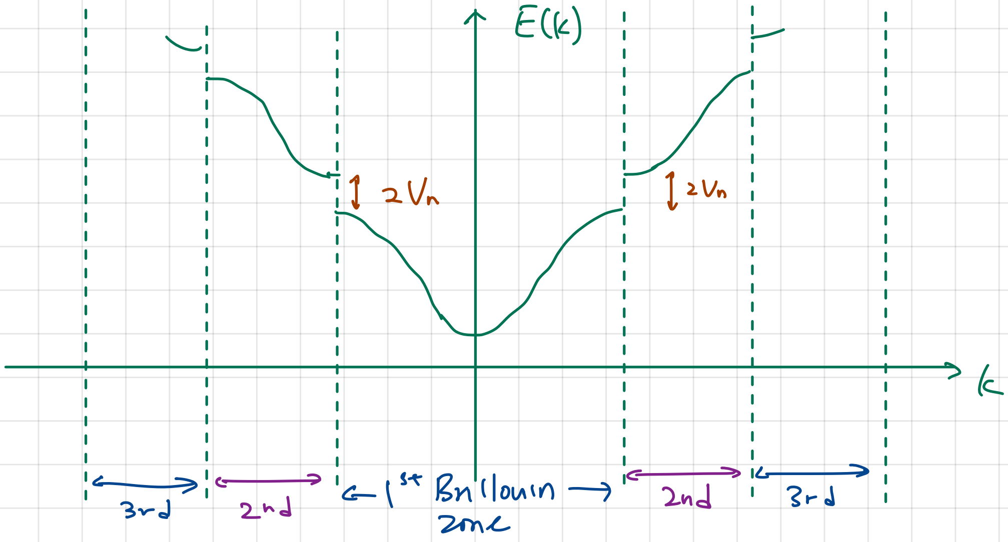
$$\left(E - (V_0 + \tfrac{1}{2} E_0(k') + \tfrac{1}{2} E_0(k)\right)^2 = |V_n|^2 + \tfrac{1}{4}\left(E_0(k) - E_0(k')\right)^2 .$$

Then for small δ,

$$E_{\pm} = \underbrace{V_0 + \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n|}_{\text{At the edge}} + \underbrace{\frac{\hbar^2}{2m}\left(1 \pm \frac{1}{|V_n|}\frac{n^2\hbar^2\pi^2}{ma^2}\right)\delta^2}_{\text{quadratic correction.}} + \dots$$

Remarks :

- Relationship between E and k is called a <u>dispersion relation</u>.
- No potential ⇒ $E_0 = \frac{\hbar^2}{2m} k^2$
- When we added a bit on potential
  - low k, basically no diff.
  - At the edge we have a gap.
  - Near the edge, spectrum is quadratic. $\frac{dE}{dk} \to 0$.



3.1.3 Floquet matrix

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

What can we say about sol^{n}s ?

- Two LI sol^n
- If $\psi_1(x), \psi_2(x)$ are sol^n. then $\psi_1(x+a), \psi_2(x+a)$ are also sol^n.
  Since $V(x)$ periodic.

All of these have to be related

$$\begin{pmatrix} \psi_1(x+a) \\ \psi_2(x+a) \end{pmatrix} = \underbrace{F(E)}_{\substack{2\times 2 \text{ matrix}: \\ \text{Floquet matrix}}} \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}. \qquad (*)$$

Study some properties of $F(E)$.

Claim det $F = 1$.

Pf: Take derivative.

$$\begin{pmatrix} \psi_1(x+a) & \psi_1'(x+a) \\ \psi_2(x+a) & \psi_2'(x+a) \end{pmatrix} = F(E) \begin{pmatrix} \psi_1(x) & \psi_1'(x) \\ \psi_2(x) & \psi_2'(x) \end{pmatrix} \qquad (**)$$

$$\det \begin{pmatrix} \psi_1(x+a) & \psi_1'(x+a) \\ \psi_2(x+a) & \psi_2'(x+a) \end{pmatrix} = \psi_1(x)\psi_2'(x) - \psi_1'(x)\psi_2(x).$$

=: Wronskian of ODE.

Simple to show $W'(x) = 0$ (cons. of prob.)

Then det of $(**)$

$$W(x+a) = \det F \; W(x)$$

but $W(x+a) = W(x) \Rightarrow \det F = 1$ □

Claim $\mathrm{Tr}\, F \in \mathbb{R}$.

Pf: In $(*)$ we can always choose a basis where ψ_1, ψ_2 are real. In this basis F is real $(\mathrm{Tr}\, F \in \mathbb{R})$.

Then if you change basis

$$F \to A F^{-1} A .$$

$$\mathrm{Tr}(F) \to \mathrm{Tr}(F).$$

☐

With these claims, say something about evals, evecs of $F(E)$.

Evals:

$$\lambda^2 - \mathrm{Tr}(F)\, \lambda + \underbrace{\det F}_{=1} = 0$$

$$\Rightarrow \quad \lambda_\pm = \frac{1}{2}\left(\mathrm{Tr}(F) - \sqrt{(\mathrm{Tr}\, F)^2 - 4}\right)$$

Based on $\mathrm{Tr}\, F \in \mathbb{R}$, have 3 cases.

Case 1: $(\mathrm{Tr}\, F)^2 > 4$

In this case, $\lambda_+ = e^{\mu a}$, $\lambda_- = e^{-\mu a}$; with $\mu \in \mathbb{R}$.

Estates: linear combinations of ψ_1, ψ_2.

$$\psi_\pm (x+a) = e^{\pm \mu a} \psi_\pm (x). \qquad \text{from } (*).$$

This tells us that estates not normalisable in this case, since F depends on E, it tells us that certain values of E are not allowed.

Case 2: $(\mathrm{Tr}\, F)^2 < 4$.

Here we have $\lambda_+ = e^{ika}$, $\lambda_- = e^{-ika}$ for some $k \in \mathbb{R}$.

and $k \in [-\pi/a, \pi/a)$.

Evecs:

$$\psi_\pm (x+a) = e^{\pm ika} \psi_\pm (x).$$

Case 3 : $(\mathrm{Tr}\ F)^2 = 4.$

$$\Rightarrow \lambda_+ = \lambda_- = \pm 1$$

Take $\lambda_+ = \lambda_- = 1.$

$$\Rightarrow \quad \underset{\substack{\big\downarrow \\ \text{Edge of band.}}}{F = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \quad \text{or} \quad \underbrace{\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}}_{\text{not normalisable}}$$

3.1.4 Blochs theorem 1D

In both models + Floquet, we saw k. Why?

Usually in QM, it is useful to look / identify symmetries since their operations might have the property $[H, Q] = 0$

Example $V(x) = 0$

- Symmetry : translation invariance
- mom. conserved.
- $[H, P] = 0$ simultaneously diagonalise both.

Now, we have $V(x) = V(x+a)$.

- this breaks the cts translational sym.

$$[H, P] \neq 0.$$

- not everything is lost. We need to formalise residual trans. sym.

Def^n Translation operator

$$T_\ell \psi(x) = \psi(x+\ell)$$

Claim T_ℓ unitary

Pf:
$$\langle\phi|T_\ell|\psi\rangle = \int dx\ \phi^*(x)\ T_\ell\psi(x)$$
$$= \int dx\ \phi^*(x)\ \psi(x+\ell)$$
$$= \int dx\ \phi^*(x-\ell)\ \psi(x).$$
$$= \int dx\ \left(T_{-\ell}(x)\right)^*\psi(x).$$
$$\Rightarrow\ T_{-\ell} = T_\ell^*$$
$$\Rightarrow\ T_{-\ell} = (T_\ell)^{-1}\ \Rightarrow\ T_\ell^\dagger = (T_\ell)^{-1}\ \text{unitary.}$$ □

Claim T_ℓ forms an abelian group.

Pf: Group: $T_{\ell_1}T_{\ell_2} = T_{\ell_1+\ell_2}$

Abelian: $[T_{\ell_1}, T_{\ell_2}] = 0.$ □

mom. operator.

Claim $T_\ell = e^{i\ell P/\hbar}$, where $P = -i\hbar\frac{d}{dx}$.

Pf:
$$T_\ell\psi(x) = e^{i\ell P/\hbar}\psi(x)$$
$$= \left(1 + \frac{i\ell P}{\hbar} + \frac{1}{2}\left(\frac{i\ell P}{\hbar}\right)^2 + \dots\right)\psi(x)$$
$$= \left(1 + \ell\frac{d}{dx} + \frac{1}{2}\left(\ell\frac{d}{dx}\right)^2 + \dots\right)\psi(x)$$
$$= \psi(x+\ell).$$ □

Def^n A system is said to be invariant under translation if
$$[H, T_\ell] = 0.$$

Note: • If $[H, T_\ell] = 0\ \forall\ \ell$, then $[H, P] = 0$.

• However, if it only hold for $\ell = na$, $n \in \mathbb{Z}$, then $[H, P] \neq 0$.

With this, characterise evecs and eval of T_ℓ.

T_ℓ unitary ⇒ evals are $e^{i\theta}$, $\theta \in \mathbb{R}$.

Convenient to write

$$T_{na} \sim e^{ikan} = (e^{ika})^n \sim (T_a)^n.$$

Consider $[H, T_a] = 0 \Rightarrow$ evecs of T_ℓ form a good basis.

Estates of T_a.

$$T_a \psi_k(x) = e^{ika}\psi_k(x) = \psi_k(x+a).$$

We can restrict $k \sim k + 2\pi/a$,

$$k \in [-\pi/a, \pi/a)$$ 1st Brillouin zone

Thm (Bloch's thm 1D) Given a periodic potential $V(x) = V(x+a)$, $\exists$ a basis of estates for H that can be written as

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

where $u_k(x+a) = u_k(x)$, $k \in [-\pi/a, \pi/a)$.

Pf: Take estates of T_a.

$$\psi_k(x+a) = e^{ika}\psi_k(x)$$

Then $u_k(x) = e^{-ika}\psi_k(x+a)$

$$u_k(x+a) = e^{-ik(x+a)} \psi_k(x+a)$$

$$= e^{-ikx} u_k(x)$$

$$= u_k(x)$$ □

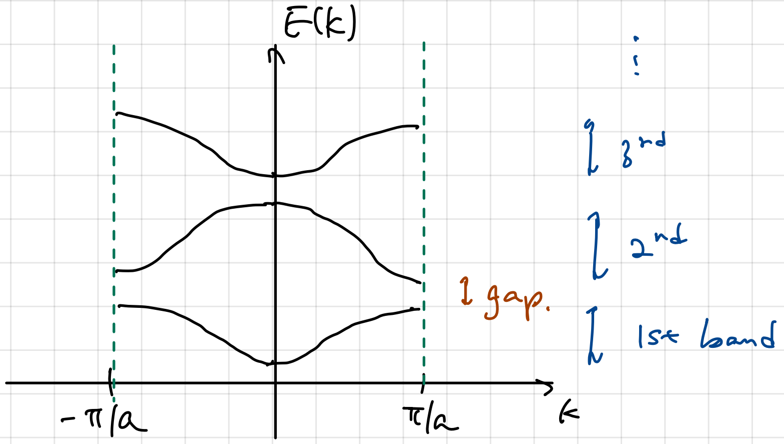
$$\psi_k(x) = \underbrace{e^{ikx}}_{\substack{\text{plane wave} \\ (\text{sol}^n\ V=0)}} \underbrace{u_k(x)}_{\substack{\text{periodic } f^n \\ \text{when } V \neq 0. \\ (\text{modification due to lattice})}}, \quad k \in [-\pi/a, \pi/a).$$

Lattice doesn't dramatically change the e^-. In particular, it is not localised at a single site.

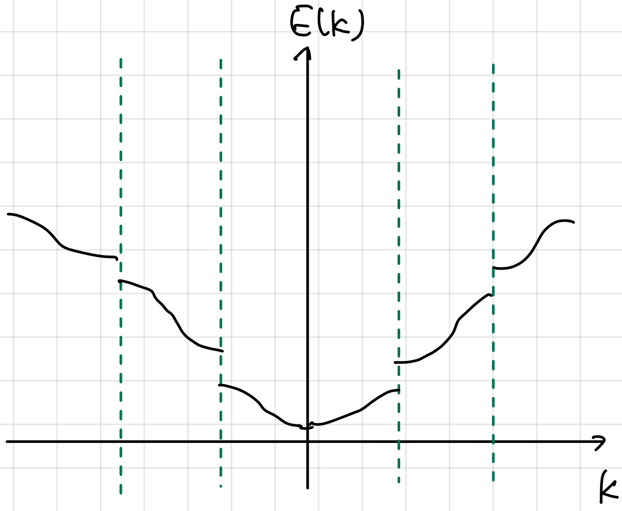
Nomenclature : k is called the crystal momentum.

Note : $k \neq$ mass × vel.

Re-think : energy spectrum.



Reduced zone scheme



Extended scheme

3.2 Band Structure 3D

Lattices

Goal : Describe periodic structures in 3D (2D).

3.2.1 Bravais lattice

Simplest extension of 1D to higher dim

Def^n (i) BL is an infinite set of points defined by an integer sum of LI primitive vectors.

In 2D : $\Lambda = \{ \underline{r} = n_1 \underline{a_1} + n_2 \underline{a_2} ,\ n_i \in \mathbb{Z} \}$. $\underline{a_1}, \underline{a_2}$ primitive vecs

3D : $\Lambda = \{ \underline{r} = n_1 \underline{a_1} + n_2 \underline{a_2} + n_3 \underline{a_3} ,\ n_i \in \mathbb{Z} \}$.

(ii) BL is an infinite discrete set of vecs where addition / subtraction of any 2 gives the third.

(iii) BL is an infinite discrete set of points where the environment of any point is equivalent to the env't of any other point

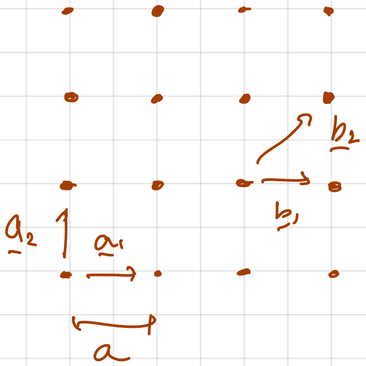
Rmk: Choice of primitive vecs not unique. Given $\underline{a}_i$,

$$\underline{b}_i = \sum_j m_{ij} \underline{a}_j$$

with m_{ij} has inverse, and entries of m_{ij}, $(m_{ij})^{-1}$ integers

→ $\det(m) = \pm 1$.

Example (2D square lattice)

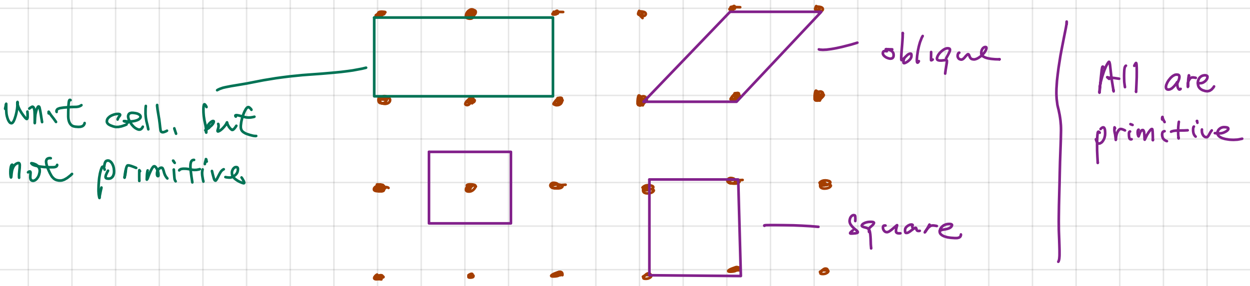


Defⁿ (Unit cell)

(i) A unit cell is a region of space s.t. when many identical cells are stacked together, it tiles (completely fills) all of the space, i.e. constructs Λ.

(ii) Are repeated motif which is the elementary building block of the periodic structure.

Defⁿ Primitive unit cell is a unit cell containing exactly one lattice point



Notes:

(1) Primitive cells are not unique

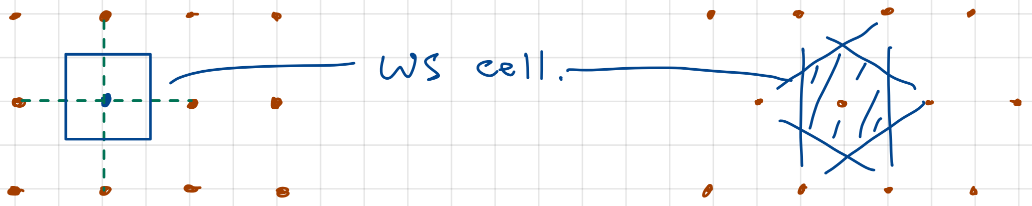
(2) Every PUC has the same area/vol. e.g. in 3D.

$$V = |\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)| = \frac{1}{n}$$

where n = density of lattice points

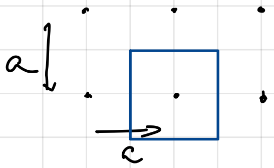
(3) One usually pick PUC that respects sym of Λ.

Def^n (Wigner-Seitz cell) Given a lattice point, the set of all points which are closer to that given lattice than any other lattice point is the WS cell. This is the canonical choice, denoted as Γ.



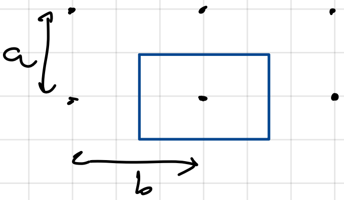
Bravais Lattices in 2D. — classification based on symmetries.

(1) Square



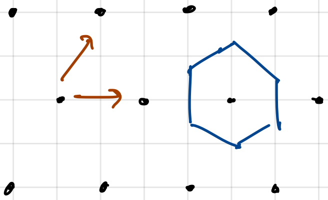
Reflections x, y
90° rot.

(2) Rectangle



$|a| \neq |b|$ → Compressed.
lost 90° rot.

(3) Hexagon

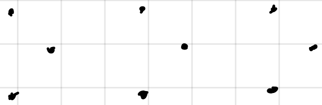


Reflections x. y
60° rot.

(4) Rectangle centred : compression of hexagon.

lost 60° rot.

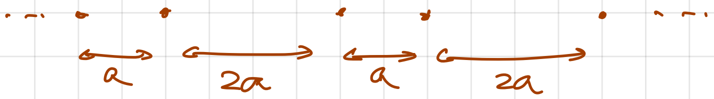
(5) Oblique:



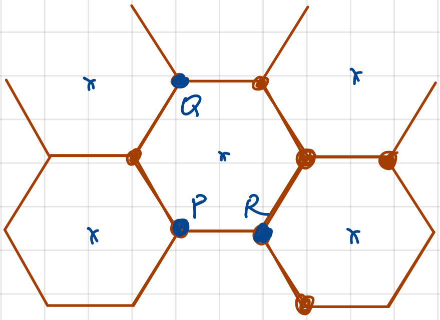
only symmetry is $\underline{L} \to -\underline{L}$.

Not all lattice are Bravais.

Example 1D .



Example 2D Honeycomb lattice



R, P inequivalent

Q, P equivalent.

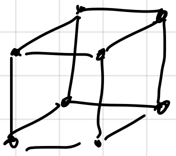
How to describe as lattice? Add × ⇒ hexagon and then decorate each × by

$$\left.\begin{aligned} \underline{V}_1 &= \alpha\left(\frac{1}{2\sqrt{3}}, 0\right) \\ \underline{V}_2 &= \alpha\left(-\frac{1}{2\sqrt{3}}, 0\right) \end{aligned}\right\} \text{basis}$$

Bravais lattice in 3D – based on sym (total 14).

3 common ones

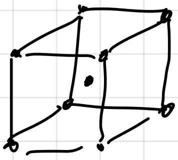
(1) Cubic



$\underline{a}_1 = a\hat{\underline{x}}$, $\underline{a}_2 = a\hat{\underline{y}}$, $\underline{a}_3 = a\hat{\underline{z}}$

WS also cube of vol a^3.

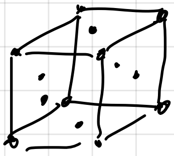
(2) Body centred cubic (BCC)



$\underline{a}_1 = a\hat{\underline{x}}$, $\underline{a}_2 = a\hat{\underline{y}}$. $\underline{a}_3 = \frac{a}{2}(\hat{\underline{x}} + \hat{\underline{y}} + \hat{\underline{z}})$

WS has vol. $V = a^3/2$

(3) Face centred cubic (FCC)



$\underline{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\underline{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$,

$\underline{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$.

Vol. of WS $= a^3/4$, also polyhedron.

Note: BCC, FCC as a lattice with a basis ⇒ still both BL.

Reciprocal Lattice

Def^n Given a BL Λ, the reciprocal (dual) lattice Λ^* is

$$\Lambda^* = \{ \underline{k} \in \mathbb{R}^3 : \underline{k}\cdot\underline{r} \in 2\pi\mathbb{Z} \quad \forall\, \underline{r} \in \Lambda \}$$

or $e^{i\underline{k}\cdot\underline{r}} = 1$

Basically,
$$\left.\begin{aligned} \underline{k} &= \sum_i n_i \underline{b}_i, \\ \underline{r} &= \sum_i n_i \underline{a}_i \end{aligned}\right\} \Rightarrow \underline{b}_i \cdot \underline{a}_j = 2\pi\,\delta_{ij}.$$

In 3D, easy to construct

$$\underline{b}_i = \frac{2\pi}{V} \cdot \frac{1}{2} \varepsilon_{ijk}\, a_j a_k$$

Reverse to get

$$a_i = \frac{2\pi}{V^*} \frac{1}{2} \varepsilon_{ijk}\, b_j b_k.$$

where $V^* = |\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)|$ volume of unit cell in Λ^*.

- $V^* = |\underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3)| = (2\pi)^3/V$
- $(V^*)^* = V \quad ((\Lambda^*)^* \sim \Lambda)$

Example

(1) Cubic $\underline{b}_1 = \frac{2\pi}{a}\hat{x}$, $\underline{b}_2 = \frac{2\pi}{a}\hat{y}$, $\underline{b}_3 = \frac{2\pi}{a}\hat{z}$

(2) $(\text{BCC})^* = \text{FCC}$.

$(\text{FCC})^* = \text{BCC}$

Fourier transforms

Consider $f(\underline{x})$ s.t. $f(\underline{x}+\underline{r}) = f(\underline{x})$ $\forall\ r \in \Lambda$

Q1 : What are properties of FT of $f(\underline{x})$?

Q2 : " of $f(\underline{x})$?

$$\hat{f}(\underline{k}) = \int_{\mathbb{R}^3} d^3x \quad e^{-i\underline{k}\cdot\underline{x}} f(\underline{x})$$

$$= \sum_{\underline{r}\in\Lambda} \int_T d^3x \quad e^{i\underline{k}\cdot(\underline{x}+\underline{r})} \underbrace{f(\underline{x}+\underline{r})}_{=f(\underline{x})} .$$

$$= \underbrace{\left(\sum_{r\in\Lambda} e^{i\underline{k}\cdot\underline{r}}\right)}_{\Delta(\underline{k})} \underbrace{\left(\int_T d^3x \quad e^{-i\underline{k}\cdot\underline{x}} f(\underline{x})\right)}_{S(\underline{k})}$$

$$= \Delta(\underline{k}) \quad S(\underline{k}) ,$$

with $\Delta(\underline{k}) = \sum_{r\in\Lambda} e^{-i\underline{k}\cdot\underline{r}}$

Claim $\Delta(\underline{k}) = 0$ unless $\underline{k} \in \Lambda^*$.

Pf:

$$\Delta(\underline{k}) = \sum_{r\in\Lambda} e^{-i\underline{k}\cdot(\underline{r}-\underline{r_0})} \qquad \text{shift by } \underline{r_0}\in\Lambda$$

$$= e^{i\underline{k}\cdot\underline{r_0}} \sum_{r\in\Lambda} e^{-i\underline{k}\cdot\underline{r}} = e^{i\underline{k}\cdot\underline{r_0}} \Delta(\underline{k}) .$$

If $\underline{k}\cdot\underline{r_0} \notin 2\pi\mathbb{Z}$, then $\Delta(\underline{k}) = 0$.

If $\underline{k}\cdot\underline{r_0} \in 2\pi\mathbb{Z}$, i.e. $\underline{k}\in\Lambda^*$, $\Delta(\underline{k}) \neq 0$. □

Claim $\Delta(\underline{k}) = V^* \sum_{q\in\Lambda^*} \delta(\underline{k}-\underline{q})$.

Pf: In 1D, consider Dirac Comb.

$$\rho(x) = \sum_{n\in\mathbb{Z}} \delta(x-an) .$$

(1D, Λ : $r = an$, $q = \frac{2\pi}{a} m$, $m, n \in \mathbb{Z}$) .

$$\tilde{\rho}(x) = \int dx\, e^{-ikx}\, \rho(x)$$
$$= \sum_n \int dx\, e^{-ikx}\, \delta(x-an)$$
$$= \sum_n e^{ikan} = \Delta(k).$$

Note ρ periodic.

$$\rho(x) = \rho(x+a) = \sum_{m\in\mathbb{Z}} C_m\, e^{i\frac{2\pi m}{a}x} .$$

with $C_m = \frac{1}{2}\int_{-a/2}^{a/2} \rho(x)\, e^{-\frac{2i\pi m x}{a}}\, dx = \frac{1}{a}$., then

$$\sum_n \delta(x-an) = \frac{1}{a} \sum_{m\in\mathbb{Z}} e^{2i\pi m x/a} .$$

This hints to

$$V^* \sum_{n\in\mathbb{Z}} \delta\left(k - \frac{2\pi n}{a}\right) \overset{?}{=} \sum_{n\in\mathbb{Z}} e^{inka}$$

$$\rho(x) = \frac{1}{2\pi}\int dk\, \tilde{\rho}(k)\, e^{ikx} = \frac{V^*}{2\pi}\int dk \sum_{n\in\mathbb{Z}} \delta\left(k-\frac{2\pi n}{a}\right) e^{ikx}$$
$$= \frac{V^*}{2\pi}\sum_{n\in\mathbb{Z}} e^{2i\pi n x/a}$$
$$\overset{!}{=} \frac{1}{a}\sum_{m\in\mathbb{Z}} e^{2i\pi n x/a}$$

$$\Rightarrow \boxed{V^* = \frac{2\pi}{a}}$$

So in 1D,

$$\Delta(k) = \sum_{n\in\mathbb{Z}} e^{-ikna} = \frac{2\pi}{a}\sum_{n\in\mathbb{Z}} \delta\left(k-\frac{2\pi n}{a}\right).$$

In 3D,

$$\rho(\underline{x}) = \sum_{\underline{r}\in\Lambda} \delta(\underline{x}-\underline{r}),$$

$$\tilde{\rho}(\underline{k}) = \Delta(\underline{k}) = \sum_{\underline{r}\in\Lambda} e^{-i\underline{k}\cdot\underline{r}} = V^* \sum_{\underline{q}\in\Lambda^*} \delta(\underline{k}-\underline{q}). \qquad \square$$

Return to original f^n

$$\tilde{f}(\underline{k}) = \Delta(\underline{k})\, S(\underline{k})$$

with $S(\underline{k}) = \int_P d^3x\, e^{-i\underline{k}\cdot\underline{x}}\, f(\underline{x})$.

Return to $f(x)$

$$f(\underline{x}) = \frac{1}{(2\pi)^3}\int d^3k\; e^{i\underline{k}\cdot\underline{x}}\,\tilde{f}(\underline{k}).$$

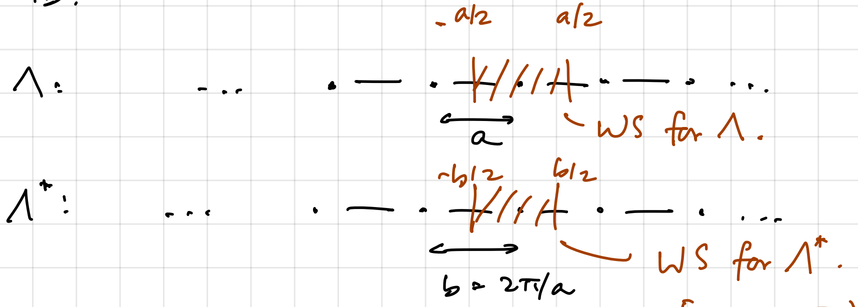
$$= \frac{V^*}{(2\pi)^3}\sum_{q\in\Lambda^*} e^{iq\cdot x}\, S(q)$$

$\Rightarrow$ periodic f^n on lattices, are sums of plane waves with mom. in Λ^*.

Brillouin zone

Def^n Brillouin zone (BZ) $\equiv$ Wigner – Seitz cell of Λ^*.

Sanity check in 1D.



3D : How to BZ (or WS) ?

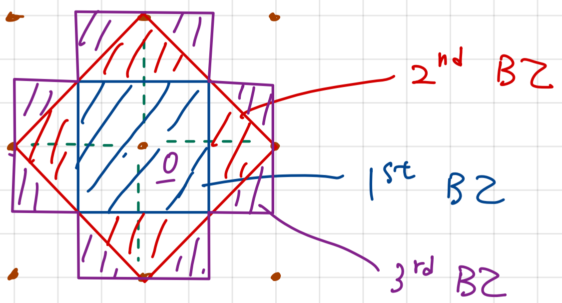
$[-\frac{\pi}{a}, \frac{\pi}{a})$ BZ

Procedure : Start with point $\underline{0}$ in Λ^*.

1st BZ : all points closest to $\underline{0}$ than other points in Λ^*.

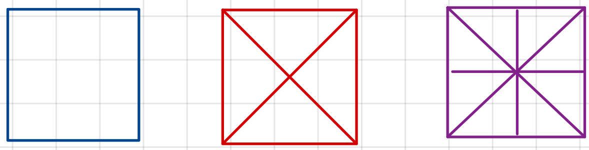
2nd BZ : all points where $\underline{0}$ is second closest in Λ^*.

Example



Comments (1) As drawn, this is called the extended scheme.

(2) Also possible to draw in reducible scheme.



(3) Every BZ has the same volume (area).

Band Structure 3D

Bloch's thm

Considering an e^- with

$$H = \underline{p}^2/2m + V(\underline{x}) \quad , \; V(\underline{x}) = V(\underline{x}+\underline{r}), \; \underline{r} \in \Lambda .$$

Thm (Bloch's thm) Energy estates for this Hamiltonian take the form

$$\psi_{\underline{k}}(\underline{x}) = e^{i\underline{k}\cdot\underline{x}}\, u_{\underline{k}}(\underline{x}),$$

with $u_{\underline{k}}(\underline{x}+\underline{r}) = u_{\underline{k}}(\underline{x}) \quad \forall \, \underline{r} \in \Lambda$,

Pf: Use symmetries! (translations by $\underline{r} \in \Lambda$)

Define $T_{\underline{r}}$ translation operator,

$$T_{\underline{r}} f(\underline{x}) = f(\underline{x}+\underline{r})$$

Properties:

(1) $T_{\underline{r}}$ unitary $\Rightarrow$ evals are phases

(2) Abelian group $\Rightarrow$ $T_{\underline{r}} T_{\underline{r}'} = T_{\underline{r}+\underline{r}'}$, $[T_{\underline{r}}, T_{\underline{r}'}] = 0$.

(3) For $\underline{r} \in \Lambda$, we have $[H, T_{\underline{r}}] = 0 \Rightarrow$ can label estates of H by estates of $T_{\underline{r}}$.

Task: characterise evals, estates of $T_{\underline{r}}$.

$$T_{\underline{r}} \psi = c(\underline{r})\, \psi, \quad \text{with } c(\underline{r}) \text{ eval}$$

$$\left.\begin{aligned} T_{\underline{r}} T_{\underline{r}'} \psi &= c(\underline{r}) c(\underline{r}') \psi \\ \| \quad & \\ T_{\underline{r}+\underline{r}'} \psi &= c(\underline{r}+\underline{r}') \psi . \end{aligned}\right\} \Rightarrow c(\underline{r}) c(\underline{r}') = c(\underline{r}+\underline{r}')$$

Choose $\underline{r} = \underline{a}_i$ (one primitive vector)

$$c(\underline{a}_i) = e^{2\pi i \theta_i} \quad , \; \theta_i \in \mathbb{R} .$$

then $\underline{r} = \sum_i n_i \underline{a}_i$, $\quad c(\underline{r}) = c(\underline{a}_1)^{n_1} c(\underline{a}_2)^{n_2} c(\underline{a}_3)^{n_3} = e^{i\underline{k}\cdot\underline{r}}$,

$$\underline{k} = \sum_i \theta_i \underline{b}_i \, , \quad \underline{b}_i \cdot \underline{a}_j = 2\pi \delta_{ij}$$

primitive of Λ^*.

Then estate satisfy

$$T_{\underline{r}}\,\psi(\underline{x}) = e^{i\underline{k}\cdot\underline{r}}\,\psi(\underline{x})$$

Then look back to statement in Bloch's thm :

$$u_{\underline{k}}(\underline{x}) = e^{-i\underline{k}\cdot\underline{x}}\,\underbrace{\psi_{\underline{k}}(\underline{x})}_{\text{estate of } T_{\underline{r}}}.$$

$$T_{\underline{r}}\,u_{\underline{k}}(\underline{x}) = u_{\underline{k}}(\underline{x}+\underline{r}) = e^{-i\underline{k}\cdot(\underline{x}+\underline{r})}\,\psi_{\underline{k}}(\underline{x}+\underline{r})$$
$$= e^{-i\underline{k}\cdot\underline{x}}\,\psi_{\underline{k}}(\underline{x}) = u_{\underline{k}}(\underline{x}) .$$

Alternatively, an estate of $T_{\underline{r}}$ is of the form

$$\psi_{\underline{k}}(\underline{x}) = e^{i\underline{k}\cdot\underline{x}}\,u_{\underline{k}}(\underline{x}) ,$$

with $u_{\underline{k}}(\underline{x}) = u_{\underline{k}}(\underline{x}+\underline{r})$. □

Defn $\underline{k}$ (eval of $T_{\underline{r}}$) is called the crystal momentum .

Property: let $\underline{k}' = \underline{k} + \underline{g}$ with $\underline{g} \in \Lambda^*$, then eval of $T_{\underline{r}}$ unchanged.

- Reduced zone scheme: choose $\underline{k}$ to lie in 1st BZ ⇒ many states with the same $\underline{k}$ and different energies

$$\psi_{\underline{k},n} \quad , \quad n: \text{ band index}$$

- Extended zone scheme : $\underline{k} \in \mathbb{R}^d$, but if $\underline{k}' = \underline{k} + \underline{g}$, $\underline{g} \in \Lambda^*$, we have same crystal mom.

Tight - Binding model 3D

$$H = \underbrace{\sum_{\underline{r}\in\Lambda} E_0\,|\underline{r}\rangle\langle\underline{r}|}_{\substack{e^- \text{ can only be} \\ \text{at 1 site}}} - \underbrace{\sum_{\underline{a}} t_{\underline{a}}}_{\substack{\text{jumping to other} \\ \text{states, simple choice,} \\ \text{e.g. } \underline{a} \text{ are nearest} \\ \text{neighbours}}}\Big(|\underline{r}\rangle\langle\underline{r}+\underline{a}| + |\underline{r}+\underline{a}\rangle\langle\underline{r}|\Big) .$$

This gives an example of a Hamiltonian with periodic potential.

Sol^n to sys:

$$|\psi(\underline{k})\rangle = \frac{1}{\sqrt{N}} \sum_{\underline{r}\in\Lambda} e^{i\underline{k}\cdot\underline{r}} |\underline{r}\rangle \qquad \text{estates}$$

$$E(\underline{k}) = E_0 - \sum_{\underline{a}} 2t_{\underline{a}} \cos(\underline{k}\cdot\underline{a}) \qquad \text{evals} .$$

where $\underline{k} \in$ 1st BZ since

$$e^{i(\underline{k}+\underline{q})\underline{r}} = e^{i\underline{k}\cdot\underline{r}} \quad , \text{ where } \underline{q} \in \Lambda^*$$

Note: BC of $t_{\underline{a}}$ states are not localised at one site.

Nearly free electron

Consider $V(\underline{x}) = V(\underline{x}+\underline{r})$ and solve evals using pert. theory.

In the free theory $(V=0)$, we have plane waves

$$\langle \underline{x} | \underline{k} \rangle \sim e^{i\underline{k}\cdot\underline{x}} \quad , \quad E_0(\underline{k}) = \hbar^2 k^2 / 2m$$

In pert. theory. we need

$$\langle \underline{k} | V | \underline{k}' \rangle = \underbrace{\underset{\nearrow\, V:\ \text{volume}}{\frac{1}{V}} \int_V d^3x \, e^{i(\underline{k}'-\underline{k})\cdot\underline{x}} \underset{\uparrow\, V:\ \text{potential}}{V(\underline{x})}}_{\text{FT } \tilde{V}(\underline{q}) \text{ with } \underline{q} = \underline{k}'-\underline{k}} = V_{\underline{k}'-\underline{k}} .$$

$\Rightarrow$ $V_{\underline{q}}$ non-vanishing only if $\underline{q} = \underline{k}' - \underline{k} \in \Lambda^*$.

Corrections to evals: two cases

(1) Non-degenerate

$$E(\underline{k}) = E_0(\underline{k}) + \langle \underline{k} | V | \underline{k} \rangle + \sum_{\substack{\underline{k}'=\underline{k}+\underline{q}, \\ \underline{q}\in\Lambda^*}} \frac{|\langle \underline{k} | V | \underline{k}' \rangle|^2}{E_0(\underline{k}) - E_0(\underline{k}')}$$

Applicable for low $\underline{k}$ modes.

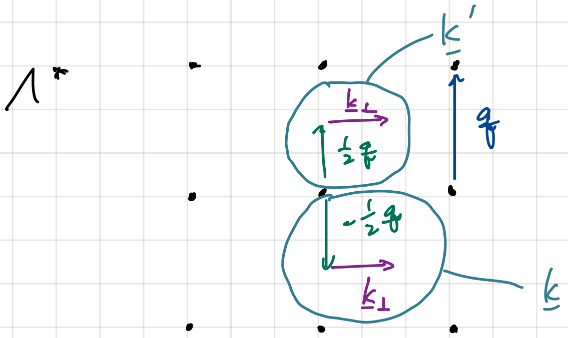
(2) Degenerate states.

If $\underbrace{E_0(\underline{k}) = E_0(\underline{k}')}_{k^2 = k'^2}$ and $\underbrace{V_{\underline{k}-\underline{k}'} \neq 0}_{\Rightarrow\ \underline{q} = \underline{k} - \underline{k}' \in \Lambda^*.}$, then

$$k^2 = (\underline{k} + \underline{q})^2 \Rightarrow 2\underline{k}\cdot\underline{q} + \underline{q}^2 = 0$$

$$\Rightarrow \underline{k} = -\frac{1}{2}\underline{q} + \underline{k}_1 , \quad \text{with } \underline{k}_1 \cdot \underline{q} = 0$$

In drawings, consider square lattice



Conclusion: we have degenerate states at the edge of BZ.

To find corrections, $|\psi\rangle = \alpha|\underline{k}\rangle + \beta|\underline{k}'\rangle$.

$$\underbrace{\begin{pmatrix} \langle \underline{k}|H|\underline{k}\rangle & \langle \underline{k}|H|\underline{k}'\rangle \\ \langle \underline{k}'|H|\underline{k}\rangle & \langle \underline{k}'|H|\underline{k}'\rangle \end{pmatrix}}_{= \begin{pmatrix} E_0(\underline{k}) & V_{-\underline{q}} \\ V_{\underline{q}} & E_0(\underline{k}') \end{pmatrix}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Evals:

$$E_\pm = E_0(\underline{k}) \pm |V_{\underline{q}}|$$

gap at edge of BZ

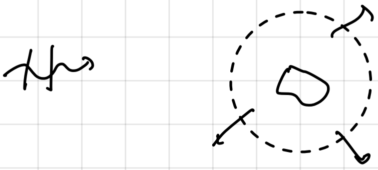
Note: Be careful at special points (usually corners) of BZ.

In square lattice, this occurs, e.g. $(\pm\pi/a, \pm\pi/a)$.

Scattering off lattice

How do we know that solid are described by lattice? Experimentalists shinning light (neutrons) to materials

Before: scattering for a single atom.



$$\psi \sim A e^{-i\omega t}\left[\underbrace{e^{i\underline{k}\cdot\underline{x}}}_{\text{incident}} + \underbrace{f(\theta,\phi)}_{\text{scattering amplitude}}\frac{e^{ikr}}{r}\right] \quad \text{as } r\to\infty$$

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 .$$

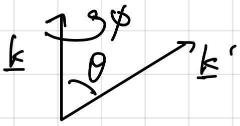
Now: many atoms

target: $V(\underline{x}) = V(\underline{x}+\underline{r})$

From Born approximation,

$$f(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2}\tilde{V}(\underline{q}) ,$$

where $\tilde{V}(\underline{q}) = \int d^3x' \, e^{i\underline{q}\cdot\underline{x}'} V(\underline{x}')$, $\quad \underline{q} = \underline{k} - k\hat{\underline{r}} = \underline{k} - \underline{k}'$



We know:

(1) Scattering amplitude is controlled by FT of potential

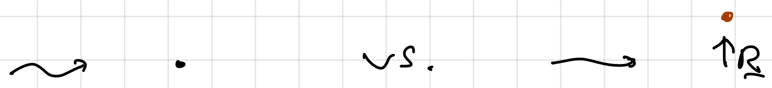
(2) FT of periodic f^n s have non-trivial prop.

$$V(\underline{q}) = \Delta(\underline{q})\, S(\underline{q})$$

with $\Delta(\underline{q}) = \sum_{\underline{r}\in\Lambda} e^{i\underline{q}\cdot\underline{r}}$, $\quad S(\underline{q}) = \int_P d^3x' \, e^{-i\underline{q}\cdot\underline{x}} V(\underline{x})$, $\quad \underline{q}\in\Lambda^*$.

UPSHOT: Scattering only take place if $\boxed{\underline{k} - \underline{k}' \in \Lambda^*}$ (Laue condition)

Another way to argue this



Then for the target displaced

$$\psi(\underline{x}) \sim e^{i\underline{k}\cdot(\underline{x}-\underline{R})} + f(\theta,\phi)\frac{e^{ik|\underline{x}-\underline{R}|}}{|\underline{x}-\underline{R}|}$$

$$\underset{r\gg R}{\underset{r\to\infty}{\approx}} e^{-i\underline{k}\cdot\underline{R}}\left[e^{i\underline{k}\cdot\underline{x}} + \underbrace{f(\theta,\phi)\,e^{-i(\underline{k}'-\underline{k})\cdot\underline{R}}}_{f_{\underline{R}}(\theta,\phi)}\frac{e^{ikr}}{r}\right]+\dots$$

If we ignore multiple scatterings from each site

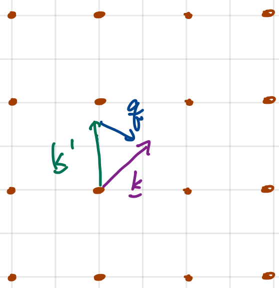
$$f_n(\theta,\phi) = f(\theta,\phi)\sum_{\underline{R}\in\Lambda} e^{i\underline{q}\cdot\underline{R}}, \quad \underline{q} = \underline{k}-\underline{k}'$$

$$\Rightarrow f_n(\underline{k},\underline{k}') = f(\underline{k},\underline{k}')\underbrace{\sum_{\underline{R}\in\Lambda} e^{i\underline{q}\cdot\underline{R}}}_{\Delta(\underline{q})}.$$

Also arrive to Laue condition.

Then when you take a picture (shine light) of a solid, you see the reciprocal lattice.

Example Square lattice, Λ^*



Bragg Condition

Rewriting of Laue condition

$$\underline{k}-\underline{k}' = \underline{q}\in\Lambda^*, \quad \underline{k}\cdot\underline{k}' = k^2\cos\theta$$

Combine both, $(\underline{k}-\underline{k}')^2 = \underline{q}^2 \Rightarrow \boxed{q = 2k\sin\frac{\theta}{2}}$

Rewrite in terms of Λ data (instead of Λ^*).

(1) $\underline{q} \cdot \underline{r} = 2\pi n$, $n \in \mathbb{Z}$, $r \in \Lambda$, $q \in \Lambda^*$.

⇒ read off separation between layers in lattice

$$q = \frac{2\pi}{d},$$

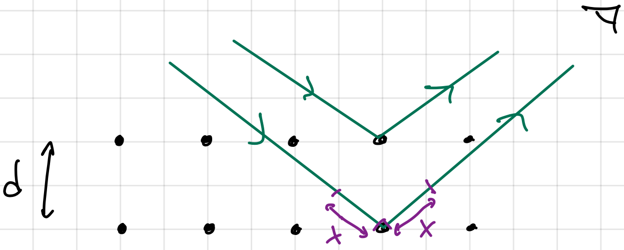
where d is the magnitude of a primitive $|\underline{a}_i| = d$

(2) Trade frequency for wavelength (λ).

$$k = 2\pi/\lambda.$$

$$\Rightarrow n\lambda = 2d\sin\frac{\theta}{2}$$

For $n=1$,



Extra distance travelled by beam is $2x = 2d\sin\theta/2$, then Bregg condition is the assurance of wave interfering constructively.

Structure factor

$$f_n(\underline{k}, \underline{k}') = \Delta(\underline{q})\ \underbrace{S(\underline{q})}_{\text{structure factor.}}$$

In many materials, we have BL + basis

$$\underline{r} = \sum_i n_i \underline{a}_i + \underline{d}_i.$$

$$S(\underline{q}) = \sum_i f_i(\underline{k}, \underline{k}')\, e^{i\underline{q}\cdot \underline{d}_i}.$$

Electron Dynamics in a Solid

Many particles (e^-) in the presence of a lattice.

Assumption: ignore interactions between e^-.

$\hookrightarrow$ effective description — Landau–Fermi description

Free system		Interactions
spin, charge, momentum	$\xrightarrow[\text{on}]{\text{turn}}$	unchanged
mass, magnetic moment	$\longrightarrow$	changed effectively renormalised

Fermi Surface

Goal: understand many e^- in solid

Q: How many e^- can we fit in a BZ ?

Claim: # of states in a BZ $= N$, where N is the no. of lattice sites (Λ)

Pf: Consider a lattice Λ, with a finite no. of sites

$$\underline{r} \in \Lambda, \qquad \underline{r} = \sum_i n_i \underline{a}_i$$

We restrict $0 \leq n_i \leq N_i$. Then

$$N = N_1 N_2 N_3 .$$

Since the system is finite, need to impose BC

$$\psi(\underline{x} + N_i \underline{a}_i) = \psi(\underline{x}) \quad , \quad i = 1, 2, 3 . \qquad (1)$$

We also have Bloch's thm

$$\psi_{\underline{k}}(\underline{x}) = e^{i\underline{k}\cdot\underline{x}} u_{\underline{k}}(\underline{x}) \qquad (2)$$

$$(1), (2) \Rightarrow \quad e^{iN_i \underline{a}_i \cdot \underline{k}} = 1 \qquad \text{restriction on } \underline{k}.$$

$$\Rightarrow \underline{k} = \sum_i \frac{m_i}{N_i} \underline{b}_i , \quad m_i \in \mathbb{Z} , \quad \underline{b}_i \in \Lambda^* .$$

$\underline{k}$ sits within BZ. hence in one zone, $0 \leq m_i \leq N_i$

$$\Rightarrow \# \text{ states in a BZ} = N_1 N_2 N_3 = N . \text{ (no. of states)}. \quad \square$$

Q: How will e^- organise in BZ?

We will use

(i) Ignore interactions between e^-

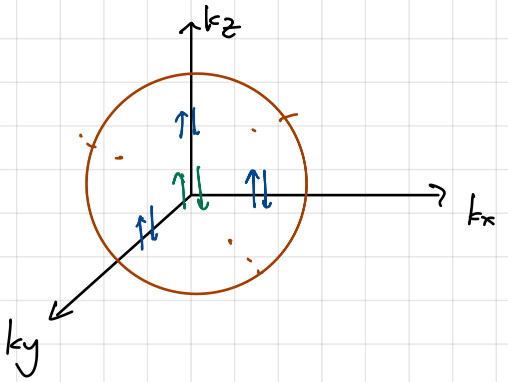
(ii) Pauli exclusion principles : no two e^- occupy same estate

(iii) We have a finite # of available sites in BZ.

Focus on (i) + (ii) first. If e^- are free ($V=0$). and we place them in a box, $E = \frac{\hbar^2}{2m} k^2$, with $k_i = \frac{2\pi n_i}{L}$, $n_i \in \mathbb{Z}$.

We also know they carry spin : $|\uparrow\rangle$, $|\downarrow\rangle$.

How do free e^- organise themselves?



Ball that describes occupation ≡ Fermi sea

Surface 〃 ≡ Fermi surface.

States on Fermi surface have

- Fermi momentum : $\hbar \underline{k}_F$
- Fermi energy : $E_F = \frac{\hbar^2}{2m} k_F^2$.

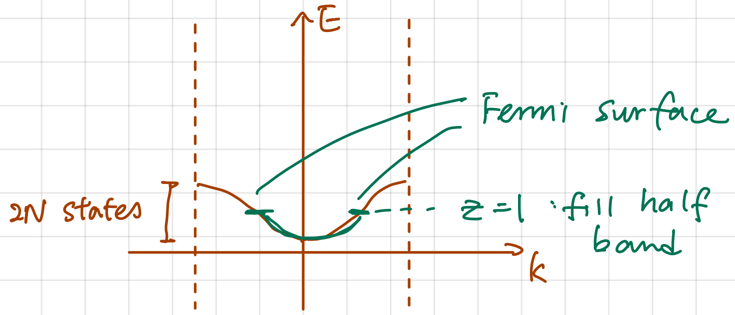
How does lattice change this? What do we know about lattices?

- energy spectrum splits in bands
- Each band can accomodate $2N$ e^-s.

One more fact / terminology: e^-s are donations from atoms. each atom donates Z e^-: valency.

In our system, hence we will have ZN e^- for N atoms in lattice.

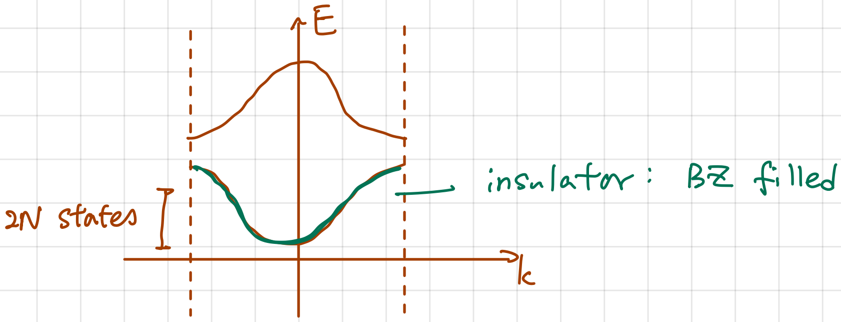
Example 1D, $Z=1$.



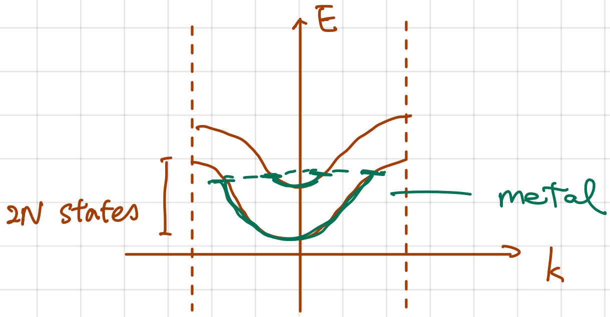
Because band is half filled ⇒ metal. (we still have available states. If a current is applied, e^- can move easily).

1D, $Z=2$

1st option

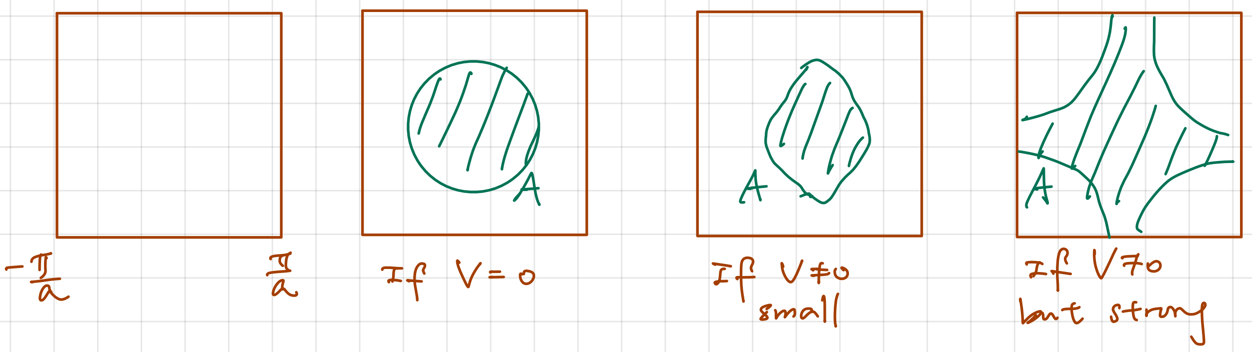


2nd option



Example 2D $Z=1$, consider square lattice.

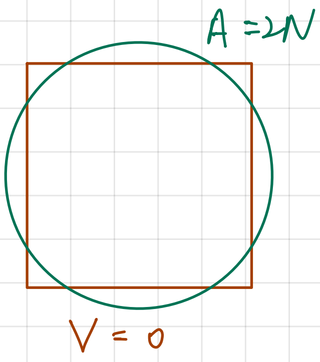
1st BZ:



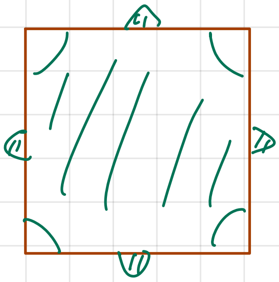
Metals

Note: Fermi-surface always hits a edge of BZ at 90°.

2D, $Z=2$



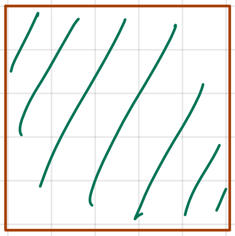
Option 1



E_{min} of 2nd BZ $< E_{max}$ of 1st BZ

Metal / conductor

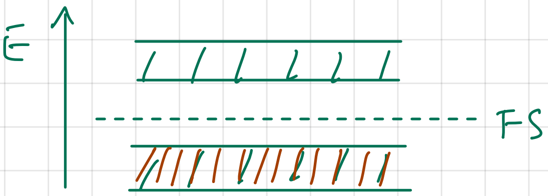
Option 2



E_{min} of 2nd BZ $> E_{max}$ of 1st BZ

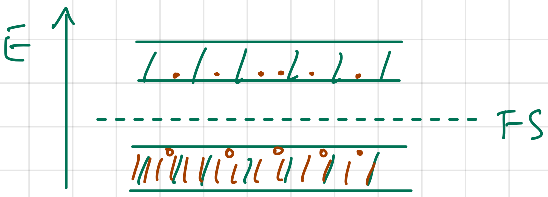
Insulator

Note: Semi-conductor



$T=0$

Insulator



$T>0$

Metal.

Dynamics of Bloch's electrons

Idea: implement quasi-particle picture.

"electron": Bloch's e^- — effective description of the collective

Consider a system, where a single B e^- has energy $E(\underline{k})$, $\underline{k} \in BZ$.

Claim Average velocity is $\underline{v} = \frac{1}{\hbar}\frac{\partial E}{\partial \underline{k}}$

Pf: In QM, avg velocity defined as $\underline{v} = \frac{1}{m}\langle \psi | -i\hbar\nabla|\psi\rangle$.

From Bloch's thm,

$$\psi_{\underline{k}}(\underline{x}) = e^{i\underline{k}\cdot\underline{x}}\, u_{\underline{k}}(\underline{x}), \qquad u_{\underline{k}}(\underline{x}+\underline{r}) = u_{\underline{k}}(\underline{x}),\ \underline{k}\in BZ$$

and

$$H\psi_{\underline{k}}(\underline{x}) = E(\underline{k})\,\psi_{\underline{k}}(\underline{x}).$$

This implies

$$H_{\underline{k}}\, u_{\underline{k}}(\underline{x}) = E(\underline{k})\, u_{\underline{k}}(\underline{x}), \qquad (1)$$

with $H = \frac{\hbar^2}{2m}(-i\nabla)^2 + V(\underline{x})$, $H_{\underline{k}} = \frac{\hbar^2}{2m}(-i\nabla + \underline{k})^2 + V(\underline{x})$.

Consider

$$H_{\underline{k}+\underline{q}} = H_{\underline{k}} + \frac{\partial H_{\underline{k}}}{\partial \underline{k}}\,\underline{q} + \dots$$

$$E(\underline{k}+\underline{q}) = E(\underline{k}) + \frac{\partial E}{\partial \underline{k}}\cdot\underline{q} + \dots$$

Replacing on (1):

$$\frac{\partial E}{\partial \underline{k}} = \langle u_{\underline{k}} | \frac{\partial H_{\underline{k}}}{\partial \underline{k}} | u_{\underline{k}}\rangle$$

$$= \langle u_{\underline{k}} | \frac{\hbar^2}{2m}(-i\nabla + \underline{k}) | u_{\underline{k}}\rangle$$

$$= \frac{\hbar}{m}\langle \psi_{\underline{k}} | -i\hbar\nabla | \psi_{\underline{k}}\rangle$$

$$\Rightarrow \underline{v} = \frac{1}{\hbar}\frac{\partial E}{\partial \underline{k}}. \qquad \square$$

Claim: A filled band carries no electric current.

Pf: A single B e^-: $\underline{j} = -e\,\underline{v}(\underline{k})$. Total current is

$$\underline{j}^T = \underset{\substack{\uparrow \\ \text{spin}}}{2}(-e)\int_{BZ}\frac{d^3k}{(2\pi)^3}\,\underline{v}$$

for occupied / filled band.

$$\Rightarrow \underline{j}^T = -\frac{2e}{\hbar}\int_{BZ}\frac{d^3k}{(2\pi)^3}\frac{\partial E}{\partial \underline{k}} = 0$$

because energy is periodic. □

Claim A filled band carries no heat current (transport energy)

Pf: Kinetic theory.

$$j_Q = \underbrace{\frac{1}{3}C_v T}_{\text{KE per particle}}\ \underline{v}\cdot \overset{\text{density}}{n} = E n \underline{v}.$$

For our model.

$$j_{Q,T} = 2\int_{BZ} E\,\underline{v}\,\frac{d^3k}{(2\pi)^3}$$

$$= \frac{2}{\hbar}\int_{BZ} E\,\frac{\partial E}{\partial \underline{k}}\,\frac{d^3k}{(2\pi)^3}$$

$$= \frac{1}{\hbar}\int_{BZ}\frac{\partial E^2}{\partial \underline{k}}\cdot\frac{d^3k}{(2\pi)^3} = 0$$ □

⇒ Insulators conduct neither electricity nor heat.

Def^n The effective mass tensor m^*_{ij}

$$m^*_{ij} := \hbar^2\left(\frac{\partial E}{\partial k_i\,\partial k_j}\right)^{-1}$$

If sys. is isotropic, $m^*_{ij} = m^*\delta_{ij}$.

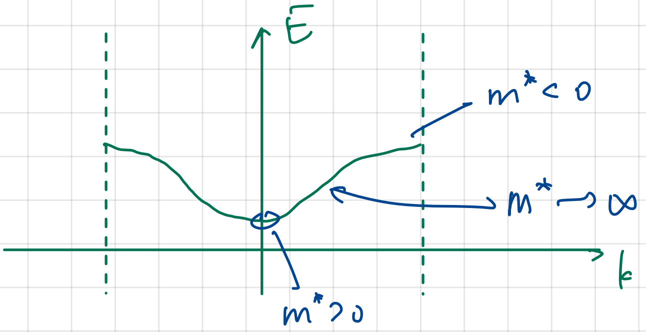
Useful def^n due to what we learned from $\underbrace{\text{nearly free}}_{\text{values of } \underline{k} \text{ sys. is free}}$ e^-.

$$E = E_{min} + \frac{\hbar^2}{2m^*}|\underline{k}-\underline{k}_{min}|^2 + \dots$$

Apply this to tight-binding in 1D.

$$E = E_0 - 2t\cos(ka) \approx \underbrace{E_0 - 2t}_{E_{min}} + ta^2k^2 + \dots \Rightarrow m^* = \frac{\hbar^2}{2ta}.$$

Note Funny things happen with m_{ij}.



Semi-classical e.o.m.

Suppose we apply an external force to the solid

$$\underline{F} = -\nabla U(\underline{x}),$$

where $U(\underline{x})$: potential, e.g. electric field.

Assumption:

(1) $U(\underline{x})$ is small

(2) Semi-classical view : $\underline{v} = \frac{1}{\hbar}\frac{\partial E}{\partial \underline{k}} = \frac{d\underline{x}}{dt}$. ⇒ consider wave packets.

Assumption (1) implies

$$\underset{\text{Total energy}}{E_T} = \underset{\text{lattice}}{E(\underline{k})} + \underset{\text{external}}{U(\underline{k})}.$$

$$\frac{dE_T}{dt} = \frac{dE(\underline{k})}{dt} + \frac{dU(\underline{k})}{dt} = 0 \quad \text{conserved}$$

$$\Rightarrow \frac{\partial E}{\partial \underline{k}}\frac{d\underline{k}}{dt} + \nabla U \frac{d\underline{x}}{dt} = 0$$

$$\Rightarrow \underline{v}\left(\hbar\frac{d\underline{k}}{dt} + \nabla U\right) = 0$$

$$\Rightarrow \boxed{\hbar\frac{d\underline{k}}{dt} = -\nabla U = \underline{F}}$$

2nd law for particles in a solid.

Rewrite as

$$m^* \frac{d\underline{v}}{dt} = \frac{m^*}{\hbar}\frac{d}{dt}\left(\frac{\partial E}{\partial k}\right)$$

$$= \frac{m^*}{\hbar}\frac{dk_i}{dt}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

$$= \frac{m^*}{\hbar}\cdot\frac{dk_i}{dt}\cdot\frac{\hbar^2}{m_*}\delta_{ij} \qquad \text{(isotropy)}$$

$$\Rightarrow \boxed{m^* \frac{d\underline{v}}{dt} = \hbar \frac{d\underline{k}}{dt}}$$

$$\Rightarrow \underline{F} = m^* \frac{d\underline{v}}{dt}$$

Then when we solve for sys,

$$\underline{v} = \frac{1}{\hbar}\frac{\partial E}{\partial \underline{k}}, \qquad \underline{F} = \hbar\frac{\partial \underline{k}}{\partial t}$$

Example An e^- in a const. E field $\underline{\mathcal{E}}$.

$$\underline{F} = -e\underline{\mathcal{E}}$$

$$\Rightarrow \hbar\dot{\underline{k}} = -e\underline{\mathcal{E}}$$

$$\Rightarrow \underline{k}(t) = \underline{k}(0) - \frac{e}{\hbar}\underline{\mathcal{E}}t.$$

Study further in 1D, where boundary is

$$E(k) = -C\cos(ka)$$

Set $\underline{k}(0) = 0$, then we have

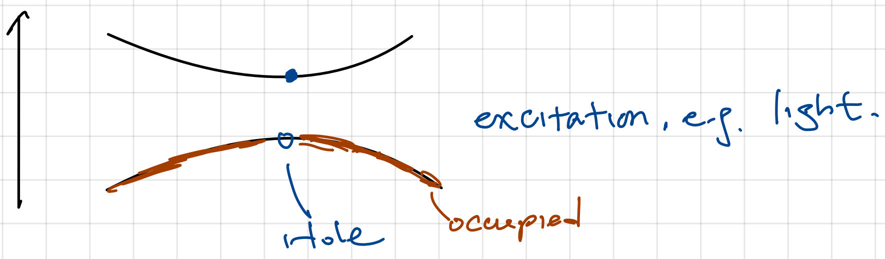
$$v = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{Ca}{\hbar}\sin(ka) = -\frac{Ca}{\hbar}\sin\left(\frac{e\mathcal{E}at}{\hbar}\right)$$

Particles move back and forth: Bloch's oscillations.

Curiosity: applied const. E field ⇒ $\underbrace{\text{outcome is AC current.}}_{\substack{\text{seen in optical lattices,} \\ \text{fragile} \because \text{material has impurities.}}}$

Holes

Consider a completely filled band and we excite one e-



First look at current

$$\underline{j} = 2(-e)\int_{\text{occupied}} \frac{d^3k}{(2\pi)^3}\,\underline{v}$$

Recall

$$0 = \int_{BZ} \frac{d^3k}{(2\pi)^3}\,\underline{v} = \int_{\text{occupied}} + \int_{\text{unoccupied}}.$$

$$\Rightarrow \underline{j} = -2(-e)\int_{\text{unoccupied}} \frac{d^3k}{(2\pi)^3}\,\underline{v} = 2(+e)\int_{\text{unoccupied}} \frac{d^3k}{(2\pi)^3}\,\underline{v}.$$

⇒ Holes behaves as a particle with +e.

We have now a fictitious particle with +e which we call <u>hole</u>.

Energy hole: near the top of the band

$$E(k) = E_{max} + \frac{\hbar^2}{2m^*}|\underline{k}-\underline{k}_{max}|^2 + \dots$$

$\hookrightarrow$ with $m^* < 0$.

As the hole moves away from the top, it costs more energy

This suggests to write

$$E_{hole} = -E(k) = -E_{max} + \frac{\hbar^2}{2m_{hole}}|\underline{k}-\underline{k}_{max}|^2 + \dots$$

with $m_{hole} = -m^* > 0$: effective mass of the hole.

Momentum hole: we removed a state with $\underline{k}$

$$\underline{k}_{hole} = -\underline{k}.$$

Velocity hole:

$$\underline{v}_{hole} = \frac{1}{\hbar} \frac{\partial E_{hole}}{\partial \underline{k}_{hole}} = \frac{1}{\hbar} \frac{\partial E}{\partial \underline{k}} = \underline{v} \quad \text{unchanged.}$$

EoM:

$$\underline{F} = m^* \frac{d\underline{v}}{dt} \overset{(e.g.)}{=} -e\underline{\mathcal{E}}$$

$$= -m_{hole} \frac{d\underline{v}_{hole}}{dt}$$

$$\Rightarrow -\underline{F} = m_{hole} \frac{d\underline{v}_{hole}}{dt} = +e\underline{\mathcal{E}}$$

Again holes behaves as a particle with +ve charge.

Lesson: in materials, more convenient or natural to think in terms of the hole. But there are no +ve charge! All charge is carried by e^- with $(-e)$.

Curiosity: this resembles in QFT the appearance of anti-particle.

3.4 Phonons

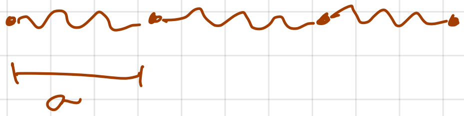
Until now, in studied solids, we fixed the positions / dynamics of atoms. They only play a role by defining Λ

$$\Rightarrow V(\underline{x}+\underline{r}) = V(\underline{x}), \quad \underline{r} \in \Lambda.$$

Dynamics of atoms $\Rightarrow$ phonons. Only do in 1D.

Classical Vibrations

Example mono atomic lattice in 1D



The n-th atom is at pos^n x_n, with $n=1,\dots,N$.

If sys in eqm,

$$x_n = na.$$

Next we will assume there is an interaction of the form

$$\sum_n V(x_n - x_{n-1}) \qquad \text{(nearest neighbour)}$$

A small deviation away from eqm, we will have.

$$u_n(t) = x_n(t) - na.$$

and then

$$H = \sum_n \overset{m\dot{u}_n}{P_n^2}/2m + \frac{\overset{\lambda \sim \partial^2 V .}{\lambda}}{2} \sum_n (u_n - u_{n-1})^2 + \dots$$

with λ the effective spring const. (not wavelength).

Solve for sys. EoM:

$$m\ddot{u}_n = -\lambda(2u_n - u_{n-1} - u_{n+1})$$

The sol^n will take the form

$$u_n = \underset{\uparrow \text{ amplitude, arbitrary but small}}{A} \exp[-i(\omega(k)t + kna)] \qquad (1)$$

Lattice will impose constraints on the sol^n.

1) BZ: sol^n invar. under $k \longrightarrow k + \frac{2\pi}{a} \Rightarrow k \in [-\frac{k}{a}, \frac{k}{a})$.

2) Periodicity: $u_{N+1} = u_1$, $k = \frac{2\pi}{na} l$, $l = -\frac{N}{2}, \dots, \frac{N}{2}$.

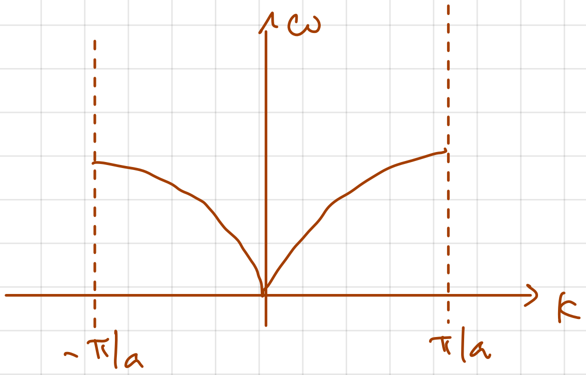
Sub (1) into EoM:

$$m\omega^2(k) = \lambda(2 - e^{ika} - e^{-ika})$$

$$\Rightarrow m\omega^2 = 4\lambda \sin^2\left(\frac{ka}{2}\right)$$

$$\Rightarrow \omega(k) = 2\sqrt{\frac{\lambda}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| .$$

This is the dispersion relation.



At small $k \to 0$.

$$\omega(k) \sim \sqrt{\frac{\lambda}{m}}\, ak \qquad \text{(relativistic dispersion)}$$

$$\Rightarrow \qquad \omega = c_s k + \dots ,$$

where $c_s = \sqrt{\frac{\lambda}{m}}\, a$ is speed of sound in the solid.

Quantum vibrations

In classical theory.

$$u_n(t) = \underbrace{X_n(t)}_{\substack{\text{centre of}\\ \text{mass motion}\\ (l=0)}} + \sum_{l\neq 0}\Big(\underbrace{\alpha_l}_{\substack{\text{Amplitude}\\ \text{(const.)}}}\, e^{-i(\omega_l t - k_l na)} + \alpha_l^* e^{i(\omega_l t - k_l na)}\Big) , \qquad (2)$$

$$k_l = \frac{2\pi}{na}\, l , \qquad l = -N/2, \dots, N/2 .$$

$$\omega_l = 2\sqrt{\frac{\lambda}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| .$$

$$p_n(t) = m\dot{u}_n = p_0(t) + \sum_{l\neq 0}\left(-im\omega_l\alpha_l\, e^{-i(\omega_l - k_l na)} + im\omega_l\alpha_l^* e^{i(\omega_l t - k_l na)}\right) .$$

(3)

Quantum theory: promote $u_n(t), p_n(t)$ to be operators.

In Schr. picture $(t=0)$,

$$[u_n, p_{n'}] = i\hbar\,\delta_{nn'}, \quad [u_n, u_{n'}] = [p_n, p_{n'}] = 0 \qquad (1)$$

Then α_ℓ becomes operators, and write $\alpha_\ell^* \to \alpha_\ell^\dagger$.

Understand the reparaission of imposing (1) on $\alpha_\ell, \alpha_\ell^\dagger$.

First invert (2), (3) at $t=0$,

$$(2): \quad \sum_{n=1}^{N} u_n e^{-ik_\ell na} = N(\alpha_\ell + \alpha_{-\ell}^\dagger)$$

$$(3): \quad \sum_{n=1}^{N} p_n e^{-ik_\ell na} = -iN\omega_\ell(\alpha_\ell - \alpha_\ell^\dagger)$$

$$\Rightarrow \quad \alpha_\ell = \frac{1}{2m\omega_\ell N}\sum_n e^{-ik_\ell na}(m\omega_\ell u_n + ip_n)$$

$$\alpha_\ell^\dagger = \frac{1}{2m\omega_\ell N}\sum_n e^{ik_\ell na}(m\omega_\ell u_n - ip_n)$$

Then from (1),

$$[\alpha_\ell, \alpha_{\ell'}^\dagger] = \frac{\hbar}{2m\omega_\ell N}\delta_{\ell\ell'}, \quad [\alpha_\ell, \alpha_{\ell'}] = [\alpha_\ell^\dagger, \alpha_{\ell'}^\dagger] = 0$$

Rescaling $\alpha_\ell = \sqrt{\frac{\hbar}{2m\omega_\ell N}}\, a_\ell$,

$$\Rightarrow [a_\ell, a_{\ell'}^\dagger] = \delta_{\ell\ell'}, \quad [a_\ell, a_{\ell'}] = [a_\ell^\dagger, a_{\ell'}^\dagger] = 0$$

A system of N harmonic oscillators.

The Hamiltonian then becomes

$$H = \underbrace{\frac{p_0^2}{2M}}_{\substack{\text{CoM motion} \\ M = Nm}} + \sum_\ell \hbar\omega_\ell\Big(a_\ell^\dagger a_\ell + \underbrace{\tfrac{1}{2}}_{\text{zero point energy}}\Big). \approx \sum_{\ell\neq 0}\hbar\omega_\ell a_\ell^\dagger a_\ell.$$

— ignore —

the <u>decoupled harmonic oscillators</u>.

- Ground state $|0\rangle$, it obeys

$$a_\ell|0\rangle = 0 \quad \forall \ell \Rightarrow E=0.$$

- Excited states:
  - Single particle state

$$|k_\ell\rangle = a_\ell^\dagger|0\rangle \Rightarrow E=\hbar\omega_\ell, \quad p=\hbar k_\ell.$$

Called phonons.

  - multiparticle states

$$|\psi\rangle = \prod_{\ell=0} \frac{(a_\ell^\dagger)^{n_\ell}}{\sqrt{n_\ell!}}|0\rangle, \quad n_\ell\in\mathbb{Z}_{\geq 0}, \Rightarrow E=\sum_\ell \hbar\omega_\ell n_\ell.$$

Superposition of phonons.

From atoms to fields.

We initially had $\underbrace{u(x=na)}_{\text{cts}} = \underbrace{u_n}_{\text{discrete}}$.

From discrete point of view,

$$m\ddot{u}_n = \lambda(2u_n - u_{n-1} - u_{n+1})$$

In the continuum

$$\rho\frac{\partial^2 u}{\partial t^2} = -\lambda'\frac{\partial^2 u}{\partial x^2}.$$

where $\rho = m/a$, $\lambda' = \lambda a \Rightarrow c_s^2 = \lambda'/\rho$.

The dynamics are derived from action

$$S=\int dt\,dx\left[\frac{\rho}{2}\left(\frac{\partial u}{\partial t}\right)^2 - \frac{\lambda'}{2}\left(\frac{\partial u}{\partial x}\right)^2\right] \qquad (*)$$

Now $u(x,t)$ (field) contains the dynamics.

(1) $(*)$ is a QFT in $(1+1)$-d, where $u(x,t)$ is a field and describes the collective of all phonons

(2) Quantisation of fields result in particles. Here the particles are phonons ⇒ all fund. particles arise from quantisation of a field.

4. Particles in a Magnetic Field

4.1 Gauge Fields

Recap IB EM:

$$\underline{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \underline{A}}{\partial t}, \qquad \phi : \text{scaler potential}$$

$$\underline{B} = \nabla \times \underline{A}. \qquad \underline{A} : \text{vector potential}$$

$\left.\right\}$ Gauge fields

The Lagrangian for a particle in the presence of $\underline{E}, \underline{B}$ is

$$L = \frac{1}{2}m\dot{\underline{x}}^2 + \frac{q}{c}\dot{\underline{x}}\cdot\underline{A} - q\phi(\underline{x}).$$

⇒ EoM:

$$m\ddot{\underline{x}} = q\left(\underline{E} + \frac{1}{c}\dot{\underline{x}}\cdot\underline{B}\right) \qquad (1)$$

Set $c=1$.

Canonical momenta:

$$\underline{p} = \frac{\partial L}{\partial \dot{\underline{x}}} = m\dot{\underline{x}} + q\underline{A} \longleftarrow \text{depends on } \underline{A}$$

Hamiltonian:

$\underline{A}$ does no work in the sys.

$$H = \dot{\underline{x}}\cdot\underline{p} - L = \frac{1}{2m}(\underline{p} - q\underline{A})^2 + q\phi \quad \left(= \frac{1}{2}m\dot{\underline{x}}^2 + q\phi\right)$$

Example $\underline{E} = 0$, $\underline{B} = (0, 0, B)$.

$$\begin{aligned} m\ddot{x} &= qB\dot{y} \\ \Rightarrow \quad m\ddot{y} &= -qB\dot{x} \\ m\ddot{z} &= 0 \end{aligned} \quad \Rightarrow \quad \begin{aligned} \dot{z} &= \text{const.} \\ x(t) &= x_0 + R\sin(\omega_B(t-t_0)) \\ y(t) &= z_0 + R\cos(\omega_B(t-t_0)) \end{aligned}$$

where x_0, y_0, R, t_0 const., $\omega_B = \dfrac{qB}{m}$.

Gauge Transformations

$\underline{A}$ and ϕ are not unique. Under trans^n

gauge parameter ↓

$$\left.\begin{aligned}\phi &\longmapsto \phi' = \phi - \partial_t\alpha,\\ \underline{A} &\longmapsto \underline{A}' = \underline{A} + \nabla\alpha\end{aligned}\right\}\ \text{gauge trans}^n$$

with $\alpha(\underline{x}, t)$ a smooth f^n. $\underline{E}$ and $\underline{B}$ unchanged.

Note: (1) EoM unaffected by gauge trans^n

(2) Lagrangian trans^n

$$L = \frac{1}{2}m\dot{\underline{x}}^2 + q\dot{\underline{x}}\cdot\underline{A} - q\phi \longmapsto L' = L + q\dot{\underline{x}}\cdot\nabla\alpha + q\,\partial_t\alpha$$

$$= L + q\underbrace{\frac{d\alpha}{dt}}$$

boundary term in action.

can be removed / $\alpha(\underline{x}, t \to \pm\infty) \to 0$

(3) $\underline{x}$ unaffected

$\underline{p}$ does transform under gauge trans^n.

→ In classical theory, gauge trans^n are redundancies.

Schrodinger eqn

In q. theory, we impose

$$[x_i, p_j] = i\hbar\,\delta_{ij}, \quad [x_i, x_j] = [p_i, p_j] = 0$$

and

$$\underline{p} \to -i\hbar\nabla.$$

Then Hamiltonian

$$H = \frac{1}{2m}(\underline{p} - q\underline{A})^2 + q\phi = \frac{1}{2m}(-i\hbar\nabla - q\underline{A})^2 + q\phi.$$

and TDSE

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi.$$

Convenient to introduce <u>covariant derivative</u>.

$$D_t\psi = \frac{\partial\psi}{\partial t} + \frac{iq}{\hbar}\phi\psi$$

$$D_i\psi = \frac{\partial\psi}{\partial x_i} - \frac{iq}{\hbar}A_i\psi.$$

Then Schr. eqn becomes

$$i\hbar D_t\psi = -\frac{\hbar^2}{2m}D^2\psi. \qquad , \quad D^2 = D_iD_i.$$

<u>Note</u>: In GR, $\nabla V = \partial V + \Gamma V$. Here $\Gamma \sim q(\phi, A_i)$.

What happens to Sch. eqn if we do a gauge trans^n?

Look at Hamiltonian

$$H \xrightarrow[\text{g.t.}]{} H' = \frac{1}{2m}(-i\hbar\nabla - qA')^2 + q\phi'$$

$$= UHU^{-1} + i\hbar\frac{\partial U}{\partial t}U^{-1},$$

where $U \equiv \exp\left(\frac{iq}{\hbar}\alpha(\underline{x},t)\right)$. We can see that if

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi,$$

then

$$i\hbar\frac{\partial\psi'}{\partial t} = H'\psi',$$

where $\psi' = U\psi = e^{iq\alpha/\hbar}\psi.$

<u>Notes</u>: (1) ψ', ψ differ by a phase $\Rightarrow$ under g.t., prob. ($|\psi|^2$) are unchanged $\Rightarrow$ sys. is <u>gauge invariant</u>.

(2) If H is time-indpt, it is natural to consider time-indep. gauge trans^n

$$H \to UHU^{-1}.$$

$\Rightarrow$ energies / evals are unaffected.

(3) Covariant derivatives transform nicely.

$$D_t\psi \to e^{iq\alpha/\hbar}D_t\psi, \qquad D_i\psi \to e^{iq\alpha/\hbar}D_i\psi.$$

4.2 Landau levels

need $\underline{A}$.

Solve Schr. eqn in a simple situation.

Consider $\underline{B} = (0, 0, B)$, B const.

$$\underline{B} = \nabla \times \underline{A} \xrightarrow[\text{gauge}]{\text{choice of}} \underline{A} = (0, xB, 0) \quad \left(\begin{matrix}\text{Landau}\\ \text{gauge}\end{matrix}\right)$$

In this gauge, Hamiltonian is

$$H = \frac{1}{2m}\left(p_x^2 + (p_y - qBx)^2 + p_z^2\right)$$

We want to determine wavef^n and energy evals.

$$[p_z, H] = 0, \quad [p_y, H] = 0.$$

$\Rightarrow$ evals of $p_{z,y}$ are good choice, but

$$[p_x, H] \neq 0.$$

$$\Rightarrow \quad \psi(x) = e^{ik_y y} e^{ik_z z} \chi(x).$$

$$p_y \psi = \hbar k_y \psi, \quad p_y = -i\hbar \partial_y$$

$$p_z \psi = \hbar k_z \psi. \quad p_z = -i\hbar \partial_z.$$

Replace ψ in Hamiltonian

$$H\psi = E\psi$$

$$\Rightarrow \frac{1}{2m}\left(p_x^2 + (\hbar k_y - qBx)^2 + \hbar^2 k_z^2\right)\psi = E\psi.$$

Rewrite as

$$\hat{H}\chi = E\chi.$$

with $\hat{H} = \frac{1}{2m}p_x^2 + \frac{m\omega_B^2}{2}(x - k_y l_B^2)^2$, and

Harmonic oscillator w/ centre shifted

$$\omega_B = \frac{qB}{m} \quad \text{cyclotron frequency}$$

$$l_B^2 = \frac{\hbar}{qB} \quad \text{magnetic length.}$$

Therefore, we have

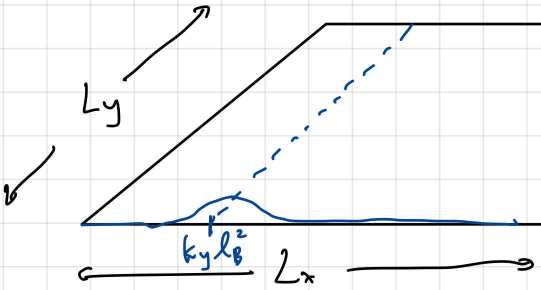
$$E = \underbrace{\hbar\omega_B\left(n+\tfrac{1}{2}\right)}_{\text{Landau levels}} + \frac{\hbar^2 k_z^2}{2m} \quad , n=0,1,2,\dots$$

Up to normalisation,

$$\chi(x) = \underset{\uparrow\ \text{Hermite poly.}}{H_n}\left(x-k_y l_B^2\right) e^{-(x-k_y l_B^2)^2/2l_B}$$

Important to note $E(n,k_z)$ indpt of k_y $\Rightarrow$ big degeneracy

Quantify this degeneracy. For simplicity, $k_z=0$. Place the sys. on a square.



Wavef^n extends in y. localises in x.

L_y finite $\Rightarrow$ $k_y = \frac{2\pi}{L_y} n$, $n \in \mathbb{Z}$.

L_x finite $\Rightarrow$ localise around $k_y l_B^2$. We can only have $0 \leq k_y \leq \frac{L_x}{l_B^2}$.

Combine both statements

$$\Rightarrow \quad 0 < n \leq \frac{L_y L_x}{2\pi l_B^2} = \frac{A}{2\pi l_B^2}.$$

$\Rightarrow$ total no. of states $N = \left\lfloor \frac{qB}{2\pi\hbar} A \right\rfloor$ degeneracy!

This number is huge. if $B \sim 0.1\,\mathrm{T}$, $A \sim 1\,\mathrm{cm}^2 \Rightarrow N \sim 10^{10}$.

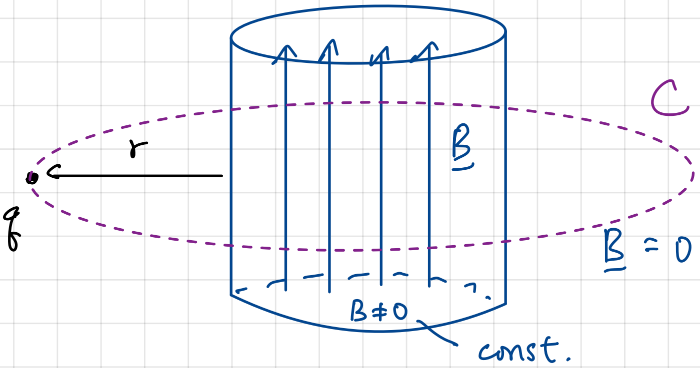
4.3 Aharonov – Bohm effect

Claim A quantum particle can be can be affected by $\underline{A}$ even in regions where $\underline{B} = 0$.

Gauge fields → classical : convenient relabelling that introduces redundancies

Gauge fields → quantum : essential !

To see this, consider the following



Path 1 : Although $\underline{B} = 0$, $\underline{A} \neq 0$ since

$$\oint_C \underline{A} \cdot d\underline{x} = \int \underline{B} \cdot d\underline{S} = BA = \Phi. \quad \text{magnetic flux.}$$

One choice of $\underline{A}$ is

$$\underline{A} = \frac{\Phi}{2\pi r} \hat{\phi} .$$

With this,

$$H = \frac{1}{2m} \left(p_\phi - qA_\phi \right)^2 = \frac{1}{2m} \cdot \frac{1}{r^2} \left(-i\hbar \frac{\partial}{\partial \phi} - \frac{q\Phi}{2\pi} \right)^2 .$$

Eigenstate

$$\psi = \frac{1}{\sqrt{2\pi}} e^{in\phi} , \quad n \in \mathbb{Z}$$

because ψ has to be single valued.

Energy:

$$E = \frac{\hbar^2}{2mr^2} \left(n - \frac{\Phi}{\Phi_0} \right)$$

energy eval affected by choice of $\underline{A}$.

where $\Phi_0 = 2\pi\hbar / q$ is the quantum flux.

Note : If $\boxed{\Phi = n'\Phi_0}$, then energy is not affected.

Path 2 : Isn't this all a gauge artifact?

$$\underline{B} = 0 \Rightarrow \underline{A} = \nabla\alpha = \frac{\Phi}{2\pi r}\hat{\phi}.$$

In this case, $\alpha = \frac{\Phi}{2\pi}\phi$.

$$\Rightarrow \psi \mapsto \psi' = e^{iq\alpha/\hbar}\psi = e^{-i\phi(\Phi/\Phi_0)}\psi.$$

not single valued. unless $\Phi = n'\Phi_0$

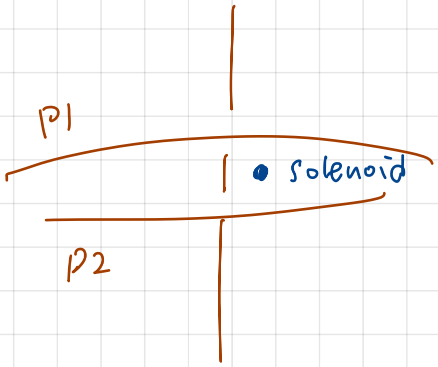
Lesson: two types of gauge trans^n.

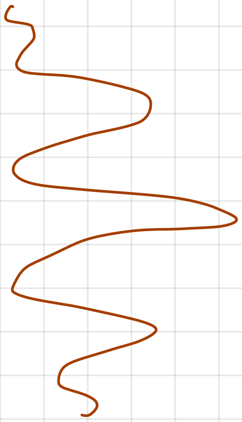
- Trivial — when α smooth and single-valued.
- Large — not single-valued and change the physics.

There is a global condition ψ, which then differentiates between trivial and large gauge trans^n. It is an example where topology enters in QM : when Hamiltonian are smoothly connected or not.

$$H' = U^{-1}HU. \qquad U = e^{iq\alpha/\hbar}.$$

Example Double Slit expt.





Q : Is the interference pattern affected by the solenoid?

A: Particle obeys

$$H\psi = \frac{1}{2m}\left(-i\hbar\nabla - q\underline{A}\right)^2\psi = E\psi.$$

Subject to boundary conditions. Formally,

$$\psi = \exp\left(\frac{iq}{\hbar}\int^{x}\underline{A}(\underline{x}')\cdot d\underline{x}'\right)\tilde{\psi}(\underline{x}).$$

Compare paths P_1 and P_2, the phase difference is

$$\begin{aligned}\Delta\theta &= \frac{q}{\hbar}\int_{P_1}\underline{A}\cdot d\underline{x} - \frac{q}{\hbar}\int_{P_2}\underline{A}\cdot d\underline{x} \\ &= \frac{q}{\hbar}\oint\underline{A}\cdot d\underline{x} \\ &= \frac{q}{\hbar}\int\underline{B}\cdot d\underline{S} = \frac{q\Phi}{\hbar}.\end{aligned}$$

4.4 Magnetic monopoles

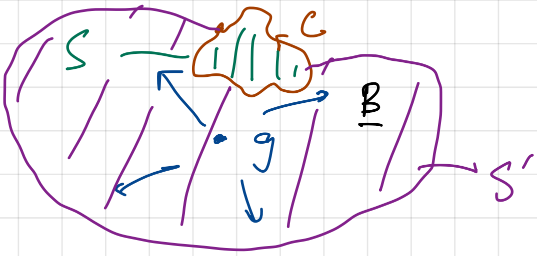
Dreams of a theorist → pretend that magnetic monopole exists, then pretty things happen.

Hypothetical:

$$\underline{B} = \frac{g}{4\pi r^2}\,\hat{\underline{r}} \Rightarrow \int_{S^2}\underline{B}\cdot d\underline{S} = g \quad \text{(magnetic charge/monopole)}$$

This goes against $\nabla\cdot\underline{B} = 0$, $\underline{B} = \nabla\times\underline{A}$.

Still, push this and consider a single magnetic monopole.



$$\psi \longrightarrow e^{iq\alpha/\hbar}\psi.$$

A-B effect: wavef^n changes around loop.

Here, $\alpha = \oint_C \underline{A}\cdot d\underline{x} = \int\underline{B}\cdot d\underline{S} \underset{\substack{\uparrow \\ \text{if } g \text{ exists}}}{=} \frac{\Omega}{4\pi}g$, where Ω is solid angle that supports S.

But now, we could have also done.

$$\alpha' = \int_{S'} \underline{B} \cdot d\underline{S} = -\left(\frac{4\pi - \Omega}{4\pi}\right) g .$$

consistency says $e^{iq\alpha/\hbar} = e^{iq\alpha'/\hbar} \Rightarrow e^{iqg/\hbar} = 1$

$$\Rightarrow \boxed{qg/\hbar = 2\pi n, \quad n \in \mathbb{Z}.} \qquad \text{(Dirac quantisation).}$$

Caution: how can we here have $\underline{B} = \nabla \times \underline{A}$ and $\nabla \cdot \underline{B} \neq 0$?

What's happening is using a singular $\underline{A}$. To see this, consider

$$A_\phi^N = \frac{g}{4\pi r} \frac{1-\cos\theta}{\sin\theta} \Rightarrow \underline{B} = \nabla \times \underline{A}^N = \frac{g}{4\pi r^2} \hat{\underline{r}} .$$

But cheating since singular at $\theta = \pi$.

Try to fix by defining on North hemisphere, and then

$$A_\phi^S = -\frac{g}{4\pi r} \frac{1+\cos\theta}{\sin\theta} \Rightarrow \underline{B} = \nabla \times \underline{A}^S = \frac{g}{4\pi r^2} \hat{\underline{r}} .$$

Still,

$$A_\phi^N = A_\phi^S + \frac{1}{r\sin\theta} \partial_\phi \alpha ,$$

with $\alpha = g\phi/2\pi$. not single valued, hence a large gauge transⁿ. Alternatively, we are seeing an effect of a large g.t.

$$\psi \to e^{iq\alpha/\hbar} \psi \Rightarrow qg = 2\pi n \hbar$$

4.5 Spin in magnetic field

In EM, magnetic fields like to couple to ang. mom.

Force: $\underline{F} = \nabla(\underline{B} \cdot \underline{m})$

Energy: $U = -\underline{B} \cdot \underline{m}$

where $\underline{m}$ is magnetic momentum (dipole expansion)

In currents : $\underline{m} = -\frac{1}{2}\int \underline{r}\times\underline{J}$

point particle : $\underline{m} = -\frac{q}{2}\,\underline{r}\times\underline{v} = \frac{q}{2m}\underline{L}$, $\underline{L}$: ang mom

In QM, have some intrinsic ang. mom. ⇒ spin

For e^-,

$$\underline{S} = \frac{\hbar}{2}\underline{\sigma},$$

where σ_i are Pauli matrices.

In classical mech, $H = -\underline{m}\cdot\underline{B}$.

In QM,

$$H = \underbrace{-g\frac{q}{2m}\underline{S}}_{=\underline{m}}\cdot\underline{B},$$

where we introduce g is coupling between spin and $\underline{B}$ (not magnetic monopole).

In QFT, this term arises "naturally", there

$$\text{electron} : g_e = \underset{\uparrow\atop\text{free } e^-}{2} + \underset{\nwarrow}{\frac{2\alpha}{2\pi}} + \dots = 2.00232.$$

QED, $\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \sim \frac{1}{137}$

proton : $g_p \approx 5.5$

neutron : $g_n \approx -3.8$.

} Differ a lot from 2
⇒ p, n not fund. particles

Spin precession

Consider e^- $q = -e$, $g = 2$, with

$$H = \frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}, \quad \underline{B} = (0,0,B),\ B \text{ const.}$$

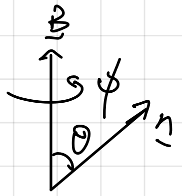
$$= \frac{e\hbar}{2m}\begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix}$$

Estates

$$H|\uparrow\rangle = \frac{\hbar\omega_B}{2}|\uparrow\rangle, \quad H|\downarrow\rangle = -\frac{\hbar\omega_B}{2}|\downarrow\rangle, \quad \omega_B = \frac{eB}{m}.$$

In general, spin of particle might point in $\hat{\underline{n}}$,

$$\hat{\underline{n}} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta)$$



Then

$$|\psi\rangle = e^{i\phi/2}\cos\frac{\theta}{2}\,|\uparrow\rangle + e^{i\phi/2}\sin\frac{\theta}{2}\,|\downarrow\rangle$$

which is an estate of $\hat{\underline{n}}\cdot\underline{\underline{\sigma}}$

Now if we evolve $|\psi\rangle$

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$$

$$\Rightarrow\ |\psi(t)\rangle = e^{i\phi/2}e^{i\omega_B t/2}\cos\frac{\theta}{2}\,|\uparrow\rangle + e^{i\phi/2}e^{-i\omega_B t/2}\sin\frac{\theta}{2}\,|\downarrow\rangle$$

So effect of $\underline{B}$ is to make $|\psi\rangle$ precess.

Last thing: $H = -\underline{m}\cdot\underline{B}$ also has an important effect for hydrogen atom.

$$\underline{m} = \frac{e}{2m}(\underline{L} + g_e\,\underline{S})$$

- proton moving $\Rightarrow$ create $\underline{B}$.
- external $\underline{B}$

$$\Rightarrow\ E_n = -\frac{E_0}{n^2} + \frac{e}{2m}(\underbrace{m_\ell}_{-l,\dots,l} + 2\underbrace{m_s}_{\pm\frac{1}{2}})B \qquad \text{(Zeeman effect)}$$