# Contents

# Chapter 1: PHYS20141 Electromagnetism

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## 1.1 Maxwell's equations

(1) Divergence theorem $\int_V \nabla\cdot\mathbf{v}\,\mathrm{d}V = \int_S \mathbf{v}\cdot\mathrm{d}\mathbf{S}$. Stoke's theorem $\int_S \nabla\times\mathbf{v}\cdot\mathrm{d}\mathbf{S} = \oint_L \mathbf{v}\cdot\mathrm{d}\mathbf{l}$.

(1) $Q = \int\rho(\mathbf{r},t)\mathrm{d}V$, $I = \int\mathbf{j}(\mathbf{r},t)\cdot\mathrm{d}\mathbf{S}$. The conservation of charge $\int_V \dot{\rho}\,\mathrm{d}V = \dot{Q} = -I = -\int_S \mathbf{j}\cdot\mathrm{d}\mathbf{S} = -\int_V \nabla\cdot\mathbf{j}\,\mathrm{d}V \Rightarrow \dot{\rho} + \nabla\cdot\mathbf{j} = 0$.

• Define $\mathbf{j} = \rho\mathbf{v}$, $I = \int\mathrm{d}I = \int\mathbf{j}\cdot\mathrm{d}\mathbf{S} = \int\rho\mathbf{v}\cdot\hat{\mathbf{n}}\,\mathrm{d}S = -nev_{\text{drift}}\int\mathrm{d}S$.

(2) *Gauss' law*. *The flux of electric field through a closed surface $S$ is proportional to the amount of charge in a volume $V$ that the surface encloses.* $\int_S \mathbf{E}\cdot\mathrm{d}\mathbf{S} = \Phi_E = \frac{Q}{\varepsilon_0} = \frac{1}{\varepsilon_0}\int_V \rho\,\mathrm{d}V$. $\int_S \mathbf{E}\cdot\mathrm{d}\mathbf{S} = \int_V \nabla\cdot\mathbf{E}\,\mathrm{d}V \Rightarrow \nabla\cdot E = \frac{1}{\varepsilon_0}\rho$.

(3) No magnetic monopoles. *The flux of magnetic field through any closed surface is zero.* $\int_S \mathbf{B}\cdot\mathrm{d}\mathbf{S} = \Phi_B = 0$. $\nabla\cdot\mathbf{B} = 0$.

(4) *Farady-Lenz law*. *The EMF induced in a closed loop is equal to the rate of change of magnetic flux linked in the loop.* $\mathcal{E} = -\frac{\mathrm{d}}{\mathrm{d}t}\Phi_B$. $\int_L \mathbf{E}\cdot\mathrm{d}\mathbf{l} = \int_S \nabla\times\mathbf{E}\cdot\mathrm{d}\mathbf{S} = -\int_S \dot{\mathbf{B}}\cdot\mathrm{d}\mathbf{S}$. Differential form $\nabla\times\mathbf{E} + \dot{\mathbf{B}} = 0$.

(5) *Ampere's law*. *The circulation of the magnetic field around a closed loop $L$ is proportional to the current passing through the surface that the loop encloses.* $\oint\mathbf{B}\cdot\mathrm{d}\mathbf{l} = \mu_0\sum I_i = \mu_0\int_S \mathbf{j}\cdot\mathrm{d}\mathbf{S}$. Differential form $\nabla\times\mathbf{B} = \mu_0\mathbf{j}$.

• $\nabla\cdot\nabla\times\mathbf{B} = 0 \Rightarrow \nabla\cdot\mathbf{j} = 0 \Rightarrow \dot{\rho} = 0 \Rightarrow$ Only valid for time independent charge density.

(6) *Ampere-Maxwell law*. $\mathbf{j}_{\text{eff}} = \mathbf{j} + \mathbf{j}_{\text{disp}} = \mathbf{j} + \varepsilon_0\dot{\mathbf{E}}$. $\oint_L \mathbf{B}\cdot\mathrm{d}\mathbf{l} = \mu_0\int_S\left(\mathbf{j} + \varepsilon_0\dot{\mathbf{E}}\right)\cdot\mathrm{d}\mathbf{S}$ . Differential form $\nabla\times\mathbf{B} - \mu_0\varepsilon_0\dot{\mathbf{E}} = \mu_0\mathbf{j}$.

(7) $\begin{cases}\int_S \mathbf{E}\cdot\mathrm{d}\mathbf{S} = \frac{1}{\varepsilon_0}\int_V \rho\,\mathrm{d}V \\ \int_S \mathbf{B}\cdot\mathrm{d}\mathbf{S} = 0 \\ \mathcal{E} = -\frac{\mathrm{d}}{\mathrm{d}t}\Phi_B \\ \oint_L \mathbf{B}\cdot\mathrm{d}\mathbf{l} = \mu_0\int_S\left(\mathbf{j} + \varepsilon_0\dot{\mathbf{E}}\right)\cdot\mathrm{d}\mathbf{S}\end{cases}$ $\begin{cases}\nabla\cdot\mathbf{E} = \frac{1}{\varepsilon_0}\rho \\ \nabla\cdot\mathbf{B} = 0 \\ \nabla\times\mathbf{E} + \dot{\mathbf{B}} = 0 \\ \nabla\times\mathbf{B} - \mu_0\varepsilon_0\dot{\mathbf{E}} = \mu_0\mathbf{j}\end{cases}$ sourceless $\begin{cases}\nabla\cdot\mathbf{B} = 0 \\ \nabla\times\mathbf{E} + \dot{\mathbf{B}} = 0\end{cases}$ spatial $\begin{cases}\nabla\cdot\mathbf{E} = \frac{1}{\varepsilon_0}\rho \\ \nabla\cdot\mathbf{B} = 0\end{cases}$ sourced $\begin{cases}\nabla\cdot\mathbf{E} = \frac{1}{\varepsilon_0}\rho \\ \nabla\times\mathbf{B} - \mu_0\varepsilon_0\dot{\mathbf{E}} = \mu_0\mathbf{j}\end{cases}$ time $\begin{cases}\dot{\mathbf{B}} = -\nabla\times\mathbf{E} \\ \dot{\mathbf{E}} = \frac{1}{\mu_0\varepsilon_0}(\nabla\times\mathbf{B} - \mu_0\mathbf{j})\end{cases}$

(8) Ampere's law $\longrightarrow$ charge conservation: $\nabla\cdot\left(\nabla\times\mathbf{B} - \mu_0\varepsilon_0\dot{\mathbf{E}}\right) = -\mu_0\varepsilon_0\nabla\cdot\dot{\mathbf{E}} = -\mu_0\dot{\rho} = \mu_0\nabla\cdot\mathbf{j} \Rightarrow \dot{\rho} = \nabla\cdot\mathbf{j}$.

(9) Time independent form. $\nabla\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0}$, $\nabla\times\mathbf{E} = 0$ (irrotational), $\nabla\cdot\mathbf{B} = 0$, $\nabla\times\mathbf{B} = \mu_0\mathbf{j} \Rightarrow \nabla\cdot\mathbf{j} = 0$ (incompressible).

• Electric fields satisfy $\oint_S \mathbf{E}\cdot\mathrm{d}\mathbf{S} = \frac{Q}{\varepsilon_0}$, $\oint_L \mathbf{E}\cdot\mathrm{d}\mathbf{l} = 0$. $\nabla\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0}$, $\nabla\times\mathbf{E} = 0 \Rightarrow$ Electric field lines end on point charges.

• Magnetic fields satisfy $\oint_S \mathbf{B}\cdot\mathrm{d}\mathbf{S} = 0$, $\oint\mathbf{B}\cdot\mathrm{d}\mathbf{l} = \mu_0\sum I_i$. $\nabla\cdot\mathbf{B} = 0$, $\nabla\times\mathbf{B} = \mu_0\mathbf{j} \Rightarrow$ Magnetic field lines never end.

(10) Set $\mathbf{B} = \nabla\times\mathbf{A}$, $\mathbf{E} = -\nabla\phi \Rightarrow$ Automatically satisfy the sourceless equations $\nabla\cdot\mathbf{B} = 0$ and $\nabla\times\mathbf{E} = 0$.

• $\mathbf{A}' = \mathbf{A} + \nabla\psi$ gives the same magnetic field. The freedom can be removed by setting $\nabla\cdot\mathbf{A} = 0$ (*Coulomb gauge*).

• Substituting into the sourced equations: $\nabla^2\phi = -\frac{\rho}{\varepsilon_0}$, $\nabla^2\mathbf{A} = -\mu_0\mathbf{j}$.

(11) Define the *potential difference* $\mathrm{d}V = \phi(\mathbf{r} + \mathrm{d}\mathbf{l}) - \phi(\mathbf{r}) = \nabla\phi\cdot\mathrm{d}\mathbf{l} = -\mathbf{E}\cdot\mathrm{d}\mathbf{l} \Rightarrow \Delta V_{A\to B} = \int_A^B \mathrm{d}V = -\int_A^B \mathbf{E}\cdot\mathrm{d}\mathbf{l}$.

(12) The magnetic flux $\phi_B = \int_S \mathbf{B}\cdot\mathrm{d}\mathbf{S} = \int_S \nabla\times\mathbf{A}\cdot\mathrm{d}\mathbf{S} = \oint_L \mathbf{A}\cdot\mathrm{d}\mathbf{l}$. $\oint_L \nabla\psi\cdot\mathrm{d}\mathbf{l} = 0 \Rightarrow$ invariant under $\mathbf{A}' = \mathbf{A} + \nabla\psi$.

## 1.2 E, B fields and potentials

(1) $\nabla^2\phi = -\frac{\rho}{\varepsilon_0} \Rightarrow \phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int_V \mathrm{d}V'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$. $\mathbf{E}(\mathbf{r}) = -\nabla_{\mathbf{r}}\phi = \frac{1}{4\pi\varepsilon_0}\int_V \mathrm{d}V'\frac{\rho(\mathbf{r}')(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3}$.

(2) A set of point charges $\rho(\mathbf{r}) = \sum_i q_i\delta^{(3)}(\mathbf{r}-\mathbf{r}_i) \Rightarrow \phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\sum_i\frac{q_i}{|\mathbf{r}-\mathbf{r}_i|}$, $\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\sum_i\frac{q_i(\mathbf{r}-\mathbf{r}_i)}{|\mathbf{r}-\mathbf{r}_i|^3}$.

• For a system with two point charges, $\mathbf{E}_2(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\frac{q_2(\mathbf{r}-\mathbf{r}_2)}{|\mathbf{r}-\mathbf{r}_2|^3}$, $\mathbf{F}_{12} = q_1\mathbf{E}_2(\mathbf{r}_1) = \frac{q_1q_2}{4\pi\varepsilon_0}\frac{\mathbf{r}_1-\mathbf{r}_2}{|\mathbf{r}_1-\mathbf{r}_2|^3} = -\mathbf{F}_{21}$.

(3) $\nabla^2\mathbf{A} = -\mu_0\mathbf{j} \Rightarrow \mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi}\int_V \mathrm{d}V'\frac{\mathbf{j}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$. $\mathbf{B}(\mathbf{r}) = \nabla\times\mathbf{A} = \frac{\mu_0}{4\pi}\int_V \mathrm{d}V'\nabla_{\mathbf{r}}\left(\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right)\times\mathbf{j}(\mathbf{r}') = \frac{\mu_0}{4\pi}\int_V \mathrm{d}V'\frac{\mathbf{j}(\mathbf{r}')\times(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3}$.

• $\mathbf{j}\,\mathrm{d}V = I\,\mathrm{d}\mathbf{l} \Rightarrow \mathbf{B}(\mathbf{r}) = \frac{\mu_0 I}{4\pi}\int\frac{\mathrm{d}\mathbf{l}\times(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3}$ (*Biot-Savart law*).

(4) Define the electric dipole moment $\mathbf{p}(\mathbf{r}) = \int\mathrm{d}V'(\mathbf{r}'-\mathbf{r})\rho(\mathbf{r}')$, for $q_{1,2} = \pm q$ at $\mathbf{r}_{1,2} = \pm\mathbf{a}$, $\mathbf{p}(\mathbf{r}) = 2q\mathbf{a}$.

• $\phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{|\mathbf{r}-\mathbf{a}|} - \frac{1}{|\mathbf{r}+\mathbf{a}|}\right)$. $|\mathbf{r}-\mathbf{a}| = \sqrt{r^2 + a^2 - 2\mathbf{r}\cdot\mathbf{a}} = r\sqrt{1 + \frac{a^2}{r^2} - \frac{2\mathbf{r}\cdot\mathbf{a}}{r^2}} \approx r\sqrt{1 - \frac{2\mathbf{r}\cdot\mathbf{a}}{r^2}}$. $\frac{1}{|\mathbf{r}-\mathbf{a}|} \approx \frac{1}{r}\left(1 + \frac{\mathbf{r}\cdot\mathbf{a}}{r^2}\right) \Rightarrow \phi(\mathbf{r}) \approx \frac{q}{4\pi\varepsilon_0 r}\left[1 + \frac{\mathbf{r}\cdot\mathbf{a}}{r^2} - \left(1 - \frac{\mathbf{r}\cdot\mathbf{a}}{r^2}\right)\right]$
$\Rightarrow \phi(\mathbf{r}) \approx \frac{\mathbf{p}\cdot\hat{\mathbf{r}}}{4\pi\varepsilon_0 r^2}$. $\frac{1}{|\mathbf{r}-\mathbf{a}|^3} \approx \frac{1}{r^3}\left(1 + 3\frac{\mathbf{r}\cdot\mathbf{a}}{r^2}\right) \Rightarrow \mathbf{E}(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0}\left(\frac{\mathbf{r}-\mathbf{a}}{|\mathbf{r}-\mathbf{a}|^3} - \frac{\mathbf{r}+\mathbf{a}}{|\mathbf{r}+\mathbf{a}|^3}\right) = \frac{1}{4\pi\varepsilon_0 r^3}[3(\hat{\mathbf{r}}\cdot\mathbf{p})\hat{\mathbf{r}} - \mathbf{p}]$.

• Example: for $\mathbf{a} = \frac{d}{2}(0,0,1)$, $\mathbf{p} = qd(0,0,1)$, $\hat{\mathbf{r}} = (\sin\theta, 0, \cos\theta) \Rightarrow \phi = \frac{qd\cos\theta}{4\pi\varepsilon_0 r^2}$.

(5) The magnetic dipole moment is defined as $\mathbf{m}(\mathbf{r}) = \frac{I}{2}\oint(\mathbf{r}'-\mathbf{r})\times\mathrm{d}\mathbf{l}$. $\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi}\frac{\mathbf{m}\times\hat{\mathbf{r}}}{r^2}$. For a closed loop $\mathbf{m} = I\mathbf{a}$.

(6) $\mathbf{B} = \nabla\times\mathbf{A}, \nabla\times\mathbf{E} + \dot{\mathbf{B}} = 0 \Rightarrow \nabla\times\left(\mathbf{E} + \dot{\mathbf{A}}\right) = 0 \Rightarrow$ satisfied by choosing $\mathbf{E} + \dot{\mathbf{A}} = -\nabla\phi \Rightarrow \mathbf{E} = -\dot{\mathbf{A}} - \nabla\phi$.

(7) Gauge freedom $\begin{cases}\phi\to\phi' = \phi - \dot{\Psi} \\ \mathbf{A}\to\mathbf{A}' = \mathbf{A} + \nabla\Psi\end{cases}$. $\mathbf{E}' = -\dot{\mathbf{A}}' - \nabla\phi' = -(\dot{\mathbf{A}} + \nabla\dot{\Psi}) - \nabla\left(\phi - \dot{\Psi}\right) = -\dot{\mathbf{A}} - \nabla\phi = \mathbf{E}$.

• Fixing the gauge. *Lorenz gauge* $\frac{1}{c^2}\dot{\phi} + \nabla\cdot\mathbf{A} = 0$. *Coulomb gauge* $\nabla\cdot\mathbf{A} = 0$.

• $\frac{1}{c^2}\dot{\phi}' + \nabla\cdot\mathbf{A}' = \frac{1}{c^2}\dot{\phi} + \nabla\cdot\mathbf{A} - \left(\frac{1}{c^2}\ddot{\Psi} - \nabla^2\Psi\right) = 0 \Rightarrow \frac{1}{c^2}\ddot{\Psi} - \nabla^2\Psi = \frac{1}{c^2}\dot{\phi} + \nabla\cdot\mathbf{A} \Rightarrow \Psi$ can be found to satisfy the Lorenz gauge.

(8) In Lorenz gauge, $\nabla\cdot\mathbf{E} = -\nabla\cdot\left(\nabla\phi + \dot{\mathbf{A}}\right) = -\nabla^2\phi - \nabla\cdot\dot{\mathbf{A}} \xlongequal{\nabla\cdot\mathbf{A}=-1/c^2\dot{\phi}} -\nabla^2\phi + \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = \frac{1}{\varepsilon_0}\rho$.

• $\nabla\times\mathbf{B} - \mu_0\varepsilon_0\dot{\mathbf{E}} = \nabla\times\nabla\times\mathbf{A} + \mu_0\varepsilon_0\left(\nabla\dot{\phi} + \ddot{\mathbf{A}}\right) = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A} + \mu_0\varepsilon_0\left[(-c^2\nabla(\nabla\cdot\mathbf{A}) + \ddot{\mathbf{A}}\right] = -\nabla^2\mathbf{A} + \frac{1}{c^2}\ddot{\mathbf{A}} = \mu_0\mathbf{j}$.

• Define $\square = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 \Rightarrow \square\phi = \frac{\rho}{\varepsilon_0}, \square\mathbf{A} = \mu_0\mathbf{j}$.

## 1.3 Electromagnetic effects in materials

### 1.3.1 Polarization and electric susceptibility

(1) $I = \frac{V}{R} = \frac{1}{R}\int\mathbf{E}\cdot\mathrm{d}\mathbf{l}$. Define the *conductivity* $\sigma$ by $\sigma\mathrm{d}\mathbf{S} = \frac{1}{R}\mathrm{d}\mathbf{l} \Rightarrow \mathbf{j} = \sigma\mathbf{E}$.

• $\dot{\rho} + \nabla\cdot\mathbf{j} = \dot{\rho} + \sigma\nabla\cdot\mathbf{E} = \dot{\rho} + \frac{\sigma}{\varepsilon_0}\rho = 0 \Rightarrow \rho(\mathbf{r},t) = \rho(\mathbf{r},0)e^{-t/t_R}$, $t_R = \frac{\varepsilon_0}{\sigma}$ is the relaxation time scale for the movement of the conduction electrons to smooth out non-unifomities in the charge density. $t_R \approx 8\times10^{-19}$ s (metal), $8\times10^{3}$ s (insulator).

(2) *Method of images*. Consider a point charge at $(0,0,a)$ above an earthed infinite conducting plane in the $x,y-$plane.

$\Rightarrow \phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0}\left[\frac{1}{|\mathbf{r}-\mathbf{a}|} - \frac{1}{|\mathbf{r}+\mathbf{a}|}\right] = \frac{q}{4\pi\varepsilon_0}\left[\frac{1}{\sqrt{x^2+y^2+(z-a)^2}} - \frac{1}{\sqrt{x^2+y^2+(z+a)^2}}\right]$. $\phi(x,y,0) = 0$.

(3) Consider a parallel place capacitor. Gauss' law: $E_z = \frac{Q}{A\varepsilon_0}$, $\Delta V = E_z d$, *capacitance* $C = \frac{Q}{\Delta V} = \frac{\varepsilon_0 A}{d}$.

• Energy of a parallel plate capacitor $U = \frac{1}{2}\varepsilon_0\int|\mathbf{E}|^2\mathrm{d}V = \frac{1}{2}C(\Delta V)^2$.

(4) Add a material between the plates. Define the *relative permittivity* of the material to be $\varepsilon_r = C/C_{\text{vacuum}}$.

• The class of materials are known as *dielectrics*, which are electrical insulators (low conductivity).

(5) *Polarization* of a material occurs when the constituents of the substance align in some preferred direction.

(6) Potential energy of the dipole $U = -qEd\cos\theta = -\mathbf{p}\cdot\mathbf{E}$. If an electric field is applied to a material:

• Intrisic dipoles will align to minimize energy and elminiate torques.

• Atoms and molecules can be polarized, inducing a dipole moment.

(7) Define a macroscopic vector field, the *polarization* $\mathbf{P}$ [$\mathrm{Cm}^{-2}$] as $\mathbf{P} = n\mathbf{p}$, where $n$ is the density of atoms and $\mathbf{p}$ the average dipole moment. The polarization in general is a function of $\mathbf{E}$. For *linear isotropic material* $\mathbf{P} = \chi_E\varepsilon_0\mathbf{E}$.

(8) When the atoms or molecules have an intrinsic dipole moment $\mathbf{p}_{\text{int}}$, the polarization in an external field $\mathbf{P}_{\text{align}} = \frac{np_{\text{int}}^2}{3k_BT}\mathbf{E}$.

• The *susceptibility* $\chi_E \propto \frac{1}{T}$. At room temperature, $\Delta U_{\max} = 2pE \approx 2\times10^{-4}$ eV $\ll \frac{3}{2}k_BT$. The largest field in air is $\approx 10^6$ $\mathrm{Vm}^{-1}$. The complete alignment will not take place even at large electric field. However the fact that the amount of atoms is large means there will be an observable polarization even at relative low values of the electric field.

(9) When a material does not have intrinsic dipoles, the external field will induce dipoles.

• If the external field causes an offset $d$ for a distribution of radius $R_0$, $qE_{\text{ext.}} = \frac{q^2}{4\pi\varepsilon_0 d^2}\frac{d^3}{R_0^3} \Rightarrow qd = 4\pi\varepsilon_0 R_0^3 E_{\text{ext.}}$.

$\Rightarrow \mathbf{P}_{\text{induced}} = n\alpha\varepsilon_0\mathbf{E}$, where $\alpha \equiv 4\pi R_0^3 \Rightarrow \mathbf{P} = \mathbf{P}_{\text{align}} + \mathbf{P}_{\text{induced}} = n\varepsilon_0\left(\alpha + \frac{p_{\text{int}}^2}{3k_BT\varepsilon_0}\right)\mathbf{E}$.

• Consider $\mathbf{P} = P_x(x)\hat{\mathbf{i}}$, $P_x > 0$. $\Delta Q = -[P_x(x+\delta x) - P_x(x)]\delta y\delta z \approx -\frac{\partial P_x}{\partial x}\delta x\delta y\delta z \Rightarrow \rho_{\text{bound}} = -\frac{\partial P_x}{\partial x}$. In 3D, $\rho_{\text{bound}} = -\nabla\cdot\mathbf{P}$.

• $Q_{\text{bound}} = \int_V\rho_{\text{bound}}\mathrm{d}V + \int_S\sigma\mathrm{d}S = 0$, $\int_V\nabla\cdot\mathbf{P}\mathrm{d}V = \int_S\mathbf{P}\cdot\hat{\mathbf{n}}\mathrm{d}S = \int_S\sigma\mathrm{d}S \Rightarrow \sigma_P = \mathbf{P}\cdot\hat{\mathbf{n}}$.

(10) $\nabla\cdot\mathbf{E} = \frac{1}{\varepsilon_0}\rho = \frac{1}{\varepsilon_0}(\rho_{\text{bound}} + \rho_{\text{free}}) = \frac{1}{\varepsilon_0}(-\nabla\cdot\mathbf{P} + \rho_{\text{free}}) \Rightarrow \nabla\cdot(\varepsilon_0\mathbf{E} + \mathbf{P}) = \rho_{\text{free}}$. Define $\mathbf{D} \equiv \varepsilon_0\mathbf{E} + \mathbf{P} \xlongequal[\text{isotropic}]{\text{linear}} (1+\chi_E)\varepsilon_0\mathbf{E} \Rightarrow$ The integral form of Guass' law: $\int_S\mathbf{D}\cdot\mathrm{d}\mathbf{S} = Q_{\text{free}}$.

(11) Consider a parallel plate capacitor with a dielectric. $\sigma_{\text{plate}} = \frac{Q}{A}$, $\int\mathbf{D}\cdot\mathrm{d}\mathbf{S} = D_zA = Q$, $D_z = (1+\chi_E)\varepsilon_0E_z \Rightarrow E_z = \frac{Q}{(1+\chi_E)\varepsilon_0A}$, $P_z = \frac{\chi_EQ}{(1+\chi_E)A}$, $V = E_zd = \frac{Qd}{(1+\chi_E)\varepsilon_0A} \Rightarrow C = \frac{Q}{V} = (1+\chi_E)\frac{\varepsilon_0A}{d} = (1+\chi_E)C_0$. Define the relative permittivity $\varepsilon_r \equiv 1+\chi_E$

$\Rightarrow \mathbf{D} = \varepsilon_r\varepsilon_0\mathbf{E}$. $\sigma_{\text{top}} = \mathbf{P}\cdot\hat{\mathbf{n}}_{\text{top}} = -\frac{\varepsilon_r-1}{\varepsilon_r}\sigma_{\text{plate}}$, $\sigma_{\text{bottom}} = +\frac{\varepsilon_r-1}{\varepsilon_r}\sigma_{\text{plate}}$. $U = \frac{1}{2}CV^2 = \frac{1}{2}\frac{\varepsilon_r\varepsilon_0A}{d}(E_zd)^2 = \frac{1}{2}AdD_zE_z = \frac{1}{2}\int\mathbf{D}\cdot\mathbf{E}\mathrm{d}V$.

(12) Consider the boundary between two regions with $\varepsilon_r^{(1)}$ and $\varepsilon_r^{(2)}$ and with no free charge on the boundary, as $d\to0$

$\Rightarrow 0 = \int\mathbf{D}\cdot\mathrm{d}\mathbf{S} = -D_\perp^{(1)}\delta S + D_\perp^{(2)}\delta S \Rightarrow D_\perp$ is continuous.

(13) Consider a loop which encompasses a boundary, as $d\to0 \Rightarrow \oint\mathbf{E}\cdot\mathrm{d}\mathbf{l} = -E_{//}^{(1)}\delta l + E_{//}^{(2)}\delta l \Rightarrow E_{//}$ is continuous.

• Assume the fields in the regions are $\mathbf{E}^{(1)} = E_1\begin{pmatrix}\sin\theta_1\\ \cos\theta_1\end{pmatrix}$, $\mathbf{E}^{(2)} = E_2\begin{pmatrix}\sin\theta_2\\ \cos\theta_2\end{pmatrix}$. $E_{//}$ being continuous $\Rightarrow E_1\sin\theta_1 = E_2\sin\theta_2$. $D_\perp$ being continuous $\Rightarrow D_1\cos\theta_1 = D_2\cos\theta_2 \Rightarrow \frac{D_1}{E_1}\cot\theta_1 = \frac{D_2}{E_2}\cot\theta_2 \Rightarrow \varepsilon_r^{(1)}\cot\theta_1 = \varepsilon_r^{(2)}\cot\theta_2$.

### 1.3.2 Magnetization and magnetic susceptibility

(1) Consider a solenoid. Ampere's law $\Rightarrow Bl = \int\mathbf{B}\cdot\mathrm{d}\mathbf{l} = Nl\mu_0I \Rightarrow B = \mu_0NI$, $\Phi_B = \int\mathbf{B}\cdot\mathrm{d}\mathbf{S} = \pi r^2\mu_0NI$. $\mathcal{E} = -\frac{\partial\Phi_B}{\partial t} = -L\frac{\partial I}{\partial t}$, which is the definition of the *inductance*. If a magnetic material is added, define the *relative permeability* $\mu_r \equiv \frac{L}{L_{\text{vaccum}}}$.

(2) Define the *magnetization* $\mathbf{M} = n\mathbf{m}$, where $\mathbf{m} = IA\hat{\mathbf{n}}$ is the *average magnetic dipole moment*. $U = -\mathbf{m}\cdot\mathbf{B}$ in external field.

(3) Define the *magnetic susceptibility* $\mathbf{M} = \frac{\chi_B}{\mu_0}\mathbf{B}$ for a linear isotropic medium. $\chi_B < 0$ corresponds to *diamagnetism*, equivalent to induced polarization. $\chi_B < 0$ corresponds to *paramagnetism*, equivalent to alignment polarization.
(4) Consider an electron orbiting a nucleus. $I = \frac{ev}{2\pi r}$, $m = \frac{ev}{2\pi r}\pi r^2 = \frac{e}{2m_e}L$, where $L = m_e v r \Rightarrow \mathbf{m} = -\frac{e}{2m_e}\mathbf{L}$.
• For more than one electrons, $\mathbf{m}_{\text{tot}} = -\frac{e}{2m_e}\sum_i \mathbf{L}_i$. If $\sum_i \mathbf{L}_i = 0$ then there's no intrinsic dipole moment.
• In the absence of an external $\mathbf{B}$ field, the electrostatic force $F = \frac{Ze^2}{4\pi\varepsilon_0 r^2} = m_e\omega_0^2 r \Rightarrow \omega_0 = \sqrt{\frac{Ze^2}{4m_e\pi\varepsilon_0 r^3}}$. With external $\mathbf{B}$ field, $m_e\omega^2 r = \frac{Ze^2}{4\pi\varepsilon_0 r^2} + e\omega r\Delta B \Rightarrow m_e\omega^2 r = m_e\omega_0^2 r + e\omega r\Delta B \Rightarrow \omega^2 - \frac{e\omega}{m_e}\Delta B = \omega_0^2 \Rightarrow \left(\omega - \frac{e\Delta B}{2m_e}\right)^2 \approx \omega_0^2 \Rightarrow \omega \approx \omega_0 + \frac{e}{2m_e}\Delta B$.
• $\omega_L \approx \frac{e}{2m_e}\Delta B$ is the *Larmor frequency*. $\mathbf{m}_{\text{induced}} = -\frac{e}{2m_e}\mathbf{L}_{\text{Larmor}} = -\frac{e^2r^2}{4m_e}\Delta B$. For $Z$ electrons, $\mathbf{m} = -\frac{ne^2Z\langle r^2\rangle}{6m_e}\mathbf{B}$.
(5) If $\sum_i \mathbf{L}_i \neq 0$, there's an intrinsic dipole moment $\mathbf{m}_{\text{int}}$. The imposition of an external field $\mathbf{B}$ will create an alignment $\Rightarrow \mathbf{M} = \frac{nm_{\text{int}}^2}{3k_BT}\mathbf{B}$ (*paramagnetism*). The overall susceptibility $\chi_B = \mu_0 n\left(\frac{m_{\text{int}}^2}{3k_BT} - \frac{Ze^2\langle r^2\rangle}{6m_e}\right)$.
(6) In a magnet, $\mathbf{j}_{\text{bound}} = \nabla\times\mathbf{M}$, $\mathbf{j}_{\text{surface}} = \mathbf{M}\times\hat{\mathbf{n}}$, $\mathbf{j} = \mathbf{j}_{\text{bound}} + \mathbf{j}_{\text{free}}$.
(7) The Ampere's law $\nabla\times\mathbf{B} = \mu_0(\mathbf{j}_{\text{bound}} + \mathbf{j}_{\text{free}}) = \mu_0(\nabla\times\mathbf{M} + \mathbf{j}_{\text{free}})$. Define the magnetic intensity vector $\mathbf{H} \equiv \frac{1}{\mu_0}\mathbf{B} - \mathbf{M}$ $\Rightarrow \nabla\times\mathbf{H} = \mathbf{j}_{\text{free}}$, $\oint_l \mathbf{H}\cdot d\mathbf{l} = I_{\text{free}}$. In mateirals, $\mathbf{M} = \frac{\chi_B}{\mu_0}\mathbf{B}$, $\mathbf{H} = \frac{1-\chi_B}{\mu_0}\mathbf{B}$. The magnetic energy $U = \frac{1}{2}\int \mathbf{B}\cdot\mathbf{H}\,dV$.
• Define the *relative permeability* $\mu_r \equiv \frac{1}{1-\chi_B} \Rightarrow \mathbf{B} = \mu_r\mu_0\mathbf{H}$.
• Consider the solenoid, $\oint \mathbf{H}\cdot d\mathbf{l} = Hl = NlI \Rightarrow H = NI$.
(8) Consider a boundary with no free currents. $\oint \mathbf{H}\cdot d\mathbf{l} = 0 \Rightarrow H_{//}$ continuous. $\int \mathbf{B}\cdot d\mathbf{A} = 0 \Rightarrow B_\perp$ continuous.
(9) In certain magnetic materials, interactions do occur and can lead to the formation of *domains*, where all magnetic moments have the same alignment $\Rightarrow$ *ferromagnetism*. For ferromagnets, $\mathbf{M} = \mathbf{M}(\mathbf{B})$, $\mu_r = \frac{1}{\mu_0}\frac{\partial B}{\partial H}$.
(10) Estimation of magnetization of Fe. Number density of magnetic dipoles $nV = N_A\frac{m}{M} \Rightarrow n = \frac{N_A\rho}{M} \approx 8.4\times10^{28}\ \text{m}^{-3}$. $n\mu_B \approx 8\times10^5\ \text{A}\cdot\text{m}^{-1}$, $|\mathbf{M}| \approx \text{few}\times n\mu_B$, $|\mathbf{B}| \approx \mu_0|\mathbf{M}| \approx \text{few T}$.
(11) *Ideal ferromagnets*: a substance with constant $\mathbf{M}$ (single magnetic domain) $\Rightarrow \nabla\times\mathbf{M} = 0$, no bound currents. $\mathbf{j}_{\text{surface}} = \mathbf{M}\times\hat{\mathbf{n}}$. No free currents: $\nabla\times\mathbf{H} = 0$, $\nabla\cdot\mathbf{H} = -\nabla\cdot\mathbf{M} = \rho_m$. Write $\mathbf{H} = -\nabla\psi \Rightarrow \nabla^2\psi = -\rho_m = \nabla\cdot\mathbf{M} \Rightarrow \psi(\mathbf{r}) = -\frac{1}{4\pi}\int dV'\frac{\nabla_{\mathbf{r}'}\cdot\mathbf{M}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \Rightarrow$ magnetic scalar potential $\psi(\mathbf{r}) = -\frac{1}{4\pi}\nabla\cdot\int dV'\frac{\mathbf{M}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$.
• Consider a uniformly magnetized sphere whose $\mathbf{M} = \begin{cases} M_0\hat{\mathbf{z}}, & r < a \\ \mathbf{0}, & r > a \end{cases} \Rightarrow \psi = \frac{1}{3}M_0\begin{cases} z, & r < a \\ \frac{1}{r^2}a^3\cos\theta, & r > a \end{cases}$.
For $r > a$, $\mathbf{B} = \mu_0\mathbf{H}$. For $r < a$, $\mathbf{H} = -\nabla\psi = -\frac{1}{3}M_0\hat{\mathbf{z}}$, $\mathbf{B} = \mu_0(\mathbf{H}+\mathbf{M}) = \frac{2}{3}\mu_0M_0\hat{\mathbf{z}}$.

## 1.4 Electromagnetic waves

(1) In free sapce, $\nabla\cdot\mathbf{E} = 0$, $\quad \nabla\cdot\mathbf{B} = 0$, $\quad \dot{\mathbf{B}} = -\nabla\times\mathbf{E}$, $\quad \dot{\mathbf{E}} = c^2\nabla\times\mathbf{B}$.
• $\ddot{\mathbf{E}} = c^2\nabla\times\dot{\mathbf{B}} = -c^2\nabla\times(\nabla\times\mathbf{E}) = -c^2\left[\nabla(\nabla\cdot\mathbf{E}) - \nabla^2\mathbf{E}\right] \Rightarrow \frac{1}{c^2}\ddot{\mathbf{E}} - \nabla^2\mathbf{E} = 0$. Similarly, $\frac{1}{c^2}\ddot{\mathbf{B}} - \nabla^2\mathbf{B} = 0$.
• A solution to these wave equations: monochromatic plane waves. $\mathbf{E} = \mathbf{E}_0e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ or $\mathbf{E} = \mathbf{E}_0\cos(\mathbf{k}\cdot\mathbf{r}-\omega t)$, $\omega = \pm ck$.
• For $\mathbf{E} = E_0\hat{\mathbf{x}}\cos(kz-\omega t)$, $\mathbf{B} = \frac{kE_0}{\omega}\hat{\mathbf{y}}\cos(kz-\omega t)$.
(2) Generally for $\mathbf{E} = \mathbf{E}_0e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$, $\nabla\cdot\mathbf{E} = i\mathbf{k}\cdot\mathbf{E}$, $\nabla\times\mathbf{E} = i\mathbf{k}\times\mathbf{E} \Rightarrow -\dot{\mathbf{B}} = \nabla\times\mathbf{E} = i\mathbf{k}\times\mathbf{E} \Rightarrow \mathbf{B} = \frac{\mathbf{k}\times\mathbf{E}_0}{\omega}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$.
• $\mathbf{E}_0\cdot\mathbf{B}_0 = \mathbf{k}\cdot\mathbf{E}_0 = \mathbf{k}\cdot\mathbf{B}_0 = 0$ (mutually orthogonal). $\mathbf{B}_0 = \frac{\mathbf{k}\times\mathbf{E}_0}{\omega}$, $B_0 = \frac{kE_0}{\omega} = \frac{E_0}{c}$. $\mathbf{E}_0\times\mathbf{B}_0 = \frac{E_0^2}{\omega}\mathbf{k} \Rightarrow \hat{\mathbf{k}} = \hat{\mathbf{E}}_0\times\hat{\mathbf{B}}_0$.
• $\mathbf{E}$ and $\mathbf{B}$ are in phase.
(3) The energy density for an EM field $u = \frac{1}{2}\varepsilon_0|\mathbf{E}|^2 + \frac{1}{2\mu_0}|\mathbf{B}|^2$. For plane waves $u = \varepsilon_0E_0^2\left[\Re\left(e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t+\theta)}\right)\right]^2$.
• For plane waves, $\langle u\rangle = \frac{1}{2}\varepsilon_0E_0^2$. Consider the volume covered by a wave in $\Delta t$ through surface $\Delta A$. The average energy density enclosed by this volume $\Delta U_{\text{tot}} = \langle u\rangle c\Delta t\Delta A = \frac{1}{2}\varepsilon_0^2E_0^2c\Delta t\Delta A$. The average flux $\mathcal{F} = \frac{\Delta U_{\text{tot}}}{\Delta t\Delta A} = \frac{E_0^2}{2Z_0}$, $Z_0 \equiv \sqrt{\frac{\mu_0}{\varepsilon_0}} = 377\Omega$.
(4) The rate of change $\dot{u} = \varepsilon_0\mathbf{E}\cdot\dot{\mathbf{E}} + \frac{1}{\mu_0}\mathbf{B}\cdot\dot{\mathbf{B}} = \frac{1}{\mu_0}(\mathbf{E}\cdot\nabla\times\mathbf{B} - \mathbf{B}\cdot\nabla\times\mathbf{E}) = -\nabla\cdot\mathbf{N}$, where the *Poynting vector* $\mathbf{N} = \frac{1}{\mu_0}\mathbf{E}\times\mathbf{B}$.
• $[\mathbf{N}] = \text{W}\cdot\text{m}^{-2}$. $\dot{U} = -\int\nabla\cdot\mathbf{N}\,dV = -\int\mathbf{N}\cdot d\mathbf{S}$.
• For plane wave solutions, $\mathbf{N} = \frac{E_0^2}{Z_0}\hat{\mathbf{k}}\cos^2(\mathbf{k}\cdot\mathbf{r}-\omega t+\theta)$. $N_{\max} = \frac{E_0^2}{Z_0}$, $\langle N\rangle = \frac{E_0^2}{2Z_0}$. In materials $\mathbf{N} = \mathbf{E}\times\mathbf{H}$.
(5) In the presence of current, $\dot{\mathbf{E}} = c^2(\nabla\times\mathbf{B} - \mu_0\mathbf{j}) \Rightarrow \frac{1}{c^2}\ddot{\mathbf{B}} - \nabla^2\mathbf{B} = \mu_0\nabla\times\mathbf{j}$, $\quad \frac{1}{c^2}\ddot{\mathbf{E}} - \nabla^2\mathbf{E} = -\mu_0\frac{\partial\mathbf{j}}{\partial t}$.
• In a conductor, $\mathbf{j} = \sigma\mathbf{E} \Rightarrow \frac{1}{c^2}\ddot{\mathbf{E}} + \mu_0\sigma\dot{\mathbf{E}} = \nabla^2\mathbf{E} \Rightarrow$ damped wave equation. $\mathbf{E} = \mathbf{E}_0\Re\left[e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\right] \Rightarrow -\frac{\omega^2}{c^2} - i\mu_0\sigma\omega = -k^2$.
Define $R = \frac{\mu_0\sigma\omega}{\omega^2/c^2} = \frac{\sigma}{2\pi\varepsilon_0 f}$. For most cases $R \gg 1$, $\frac{\omega^2}{c^2} \ll \mu_0\sigma\omega \Rightarrow k^2 = i\mu_0\sigma\omega = e^{i\pi/2}\mu_0\sigma\omega \Rightarrow k = \pm e^{i\pi/4}\sqrt{\mu_0\sigma\omega}$
$\Rightarrow \mathbf{E} = \mathbf{E}_0e^{-z/\delta}\exp\left[i\left(\sqrt{\frac{\mu_0\sigma\omega}{2}}z - \omega t\right)\right]$, where $\delta = \sqrt{\frac{2}{\mu_0\sigma\omega}}$ is the *skin depth*, the length scale over which the amplitude of an EM wave decays inside a conductor.

(6) *Plasma* is a state of matter which is partially ionised and electrons move under the influence of the electric field, ignoring much weaker magnetic field. $\mathbf{F}_e = m_e\ddot{\mathbf{r}} = -e\mathbf{E}$. $\mathbf{j} = -en_e\dot{\mathbf{r}} \Rightarrow \frac{\partial \mathbf{j}}{\partial t} = \frac{e^2 n_e}{m_e}\mathbf{E} \Rightarrow \frac{1}{c^2}\ddot{\mathbf{E}} + \frac{\mu_0 e^2 n_e}{m_e}\mathbf{E} = \nabla^2\mathbf{E}$.

• Ansatz $\Rightarrow -\frac{\omega^2}{c^2} + \frac{\mu_0 e^2 n_e}{m_e} = -k^2 \Rightarrow ck = \pm\sqrt{\omega^2 - \omega_p^2}$, where $\omega_p^2 = \frac{e^2 n_e}{\varepsilon_0 m_e}$. If $\omega < \omega_p$ the waves don't propagate.

# Chapter 2: PHYS20101 Introduction to Quantum Mechanics

## 2.1 Basic elements of quantum mechanics

### 2.1.1 Wave mechanics and the Schrodinger equation

(1) Plane waves are described by $\Psi(x,t) = Ae^{i(kx-\omega t)}$, where $k = \frac{2\pi}{\lambda}$ is the *wave number*. $\lambda = \frac{h}{p} \Rightarrow k = \frac{2\pi p}{h} = \frac{p}{\hbar}$.
• A particle with kinetic energy $E$ behaves as a wave with angular frequency $\omega = 2\pi\nu = 2\pi\frac{E}{h} = \frac{E}{\hbar}$.
• For a non-relativistic particle $E = \frac{p^2}{2m}$ or $\frac{\hbar^2 k^2}{2m} = \hbar\omega$.
(2) $\frac{\partial^2}{\partial x^2}\Psi = -k^2\Psi,\ \frac{\partial}{\partial t}\Psi = -i\omega\Psi,\ \frac{\hbar^2 k^2}{2m}\Psi = \hbar\omega\Psi \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial\Psi}{\partial t}$ (TDSE in free space).
• If the particle experiences a potential $V(x,t)$, $\frac{p^2}{2m} + V(x,t) = E \Longrightarrow$ *TDSE*: $\left[-\frac{\hbar^2}{2m} + V(x,t)\right]\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$.
• TDSE in 3D: $\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right)\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)$
(3) *Interpretation*: The TDSE is motivated by plane waves. The general solution for $\Psi$ has a wave structure, but does not consist of plane waves in general. We call it the wavefunciton, which fully describes the behaviour of the particle.
• While $\Psi$ is not directly observable, it contains *all the information needed to make a prediction* for any physical observable.
• *Born interpretation*: $|\Psi(x,t)|^2$ is a probability density. $|\Psi|^2 \mathrm{d}x$ is the probability that the particle described by $\Psi$ is between $x$ and $x+\mathrm{d}x$ at time $t$.
• Like any wave, we expect interference $\Rightarrow$ probabilities are not additive, the phase of $\Psi$ matters.
(4) Properties of the wavefunction.
• Normalization: $\int_{\text{space}} |\Psi(\underline{r},t)|^2\, \mathrm{d}V = 1$. $\Psi$ is single-valued, finite everywhere, continuous and smooth. $\Psi$ is fragile.
(5) $\Psi(x,t) = \psi(x)T(t) \Rightarrow \frac{1}{\psi(x)}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi(x)\right) = \frac{i\hbar}{T(t)}\frac{\mathrm{d}T}{\mathrm{d}t} \Rightarrow$ eigenfunction $\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)\psi(x) = E\psi(x)$ (*TISE*).
• In most cases, the form of $V(x)$ and/or the b.c.s imply that it has a set of discrete solutions $\{\psi_i(x)\}$ with $E_i$.
• $i\hbar\frac{\mathrm{d}T}{\mathrm{d}t} = ET(t) \Rightarrow T(t) = Ae^{-iEt/\hbar} \Rightarrow$ General solution of TDSE $\Psi(x,t) = \sum_i A_i\psi_i(x)e^{-iE_i t/\hbar}$.
• If only one $A_n \neq 0$, $|\Psi(x,t)|^2 = \left|A_n\psi_n(x)e^{-iE_n t/\hbar}\right|^2 = |A_n|^2\left|\psi_n(x)\right|^2$. The probability does not chagne with time $\Rightarrow$ The eigenfunctions of the TISE $\psi_i(x)$ are called the *stationary states*.
(6) Infinite square wall $V(x) = \begin{cases} 0, & x \in [0,a] \\ \infty, & x \notin [0,a] \end{cases}$. $-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x) \Rightarrow \psi(x) = A\sin kx + B\cos kx$, with $k^2 = \frac{2mE}{\hbar^2}$
• Boundary conditions $\psi(0) = 0 \Rightarrow B = 0, \psi(a) = 0 \Rightarrow k = \frac{n\pi}{a} \Rightarrow \psi(x) = A\sin\left(\frac{n\pi x}{a}\right)$, $E_n = \frac{1}{2m}\left(\frac{n\pi\hbar}{a}\right)^2, n \geq 1$.
• Zero-point-enery: $n = 1$, $E = \frac{1}{2m}\left(\frac{\pi\hbar}{a}\right)^2$. Uncertainty principle: $\Delta x \sim a$, $\Delta p \sim \frac{\hbar}{a}$, $E \sim \frac{1}{2m}\left(\frac{\hbar}{a}\right)^2$.
(7) Misc: (i) Particles are described by wavefunctions, they exhibit interference, diffraction, etc. (ii) The wavefunctions are solutions of the TDSE, which can be built from solutions to the TISE, each with time dependence given by an oscillating exponential.

### 2.1.2 Operators, Commutators and Compatibility

(1) Hamiltonian operator: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$. Eigenfunctions $\hat{H}\psi_i(x) = E_i\psi_i(x)$ are the stationary states.
(2) The expectation value of a stationary state $\langle E\rangle = E_n\int_{-\infty}^{\infty}\Psi_n(x,t)^*\Psi_n(x,t)\mathrm{d}x = \int_{-\infty}^{\infty}\Psi_n(x,t)^*\hat{H}\Psi_n(x,t)\mathrm{d}x$.
(3) Consider the linear combination of two stationary states $\Psi(x,t) = A_1\psi_1(x)\mathrm{e}^{-iE_1 t/\hbar} + A_2\psi_2(x)\mathrm{e}^{-iE_2 t/\hbar}$
$\Longrightarrow \langle E\rangle = \int_{-\infty}^{\infty}\Psi(x,t)^*\hat{H}\Psi(x,t)\mathrm{d}x = E_1|A_1|^2 + E_2|A_2|^2$ and $\left\langle E^2\right\rangle = \int_{-\infty}^{\infty}\Psi(x,t)^*\hat{H}(\hat{H}\Psi(x,t))\mathrm{d}x = E_1^2|A_1|^2 + E_2^2|A_2|^2$.
• Whatever energy was measured the first time, the same energy is measured the second time.
(4) Measurements: $\hat{A}\psi_n = a_n\psi_n$, $\langle A\rangle = \int\psi^*\hat{A}\psi\mathrm{d}x$.
• If the system is in state $\psi_n$, the measurement of $A$ will always give the value $a_n$
• If the system is in a mixed state $\psi$, the measurement of $A$ gives one of the values $\{a_n\}$ with expectation value $\langle A\rangle$
• After measuring $a_n$, the system is left in state $\psi_n$.
(5) Hermitian conjugate of $\hat{A}: \int\Phi^*\hat{A}^\dagger\Psi\mathrm{d}x = \int(\hat{A}\Phi)^*\Psi\mathrm{d}x$. Hermitian operator: $\hat{A}^\dagger = \hat{A}$.
• All eigenvalues of a Hermitian operator are real. Hermitian operators correspond naturally to physical observables.
• Eigenfunctions of a Hermitian operator with different eigenvalues are orthogonal.
(6) commutator of $\hat{A}$ and $\hat{B}: [\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$.
• If $[\hat{A},\hat{B}] = 0 \Rightarrow \hat{A}\hat{B}\Psi = \hat{B}\hat{A}\Psi$ for any $\Psi \Rightarrow A$ and $B$ can be measured in either order and give the same answer (*compatible*).
• If $[\hat{A},\hat{B}] \neq 0$, $A$ and $B$ are incompatible. Measurements of one affect the other. It is not possible to know both simultaneously and they do not share eigenfunctions.
(7) $[\hat{x},\hat{p}_x] = i\hbar$.

(8) *Uncertainty* of the measurement $(\Delta A)^2 = \left\langle A^2 \right\rangle - \langle A \rangle^2$. *Generalised uncertainty principle* $(\Delta A)(\Delta B) \geq \left| \frac{i}{2} \left\langle [\hat{A}, \hat{B}] \right\rangle \right|$.

## 2.2 Quantum harmonic oscillators and angular momentum

### 2.2.1 Quantum harmonic oscillators

(1) Hamiltonian for 1D QHO $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$. The TISE is $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi$. Boundary conditions: $\psi(\pm\infty) = 0$.

(2) Solutions of 1D QHO: $\psi_n(x) = AH_n\left(\frac{x}{a}\right)\mathrm{e}^{-x^2/2a^2}$, $a = \sqrt{\frac{\hbar}{m\omega}}$, $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$.

• The lowest solution is a Gaussian with no nodes. The $n$th excited level has $n$ nodes. For even/odd $n$, the solutions are even/odd functions.

• The fact that the zero-point energy is non-zero corresponds to the statement that a particle in a potential can never be at rest, since its $x$ position is confined near the bottom of the potential, its momentum values are spread out.

(3) *Diatomic molecules*. As atoms become closer their electron clouds induce dipoles in each other, giving rise to an attractive force. When they are very close together, their electron clouds start to overlap and they repel each other.

• Around equilibrium position, $V(r) \approx V(r_0) + (r - r_0)\frac{\partial V}{\partial r}\Big|_{r=r_0} + \frac{1}{2}(r - r_0)^2 \frac{\partial^2 V}{\partial r^2}\Big|_{r=r_0} = -V_0 + \frac{1}{2}kx^2$.

• In the center-of-mass frame $E = \frac{1}{2}kx^2 + \frac{p^2}{2\mu}$. Expect photons to be absorbed or emitted by molecules at $\omega = \frac{k}{\mu}$.

• Example: CO. Observed frequency of EM radiation from transitions between adjacent vibrational levels in CO is $6.43\times10^{13}$ Hz. $\mu = \frac{m_1 m_2}{m_1 + m_2} = 6.86$ amu $= 1.14\times10^{-26}$ kg. $\omega = 2\pi\nu = 4.04\times10^{14} \sim 0.266$ eV (infrared). $k = \mu\omega^2 = 1860$ Nm$^{-1}$.

(4) Hamiltonian for 2D QHO: $\hat{H} = \hat{H}_x + \hat{H}_y$, $\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$, $\hat{H}_y = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2 y^2$.

(5) TISE for 2D QHO: $-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right) + \frac{1}{2}m\omega^2(x^2 + y^2)\psi(x,y) = E\psi(x,y)$. Eigenvalues $E_{n_x,n_y} = (n_x + n_y + 1)\hbar\omega$.

(6) *Superposition*: $\psi_{10}(x,y)$ and $\psi_{01}(x,y)$ have the same energy $2\hbar\omega$, any linear comb. $a\psi_{10} + b\psi_{01}$ has the same energy.

### 2.2.2 Angular momentum

(1) In classical mechanics, motion in a central potential conserves angular momentum. $\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \mathbf{r}\times\mathbf{F} = 0$, $\mathbf{L} = \mathbf{r}\times\mathbf{p} = $ const.

(2) $\hat{\mathbf{L}} = \hat{\mathbf{r}}\times\hat{\mathbf{p}}$. $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = (-i\hbar)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\phi}$.

(3) Suppose $\psi(r,\phi) = R(r)\Phi(\phi)$. Eigenfunctions of $\hat{L}_z$: $\hat{L}_z\Phi(\phi) = L_z\Phi(\phi) \Rightarrow \Phi(\phi) = \mathrm{e}^{iL_z\phi/\hbar} \xrightarrow{\Phi(\phi+2\pi)=\Phi(\phi)} L_z = m\hbar,\ m\in\mathbb{Z}$.

(4) Consider $\psi_{00} = Ae^{-r^2/2a^2}$ and $\psi_{10} = Ar\cos\phi e^{-r^2/2a^2}$. $\psi_{00}$ is a trivial eigenfunction of $\hat{L}_z$, but $\psi_{10}$, $\psi_{01}$ are not.

(5) Consider $\psi = a\psi_{01} + b\psi_{10}$, $\psi_{10} \pm i\psi_{01}$ is an eigenfunction of $\hat{L}_z$ with eigenvalue $L_z = \pm\hbar$.

(6) $\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right) + \frac{1}{2}m\omega^2 r^2$, $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi} \Rightarrow [\hat{L}_z, \hat{H}] = 0$.

(7) Define $n = n_x + n_y$ and $m$ are *good quantum numbers* for the 2D QHO. They can be known simultaneously and they fully specify the state of the system. An $(n,m)$ pair uniquely describes a state of definite energy $E = (n+1)\hbar\omega$, $L_z = m\hbar$.

(8) $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$, $[\hat{L}^2, \hat{L}_z] = 0$. We can know $|\mathbf{L}|$ and $L_z$ simultaneously, but not $\mathbf{L}$.

(9) The total angular momentum operator $\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta^2}\frac{\partial^2}{\partial\phi^2}\right)$.

(10) The TISE for a particle in a central potential. $\left(-\frac{\hbar^2}{2m} + V(r)\right)\psi = E\psi$.

• $\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \Rightarrow \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\psi + \frac{\hat{L}^2}{2mr^2}\psi + V(r)\psi = E\psi$.

(11) $\left(\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right)\psi = E\psi \Longrightarrow \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\psi + \frac{\hat{L}^2}{2mr^2}\psi + V(r)\psi = E\psi$

(12) $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$. Consider the eigenfunction equation $\hat{L}^2\psi = L^2\psi$ and let $Y$ be the eigenfunction of $\hat{L}^2$.

$\Longrightarrow -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y(\theta,\phi) = L^2 Y(\theta,\phi)$. Let $Y$ to be an eigenfunction of $\hat{L}_z$ as well $\Rightarrow Y(\theta,\phi) = P(\theta)e^{im\phi}$.

$\Longrightarrow -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} - \frac{m^2}{\sin^2\theta}\right)P(\theta) = L^2 P(\theta)$. Define $L^2 = \lambda\hbar^2 \Rightarrow \frac{\mathrm{d}^2 P}{\mathrm{d}\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\mathrm{d}P}{\mathrm{d}\theta} + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)P = 0. \Rightarrow Y(\theta,\phi) = P_l^m(\theta)e^{im\phi}$.

• Eigenvalues $L^2 = \lambda\hbar^2 = l(l+1)\hbar^2$ and $L_z = m\hbar$, $|m| \leq l$. $l$ and $m$ are good quantum numbers.

### 2.2.3 Rotational motion of diatomic molecules

(1) Consider two atoms separated by a distance $r_0$ and are free to rotate around their center of mass.

• $I = m_1\left(\frac{m_2}{m_1+m_2}r_0\right)^2 + m_2\left(\frac{m_1}{m_1+m_2}r_0\right)^2 = \frac{m_1 m_2}{m_1+m_2}r_0^2 = \mu r_0^2$. $L = I\omega$, $E = \frac{1}{2}I\omega^2 = \frac{L^2}{2I} \Rightarrow \hat{H} = \frac{1}{2I}\hat{L}^2 \Rightarrow E_l = \frac{\hbar^2}{2I}l(l+1)$.

(2) For an $H_2$ molecule, $\mu = \frac{m}{2} = 0.84\times10^{-27}$ kg, $r_0 = 0.74$ Å $\Rightarrow \frac{\hbar^2}{2I} = 7.5\times10^{-3}$ eV.

• $E \sim kT \Rightarrow T \sim 90K \Rightarrow$ rotational excited states are populated at room temperature, unlike vibrational states.

• $E \sim$ photon wavelength $\lambda \approx 0.16$ mm (far infrared towards microwaves). $\widetilde{\nu} = \frac{1}{\lambda} = \frac{f}{c} = \frac{E}{hc} = \frac{h}{8\pi^2 cI}l(l+1) = Bl(l+1)$.

## 2.3 One electron atoms

### 2.3.1 The Hydrogen atom

(1) A H atom consists of a single electron in a bound state around a single proton, held together by the Coulomb force.
(2) TDSE: $\left[\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\hat{L}^2}{2mr^2}-\frac{e^2}{4\pi\varepsilon_0 r}\right]\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$.
• $V(r)=-\frac{e^2}{4\pi\varepsilon_0 r}$ is negative corresponds to this being an attractive force and we expect to find bound states.
(3) $\psi(r,\theta,\phi)=R(r)Y_{lm}(\theta,\phi)\Longrightarrow\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{\ell(\ell+1)\hbar^2}{2mr^2}-\frac{e^2}{4\pi\varepsilon_0 r}\right)R(r)Y_{\ell m}(\theta,\phi)=ER(r)Y_{\ell m}(\theta,\phi)$. Write $R(r)=\frac{U(r)}{r}$.
$\Longrightarrow -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2U}{\mathrm{d}r^2}+\frac{\ell(\ell+1)\hbar^2}{2mr^2}U-\frac{e^2}{4\pi\varepsilon_0 r}U=EU$. Define $\rho=\frac{r}{a_0}$, $\widetilde{E}=\frac{E}{E_R}$ with $E_R=\frac{m_e e^4}{2(4\pi\varepsilon_0)^2\hbar^2}=13.6$ eV, $a_0=\frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}=0.53$ Å.

$$\Longrightarrow -\frac{\mathrm{d}^2U}{\mathrm{d}\rho^2}+\frac{l(l+1)}{\rho^2}U-\frac{2}{\rho}U=\widetilde{E}U\begin{cases}\text{For large }\rho,\ -\frac{\mathrm{d}^2U}{\mathrm{d}\rho^2}\approx\widetilde{E}U.\ \text{Define }\widetilde{E}=-b^2\Rightarrow U(\rho)=e^{\pm b\rho}.\ \text{Since }\lim\limits_{\rho\to+\infty}U(\rho)=0,\ U(\rho)\to e^{-b\rho}.\\ \text{For small }\rho.\ -\frac{\mathrm{d}^2U}{\mathrm{d}\rho^2}+\frac{l(l+1)}{\rho^2}\approx 0.\ U(0)=0\Rightarrow\text{try }U(\rho)\sim\rho^\alpha\Rightarrow U(\rho)\to\rho^{l+1}.\end{cases}$$

$\Longrightarrow U(\rho)=\rho^{l+1}e^{-b\rho}f(\rho)$ with $\widetilde{E}=-b^2$. Substitution $\Rightarrow \rho\frac{\mathrm{d}^2f}{\mathrm{d}\rho^2}+2(\ell+1-b\rho)\frac{\mathrm{d}f}{\mathrm{d}\rho}+2(1-b(\ell+1))f=0$.
• Let $f(\rho)=\sum\limits_{k=0}^{\infty}c_k\rho^k\Rightarrow\sum\limits_{k=1}^{\infty}k(k+1)c_{k+1}\rho^k+2(l+1)\sum\limits_{k=0}^{\infty}(k+1)c_{k+1}\rho^k-2b\sum\limits_{k=0}^{\infty}(k+1)c_{k+1}\rho^{k+1}+2[1-b(l+1)]\sum\limits_{k=0}^{\infty}c_k\rho^k=0$.
$\Longrightarrow 2(l+1)(k+1)c_1+2[b(k+l+1)-1]c_0=0$, $[k(k+1)+2(k+1)(l+1)]c_{k+1}=2[b(k+l+1)-1]c_k$. The series doesn't converge.

$$c_{p+1}=0\Longrightarrow b=\frac{1}{l+p+1},\ \widetilde{E}=-\frac{1}{(l+p+1)^2}\Longrightarrow\begin{cases}E=-\frac{E_R}{(l+1)^2}\ \text{described by } p=0\text{th order polynomial and } l=0,1,2,\cdots\\ E=-\frac{E_R}{(l+2)^2}\ \text{described by } p=1\text{th order polynomial and } l=0,1,2,\cdots,\ \text{etc.}\end{cases}$$

• Define a quantum number $n$ such that $E_n=-\frac{E_R}{n^2}$, $n\geq 1$ and $0\leq l\leq n-1$ with a $p=(n-1-l)$th order polynomial.

$$\psi(r,\theta,\phi)=R_{nl}(r)Y_{lm}(\theta,\phi)=\frac{U_{nl}(r)}{r}Y_{lm}(\theta,\phi)$$
$$\propto\left(\frac{r}{a_0}\right)^l e^{-r/na_0}f_{nl}\left(\frac{r}{a_0}\right)Y_{lm}(\theta,\phi)$$

| $n$ | $l=0$ | $l=1$ | $l=2$ |
|---|---|---|---|
| 1 | $e^{-r/a_0}$ | | |
| 2 | $\left(1-\frac{r}{a_0}\right)e^{-r/2a_0}$ | $\frac{r}{a_0}e^{-r/2a_0}$ | |
| 3 | $\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}$ | $\frac{r}{a_0}\left(1-\frac{r}{6a_0}\right)e^{-r/3a_0}$ | $\left(\frac{r}{a_0}\right)^2e^{-r/3a_0}$ |

• Normalization: $\int_0^\infty\mathrm{d}r\int_0^\pi\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi r^2\sin\theta\left|\psi\right|^2=\int_0^\infty\mathrm{d}rr^2|R(r)|^2\times\int_0^\pi\mathrm{d}\theta\sin\theta\int_0^{2\pi}\mathrm{d}\phi|Y_{lm}|^2=\int_0^\infty\mathrm{d}rr^2|R(r)|^2=1$.
(4) Transitions between energy levels: $h\nu=E_R\left(\frac{1}{n'^2}-\frac{1}{n^2}\right)$, $n'<n$.
(5) For ions with the same structure with Hydrogen ($H_e^+, Li^{2+}$) $V(r)=-\frac{Ze^2}{4\pi\varepsilon_0 r}$, $E_n=-\frac{Z^2E_R}{n^2}$.
• Classically, $E_n=-\frac{Z^2E_R}{n^2}\frac{\mu}{m_e}$, where $\mu=\frac{m_eM_N}{m_e+M_n}$. For positronium, $\mu=\frac{m_e}{2}$.

### 2.3.2 Electron spin

(1) *Magnetic moment* $\boldsymbol{\mu}=I\mathbf{A}$, $A=\int_0^{2\pi}\frac{1}{2}r^2\mathrm{d}\theta=\int_0^T\frac{1}{2}r^2\frac{\mathrm{d}\theta}{\mathrm{d}t}\mathrm{d}t=\int_0^T\frac{1}{2}\frac{L}{m_e}\mathrm{d}t=\frac{T}{2m_e}L$. $I=-\frac{e}{T}\Rightarrow\boldsymbol{\mu}=-\frac{e}{2m_e}\mathbf{L}$.
(2) QM: $\hat{\mu}_z=-\frac{e}{2m_e}\hat{L}_z$ with eigenvalues $-\frac{e\hbar}{2m_e}m_l=m_l\mu_B$, where $\mu_B=\frac{e\hbar}{2m_e}$.
(3) Stern-Gerlach: The magnetic moments measured did not fit the pattern predicted by $\mu_z=-\frac{\mu_B}{\hbar}L_z$. In particular, it was found that even electrons in $s$ orbitals ($l=0$) have a magnetic moment $\Rightarrow$ electrons have intrinsic angular momentum.
(4) All electrons have a spin quantum number $s=\frac{1}{2}$, with $S^2=s(s+1)\hbar^2$, $S_z=m_s\hbar$, $m_s=-s,\cdots,s$. $\mu_z=-g_s\mu_Bm_s$.
(5) Define spin wavefunction $\chi_\pm$ to be the eigenfunctions of $\hat{S}_z$, $\hat{S}_z\chi_\pm=\pm\frac{\hbar}{2}\chi_\pm$.
• The Hydrogen wavefunction $\Psi_{n,l,m_l,m_s}=\psi_{n,l,m_l}\chi_{m_s}$. $(n,l,m_l,m_s)$ is the complete set of good quantum numbers.
(6) In quantum mechanics, we cannot know all the components of $\mathbf{L}_1$ or $\mathbf{L}_2$ simultaneously, so we cannot simply add $\mathbf{J}=\mathbf{L}_1+\mathbf{L}_2$. *Angular momentum addition theorem*: states with $l_1$ and $l_2$ combine to give a set of states with $j=l_1+l_2,\cdots,|l_1-l_2|$.

### 2.3.3 First order perturbation theory

(1) Suppose the Hamiltonian of a system $\hat{H}=\hat{H}_0+\hat{V}$ and $\hat{H}_0\psi_n=E_n\psi_n$, where $\{\psi_n\}$ are eigenfunctions. $\hat{V}$ is small.
(2) Suppose $\Phi_n=\psi_n+\sum\limits_{i\neq n}a_i^{(n)}\psi_n$. $\left(\hat{H}_0+\hat{V}\right)\Psi_n=(E_n+\Delta E_n)\Psi_n\Rightarrow\left(\hat{H}_0+\hat{V}\right)\psi_n+\sum\limits_{i\neq n}a_i^{(n)}\left(\hat{H}_0+\hat{V}\right)\psi_i=(E_n+\Delta E_n)\left(\psi_n+\sum\limits_{i\neq n}a_i^{(n)}\psi_i\right)$
$\Longrightarrow E_n\psi_n+\hat{V}\psi_n+\sum\limits_{i\neq n}a_i^{(n)}E_i\psi_i=E_n\psi_n+\Delta E_n\psi_n+E_n\sum\limits_{i\neq n}a_i^{(n)}\psi_i\xrightarrow{\text{orthogonality}}\Delta E_n=\int\psi_n^*\hat{V}\psi_n\,\mathrm{d}^3x$.
(3) Consider $\hat{H}=\hat{H}_{QHO}+\alpha x^4$. $\psi_n(x)=A_nH_n\left(\frac{x}{a}\right)e^{-x^2/2a^2}\Rightarrow\Delta E_n=A_n^2\int\left[H_n\left(\frac{x}{a}\right)\right]^2\alpha x^4e^{-x^2/a^2}\mathrm{d}x$. For $n=0$, $\Delta E_0=\frac{3}{4}\alpha\left(\frac{\hbar}{m\omega}\right)^2$.
• Condition to use P.T.: $\alpha\left(\frac{\hbar}{m\omega}\right)^2\ll\hbar\omega\Rightarrow\alpha\ll\frac{m\omega}{\hbar}k=\frac{k}{a^2}$. Classically if $V(x)=\frac{1}{2}kx^2+\alpha x^4$, $\alpha a^4\ll ka^2\Rightarrow\alpha\ll\frac{k}{a^2}$.

(4) Consider $\hat{H} = \hat{H}_{\rm QHO} + \beta x$. In first order P.T., none of the energy levels are shifted.

### 2.3.4 Spin-orbit interaction

(1) $\hat{H} = \hat{H}_0 + \hat{V}_{\rm S.O.} = \hat{H}_0 + f(r)\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$, $f(r) = \frac{1}{2m_e^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r} = \frac{e^2}{8\pi\varepsilon_0 m_e^2c^2r^3}$.

• Estimate $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} \sim \hbar^2$, $r \sim a_0 \Rightarrow \langle V_{\rm S.O.}\rangle \sim 10^{-3}$ eV, which is much smaller than the spacing between H levels (few eV).

• $[\hat{L}_z, \hat{H}] \neq 0$. $[\hat{\mathbf{J}}^2, \hat{\mathbf{L}}^2] = 0$. $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} \Rightarrow \hat{\mathbf{J}}^2 = \hat{\mathbf{L}}^2 + 2\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} + \hat{\mathbf{S}}^2 \Rightarrow \hat{\mathbf{L}}\cdot\hat{\mathbf{S}} = \frac{1}{2}\left(\hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2\right)$

$\Longrightarrow$ If we are in definite states of $J^2, L^2, S^2 \Rightarrow \left\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right\rangle = \frac{1}{2}(j(j+1) - l(l+1) - s(s+1))\hbar^2$.

• On this basis, $(n, l, j, m_j)$ are good quantum numbers.

(2) Consider the $2s$ and $2p$ states with $l = 0$ or $l = 1 (m_l = -1, 0, 1)$. The $4 \times 2$ states are all degenerate with $E_n = -\frac{E_R}{4}$.

• For $l = 0$, $\left\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right\rangle = 0 \Rightarrow \Delta E = 0$.

• For $l = 1$, $j = \frac{3}{2}$ or $j = \frac{1}{2}$. With $j = \frac{3}{2}$, $\left\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right\rangle = \frac{1}{2}\hbar^2$. With $j = \frac{1}{2}$, $\left\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right\rangle = -\hbar^2$.

• $\Delta E = \left\langle f(r)\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right\rangle = \frac{e^2}{8\pi\varepsilon_0 m_e^2c^2}\left\langle\frac{1}{r^3}\right\rangle\frac{1}{2}(j(j+1) - l(l+1) - s(s+1))\hbar^2 = \frac{E_n^2}{m_ec^2}n\frac{j(j+1)-l(l+1)-s(s+1)}{l(l+\frac{1}{2})(l+1)}$. $\Delta E_2 = 1.51 \times 10^{-5}\text{ eV} \times \begin{cases} +1 \\ 0 \\ -2 \end{cases}$.

### 2.3.5 The strong and weak Zeeman effect

(1) If the magnetic field is strong enough, the spin-orbit interaction is a small correction to the magnetic energy. We can therefore calculate the magnetic energy as a perturbation of the unperturbed hydrogen orbitals.
(2) If the magnetic field is weak enough, the magnetic energy is a small correction to the spin-orbit interaction.

$\Longrightarrow$ Strong Zeeman $\left\langle \hat{V}_{\rm mag}\right\rangle = \mu_B B(m_l + 2m_s)$. Weak Zeeman $\left\langle \hat{V}_{\rm mag}\right\rangle = \mu_B B\left(\left\langle \hat{L}_z\right\rangle + 2\left\langle \hat{S}_z\right\rangle\right)/\hbar = \mu_B B\left(\left\langle \hat{J}_z\right\rangle + \left\langle \hat{S}_z\right\rangle\right)/\hbar$.

• $\left\langle \hat{S}_z\right\rangle = \frac{j(j+1)+s(s+1)-\ell(\ell+1)}{2j(j+1)}m_j\hbar$. $\Rightarrow \left\langle \hat{V}_{\rm mag}\right\rangle = g_L\mu_B B m_j$, where $g_L = 1 + \frac{j(j+1)+s(s+1)-l(l+1)}{2j(j+1)}$.

### 2.3.6 Miscellaneous

(1) Define the parity operator $\hat{P}\psi(\mathbf{r}) = \psi(-\mathbf{r})$. $[\hat{H}, \hat{P}] = 0$, parity is conserved, its eigenvalues are good quantum numbers.

• For Hydrogen, $\psi(\mathbf{r}) = R(r)Y_{lm}(\theta,\phi)$, $\psi(-\mathbf{r}) = R(r)Y_{lm}(\pi-\theta, \phi+\pi) = (-1)^l R(r)Y_{lm}(\theta,\phi) \Rightarrow l$ is even/odd $\Rightarrow \psi(\mathbf{r})$ is even/odd.

(2) *Radiative transitions*. If a hydrogen atom is in an EM field, the separation of the negatively-charged electron from the positively-charged nucleus corresponds to an electric dipole. Define an operator $\hat{\mathbf{d}} = -e\hat{\mathbf{r}}$ as a measurement of this dipole moment. We can think of the interaction of a photon with the atom as a measurement of this dipole moment. The measurement can change the wavefunction and flip it into another state.

• The transition rate $\int \mathrm{d}^3r\psi_f^*(\mathbf{r})\hat{\mathbf{d}}\psi_i(\mathbf{r}) = -e\int \mathrm{d}^3r\psi_f^*(\mathbf{r})\hat{\mathbf{r}}\psi_i(\mathbf{r})$. The result is non-zero only if the transition is between an odd and an even function. Actual transitions can only take place between states that differ only by $\Delta l = 1$.

• There is no single-photon transition from $2s$ to $1s$. The $2s$ state is stable.

## 2.4 Multi-electron atoms

### 2.4.1 Multi-particle wavefunctions

(1) Fundamental particles are all *identical* or *indistinguishable*. Consider a two-electron system, $\left|\psi(\mathbf{r}_1, \mathbf{r}_2)\right|^2 = \left|\psi\mathbf{r}_2, \mathbf{r}_1\right|^2$.

(2) Define the *spin-parity* operator $\hat{P}\psi(\{\mathbf{r}_1, s_1\}, \{\mathbf{r}_2, s_2\}) = \psi(\{\mathbf{r}_2, s_2\}, \{\mathbf{r}_1, s_1\})$. $\hat{P}$ has eigenvalues $\pm 1$ : $\psi(1,2) = \pm\psi(2,1)$.

• Particles that have $\psi(1,2) = +\psi(2,1)$ are called *bosons* ($\gamma$, He). Particles that have $\psi(1,2) = -\psi(2,1)$ are called *fermions*.

(3) Consider a system with single-particle wavefunctions $\psi_\alpha(\mathbf{r})$ and $\psi_\beta(\mathbf{r})$, where $\alpha \neq \beta$ are sets of quantum numbers fully describing the state.

• Two-particle wavefunction $\begin{cases} \psi^{(S)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left[\psi_\alpha(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2) + \psi_\alpha(\mathbf{r}_2)\psi_\beta(\mathbf{r}_1)\right] \\ \psi^{(A)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left[\psi_\alpha(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2) - \psi_\alpha(\mathbf{r}_2)\psi_\beta(\mathbf{r}_1)\right] \end{cases}$

• If $\alpha = \beta$, then $\psi^{(S)}(\mathbf{r}_1, \mathbf{r}_2) = \psi_\alpha(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2)$ is allowed, but $\psi^{(A)}(\mathbf{r}_1, \mathbf{r}_2) = 0$.

(3) *Pauli Exclusion Principle*: Identical fermions are not allowed to be in the same state.

(4) *The Quasi-Independent Particle Approximation*: Each electron's wavefunction is independent, apart from the antisymmetrization due to the fact that electrons are identical fermions.

### 2.4.2 The Helium Atom

(1) The Hamiltonian for He/Li$^+$/Be$^{2+}$: $\hat{H} = \frac{\hat{p}_1^2}{2m_e} + \frac{\hat{p}_2^2}{2m_e} - \frac{Ze^2}{4\pi\varepsilon_0 r_1} - \frac{Ze^2}{4\pi\varepsilon_0 r_2} + \frac{e^2}{4\pi\varepsilon_0 r_{12}} = \hat{H}_1 + \hat{H}_2 + \hat{V}(r_{12})$.

• $\psi^{(S)}(\mathbf{r}_1, \mathbf{r}_2)$ and $\psi^{(A)}(\mathbf{r}_1, \mathbf{r}_2)$ are eigenfunctions of $\hat{H}_1 + \hat{H}_2$ with eigenvalues $E_\alpha + E_\beta$, $E_{\alpha,\beta} = -\frac{Z^2E_R}{n^2}$.

(2) The wavefunction $\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = \psi(\mathbf{r}_1, \mathbf{r}_2)\chi(s_1, s_2)$. Consider the $\chi$ part.

• The total spin of the two electrons $\begin{cases} S=0 \Rightarrow M_S = 0 \Rightarrow \chi^{(A)} = \frac{1}{\sqrt{2}}(\chi_+(1)\chi_-(2) - \chi_-(1)\chi_+(2)) \\ S=1 \Rightarrow M_S = -1,0,+1 \Rightarrow \begin{cases} \chi^{(S)}_{+1} = \chi_+(1)\chi_+(2) \\ \chi^{(S)}_{0} = \frac{1}{\sqrt{2}}(\chi_+(1)\chi_-(2) + \chi_-(1)\chi_+(2)) \\ \chi^{(S)}_{-1} = \chi_-(1)\chi_-(2) \end{cases} \end{cases}$

(3) For $S = 0$. $\chi$ is antisymmetric, so $\psi$ must be symmetric $\Rightarrow$ ground state $\psi^{(S)}_{1s1s}(\mathbf{r}_1,\mathbf{r}_2) = \psi_{1s}(\mathbf{r}_1)\psi_{1s}(\mathbf{r}_2)$. Its energy

$$E = \int d^3r_1 d^3r_2 (\psi^*_{1s}(\mathbf{r}_1)\psi^*_{1s}(\mathbf{r}_2))\big(\hat{H}_1 + \hat{H}_2 + \hat{V}\big)(\psi_{1s}(\mathbf{r}_1)\psi_{1s}(\mathbf{r}_2)) = 2E_{1s} + \frac{e^2}{4\pi\varepsilon_0}\int d^3r_1 d^3r_2 \frac{1}{r_{12}}\left|\psi_{1s}(r_1)\right|^2\left|\psi_{1s}(r_2)\right|^2 \tag{2.1}$$

$$= -2Z^2E_R + \frac{5}{4}ZE_R = -74.8\text{eV}. \tag{2.2}$$

• The last integral is the energy shift due to the classical Coulomb repulsion between two electrons.
• The double-ionization energy of helium is 79.0 eV (1st order P.T. is accurate).
• For $Z = 1$, the $H^-$ ion, $E = -10.2$ eV. This is higher than the ground state energy of the H atom $\Rightarrow$ The ion cannot exist. However, 2nd-order P.T. gives $E = -14.4$ eV and the $H^-$ does exist.
(4) For $S = 1$, $\chi$ is symmetric $\Rightarrow$ $\psi$ is antisymmetric. Electrons can't both be in the $1s$ state. The ground state is $1s2s$.

$$E = \frac{1}{2}\int d^3r_1 d^3r_2 (\psi^*_{1s}(\mathbf{r}_1)\psi^*_{2s}(\mathbf{r}_2) - \psi^*_{2s}(\mathbf{r}_1)\psi^*_{1s}(\mathbf{r}_2))\big(\hat{H}_1 + \hat{H}_2 + \hat{V}\big)(\psi_{1s}(\mathbf{r}_1)\psi_{2s}(\mathbf{r}_2) - \psi_{2s}(\mathbf{r}_1)\psi_{1s}(\mathbf{r}_2)) = E_{1s} + E_{2s} + E_C - E_{\text{ex}}$$

• $E_C = \frac{e^2}{4\pi\varepsilon_0}\int d^3r_1 d^3r_2 \frac{1}{r_{12}}\left|\psi_{1s}(r_1)\right|^2\left|\psi_{2s}(r_2)\right|^2$ is the classical Coulomb repulsion.
• $E_{\text{ex}} = \frac{e^2}{4\pi\varepsilon_0}\int d^3r_1 d^3r_2 \frac{1}{r_{12}}\psi^*_{1s}(\mathbf{r}_1)\psi^*_{2s}(\mathbf{r}_2)\psi^*_{2s}(\mathbf{r}_1)\psi^*_{1s}(\mathbf{r}_2)$ lowers the energy of the ground state. Due to the exclusion principle, the electrons are pushed furthur apart than they would be and results in a lower electrostatic repulsion.
(5) Consider the first excited state of the parahelium ($S = 0$) $\psi^{(S)}_{1s2s}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}(\psi_{1s}(\mathbf{r}_1)\psi_{2s}(\mathbf{r}_2) + \psi_{2s}(\mathbf{r}_1)\psi_{1s}(\mathbf{r}_2))$.
• $E = E_{1s} + E_{2s} + E_C + E_{\text{ex}}$. The parahelium's first excited state is higher than orthohelium's ground state, because electrons spend more time near each other in the symmetric state and thus the Coulomb repulsion is stronger.

### 2.4.3 The Periodic table

(1) Consider the Li atom. The $1s$ orbital has $\langle r\rangle \sim a_0/3$ and the $n = 2$ orbitals have $\langle r\rangle \sim 4a_0$. The *shell model* assumes there is almost no overlap between two levels. The $n = 2$ electron *sees* a total charge $(Z-2)e = 1e$ (an approx. of H atom).
• The Hydrogen wavefunctions $\psi \sim r^l$ for small $r$. In the $2s$ orbital, the electron spends a higher fraction of its time *inside the shell* of the $1s$ electrons. Thus the energy of the $2s$ state is slightly lowered $\Rightarrow$ the 3rd electron occupies the $2s$ orbital.
(2) For atomic number $Z$ = 3-10. Li = (He)$(1s)$, Be = (He)$(1s)^2$, B = (He)$(1s)^2(2p)$, $\cdots$, Ne = (He)$(1s)^2(2p)^6$.
(3) $\sum_m \left|Y_{lm}(\theta,\phi)\right|^2 = \frac{1}{4\pi}$ for all $l \Rightarrow$ A *full* orbital is spherically symmetric.
• For Na, the two $n = 1$ electrons are at $\langle r\rangle \sim a_0/11 \sim 0.1a_0$, the eight $n = 2$ electrons are at $\langle r\rangle \sim \frac{4a_0}{9} \sim 0.4a_0$, the $n = 3$ orbitals have $\langle r\rangle \sim 9a_0$.
(3) For atomic number $Z$ = 11-18. Na = (Ne)$(3s)$, Mg = (Ne)$(3s)^2$, Al = (Ne)$(3s)^2(3p)$, $\cdots$, Ar = (Ne)$(3s)^2(3p)^6$.
(4) As $n$ increases, the energy levels of hydrogen get closer and the advantage of low $l$ orbitals *penetrating* inner shells remains and eventually *wins*. For atomic number $Z$ = 19-30. K = (Ar)$(4s)$, Ca = (Ar)$(4s)^2$, Sc = (Ar)$(4s)^2(3d)$, Ti = (Ar)$(4s)^2(3d)^2$, V = (Ar)$(4s)^2(3d)^3$, Cr = (Ar)$(4s)(3d)^5$, Mn = (Ar)$(4s)^2(3d)^5$, Fe = (Ar)$(4s)^2(3d)^6$, Co = (Ar)$(4s)^2(3d)^7$, Ni = (Ar)$(4s)^2(3d)^8$, Cu = (Ar)$(4s)(3d)^{10}$, Zn = (Ar)$(4s)^2(3d)^{10}$.
(5) A negative exchange energy will give the lowest possible total energy $\Rightarrow$ The lowest energy state has to have an antisymmetric spatial wavefunction $\Rightarrow$ The spin wavefunction must be symmetric.
$\Longrightarrow$ *Hund's rule 1*: The ground state has the highest possible $S$ value.
• Carbon $(2p)^2$: $\uparrow\ \uparrow\ \_\ \ \ \uparrow\ \_\ \uparrow\ \ \ \_\ \uparrow\ \uparrow$ $\Longrightarrow M_L = +1, 0, -1$. Carbon has $S = 1$, $L = 1$.
• Nitrogen $(2p)^3$: $\uparrow\ \uparrow\ \uparrow$ $\Longrightarrow M_L = 0$. Nitrogen has $S = \frac{3}{2}$, $L = 0$.
• Similarly, Oxygen has $S = 1$, $L = 1$. Fluorine has $S = \frac{1}{2}$, $L = 1$. Neon has $S = 0$, $L = 0$.
(6) Electrons with similar momenta spend less time near each other (eg: $m_l = 2, 1$ spend less time than $m_l = 2, -1$).
$\Longrightarrow$ *Hund's rule 2*: The ground state has the highest possible $L$ value.
• Ti (Ar)$(4s)^2(3d)^2$ has $S = 1$ and $L = 3$.
(7) The spin-orbit interaction for a single electron $\propto j(j+1) - l(l+1) - s(s+1) \Rightarrow$ The energy is minimized by taking the smallest possible $j$, $|l-s| \Longrightarrow$ *Hund's rule 3a*: If the orbital is less than half full, the ground state has the lowest possible $J$ value, $|L-S|$.
(8) *Hund's rule 3b*: If the orbital is more than half full, the ground state has the highest possible $J$ value, $L+S$.

## Chapter 3: PHYS 20672 Complex Variables and Vector Spaces

### 3.1 Complex numbers and complex variables

(1) $z = x+iy = r\cos\theta + i\sin\theta = re^{i\theta}$, where $r^2 = x^2+y^2 = (x+iy)(x-iy) = z\bar{z}$.

• *Modulus* of $z$: $r = |z|$. *Argument* of $z$: $\theta = \arctan\left(\frac{y}{x}\right) = \arg z$. $\theta = \mathrm{Arg}z \in (-\pi,\pi]$ is the *principle value* of $\arg z$.

(2) *Region*: A connected open set. eg: $|z| < 1$.

(3) $f(z)$ defines for each $z = x+iy$ in its domain, a new complex number $w = f(z) = u(x,y)+iv(x,y)$.

(4) Functions based on exponentials: $e^z = e^{x+iy} = e^x e^{iy} = e^x\cos y + ie^x \sin y$. $\sin z = \frac{1}{2}\left(e^{iz}-e^{-iz}\right)$, $\cos z = \frac{1}{2}\left(e^{iz}+e^{-iz}\right)$.

(5) Inverse functions and multi-valued functions. If $w = f(z)$, then $z = f^{-1}(w)$.

• $f(z) = z^{\frac{1}{2}} = \left(re^{i\theta}\right)^{\frac{1}{2}} = \left[re^{i(\theta+2\pi k)}\right]^{\frac{1}{2}} = \sqrt{r}e^{i\frac{\theta}{2}}e^{i\pi k} = (-1)^k\sqrt{r}e^{i\frac{\theta}{2}}$.

• $f(z) = z^n$. $f^{-1}(z) = z^{\frac{1}{n}} = \left[re^{i(\theta+2\pi k)}\right]^{\frac{1}{n}} = r^{\frac{1}{n}}e^{i\frac{\theta}{n}}e^{i\frac{2\pi k}{n}} \Rightarrow n$ values functions.

• $f(z) = e^z$. $f^{-1}(z) = \ln z = \ln\left[re^{i(\theta+2\pi k)}\right] = \ln r + i(\theta+2\pi k)$, $k\in\mathbb{Z} \Rightarrow$ Infinitely many values function. Functions defined by different values of $k$ are different branches of $\ln z$. The principle value $\mathrm{Ln}z = \ln r + i\theta = \ln r + i\mathrm{Arg}z$, $\theta\in(-\pi,\pi]$.

(6) Functions of mapping. Consider $w = f(z) = \frac{1}{z}$. $z = x+iy$, $w = u+iv \Rightarrow z = \frac{1}{u+iv} = \frac{u}{u^2+v^2} - i\frac{v}{u^2+v^2}$.

• For $x$ =const, $\frac{u}{u^2+v^2} = x = \text{const} \Rightarrow \left(u-\frac{1}{2x}\right)^2 + v^2 = \left(\frac{1}{2x}\right)^2$.

(7) A function $f(z)$ is *continuous* if a *continuous path* in the the $z-$plane maps to a *continuous path* in the plane of $w = f(z)$.

• Polynomials are continuous.

• $f(z) = \frac{\bar{z}}{z} = \frac{x-iy}{x+iy}$ is not continuous at $z=0$. $\lim\limits_{y=0,x\to 0} = 1$, $\lim\limits_{x=0,y\to 0} = -1$.

(8) *Argument theorem* (for continuous single-valued functions): Consider $w = f(z)$, $f(z_1) = f(z_2) = \cdots = 0$ and $C$ is a path in the $z$ plane. If $n$ zeros are enclosed by $C$, then $\Delta\arg w = \Delta\arg f(z) = 2\pi n$.

(9) *Differentiation*. Define $\frac{\mathrm{d}f}{\mathrm{d}z} = \lim\limits_{\delta z\to 0} = \frac{f(z+\delta z)-f(z)}{\delta z}$. If $\frac{\mathrm{d}f}{\mathrm{d}z}$ exist (independent of how $\delta z\to 0$) at $z$ and in a small neighbourhood of $z$, $f(z)$ is an *analytic function* of $z$. $f(z) = f(x+iy) = u(x,y)+iv(x,y)$, $\mathrm{d}f = \mathrm{d}u + i\,\mathrm{d}v = \left(\frac{\partial u}{\partial x}\mathrm{d}x + \frac{\partial u}{\partial y}\mathrm{d}y\right) + i\left(\frac{\partial v}{\partial x}\mathrm{d}x + \frac{\partial v}{\partial y}\mathrm{d}y\right)$.

$$\mathrm{d}z = \mathrm{d}x + i\,\mathrm{d}y \Longrightarrow \frac{\mathrm{d}f}{\mathrm{d}z} = \begin{cases} \frac{\frac{\partial u}{\partial x}\mathrm{d}x + i\frac{\partial v}{\partial x}\mathrm{d}x}{\mathrm{d}x} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} \\ \frac{\frac{\partial u}{\partial y}\mathrm{d}y + i\frac{\partial v}{\partial y}\mathrm{d}y}{i\,\mathrm{d}y} = \frac{\partial v}{\partial y} - i\frac{\partial u}{\partial y} \end{cases} \Rightarrow \begin{cases} \frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \end{cases} \quad \text{(\textit{Cauchy-Riemann equations})}.$$

• If $\frac{\mathrm{d}f}{\mathrm{d}z}$ exists, $\frac{\mathrm{d}f}{\mathrm{d}z} = \frac{\partial f}{\partial x} = \frac{1}{i}\frac{\partial f}{\partial y}$. If $f$ is analytic, then $\frac{\mathrm{d}f}{\mathrm{d}z}$ and all higher derivatives exist.

• $f(z) = z^n \begin{cases} n\in\mathbb{Z},\ n\geq 0. & z^n \text{ is analytic for any finite } n. \\ n\in\mathbb{Z},\ n<0. & z^n \text{ is analytic except at } z=0. \\ n\in\mathbb{R},\ n\notin\mathbb{Z}. & z^n \text{ is analytic except at } z=0. \end{cases}$ (For $n\in\mathbb{R}$, $n\notin\mathbb{Z}$. The derivative may exist at $z=0$ But doesn't exist throughout a small neightborhood of $z=0$ as a result of $z=0$ is a branch point.)

• $f(z) = e^z = e^x\cos y + ie^x\sin y$ is differentiable and analytic throughout the complex plane.

(10) If $f(z) = u+iv$ is analytic, then $\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$, $\nabla^2 v = 0$. $u$ and $v$ are called *conjugate functions*.

• $f(z) = u+iv$ is analytic, $v(x,y) = 4x^3y - 4xy^3 \Longrightarrow u(x,y) = x^4 = 6x^2y^2 + y^4 + C$, $f(z) = z^4 + C$.

• Analytic functions of $z$ can be written as a function of $z$ alone. eg: $f(z) = |z|^2 = z\bar{z}$ is not analytic.

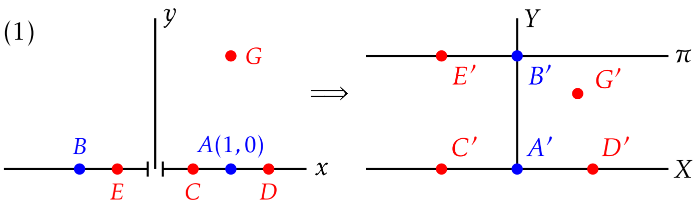
(11) $\nabla u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$, $\nabla v = \left(\frac{\partial v}{\partial x}, \frac{\partial u}{\partial y}\right) \Rightarrow$ For analytic functions, $\nabla u\cdot\nabla v = 0$. For an analytic mapping $w = f(z)$, the contours of $x,y$ =const intersect at right angles. In general, an analytic function $f$ preserves angles if $\frac{\mathrm{d}f}{\mathrm{d}z} \neq 0$.

> *Proof*: Let $f(z)$ be analytic at $z_0$, $w_0 = f(z_0)$, $w_0 + \Delta w = f(z_0+\Delta z)$, $\Delta z = \varepsilon e^{i\theta} \Rightarrow \Delta w = f(z_0+\Delta z) - f(z_0) \approx \Delta z\frac{\mathrm{d}f}{\mathrm{d}z}\Big|_{z_0}$.
> Write $\frac{\mathrm{d}f}{\mathrm{d}z}\Big|_{z_0} = me^{i\alpha}$, then $\Delta w \approx \left(\varepsilon e^{i\theta}\right)\left(me^{i\alpha}\right) = \varepsilon me^{i(\theta+\alpha)}$. So locally $f$ scales $\Delta z$ by $m$ and rotates by $\alpha$.

(12) A sourceless electric field $\mathbf{E} = -\nabla U$, $\nabla\cdot\mathbf{E} = 0 \Rightarrow \nabla^2 U = 0$. $U$ is determined uniquely by the b.c.s

• Consider a pair of infinite conducting plates. $u(x,0) = 0$, $u(x,L) = V_0$, $u(x,y) = \frac{V_0}{L}y$. Define a complex potential $w = u+iv$. choose $v = -\frac{V_0}{L}x$ to make $w$ analytic $\Rightarrow w = -\frac{iV_0}{L}z$.

(13) *General strategy of using conformal mapping to solve the potential*: (i) Define the problem in the $x,y$ plane. (ii) Find a mapping that takes unknown equipotentials to a simpler geometry in the plane $Z = X(x,y)+iY(x,y)$. (iii) Solve by inspection in the $XY$ plane. (iv) $u(x,y)+iv(x,y) = \Phi(X,Y)+i\Psi(x,y)$.

(1)
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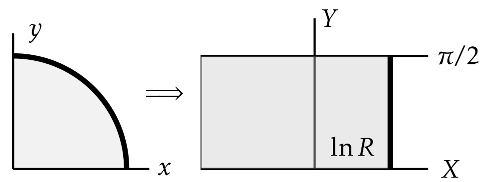
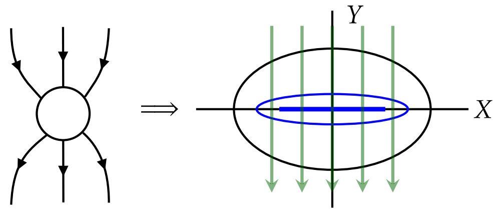
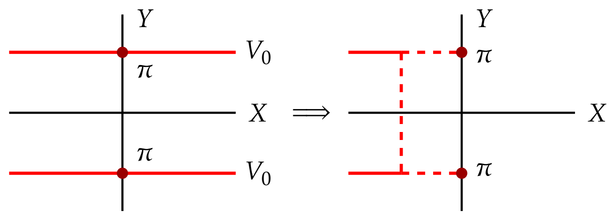



• Consider two conducting semi-plane separated by two small insulators.
Transformation: $Z = \text{Ln}z = \ln|z| + i\text{Arg}z$. Solution in the $XY$ plane: $\Phi + i\Psi = -\frac{iV_0}{\pi}Z = -\frac{iV_0}{\pi}\text{Ln}z = -\frac{iV_0}{\pi}[\ln|z| + i\text{Arg}z]$.
$\Longrightarrow \Phi + i\Psi = -\frac{iV_0}{\pi}\left[\ln\sqrt{x^2+y^2}\right] + i\arctan\left(\frac{y}{x}\right) \Longrightarrow u(x,y) = \frac{V_0}{\pi}\arctan\left(\frac{y}{x}\right)$, $v(x,y) = -\frac{V_0}{2\pi}\ln\left(x^2+y^2\right)$.
• Heat flow: $\frac{\partial u}{\partial t} = D\nabla^2 u$, in the steady state $\nabla^2 u = 0$. $u(x,0) = 0$, $u(0,y) = T_0$. The quarter-circle is insulated.
Transformation: $Z = \text{Ln}z = \ln|z| + i\text{Arg}z \Longrightarrow$ Heat flows along circular arcs.

(3)



(4)



• Conducting cylinder in uniform electric field, $\mathbf{E} = -E\hat{\mathbf{y}}$. $u = 0$ at $|z| = a$. Expect $u = Ey + Eyg(r)$, $\lim_{r\to\infty} g(r) = 0$, $g(a) = -1$.
Inspection: $u = Ey - Ey\frac{a^2}{x^2+y^2} = \Im\left(z + \frac{a^2}{z}\right) = \Re\left[-iE\left(z + \frac{a^2}{z}\right)\right]$. Transformation: $Z = z + \frac{a^2}{z} = X + iY$. Solution $\Phi = -eY$.

For $z = re^{i\theta}$, $Z = \left(r + \frac{a^2}{r}\right)\cos\theta + i\left(r - \frac{a^2}{r}\right)\sin\theta \Rightarrow \begin{cases} X = \left(r + \frac{a^2}{r}\right)\cos\theta = \alpha(r)\cos\theta \\ Y = \left(r - \frac{a^2}{r}\right)\sin\theta = \beta(r)\sin\theta \end{cases} \Rightarrow \left(\frac{X}{\alpha}\right)^2 + \left(\frac{Y}{\beta}\right)^2 = 1.$

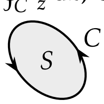
As $r \to a$, $\beta \to 0$, $\alpha \to 2a$. A conducting strip of width $4a$ doesn't affect the uniform field in the $Z$ plane.
• End of parallel plate capacitor. Consider $z = f^{-1}(Z) = Z + e^{-Z}$ for $X \in (-\infty,\infty)$, $Y \in [-\pi,\pi]$.

$z = x + iy = X + iY + e^{X+iY} \Rightarrow \begin{cases} x = X + e^X\cos Y \\ y = Y + e^X\sin Y \end{cases}$. $Y = 0$ maps to $\begin{cases} y = 0 \\ x = X + e^X \end{cases}$, $Y = \pm\pi$ maps to $\begin{cases} y = Y \\ x = X - e^X \end{cases}$.

$\Phi(X,Y) + i\Psi(X,Y) = -i\frac{V_0}{\pi}Z$. Equipotentials $Y = b \Rightarrow x = X + e^X\cos b$, $y = b + e^X\sin b$.

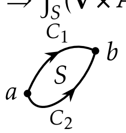
## 3.2 Complex integration

(1) Define points $z_0 = a$, $z_N = b$ to be end points of a path $C$, define $t_k$ to be a point on $C$ between $z_{k-1}$ and $z_k$. $f(z) = u + iv$.
Let $S_N = \sum_{k=1}^{N} f(t_k)(z_k - z_{k-1}) = \sum_{k=1}^{N} f(t_k)\Delta z_k$. Define $\int_C f(z)\,\text{d}z = \lim_{N\to\infty} S_N$. $z_k = x_k + iy_k \Rightarrow S_N = \sum_{k=1}^{N}(u_k + iv_k)(\Delta x_k + i\Delta y_k)$
$\Rightarrow S_N = \sum_{k=1}^{N}(u_k\Delta x_k + iv_k\Delta x_k + iu_k\Delta y_k - v_k\Delta y_k) \Rightarrow \lim_{N\to\infty} S_N = \int_C f(z)\,\text{d}z = \int u\,\text{d}x - \int v\,\text{d}y + i\int v\,\text{d}x + i\int u\,\text{d}y$.
• If we write $\mathbf{dr} = (\text{d}x, \text{d}y)$, $\int_C f(z)\,\text{d}z = \int (u+iv)\,\text{d}x + i(u+iv)\,\text{d}y = \int (f, if)\cdot\mathbf{dr}$.
(2) $\int_0^{1+i} z^2\,\text{d}z$ along $y = x$. $f(z) = z^2 = x^2 - y^2 + 2ixy$, $\text{d}z = \text{d}x + i\,\text{d}x$. $\int_C z^2\,\text{d}z = \int_0^1 (i2x^2)(1+i)\,\text{d}x = \frac{2}{3}(-1+i)$.
(3) $\oint_C \frac{1}{z}\,\text{d}z$, $C$ is a circle centered at the origin. $z = Re^{i\theta}$, $\text{d}z = Rie^{i\theta}\,\text{d}\theta = iz\,\text{d}\theta$. $\oint \frac{1}{z}\,\text{d}z = \int_0^{2\pi} \frac{1}{z} iz\,\text{d}\theta = 2\pi i$.

(4) 

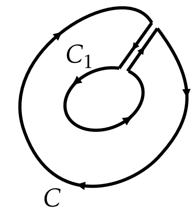
*Cauchy's theorem*: If $f(z)$ is analytic in a region $S$, then $\oint_C f(z)\,\text{d}z = 0$.

> *Proof*: From Stoke's theorem $\oint \mathbf{A}\cdot\text{d}\mathbf{r} = \int (\nabla\times\mathbf{A})\cdot\text{d}\mathbf{S}$. In terms of $\text{d}\mathbf{r} = (\text{d}x, \text{d}y, 0)$, $\text{d}\mathbf{S} = (0, 0, \text{d}x\,\text{d}y)$
> $\Rightarrow \int_S (\nabla\times\mathbf{A})\cdot\text{d}\mathbf{S} = \iint\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\text{d}x\,\text{d}y$. $\oint f(z)\,\text{d}z = \oint (f\,\text{d}x + if\,\text{d}y) = \oint (f, if)\cdot(\text{d}x, \text{d}y) = \iint\left(i\frac{\partial f}{\partial x} - \frac{\partial f}{\partial y}\right)\text{d}x\,\text{d}y = 0$.

• 

Corollary: If $f(z)$ is analytic in $S$, then $\oint_{C_1 - C_2} = \int_{C_1} - \int_{C_2} = 0 \Rightarrow \int_{C_1} = \int_{C_2} \Rightarrow \int_a^b$ is independent of path.

• Converse of Cauchy's theorem: If $\oint_C f(z)\,\text{d}z = 0$ for all closed path in a region $D$, then $f(z)$ is analytic in $D$.
(5) Define $F(z) = \int_a^z f(s)\,\text{d}s$ for paths in region of analyticity of $f$.
• $F(z + \text{d}z) - F(z) = \int_a^{z+\Delta z} f(s)\,\text{d}s - \int_a^z f(s)\,\text{d}s = \int_z^{z+\Delta z} f(s)\,\text{d}s \approx f(z)\Delta z$ (continuity) $\Rightarrow f(z) = \lim_{\Delta z\to 0}\frac{F(z+\text{d}z)-F(z)}{\Delta z} = \frac{\text{d}F}{\text{d}z}$. This also shows that $F(z)$ is analytic: it derivative exits.




• Definite integral: $\int_{z_1}^{z_2} f(z)\,\mathrm{d}z = \int_a^{z_2} f(z)\,\mathrm{d}z - \int_a^{z_1} f(z)\,\mathrm{d}z = F(z_2) - F(z_1)$. Indefinite integral $F(z) = \int f(z)\,\mathrm{d}z$.

• $\int z^n = \frac{z^{n+1}}{n+1} + C$, $\int \frac{1}{z}\,\mathrm{d}z = \ln z + C$ (the path doesn't enclose $z = 0$).

(6) *Path deformation*: If $f$ is analytic between $C$ and $C_1$, then $\oint_C f(z)\,\mathrm{d}z = \oint_{C_1} f(z)\,\mathrm{d}z$. Proof: consider the path

• If there are several regions of non-analyticity, we can deform the path to several loop containing the regions of non-analyticity: $\oint_C = \oint_{C_1} + \oint_{C_2} + \cdots$.

(7) *Cauchy's integral formula*. Let $f(z)$ be analytic on and within a closed path $C$ and $a$ be a point enclosed by $C$. Then

$$f(a) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z-a}\,\mathrm{d}z, \quad f'(a) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-a)^2}\,\mathrm{d}z, \quad f^{(n)}(a) = \frac{n!}{2\pi i}\oint_C \frac{f(a)}{(z-a)^{n+1}}\,\mathrm{d}z$$

> *Proof*: Take $C$ to be circle of radius $\rho$ centered on $a$, so $z = a + \rho e^{i\theta} \Rightarrow \mathrm{d}z = i\rho e^{i\theta}\,\mathrm{d}\theta \Rightarrow \oint_C \frac{f(z)}{z-a}\,\mathrm{d}z = \int_0^{2\pi} \frac{f(a+\rho e^{i\theta})}{\rho e^{i\theta}} i\rho e^{i\theta}\,\mathrm{d}\theta = i\int_0^{2\pi} f(a+\rho e^{i\theta})\,\mathrm{d}\theta \xlongequal{\rho\to 0} i\int_0^{2\pi} f(a)\,\mathrm{d}\theta = 2\pi i f(a)$. $f'(a) = \lim_{\Delta a\to 0} \frac{f(a+\Delta a) - f(a)}{\Delta a} = \lim_{\Delta a\to 0} \frac{1}{\Delta a}\frac{1}{2\pi i}\left[\oint_C \frac{f(z)}{z-a-\Delta a}\,\mathrm{d}z - \oint_C \frac{f(z)}{z-a}\,\mathrm{d}z\right] = \lim_{\Delta a\to 0} \frac{1}{\Delta a}\frac{1}{2\pi i}\oint_C \left[\frac{1}{z-a-\Delta a} - \frac{1}{z-a}\right] f(z)\,\mathrm{d}z = \lim_{\Delta a\to 0}\frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-a-\Delta a)(z-a)}\,\mathrm{d}z = \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-a)^2}\,\mathrm{d}z$.

(8) *Estimation lemma*: If $|f(z)| \le M$ on $C$, then $\left|\int_C f(z)\,\mathrm{d}z\right| \le ML$, where $L$ is the length of $C$.

> *Proof*: $S_N = \left|\sum_{k=1}^N f(t_k)\Delta z_k\right| \le \sum_{k=1}^N |f(t_k)||\Delta z_k| \le \sum_{k=1}^N M|\Delta z_k| \xrightarrow{N\to\infty} \left|\int_C f(z)\,\mathrm{d}z\right| \le ML$.

(9) *Liouville's theorem*: If an analytic function is bounded, $|f(z)| \le M$ for all $z$, then $f$ is constant.

> *Proof*: $f'(a) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-a)^2}\,\mathrm{d}z$, $C$ is a circle of $R$ at $z = a$. $|f'(a)| \le \frac{1}{2\pi}\oint_C \frac{|f(a)|}{R^2}|\mathrm{d}z| \le \frac{1}{2\pi}\frac{m}{R^2} 2\pi R = \frac{m}{R} \xrightarrow{R\to\infty} 0$.

• Any function $f(z)$ that is not constant becomes arbitrary big somewhere in $\mathbb{C}$.

(10) *Fundamental theorem of algebra*. $P_n(z) = c_0 + c_1 z + \cdots + c_n z^n$ has $n$ roots in $\mathbb{C}$.

> If $P_n(z)$ has no roots, then $\frac{1}{P_n(z)}$ is analytic in $\mathbb{C}$ and has some max value $\xrightarrow{\text{Liouville}} \frac{1}{P_n(z)} = \text{const} \Rightarrow$ contradiction.
>
> $\Longrightarrow P_n(z)$ must have at least one root $z_1 \Rightarrow P_n(z) = (z-z_1)P_{n-1}(z) \xRightarrow{\text{repeat...}} P_n(z) = (z-z_1)(z-z_2)\cdots(z-z_n P_0(z)$.

(11) If analytic function $f(z)$ vanishes as $(z-z_0)^n$, $n \in \mathbb{Z}$, we say $f$ has a *zero* of order $n$ and we can write $f(z) = (z-z_0)^n g(z)$, where $g(z)$ is analytic and $g(z_0) \ne 0$. If $f$ is non-analytic at $z_0$, but $h(z) = (z-z_0)^p f(z)$ is analytic and non-zero at $z = z_0$, then $f$ has a *pole* of order $p$ at $z = z_0$. A function that is analytic except at isolated poles is *meromorphic*.

(12) *The argument theorem* $f(z)$ is meromorphic within a closed contour $C$ and analytic and non-zero on $C$, then $\oint_C \frac{f'(z)}{f(z)}\,\mathrm{d}z = 2\pi i(N-P)$, where $N$, $P$ is the sum of orders of zeros/poles of $f$ within C.

> *Proof*: Consider a pole of order $p$ at $z_0$. $f(z) = (z-z_0)^{-p}g(z)$, with $g(z)$ being analytic and non-zero at $z_0$.
> $\Longrightarrow f'(z) = -p(z-z_0)^{p-1}g(z) + (z-z_0)^{-p}g'(z) \Rightarrow \frac{f'(z)}{f(z)} = -\frac{p}{z-z_0} + \frac{g'(z)}{g(z)}$. Consider a loop $C_0$ with radius $\rho$ centered at $z_0$, $\oint_{C_0} \frac{f'}{f}\,\mathrm{d}z = -p\oint_{C_0} \frac{1}{z-z_0}\,\mathrm{d}z + \oint_{C_0} \frac{g'(z)}{g(z)}\,\mathrm{d}z = -2\pi i p$. Similarly for zeors, $\oint_{C_1} \frac{f'}{f}\,\mathrm{d}z = +2\pi i n$.

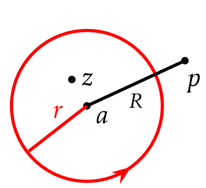
• $\frac{f'}{f} = \frac{\mathrm{d}}{\mathrm{d}z}(\ln f) \Rightarrow \oint \frac{f'(z)}{f(z)}\,\mathrm{d}z = (\ln|f| + i\arg f)\Big|_{\text{begin}}^{\text{end}} = 0 + i\Delta(\arg f)$.

## 3.3 Taylor and Laurent series

(1) If $f(z)$ is analytic within a circle of radius $R$ centered at $z = a$, then for any $z$ such that $|z-a| < R$,

$$f(z) = f(a) + (z-a)f'(a) + \frac{(z-a)^2}{2!}f''(a) + \cdots$$

> *Proof*: Consider a contour $C$ of radius $r$ such that $|z-a| < r < R$.




> $f(z) = \frac{1}{2\pi i}\oint_C \frac{f(s)}{s-z}\,\mathrm{d}s = \frac{1}{2\pi i}\oint_C \frac{f(s)}{(s-a)-(z-a)}\,\mathrm{d}s = 2\pi i\oint_C \frac{f(s)}{(s-a)\left[1-\frac{z-a}{s-a}\right]}\,\mathrm{d}s = \frac{1}{2\pi i}\oint_C \frac{f(s)}{(s-a)(1-t)}$, $t = \frac{z-a}{s-a}$.
>
> $\Rightarrow f(z) = \frac{1}{2\pi i}\oint_C \frac{1}{s-a}\left[\sum_{k=1}^n t^k + \frac{t^{n+1}}{1-t}\right] f(s)\,\mathrm{d}s = \sum_{k=0}^n \frac{1}{2\pi i}(z-a)^k \oint_C \frac{f(s)}{(s-a)^{k+1}}\,\mathrm{d}s + \frac{1}{2\pi i}\oint_C \frac{(z-a)^{n+1}}{(s-a)^{n+1}}\frac{f(s)}{1-\left(\frac{z-a}{s-a}\right)}\,\mathrm{d}s$
>
> $= \sum_{k=0}^n \frac{f^{(k)}(a)}{k!}(z-a)^k + R_n(z,a)$. $|R_n| = \frac{1}{2\pi}\left|\oint_C \frac{(z-a)^{n+1}}{(s-a)^{n+1}} \cdot \frac{f(s)}{s-z}\,\mathrm{d}s\right| \le \frac{1}{2\pi}\frac{|z-a|^{n+1}}{r^{n+1}}\frac{m}{r-|z-a|} \cdot 2\pi r \to 0$

• Expand $f(z)=\frac{1}{z+2}$ about $z=1$. $f'(z)=-\frac{1}{(z+2)^2}$, $f'(1)=-\frac{1}{3^2}$. $f''(z)=\frac{2}{(z+2)^2}$, $f''(1)=\frac{2}{3^3}$. $f(z)=\frac{1}{3}-\frac{1}{3^2}(z-1)+\frac{1}{3^3}(z-1)^2-\cdots$.

• Expand $f(z)=\sin z$ about $z=\frac{\pi}{2}$. $f(z)=1-\frac{1}{2!}\left(z-\frac{\pi}{2}\right)^2+\frac{1}{4!}\left(z-\frac{\pi}{2}\right)^4-\cdots$.

(2) Suppose $f(z)$ is analytic on and between closed contours $C_1$ and $C_2$ with radii $r_1<r_2$, enclosing $z=a$, then

$$f(z)=\sum_{k=1}^{\infty}a_k(z-a)^k+\sum_{k=1}^{\infty}b_k(z-a)^{-k}=\sum_{k=-\infty}^{\infty}a_k(z-a)^k,\text{ where } a_k=\frac{1}{2\pi i}\oint_C\frac{f(s)}{(s-a)^{k+1}}\,\mathrm{d}s,\, b_k=\frac{1}{2\pi i}\oint_C f(s)(s-a)^{k-1}\,\mathrm{d}s.$$

• We can choose $a$ to be an isolated singular point of $f$ (not a branch point). The regular part will converge to the next singularity of $f(z)$. If the principle series terminates at $k=n$, $f(z)$ has a pole of order $n$ at $z=a$. If the series doesn't terminate, then $a$ is called an *essential singularity*.

• Expand $f(z)=\frac{1}{z(1-z)}$ about $z=0$. $f(z)=\frac{1}{z}(1-z)^{-1}=\frac{1}{z}(1+z+z^2+\cdots)=\frac{1}{z}+1+z+z^2+\cdots$.

• Expand $f(z)=\frac{\sin z}{z^3}$ about $z=0$. $f(z)=\frac{1}{z^3}\left(z-\frac{z^3}{6}+\frac{z^3}{120}\right)=\frac{1}{z^2}-\frac{1}{6}+\frac{z^2}{120}-\cdots$.

• Expand $f(z)=e^{1/z}$ about $z=0$. $f(z)=1+\frac{1}{z}+\frac{1}{2}\frac{1}{z^2}+\cdots\Longrightarrow$ Essential singularity at $z=0$.

(3) Consider $f(z)=\frac{1}{\sin z}$. Find and classify its singularities. $\sin z=0$ for $z=n\pi$. Write $z=n\pi+s$, $\sin z=\sin(n\pi+s)=\cos n\pi\sin s=(-1)^n\sin s=(-1)^n\left(s-\frac{1}{6}s^3+\cdots\right)\Rightarrow f(n\pi+s)=\frac{(-1)^n}{s-\frac{1}{6}s^3+\cdots}=\frac{(-1)^n}{s}\left(1-\frac{1}{6}s^2+\cdots\right)^{-1}=\frac{(-1)^n}{s}+\frac{(-1)^n}{6}s+\cdots$ (simple pole).

## 3.4 Residue theorem

(1) The *residue* of $f(z)$ at $z=a$ is the coefficient $b_1$ of the Laurent series of $f$ about $z=a$.

(2) The *residue theorem*. Suppose $f(z)=\sum_{k=0}^{\infty}a_k(z-a)^k+\sum_{k=1}^{\infty}b_k(z-a)^{-k}$, consider the integral around $z=a$, with no other singularities within the contour. $\oint(z-a)^k\,\mathrm{d}z=0$ for $k\neq-1$, $\oint(z-a)^{-1}\,\mathrm{d}z=2\pi i$. Thus $\oint f(z)\,\mathrm{d}z=2\pi i b_1=2\pi i\,\mathrm{res}(a)$. In general, if $f(z)$ has singularities at $z_1,z_2,\cdots$ within $C$, then $\oint f(z)\,\mathrm{d}z=2\pi i\sum_j\mathrm{res}(z_j)$.

(3) Suppose $f(z)$ has a simple pole at $z=a$. Then $g(z)=(z-a)f(z)$ is analytic at $z=a\Rightarrow g(z)=g_0+(z-a)g_1+\cdots$
$\Longrightarrow f(z)=\frac{g_0}{z-a}+g_1+\mathcal{O}(z-a)\Rightarrow b_1=g_0=g(a)=\lim_{z\to a}\{(z-a)f(z)\}$.

(4) Example.

• $\oint_C\frac{z-1}{z(z-2)}\,\mathrm{d}z=\oint_{C_1}\frac{1}{2}\left(\frac{1}{z}+\frac{1}{z-2}\right)\mathrm{d}z+\oint_{C_2}\frac{1}{2}\left(\frac{1}{z}+\frac{1}{z-2}\right)\mathrm{d}z=\frac{1}{2}(2\pi i+0+0+2\pi i)=2\pi i.$ $\left(\text{Using properties of }\oint_C\frac{1}{z}\,\mathrm{d}z\right)$

• $\oint_C\frac{z-1}{z(z-2)}\,\mathrm{d}z=\oint_{C_1}\frac{1}{z}\left(\frac{z-1}{z-2}\right)\mathrm{d}z+\oint_{C_2}\frac{1}{z-2}\left(\frac{z-1}{z}\right)\mathrm{d}z=\oint_{C_1}\frac{f_1}{z-0}\,\mathrm{d}z+\oint_{C_2}\frac{f_2}{z-2}\,\mathrm{d}z=\pi i+\pi i=2\pi i.$ (Cauchy's theorem)

• $\oint_C\frac{z-1}{z(z-2)}\,\mathrm{d}z=2\pi i(\mathrm{res}(0)+\mathrm{res}(2))=2\pi i\left\{\lim_{z\to0}\left(z\frac{z-1}{z(z-2)}\right)+\lim_{z\to2}\left[(z-2)\frac{z-1}{z(z-2)}\right]\right\}=2\pi i\left(\frac{1}{2}+\frac{1}{2}\right)=2\pi i.$ (Residue theorem)

(5) Consider $f(z)=\frac{g(z)}{h(z)}$, $g(a)\neq0$, $h(a)=0$. Expand $h(z)=(z-a)h'(a)+\frac{1}{2}(h-a)^2h''(a)+\cdots$, then $\mathrm{res}(a)=\lim_{z\to a}\left\{\frac{(z-a)g(z)}{(z-a)h'(a)+\frac{1}{2}(z-a)^2h''(a)+\cdots}\right\}$ $=\lim_{z\to a}\frac{g(z)}{h'(a)+\frac{1}{2}(z-a)h''(a)+\cdots}=\frac{g(a)}{h'(a)}$. $\Longrightarrow$ Suppose $f(z)=\frac{g(z)}{h(z)}$, if $z_0$ is a simple zero of $h(z)$, then $\mathrm{res}(f(z_0))=\frac{g(z_0)}{h'(z_0)}$.

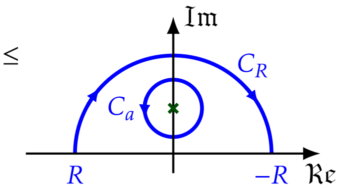
• $f(z)=\frac{1}{\sin z}$, $\mathrm{res}(0)=\lim_{z\to0}\frac{z}{\sin z}=1$. For residues at $z=n\pi$, write $z=n\pi+\varepsilon$, $\sin z=(-1)^n\sin\varepsilon$, $\mathrm{res}(n\pi)=\lim_{z\to n\pi}\frac{(z-n\pi)}{\sin z}=(-1)^n$.
Consider $f(z)=\frac{1}{\sin z}=\frac{g(z)}{h(z)}\Rightarrow\mathrm{res}(n\pi)=\frac{1}{\cos(n\pi)}=(-1)^n$.

(6) Suppose $f(z)$ has pole of order $n$ at $z=a$. Then $g(z)=(z-a)^nf(z)$ is analytic at $z=a$ and has expansion $g(z)=g(a)+(z-a)g'(a)+\cdots+\frac{(z-a)^{n-1}}{(n-1)!}g^{(n-1)}(a)+\cdots\Rightarrow f(z)=\frac{g(z)}{(z-a)^n}=\frac{g(a)}{(z-a)^n}+\cdots+\frac{(z-a)^{-1}}{(n-1)!}g^{(n-1)}(a)+\cdots\Rightarrow\mathrm{res}(a)=\frac{g^{(n-1)(a)}}{(n-1)!}$.

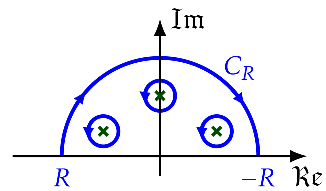
$$\mathrm{res}(a)=\frac{1}{(n-1)!}\lim_{z\to a}\left\{\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}}[(z-a)^nf(z)]\right\}$$

(7) Consider $f(z)=\frac{\ln(1-z)}{(e^z-1)^2}$. $\ln(1-z)=-z-\frac{z^2}{2}-\cdots=z\left(1+\frac{1}{2}z+\cdots\right)$, $e^z-1=z+\frac{z^2}{2!}+\cdots=z\left(1+\frac{1}{2}z+\cdots\right)\Rightarrow(e^z-1)^2=z^2(1+z+\cdots)$.
$\Rightarrow f(z)=-\frac{z\left(1+\frac{1}{2}z+\cdots\right)}{z^2(1+z+\cdots)}=-\frac{1}{z}\left(1+\frac{1}{2}z+\cdots\right)(1-z+\cdots)=-\frac{1}{z}+\frac{1}{2}+\mathcal{O}(z)\Rightarrow$ A simple pole at $z=0$, with residue -1.

## 3.5 Definite integrals




(1) $I=\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{x^2+a^2}=\lim_{R\to\infty}\int_{-R}^{R}\frac{\mathrm{d}x}{x^2+a^2}.\ \int_{-R}^{R}=\oint_{C_a}+\int_{C_R}$. On $C_R$ write $z=Re^{i\theta}$, $\left|\frac{1}{z^2+a^2}\right|\le\frac{1}{|z^2|-a^2}=\frac{1}{R^2-a^2}.\ \left|\oint_{C_R}\frac{\mathrm{d}z}{z^2+a^2}\right|\le\frac{\pi R}{R^2-a^2}\xrightarrow{R\to\infty}0\Rightarrow I=\oint_{C_a}\frac{\mathrm{d}z}{z^2+a^2}=2\pi i\,\mathrm{res}(ia)=\frac{\pi}{a}$.

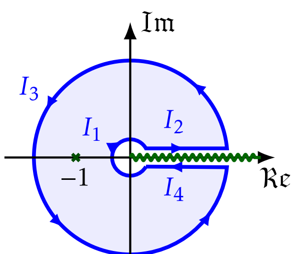



(2) $I=\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{x^6+a^6}=\oint_{C_1}+\oint_{C_2}+\oint_{C_3}=2\pi i\left[\mathrm{res}\left(ae^{i\pi/6}\right)+\mathrm{res}\left(ae^{i\pi/2}\right)+\mathrm{res}\left(ae^{i5\pi/6}\right)\right]=\frac{2\pi}{3a^5}$.

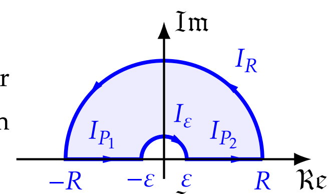
(3) *Fourier integrals*. $I=\int_{-\infty}^{\infty}f(x)e^{ikx}\,\mathrm{d}x$, $k>0$, with $\lim_{z\to\infty}|f(z)|\to 0$ in the upper half plane of $z$. Assume also $f(z)$ is meromorphic in the UHP. Then $I=\lim_{R\to\infty}\int_{-R}^{R}=\lim_{R\to\infty}I_R$. On $C_R$, write $z=Re^{i\theta}$ and suppose that $\left|f\left(Re^{i\theta}\right)\right|\le\varepsilon$ for sufficiently large $R\Rightarrow\left|\int_{C_R}f(z)e^{ikz}\,\mathrm{d}z\right|=\left|\int_{C_R}f\left(Re^{i\theta}\right)e^{ikR(\cos\theta+i\sin\theta)}iRe^{i\theta}\,\mathrm{d}\theta\right|$ $\le\varepsilon R\int_0^{\pi}e^{-kR\sin\theta}\,\mathrm{d}\theta=2\varepsilon R\int_0^{\pi/2}e^{-ikR\sin\theta}\,\mathrm{d}\theta\le 2\varepsilon R\int_0^{\pi/2}e^{-2kR\theta/\pi}=\frac{\varepsilon\pi}{R}\left(1-e^{-kR}\right)\xrightarrow{\varepsilon\to 0,R\to\infty}0.\ \int_{-\infty}^{\infty}f(x)e^{ikz}\,\mathrm{d}x=\oint_{C_1}+\oint_{C_2}+\cdots$.
$\Longrightarrow\int_{-\infty}^{\infty}f(x)e^{ikx}\,\mathrm{d}x=2\pi i(\text{sum of residues from poles in UHP})$, in the condition (i) $k>0$, (ii) $f(z)$ is meromorphic in UHP, (iii) $f(z)\to 0$ for $|z|\to\infty$ in UHP.

- *Jordan's Lemma*: Consider a continuous $g(z)$ defined on a semicircular contour $C_R=\left\{Re^{i\theta}|\theta\in[0,\pi]\right\}$ in the UHP. If the function is of the form $g(z)=f(z)e^{ikz}$ with $k>0$ and $\lim_{|z|\to\infty}f(z)=0$, then $\lim_{R\to\infty}\int_{C_R}f(z)e^{ikz}=0$.
- $I=\int_{-\infty}^{\infty}\frac{e^{ikx}}{x^2+a^2}\mathrm{d}x$, $k>0$, $a>0$. $I=2\pi i(ia)=\frac{e^{-ka}}{2ia}=\frac{\pi}{a}e^{-ka}$. For $k<0$ consider the LHP. $\int_{-\infty}^{\infty}\frac{e^{ikx}}{x^2+a^2}\mathrm{d}x=\frac{\pi}{a}e^{-|k|a}$.

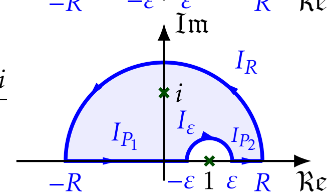
(4) *Integrand with branch point*. Consider $I=\int_0^{\infty}\frac{x^{-\alpha}}{1+x}\mathrm{d}x$, $0<\alpha<1$. $f(z)=\frac{z^{-\alpha}}{1+z}$ has branch point at $z=0$.



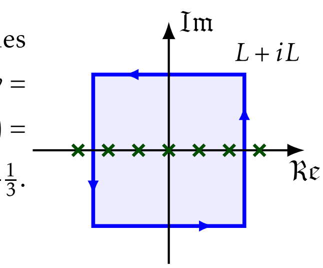

$I_1=\int_{2\pi}^{0}\frac{\varepsilon^{-\alpha}e^{-i\alpha\theta}}{1+\varepsilon e^{i\theta}}i\varepsilon e^{i\theta}\,\mathrm{d}\theta$. $|I_1|\le\frac{\varepsilon^{1-\alpha}}{1-\varepsilon}2\pi\to 0$. $I_3=\int_0^{2\pi}\frac{R^{-\alpha}e^{-i\alpha\theta}}{1+Re^{i\theta}}iRe^{i\theta}\,\mathrm{d}\theta$. $|I_3|\le\frac{R^{1-\alpha}}{R-1}2\pi\sim 2\pi R^{-\alpha}\to 0$. Write $z=xe^{2\pi i}$, $I_4=\int_R^{\varepsilon}\frac{x^{-\alpha}e^{-2\pi i\alpha}}{1+x}\mathrm{d}x=-e^{2\pi i\alpha}\int_{\varepsilon}^{R}\frac{x^{-\alpha}}{1+x}\mathrm{d}x=-e^{2\pi i\alpha}I_2$.
For $R\to\infty$, $\varepsilon\to 0$. $I_1+I_2+I_3+I_4\to I_2+I_4=I_2\left(1-e^{2\pi i\alpha}\right)=2\pi i\,\mathrm{res}(-1)=2\pi i e^{-i\pi\alpha}$.
$\Longrightarrow I_2\left(e^{i\pi\alpha}-e^{-i\pi\alpha}\right)=2i\sin(\pi\alpha)I_1=2\pi i\Longrightarrow I=I_2=\frac{\pi}{\sin\pi\alpha}$.




(5) *Cauchy principle value integrals*. $J=\int_{-\infty}^{\infty}\frac{\sin x}{x}$. The integrand is analytic at $x=0$. Consider $I=\int_{-\infty}^{\infty}\frac{e^{ix}}{x}$ such that $J=\mathfrak{Im}(I)$, where $\int_{-\infty}^{\infty}$ is defined as $\lim_{\varepsilon\to 0}\left(\int_{-\infty}^{-\varepsilon}+\int_{\varepsilon}^{\infty}\right)$. Consider the path integral $I_{P_1}+I_\varepsilon+I_{P_2}+I_R=0$. Jordan's Lemma $\Rightarrow I_R=0$, $I_\varepsilon=\int_\pi^0\frac{e^{i\varepsilon e^{i\theta}}i\varepsilon e^{i\theta}\,\mathrm{d}\theta}{\varepsilon e^{i\theta}}=-i\pi$.
$\Longrightarrow I=I_{P_1}+I_{P_2}=-I_\varepsilon=i\pi$, $J=\mathfrak{Im}(I)=\pi$.




- $I_P=\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{(x-1)(x^2+1)}$. $I_{P_1}+I_{P_2}+I_\varepsilon+I_R=2\pi i\,\mathrm{res}(i)=-\frac{\pi}{2}(1+i)$. $I_R\to 0$, $I_\varepsilon=-\pi i\,\mathrm{res}(1)=-\frac{\pi i}{2}$
$\Longrightarrow I_P=-\frac{\pi}{2}(1+i)+\frac{\pi i}{2}=-\frac{\pi}{2}$.




(6) *Summation of series*. Consider $f(z)=\frac{1}{z^2}\cot z$, which has order-3 pole at $z=0$ and simple poles at $z=n\pi$, $n\ne 0$. For residues at $n\pi, n\ne 0$, write $z=n\pi+w$. $\cot z=\frac{\cos(n\pi+w)}{\sin(n\pi+w)}=\frac{(-1)^n\cos w}{(-1)^n\sin w}=\cot w=\frac{1}{w}-\frac{1}{3}w-\frac{1}{45}w^3+\mathcal{O}(w^5)$. $\frac{1}{z^2}\cot z=\frac{1}{(n\pi+w)^2}\left(\frac{1}{w}-\frac{1}{3}w+\cdots\right)\Rightarrow\mathrm{res}(n\pi)=\lim_{w\to 0}\frac{w}{(n\pi+w)^2}\left(\frac{1}{w}-\frac{1}{3}w+\cdots\right)=\frac{1}{n^2\pi^2}$, $n\ne 0$. For residues at $z=0$, $\frac{1}{z^2}\cot z=\frac{1}{z^2}\left(\frac{1}{z}-\frac{1}{3}z+\mathcal{O}(z^3)\right)=\frac{1}{z^3}-\frac{1}{3z}+\mathcal{O}(z)\Rightarrow\mathrm{res}(0)=-\frac{1}{3}$. Consider a square contour with $L=\left(N+\frac{1}{2}\right)\pi$. On the contour,

$\frac{1}{|z|^2}=\frac{1}{x^2+y^2}\le L^2$. On the vertical side $z=L+iy$, $\cot z=\frac{\cos(L+iy)}{\sin(L+iy)}=\frac{-\sin L\sin(iy)}{\sin L\cos(iy)}=-\tan(iy)=-i\tanh y$
$\Rightarrow|\cot z|=|\tanh z|<1$. Similarly for the vertical side $L-iy$. On the horizontal side $z=x+iL$, $\cot z=\frac{\frac{1}{2}\left[e^{i(x+iL)}+e^{-i(x+iL)}\right]}{\frac{1}{2i}\left[e^{i(x+iL)}-e^{-i(x+iL)}\right]}=$
$i\frac{e^{ix}e^{-L}+e^{-ix}e^{L}}{e^{ix}e^{-L}-e^{-ix}e^{L}}\approx\frac{ie^{-ix}e^{L}}{-e^{-ix}e^{L}}\to -i$ ($e^L\gg e^{-L}$ for $L\to\infty$) $\Longrightarrow\left|\oint\frac{1}{z^2}\cot z\,\mathrm{d}z\right|\le\frac{1}{L^2}\cdot 8L\to 0$. $\oint\frac{1}{z^2}\cot z=\mathrm{res}(0)+\sum_{n\ne 0}\mathrm{res}(n\pi)=2\pi i\left(-\frac{1}{3}+\sum_{n\ne 0}\frac{1}{n^2\pi^2}\right)\Rightarrow$
$\sum_{n\ne 0}\frac{1}{n^2}=\frac{\pi^2}{6}$.

# Chapter 4: PHYS20171 Mathematics of Waves and Fields

## 4.1 Introduction to differential equations

(1) *First-order linear equation* $y' + P(x)y = Q(x)$. Let $I = \int P\mathrm{d}x$, $\frac{\mathrm{d}}{\mathrm{d}x}\left(ye^I\right) = e^I(y + Py) = Qe^I \Rightarrow ye^I = \int Qe^I\mathrm{d}x + C$.

• The Bernoulli equation $y' + P(x)y = Q(x)y^n$. Let $z = y^{1-n}$, $z' = (1-n)y^{-n}y'$. Multiply the equation by $(1-n)y^{-n}$ $\Longrightarrow (1-n)y^n y' + (1-n)Py^{1-n} = (1-n)Q \Rightarrow z' + (1-n)Pz = (1-n)Q \Rightarrow$ linear first order equation.

(2) The differential equation $P(x,y)\mathrm{d}x + Q(x,y)\mathrm{d}y = 0$ or $y' = -\frac{P}{Q}$ is called *exact* if $\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}$. In this case there exists a function $F(x,y)$ such that $P = \frac{\partial F}{\partial x}$, $Q = \frac{\partial F}{\partial y}$, $\mathrm{d}F = P\mathrm{d}x + Q\mathrm{d}y$. The equatoion $P\mathrm{d}x + Q\mathrm{d}y = 0 = \mathrm{d}F \Rightarrow F(x,y) = \text{const}$.

• The equation $x\mathrm{d}y - y\mathrm{d}x = 0$ is not exact. but $\frac{x\mathrm{d}y - y\mathrm{d}x}{x^2} = \mathrm{d}\left(\frac{y}{x}\right) = 0$ is $\Rightarrow \frac{y}{x} = \text{const}$.

(3) A *homogeneous function* of $x$ and $y$ oof degree $n$ means a function which can be written as $x^n f\left(\frac{y}{x}\right)$. An equation of the form $P(x,y)\mathrm{d}x + Q(x,y)\mathrm{d}y = 0$ where $P$ and $Q$ are homogeneous functions of the same degree is called *homogeneous*.
It can be written as $y' = \frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{P(x,y)}{Q(x,y)} = f\left(\frac{y}{x}\right)$. Substitute $v = \frac{y}{x} \Rightarrow x\frac{\mathrm{d}v}{\mathrm{d}x} + v = f(v) \Rightarrow \frac{\mathrm{d}v}{f(v)-v} = \frac{\mathrm{d}x}{x}$ (Separable form).

(4) *Second-order differential equation* $a_2\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + a_1\frac{\mathrm{d}y}{\mathrm{d}x} + a_0 y = 0$.

| Equation | Auxiliary equation | Solution |
|---|---|---|
| $y'' + 5y' + 4y = 0$ | $\lambda^2 + 5\lambda + 4 = 0,\ \lambda = -1, -4$ | $y = c_1e^{-4x} + c_2e^{-x}$ |
| $y'' - 6y' + 9y = 0$ | $(\lambda - 3)^2 = 0,\ \lambda = 3$ | $y = (Ax + B)e^{3x}$ |
| $my'' = -ky$ or $y'' + \omega^2 y = 0$ | $\lambda^2 + \omega^2 = 0,\ \lambda = \pm i\omega$ | $y = Ae^{i\omega t} + Be^{-i\omega t} = c_1\sin\omega t + c_2\cos\omega t$ |

(5) The *wave equation* $\nabla^2\phi = \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}$. In 1D, $\frac{\partial^2\phi}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}$. The general solution: $\phi = f(x - ct) + g(x + ct)$.

• Consider the boundary condition $\phi(0,t) = \phi(L,t) = 0$ (vibrating stretched string). Seperation of variables: $\phi = X(x)T(t)$
$\Rightarrow \frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = \frac{1}{c^2}\frac{1}{T}\frac{\mathrm{d}^2T}{\mathrm{d}t^2} = -k^2$. $\begin{cases}\phi(0,t) = 0 \Rightarrow X \propto \sin(kx),\ \phi(L,t) = 0 \Rightarrow k_n = \frac{n\pi}{L} \\ T(t) = A_n\cos(ck_nt) + B_n\sin(ck_nt)\end{cases} \Rightarrow \phi(x,t) = \sum_{n=1,2,\cdots}\sin k_nx(A_n\cos\omega_nt + B_n\sin\omega_nt)$.

## 4.2 Fourier series

(1) The functions $\sin\frac{n\pi x}{L}$ and $\cos\frac{n\pi x}{L}$ form a *complete basis*.

$$\int_{-L}^{L}\sin\frac{n\pi x}{L}\cos\frac{n\pi x}{L}\mathrm{d}x = 0, \quad \int_{-L}^{L}\sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}\mathrm{d}x = L\delta_{nm}, \quad \int_{-L}^{L}\cos\frac{n\pi x}{L}\cos\frac{m\pi x}{L}\mathrm{d}x = L\delta_{nm}\ (m = n \neq 0).$$

(2) Given a function $f(x)$ with period $2L$ in the range $[-L, +L]$, the Fourier expansion:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(a_n\cos\frac{n\pi x}{L} + b_n\sin\frac{n\pi x}{L}\right), \quad a_n = \frac{1}{L}\int_{-L}^{L}f(x)\cos\frac{n\pi x}{L}\mathrm{d}x, \quad b_n = \frac{1}{L}\int_{-L}^{L}f(x)\sin\frac{n\pi x}{L}\mathrm{d}x.$$

• If $f(t)$ is periodic in $[0,T]$, write $\omega = \frac{2\pi}{T}$. $f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(a_n\cos\frac{n\pi t}{T/2} + b_n\sin\frac{n\pi t}{T/2}\right) \Rightarrow f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_n\cos(n\omega t) + b_n\sin(n\omega t))$.

• The expansion is valid for any function satisfying *Dirichlet's conditions*.
(i) The function is *single-valued*. (ii) The function has *finite number of discontinuities*. (iii) $\int_{-L}^{L}|f(x)|\mathrm{d}x$ must be *finite*.

(3) Writing $\cos\frac{n\pi x}{L}$ and $\sin\frac{n\pi x}{L}$ as exponentials, define $c_n = \frac{a_n - ib_n}{2}$, $c_{-n} = \frac{a_n + ib_n}{2}$.

$$f(x) = \sum_{-\infty}^{+\infty}c_n\exp\left(i\frac{n\pi x}{L}\right), \quad c_n = \frac{1}{2L}\int_{-L}^{L}f(x)\exp\left(-i\frac{n\pi x}{L}\right).$$

(4) For non-periodic functions, consider the period $(-L, L)$ to an infinite extent. Write $k_n = \frac{n\pi}{L}$, $\Delta k = \frac{\pi}{L}$
$f(x) = \sum_{n=-\infty}^{\infty}c_n\exp(ik_nx) = \frac{1}{2\pi a}\sum_{n=-\infty}^{\infty}2Lac_n\exp(ik_nx)\Delta k = \frac{1}{2\pi a}\sum_{n=-\infty}^{\infty}F(k_n)\exp(ik_nx)\Delta k$, $F(k_n) = 2Lac_n = a\int_{-L}^{L}f(x)\exp(-k_nx)\mathrm{d}x$.

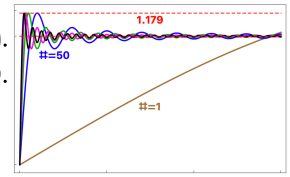
$$L \to \infty : F(k) = a\int_{-\infty}^{\infty}f(x)e^{-ikx}\mathrm{d}x, f(x) = \frac{1}{2\pi a}\int_{-\infty}^{\infty}F(k)e^{ikx}\mathrm{d}k. \quad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-ikx}\mathrm{d}x, f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}F(k)e^{ikx}\mathrm{d}k.$$

(5) Consider the square function $f(x) = \begin{cases}1, & x \in (0,1) \\ -1, & x \in (-1,0)\end{cases} \Rightarrow a_n = 0$, $b_n = -\int_{-1}^{0}\sin(n\pi x)\mathrm{d}x + \int_{0}^{1}\sin(n\pi x)\mathrm{d}x = \frac{2}{n\pi}(1 - \cos(n\pi))$.

$\Longrightarrow f(x) = 2\sum_{n=1}^{\infty}\frac{1-(-1)^n}{n\pi}\sin n\pi x = \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{\sin[(2n-1)\pi x]}{(2n-1)} = \frac{4}{\pi}\left(\frac{\sin[\pi x]}{1}+\frac{\sin[3\pi x]}{3}+\cdots+\frac{\sin[(2N-1)\pi x]}{2N-1}+\cdots\right).$

(6) Consider $f(x) = x^2$ confined to $[-L, L]$ and repeats outside the region. $b_n = 0$, $a_n = \frac{1}{L}\int_{-L}^{L} x^2\cos\frac{n\pi x}{L}\mathrm{d}x$. $a_0 = \frac{2}{3}L^2$. Let $g(\alpha) = \frac{1}{L}\int_{-L}^{L} -\cos(\alpha x)\mathrm{d}x = -\frac{2}{L}\frac{\sin(\alpha L)}{\alpha}$. $g''(\alpha) = \frac{1}{L}\int_{-L}^{L} x^2\cos(\alpha x)\mathrm{d}x = -\frac{1}{L}\left[-\frac{2L^2\sin(\alpha L)}{\alpha}+\frac{4\sin(\alpha L)}{\alpha^3}-\frac{4L\cos(\alpha L)}{\alpha^2}\right]$. Let $\alpha = \frac{n\pi}{L}$, $a_n = \frac{4L^2(-1)^n}{\pi^2 n^2}$ $(n>0) \Longrightarrow f(x) = x^2 = \frac{L^3}{3}+\frac{4L^2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\cos\frac{n\pi x}{L}$.

(7) *Gibbs phenomena*. Consider the square function $f(x) = \frac{4}{\pi}\left(\frac{\sin[\pi x]}{1}+\frac{\sin[3\pi x]}{3}+\cdots+\frac{\sin[(2N-1)\pi x]}{2N-1}\right)$. The *overshoots* occur at the turning points $f'(x) = 4(\cos[\pi x]+\cos[3\pi x]+\cdots+\cos[(2N-1)x]) = 0$.




$f'(x) = 4\mathfrak{Re}\left[\sum_{n=1}^{N} e^{i(2n-1)\pi x}\right] = 4\mathfrak{Re}\left[\frac{\sin N\pi x}{\sin \pi x}e^{iN\pi x}\right] = 2\frac{\sin(2N\pi x)}{\sin(\pi x)} = 0 \Rightarrow$ The first maxima is $x = \frac{1}{2N}$.

$$f\left(\frac{1}{2N}\right) = 4\left(\frac{\sin\left[\frac{\pi}{2N}\right]}{\pi}+\frac{\sin\left[\frac{3\pi}{2N}\right]}{3\pi}+\cdots\frac{\sin\left[\frac{(2N-1)\pi}{2N}\right]}{(2N-1)\pi}\right) = \frac{2}{N}\left(\mathrm{sinc}\left[\frac{\pi}{2N}\right]+\mathrm{sinc}\left[\frac{3\pi}{2N}\right]+\cdots+\mathrm{sinc}\left[\frac{(2N-1)\pi}{2N}\right]\right).$$

$$\lim_{N\to\infty} f\left(\frac{1}{2N}\right) = \lim_{N\to\infty}\frac{2}{\pi}\left(\frac{\pi}{N}\mathrm{sinc}\left[\frac{\pi}{2N}\right]+\frac{\pi}{N}\mathrm{sinc}\left[\frac{3\pi}{2N}\right]+\cdots+\frac{\pi}{N}\mathrm{sinc}\left[\frac{(2N-1)\pi}{2N}\right]\right) = \frac{2}{\pi}\int_0^{\pi}\mathrm{sinc}(x)\mathrm{d}x \approx 1.17898.$$

(8) The parabola at $x = 0$, $\frac{L^3}{3}+\frac{4L^2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2} = 0 \Rightarrow \pi^2 = 12\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2}$. At $x = L$, $\frac{L^3}{3}+\frac{4L^2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} = L^2 \Rightarrow \pi^2 = \sum_{n=1}^{\infty}\frac{1}{n^2} = 6\zeta(2)$.

(9) The mean value $\overline{f} = \frac{1}{2L}\int_{-L}^{L} f(x)\mathrm{d}x = \frac{a_0}{2}$. $\int_{-L}^{L}[f(x)]^2\mathrm{d}x = \frac{1}{2}a_0\int_{-L}^{L} f(x)\mathrm{d}x+\int_{-L}^{L}\sum_{n=1}^{\infty} f(x)a_n\cos\frac{n\pi x}{L}\mathrm{d}x+\int_{-L}^{L}\sum_{n=1}^{\infty} f(x)b_n\sin\frac{n\pi x}{L}\mathrm{d}x$

$\Rightarrow \overline{f^2} = \frac{1}{2L}\int_{-L}^{L}[f(x)]^2\mathrm{d}x = \left(\frac{a_0}{2}\right)^2+\frac{1}{2}\sum_{n=1}^{\infty}\left(a_n^2+b_n^2\right).$

(10) Consider the second order differential equation $\frac{\mathrm{d}^2y}{\mathrm{d}t^2}+p\frac{\mathrm{d}y}{\mathrm{d}t}+ry = f(t)$, where $f(t) = f(t+T)$. Drive frequency $\omega = \frac{2\pi}{T}$. Expand $f(t) = \frac{A_0}{2}+\sum_{n=1}^{\infty}(A_n\cos(n\omega t)+B_n\sin(n\omega t))$ and $y(t) = \frac{a_0}{2}+\sum_{n=1}^{\infty}(a_n\cos(n\omega t)+b_n\sin(n\omega t)) \Rightarrow y'(t) = -\sum_{n=1}^{\infty} n\omega(a_n\sin(n\omega t)-b_n\cos(n\omega t))$, $y''(t) = -\sum_{n=1}^{\infty}(n\omega)^2(a_n\cos(n\omega t)+b_n\sin(n\omega t))$. Substitution $\Rightarrow ra_0 = A_0$, $\begin{pmatrix}-n^2\omega^2+r & pn\omega\\ -pn\omega & -n^2\omega^2+r\end{pmatrix}\begin{pmatrix}a_n\\ b_n\end{pmatrix} = \begin{pmatrix}A_n\\ B_n\end{pmatrix}$.

$\Rightarrow \begin{pmatrix}a_n\\ b_n\end{pmatrix} = \frac{1}{\Delta}\begin{pmatrix}-n^2\omega^2+r & -pn\omega\\ pn\omega & -n^2\omega^2+r\end{pmatrix}\begin{pmatrix}A_n\\ B_n\end{pmatrix}$, $\Delta = (-n^2\omega^2+r)^2+(pn\omega)^2$. Notice that $\left(a_n^2+b_n^2\right) = \left(\frac{A_n^2+B_n^2}{\Delta}\right)^2$.

- For large values of $n$, $\Delta \propto n^4 \Rightarrow$ High frequency harmonics are strongly damped.
- Set $r = \omega_0^2$. For $p = 0$ and the drive frequency is much larger than the natural resonance frequency ($n\omega \gg \omega_0$), $a_n \to -\frac{1}{n^2\omega^2}A_n$. The amplitude is strongly damped $\Rightarrow$ The system cannot respond to be driven faster than its natural frequency of vibration. For small $p$, the maximum amplitude excited corresponds to $n\omega \approx \omega_0$.
- When $A_n = 1$, $A_{m\neq n} = B_n = 0$. $a_n = \frac{1}{\Delta}\left(\omega_0^2-n^2\omega^2\right)$, $b_n = \frac{1}{\Delta}pn\omega$.

| Frequency | Result |
|---|---|
| $n\omega < \omega_0$ | $a_n$ and $A_n$ have the same sign and the oscillations are in phase with the driving force. |
| $n\omega > \omega_0$ | $a_n < 0$ and the motion is out of phase with the driving force. |
| $n\omega = \omega_0$ | $a_n = 0$ and the motion is confined to $b_n$. The motion is $\frac{\pi}{2}$ out of phase. |

## 4.3 Laplace and diffusion equations

(1) The *Laplace's equation* is of the form $\nabla^2\phi = 0$. In 2D $\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2} = 0$. $\phi(x,y) = X(x)Y(y) \Rightarrow \frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2}+\frac{1}{Y}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} = 0$.

(2) Consider the boundary conditions $\phi(x,0) = \phi(x,L) = \phi(0,y) = 0$, $\phi(L,y) = V$. Letting $\frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = -\frac{1}{Y}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} = k^2$

$\Rightarrow Y(y) = B\sin\frac{n\pi y}{L}$. $X(x) = A_n\exp\left(\frac{n\pi x}{L}\right)+B_n\exp\left(-\frac{n\pi x}{L}\right) \Rightarrow \phi(x,y) = \sum_{n=1}^{\infty}\sin\frac{n\pi y}{L}\left[A_n\exp\left(\frac{n\pi x}{L}\right)+B_n\exp\left(-\frac{n\pi x}{L}\right)\right]$.

$\phi(0,y) = \sum_{n=1}^{\infty}(A_n+B_n)\sin\frac{n\pi y}{L} = 0 \Rightarrow A_n = -B_n \Rightarrow X_n = 2A_n\sinh\left(\frac{n\pi x}{L}\right)$. $\phi(L,y) = \sum_{n=1}^{\infty}2A_n\sinh(n\pi)\sin\left(\frac{n\pi y}{L}\right) = V$.

$2A_n\sinh(n\pi)\frac{L}{2} = \int_0^L V\sin\left(\frac{n\pi y}{L}\right)\mathrm{d}x = \frac{VL}{n\pi}(1-(-1)^n) \Rightarrow \phi(x,y) = \frac{4V}{\pi}\sum_{\text{odd } n}\frac{1}{n\sinh n\pi}\sinh\frac{n\pi x}{L}\sin\frac{n\pi y}{L}$.

(3) The *diffusion equation* is of the form $\nabla^2T = \frac{1}{\alpha^2}\frac{\partial T}{\partial t}$. $T$ can refer the the temperature or the density of particles.

(4) The heat energy $Q = cmT$. The *Fourier's law of heat transfer*: $\dot{Q}\frac{1}{A} = -K\frac{\partial T}{\partial x}$, where $K$ is the thermal conductivity.

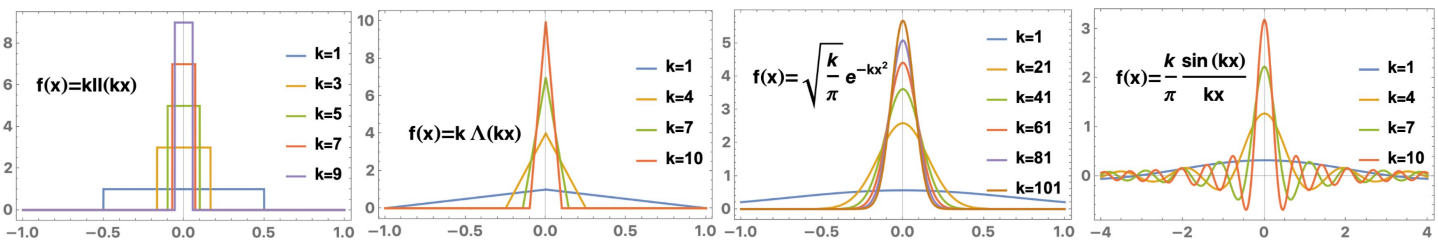
- Consider a uniform rod with density $\rho$ and non-uniform temperature. The heat energy of segment $[x, x+\mathrm{d}x]$ is given by $Q = c\rho A\Delta xT(x,t) \Rightarrow c\rho A\Delta x[T(x,t+\Delta t)-T(x,t)] = \Delta tAK\left(-\frac{\partial T}{\partial x}\Big|_x+\frac{\partial T}{\partial x}\Big|_{x+\Delta x}\right) \Rightarrow \frac{T(x,t+\Delta t)-T(x,t)}{\Delta t} = \frac{K}{c\rho}\left[\frac{\frac{\partial T}{\partial x}\big|_{x+\Delta x}-\frac{\partial T}{\partial x}\big|_x}{\Delta x}\right]$.

In the limit $\Delta x \to 0$, $\Delta t \to 0$, $\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha^2}\frac{\partial T}{\partial t}$. $\alpha^2 = \frac{K}{c\rho}$ is the thermal diffusivity. In the steady state $\frac{\partial T}{\partial t} = 0$ and reduces to the Laplacian equation. Boundary conditions: (i) fix $T$ on some surface; (ii) fix the rate of heat flow across a surface.

> *Example*: A wall of a refrigerator is initially in steady-state with the inside at $T_0$ and the outside at $T_1$. Suddenly the wall is moved outside where the air temperature is also $T_0$. What is $T(x,t)$?
> $T(x,t) = X(x)\Theta(t) \Rightarrow \frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = \frac{1}{\alpha^2\Theta}\frac{\mathrm{d}\Theta}{\mathrm{d}t} = -k^2 \Rightarrow X = A\sin kx + B\cos kx$, $\Theta(t) = e^{-\alpha^2k^2t} \to 0$. Let $T = T_0 + \widetilde{T}$.
> $\Longrightarrow \nabla^2\widetilde{T} = \frac{1}{\alpha^2}\frac{\partial\widetilde{T}}{\partial t}$ and $\nabla^2 T_0 = 0$. Boundary and initial conditions: $\widetilde{T}(0,t) = 0$, $\widetilde{T}(d,t) = 0$, $\widetilde{T}(x,0) = \frac{(T_1-T_0)x}{d}$.
> $\Longrightarrow X_n(x) = A_n\sin k_nx$, $k_n = \frac{n\pi}{d}$. $\widetilde{T}(x,t) = \sum\limits_{n=1}^{\infty} A_n\exp\left(-\alpha^2k_n^2t\right)\sin k_nx$. $\widetilde{T}(x,0) \Rightarrow A_n = (T_1-T_0)\frac{2}{n\pi}(-1)^{n+1}$.
> $\Longrightarrow T(x,t) = \frac{2}{\pi}(T_1-T_0)\sum\limits_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}e^{-(\alpha n\pi/d)^2t}\sin\frac{n\pi x}{d} + T_0$.
> Consider a shift in the *right hand boundary* $T(d,t) = T_0 + \Delta T$. Now define $T = \widetilde{T} + T_0 + \Delta T\frac{x}{d}$. $\widetilde{T}(0,t) = 0, \widetilde{T}(d,t) = 0$.
> $T(x,0) = T_0 + \frac{T_1-T_0}{d}x \Rightarrow \widetilde{T}(x,0) = \frac{T_1-T_0-\Delta T}{d}x$. $\Longrightarrow T(x,t) = \frac{2}{\pi}(T_1-T_0-\Delta T)\sum\limits_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}e^{-(\alpha n\pi/d)^2t}\sin\frac{n\pi x}{d} + T_0 + \frac{\Delta T}{d}x$.

## 4.4 Fourier transform

### 4.4.1 Dirac function




(1) $\delta(x) = \lim\limits_{k\to\infty} k\Pi(kx)$. $\delta(x) = \lim\limits_{k\to\infty} k\Lambda(kx)$, where $\Lambda(x) = \begin{cases} 1-|x|, & x\in[-1,1] \\ 0 \end{cases}$. $\delta(x) = \lim\limits_{k\to\infty}\sqrt{\left(\frac{k}{\pi}\right)}e^{-kx^2}$. $\delta(x) = \lim\limits_{k\to\infty}\frac{k}{\pi}\mathrm{sinc}(kx)$.

(2) **Essential properties**: $\lim\limits_{x\to 0}\delta(x) = \infty$, $\int_{-\infty}^{\infty}\delta(x)\mathrm{d}x = 1$. $\int_{-\infty}^{\infty}\delta(x-x_0)f(x)\mathrm{d}x = f(x_0)$. $\delta'(x) = -\delta'(-x)$.

(3) $\lim\limits_{k\to\infty}\int_{-k}^{k}e^{-ikx}\mathrm{d}k = \lim\limits_{k\to\infty}\frac{1}{-ix}\left(e^{-ikx}-e^{ikx}\right) = \lim\limits_{k\to\infty}\frac{2}{x}\sin(kx) = \lim\limits_{k\to\infty}2k\mathrm{sinc}(kx) = 2\pi\delta(x) \Rightarrow \delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-ikx}\mathrm{d}k = \delta(-x)$.

• $f(x) = \int_{-\infty}^{\infty}f(x')\delta(x'-x)\mathrm{d}x' = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-ik(x'-x)}f(x')\mathrm{d}k\mathrm{d}x' = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}f(x')e^{-ikx'}\mathrm{d}x'e^{ikx}\mathrm{d}k = \frac{1}{2\pi}\int_{-\infty}^{\infty}F(k)e^{ikx}\mathrm{d}k$.

(4) The Fourier transform pair: $f(x) = \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{\infty}F(k)e^{ikx}\mathrm{d}k$, $F(k) = \displaystyle\int_{-\infty}^{\infty}f(x)e^{-ikx}\mathrm{d}x$ (Physics definition).

• Note that $F(0) = \int_{-\infty}^{\infty}f(x)\mathrm{d}x$. The total area under $f(x)$ is given by the Fourier transform at the origin.

(5) Consider $f(x) = \sum\limits_{n=-\infty}^{\infty}c_ne^{in\pi x/L} \xrightarrow[L=\pi]{T=2\pi} \sum\limits_{n=-\infty}^{\infty}c_ne^{inx}$. The function $f(x) = \sum\limits_{n=-\infty}^{\infty}\delta(x-2n\pi)$ has period $2\pi$. The coefficients $c_n = \frac{1}{2\pi}\int_0^{2\pi}f(x)e^{-inx}\mathrm{d}x = \frac{1}{2\pi} \Rightarrow \sum\limits_{n=-\infty}^{\infty}\delta(x-2n\pi) = \frac{1}{2\pi}\sum\limits_{n=-\infty}^{\infty}e^{inx}$. For period $L$, $\sum\limits_{n=-\infty}^{\infty}\delta(x-nL) = \frac{1}{L}\sum\limits_{n=-\infty}^{\infty}e^{i2n\pi x/L}$.

(6) $\int_{-\infty}^{\infty}\delta'(x-a)f(x)\mathrm{d}x = \int_{-\infty}^{\infty}f(x)\mathrm{d}\delta(x-a) = f(x)\delta(x-a)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\delta(x-a)f'(x) \Rightarrow \int_{-\infty}^{\infty}\delta'(x-a)f(x)\mathrm{d}x = f'(a)$.

• Let $f(x) = xg(x)$, $\int_{-\infty}^{\infty}xg(x)\delta'(x)\mathrm{d}x = -\int_{-\infty}^{\infty}\delta(x)\mathrm{d}[xg(x)] = -\int_{-\infty}^{\infty}\delta(x)[g(x)+xg'(x)]\mathrm{d}x = -\int_{-\infty}^{\infty}\delta(x)g(x)\mathrm{d}x \Rightarrow x\delta'(x) = -\delta(x)$.

• In general, $\int_{-\infty}^{\infty}f(x)\delta^{(n)}(x)\mathrm{d}x = -\int_{-\infty}^{\infty}\frac{\mathrm{d}f}{\mathrm{d}x}\delta^{n-1}(x)\mathrm{d}x$, $x^n\delta^{(n)}(x) = (-1)^n n!\delta(x)$.

(7) For $a>0$, $\int_{-\infty}^{\infty}\delta(ax)f(x)\mathrm{d}x \overset{y=ax}{=\!=\!=} \frac{1}{a}\int_{-\infty}^{\infty}\delta(y)f\left(\frac{y}{a}\right)\mathrm{d}y = \frac{1}{a}f(0) = \frac{1}{a}\int_{-\infty}^{\infty}\delta(x)f(x)\mathrm{d}x$. Generally $\delta(ax) = \frac{1}{|a|}\delta(x)$.

(8) $\delta(g(x)) = \sum\limits_i\frac{1}{|g'(x_i)|}\delta(x-x_i)$, where $g(x_i) = 0$ and $g'(x_i) \neq 0$. $\delta(x^2-a^2) = \frac{1}{|2a|}[\delta(x-a)+\delta(x+a)]$. $\delta((x-a)(x-b)) = \frac{1}{|a-b|}[\delta(x-a)+\delta(x-b)]$.

### 4.4.2 Fourier transformation

(1) $\Pi(x) = \begin{cases} 1, & x\in[-a,a] \\ 0, & \text{elsewhere} \end{cases}$. $F(k) = \frac{1}{\sqrt{2\pi}}\int_{-a}^{a}e^{-ikx}\mathrm{d}x = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{-ik}\right)\left(e^{-ika}-e^{ika}\right) = \sqrt{\frac{2}{\pi}}\frac{\sin ka}{k} = \sqrt{\frac{2}{\pi}}a\mathrm{sinc}(ka)$.

• Width of the distribution $\Delta k \approx \frac{2\pi}{a}$, $\Delta x \approx 2a \Rightarrow \Delta k\Delta x \approx \pi$. In general $\Delta k\Delta x \geq \frac{1}{2}$.

(2) $f(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{x^2}{2\sigma^2}\right)$. $F(k) = \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{2\sigma^2}\right)\exp(-ikx)\mathrm{d}x = \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty}\exp\left[-\left(\frac{x}{\sqrt{2}\sigma}+i\frac{k\sigma}{\sqrt{2}}\right)^2 - \frac{k^2\sigma^2}{2}\right]\mathrm{d}x$

$= \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{k^2\sigma^2}{2}\right)\int_{-\infty}^{\infty}\exp\left(-\xi^2\right)\sqrt{2}\sigma\mathrm{d}\xi = \exp\left(-\frac{\sigma^2 k^2}{2}\right)$.

(3) *Parseval's theorem*: $\int_{-\infty}^{\infty}|f(x)|^2\mathrm{d}x = \int_{-\infty}^{\infty}\left|F(k)^2\right|\mathrm{d}k$ (Math defn.)

$\int_{-\infty}^{\infty}|f(x)|^2\mathrm{d}x = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}F(k)e^{ikx}\mathrm{d}k\int_{-\infty}^{\infty}F^*(k')e^{-ik'x}\mathrm{d}k'\mathrm{d}x = \int_{-\infty}^{\infty}F(k)\mathrm{d}k\int_{-\infty}^{\infty}F^*(k')\mathrm{d}k'\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i(k-k')}\mathrm{d}x = \int_{-\infty}^{\infty}|F(k)|^2\mathrm{d}k$.

(4) *Convolution*. $h(x) = f(x)*g(x) = \int_{-\infty}^{\infty}f(x-x')g(x')\mathrm{d}x' = \int_{-\infty}^{\infty}f(x')g(x-x')\mathrm{d}x'$. $H(k) = aF(k)G(k)$. $a = 1/\sqrt{2\pi}$ (Phys./Math.)

$H(k) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}x\mathrm{d}x' f(x-x')g(x')e^{-ikx} \xrightarrow[\mathrm{d}\zeta=\mathrm{d}x]{\zeta=x-x'} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}x'\mathrm{d}\zeta f(\zeta)g(x')e^{-ik(\zeta+x')} = \int_{-\infty}^{\infty}g(x')e^{-ikx'}\mathrm{d}x'\int_{-\infty}^{\infty}f(\zeta)e^{-ik\zeta}\mathrm{d}\zeta$.

- $h'(x) = f'(x)*g(x) = f(x)*g'(x)$.
- For $a = \frac{1}{2}$, $h(x) = \Pi(x)*\Pi(x) = \int_{-\infty}^{\infty}\Pi(x')\Pi(x-x')\mathrm{d}x' = \Lambda(x)$, $H(k) = \mathrm{sinc}^2\left(\frac{k}{2}\right)$ (Math.).

(5) $f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}F(k)e^{ikx}\mathrm{d}k$, $\frac{\mathrm{d}}{\mathrm{d}x}f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}ikF(k)e^{ikx}\mathrm{d}k \Rightarrow \mathcal{F}\left[\frac{\mathrm{d}}{\mathrm{d}x}f(x)\right] = ikF(k)$. $\mathcal{F}\left[f^{(n)}(x)\right] = (ik)^n F(k)$.

(5) Define $U = \int_{-\infty}^{\infty}|f(x)|^2\mathrm{d}x = \int_{-\infty}^{\infty}|F(k)|^2\mathrm{d}k$, $\begin{cases}\overline{x} = \left(\frac{1}{U}\int_{-\infty}^{\infty}x|f(x)|^2\mathrm{d}x\right)^{1/2}, \Delta x = \left[\frac{1}{U}\int_{-\infty}^{\infty}(x-\overline{x})^2|f(x)|^2\mathrm{d}x\right]^{1/2} \\ \overline{k} = \left(\frac{1}{U}\int_{-\infty}^{\infty}k|F(k)|^2\mathrm{d}k\right)^{1/2}, \Delta k = \left[\frac{1}{U}\int_{-\infty}^{\infty}(k-\overline{k})^2|F(k)|^2\mathrm{d}k\right]^{1/2}\end{cases}$.

Assume $\overline{x} = \overline{k} = 0$. $\mathcal{F}[f'(x)] = ikF(k) \Rightarrow \int_{-\infty}^{\infty}|f'(x)|^2\mathrm{d}x = \int_{-\infty}^{\infty}k^2|F(k)|^2\mathrm{d}k$. $(\Delta x)^2(\Delta k)^2 = \frac{1}{U^2}\left(\int_{-\infty}^{\infty}x^2|f(x)|^2\mathrm{d}x\right)\left(\int_{-\infty}^{\infty}|f'(x)|\mathrm{d}x\right)$.

$\int_a^b|a(x)|^2\mathrm{d}x\int_a^b|b(x)|^2\mathrm{d}x \geq \left|\int_a^b a^*(x)b(x)\mathrm{d}x\right|^2 \Rightarrow (\Delta x)^2(\Delta k)^2 \geq \frac{1}{U^2}\left|\int_{-\infty}^{\infty}xf^*(x)f'(x)\mathrm{d}x\right|^2 = \frac{1}{4U^2}\left|\int_{-\infty}^{\infty}x\frac{\mathrm{d}}{\mathrm{d}x}|f(x)|^2\mathrm{d}x\right|^2 = \frac{1}{4U^2}\left|\int_{-\infty}^{\infty}x\mathrm{d}|f(x)|^2\right|^2$
$= \frac{1}{4U^2}\left|x|f(x)|^2\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}|f(x)|^2\mathrm{d}x\right|^2 = \frac{1}{4U^2}U^2 = \frac{1}{4} \Rightarrow (\Delta x)^2(\Delta k)^2 \geq \frac{1}{4}$.

### 4.4.3 Wave packets

(1) Substitute a forward travelling wave $\phi(x,t) = e^{-i(kx-\omega t)}$ to the 1D wave equation $\Rightarrow w = ck$. For a plane wave $\phi(\mathbf{r},t) = e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ we have $\frac{\omega}{|\mathbf{k}|} = c$ and $\mathbf{k}\cdot\mathbf{r} = \alpha$ is the equation of a plane perpendicular to $\mathbf{k}$.

(2) General 1D wave equation can be written as $\phi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}G(k)e^{i(kx-\omega(k)t)}\mathrm{d}k$. $G(k)$ is the Fourier transform of $\phi(x,0)$.

- Waves travelling in the same speed $c$: $\phi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}G(k)e^{ik(x-ct)}$. The shape of the wave is unchanged.

(3.1) Example: Gaussian wave packet $\phi(x,0) = e^{ik_0x}e^{-x^2/\Delta^2}$. $G(k) = \mathcal{F}[\phi] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{ik_0x}e^{-x^2/\Delta^2}e^{-ikx}\mathrm{d}x = \frac{\Delta}{\sqrt{2}}e^{-\frac{\Delta^2(k-k_0)^2}{4}}$

$\Rightarrow \phi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\Delta}{\sqrt{2}}e^{-\frac{\Delta^2(k-k_0)^2}{4}}e^{i(kx-\omega(k)t)}\mathrm{d}k$. Suppose $\omega(k)$ is dominated by the region in the vicinity of $k = k_0$,
$\omega(k) \approx \omega(k_0) + \omega'(k_0)(k-k_0) = k_0v_p + v_g(k-k_0)$. Thus $\phi(x,t) \approx \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}G(k)e^{i(kx-\omega_0t-\omega_0'(k-k_0)t)}\mathrm{d}k$
$\approx \frac{1}{\sqrt{2\pi}}e^{i(k_0x-\omega_0t)}\int_{-\infty}^{\infty}G(k)e^{i(-k_0x+kx-\omega_0'(k-k_0)t)}\mathrm{d}k \approx e^{i(k_0x-\omega_0t)}\int_{-\infty}^{\infty}G(k)e^{i(k-k_0)(x-\omega_0't)}\frac{\mathrm{d}k}{\sqrt{2\pi}}$.

- The first factor corresponds to a wave with $k = k_0$ and phase velocity $v_p = \frac{\omega(k_0)}{k_0}$.
- The second factor $\int_{-\infty}^{\infty}G(k)e^{i(k-k_0)(x-\omega_0't)}\frac{\mathrm{d}k}{\sqrt{2\pi}} \xrightarrow{y=x-\omega_0't} e^{-ik_0y}\int_{-\infty}^{\infty}G(k)e^{iky}\frac{\mathrm{d}k}{\sqrt{2\pi}} = e^{-ik_0y}\phi(y,0) = e^{-ik_0y}e^{ik_0y}e^{-y^2/\Delta^2} = e^{-\frac{(x-\omega_0't)^2}{\Delta^2}}$, which is the envelope of a wave moving with speed $v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k}\Big|_{k_0} = \omega_0'$.
- The overall integral $\phi(x,t) = e^{i(k_0x-\omega_0t)}e^{-(x-\omega_0't)^2/\Delta^2} = e^{i(k_0x-k_0v_pt)}e^{-(x-v_gt)^2/\Delta^2}$.
- In general, $v_p = \frac{\omega}{k}$, $\frac{\mathrm{d}v_p}{\mathrm{d}k} = \frac{1}{k}\frac{\mathrm{d}\omega}{\mathrm{d}k} - \frac{\omega}{k^2} = \frac{v_g}{k} - \frac{v_p}{k} \Rightarrow v_g = v_p + k\frac{\mathrm{d}v_p}{\mathrm{d}k}$.

(3.2) Consider a higher order expansion $\omega(k) \approx \omega(k_0) + \omega'(k_0)(k-k_0) + \frac{1}{2}\omega''(k_0)(k-k_0)^2 = v_pk_0 + v_g(k-k_0) + \frac{1}{2}\Gamma(k-k_0)^2$.

In this case $\phi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\Delta}{\sqrt{2}}e^{-\frac{\Delta^2(k-k_0)^2}{4}}e^{i[kx-(k_0v_p+(k-k_0)v_g+\frac{1}{2}\Gamma(k_0)(k-k_0)^2)t]} = \frac{\Delta}{\sqrt{\Delta^2+2i\Gamma t}}e^{ik_0(x-v_pt)}\exp\left[-\left(\frac{x-v_gt}{\sqrt{\Delta^2+2i\Gamma t}}\right)^2\right]$.

Write $\sigma_x = \sqrt{2}\Delta$, $\sigma(t) = \sigma_x\sqrt{1+\frac{t^2\Gamma^2}{\sigma_x^4}}$, then $\phi(x,t) = e^{ik_0(x-v_pt)}\frac{\sigma_x}{\sigma(t)}\exp\left[-\left((x-v_gt)(1-\frac{it\Gamma}{2\sigma_x^2})\right)\Big/\sqrt{2\sigma(t)}\right]^2\left(1-\frac{it\Gamma}{\sigma_x^2}\right)^{1/2}$.

- The envelope $\phi(x,t) = \frac{\sigma_x}{\sigma(t)}\left(1+\frac{t^2\Gamma^2}{\sigma_x^4}\right)^{1/4}e^{-\frac{(x-v_gt)^2}{2\sigma^2(t)}}$. As wave propagates in time $\sigma(t)$ grows $\Rightarrow$ The wave broadens.

(4) Example: Exponential damped cosine $f(t) = \begin{cases}e^{-\alpha t}e^{i\omega_0t}, & 0 \leq t \leq \infty \\ 0, & t < 0\end{cases}$. $G(\omega) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty}e^{-(\alpha+i(\omega-\omega_0))t}\mathrm{d}t = \frac{1}{\sqrt{2\pi}}\frac{1}{\alpha+i(\omega-\omega_0)}$.

- The intensity $|G(\omega)| = \frac{1}{2\pi(\alpha^2+(\omega-\omega_0)^2)}$ (*Lorentz distribution*). It is also the spectrum emitted by an atom as it decays to a lower energy state with lifetime $\sim 1/\alpha$. In this instance, we cannot measure the frequency better than $\sim$ 1/lifetime (width). For an atomic transition we have $\Delta E\Delta t \sim \hbar$ or $\Delta\omega\Delta t \sim 1$.

(5) The diffusion equation of particles $n(x,t)$ is given by $\frac{\partial^2 n(x,t)}{\partial x^2} = \frac{1}{D}\frac{\partial n(x,t)}{\partial t}$. Consider a drop of ink, $n(x,0) = S\delta(x)$

- Take the Fourier transform of the equation $\Rightarrow -k^2N(k,t) = \frac{1}{D}\frac{\partial N(k,t)}{\partial t} \Rightarrow \frac{\mathrm{d}\ln N}{\mathrm{d}t} = -k^2D \Rightarrow N(k,t) = N_0(k)e^{-Dk^2t}$

$\Longrightarrow n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} N(k,t)e^{ikx}\mathrm{d}k = \frac{1}{2\pi}\int_{-\infty}^{\infty} N_0(k)e^{ikx-Dk^2t}\mathrm{d}k$. $N_0(k) = N(k,0) = \int_{-\infty}^{\infty} n(x,0)e^{-ikx}\mathrm{d}x = S\int_{-\infty}^{\infty}\delta(x)e^{-ikx}\mathrm{d}x = S$.

$\Longrightarrow n(x,t) = \frac{S}{2\pi}\int_{-\infty}^{\infty} e^{ikx-Dk^2t}\mathrm{d}k = \frac{S}{2\pi}\int_{-\infty}^{\infty}\exp\left[-\left(\sqrt{Dt}k - \frac{ix}{2\sqrt{Dt}}\right)^2 - \frac{x^2}{4Dt}\right]\mathrm{d}k$. Let $\xi = \sqrt{Dt}k - \frac{ix}{2\sqrt{Dt}}$, $\mathrm{d}\xi = \sqrt{Dt}\mathrm{d}k$.

$\Longrightarrow n(x,t) = \frac{S}{2\pi}\int_{-\infty}^{\infty} e^{-\xi^2}e^{-\frac{x^2}{4Dt}}\frac{\mathrm{d}\xi}{\sqrt{Dt}} = \frac{Se^{-\frac{x^2}{4Dt}}}{2\pi\sqrt{Dt}}\int_{-\infty}^{\infty} e^{-\xi^2}\mathrm{d}\xi \Longrightarrow n(x,t) = \frac{S}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}$.

### 4.4.4 Green's function

(1) Consider $f(x) = -\frac{e^{-a|x|}}{2a}$, $F(k) = \mathcal{F}[f(x)] = -\frac{1}{2a}\int_{-\infty}^{0} e^{ax}e^{-ikx}\mathrm{d}x - \frac{1}{2a}\int_0^{\infty} e^{-ax}e^{-ikx} = -\frac{1}{k^2+a^2} \Rightarrow \mathcal{F}\left[-\frac{e^{-a|x|}}{2a}\right] = -\frac{1}{k^2+a^2}$.

• $\int_{-\infty}^{\infty} g(x-x_0)e^{-ikx}\mathrm{d}x = e^{-ikx_0}\int_{-\infty}^{\infty} g(x)e^{-ikx}\mathrm{d}x \Rightarrow \mathcal{F}[g(x-x_0)] = e^{-ikx_0}\mathcal{F}[g(x)] \Rightarrow \mathcal{F}\left[-\frac{e^{-a|x-x'|}}{2a}\right] = -\frac{e^{-ikx'}}{k^2+a^2}$.

(2) Consider the differential equation $\frac{\mathrm{d}^2 g(x,x')}{\mathrm{d}x^2} - a^2 g(x,x') = \delta(x-x') \overset{\mathcal{F}}{\Rightarrow} G(k) = -\frac{e^{-ikx'}}{k^2+a^2} \Rightarrow g(x) = -\frac{e^{-a|x-x'|}}{2a}$.

• Convolute both sides by $f(x) \Rightarrow \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - a^2\right)\int_{-\infty}^{\infty} g(x-x')f(x')\mathrm{d}x = \int_{-\infty}^{\infty}\delta(x-x')f(x') = f(x)$. Let $y(x) = \int_{-\infty}^{\infty} f(x')g(x-x')\mathrm{d}x'$

$\Longrightarrow \frac{\mathrm{d}^2}{\mathrm{d}x^2}y(x) - a^2 y(x) = f(x)$. $y(x)$ is a solution for a general RHS $f(x)$.

(3) $g(x) = -\frac{e^{-a|x-x'|}}{2a}$ is the *Green's function*.

(4) Consider the *Poisson equation* $\nabla^2 g(\mathbf{r}) = -\frac{\delta(\mathbf{r})}{\varepsilon}$. Taking the Fourier transform $\Rightarrow -k^2 G(\mathbf{k}) = -\frac{1}{\varepsilon} \Rightarrow G(\mathbf{k}) = \frac{1}{\varepsilon k^2}$.

$\Longrightarrow g(\mathbf{r}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} G(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}\mathrm{d}^3\mathbf{k} = \frac{1}{(2\pi)^3}\int_0^{\infty} k^2\mathrm{d}k\int_0^{\pi}\sin\theta\mathrm{d}\theta\int_0^{2\pi}\frac{1}{\varepsilon k^2}e^{i\mathbf{k}\cdot\mathbf{r}}\mathrm{d}\phi = -\frac{1}{(2\pi)^2}\frac{1}{\varepsilon}\int_0^{\infty}\mathrm{d}k\int_0^{\pi} e^{ikr\cos\theta}\mathrm{d}\cos\theta$

$= -\frac{1}{(2\pi)^2\varepsilon}\int_0^{\infty}\frac{\mathrm{d}k}{ikr}\left[e^{ikr\cos\theta}\right]_1^{-1} = \frac{1}{(2\pi)^2\varepsilon}\int_0^{\infty}\frac{2\sin(kr)\mathrm{d}k}{kr}\,\frac{y=kr}{\overline{\mathrm{d}y=r\mathrm{d}k}}\,\frac{1}{(2\pi)^2\varepsilon r}\int_0^{\infty}\frac{2\sin y}{y}\mathrm{d}y = \frac{1}{4\pi\varepsilon r} = \frac{1}{4\pi\varepsilon|\mathbf{r}|}$.

• The solution of $\nabla^2 g(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon}$ is given by the convolution $\phi(\mathbf{r}) = \rho(\mathbf{r}) * g(\mathbf{r}) = \int\frac{\rho(\mathbf{r}')}{4\pi\varepsilon|\mathbf{r}-\mathbf{r}'|}\mathrm{d}\mathbf{r}'$.

### 4.4.5 Fourier transform pairs and misc

(1) The Heaviside function $H(x) = \begin{cases}1, & x \geq 0\\ 0, & x < 0\end{cases} = \begin{cases}\lim\limits_{\alpha\to 0} e^{-\alpha x}, & x \geq 0\\ 0, & x < 0\end{cases}$. $F(k) = \int_0^{\infty} e^{-\alpha x}e^{-ikx}\mathrm{d}x = \int_0^{\infty} e^{-(\alpha+ik)x}\mathrm{d}x = \frac{-1}{\alpha+ik}e^{-(\alpha+ik)x}\Big|_0^{\infty}$

$= \frac{\alpha}{\alpha^2+k^2} - i\frac{k}{\alpha^2+k^2}$. $\int_{-\infty}^{\infty}\frac{\alpha}{\alpha^2+k^2}\mathrm{d}k = \arctan\left(\frac{k}{\alpha}\right)\Big|_{-\infty}^{\infty} = \pi \Rightarrow F(k) = \lim\limits_{\alpha\to 0}\left(\frac{\alpha}{\alpha^2+k^2} - i\frac{k}{\alpha^2+k^2}\right) = \pi\delta(k) + \frac{1}{ik}$. $\mathcal{F}[H(x)] = \pi\delta(k) + \frac{1}{ik}$.

(2) $\mathrm{sgn}(x) = \begin{cases}1, & x > 0\\ -1, & x < 0\end{cases}$. $\mathrm{sgn}(x) = 2H(x) - 1$. $\mathcal{F}[\mathrm{sgn}(x)] = 2\pi\delta(k) + \frac{2}{ik} - 2\pi\delta(x) = \frac{1}{ik}$. $\mathcal{F}[\mathrm{sgn}(x)] = \frac{1}{ik}$.

(3) Top hat $\Pi(x)$ for $a = \frac{1}{2}$. $\mathcal{F}[\Pi(x)] = \mathrm{sinc}\left(\frac{k}{2}\right)$ (Phys. defn.). $\Pi(x) = H\left(x+\frac{1}{2}\right) - H\left(x-\frac{1}{2}\right)$, $\mathcal{F}[\Pi(x)] = \left(e^{ik/2} - e^{-ik/2}\right)\left(\pi\delta(k) + \frac{1}{ik}\right)$

$= 2i\sin\left(\frac{k}{2}\right)\left(\pi\delta(k) + \frac{1}{ik}\right) = 2\pi i\sin\left(\frac{k}{2}\right)\delta(k) + \frac{2\sin(k/2)}{k} = \mathrm{sinc}(k/2)$.

(4) Consider the convolution $\int_{-\infty}^{\infty} f(x')H(x-x')\mathrm{d}x' = \int_{-\infty}^{x} f(x')\mathrm{d}x'$. $\mathcal{F}\left[\int_{-\infty}^{x} f(x')\mathrm{d}x'\right] = F(k)\left(\frac{1}{ik} + \pi\delta(k)\right) = \frac{F(k)}{ik} + \pi F(0)\delta(k)$.

(5) Consider $h(x) = \Pi(x) * \Pi(x)$. $h'(x) = \Pi'(x) * \Pi(x) = \left[H'\left(x+\frac{1}{2}\right) - H'\left(x-\frac{1}{2}\right)\right] * \Pi(x) = \left[\delta\left(x+\frac{1}{2}\right) - \delta\left(x-\frac{1}{2}\right)\right] * \Pi(x)$

$\Longrightarrow h'(x) = \Pi\left(x+\frac{1}{2}\right) - \Pi\left(x-\frac{1}{2}\right) = H(x+1) - H(x) - H(x) + H(x-1) = H(x+1) - 2H(x) + H(x-1)$

$\Longrightarrow h(x) = r(x+1) - 2r(x) + r(x-1) = \Lambda(x)$, where $r(x) = xH(x)$.

• Consider $h(x) = \Pi(x) * \Lambda(x) = \Pi(x) * (\Pi(x) * \Pi(x))$. $h'(x) = \Pi'(x) * \Lambda(x) = \left(\delta\left(x+\frac{1}{2}\right) - \delta\left(x-\frac{1}{2}\right)\right) * \Lambda(x) = \Lambda\left(x+\frac{1}{2}\right) - \Lambda\left(x-\frac{1}{2}\right)$

$= r\left(x+\frac{3}{2}\right) - 2r\left(x+\frac{1}{2}\right) - r\left(x-\frac{1}{2}\right) - \left[r\left(x+\frac{1}{2}\right) - 2r\left(x-\frac{1}{2}\right) - r\left(x-\frac{3}{2}\right)\right] = r\left(x+\frac{3}{2}\right) - 3r\left(x+\frac{1}{2}\right) + 3r\left(x-\frac{1}{2}\right) - r\left(x+\frac{3}{2}\right)$

$\Longrightarrow h(x) = q\left(x+\frac{3}{2}\right) - 3q\left(x+\frac{1}{2}\right) + 3q\left(x-\frac{1}{2}\right) - q\left(x-\frac{3}{2}\right)$, where $q(x) = \frac{1}{2}x^2H(x)$.

## 4.5 Special functions

### 4.5.1 Taylor expansion

(1) $f(x) = f(a) + \int_a^x f'(t)\mathrm{d}t = f(a) + \int_a^x f'(t)\mathrm{d}(t-x) = f(a) + (t-x)f'(t)\Big|_a^x - \int_a^x (t-x)f''(t)\mathrm{d}t = f(a) - (a-x)f'(a) - \int_a^x (t-x)f''(t)\mathrm{d}t$

$= f(a) + (x-a)f'(a) - \int_a^x f''(t)\mathrm{d}\left[\frac{(t-x)^2}{2}\right] = f(a) + (x-a)f'(a) - \frac{1}{2}(t-x)^2 f''(t)\Big|_a^x + \int_a^x \frac{(t-x)^2}{2}f'''(t)\mathrm{d}t = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \ldots$

(2) Maclaurin expansions

| $f(x)$ | Series | Domain | $f(x)$ | Series | Domain |
|---|---|---|---|---|---|
| $e^x$ | $1+x+\frac{x^2}{2!}+\frac{x^3}{3!}+\cdots$ | $x\in\mathbb{R}$ | $(1+x)^\alpha$ | $1+ax+\frac{a(a-1)x^2}{2!}+\cdots=\sum\limits_{n=0}^{\infty}\binom{a}{n}x^n$ | $\|x\|<1$ |
| $\sin x$ | $x-\frac{x^3}{3}+\frac{x^5}{5!}-\cdots$ | $x\in\mathbb{R}$ | $\ln(1+x)$ | $x-\frac{x^2}{2}+\frac{x^3}{3}-\cdots$ | $\|x\|<1$ |
| $\cos x$ | $1-\frac{x^2}{2!}+\frac{x^4}{4!}-\cdots$ | $x\in\mathbb{R}$ | $\ln(1-x)$ | $-x-\frac{x^2}{2}-\frac{x^3}{3}-\cdots$ | $\|x\|<1$ |

### 4.5.2 Hermite's equation

(1) *Hermite's equation* is given by $\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+2ny=0$. Let $y=\sum\limits_{k=0}^{\infty}a_kx^k$, $y'=\sum\limits_{k=1}^{\infty}a_kkx^{k-1}$, $y''=\sum\limits_{k=2}^{\infty}a_kk(k-1)x^{k-2}$.
$\Longrightarrow \sum\limits_{k=0}^{\infty}a_{k+2}(k+2)(k+1)x^k-2\sum\limits_{k=0}^{\infty}a_kkx^k+2n\sum\limits_{k=0}^{\infty}a_kx^k=0\Rightarrow\sum\limits_{k=0}^{\infty}[a_{k+2}(k+2)(k+1)-2ka_k+2na_k]x^k=0$
$\Longrightarrow a_{k+1}=\frac{2(k-n)}{(k+2)(k+1)}a_k\Longrightarrow y=a_0\Big[1-\frac{2n}{2!}x^2-\frac{2n(4-2n)}{4!}x^4-\cdots\Big]+a_1\Big[x+\frac{(2-2n)}{3!}x^3+\frac{(2-2n)(6-2n)}{5!}x^5+\cdots\Big]$.

- If $a_0=1$, $a_1=0$ and $n$ is even. $h_0(x)=1$, $h_2(x)=1-2x^2$, $h_4(x)=1-4x^2+\frac{4}{3}x^4$.
- If $a_0=0$, $a_1=1$ and $n$ is odd. $h_1(x)=x$, $h_3(x)=x-\frac{2}{3}x^3$, $h_5(x)=x-\frac{4}{3}x^3+\frac{4}{15}x^5$.

(2) The schrodinger equation of QHO: $-\frac{\hbar^2}{2m}\psi''+\frac{1}{2}m\omega^2x^2\psi=E\psi\Rightarrow\psi''+\Big[\frac{2mE}{\hbar^2}-\Big(\frac{m\omega}{\hbar}\Big)^2x^2\Big]\psi=0$. Define $\alpha=\frac{m\omega}{\hbar}$, $\beta=\frac{2mE}{\hbar^2}$
$\Longrightarrow\frac{d^2\psi}{dx^2}+(\beta^2-\alpha^2x^2)\psi=0$. Let $\xi=\sqrt{\alpha}x\Rightarrow\frac{d^2\psi}{d\xi^2}+\Big(\frac{\beta}{\alpha}-\xi^2\Big)\psi=0$. If $\psi(\xi)=Ae^{-\xi^2/2}H(\xi)$ then $\frac{d^2H}{d\xi^2}-2\xi\frac{dH}{d\xi}+\Big(\frac{2E}{\hbar\omega}-1\Big)H=0$.

### 4.5.3 Legendre's equation

(1) *Legendre's equation* is given by $\big(1-x^2\big)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+l(l+1)y=0$. Let $y=\sum\limits_{n=0}^{\infty}a_nx^n$, $y'=\sum\limits_{n=1}^{\infty}na_nx^{n-1}$, $y''=\sum\limits_{n=0}^{\infty}n(n-1)a_nx^{n-2}$.
$\Longrightarrow a_{n+2}=\frac{n(n+1)-l(l+1)}{(n+1)(n+2)}a_n=\frac{(n-l)(n+l+1)}{(n+1)(n+2)}a_n\Rightarrow y=a_0\Big[1-l(l+1)\frac{x^2}{2!}+(l-2)l(l+1)(l+3)\frac{x^4}{4!}\Big]+a_1\Big[x-(l-1)(l+2)\frac{x^3}{3!}+\cdots\Big]$.
(2) Consider the expansion of electrostatic potential $S=\frac{1}{|\mathbf{R}-\mathbf{r}|}=\frac{1}{\sqrt{R^2+r^2-2Rr\cos\theta}}=\frac{1}{R}\frac{1}{\sqrt{1+(r/R)^2-2(r/R)\cos\theta}}=\frac{1}{R}(1-\beta)^{-1/2}$
$=\frac{1}{R}\Big(1+\frac{1}{2}\beta+\frac{3}{8}\beta^2+\frac{5}{16}\beta^3+\frac{35}{128}\beta^4+\cdots\Big)$. Let $x=\cos\theta$ and $\alpha=\frac{r}{R}$, $S=\frac{1}{R}\Big(1+\frac{1}{2}\big(2\alpha x-\alpha^2\big)+\frac{3}{8}\big(2\alpha x-\alpha^2\big)^2+\cdots\Big)$
$\Longrightarrow S=\frac{1}{R}\Big(1+\alpha x+\frac{3x^2-1}{2}\alpha^2+\cdots\Big)=\frac{1}{R}\Big(P_0(x)+P_1(x)\alpha+P_2(x)\alpha^2+\cdots\Big)\Rightarrow\frac{1}{|\mathbf{R}-\mathbf{r}|}=\sum\limits_{l=0}^{\infty}\frac{r^l}{R^{l+1}}P_l(\cos\theta)$.

- For several charges $q_i$, the electrostatic potential at $\mathbf{R}$ is given by $\phi=\frac{1}{4\pi\varepsilon}\sum\limits_{l=0}^{\infty}\frac{1}{R^{l+1}}\Big[\sum\limits_i q_ir_i^lP_l(\cos\theta_i)\Big]$.

(3) When $l$ is even, $y=a_0+a_2x^2+a_4x^4+\cdots+a_lx^l$. When $l$ is odd, $y=a_1x+a_3x^3+a_5x^5+\cdots+a_lx^l$. When $y(1)=1$, the solutions are known as *Legendre polynomials*. $P_0(x)=1$, $P_1(x)=x$, $P_2(x)=\frac{1}{2}\big(3x^2-1\big)$.
(4) Let $\hat{L}^2=-(1-x^2)\frac{d^2}{dx^2}+2x\frac{d}{dx}$. Then the eigenvalue equation $\hat{L}^2P_l(x)=\lambda P_l(x)$ has eigenvalues $\lambda=l(l+1)$.
(5) *Orthogonality*: $\int_{-1}^{1}P_l(x)P_m(x)dx=\frac{2}{2l+1}\delta_{lm}$.
(6) Legendre series expansion $f(x)=\sum\limits_{l=0}^{\infty}c_lP_l(x)$, $x\in[-1,1]$, $c_l=\frac{1}{2}(2l+1)\int_{-1}^{1}f(x)P_l(x)dx$.

- Consider $f(x)=\begin{cases}1, & x\in[0,1]\\ 0, & x\in[-1,0)\end{cases}$. $c_l=\frac{2l+1}{2}\int_{-1}^{l}f(x)P_l(x)dx\Rightarrow f(x)=\frac{1}{4}P_0(x)+\frac{1}{2}P_1(x)+\frac{5}{16}P_2(x)+\cdots$.

(7) *Rodrigue's formula*. $P_l(x)=\frac{1}{2^ll!}\frac{d^l}{dx^l}\big(x^2-1\big)^l$.

### 4.5.4 Bessel's equation

(1) *Bessel's equation* is given by $x^2\frac{d^2y}{dx^2}+x\frac{dy}{dx}+\big(x^2-m^2\big)y=0$ subject to boundary conditions: $y$ is finite at $x=0$.
Let $y=x^s\sum\limits_{n=1}^{\infty}a_nx^n\Rightarrow\sum\limits_{n=0}^{\infty}a_n(n+s)(n+s-1)x^{n+s}+\sum\limits_{n=0}^{\infty}a_n(n+s)x^{n+s}+\sum\limits_{n=2}^{\infty}a_nx^{n+s}-m^2\sum\limits_{n=0}^{\infty}a_nx^{n+s}=0$

- For $n=0$, $s=\pm m$. For $n=1$, $a_1=0$ unless $s=\pm m=-\frac{1}{2}$. For $n\geq 2$, $\Big[(n+s)^2-m^2\Big]a_n+a_{n-2}=0$. Take $s=+m>0$.

$\Rightarrow a_{2j}=\frac{(-1)^ja_0m!}{2^{2j}j!(m+j)!}\Longrightarrow y(x)=\sum\limits_{n=1}^{\infty}a_nx^{m+n}=\cdots=a_0m!2^m\sum\limits_{j=0}^{\infty}\frac{(-1)^j}{j!(m+j)!}\Big(\frac{x}{2}\Big)^{m+j}\Rightarrow y(x)=a_02^mm!J_m(x)$, $J_m(x)=\sum\limits_{j=0}^{\infty}(-1)^j\frac{1}{j!(m+j)!}\Big(\frac{x}{2}\Big)^{m+2j}$.

- $J_m(x)=\frac{1}{m!}\Big(\frac{x}{2}\Big)^m-\frac{1}{(m+1)!}\Big(\frac{x}{2}\Big)^{m+2}+\frac{1}{2!(m+2)!}\Big(\frac{x}{2}\Big)^{m+4}+\cdots\Rightarrow J_0(0)=1$, $J_m(0)=0$ for $m\geq 0$.

(2) *Orthogonality*: $\int_0^lJ_p\Big(\frac{\chi_n}{l}x\Big)J_p\Big(\frac{\chi_m}{l}x\Big)dx=\frac{l^2}{2}J_{p+1}^2(\chi_m)$, where $J_p(\chi_n)=0$.

## 4.6 Miscellaneous

### 4.6.1 Rectangular membranes

(1) Consider the transverse displacement of the membrane satisfying $\frac{d^2\phi}{dx^2}+\frac{d^2\phi}{dy^2}=\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}$ with boundary $\phi_{\text{boundary}}=0$.

• $\phi(x,y,t)=X(x)Y(y)T(t)\Rightarrow\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}=\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}=-k^2$. Let $\frac{1}{X}\frac{d^2X}{dx^2}=-k^2-\frac{1}{Y}\frac{d^2Y}{dy^2}=-k_x^2$, $\frac{1}{Y}\frac{d^2Y}{dy^2}=-k_y^2$.

$\Longrightarrow X(x)=\sin k_x x=\sin\frac{n_x\pi x}{a}$, $Y(y)=\sin k_y y=\sin\frac{n_y\pi y}{b}$, $T(t)=A\cos\omega t+B\sin\omega t$, where $\omega=ck$.

$\Longrightarrow \phi(x,y,t)=\sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\left[A_{n_x,n_y}\cos\left(\omega_{n_x,n_y}t\right)+B_{n_x,n_y}\sin\left(\omega_{n_x,n_y}t\right)\right]\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)$.

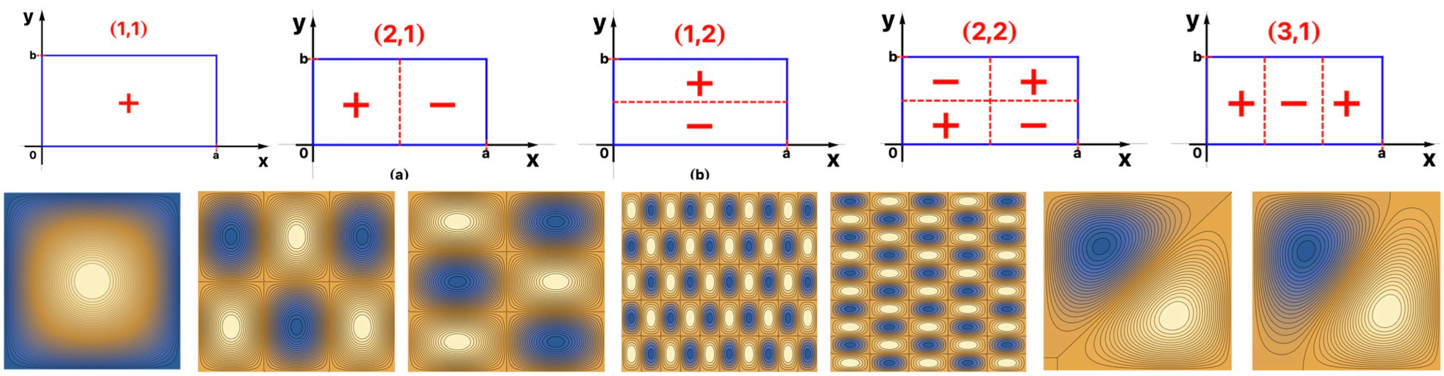
• $\phi(0)=f(x,y)\Rightarrow\sum A_{n_x,n_y}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)=f(x,y)$. $\dot\phi(0)=g(x,y)\Rightarrow\sum\omega_{n_x,n_y}B_{n_x,n_y}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)=g(x,y)$.

$\Longrightarrow A\int_0^a\sin^2\left(\frac{n_x\pi x}{a}\right)dx\int_0^b\sin^2\left(\frac{n_y\pi y}{b}\right)dy=\int_0^a dx\int_0^b dy\,f(x,y)\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)\Rightarrow A=\frac{4}{ab}\int_0^a dx\int_0^b dy\,f(x,y)\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)$.

• Spatial normal modes are specified by $k_x=\frac{n_x\pi}{a}$ and $k_y=\frac{n_y\pi}{b}$ and oscillates with $\omega=ck=c\sqrt{k_x^2+k_y^2}$.

• Lowest order: $\phi_{11}=(A_{11}\cos\omega_{11}t+B_{11}\sin\omega_{11}t)\sin\frac{\pi x}{a}\sin\frac{\pi y}{b}$. $\omega_{11}=ck=c\pi\sqrt{\frac{1}{a^2}+\frac{1}{b^2}}$.

• Consider a square membrane, $\omega_{21}=\omega_{12}$. Consider the linear combination $\phi_{12}-\phi_{21}\propto\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a}-\sin\frac{\pi y}{a}\sin\frac{2\pi x}{a}$.
$\Rightarrow$ The mode vanishes along $y=x$, which is referred toas a *nodal line*.




### 4.6.2 Waveguide

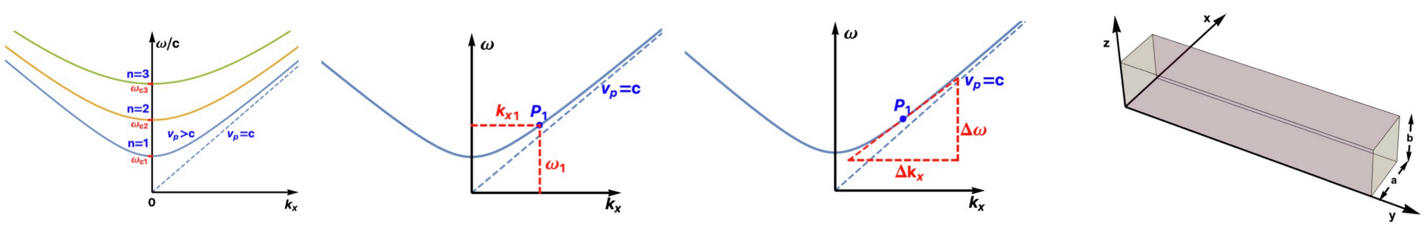
(1) Consider a rectangular stretched membrane attached at $y=0$ and $y=b$, and the wave is free to move along $\pm x$.

• Wave equation $\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}$. $\phi(x,y,t)=X(x)Y(y)T(t)\Rightarrow\frac{\partial^2X}{\partial x^2}=-k_x^2X$, $\frac{\partial^2Y}{\partial y^2}=-k_y^2Y$, $\frac{1}{c^2}\frac{\partial^2T}{\partial t^2}=-k^2T$, $k_x^2+k_y^2=k^2$.

$\Rightarrow Y=\sin k_y y=\sin\frac{n\pi y}{b}$, $X(x)=e^{ik_x x}$, $T(t)=Ae^{i\omega t}+Be^{-i\omega t}\Rightarrow\phi(x,y,t)=\sin\frac{n\pi y}{b}\left[Ae^{i(k_x x+\omega t)}+Be^{i(k_x x-\omega t)}\right]$ and $\frac{\omega^2}{c^2}=k_x^2+\left(\frac{n\pi}{b}\right)^2$.

$\Longrightarrow$ General solution $\phi(x,t)=\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{dk_x}{\sqrt{2\pi}}\sin\frac{n\pi y}{b}\left[A(k_x)e^{i(k_x x+\omega t)}+B(k_x)e^{i(k_x x-\omega t)}\right]$. $v_p=\frac{\omega}{k_x}=c\sqrt{1+\frac{n^2\pi^2}{k_x^2b^2}}$, $v_g=\frac{d\omega}{dk_x}=\frac{c}{\sqrt{1+\frac{n^2\pi^2}{k_x^2b^2}}}$.

• Waves can propagate provided $\omega>c\frac{n\pi}{b}$ ($\lambda<\frac{2b}{n}$), otherwise $k_x$ is imaginary and will be exponentially damped.




(2) Consider the electric field for a Transverse Magnetic (TM) mode. The equation along $y$ is $\frac{\partial^2E_y}{\partial x^2}+\frac{\partial^2E_y}{\partial y^2}+\frac{\partial^2E_y}{\partial z^2}=\frac{1}{c^2}\frac{\partial^2E_y}{\partial t^2}$.

• $E_y=X(x)Y(y)Z(z)T(t)\Rightarrow\frac{d^2X}{dx^2}=-k_x^2X$, $\frac{d^2Y}{dy^2}=-k_y^2Y$, $\frac{d^2Z}{dz^2}=-k_z^2Z$, $\frac{1}{c^2}\frac{d^2T}{dt^2}=-k^2T$ and $k_x^2+k_y^2+k_z^2=k^2=\frac{\omega^2}{c^2}$.

For conducting walls $E_y(0,z)=E_y(a,z)=E_y(x,0)=E_y(x,b)=0\Rightarrow X(x)\sim\sin k_x x=\sin\frac{n\pi x}{a}$, $Z(z)\sim\sin k_z z=\sin\frac{m\pi z}{b}$.

$\Rightarrow\left(\frac{n\pi}{a}\right)^2+\left(\frac{m\pi}{b}\right)^2+k_y^2=\left(\frac{\omega}{c}\right)^2$. The field $E_y=\mathfrak{Re}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left(A_{mn}e^{i\beta_{mn}y}+B_{mn}e^{-i\beta_{mn}y}\right)\sin\frac{n\pi x}{a}\sin\frac{m\pi z}{b}e^{-i\omega t}$, where $\beta_{mn}=k_{ymn}$.

### 4.6.3 Heat flow

(1) Consider a thin circular plate with insulated edges. The temperature distribution satiesfies $\nabla^2 T = \frac{1}{\alpha^2}\frac{\partial T}{\partial t}$.

• In the polar coordinates, $\nabla^2 T = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} = \frac{1}{\alpha^2}\frac{\partial T}{\partial t}$ with boundary condition $\frac{\partial T}{\partial r}\Big|_{r=a} = 0$ and $T(\theta) = T(\theta + 2\pi)$.

$$T(r,\theta,t) = R(r)\Theta(\theta)\tau(t) \Rightarrow \frac{1}{Rr}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{1}{\Theta r^2}\frac{\partial^2\Theta}{\partial\theta^2} = \frac{1}{\alpha^2\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t} = -k^2 \Rightarrow \frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + k^2r^2 + \frac{1}{\Theta}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2} = 0 \Rightarrow \begin{cases} \frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + k^2r^2 = m^2 \\ \frac{1}{\Theta}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2} = -m^2 \end{cases}$$

$\Longrightarrow \Theta(\theta) = A\cos m\theta + B\sin m\theta$, $m \in \mathbb{Z}$ and $r^2\frac{\mathrm{d}^2R}{\mathrm{d}r^2} + r\frac{\mathrm{d}R}{\mathrm{d}r} + \left(k^2r^2 - m^2\right)R = 0 \Rightarrow R(r) = J_m(kr)$ and $J_m'(ka) = 0$ ($k_{mn}$, $n$-th root)

$\Longrightarrow T_{mn} = J_m(k_{mn}r)(A_{mn}\cos m\theta + B_{mn}\sin m\theta)e^{-\alpha^2 k_{mn}^2 t}$, $T(r,\theta,t) = \sum_{mn} T_{mn}(r,\theta,t)$.

### 4.6.4 Spherical waves

(1) Consider the wave on the surface of a sphere $r = a$. $\nabla^2 f(\theta,\phi,t) = \frac{1}{a^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{a^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2} = \frac{1}{c^2}\frac{\partial^2 f}{\partial t^2}$.

• $f = Y(\theta,\phi)T(t) \Rightarrow \frac{1}{Ya^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Ya^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = \frac{1}{c^2T}\frac{\mathrm{d}^2T}{\mathrm{d}t^2} = -\frac{\ell(\ell+1)}{a^2} \Rightarrow T(t) = A\cos\omega t + B\sin\omega t$, $\omega = \frac{c}{a}\sqrt{l(l+1)}$.

$\Longrightarrow \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)Y$. The eigenfunctions $Y(\theta,\phi)$ are known as *spherical harmonics*. $Y = \Theta(\theta)\Phi(\phi)$

$\Longrightarrow \frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \ell(\ell+1)\sin^2\theta = -\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = m^2$. For azimuthally symmetric case, $m = 0$. $f(\theta,t) = \Theta(\theta)T(t)$.

$\Longrightarrow \frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \ell(\ell+1)\sin^2\theta = 0 \xrightarrow{x=\cos\theta} \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)\frac{\mathrm{d}\Theta}{\mathrm{d}x}\right] + \ell(\ell+1)\Theta = 0 \Rightarrow \Theta = P_l(x)$, $l \in \mathbb{Z}$.

$\Longrightarrow f(\theta,t) = \sum_{l=0}^{\infty} P_l(\cos\theta)(A_l\cos\omega_l t + B_l\sin\omega_l t)$, $\omega_l = \frac{c}{a}\sqrt{l(l+1)}$. $\dot{f}(\theta,0) = 0 \Rightarrow B_l = 0$. $f(\theta,0) = g(x) \Rightarrow g(x,0) = \sum_{l=0}^{\infty} P_l(x)A_l$.

$\Longrightarrow \int_{-1}^{1} g(x)P_l(x)\mathrm{d}x = A_l\int_{-1}^{1} P_l^2(x)\mathrm{d}x = \frac{2A_l}{2l+1} \Rightarrow A_l = \frac{2l+1}{2}\int_{-1}^{1} g(x)P_l(x)\mathrm{d}x$.

• Consider an initial condition $g(x) = I\delta(x-1) \Rightarrow A_l = \frac{2l+1}{2}I$, $f(\theta,t) = \frac{I}{2}\sum_{l=0}^{\infty}(2l+1)P_l(x)\cos\omega_l t$ with $\omega_l = \frac{c}{a}\sqrt{l(l+1)}$.

$\Longrightarrow$ At the opposite side $x = -1$, $P_l(-1) = (-1)^l \Rightarrow$ oscillate in sign and interfere destructively except when $\cos\omega_l t = (-1)^l$, which will occur at $\omega_l t = l\pi$. At large $l$, $\omega_l \sim \frac{cl}{a} \Rightarrow t = \frac{\pi a}{c}$ (time taken to travel halfway around the globe at speed $c$).

(2) If the equation retained the $\phi$ dependence ($m \neq 0$).

$\Longrightarrow \Phi(\phi) = A\exp(im\phi)$, $m \in \mathbb{Z}$ and $\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]\Theta = 0 \xrightarrow{x=\cos\theta} \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)\frac{\mathrm{d}\Theta}{\mathrm{d}x}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]\Theta = 0$

$\Longrightarrow \Theta = P_l^m(x)$ (*associated Legendre functions*), $|m| \le l$.

(3) Consider waves inside a sphere $\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2} = \frac{1}{c^2}\frac{\partial^2 f}{\partial t^2}$ with $f(a,\theta,\phi,t) = 0$.

• $f(r,\theta,\phi,t) = R(r)Y(\theta,\phi)T(r) \Rightarrow Y(\theta,\phi) = Y_{lm}$ and $\frac{1}{Rr^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - \frac{l(l+1)}{r^2} = \frac{1}{c^2T}\frac{\mathrm{d}^2T}{\mathrm{d}t^2} = -k^2 \Rightarrow T(t) = A\cos\omega t + B\sin\omega t$

$\Longrightarrow \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \left[k^2r^2 - l(l+1)\right]R = 0 \xrightarrow{x=kr} x^2\frac{\mathrm{d}^2R}{\mathrm{d}x^2} + 2x\frac{\mathrm{d}R}{\mathrm{d}x} + \left[x^2 - l(l+1)\right]R = 0$ (*Spherical Bessel functions*) $\Rightarrow R(r) = j_l(kr)$.

Boundary conditions $\Rightarrow j_l(ka) = 0 \Rightarrow k = k_{ln} \Longrightarrow f_{nlm}(r,\theta,\phi,t) = j_l(k_{ln}r)Y_{lm}(\theta,\phi)(A_{nlm}\cos\omega_{ln}t + B_{nlm}\sin\omega_{ln}t)$.

• $j_l(x) = \sqrt{\frac{\pi}{2x}}J_{l+1/2}(x)$.

# Chapter 5: PHYS30201 Mathematical Foundamentals of Quantum Mechanics

## 5.1 The fundamentals of quantum mechanics

0. Postulates of Quantum Mechanics

(1) The state of a particle is given by a vector $\left|\psi(t)\right\rangle$ in a Hilbert space. The state is normalised: $\langle\psi(t)|\psi(t)\rangle = 1$.

• Consequence: superposition.

(2) There is a Hermitian operator corresponding to each observable property of the particle. Those corresponding to position $\boldsymbol{x}$ and momentum $\boldsymbol{p}$ satisfy $[x_i, p_j] = i\hbar\delta_{ij}$.

• The commutation relation for $\boldsymbol{x}$ and $\boldsymbol{p}$ is a formal expression of Heisenberg's uncertainty principle.

(3) Measurement of the observable associated with the operator $\Omega$ will result in on of the eigenvalues $\omega_i$ of $\Omega$. Immediately after the measurement the particle will be in the corresponding eigenstate $|\omega_i\rangle$.

• Ensures reproducibility of measurements.

(4) The probability of obtaining the result $\omega_i$ in the above measurement (at time $t_0$) is $\left|\langle\omega_i|\psi(t_0)\rangle\right|^2$.

• The postulate expressed this way has the same content as saying that the average value of $\omega$ is given by $\langle\psi(t_0)|\Omega|\psi(t_0)\rangle$.

(5) The time evolution of the state $|psi(t)\rangle$ is given by $i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle$, where $H$ is the operator corresponding to the classical Hamiltonian.

(6) The Hilbert space for a system of two or more subsystems is a product space.

• This is true whether the subsystems interact or not.

1. The propagator: $U(t,t_0) = e^{-iH(t-t_0)/\hbar}$, $U(t,t_0) = \sum_n e^{-iE_n(t-t_0)/\hbar}|n\rangle\langle n|$, $U(t,t_0) = T\exp\left\{-i\int_{t_0}^{t} H(t')\mathrm{d}t'/\hbar\right\}$.

• $i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle \Rightarrow \left|\psi(t+\mathrm{d}t)\right\rangle = \left(1-\frac{i}{\hbar}H\mathrm{d}t\right)\left|\psi(t)\right\rangle \Rightarrow \left|\psi(t)\right\rangle = \lim_{N\to\infty}\left(1-\frac{i}{\hbar}H\frac{(t-t_0)}{N}\right)^N\left|\psi(t_0)\right\rangle = e^{-iH(t-t_0)/\hbar}\left|\psi(t_0)\right\rangle = U(t.t_0)\left|\psi(t_0)\right\rangle$.

• If $\left|\psi(t_0)\right\rangle = \sum_n c_n|n\rangle$, then $\left|\psi(t)\right\rangle = \sum_n c_n e^{-iE_n(t-t_0)/\hbar}|n\rangle$.

2. An example: two state system with $A|a\pm\rangle = \pm|a\pm\rangle$, $B|a\pm\rangle = |a\mp\rangle$.

• Representations under basis $\{|a\pm\rangle\}$: $|a+\rangle \to \begin{pmatrix}0\\1\end{pmatrix}$, $|a-\rangle \to \begin{pmatrix}1\\0\end{pmatrix}$, $A \to \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$, $B \to \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$, $|b\pm\rangle = \sqrt{\frac{1}{2}}(|a+\rangle \pm |a-\rangle) \to \sqrt{\frac{1}{2}}\begin{pmatrix}1\\\pm 1\end{pmatrix}$.

• Possible outcomes after measuring $a = +1$: $\mathcal{P}(b=+1) = |\langle b+|a+\rangle|^2$, $\mathcal{P}(b=-1) = |\langle b-|a+\rangle|^2$

• Consider $H = \hbar\gamma B$. Then $U(t,0) = e^{-i\gamma B} = I - i\gamma tB - \frac{1}{2!}\gamma^2t^2B^2 + i\frac{1}{3!}\gamma^3t^3B^3 + \cdots = \cos\gamma t I - i\sin\gamma t B \to \begin{pmatrix}\cos\gamma t & -i\sin\gamma t\\ -i\sin\gamma t & \cos\gamma t\end{pmatrix}$.

If we start with $\left|\psi(0)\right\rangle = |a+\rangle$, then $\left|\psi(t)\right\rangle = \cos\gamma t|a+\rangle - i\sin\gamma t|a-\rangle = \sqrt{\frac{1}{2}}(e^{-i\gamma t}|b+\rangle + e^{i\gamma t}|b-\rangle)$.

• $\langle A\rangle = \langle\psi(t)|A|\psi(t)\rangle = \cos 2\gamma t$. The system oscillates between $|a\pm\rangle$ with a frequency $2\gamma$.

3. Propagator in the free space. $\psi(\mathbf{r},t) = \langle\mathbf{r}|\psi(t)\rangle = \langle\mathbf{r}|U(t,0)|\psi(0)\rangle = \int\langle\mathbf{r}|U(t,0)|\mathbf{r}'\rangle\psi(\mathbf{r}',0)\mathrm{d}^3\mathbf{r}'$

• $U(\mathbf{r},\mathbf{r}';t,0) = \langle\mathbf{r}|U(t,0)|\mathbf{r}'\rangle$ is the probability of finding the particle at position $\mathbf{r}'$ at time $t$, given that at $t=0$ it was at $\mathbf{r}'$.

$$\left\langle\mathbf{r}|U(t,0)|\mathbf{r}'\right\rangle = \iint\langle\mathbf{r}|\mathbf{p}\rangle\left\langle\mathbf{p}|U(t,0)|\mathbf{p}'\right\rangle\left\langle\mathbf{p}'|\mathbf{r}'\right\rangle\mathrm{d}^3\mathbf{p}\mathrm{d}^3\mathbf{p}' = \iint\langle\mathbf{r}|\mathbf{p}\rangle\left\langle\mathbf{p}\left|\exp\left(\frac{-i\hat{\mathbf{p}}^2t}{2m\hbar}\right)\right|\mathbf{p}'\right\rangle\left\langle\mathbf{p}'|\mathbf{r}'\right\rangle\mathrm{d}^3\mathbf{p}\mathrm{d}^3\mathbf{p}'$$

$$= \frac{1}{(2\pi\hbar)^3}\iint\exp\left(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right)\exp\left(\frac{-i\mathbf{p}^2t}{2m\hbar}\right)\delta\left(\mathbf{p}-\mathbf{p}'\right)\exp\left(\frac{-i\mathbf{p}'\cdot\mathbf{r}'}{\hbar}\right)\mathrm{d}^3\mathbf{p}\mathrm{d}^3\mathbf{p}' = \frac{1}{(2\pi\hbar)^3}\int\exp\left(\frac{-i\mathbf{p}^2t}{2m\hbar} + \frac{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}{\hbar}\right)\mathrm{d}^3\mathbf{p} = \left(\frac{m}{2i\pi\hbar t}\right)^{3/2}\exp\left(\frac{im\left|\mathbf{r}-\mathbf{r}'\right|^2}{2\hbar t}\right)$$

• Suppose $\psi(\mathbf{r},0) = (\pi\Delta^2)^{-3/4}\exp\left(-\frac{|\mathbf{r}|^2}{2\Delta^2}\right)$, then $\psi(\mathbf{r},t) = \pi^{\frac{3}{2}}(\Delta^2 + (\hbar t/m\Delta)^2)^{-\frac{3}{2}}\exp\left(-\frac{|\mathbf{r}|^2}{\Delta^2+(\hbar t/m\Delta)^2}\right)$

$\Longrightarrow$ The narrower the initial wavepacket (in position space), the faster the subsequent spread.

4. Ehrenfest's Thoerem: $\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle = \frac{1}{i\hbar}\langle[\Omega,H]\rangle + \left\langle\frac{\partial\Omega}{\partial t}\right\rangle$. For $H = \frac{p^2}{2m} + V(x)$, $\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \left\langle\frac{p}{m}\right\rangle$, $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\left\langle\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right\rangle$

• Anything that commutes with the Hamiltonian is a constant of motion (a conserved quantity).

• Even if $[\Omega,H] \neq 0$, if the system is in an eigenstate of $H$, the expectation value of $\Omega$ will not change with time: $\langle\psi|[\Omega,H]|\psi\rangle = \langle\psi|\Omega E - E\Omega|\psi\rangle = 0$ (eigenstates).

• If $\Delta x$ and $\Delta p$ are sufficiently small, the quantum motion will approximate the classical path.

5. Harmonic Oscillator

(1) $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$. Define $x_0 = \sqrt{\frac{\hbar}{m\omega}}$, $\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + i\frac{x_0}{\hbar}\hat{p}\right)$, $\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} - i\frac{x_0}{\hbar}\hat{p}\right)$, $[\hat{a},\hat{a}^\dagger] = 1$

• $\hat{H} = \hbar\omega(\hat{a}\hat{a}^\dagger + \frac{1}{2})$, $[\hat{H},\hat{a}] = -\hbar\omega\hat{a}$, $[\hat{H},\hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger$.

• $E_n = \langle n|\hat{H}|n\rangle = \hbar\omega\langle n|\hat{a}^\dagger\hat{a} + \frac{1}{2}|n\rangle = \hbar\omega\langle n|\hat{a}^\dagger\hat{a}|n\rangle + \frac{1}{2}\hbar\omega = \langle\hat{a}n|\hat{a}n\rangle + \frac{1}{2}\hbar\omega \geq \frac{1}{2}\hbar\omega$.

• $\hat{H}(\hat{a}|n\rangle) = \hat{a}\hat{H}|n\rangle - \hbar\omega\hat{a}|n\rangle = (E_n - \hbar\omega)\hat{a}|n\rangle \Longrightarrow \hat{a}^\dagger|n\rangle/\hat{a}|n\rangle$ is an eigenstate with energy $E_n \pm \hbar\omega$.

• $\hat{H}\left(\hat{a}^\dagger\right)^n|0\rangle \equiv \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\left(\hat{a}^\dagger\right)^n|0\rangle = \left(n+\frac{1}{2}\right)\hbar\omega\left(\hat{a}^\dagger\right)^n|0\rangle$. $E_n = (n+\frac{1}{2})\hbar\omega$, $\hat{N} = \hat{a}^\dagger\hat{a}$ is the number operator.

• Normalisation: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$.

• $\phi_0(x) = \langle x|0\rangle$, $\langle x|\hat{a}|0\rangle = 0 \Longrightarrow \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + x_0\frac{\mathrm{d}}{\mathrm{d}x}\right)\phi_0(x) = 0 \Longrightarrow \phi_0(x) = Ne^{-x^2/(2x_0^2)}$. $\phi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{x}{x_0} - x_0\frac{\mathrm{d}}{\mathrm{d}x}\right)^n\phi_0(x)$.

## 5.2 Angular momentum

### 5.2.1 General properties of angular momentum

(1) $[\hat{J}_1,\hat{J}_2] = i\hbar\hat{J}_3$, $[\hat{\mathbf{J}}^2,\hat{J}_i] = 0$. Denote the normalised states $|\lambda,\mu\rangle$ with eigenvalue $\hbar^2\lambda$ of $\hat{\mathbf{J}}^2$ and eigenvalue $\hbar\mu$ of $\hat{J}_3$.

(2) $\hbar^2(\lambda-\mu^2) = \langle\lambda,\mu|\hat{\mathbf{J}}^2 - \hat{J}_3^2|\lambda,\mu\rangle = \langle\lambda,\mu|\hat{J}_1^2 + \hat{J}_2^2|\lambda,\mu\rangle \geq 0 \Longrightarrow |\mu| \leq \sqrt{\lambda}$.

(3) Define $\hat{J}_+ = \hat{J}_1 + i\hat{J}_2$, $\hat{J}_- = \hat{J}_1 - i\hat{J}_2$. $[\hat{J}_+,\hat{J}_-] = 2\hbar J_3$, $[\hat{J}_3,\hat{J}_\pm] = \pm\hbar\hat{J}_\pm$, $[\hat{\mathbf{J}}^2,\hat{J}_\pm] = 0$. $\hat{\mathbf{J}}^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_3^2 = \hat{J}_\pm\hat{J}_\mp + \hat{J}_3^2 \mp \hbar\hat{J}_3$.

(4) $\hat{J}_3\left(\hat{J}_+|\lambda,\mu\rangle\right) = \hat{J}_+\hat{J}_3|\lambda,\mu\rangle + \hbar\hat{J}_+|\lambda,\mu\rangle = \hbar(\mu+1)\left(\hat{J}_+|\lambda,\mu\rangle\right) \Longrightarrow \hat{J}_\pm|\lambda,\mu\rangle$ is another eigenstate of $\hat{J}_3$ with eigenvalue $\hbar(\mu\pm1)$

(5) Suppose $\hat{J}_+|\lambda,\mu\rangle = C_{\lambda\mu}|\lambda,\mu+1\rangle$. $|C_{\lambda\mu}|^2 = \langle\lambda,\mu|\hat{J}_-\hat{J}_+|\lambda\mu\rangle = \langle\lambda,\mu|\hat{\mathbf{J}}^2 - \hat{J}_3^2 - \hbar\hat{J}_3|\lambda,\mu\rangle = \hbar^2(\lambda-\mu^2-\mu) \Rightarrow C_{\lambda\mu} = \hbar\sqrt{\lambda-\mu^2-\mu}$.

(6) $\lambda - \mu_{\max}(\mu_{\max}+1) = 0$, $\lambda - \mu_{\min}(\mu_{\min}+1) = 0$, $\mu_{\max} - \mu_{\min} = N$, $\Longrightarrow \mu_{\max} = \frac{N}{2}$.

(7) $\boxed{\hat{\mathbf{J}}^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle, \quad \hat{J}_3|j,m\rangle = m\hbar|j,m\rangle, \quad \hat{J}_\pm = \hbar\sqrt{j(j+1)-m(m\pm1)}|j,m\pm1\rangle}$

### 5.2.2 Spin$-\frac{1}{2}$ system

(1) Whereas with orbital angular momentum we were talking about an infinite-dimension space which could be considered as a sum of subspaces with $l = 0,1,2,\cdots$, when we talk about intrinsic angular momentum, we are confined to a single subspace with fixed $j(s)$. In the case $s = \frac{1}{2}$, $m = \pm\frac{1}{2}$, the space is 2D with bases denoted by $\left\{\left|\frac{1}{2},\frac{1}{2}\right\rangle,\left|\frac{1}{2},-\frac{1}{2}\right\rangle\right\} = \{|\hat{\mathbf{z}}+\rangle,|\hat{\mathbf{z}}-\rangle\}$.

(2) $\hat{S}_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\sqrt{\frac{3}{4}+\frac{1}{4}}\left|\frac{1}{2},\frac{1}{2}\right\rangle$, $\quad \hat{S}_+\left|\frac{1}{2},\frac{1}{2}\right\rangle = 0$, $\quad \hat{S}_x = \frac{1}{2}\left(\hat{S}_+ + \hat{S}_-\right)$, $\quad \hat{S}_y = -\frac{1}{2}i\left(\hat{S}_+ - \hat{S}_-\right)$.

$\Rightarrow |\hat{\mathbf{z}}+\rangle \xrightarrow{S_z} \begin{pmatrix}1\\0\end{pmatrix}$, $\quad |\hat{\mathbf{z}}-\rangle \xrightarrow{S_z} \begin{pmatrix}0\\1\end{pmatrix}$, $\quad \hat{S}_+ \xrightarrow{S_z} \hbar\begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$, $\quad \hat{S}_- \xrightarrow{S_z} \hbar\begin{pmatrix}0 & 0\\1 & 0\end{pmatrix}$, $\quad \hat{S}_x \xrightarrow{S_z} \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$, $\quad \hat{S}_y \xrightarrow{S_z} \frac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix}$, $\quad \hat{S}_z \xrightarrow{S_z} \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$.

• *Pauli matrices*: $\sigma_1 = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$, $\sigma_2 = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}$, $\sigma_3 = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$.

• $[\sigma_1,\sigma_2] = 2i\sigma_3$, $\quad \sigma_i\sigma_j = \delta_{ij}\mathbf{I} + i\sum_k \varepsilon_{ijk}\sigma_k$, $\quad \sigma_i^2 = \mathbf{I}$.

• $\mathbf{a}\cdot\boldsymbol{\sigma}$ is Hermitian. $\quad (\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b}\mathbf{I} + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}$.

• Together with the identity matrix, they form a basis (with real coefficients) for all Hermitian $2\times2$ matrices.

• The eigenvectors of a $\sigma_1$: $|\hat{\mathbf{x}}+\rangle = \frac{1}{\sqrt{2}}(|\hat{\mathbf{z}}-\rangle + |\hat{\mathbf{z}}+\rangle) \to \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$, $\quad |\hat{\mathbf{x}}-\rangle = \frac{1}{\sqrt{2}}(|\hat{\mathbf{z}}-\rangle - |\hat{\mathbf{z}}+\rangle) \to \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$.

• $\mathbf{n} = \sin\theta\cos\varphi\mathbf{e}_x + \sin\theta\sin\varphi\mathbf{e}_y + \cos\theta\mathbf{e}_z$. Then $\hat{\mathbf{S}}\cdot\mathbf{n} \xrightarrow{S_z} \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\\\sin\theta e^{i\varphi} & -\cos\theta\end{pmatrix}$ with eigenvector $|\mathbf{n}+\rangle \xrightarrow{S_z} \begin{pmatrix}\cos\frac{\theta}{2}e^{-i\varphi/2}\\\sin\frac{\theta}{2}e^{i\varphi/2}\end{pmatrix}$.

(3) The Hamiltonian of a spin$-\frac{1}{2}$ electron in a uniform magnetic field $\hat{H} = -\boldsymbol{\mu}\cdot\mathbf{B} = \frac{g_s\mu_B}{\hbar}\hat{\mathbf{S}}\cdot\mathbf{B} \xrightarrow{S_z} \mu_B\boldsymbol{\sigma}\cdot\mathbf{B}$.

• Assume $|\psi(0)\rangle = |\hat{\mathbf{z}}+\rangle = \frac{1}{\sqrt{2}}(|\hat{\mathbf{x}}+\rangle + |\hat{\mathbf{x}}-\rangle)$, then $|\psi(t)\rangle = \frac{1}{\sqrt{2}}(e^{-i\omega t/2}|\hat{\mathbf{x}}+\rangle + e^{i\omega t/2}|\hat{\mathbf{x}}-\rangle) = \cos\frac{\omega t}{2}|\hat{\mathbf{z}}+\rangle - \sin\frac{\omega t}{2}|\hat{\mathbf{z}}-\rangle$, $\omega = 2\gamma = \frac{2\mu_B B}{\hbar}$.

• $\langle\psi(t)|\hat{S}_z|\psi(t)\rangle = \frac{\hbar}{2}\cos\omega t$, $\langle\psi(t)|\hat{S}_y|\psi(t)\rangle = -\frac{\hbar}{2}\sin\omega t$, $\langle\psi(t)|\hat{S}_x|\psi(t)\rangle = 0$. So $\langle\hat{\mathbf{S}}\rangle$ is a vector of length $\frac{\hbar}{2}$ in the $yz$ plane which rotates with frequency $\omega = 2\mu_B B/\hbar$.

### 5.2.3 Addition of angular momenta

(1) $\hat{\mathbf{J}} = \hat{\mathbf{L}}\otimes\hat{I} + \hat{I}\otimes\hat{\mathbf{S}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$, $\hat{\mathbf{J}}^2 = \hat{\mathbf{L}}^2\otimes\hat{I} + \hat{I}\otimes\hat{\mathbf{S}}^2 + 2\hat{\mathbf{L}}\otimes\hat{\mathbf{S}} = \hat{\mathbf{L}}^2 + \hat{\mathbf{S}}^2 + 2\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$.

(2) $[\hat{\mathbf{L}}^2,\hat{J}_i] = 0, [\hat{\mathbf{S}}^2,\hat{J}_i] = 0 \Longrightarrow (l,s,m_l,m_s), m_j = m_l + m_s$. $\quad [\hat{\mathbf{J}}^2,\hat{L}_i] \neq 0, [\hat{\mathbf{J}}^2,\hat{S}_i] \neq 0 \Longrightarrow (l,s,j,m_j)$. $|l,m_l\rangle\otimes|s,m_s\rangle \to |l,s,j,m_j\rangle$.

(3) The state of maximal $m$ in a multiplet $|j,j\rangle$ is called the *stretched state*. Denote $j_> = l+s$.

• $|j_>,j_>\rangle = |l,l\rangle\otimes|s,s\rangle \Rightarrow \hat{J}_-|j_>,j_>\rangle = (\hat{L}_-|l,l\rangle)\otimes|s,s\rangle + |l,l\rangle\otimes(\hat{S}_-|s,s\rangle) \Rightarrow \sqrt{2j_>}|j_>,j_>-1\rangle = \sqrt{2l}|l,l-1\rangle\otimes|s,s\rangle + \sqrt{2s}|l,l\rangle\otimes|s,s-1\rangle$. After $2j_>$ steps we will reach the bottom of the latter $|j_>,-j_>\rangle = |l,-l\rangle\otimes|s,-s\rangle$. Whichever is the smaller of $l$ or $s$ will govern the maximum number of $\{m_l,m_s\}$ that can equal any $m_j$.

• $\begin{cases}|j_>,j_>-1\rangle = \sqrt{\frac{l}{l+s}}|l,l-1\rangle\otimes|s,s\rangle + \sqrt{\frac{s}{l+s}}|l,l\rangle\otimes|s,s-1\rangle.\\|j_>-1,j_>-1\rangle = -\sqrt{\frac{s}{l+s}}|l,l-1\rangle\otimes|s,s\rangle + \sqrt{\frac{l}{l+s}}|l,l\rangle\otimes|s,s-1\rangle.\end{cases}$

• When we add angular momenta with quantum numbers $l$ and $s$, the quantum number $j$ that gives the magnitude of the total runs in steps of one over the range $|l-s| \leq j \leq l+s$.

(4) An example for $l = 2, s = 1$:

$$|3,3\rangle = |2,2\rangle\otimes|1,1\rangle$$
$$|3,2\rangle = \sqrt{\frac{2}{3}}|2,1\rangle\otimes|1,1\rangle + \sqrt{\frac{1}{3}}|2,2\rangle\otimes|1,0\rangle,$$
$$|3,1\rangle = \sqrt{\frac{2}{5}}|2,0\rangle\otimes|1,1\rangle + \sqrt{\frac{8}{15}}|2,1\rangle\otimes|1,0\rangle,$$
$$|3,0\rangle = \sqrt{\frac{1}{5}}|2,-1\rangle\otimes|1,1\rangle + \sqrt{\frac{3}{5}}|2,0\rangle\otimes|1,0\rangle + \sqrt{\frac{1}{5}}|2,1\rangle\otimes|1,-1\rangle$$
$$|3,-1\rangle = \sqrt{\frac{1}{15}}|2,-2\rangle\otimes|1,1\rangle + \sqrt{\frac{8}{15}}|2,-1\rangle\otimes|1,0\rangle + \sqrt{\frac{2}{5}}|2,0\rangle\otimes|1,-1\rangle$$
$$|3,-2\rangle = \sqrt{\frac{1}{3}}|2,-2\rangle\otimes|1,0\rangle + \sqrt{\frac{2}{3}}|2,-1\rangle\otimes|1,-1\rangle,$$
$$|3,-3\rangle = |2,-2\rangle\otimes|1,-1\rangle$$

$$|2,2\rangle = -\sqrt{\frac{1}{3}}|2,1\rangle\otimes|1,1\rangle + \sqrt{\frac{2}{3}}|2,2\rangle\otimes|1,0\rangle,$$
$$|2,1\rangle = -\sqrt{\frac{1}{2}}|2,0\rangle\otimes|1,1\rangle + \sqrt{\frac{1}{6}}|2,1\rangle\otimes|1,0\rangle,$$
$$|2,0\rangle = -\sqrt{\frac{1}{2}}|2,-1\rangle\otimes|1,1\rangle + 0|2,0\rangle\otimes|1,0\rangle + \sqrt{\frac{1}{2}}|2,1\rangle\otimes|1,-1\rangle$$
$$|2,-1\rangle = -\sqrt{\frac{1}{3}}|2,-2\rangle\otimes|1,1\rangle - \sqrt{\frac{1}{6}}|2,-1\rangle\otimes|1,0\rangle + \sqrt{\frac{1}{2}}|2,0\rangle\otimes|1,-1\rangle$$
$$|2,-2\rangle = -\sqrt{\frac{2}{3}}|2,-2\rangle\otimes|1,0\rangle + \sqrt{\frac{1}{3}}|2,-1\rangle\otimes|1,-1\rangle$$

$$|1,1\rangle = \sqrt{\frac{1}{10}}|2,0\rangle\otimes|1,1\rangle - \sqrt{\frac{3}{10}}|2,1\rangle\otimes|1,0\rangle$$
$$|1,0\rangle = \sqrt{\frac{3}{10}}|2,-1\rangle\otimes|1,1\rangle - \sqrt{\frac{2}{5}}|2,0\rangle\otimes|1,0\rangle\sqrt{\frac{3}{10}}|2,1\rangle\otimes|1,-1\rangle$$
$$|1,-1\rangle = \sqrt{\frac{3}{5}}|2,-2\rangle\otimes|1,1\rangle - \sqrt{\frac{3}{10}}|2,-1\rangle\otimes|1,0\rangle + \sqrt{\frac{1}{10}}|2,0\rangle\otimes|1,-1\rangle$$

• The coefficients (*Clebsch-Gordan coefficients*) are inner products ($\left\langle l,s,m_l,m_s \middle| j,m_j \right\rangle$)
(5) The general form: $|J,M\rangle = \sum_{m_1,m_2} \langle j_1,m_1;j_2,m_2|J,M\rangle |j_1,m_1\rangle\otimes|j_2,m_2\rangle$, $\quad |j_1,m_1\rangle\otimes|j_2,m_2\rangle = \sum_{J,M}\langle j_1,m_1;j_2,m_2|J,M\rangle|J,M\rangle$.
• For $s=\frac{1}{2}, j=l\pm\frac{1}{2}$: $\left|l\pm\frac{1}{2},m_j\right\rangle = \sqrt{\frac{l\mp m_j+\frac{1}{2}}{2l+1}}\left|l,m_j+\frac{1}{2}\right\rangle\otimes\left|\frac{1}{2},-\frac{1}{2}\right\rangle \pm \sqrt{\frac{l\pm m_j+\frac{1}{2}}{2l+1}}\left|l,m_j-\frac{1}{2}\right\rangle\otimes\left|\frac{1}{2},\frac{1}{2}\right\rangle$.
• $\mathbb{V}^{2j_1+1}\otimes\mathbb{V}^{2j_2+1} = \mathbb{V}^{2|j_1-j_2|+1}\oplus\mathbb{V}^{2(j_1+j_2)+1}$. In particular for $s=\frac{1}{2}$: $\mathbb{V}^{2l+1}\otimes\mathbb{V}^2 = \mathbb{V}^{2l+2}\oplus\mathbb{V}^{2l}$.
(6) Example: spin-1 particles. The basis are $|1,1\rangle, |1,0\rangle, |1,-1\rangle$.

## 5.3 Approximation method – Variational method

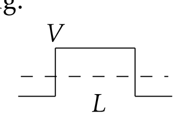
### 5.3.1 Ground state

(1) Suppose we know the Hamiltonian of a bound system but don't know the energy of the ground state: $\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0$.
• $|\Psi\rangle = \sum_n c_n|n\rangle$, $\langle\Psi|\hat{H}|\Psi\rangle = \sum_{n,m} c_m^* c_n \langle m|\hat{H}|n\rangle = \sum_n |c_n|^2 E_n$, $\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum_n |c_n^2| E_n}{\sum_n |c_n|^2} \geq E_0$.
(2) Example: Infinite square well with $V\big|_{0<x<a} = 0$. Trial function $\Psi(x)\big|_{0<x<a} = x(a-x)$.
$\Longrightarrow \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{1}{2m}\frac{\langle\Psi|\hat{p}^2|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{1}{2m}\frac{\langle\hat{p}\Psi|\hat{p}\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{10\hbar^2}{2ma^2} = 1.013\frac{\pi^2\hbar^2}{2ma^2}$.
• Use an adjustable parameter $\Rightarrow \Psi(x) = x(a-x) + bx^2(a-x)^2$.

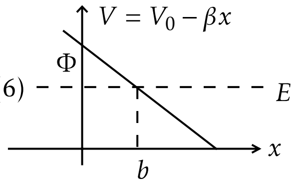
### 5.3.2 Excited states

(1) $\left\langle\hat{H}\right\rangle = \sum_n P_n E_n$, where $P_n$ are the squares of the overlap between the trial function and the actual eigenstates of the system $\Rightarrow$ We can only find bounds on excited states if we can *arrange for the overlap of the trial wave function with all lower states to be zero.*
• The lowest state with odd parity will automatically have zero overlap with the even-parity ground state.
(2) Example: For square well. Trial function $\Psi_1(x) = x(a-x)(2x-a)$.

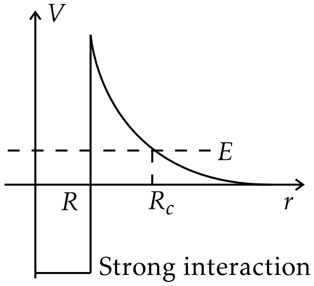
## 5.4 Approximation method – WKB approximation

(1) The one-dimensional TISE can be written as $\frac{d^2\psi}{dx^2} = -k(x)^2\psi(x)$, where $k(x) = \sqrt{2m(E-V(x))}/\hbar$.
• $k(x)$ can be thought as a *spatially-varying wavenumber* if it doesn't change too quickly with position.
(2) An approximation for the wave function is $\psi(x) = \frac{A}{\sqrt{k(x)}}\exp\left(\pm i\int^x k(x')dx'\right)$ provided $|\lambda'(x)| = \left|\frac{k'(x)}{k(x)^2}\right| \ll 1$.
(3) WKB approximation for bound states: In the classically allowed region the wave function will be oscillatory and can be written as an equal superposition of right- and left-moving waves as $\psi(x) = \frac{A}{\sqrt{k(x)}}\cos\left(\int_{x_0}^x k(x')dx' + \phi\right)$.
• For infinite well, the solution vanish at the boundaries ($x=a,b$), $\int_a^b k(x')dx' = (n+1)\pi$.
• For a general potential, outside the classically allowed region we have decaying exponentials. $\int_a^b k(x')dx' = (n+\frac{1}{2})\pi$.
(4) Example:
(5) WKB for tunnelling:
• For a square barrier 

$E$, the tunnelling probability $T = \left[\begin{matrix}\text{prefactor from}\\ \text{reflection at the ends}\end{matrix}\right]\times e^{-2\kappa L}$, $\kappa = \frac{1}{\hbar}\sqrt{2m(V-E)}$.
• Consider barrier that can be split into series of square ones, in each slice $T\propto e^{-2\kappa(x_N)\Delta L}$, define *decay length* $\lambda = \frac{1}{\kappa}$, if $|\lambda'| \ll 1$, then we can take $\Delta L \gg \lambda$ but still small on scale of variation of $V(x)$. $\Longrightarrow T = [\text{prefactor}]\times\exp\left(-2\int_a^b \kappa(x')dx'\right)$.

(6) 


Example: Field emission. Metal surface (cathode) in an electric field can emit electron. $W = 2\int_0^b \frac{1}{\hbar}\sqrt{2m(V(x)-E)}\mathrm{d}x = \frac{2}{\hbar}\int_0^b \sqrt{2m(\Phi-\beta x)}\mathrm{d}x = \frac{4\sqrt{2m}}{3\hbar}\frac{\Phi^{3/2}}{\beta}$, $T \propto e^{-W}$.

(7) 


Example: $\alpha$ decay. $V_C(r) = Z_1 Z_2 \frac{\alpha\hbar c}{r}$.
$W = 2\int_R^{R_C}\frac{1}{\hbar}\sqrt{2m(V_C(r)-E)}\mathrm{d}r = 2\sqrt{\frac{2mc^2E}{\hbar^2c^2}}\int_R^{R_C}\left(\frac{R_C}{r}-1\right)^{1/2}\mathrm{d}r = \sqrt{\frac{E_G}{E}}$, $T \propto \exp\left(-\sqrt{\frac{E_G}{E}}\right)$.

## 5.5 Approximation method – Time independent perturbation theory

### 5.5.1 Non-degenerate perturbation theory

(1) $\left(\hat{H}^{(0)} + \lambda\hat{H}^{(1)}\right)|n\rangle = E_n|n\rangle$. Then substitue in $E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$ and $|n\rangle = |n(0)\rangle + \lambda|n(1)\rangle + \lambda^2|n(2)\rangle + \cdots$.

• Match terms with $\lambda \Longrightarrow$

$$\hat{H}^{(0)}\left|n^{(0)}\right\rangle = E_n^{(0)}\left|n^{(0)}\right\rangle \qquad (4.1)$$
$$\hat{H}^{(0)}\left|n^{(1)}\right\rangle + \hat{H}^{(1)}\left|n^{(0)}\right\rangle = E_n^{(0)}\left|n^{(1)}\right\rangle + E_n^{(1)}\left|n^{(0)}\right\rangle \qquad (4.2)$$
$$\hat{H}^{(0)}\left|n^{(2)}\right\rangle + \hat{H}^{(1)}\left|n^{(1)}\right\rangle = E_n^{(0)}\left|n^{(2)}\right\rangle + E_n^{(1)}\left|n^{(1)}\right\rangle + E_n^{(2)}\left|n^{(0)}\right\rangle \qquad (4.3)$$

(2) Inner product with $\left\langle n^{(0)}\right| \Rightarrow \begin{cases}\left\langle n^{(0)}\middle|\hat{H}^{(0)}\middle|n^{(1)}\right\rangle + \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle = E_n^{(0)}\left\langle n^{(0)}\middle|n^{(1)}\right\rangle + E_n^{(1)}\left\langle n^{(0)}\middle|n^{(0)}\right\rangle \Rightarrow E_n^{(1)} = \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle. \\ \left\langle n^{(0)}\middle|\hat{H}^{(0)}\middle|n^{(2)}\right\rangle + \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(1)}\right\rangle = E_n^{(0)}\left\langle n^{(0)}\middle|n^{(2)}\right\rangle + E_n^{(1)}\left\langle n^{(0)}\middle|n^{(1)}\right\rangle + E_n^{(2)}\left\langle n^{(0)}\middle|n^{(0)}\right\rangle\end{cases}$

• Unperturbed states $\left\{\left|n^{(0)}\right\rangle\right\}$ form a basis, write $\left|n^{(1)}\right\rangle = \sum_m c_m\left|m^{(0)}\right\rangle = \sum_m\left\langle m^{(0)}\middle|n^{(1)}\right\rangle\left|m^{(0)}\right\rangle$.

• Inner product with $\left\langle m^{(0)}\right|$ for $m \neq n \Rightarrow \left\langle m^{(0)}\middle|\hat{H}^{(0)}\middle|n^{(1)}\right\rangle + \left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle = E_n^{(0)}\left\langle m^{(0)}\middle|n^{(1)}\right\rangle + E_n^{(1)}\left\langle m^{(0)}\middle|n^{(0)}\right\rangle$

$\Longrightarrow E_m^{(0)}\left\langle m^{(0)}\middle|n^{(1)}\right\rangle + \left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle = E_n^{(0)}\left\langle m^{(0)}\middle|n^{(1)}\right\rangle \Rightarrow \left\langle m^{(0)}\middle|n^{(1)}\right\rangle = \frac{\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle}{E_n^{(0)}-E_m^{(0)}} \Rightarrow |n(1)\rangle = \sum_{m\neq n}\frac{\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle}{E_n^{(0)}-E_m^{(0)}}\left|m^{(0)}\right\rangle$.

• The undetermined $\left\langle n^{(0)}\middle|n^{(1)}\right\rangle$ is imaginary and can be ignored $\Rightarrow E_n^{(2)} = \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(1)}\right\rangle = \sum_{m\neq n}\frac{\left|\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}}$.

(2) Summary results:

$$|n\rangle = |n(0)\rangle + \sum_{m\neq n}\frac{\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle}{E_n^{(0)}-E_m^{(0)}}\left|m^{(0)}\right\rangle + \cdots, \qquad E_n = E_n^{(0)} + \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle + \sum_{m\neq n}\frac{\left|\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}} + \cdots$$

(3) Perturbed harmonic oscillator: $\hat{H}^{(0)} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ with $\hat{H}^{(1)} = \lambda\hat{x}^2$. Unperturbed states $|n(0)\rangle$ with $E_0^{(0)} = (n+\frac{1}{2})\hbar\omega$.

• $\hat{x} = \frac{x_0}{\sqrt{2}}\left(\hat{a}+\hat{a}^\dagger\right) \Rightarrow E_n^{(1)} = \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle = \frac{x_0^2\lambda}{2}\left\langle n^{(0)}\middle|\left(\hat{a}^\dagger\right)^2 + \hat{a}^2 + 2\hat{a}^\dagger\hat{a} + 1\middle|n^{(0)}\right\rangle = \frac{\lambda}{m\omega^2}\hbar\omega\left(n+\frac{1}{2}\right)$

• $\left|n^{(1)}\right\rangle = \sum_{m\neq n}\frac{\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle}{E_n^{(0)}-E_m^{(0)}}\left|m^{(0)}\right\rangle = \frac{\hbar\lambda}{2m\omega}\left(\frac{\sqrt{(n+1)(n+2)}}{-2\hbar\omega}\left|(n+2)^{(0)}\right\rangle + \frac{\sqrt{n(n-1)}}{2\hbar\omega}\left|(n-2)^{(0)}\right\rangle\right)$.

• $E_n^{(2)} = \left\langle n^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(1)}\right\rangle = \sum_{m\neq n}\frac{\left|\left\langle m^{(0)}\middle|\hat{H}^{(1)}\middle|n^{(0)}\right\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}} = \left(\frac{\hbar\lambda}{2m\omega}\right)^2\left(\frac{(n+1)(n+2)}{-2\hbar\omega} + \frac{n(n-1)}{2\hbar\omega}\right) = -\frac{1}{2}\left(\frac{\lambda}{m\omega^2}\right)^2\hbar\omega\left(n+\frac{1}{2}\right)$

• Define $\omega' = \omega\sqrt{1+\frac{2\lambda}{m\omega^2}} \Rightarrow E_n = \left(n+\frac{1}{2}\right)\hbar\omega' = \left(n+\frac{1}{2}\right)\hbar\omega\left(1+\frac{\lambda}{m\omega^2} - \frac{1}{2}\left(\frac{\lambda}{m\omega^2}\right)^2 + \ldots\right)$

### 5.5.2 Degenerate perturbation theory

(1) We need to find a new set of states in the degenerate space, linear combinations of our initial choice, which are not mixed by the perturbation, i.e. $\left\langle m'^{(0)}\middle|\hat{H}^{(1)}\middle|n'^{(0)}\right\rangle = 0$ if $E_m^{(0)} = E_n^{(0)}$ for $m \neq n$. In the new basis $\hat{H}^{(1)}$ is diagonal in the degenerate subspace.

(2) Example: Suppose we have a three-state basis with degenerate energies:

$$\left|1^{(0)}\right\rangle \longrightarrow \begin{pmatrix}1\\0\\0\end{pmatrix},\quad \left|2^{(0)}\right\rangle \longrightarrow \begin{pmatrix}0\\1\\0\end{pmatrix},\quad \left|3^{(0)}\right\rangle \longrightarrow \begin{pmatrix}0\\0\\1\end{pmatrix},\quad \hat{H}^{(0)} \longrightarrow \begin{pmatrix}E_0 & 0 & 0\\0 & E_0 & 0\\0 & 0 & 2E_0\end{pmatrix},\quad \hat{H}^{(1)} \longrightarrow a\begin{pmatrix}1 & 1 & 1\\1 & 1 & 1\\1 & 1 & 1\end{pmatrix}$$

In the eigenspace of $\left|1^{(0)}\right\rangle$ and $\left|2^{(0)}\right\rangle$, $\hat{H}^{(1)} \to a\left(\begin{smallmatrix}1 & 1\\1 & 1\end{smallmatrix}\right)$ with eigenstates $\sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\-1\end{smallmatrix}\right)$, $\sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\1\end{smallmatrix}\right)$ and respective eigenvalues $0, 2a$.

We now have new basis $\left|1'^{(0)}\right\rangle \to \sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\-1\\0\end{smallmatrix}\right)$, $\left|2'^{(0)}\right\rangle \to \sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\1\\0\end{smallmatrix}\right)$, $\left|3^{(0)}\right\rangle \to \left(\begin{smallmatrix}0\\0\\1\end{smallmatrix}\right)$. Also, $\left\langle 2'^{(0)}\middle|\hat{H}^{(1)}\middle|1'^{(0)}\right\rangle = 0$

- $E^{(1)}_{1'} = \left\langle 1'^{(0)}\middle|\hat{H}^{(1)}\middle|1'^{(0)}\right\rangle = 0,\ E^{(1)}_{2'} = \left\langle 2'^{(0)}\middle|\hat{H}^{(1)}\middle|2'^{(0)}\right\rangle = \sqrt{\frac{1}{2}}(1\ 1\ 0)a\left(\begin{smallmatrix}1&1&1\\1&1&1\\1&1&1\end{smallmatrix}\right)\sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\1\\0\end{smallmatrix}\right) = 2a,\ E^{(1)}_3 = a.$
- $\left\langle 3'^{(0)}\middle|\hat{H}^{(1)}\middle|1'^{(0)}\right\rangle = (0\ 0\ 1)a\left(\begin{smallmatrix}1&1&1\\1&1&1\\1&1&1\end{smallmatrix}\right)\sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\-1\\0\end{smallmatrix}\right) = 0,\quad \left\langle 3'^{(0)}\middle|\hat{H}^{(1)}\middle|2'^{(0)}\right\rangle = (0\ 0\ 1)a\left(\begin{smallmatrix}1&1&1\\1&1&1\\1&1&1\end{smallmatrix}\right)\sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\1\\0\end{smallmatrix}\right) = \sqrt{2}a.$
- $\left|1'^{(1)}\right\rangle = 0,\ \left|2'^{(1)}\right\rangle = \frac{\left\langle 3^{(0)}\middle|\hat{H}^{(1)}\middle|2'^{(0)}\right\rangle}{E^{(0)}_2 - E^{(0)}_3}\left|3^{(0)}\right\rangle = \frac{\sqrt{2}a}{-E_0}\left|3^{(0)}\right\rangle \to -\frac{\sqrt{2}a}{E_0}\left(\begin{smallmatrix}0\\0\\1\end{smallmatrix}\right),\ \left|3^{(1)}\right\rangle = 0\left|1'^{(0)}\right\rangle + \frac{\left\langle 2'^{(0)}\middle|\hat{H}^{(1)}\middle|3^{(0)}\right\rangle}{E^{(0)}_3 - E^{(0)}_2}\left|2'^{(0)}\right\rangle = \frac{\sqrt{2}a}{E_0}\left|2'^{(0)}\right\rangle \to \frac{a}{E_0}\left(\begin{smallmatrix}1\\1\\0\end{smallmatrix}\right).$
- $E^{(2)}_{1'} = \frac{\left|\left\langle 3^{(0)}\middle|\hat{H}^{(1)}\middle|1'^{(0)}\right\rangle\right|^2}{E^{(0)}_1 - E^{(0)}_3} = 0,\ E^{(2)}_{2'} = \frac{\left|\left\langle 3^{(0)}\middle|\hat{H}^{(1)}\middle|2'^{(0)}\right\rangle\right|^2}{E^{(0)}_2 - E^{(0)}_3} = -\frac{2a^2}{E_0},\ E^{(2)}_3 = \frac{\left|\left\langle 1'^{(0)}\middle|\hat{H}^{(1)}\middle|3^{(0)}\right\rangle\right|^2}{E^{(0)}_3 - E^{(0)}_1} + \frac{\left|\left\langle 2'^{(0)}\middle|\hat{H}^{(1)}\middle|3^{(0)}\right\rangle\right|^2}{E^{(0)}_3 - E^{(0)}_2} = \frac{2a^2}{E_0}.$
- $\left|3^{(1)}\right\rangle = \frac{\left\langle 1'^{(0)}\middle|\hat{H}^{(1)}\middle|3^{(0)}\right\rangle}{E_0}\left|1'^{(0)}\right\rangle + \frac{\left\langle 2'^{(0)}\middle|\hat{H}^{(1)}\middle|3^{(0)}\right\rangle}{E_0}\left|2'^{(0)}\right\rangle = \frac{1}{E_0}\left(\left|1'^{(0)}\right\rangle\left\langle 1'^{(0)}\right| + \left|2'^{(0)}\right\rangle\left\langle 2'^{(0)}\right|\right)\hat{H}^{(1)}\left|3^{(0)}\right\rangle = \frac{1}{E_0}\left(\left|1^{(0)}\right\rangle\left\langle 1^{(0)}\right| + \left|2^{(0)}\right\rangle\left\langle 2^{(0)}\right|\right)\hat{H}^{(1)}\left|3^{(0)}\right\rangle.$

$\Rightarrow$ We could equally have used the un-diagonalised states.

### 5.5.3 The hydrogen atom

(1.1) Non-relativistic H atom: $\hat{H}^{(0)} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{\alpha\hbar c}{r}$ with eigenvalues $E^{(0)}_n = -\frac{E_R}{n^2}$, where $E_R = \frac{1}{2}\alpha^2 mc^2 \Rightarrow$ Depend only on $n$.

(1.2) The wave function of the ground state $\psi_0 \propto e^{-r/a_0}$ where $a_0 = \frac{\hbar c}{\alpha mc^2}$. Typical momentum $p_0 = \alpha mc \ll mc$.

(1.3) Full eigenstates are given by $|n,l,m_l\rangle \otimes \left|\frac{1}{2}, m_s\right\rangle = |n,l,m_l,m_s\rangle$ or $\left|n,l,j,m_j\right\rangle$.

(2) Relativistic correction: $E_{\text{KE}} = \sqrt{m^2c^4 + p^2c^2} - mc^2 = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots \Longrightarrow$ perturbation $\hat{H}^{(1)}_{\text{KE}} = -\frac{\hat{p}^4}{8m^3c^2} = -\frac{1}{2mc^2}\left(\hat{H}^{(0)} - \hat{V}^2_C\right)^2$.

$$\left\langle n,l\middle|\hat{H}^{(1)}_{\text{KE}}\middle|n,l\right\rangle = -\alpha^2\frac{\left|E^{(0)}_n\right|}{n}\left(\frac{2}{2l+1} - \frac{3}{4n}\right)$$

(3) Spin-orbit interaction $\hat{H}^{(0)}_{\text{SO}} = \frac{1}{2m^2c^2r}\frac{\mathrm{d}V_C}{\mathrm{d}r}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$. $2\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} = \hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2 \Rightarrow$ States with definite $j$ are not mixed by S.O..

$$\left\langle n,l,j,m_j\middle|\hat{H}^{(0)}_{\text{SO}}\middle|n,l,j,m_j\right\rangle = \alpha^2\frac{\left|E^{(0)}_n\right|^2}{n}\left(\frac{2}{2l+1} - \frac{2}{2j+1}\right)\quad (l \neq 0)$$

(4) For $l = 0$, the Darwin term is the same as the expression above.

$$\left\langle n,l,j,m_j\middle|\hat{H}^{(0)}_{\text{KE}} + \hat{H}^{(0)}_{\text{SO}} + \hat{H}^{(0)}_{\text{D}}\middle|n,l,j,m_j\right\rangle = \alpha^2\frac{\left|E^{(0)}_n\right|^2}{n}\left(\frac{3}{4n} - \frac{2}{2j+1}\right)$$

- All of these effects are of the same order of magnitude $\alpha^2 E^{(0)}_n$.

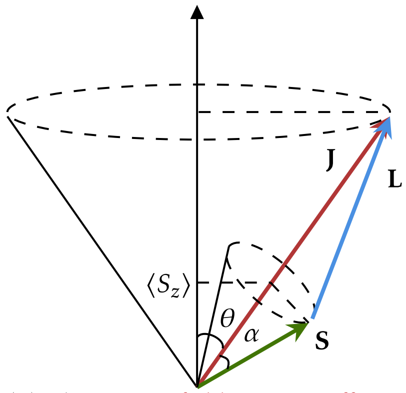
(5) For atoms spin-orbit interaction lowers energy of smaller $j$. $E_{2p_{3/2}} - E_{2p_{1/2}} = 4.5\times10^{-5}$ eV $\approx \mu_B B \Rightarrow B \approx 1$T.

(6) The proton has a magnetic moment $\mu_p = g_p\frac{e\hbar}{2m_p}$. This generates a magnetic coupling between $p$ spin and $e$ angular momentum. The splittings $\approx \frac{m_e}{m_p} \approx 10^{-3}$ smaller than electronic S.O. $\Rightarrow$ *hyperfine structure*.

(7) *Lamb shift*: A combined effect of virtual particles and the charge radius the proton.

- Breaks the degeneracy of $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ by $\Delta E \approx 4.4\times10^{-6}$ eV.

(8) The *weak-field Zeeman effect*: H atom in an external field $\mathbf{B} = B\mathbf{e}_z$, where $B \ll 1$T. The fine structure effects will be stronger; the basis is then $\left\{\left|n,l,j,m_j\right\rangle\right\}$ and states of the same $j$ but different $L$ and $m_j$ are degenerate.




The perturbing Hamiltonian $\hat{H}^{(1)}_{\rm mag} = \frac{\mu_B B}{\hbar}\left(\hat{L}_z + 2\hat{S}_z\right)$.

$E^{(1)}_{nljm_j} = \frac{\mu_B B}{\hbar}\left\langle j, m_j\middle|\hat{L}_z + \hat{S}_z\middle|j, m_j\right\rangle = \mu_B B m_j + \mu_B B\left\langle j, m_j\middle|\hat{S}_z\middle|j, m_j\right\rangle$.

$\left\langle j, m_j\middle|\hat{S}_z\middle|j, m_j\right\rangle = \cos\theta\cos\alpha|\mathbf{S}| = \frac{\langle\hat{J}_z\rangle}{|\mathbf{J}|}\frac{\langle\hat{\mathbf{S}}\cdot\hat{\mathbf{J}}\rangle}{|\mathbf{J}|} = \frac{\langle\hat{J}_z\rangle\langle\hat{\mathbf{S}}\cdot\hat{\mathbf{J}}\rangle}{|\mathbf{J}|^2} = \frac{m_j\hbar\langle\hat{\mathbf{S}}\cdot\hat{\mathbf{J}}\rangle}{j(j+1)\hbar^2} = \frac{m_j\hbar\frac{1}{2}\langle\hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 + \hat{\mathbf{S}}^2\rangle}{j(j+1)\hbar^2}$

$\Longrightarrow E^{(1)}_{nljm_j} = \mu_B B m_j\left(1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}\right) = g_j\mu_B B m_j$

- Each level splits into $2j+1$ sublevels with equal splittings $\Delta E^{(1)}_j = g_j\mu_B B$.

(9) The *strong-field Zeeman effect*: The spin-orbit effect is small compared to external field. States of definite $j$ are effectively degenerate but are mixed by $\hat{H}^{(1)}_{\rm mag} = \frac{\mu_B B}{\hbar}\left(\hat{L}_z + 2\hat{S}_z\right) \Rightarrow$ Use $|n, l, m_l, m_s\rangle$ basis $\Rightarrow E^{(1)}_{nlm_lm_s} = \mu_B(m_l + 2m_s)$.

(10) The *Stark effect*: The energy shifts of hydrogen in a strong external electric field $\mathbf{E} = \mathcal{E}\mathbf{e}_z$. Fine structure and spin can be ignored $\Rightarrow$ The unperturbed eigenstates are represented by $|n, l, m_l\rangle$.

- The perturbing Hamiltonian $\hat{H}^{(1)} = |e|\mathcal{E}\hat{z}$. $\langle n, l, m_l|\hat{z}|n, l, m_l\rangle = \int d^3r z\left|\psi_{nlm_l}\right|^2 = 0 \Rightarrow$ No first-order energy shift for the ground state. *Hydrogen atom in its ground state has no electric dipole moment*.
- Second order shift in ground state energy

$$E^{(2)}_{100} = (e\mathcal{E})^2\left[\sum_{n>1}\frac{|\langle n, l, m|\hat{z}|1, 0, 0\rangle|^2}{E^{(0)}_1 - E^{(0)}_n} + \int d^3\mathbf{k}\frac{|\langle\mathbf{k}|\hat{z}|1, 0, 0\rangle|^2}{E^{(0)}_1 - E^{(0)}_k}\right] = (e\mathcal{E})^2\left[\sum_{n>1}\frac{|\langle n, 1, 0|\hat{z}|1, 0, 0\rangle|^2}{E^{(0)}_1 - E^{(0)}_n} + \int d^3\mathbf{k}\frac{|\langle\mathbf{k}|\hat{z}|1, 0, 0\rangle|^2}{E^{(0)}_1 - E^{(0)}_k}\right]$$

$$\begin{aligned}\left|E^{(2)}_{100}\right| &\le \frac{(e\mathcal{E})^2}{\left|E^{(0)}_2 - E^{(0)}_1\right|}\left[\sum_{n\ge 1}\langle 1, 0, 0|\hat{z}|n, 1, 0\rangle\,\langle n, 1, 0|\hat{z}|1, 0, 0\rangle + \int d^3k\,\langle 1, 0, 0|\hat{z}|\mathbf{k}\rangle\,\langle\mathbf{k}|\hat{z}|1, 0, 0\rangle\right] \\ &= \frac{(e\mathcal{E})^2}{\left|E^{(0)}_2 - E^{(0)}_1\right|}\langle 1, 0, 0|\,\hat{z}\left[\sum_n |n, 1, 0\rangle\langle n, 1, 0| + \int d^3k\,|\mathbf{k}\rangle\langle\mathbf{k}|\right]\hat{z}\,|1, 0, 0\rangle \\ &= \frac{(e\mathcal{E})^2}{\left|E^{(0)}_2 - E^{(0)}_1\right|}\langle 1, 0, 0|\hat{z}^2|1, 0, 0\rangle = \frac{8}{c}(e\mathcal{E})^2\frac{a_0^3}{\alpha\hbar c}.\end{aligned}$$

(11) Stark effect for $n = 2$ level of H atom: 4 degenerate states $|2, 0, 0\rangle$, $|2, 1, 0\rangle$, $|2, 1, \pm 1\rangle$. $\langle 2, 1, 0|\hat{z}|2, 0, 0\rangle = -3a_0 \ne 0$.

- Use degenerate PT in the subspace $|2, 0, 0\rangle \to \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$ and $|2, 1, 0\rangle \to \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right) \Rightarrow$ diagonalize $\hat{H}^{(1)} \to -3e\mathcal{E}a_0\left(\begin{smallmatrix}0 & 1\\1 & 0\end{smallmatrix}\right)$.

$\Longrightarrow$ Eigenvectors $|2, \pm, 0\rangle \to \sqrt{\frac{1}{2}}\left(\begin{smallmatrix}1\\\pm 1\end{smallmatrix}\right)$ with energy shift $E^{(1)}_{\pm} = \mp 3e\mathcal{E}a_0$

- Electric field polarizes $l$, inducing an EDM.

# Chapter 6: PHYS40202 Advanced Quantum Mechanics

## 6.1 Symmetries

### 6.1.1 Symmetries in classical mechanics

(1) *Translation in space.* $\mathbf{r}'(t) = T_{\mathbf{a}}\mathbf{r}(t) = \mathbf{r}(t) - \mathbf{a}$. $T_{\mathbf{a}} f(\mathbf{r}) = f(T_{\mathbf{a}}\mathbf{r}) = f(\mathbf{r}-\mathbf{a})$. If $f(\mathbf{r}) = f(\mathbf{r}')$, it is translationally invariant.
- $(\mathbf{r},\mathbf{p}) \to (\mathbf{r}-\mathbf{a},\mathbf{p})$. The momentum is invariant under spatial translation. Newton's 2nd law $\mathbf{F} = \dot{\mathbf{p}}$ is also invariant.
- The Hamiltonian for a single particle $H = \frac{p^2}{2m} + V(\mathbf{r})$ is trans. invariant only if $V(\mathbf{r}-\mathbf{a}) = V(\mathbf{r})$.
- The Hamiltonian for a two-particle system $H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(\mathbf{r}_1,\mathbf{r}_2)$ is trans. invariant if $V(\mathbf{r}_1,\mathbf{r}_2) = V(\mathbf{r}_1 - \mathbf{r}_2)$.
- Denote $\mathbf{r} = (r_1, r_2, r_3, 1)^T$, then $T_{\mathbf{a}} = \begin{pmatrix} 1 & 0 & 0 & -a_1 \\ 0 & 1 & 0 & -a_2 \\ 0 & 0 & 1 & -a_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$. $\mathbf{r}' = \begin{pmatrix} 1 & 0 & 0 & -a_1 \\ 0 & 1 & 0 & -a_2 \\ 0 & 0 & 1 & -a_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ 1 \end{pmatrix} = \begin{pmatrix} r_1 - a_1 \\ r_2 - a_2 \\ r_3 - a_3 \\ 1 \end{pmatrix} = \mathbf{r} - \boldsymbol{a}$.

(2) *Translation in time.* $t' = T_{t_0} t = t - t_0$, $f(t') = T_{t_0} f(t) = f(t - t_0)$.
- $(\mathbf{r}(t), \mathbf{p}(t)) \to (\mathbf{r}(t-t_0), \mathbf{p}(t-t_0))$. Newton's 2nd law is invariant $\Leftarrow \frac{d\mathbf{p}}{dt} = \frac{d\mathbf{p}}{dt'}\frac{dt'}{dt} = \frac{d\mathbf{p}}{dt'}$.

(3) *Rotations in space.* $r' = \sum_j R_{ij}(\phi) r_j$. eg: $R_{(0,0,\theta)} = R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$.
- Newton's second law has the same form in the unrotated and rotated *time-independent* frames.

(4) *Parity.* $\mathbf{r} \to -\mathbf{r}, \mathbf{p} \to -\mathbf{p}$. *Pseudovectors* $\mathbf{L} = \mathbf{r} \times \mathbf{p} \to \mathbf{L}$. Symmetry under the parity transformation implies that the theory does not care whether the coordinate system is left- or right-handed.

(5) *Time reversal.* $t \to -t, \mathbf{p} \to -\mathbf{p}$.

(6) *Relativistic transformations.* Energy and momentum are not invariant under Lorentz transformations, but $|P^\mu|^2$ is.

### 6.1.2 Symmetries in quantum mechanics

(1) Define a *quantum active transformation* $\hat{T}_S \psi(\mathbf{r},t) = \psi(S\mathbf{r},t) = \psi(\mathbf{r}',t)$. Consider the matrix element

$$\int d\mathbf{r}\psi_n^*(\mathbf{r},t)\hat{O}\psi_m(\mathbf{r},t) \to \int d\mathbf{r}\psi_n^*(S\mathbf{r},t)\hat{O}\psi_m(S\mathbf{r},t) = \int d\mathbf{r}\left(\hat{T}_S\psi_n(\mathbf{r},t)\right)^* \hat{O}\hat{T}_S\psi_m(\mathbf{r},t) = \int d\mathbf{r}\psi_n^*(\mathbf{r},t)\left(\hat{T}_S^\dagger\hat{O}\hat{T}_S\right)\psi_m(\mathbf{r},t)$$

- In the *quantum passive view* $\hat{O} \to \hat{T}_S^\dagger \hat{O}\hat{T}_S$. If the system is invariant under a particular symmetry then $\hat{O} = \hat{T}_S^\dagger\hat{O}\hat{T}_S$.

(2) *Momentum generator*. Consider an Infinitesimal spatial translation $\psi(\mathbf{r}) \to T_{\boldsymbol{\varepsilon}}\psi(\mathbf{r}) = \psi(\mathbf{r}-\boldsymbol{\varepsilon}) \approx \psi(\mathbf{r}) - \varepsilon\cdot\nabla\cdot\psi(\mathbf{r}) = \psi(\mathbf{r}) - \frac{i}{\hbar}\varepsilon\cdot\hat{\mathbf{p}}\psi(\mathbf{r}) \Rightarrow T_{\boldsymbol{\varepsilon}} = \hat{I} - \frac{i}{\hbar}\varepsilon\cdot\hat{\mathbf{p}}$.
- $\int d\mathbf{r}\psi_n^*(\mathbf{r})\hat{O}\psi_m(\mathbf{r}) \to \int d\mathbf{r}\psi_n^*(\mathbf{r}-\boldsymbol{\epsilon})\hat{O}\psi_m(\mathbf{r}-\boldsymbol{\epsilon}) \approx \int d\mathbf{r}\psi_n^*(\mathbf{r})\hat{O}\psi_m(\mathbf{r}) + \frac{i}{\hbar}\sum_i \int d\mathbf{r}\psi_n^*(\mathbf{r})\left(\hat{p}_i\hat{O} - \hat{O}\hat{p}_i\right)\psi_m(\mathbf{r})$

$\Longrightarrow$ The generator commutes with the observable $\hat{O}$ if the observable is compatible with the symmetry ($[\hat{p}_i, \hat{O}] = 0$).
- The Hamiltonian $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}})$ is not in general translationally invariant.

(3) *Hamiltonian generator*. $\psi(\mathbf{r},t) \to \hat{T}_{\delta t}\psi(\mathbf{r},t) = \psi(\mathbf{r},t-\delta t) \approx \psi(\mathbf{r},t) - \delta t\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \psi(\mathbf{r},t) + \delta t\frac{i}{\hbar}\hat{H}\psi(\mathbf{r},t) \Rightarrow \hat{H}_{\delta t} = \hat{I} + \frac{i}{\hbar}\delta t\hat{H}$.
- For an observable to be time translation invariant it must satisfy $[\hat{H}, \hat{O}] = 0$.

(4) *Angular momentum generator*. Consider $R_z(\delta\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \approx \begin{pmatrix} 1 & -\delta\theta & 0 \\ \delta\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I - \delta\theta\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = I - \delta\theta S_3$.
$\psi(\mathbf{r}) \to \hat{R}_z(\delta\theta)\psi(\mathbf{r}) = \psi(\mathbf{r} - \delta\theta S_3\mathbf{r}) \approx \psi(\mathbf{r}) - \delta\theta S_3\mathbf{r}\cdot\nabla\psi(\mathbf{r})$. $S_3\mathbf{r}\cdot\nabla = -\frac{i}{\hbar}\hat{L}_z \Rightarrow \hat{R}_z(\delta\theta) = \hat{I} + \frac{i}{\hbar}\delta\theta\hat{L}_z$. In general $\hat{R}(\boldsymbol{\delta\theta}) = \hat{I} + \frac{i}{\hbar}\boldsymbol{\delta\theta}\cdot\hat{\boldsymbol{L}}$.

(5) In the passive view, $\hat{O} \to \hat{T}_\varepsilon^\dagger\hat{O}\hat{T}_\varepsilon = \left(\hat{I} + \frac{i}{\hbar}\varepsilon\cdot\hat{\mathbf{p}}\right)\hat{O}\left(\hat{I} - \frac{i}{\hbar}\varepsilon\cdot\hat{\mathbf{p}}\right) = \hat{O} + \frac{i}{\hbar}\sum_i \varepsilon_i[\hat{p}_i, \hat{O}]$. For $\hat{\mathbf{r}}$, $\hat{T}_{\boldsymbol{\varepsilon}}^\dagger\hat{\mathbf{r}}\hat{T}_{\boldsymbol{\varepsilon}} = \hat{\mathbf{r}} + \boldsymbol{\varepsilon}$.

### 6.1.3 Unitary operators

(1) Any operator that satisfies $\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{I}$ is called unitary.
- Unitary operators preserve the overlap between any two wavefunctions. $\langle\phi_U|\psi_U\rangle = \langle\phi|\hat{U}\hat{U}^\dagger|\psi_u\rangle = \langle\phi|\psi\rangle$.

(2) Symmetry transformation operators must be unitary $\hat{T}^\dagger\hat{T} = \hat{I}$.

(3) Finite spatial/time/rotation translation operators: $\hat{U}_{\boldsymbol{a}} = e^{-i\boldsymbol{a}\hat{\mathbf{p}}/\hbar}$, $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$, $\hat{U}_{\boldsymbol{\theta}} = e^{i\boldsymbol{\theta}\cdot\hat{L}/\hbar}$.

(4) Parity operator $\hat{P}\psi(\mathbf{r},t) = \psi(-\mathbf{r},t)$. By evaluating matrix element, $\left\langle\phi\left|\hat{P}^\dagger\hat{\mathbf{r}}\hat{P}\right|\psi\right\rangle = -\langle\phi|\hat{\mathbf{r}}|\psi\rangle \Rightarrow \hat{P}^\dagger\hat{\mathbf{r}}\hat{P} = -\hat{\mathbf{r}}$, $\hat{P}^\dagger\hat{\mathbf{p}}\hat{P} = -\hat{\mathbf{p}}$.
- If the system is invariant under spatial inversion then $[\hat{H}, \hat{P}] = 0$.

(5) Time reversal operator $\hat{T}\psi(\mathbf{r},t) = \psi^*(\mathbf{r},t)$. Consider $\psi(\mathbf{r},t) = U(t)\psi(\mathbf{r},0) = e^{-i\hat{H}t/\hbar}\psi(\mathbf{r},0) \Rightarrow \psi^*(\mathbf{r},t) = e^{i\hat{H}t/\hbar}\psi^*(\mathbf{r},0)$.
- $\hat{T}^\dagger[\hat{H},\hat{T}] = \hat{T}^\dagger\hat{H}\hat{T} - \hat{T}^\dagger\hat{T}\hat{H} = \hat{H}^* - \hat{H} \Rightarrow$ Time reversal is only a symmetry of the system if the Hamiltonian is real.
- $\hat{T}^\dagger\hat{\mathbf{r}}\hat{T} = \hat{\mathbf{r}}$, $\hat{T}^\dagger\hat{\mathbf{p}}\hat{T} = \hat{\mathbf{p}}$.

(6) *Antiunitary operators* satisfy $\hat{O}^\dagger\hat{O} = \hat{I}$, but with $\hat{O}\lambda = \lambda^*\hat{O}$. Unitary operators satisfy $\hat{O}\lambda = \lambda\hat{O}$.

- $\hat{P}^\dagger i\hbar\delta_{ij}\hat{P} = \hat{P}^\dagger\left[\hat{r}_i, \hat{p}_j\right]\hat{P} = \left[\hat{P}^\dagger\hat{r}_i\hat{P}, \hat{P}^\dagger\hat{p}_j\hat{P}\right] = \left[-\hat{r}_i, -\hat{p}_j\right] = i\hbar\delta_{ij}$. $\hat{T}^\dagger i\hbar\delta_{ij}\hat{T} = \hat{T}^\dagger\left[\hat{r}_i, \hat{p}_j\right]\hat{T} = \left[\hat{T}^\dagger\hat{r}_i\hat{T}, \hat{T}^\dagger\hat{p}_j\hat{T}\right] = \left[\hat{r}_i, -\hat{p}_j\right] = -i\hbar\delta_{ij}$.

(7) $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\hat{O}|\psi\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H}, \hat{O}]|\psi\rangle + \langle\psi|\frac{\partial\hat{O}}{\partial t}|\psi\rangle$. If $\hat{O}$ has no explicit time dependence, then $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\hat{O}|\psi\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H}, \hat{O}]|\psi\rangle$.

- If the observable $\hat{O}$ commutes with the Hamiltonian, its expectation value is conserved for any state $|\psi\rangle$.
- For time-independent Hamiltonians $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\hat{H}|\psi\rangle = 0 \Rightarrow$ Conservation of energy.
- For translationally-invariant Hamiltonians $[\hat{H}, \hat{\mathbf{p}}] = 0 \Rightarrow$ Conservation of momentum.

(8) Finite rotation operator $\hat{U}_{\boldsymbol{\theta}} = e^{i\boldsymbol{\theta}\cdot\hat{\mathbf{L}}/\hbar} = e^{i\left(\theta_x\hat{L}_x + \theta_y\hat{L}_y + \theta_z\hat{L}_z\right)/\hbar} \neq e^{i\theta_x\hat{L}_x/\hbar}e^{i\theta_y\hat{L}_y/\hbar}e^{i\theta_z\hat{L}_z/\hbar}$. Define the rotation in *Euler angles*: (i) rotate the system about the $z$–axis by $\gamma \in [0, 2\pi]$, (ii) rotate the system about the $x$–axis by $\beta \in [0, \pi]$, (iii) rotate the system about the $z$–axis by $\alpha \in [0, 2\pi]$. $\psi(\mathbf{r}) \to \psi(R_z(\alpha)R_x(\beta)R_z(\gamma)) = \hat{U}_{\alpha,\beta,\gamma}\psi(\mathbf{r}) = e^{i\alpha\hat{L}_z/\hbar}e^{i\beta\hat{L}_x/\hbar}e^{i\gamma\hat{L}_z/\hbar}\psi(\mathbf{r})$.

(9) In the basis $\{|l, m\rangle\}$. The matrix element

$D^l_{m,m'}(\alpha, \beta, \gamma) = \langle l, m|\hat{U}_{\alpha,\beta,\gamma}|l, m'\rangle = \langle l, m|e^{i\alpha\hat{L}_z/\hbar}e^{i\beta\hat{L}_x/\hbar}e^{i\gamma\hat{L}_z/\hbar}|l, m'\rangle = e^{i(\alpha m+\gamma m')}\langle l, m|e^{i\beta\hat{L}_x/\hbar}|l, m\rangle = e^{i(\alpha m+\gamma m')}d^l_{m,m'}(\beta)$.

- The $(2l+1)\times(2l+1)$ matrix $D^l(\alpha, \beta, \gamma)$ is known as the *Wigner D-matrix*. Its elements $D^l_{m,m'}(\alpha, \beta, \gamma) = e^{i(\alpha m+\gamma m')}d^l_{m,m'}(\beta)$.
- For $l = 1$, $\hat{L}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}$. $e^{i\beta\hat{L}_x/\hbar} = \exp\left[\frac{i\beta}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}\right] = \begin{pmatrix}\cos^2(\beta/2) & \frac{i}{\sqrt{2}}\sin(\beta) & -\sin^2(\beta/2)\\ \frac{i}{\sqrt{2}}\sin(\beta) & \cos(\beta) & \frac{i}{\sqrt{2}}\sin(\beta)\\ -\sin^2(\beta/2) & \frac{i}{\sqrt{2}}\sin(\beta) & \cos^2(\beta/2)\end{pmatrix}$.

## 6.2 Time dependent perturbation theory

### 6.2.1 Time dependent perturbation theory

(1) TDSE with perturbation $i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle = \left(\hat{H}_0 + \lambda\hat{V}(t)\right)|\psi(t)\rangle$. Write $|\psi(t)\rangle = \sum_n c_n(t)e^{-iE_nt/\hbar}|n\rangle$.

$\Longrightarrow \sum_n\left[i\hbar\frac{\mathrm{d}c_n(t)}{\mathrm{d}t} + E_nc_n(t)\right]e^{-iE_nt/\hbar}|n\rangle = \sum_n\left[E_n + \lambda\hat{V}(t)\right]c_n(t)e^{-iE_nt/\hbar}|n\rangle \Rightarrow \sum_n i\hbar\frac{\mathrm{d}c_n(t)}{\mathrm{d}t}e^{-iE_nt/\hbar}|n\rangle = \lambda\sum_n\hat{V}(t)c_n(t)e^{-iE_nt/\hbar}|n\rangle$

$\xRightarrow{\text{orthonormality}} i\hbar\frac{dc_m(t)}{dt} = \lambda\sum_n c_n(t)e^{i\omega_{mn}t}\langle m|\hat{V}(t)|n\rangle$, where $\omega_{nm} = \frac{E_m - E_n}{\hbar}$. Expand $c_n(t) = c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \lambda^2c_n^{(2)}(t) + \cdots$

$\Longrightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left[c_m^{(0)}(t) + \lambda c_m^{(1)}(t) + \lambda^2c_m^{(2)}(t) + \ldots\right] = \lambda\sum_n\left[c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \lambda^2c_n^{(2)}(t) + \ldots\right]e^{i\omega_{mn}t}\langle m|\hat{V}(t)|n\rangle \Rightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_m^{(0)}(t) = 0$.

$\Longrightarrow$ At first order in $\lambda$ $i\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_m^{(1)}(t) = \sum_n c_n^{(0)}(t)e^{i\omega_{mn}t}\langle m|\hat{V}(t)|n\rangle = \sum_n c_n^{(0)}(t_0)e^{i\omega_{mn}t}\langle m|\hat{V}(t)|n\rangle$.

- Initial condition: $|\psi(t_0)\rangle = |i\rangle$, $c_n(t_0) = c_n^{(0)}(t_0) = \delta_{ni} \Rightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_m^{(1)}(t) = e^{i\omega_{mi}t}\langle m|\hat{V}(t)|i\rangle \Rightarrow c_m^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^t\mathrm{d}t'e^{i\omega_{mi}t'}\langle m|\hat{V}(t')|i\rangle$.

$\Longrightarrow |\psi(t)\rangle \approx \sum_n\left[\delta_{ni} + c_n^{(1)}(t)\right]e^{-iE_nt/\hbar}|n\rangle$. $P_f(t) = \left|\langle f|\psi(t)\rangle\right|^2 = \left|c_f^{(1)}(t)\right|^2$.

(2) Perturbation switched on slowly. Consider $\hat{H} = \begin{cases}\hat{H}_0 & , t < 0\\ \hat{H}_0 + \hat{V}e^{t/\tau} & , t = 0\end{cases}$. $c_n^{(1)}(0) = -\frac{i}{\hbar}\langle n|\hat{V}|i\rangle\int_{-\infty}^0\mathrm{d}te^{t/\tau}e^{i\omega_{ni}t} = -\frac{i}{\hbar}\frac{\langle n|\hat{V}|i\rangle}{(1/\tau + i\omega_{ni})}$.

- $\lim_{\tau\to\infty}c_n^{(1)}(0) = \frac{\langle n|\hat{V}|i\rangle}{E_i - E_n}$ (compatible with time-independent perturbation theory).

(3) Perturbation switched on and off. Consider $\hat{H} = \hat{H}_0 + \hat{V}e^{-t^2/\tau^2}$.

$\Longrightarrow c_n^{(1)}(\infty) = -\frac{i}{\hbar}\langle n|\hat{V}|i\rangle\int_{-\infty}^\infty\mathrm{d}te^{-t^2/\tau^2}e^{i\omega_{ni}t} = -\frac{i}{\hbar}\langle n|\hat{V}|i\rangle e^{-\omega_{ni}^2/\tau^2/4}\sqrt{\pi}\tau$. $P_f(\infty) = \left|c_f^{(1)}(\infty)\right|^2 = \frac{\pi\tau^2}{\hbar^2}|\langle f|\hat{V}|i\rangle|^2e^{-\omega_{fi}^2\tau^2/2}$.

- $\lim_{\tau\to\infty}P_f(\infty) \to 0$. The system initialised in an eigenstate of $\hat{H} = \hat{H}_0$ at $t = -\infty$ will remain in an instantaneous eigenstate of $\hat{H}$ as the perturbation is slowly switched on and then off again (adiabatic).
- $\lim_{\tau\to 0}P_f(\infty) \to 0$. A sudden change to the system leaves its state unchanged.

(4) *Hydrogen atom in an external field*. In the ground state $\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}$. At $t = 0$ turn on $E(t) = E_0e^{-t/\tau}$, $E_0 > 0, \tau > 0$.

- The perturbation $\hat{V}(t) = -\mathbf{d}\cdot\mathbf{E}(t) = -(-e)zE_z = er\cos\theta E_0e^{-t/\tau}$. Consider the final state $n = 2, l = 1, m = 0$.
- $c^{(1)}(t) = -\frac{i}{\hbar}\int_0^t\mathrm{d}t'\left\langle\psi_{210}\left|\hat{V}(t')\right|\psi_{100}\right\rangle e^{i\omega t'} = -\frac{ieE_0}{\hbar}\langle\psi_{210}|r\cos\theta|\psi_{100}\rangle\int_0^t\mathrm{d}t'e^{-t'/\tau}e^{i\omega t'} = -\frac{ieE_0A}{\hbar}\left[\frac{e^{(i\omega-1/\tau)t} - 1}{i\omega - 1/\tau}\right]$, $A = \frac{2^{15/2}a_0}{3^5}$.
- $P(t) = \left|c^{(1)}(t)\right|^2 = \frac{e^2E_0^2A^2}{\hbar^2\omega^2 + \hbar^2/\tau^2}\left(1 + e^{-2t/\tau} - 2e^{-t/\tau}\cos\omega t\right)$. $P(\infty) = \frac{e^2E_0^2A^2}{\hbar^2\omega^2 + \hbar^2/\tau^2}$. $\lim_{\tau\to 0}P(\infty) \to 0$, $\lim_{\tau\to\infty}P(\infty) \to \frac{e^2E_0^2A^2}{\hbar^2\omega^2}$.

(5) *Oscillatory perturbations*. Consider $\hat{V}(t) = \begin{cases}0, & t \leq 0\\ \hat{V}_0e^{-i\omega t}, & t > 0\end{cases}$.

$\Longrightarrow c_f^{(1)}(t) = -\frac{i}{\hbar}\int_0^t\mathrm{d}t'e^{i\omega_{fi}t'}\left\langle f\left|\hat{V}(t')\right|i\right\rangle \Rightarrow P_{i\to j}(t) = \frac{4}{\hbar^2}\left|\left\langle f\left|\hat{V}_0\right|i\right\rangle\right|^2\frac{\sin^2((\omega_{fi} - \omega)t/2)}{(\omega_{fi} - \omega)^2} = \frac{t^2}{\hbar^2}\left|\left\langle f\left|\hat{V}_0\right|i\right\rangle\right|^2\mathrm{sinc}^2\left((\omega_{fi} - \omega)t/2\right)$

- For $\omega \neq \omega_{fi}$, the transition probability oscillates in time with a small amplitude.
- For $\omega = \omega_{fi}$, $P_{i\to j}(t) = \frac{2\pi t}{\hbar^2}\left|\langle f|\hat{V}_0|i\rangle\right|^2\delta(\omega_{fi} - \omega) \Rightarrow R_{i\to f}(t) = \frac{\mathrm{d}P_{i\to f}(t)}{\mathrm{d}t} = \frac{2\pi}{\hbar^2}\left|\left\langle f\left|\hat{V}_0\right|i\right\rangle\right|^2\delta\left(\omega_{fi} - \omega\right)$.

• *Fermi's Golden Rule*: $R_{i\to f}(t) = \frac{2\pi}{\hbar}\left|\left\langle f\left|\hat{V}_0\right|i\right\rangle\right|^2 \delta\left(E_{fi} - \hbar\omega\right)$. In the long-time limit, only a perturbation with frequency that matches the system transition frequency $\omega_{fi}$ can induce a transition from $|i\rangle$ to $|j\rangle$. Here the energy is absorbed from the perturbing field and $E_f > E_i$.
• If $\hat{V}(t) = \hat{V}_0 e^{i\omega t}$ then we have $\delta(E_{fi} + \hbar\omega)$. Energy is given up to the perturbing field in an emission process.

### 6.2.2 Selection rules

(1) *Emission and absorption of radiation*. Consider $\hat{V}(t) = \begin{cases} 0, & t \le 0 \\ eE_0\cos(\omega t)\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}} = \frac{eE_0}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}}, & t > 0 \end{cases}$.
• Consider a field with a range of frequencies each weighted by $E_0$,

$$R_{i\to f} = \frac{\pi}{2\hbar^2}e^2\int_0^\infty d\omega E_0(\omega)^2|\langle f|\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}}|i\rangle|^2\left[\delta\left(\omega_{fi}-\omega\right)+\delta\left(\omega_{fi}+\omega\right)\right] = \frac{\pi}{2\hbar^2}e^2 E_0\left(\left|\omega_{fi}\right|\right)^2|\langle f|\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}}|i\rangle|^2,$$

which applies both to absorption and stimulated emission.
(2) For electric dipole transitions to be allowed we require $\langle f|\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}}|i\rangle \neq 0$. For Hydrogen consider $\left\langle n', l', s', j', m_j'\left|\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}}\right|n, l, s, j, m_j\right\rangle$.
• Write $\hat{\mathbf{r}} = \sqrt{4\pi}r\left(Y_1^1\mathbf{e}_- + Y_1^0\mathbf{e}_0 + Y_1^{-1}\mathbf{e}_+\right)$, where $\mathbf{e}_\pm = \pm\sqrt{\frac{1}{2}}\left(\mathbf{e}_x \pm i\mathbf{e}_y\right) \Rightarrow$

## 6.3 Charged particles in electromagnetic fields

### 6.3.1 Hamiltonian of charged particles in electromagnetic fields

(1) Lagrangian for a charged particle in the EM field: $\mathscr{L} = \frac{1}{2}m\dot{\mathbf{r}}^2 - q\Phi(\mathbf{r},t) + q\mathbf{A}(\mathbf{r},t)\cdot\dot{\mathbf{r}} \Longrightarrow m\ddot{\mathbf{r}} = q[\mathbf{E}(\mathbf{r},\mathbf{t}) + \dot{\mathbf{r}}\times\mathbf{B}(\mathbf{r},t)]$.
(2) Canonical momentum $p_i = \frac{\partial\mathscr{L}}{\partial\dot{r}_i} = m\dot{r}_i + qA_i(\mathbf{r},t)$, $\mathbf{p} = m\dot{\mathbf{r}} + q\mathbf{A}(\mathbf{r},t)$. Kinetic momentum $m\dot{\mathbf{r}} = \mathbf{p} - q\mathbf{A}(\mathbf{r},t)$.
(3) Classical Hamiltonian: $H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A}(\mathbf{r},t))^2 + q\Phi(\mathbf{r},t)$. Quantum Hamiltonian $\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}},t))^2 + q\Phi(\hat{\mathbf{r}},t)$.
(4) In the case $\Phi(\hat{\mathbf{r}},t) = 0$, $\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}},t))^2$. $[\hat{H},\hat{p}_i]$ isn't necessarily 0. For kinetic momentum $\left[m\dot{\hat{\mathbf{r}}}, H\right] = 0$ (conserved).

### 6.3.2 Gauge transformations and gauge invariance

(1) *Gauge transformation* $\Phi(\mathbf{r},t) \to \Phi_\lambda(\mathbf{r},t) = \Phi(\mathbf{r},t) - \frac{\partial\lambda(\mathbf{r},t)}{\partial t}$, $\quad \mathbf{A}(\mathbf{r},t) \to \mathbf{A}_\lambda(\mathbf{r},t) = \mathbf{A}(\mathbf{r},t) + \nabla\lambda(\mathbf{r},t)$
(2) Hamiltonian under gauge transformation $\hat{H} \to \hat{H}_\lambda = \frac{1}{2m}[\hat{\mathbf{p}} - q(\mathbf{A}(\hat{\mathbf{r}},t) + \nabla\lambda(\hat{\mathbf{r}},t))]^2 + q\left(\Phi(\hat{\mathbf{r}},t) - \frac{\partial\lambda(\hat{\mathbf{r}},t)}{\partial t}\right)$.
(3) Define unitary operator $\hat{G}_\lambda = e^{iq\lambda(\mathbf{r},t)/\hbar}$, $\hat{G}_\lambda\hat{\mathbf{p}}\hat{G}_\lambda^\dagger = \hat{\mathbf{p}} - q\nabla\lambda(\mathbf{r},t)$.
(4) Consider $\begin{cases} \hat{G}_\lambda i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{G}_\lambda\hat{H}|\psi\rangle = \hat{G}_\lambda\hat{H}\hat{G}_\lambda^\dagger\hat{G}_\lambda|\psi\rangle \\ \frac{\partial}{\partial t}\hat{G}_\lambda|\psi\rangle = \frac{iq}{\hbar}\frac{\partial\lambda(\mathbf{r},t)}{\partial t}\hat{G}_\lambda|\psi\rangle + \hat{G}_\lambda\frac{\partial}{\partial t}|\psi\rangle \end{cases} \Rightarrow \left[i\hbar\frac{\partial}{\partial t} + q\frac{\partial\lambda(\mathbf{r},t)}{\partial t}\right]\hat{G}_\lambda|\psi\rangle = \hat{G}_\lambda\hat{H}\hat{G}_\lambda^\dagger\hat{G}_\lambda|\psi\rangle$.
$\hat{G}_\lambda\hat{H}\hat{G}_\lambda^\dagger = \frac{1}{2m}\hat{G}_\lambda[\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{r},t)]\hat{G}_\lambda^\dagger\hat{G}_\lambda[\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{r},t)]\hat{G}_\lambda^\dagger + q\Phi(\mathbf{r},t) = \frac{1}{2m}[\hat{\mathbf{p}} - q(\mathbf{A}(\mathbf{r},t) + \nabla\lambda(\mathbf{r},t))]^2 + q\Phi(\mathbf{r},t)$. Define $|\psi_\lambda\rangle = \hat{G}_\lambda|\psi\rangle$.
$\Longrightarrow i\hbar\frac{\partial}{\partial t}|\psi_\lambda\rangle = \hat{H}_\lambda|\psi_\lambda\rangle$, $\hat{H}_\lambda = \frac{1}{2m}[\hat{\mathbf{p}} - q(\mathbf{A}(\mathbf{r},t) + \nabla\lambda(\mathbf{r},t))]^2 + q\left(\Phi(\mathbf{r},t) - \frac{\partial\lambda(\mathbf{r},t)}{\partial t}\right) = \frac{1}{2m}[\hat{\mathbf{p}} - q\mathbf{A}_\lambda(\hat{\mathbf{r}},t)]^2 + q\Phi_\lambda(\hat{\mathbf{r}},t)$.
• If $|\psi\rangle$ satisfies the TDSE in the original gauge, then the unitarily transformed $|\psi_\lambda\rangle$ satisfies the TDSE in the new gauge.
(5) The expectation value of any observable $\hat{O}$ will be unchanged provided we transform both the observable and the state $\langle\psi|\hat{O}|\psi\rangle = \left\langle\psi\left|G_\lambda^\dagger G_\lambda\hat{O}G_\lambda^\dagger G_\lambda\right|\psi\right\rangle = \left\langle\psi_\lambda\left|\hat{O}_\lambda\right|\psi_\lambda\right\rangle$, where $\hat{O}_\lambda = \hat{G}_\lambda\hat{O}\hat{G}_\lambda^\dagger$.
• Any operator for which $\hat{O}_\lambda = \hat{O}$ is termed *gauge invariant*. Their expectation values are the same for $|\psi\rangle$ and $|\psi_\lambda\rangle$.
• $\hat{G}_\lambda\hat{\mathbf{r}}\hat{G}_\lambda^\dagger = \hat{\mathbf{r}}$, $\hat{G}_\lambda\hat{\mathbf{p}}\hat{G}_\lambda^\dagger = \hat{\mathbf{p}} - q\nabla\lambda(\mathbf{r},t)$. $\hat{G}_\lambda m\dot{\mathbf{r}}\hat{G}_\lambda^\dagger = \hat{\mathbf{p}} - q\nabla\lambda(\hat{\mathbf{r}},t) - q\mathbf{A}(\hat{\mathbf{r}},t) = \hat{\mathbf{p}} - q\mathbf{A}_\lambda(\hat{\mathbf{r}},t)$.
• $m\dot{\hat{\mathbf{r}}}$ represents the mechanical momentum in any gauge, though its operator representation changes in different gauges. The canonical momentum $\hat{\mathbf{p}}$ has the same operator representation in all gauges, it does not represent the same physical observable in all gauges. Position and mechanical momentum are considered *true physical quantities*.
• For a true physical quantity the direct gauge transformation of the potentials along with the transformation $\hat{G}_\lambda$ of the state will leave expectation values invariant. $\langle\psi|\hat{\mathbf{r}}|\psi\rangle \to \langle\psi_\lambda|\hat{\mathbf{r}}|\psi_\lambda\rangle = \left\langle\psi\left|\hat{G}_\lambda^\dagger\hat{\mathbf{r}}\hat{G}_\lambda\right|\psi\right\rangle = \langle\psi|\hat{\mathbf{r}}|\psi\rangle$ (Also $\langle\psi|p - q\mathbf{A}(\hat{\mathbf{r}},t)|\psi\rangle$).
(4) *Time-independent Hamiltonian*. By treating the EM field as external (time-dependent) we are approximating their influence on our system. If we were to include the dynamical variables of the field our Hamiltonian would be time independent.
• $\hat{H}_\lambda = \hat{G}_\lambda\hat{H}\hat{G}_\lambda^\dagger$. TISE $\hat{H}|\psi\rangle = E|\psi\rangle \Rightarrow \hat{G}_\lambda\hat{H}|\psi\rangle = \hat{G}_\lambda E|\psi\rangle \Rightarrow \hat{H}_\lambda|\psi_\lambda\rangle = E|\psi_\lambda\rangle$.

### 6.3.3 Dipole interactions and Goppert-Mayer transformation

(1) Consider a field which has zero scalar potential $\mathbf{E}(\hat{\mathbf{r}},t) = -\frac{\partial\mathbf{A}(\hat{\mathbf{r}},t)}{\partial t}$. For a particle of charge $q$ at the origin $\mathbf{0}$, in the long-wavelength limit $\mathbf{E}(\mathbf{0},t) = -\frac{\mathrm{d}\mathbf{A}(\mathbf{0},t)}{\mathrm{d}t}$ and $\mathbf{B}(\hat{\mathbf{r}},t) = \nabla\times\mathbf{A}(\mathbf{0},t) = 0$.
(2) In the *electric dipole approximation* $\hat{H} = \frac{1}{2m}[\hat{p} - q\mathbf{A}(\mathbf{0},t)]^2 + V(\hat{\mathbf{r}})$, where $V(\hat{\mathbf{r}})$ commutes with any gauge transformations.
(3) Chose $\lambda(\hat{\mathbf{r}},t) = -\hat{\mathbf{r}}\cdot\mathbf{A}(\mathbf{0},t)$. $\hat{G}_\lambda = e^{-iq\lambda(\mathbf{r},t)/\hbar} = e^{-iq\hat{\mathbf{r}}\cdot\mathbf{A}(\mathbf{0},t)/\hbar} \Rightarrow \hat{H}_\lambda = \frac{1}{2m}\hat{\mathbf{p}}^2 + V(\hat{\mathbf{r}}) + q\hat{\mathbf{r}}\cdot\frac{\mathrm{d}\mathbf{A}(\mathbf{0},t)}{\mathrm{d}t} = \frac{1}{2m}\hat{\mathbf{p}}^2 + V(\hat{\mathbf{r}}) - \hat{\mathbf{d}}\cdot\mathbf{E}(\mathbf{0},t)$.

### 6.3.4 Landau levels

(1) Consider a particle of charge $q$ in the homogeneous magnetic field $\mathbf{B}=(0,0,B)$, choose $\mathbf{A}=(0,Bx,0)$.

$\Longrightarrow$ The Hamiltonian $\hat{H}=\frac{1}{2m}(\hat{\mathbf{p}}-q\mathbf{A})^2=\frac{1}{2m}\left[\hat{p}_x^2+\left(\hat{p}_y-qBx\right)^2+\hat{p}_z^2\right]$.

• The $z$−component is decoupled from the $xy$−motion and $[\hat{p}_z,\hat{H}]=0\Rightarrow\psi(x,y,z)=\psi(x,y)e^{ik_zz}$.

$\Longrightarrow\hat{H}_{xy}=\frac{1}{2m}\left[\hat{p}_x^2+\left(\hat{p}_y^2-qBx\right)^2\right]=\frac{1}{2m}\left[\hat{p}_x^2+\hat{p}_y^2+q^2B^2x^2-2qBx\hat{p}_y\right]$. d $\Longrightarrow\frac{1}{2m}\left[\hat{p}_x^2+\hbar^2k_y^2+q^2B^2x^2-2qB\hbar k_yx\right]\psi_{k_y}(x)=E_{xy}\psi_{k_y}(x)\Rightarrow$ $\frac{1}{2m}\left[\hat{p}_x^2+q^2B^2\left(x-\frac{\hbar k_y}{qB}\right)^2\right]\psi_{k_y}(x)=E_{xy}\psi_{k_y}(x)$.

$\Longrightarrow\left[\frac{1}{2m}\hat{p}_x^2+\frac{1}{2}m\omega_c^2(x-x_0)^2\right]\psi_{k_y}(x)=E\psi_{k_y}(x)$, where $x_0=\frac{\hbar k_y}{qB}$, $\omega_c=\frac{qB}{m}\Rightarrow\psi_{k_y}(x)=\Phi_n(x-x_0)$, $\psi(x,y)=\Phi_n(x-x_0)e^{ik_yy}$.

• Energy eigenvalues $E_{n,k_y}=\hbar\omega_c\left(n+\frac{1}{2}\right)$. The set of degenerate states for a fixed value of $n$ is called a *Landau level*.

(2) For $\mathbf{B}=(0,0,B)$, choose $\mathbf{A}=(-yB,Bx,0)$ instead $\Rightarrow\boldsymbol{\nabla}\lambda=-(yB,Bx,0)\Rightarrow\lambda=-Bxy$. $\hat{G}_\lambda=e^{-iqBxy/\hbar}$.

$\Longrightarrow\left[\frac{1}{2m}\hat{p}_y^2+\frac{1}{2}m\omega_c^2(y+y_0)^2\right]\psi_{k_x}(y)=E\psi_{k_x}(y)$, where $y_0=\frac{\hbar k_x}{qB}\Rightarrow\psi'(x,y)=e^{ik_xx}\Phi_n(y+y_0)$, $E_{n,k_x}=\hbar\omega_c\left(n+\frac{1}{2}\right)$.

(3) For $\mathbf{A}=(0,Bx,0)$, the eigenstates $\psi(x,y,z)=\psi_{k_y}e^{ik_yy}e^{ik_zz}=\Phi_n(x-x_0)e^{ik_yy}e^{ik_zz}=NH_n(x-x_0)e^{-qB(x-x_0)^2/2\hbar}e^{ik_yy}e^{ik_zz}$

$\Longrightarrow\frac{1}{2m}\left[\hat{p}_x^2+q^2B^2\left(x-\frac{\hbar k_y}{qB}\right)^2+\hbar^2k_z^2\right]\psi_{k_y}(x)=E\psi_{k_y}(x)$, $E_{n,k_y}=\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{\hbar^2k_z^2}{2m}$.

(4) Choose a finite region with length $L_x,L_y$ in the $xy$−plane and set the b.c. $\psi(x,y,z)=\psi(x,y+L_y,z)$.

• $k_yL_y=2\pi n_y, k_y=\frac{qBx_0}{\hbar}\Rightarrow 0\le k_y\le\frac{qBL_x}{\hbar}$. Number of available states $N=\frac{L_y}{2\pi}\int_0^{qBL_x/\hbar}\mathrm{d}k=\frac{qBL_xL_y}{2\pi\hbar}=\frac{qBA}{2\pi\hbar}$.

• For $L_xL_y=1\text{cm}^2$ and $B\sim 0.1$ T. Number of degenerate states $N\sim10^{10}$ per Landau level.

# Chapter 7: PHYS40222 Particle Physics

## 7.1 The Standard Model and relativistic kinematics

(1)

| Particle | Mass | Electric Charge | Weak Isospin | Colour charge |
|---|---|---|---|---|
| $u$ | 2.2 MeV | $+2/3$ | $+1/2$ | $r,b,g$ |
| $d$ | 4.7 MeV | $-1/3$ | $-1/2$ | $r,b,g$ |
| $c$ | 1.3 GeV | $+2/3$ | $+1/2$ | $r,b,g$ |
| $s$ | 96 MeV | $-1/3$ | $-1/2$ | $r,b,g$ |
| $t$ | 172 GeV | $+2/3$ | $+1/2$ | $r,b,g$ |
| $b$ | 4 GeV | $-1/3$ | $-1/2$ | $r,b,g$ |
| $\nu_e$ | — | 0 | $+1/2$ | no |
| $e$ | 511 keV | $-1$ | $-1/2$ | no |
| $\nu_\mu$ | — | 0 | $+1/2$ | no |
| $\mu$ | 105 MeV | $-1$ | $-1/2$ | no |
| $\nu_\tau$ | — | 0 | $+1/2$ | no |
| $\tau$ | 1.78 GeV | $-1$ | $-1/2$ | no |

(2)

| Interaction | Mediators | Mass | Relative strength | Long-distance behaviour | Range(m) | Lifetime(s) |
|---|---|---|---|---|---|---|
| Strong | $g$ (8) | massless | $10^{38}$ | 1 | $10^{-15}$ | $10^{-22}-10^{-24}$ |
| Electromagnetic | $\gamma$ | massless | $10^{36}$ | $1/r^2$ | $\infty$ | $10^{-16}-10^{-21}$ |
| Weak | $W^+, W^-$<br>$Z$ | 80 GeV<br>90 GeV | $10^{25}$ | $\frac{1}{r}e^{-m_{W,Z}r}$ | $10^{-18}$ | $10^{-7}-10^{-13}$ |

• Leptons and quarks are spin-$\frac{1}{2}$ fermions. Force-mediating particles are spin-1 bosons. The Higgs is spin-0 (125 GeV).

(3) *Natural units*: $\hbar = c = 1$. $E = \gamma mc^2 = \gamma m$.

• All units are powers of energy. Energy, momentum and mass are measured in eV. Length and time are measured in $\text{eV}^{-1}$. 1 eV$=1.6\times10^{-19}$J. $\hbar = 6.58\times10^{-22}$ MeVs, $\hbar c = 1.97\times10^{-13}$ MeVm.

(4) $P^\mu = (E, \mathbf{p}) = (E, p_x, p_y, p_z)$. The *invariant mass* is given by $M^2 = |P^\mu|^2 = E^2 - p_x^2 - p_y^2 - p_z^2$.

• For a single particle, the invariant mass is simply the mass of the particle.

• For a system of $N$ particles, $P^\mu_{\text{tot}} = \sum_{j=0}^{N} P^\mu_j$. $M^2 = \left|P^\mu_{\text{tot}}\right|^2 = \left(\sum_{j=0}^{N} E\right)^2 - \left(\sum_{j=0}^{N} p_{x,j}\right)^2 - \left(\sum_{j=0}^{N} p_{y,j}\right)^2 - \left(\sum_{j=0}^{N} p_{z,j}\right)^2$. As energy and momentum must be conserved, the invariant mass must also be conserved.

(5) In the *centre-of-mass* frame, $\sum_{j=0}^{N} \mathbf{p}_j = 0$. $E^2_{\text{cm}} = M^2$.

• Example: Threshold production. The minimum beam energy for the protons for the process $pp \to ppp\overline{p}$.
*Fixed-target*: Minimum energy needed if final state particles have 0 momentum. In the c.o.m. frame, $P^\mu_{\text{tot,cm}} = (4m_p, 0)$, $M^2 = (4m_p)^2$. In the lab frame, $P^\mu_{\text{beam}} = (E_b, \mathbf{p}_b)$, $P^\mu_{\text{target}} = (m_p, 0)$, $P^\mu_{\text{tot,lab}} = (E_b + m_p, \mathbf{p}_b)$. $M^2 = (E_b + m_p)^2 - \mathbf{p}_b^2 \Rightarrow E_b = 7m_b$.

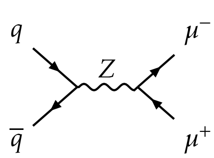
• Assume $E_b \gg m_p$, $M^2 = E_b^2 + 2E_b m_p + \cancel{m_p^2} - E_b^2 = 2E_b m_p \Rightarrow E_{\text{cm}} \propto 2E_b m_p$. If we want to double $E_{\text{cm}}$ need $4\times E_b$.

• *Collision*. $P^\mu_1 = (E_b, \mathbf{p}_b)$, $P^\mu_2 = (E_b, -\mathbf{p}_b)$. $M^2 = (2E_b)^2 - \mathbf{0}^2 = 4E_b^2$. If we want to double $E_{\text{cm}}$ need $2\times E_b$.

• Heavy particle decays. Example: $X \to AB$, $E_A = E_B = 88.39$ GeV, $\mathbf{p}_A$ and $\mathbf{p}_B$ are measured to be 88.39 GeV along the $x/z$–direction $\Rightarrow m_X^2 = (2\times 88.39)^2 - \left(\sqrt{2}\times 88.39\right)^2 \Rightarrow m_X = 125$ GeV.

(6) Particle *decay widths*: $N(t) = N_0 e^{-t/\tau}$, $\Delta E \Delta t \sim 1 \Rightarrow \Delta E = \Delta m \sim \frac{1}{\tau} = \Gamma$. The mass of the particle produced in decays will not have a well-defined mass, but have an uncertainty associated.

(7) *Bump-hunting* example: $pp \to \mu^+\mu^-$. Bumps: resonance decay.

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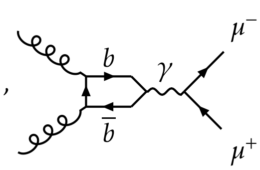
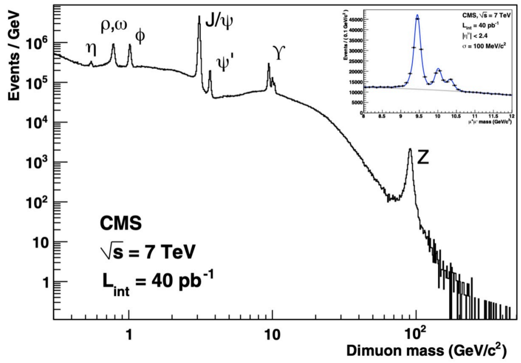
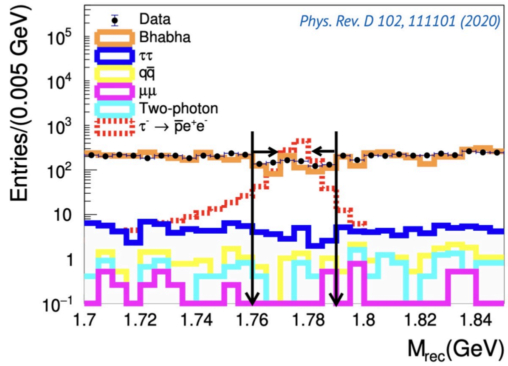
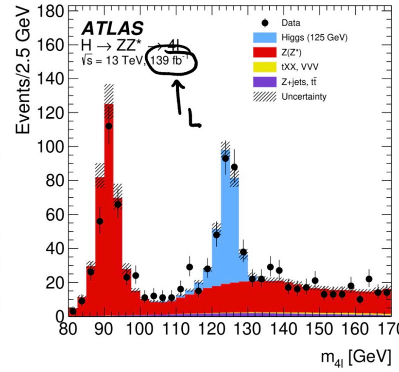



$\Upsilon(b\overline{b})$.



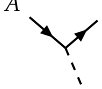




(8) Relativistic wave equation (*the Klein-Gordon equation*): $E^2 = p^2 + m^2 \xrightarrow{quantise} \hat{E}^2\psi = \hat{p}^2\psi + m^2\psi \Rightarrow -\frac{\partial^2\psi}{\partial t^2} = -\nabla^2\psi + m^2\psi$.

• Solutions: $\psi(\boldsymbol{x}, t) = Ne^{\pm i(Et - \mathbf{p}\cdot\mathbf{x})}$. The solution have positive and negative energy eigenvalues.

## 7.2 Interaction vertices

(1) Kinematic properties of a virtual process $A \to A' + X$:  . Consider the rest frame of the initial state,



$P_A^\mu = (m_A, \mathbf{0})$, $P_{A'+X}^\mu = \left(\sqrt{\mathbf{p}_f^2 + m_A^2}, \mathbf{p}_f\right) + \left(\sqrt{\mathbf{p}_f^2 + m_X^2}, -\mathbf{p}_f\right)$.

• $\Delta E = \sum E_f - \sum E_i = \sqrt{\mathbf{p}_f^2 + m_A^2} + \sqrt{\mathbf{p}_f^2 + m_X^2} - m_A$. $\begin{cases} m_X = 0 : \text{if } p_f \ll m_A \to \Delta E = p_f, & \text{if } p_f \gg m_A \to \Delta E = 2p_f \\ m_X \neq 0 : \text{if } p_f \ll m_A, m_X \to \Delta E = m_X, & \text{if } p_f \gg m_A, m_X \to \Delta E = 2p_f \end{cases}$

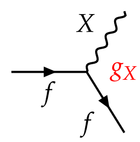
• Define the process as a *virtual process* as the energy is not conserved during this interaction and the relationship $E^2 - p^2 = m^2$ cannot hold for at least one of the particles. A particle that has $E^2 - p^2 \neq m^2$ is a *virtual particle*.

(2) Real processes have to contain at least two interactions. Consider $AB \to A'B'$ via the exchange of $X$.

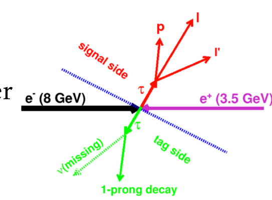
• KG equation in the static state: $\nabla^2\phi = m_X^2\phi$. For point-like particles we can rewrite it as $\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}(r\phi) = m_X^2\phi$.

• The solution $\phi(r) = -\frac{g^2}{4\pi}\frac{e^{-m_X r}}{r}$ is called the *Yukawa potential*. The normalisation constant $\frac{g^2}{4\pi}$ is related to the intrinsic strength of the interaction.

• For massless particle exchange, $\phi(r) \propto \frac{1}{r}$. For massive particle, $\phi \propto e^{-m_X r}$. $R = \frac{1}{m_X}$ is defined as the range of the force.

(3) Interactions in Feynman diagrams are represented by interaction vertices. eg:  Each interaction occurs with a *coupling strength* $g_X$. Define the dimensionless coupling $\alpha_X = \frac{g_X^2}{4\pi}$.






(4) The following quantities are conserved at each interaction vertex: electric charge $Q$, electron number $L_e$, muon number $L_\mu$, tau number $L_\tau$, baryon number $B$.

• Example: Searches for BNV and LNV: $\tau^- \to \bar{p}e^+e^-$, where $\tau$ is produced from $e^-e^+ \to \tau^-\tau^+$.

(5) The *scattering amplitude* $\mathcal{M}_{fi}$ is the probability amplitude for a scattering process, which can be calculated using Feynman diagrams. It is proportional to the product of coupling strengths defined by each interaction vertex. $\mathcal{M}_{fi} \propto \prod_i g_i$.

• Consider the scattering of a particle from a static potential: $\mathcal{M}_{fi} = \int \mathrm{d}^3r\, \psi_f^*(r)V(r)\psi_i(r)$. Assume $\psi(r) = e^{i\mathbf{p}\cdot\mathbf{r}}$,

$\Longrightarrow \mathcal{M}_{fi} = \int \mathrm{d}^3r e^{i\mathbf{q}\cdot\mathbf{r}} V(r)$, where $\mathbf{q} = \mathbf{p}_i - \mathbf{p}_f$. For the Yukawa potential, $V(r) = -\frac{g^2}{4\pi}\frac{e^{-m_X r}}{r}$, $\mathcal{M}_{fi} = -\frac{g^2}{|q|^2 + m_X^2}$. The relativistic result is $\mathcal{M}_{fi} = -\frac{g^2}{|q^\mu|^2 - m_X^2}$. $q^\mu = P_i^\mu - P_f^\mu$.

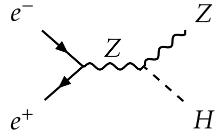
• For $|q^\mu|^2 \ll m_X^2$ (non-relativistic), $\mathcal{M}_{fi} = -\frac{g^2}{m_X^2} = \text{const}$. The probability amplitude is suppressed by the mass of the particle mediating the interaction $\Rightarrow$ The weak force is so much weaker than the EM force at low energies.

• For $|q^\mu|^2 \gg m_X^2$, $\mathcal{M}_{fi} = -\frac{g^2}{|q|^2}$. The mass of the mediating particle becomes irrelevant $\Rightarrow$ The weak force and the EM force becomes approximately equal in strength at very high energies.

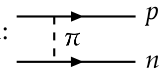
• $\mathcal{M}_{fi}$ is largest for $|q^\mu|^2 \sim m_X^2 \Rightarrow$ The virtual mediating particle are preferentially produced with an invariant mass that is close to the true mass of the particle.

(6) The *cross section* $\sigma$ is a measure of the probability of a specific interaction. The units for cross sections are *barns* (b).

• $\sigma \propto |\mathcal{M}_{fi}|^2$. The number of events in a collider experiment $N = \sigma L$, where $L$ is the *integrated luminosity*. The integrated luminosity is a measure of the size of a dataset, i.e. how many interactions have occurred in a given timeframe.

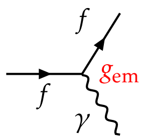
(7) Search for Higgs at LEP: $e^+e^- \to ZH$, 

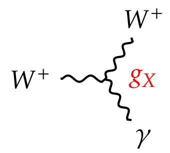
. $m_{ZH}^{\text{min}} = m_H + m_Z = 216$ GeV $> E_{\text{cm}}^{\text{LEP}} = 209$ GeV (1995).

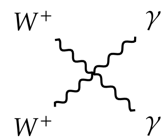
(8) Search of Higgs at LHC: $H \to ZZ^* \to 4l$. $\sigma_H \sim 55$ pb $\Rightarrow N_H \overset{139\text{fb}^{-1}}{=\!=\!=} 7.6\times 10^6$. Events observed $N = 220$. Factors: (i) Branching ratio $\mathcal{BR}(H \to 4l) = 1.29\times 10^{-4}$, (ii) Detector efficiency.
(9) Range of the strong force. $R \sim 1$fm $= 5.08$ GeV$^{-1}$ $\Rightarrow m_X = 197$ MeV. Yukawa: 

. Modern explanation: exchange of $d$ between $p$ and $n$.

## 7.3 Basics of the EM and strong interaction

(1) Between fermions and photons: 

. Between W-bosons and photons: 

, 

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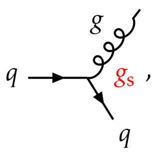
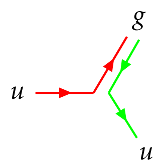
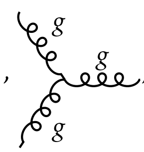
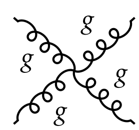
(2) The EM interaction strength $g_{\text{em}} = q_f$. The fine structure constant $\alpha_{\text{em}} = \frac{e^2}{4\pi\varepsilon_0\hbar c}$ [SI] / $\frac{e^2}{4\pi}$ [natural].
(3) Due to quantum fluctuations, the value of the coupling strength depends on the distance/momentum scale. *Quantum fluctuations* are the continuous emission and absorption of virtual particles from a real particle. Thus a real electron in a free space is surrounded by a plethora of virtual particles $\Rightarrow$ *vacuum polarisation* $\Rightarrow$ The electron charge is screened.
• $\alpha_{\text{em}} = \frac{1}{137}$ is valid only at $r \to \infty$. $\alpha_{em}$ increases as $r$ decreases.
• $\alpha_{\text{em}}^{\text{eff}} = \frac{\alpha_{\text{em}}^0}{1-\Delta\alpha(Q^2)}$, where $Q^2$ is the squared four momentum of the particle mediating the interaction (*virtuality*). Small $r$ is equivalent to large $Q^2$.
(4) Allowed vertices for QCD: 

, 

, 

, 

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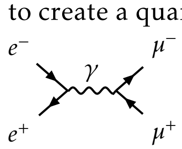
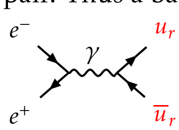
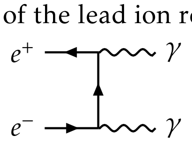
(5) Quarks carry $r, g, b$, antiquarks carry $\bar{r}, \bar{g}, \bar{b}$. Gluons carry $r\bar{g}$, $r\bar{b}$, $b\bar{r}$, $b\bar{g}$, $g\bar{r}$, $g\bar{b}$, $\frac{1}{2}(r\bar{r} - g\bar{g})$, $\frac{1}{\sqrt{6}}\left(r\bar{r} + g\bar{g} - 2b\bar{b}\right)$, ~~$\frac{1}{\sqrt{3}}\left(r\bar{r} + b\bar{b} + g\bar{g}\right)$~~.
• Each color charge can be written as $\Psi_r = \begin{pmatrix}1\\0\\0\end{pmatrix}, \Psi_g = \begin{pmatrix}0\\1\\0\end{pmatrix}, \Psi_b = \begin{pmatrix}0\\0\\1\end{pmatrix}$ in the colour space. The strong interaction can be thought as a rotation in the color space and gluons can be represented by the $3\times 3$ rotation matrices (Gellman matrices).
(6) The dimensionless coupling for the strong interaction $\alpha_s = \frac{g_s^2}{4\pi} \gg \alpha_{\text{em}}$.
• Effective QCD coupling strength is a balance between screening and antiscreening $\alpha_s(Q^2) = \frac{12\pi}{(33-2N_f)\ln\left(\frac{Q^2}{\Lambda^2}\right)}$. $N_f = 6$ is the number of colour-carrying fermions in the theory, $Q^2$ the four-momentum of the virtual gluon. That $33 > N_f$ leads to antiscreening wins and $\alpha_s$ decreases with increasing $Q^2$.
• *Asymptotic freedom*: At small $r$, $\alpha \to 0.1$, the potential $V(r) \sim \frac{\alpha_s}{r}$.
• *Colour confinement*: At large $r$, $\alpha_s$ rapidly increases. The potential $V(r) \sim r$ and eventually becomes large enough such that it is energetically favourable to create a quark-antiquark pair. Thus a bare-quark cannot be observed freely in nature.

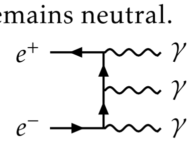
(7) Examples: $e^+e^- \to \mu^+\mu^-$: 

, $e^+e^- \to q\bar{q}$: 

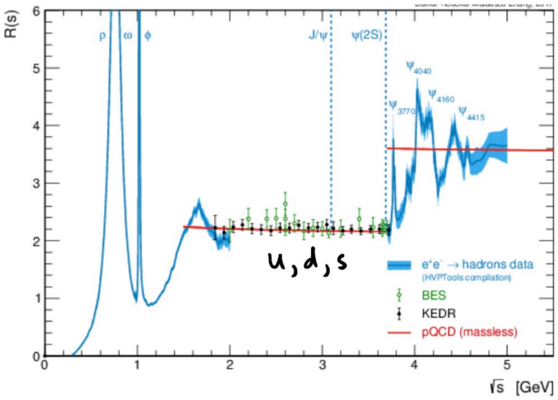
$\sum_i Q_i = 0$, $L_e^i = L_e^f = 0$, $L_\mu^i = L_\mu^f = 0$

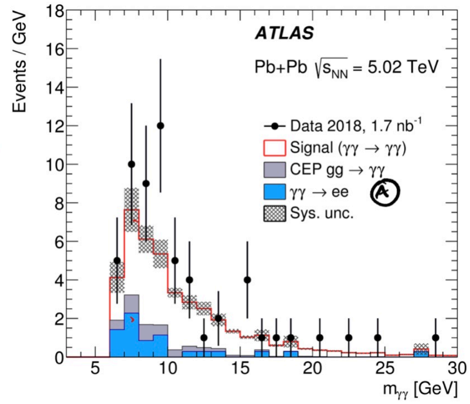
• $e^+e^- \to \mu^+\mu^-$: $\mathcal{M}_{fi} \propto e^2$. $\sigma_{e^+e^-\to\mu^+\mu^-} \propto |\mathcal{M}_{fi}|^2 = k(e^2)^2 = k\alpha_{\text{em}}^2 \overset{QFT}{=\!=\!=} \frac{4\pi\alpha_{\text{em}}^2}{3s}$, $\frac{d\sigma}{d\Omega} = \frac{\alpha_{\text{em}}^2}{4s}\left(1+\cos^2\theta\right)$.
• $e^+e^- \to q\bar{q}$: $\mathcal{M}_{fi} \propto \frac{2}{3}e^2$. $\sigma_{e^+e^-\to u_r\bar{u}_r} = k\frac{4}{9}\alpha_{\text{em}}^2$, $\sigma_{e^+e^-\to u\bar{u}} = 3k\frac{4}{9}\alpha_{\text{em}}^2$, $\sigma_{e^+e^-\to q\bar{q}} = 3k\alpha_{\text{em}}^2\sum Q_f^2$.
• $R = \frac{\sigma_{e^+e^-\to q\bar{q}}}{\sigma_{e^+e^-\to\mu^+\mu^-}} = 3\sum Q_f^2$. $R$ (i) can be used to confirm the number of colour states for quarks, (ii) or the number of active quarks that can be produced at a given $s$. (iii) $R$ will change w.r.t. $\sqrt{s}$ as more quark species become active.
gluon bkg: the net color of the lead ion remains neutral.

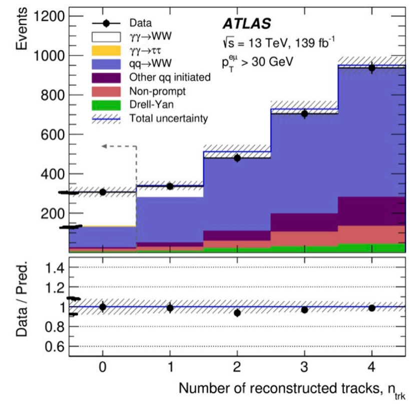
(8) Example: $e^+e^- \to 2\gamma$ 

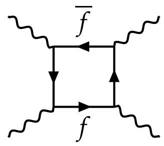
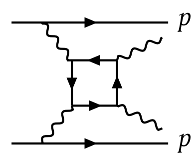
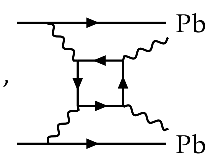
, 

. $\sigma_{\gamma\gamma} \propto |\mathcal{M}_{fi}|^2 \propto k_2\alpha_{\text{em}}^2$, $\sigma_{\gamma\gamma\gamma} \propto k_3\alpha_{\text{em}}^3$, $\frac{\sigma_{\gamma\gamma}}{\sigma_{\gamma\gamma\gamma}} \sim \frac{\alpha_{\text{em}}^2}{\alpha_{\text{em}}^3} \sim 137$.



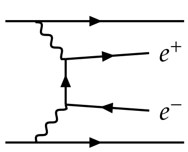
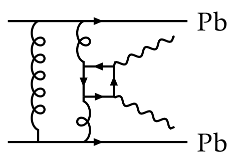



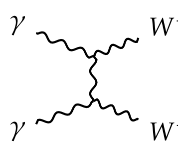
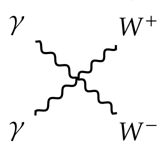

(9) *Light-by-light scattering*:  $\mathcal{M}_{fi} \propto e^4$, $\sigma_{\gamma\gamma\to\gamma\gamma} \propto \alpha_{\text{em}}^4$. Sources:  ,  .

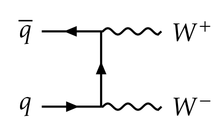
$\mathcal{M}_{fi}^{pp} \propto e^6$, $\sigma = k\alpha_{\text{em}}^6$. $\mathcal{M}_{fi}^{\text{PbPb}} \propto Z^2 e^6$, $\sigma = kZ^4\alpha_{\text{em}}^6$. $\frac{\sigma_{\text{PbPb}}}{\sigma_{pp}} \sim Z^4 = 4.5\times 10^7$. $\frac{N_{\text{PbPb}}}{N_{pp}} = \frac{\sigma_{\text{PbPb}}}{\sigma_{pp}}\frac{L_{\text{PbPb}}}{L_{pp}} \sim 1.3$ (ATLAS 2018).

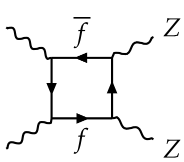
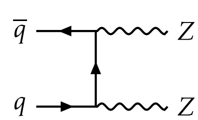
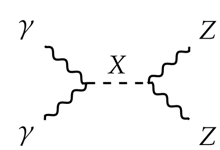
• Benefits of PbPb: We can keep a larger fraction of events in PbPb collisions because we're producing less events per second in the same disk size. Every time we read out the detector, we typically only have one PbPb interaction while in $pp$ collisions we have 60 $pp$ interactions read out.

• Backgrounds:  ,  Background: $\gamma\gamma \to e^+e^-$, $gg \to \gamma\gamma$. *Mistag rate*: The detector is not perfect, the track of the electron is somehow not seen in the tracker ($1\%^2$). $\sigma_{\gamma\gamma\to ee} \approx 10000\sigma_{\gamma\gamma\to\gamma\gamma}$. The relative rate at the end is similar between the two processes.

• Significance: After applying all selection criteria, 59 candidate events are observed for a background expectation of $12\pm3$ events $\Rightarrow$ *Excess of events over bkg* (Size of sig. events $S$): 59-12=47. *Expected bkg* (null hypothesis): 12. *Uncertainty in expectation*: $\sqrt{12}$ (stat.), 3 (syst.) $\Rightarrow$ Significance $\frac{S}{\sigma_B} = \frac{47}{\sqrt{3^2+12}} \sim 10$.

(10) $\gamma\gamma \to W^+W^-$:   . Experimental considerations: (i) ion-ion interactions disflavored for photon fusion if $m_{\gamma\gamma} \sim 200$ GeV. High momentum photon have shorter wavelength and it starts to resolve the structure of the ion. (ii) Effective detector acceptance similar in both $pp$ and PbPb.

• Signal: Number of additional charge particles produced in that $pp$ collision is zero. Background:  Since a colour charge is taken outside the proton, the proton will break up and lots of hadronisation will occur. But there's a fraction of events where no charged particles is produced.

(11) $\gamma\gamma \to ZZ$:  . Background:  . BSM possibilities:  (If you have something that interact with a photon, you kind of expect that thing to be interacting with $Z$ bosons as well) .

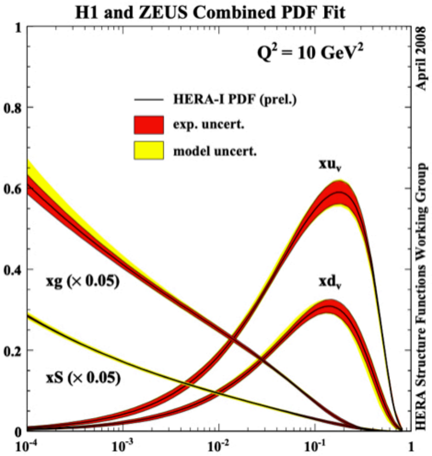
## 7.4 Hadron collisions and jets

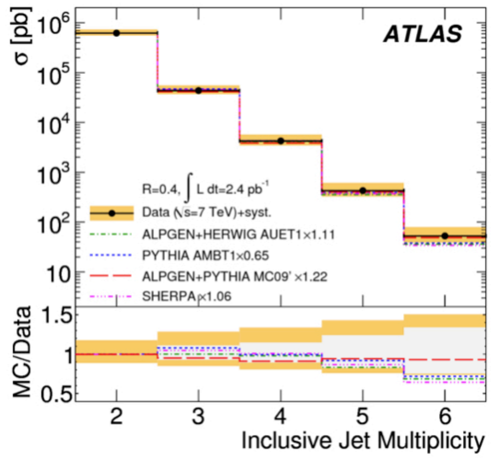
(1) The proton is made up of $uud$, which we refer to as *valence quarks*.

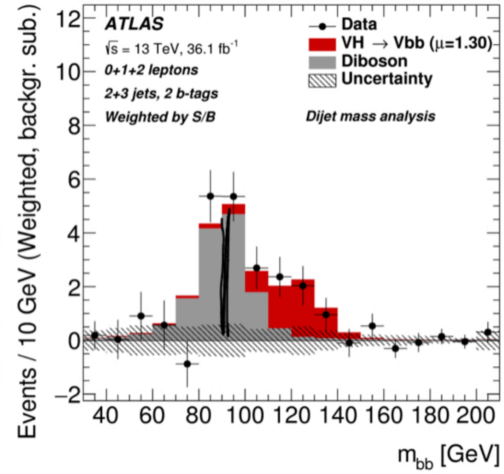
• The valence quarks are bound inside the proton by the strong force and therefore constantly interacting with each other via the exchange of *virtual gluons*. The virtual gluons can split into a *virtual quark-antiquark pair* or a gluon pair. We refer the virtual quarks and antiquarks. as *sea quarks*.

• Inside the proton there's a constant changing of color states of each of the quark but it's always in being color neutral.

(2) Hadron-hadron collision cross section:

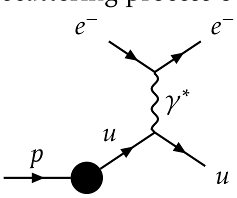



$$\sigma_{pp\to X} = \sum_{i,j}\int \mathrm{d}x_1 \int \mathrm{d}x_2 f_{i/p}\left(x_1, Q^2\right) f_{j/p}\left(x_2, Q^2\right) \hat{\sigma}_{ij\to X}\left(x_1, x_2, Q^2\right)$$

• $f_{i/p}\left(x, Q^2\right)$ is the *partonic distribution function* (PDF) which specify the probability of getting a parton of flavour $i$ out of a proton such that the parton carries a fraction $x$ of the proton momentum. $Q^2$ is the four-momentum scale at which the scattering process occurs.



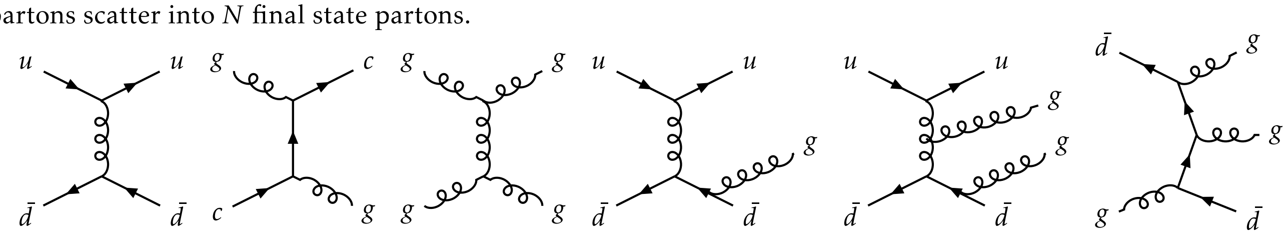

The PDFs are measured in processes such as *deep inelastic scattering* (DIS) at the HERA experiment. Consider the DIS process $e^-p \to e^-X$. In this process, $Q^2 = -|q^\mu|^2$, where $q^\mu$ is the four-momentum of the virtual photon. In DIS, $x = \frac{Q^2}{2(E_q E_p - \mathbf{q}\cdot\mathbf{p})}$, where $p^\mu = (E_p, \mathbf{p})$ is the four momentum of the proton beam. The results demonstrate that valence quarks have a peak at $x \sim 0.1 - 0.2$.

• The PDF of valence quarks have a peak slightly below a momentum fraction of $\frac{1}{3}$. At low momentum fraction there is a large contribution from additional virtual particles.

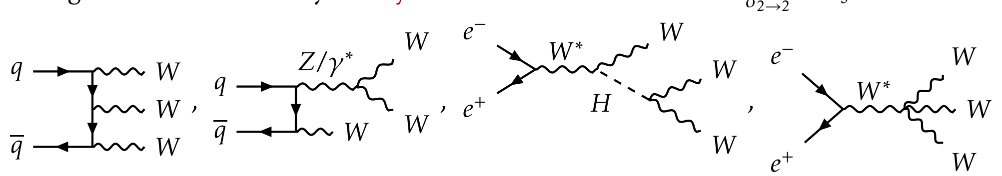
(3) If a process (eg: $u\bar{u} \to d\bar{d}$) can proceed via the strong or EM interactions, then the strong interaction will dominate. $\sigma_s \sim k\alpha_s^2$, $\sigma_{\text{em}} \sim k\alpha_{\text{em}}^2\left(\frac{2}{3}\right)^2\left(\frac{1}{3}\right)^2$. $\frac{\sigma_s}{\sigma_{\text{em}}} = \frac{81}{4}\frac{\alpha_s^2}{\alpha_{\text{em}}^2} \sim 500$.

• For each initial state color configuration, there are 3 final states for $\gamma \to d\bar{d}$ and 1 final state for $g \to d\bar{d}$.

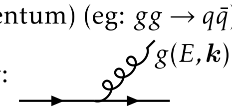
(4) The dominant parton scattering processes at hadron colliders are $2 \to N$ strong interaction processes, where two initial state partons scatter into $N$ final state partons.

• Eg: 


• The final state partons carry color charge and will eventually form *jets* of color neutral hadrons. $\frac{\sigma_{2\to 3}}{\sigma_{2\to 2}} \sim \alpha_s$.

• Electroweak $WWW$ production. 

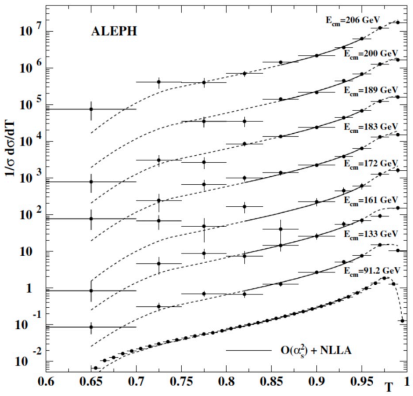

(5) *Multiple parton scattering*: (i) Double-parton scattering will occur in 4–jet production as background via two $pp \to jj$. (ii) Multiple soft partonic scattering (at low momentum) (eg: $gg \to q\bar{q}$) will accompany any hard scatter (eg: $q\bar{q} \to Z$).

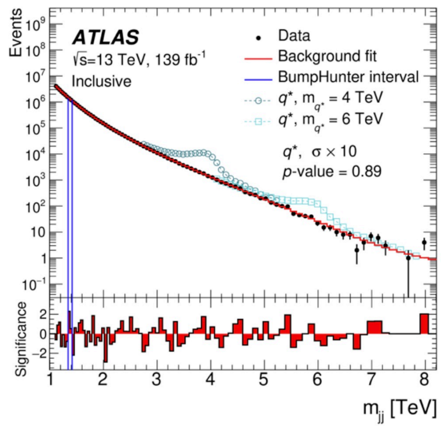
(6) *Jet formation*: Consider the processs $q \to qg$: 

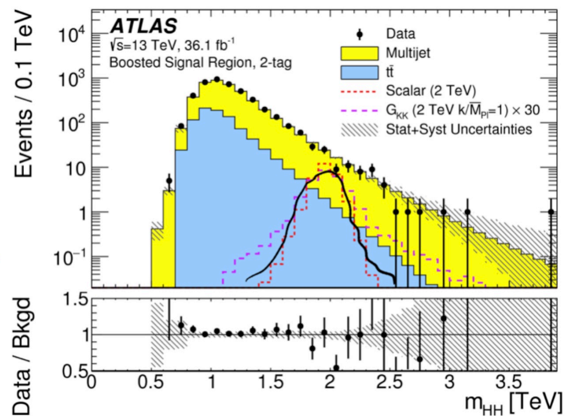
. Prob $\approx \frac{2\alpha_s C_F}{\pi}\frac{\mathrm{d}E}{E}\frac{\mathrm{d}\theta}{\theta}$ will diverge if $E \to 0$, $\theta \to 0 \Rightarrow$ Lots of soft (low-energy) or collinear (small angle) emissions $\Rightarrow$ parton shower (a stream of collinear hadrons).

• At the end of the parton shower, the partons are bound inside hadrons in process referred to as *hadronisation*.

• At large multiplicity, ⟨energy⟩ of partons decreases. Eventually $\alpha_s(Q^2)$ is large enough to form hadrons.



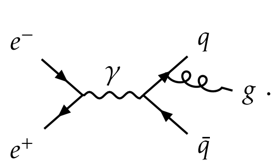



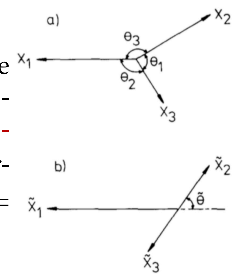

(7) Each of the partons carries a fraction of the initial quark energy → Parton-hadron duality: $\sum_i^{\text{hadrons}} \mathbf{p}_i \sim \mathbf{p}_{\text{quark}}$ in jet formation.

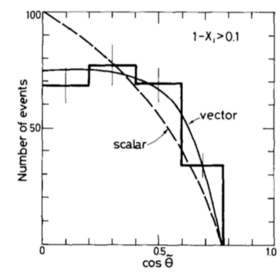
• Example: In $e^+e^-$ collisions, the measurement of $2j$ events tells us that the scattering process was $e^+e^- \to q\bar{q}$. The measurement of the differential cross section as a function of jet angle in COM frame proves that quarks are spin$-\frac{1}{2}$ particles. $\left(\frac{d\sigma}{d\Omega}\text{ is dependent on the particle spin}\right)$.

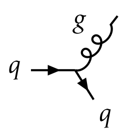
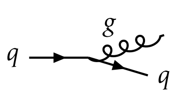
• The measurement of $3j$ events tells us the process was $e^+e^- \to q\bar{q}g$.



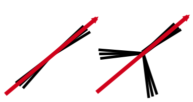

This proves the existence of the gluon. In the (b) frame (beam coming into page, products labelled according to energy) the *Ellis-Karliner angle* $\widetilde{\theta}$ is used to prove that gluons are spin−1 particles (solid/dashed line for spin−1/0). $\frac{\sigma_{jj}+\sigma_{jjj}}{\sigma_{jj}} = \left(1+\frac{\alpha_s}{\pi}\right)$.




(9) Classify  and  using event-shape observables (eg: *thrust*) and *jet algorithms*.

• Thrust $T = \max\left(\frac{\sum_i |\mathbf{p}_i \cdot \mathbf{n}_T|}{\sum_i |\mathbf{p}_i|}\right)$, where the summation runs over all hadrons and $\mathbf{n}_T$ is the *thrust axis* defined to maximise $T$.



Pencil-like events have $T \to 1$, Mercedes-like events have $T \to \frac{2}{3}$. This is useful for understanding QCD-induced effects but not useful for bump-hunting decays of heavy particles (eg: $Z/H \to b\bar{b}$).

(10) Kinematic properties: In the COM frame, $\begin{bmatrix} P_q^\mu = \left(x_q E_b, 0, 0, x_q E_b\right) \\ P_{\bar{q}}^\mu = \left(x_{\bar{q}} E_b, 0, 0, -x_{\bar{q}} E_b\right) \end{bmatrix} \Rightarrow m_{q\bar{q}}^2 = \left(P_q^\mu + P_{\bar{q}}^\mu\right)^2 = x_q x_{\bar{q}} E_{\text{cm}}^2,\ E_{\text{cm}} = 2E_b.$

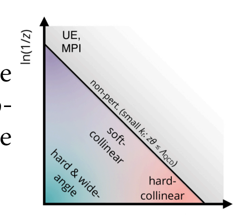
• Momentum fractions carried by the two colliding partons are typically small (PDF) $\Longrightarrow$ small invariant mass. Compounded by propagator effects $\mathcal{M}_{fi} \propto \frac{1}{|q^\mu|^2 - m_X^2} \Longrightarrow$ A falling distribution.

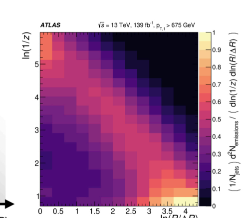
• No evidence for new hypothetical particles with mass 4/6 TeV (virtual resonance particles)

(11) Jet algorithm: particles clustered into jets if they are nearby using a predefined distance parameter and can be used for both QCD and bump-hunting (We want to work with 2/3 jets instead of 40 hadrons).

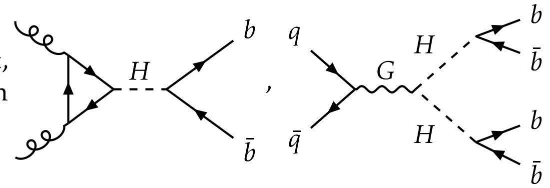
> **Iterative method**: (1) start with high−$p_T$particle and call this a pseudo-jet. (2) Add 4−momentum of nearby particle to the pseudo-jet if the distance between particle and pseudo-jet is small, i.e. if $\Delta R_{ij}^2 = (\eta_i - \eta_j)^2 - (\phi_i - \phi_j)^2 \le R_0^2$. (3) Recalculate the pseudo-jet 4−momentum. (4) Repeat steps 1-3 until all particles are merged into jets. **Key feature** is the distance measure. There are many variations for deciding that based on angular distance or relative momentum.

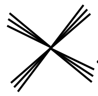
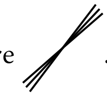
(12) The *Lund Plane*: Run jet-finding algorithms *backwards*, identify the hadrons that are being merged into a jet and test if the probability follows the theory. $P(E, \theta)$ can be represented by Lund Plane variables $\Delta R$ = angle between subjets and $Z = E_{\text{subjet}}/E_{\text{jet}}$. Large $\ln(R/\Delta R)$ stands for collinear and large $\ln(1/Z)$ stands for soft emission.



(13) Hadronically decaying boson produced at threshold (Higgs will be at rest, 2 back-to back jets). Hadronically decaying boson produced at high momentum (BSM), requires jet substructure analysis.




• Resolved boson decays: $m_G \gtrsim 2m_H$, 4 jet analysis . Bossted boson decays: $m_G \gg m_H$, 2 jet + substructure .

**V. Symmetries, conservation laws and hadron structure**

(1) *Noether's theorem*: There is a conserved quantity is the equations of motion are symmetric under a given transformation. In quantum mechanics, operators that commute with the Hamiltonian are conserved quantities.

(2) *Translational symmetry. Equation of motion*: $\psi'(x) = \hat{H}\psi(x)$. *Translation operator* $\hat{D}(x) = \psi(x + \mathrm{d}x)$. $\hat{D}\hat{H}\psi(x) = \hat{D}\psi'(x) = \psi'(x + \mathrm{d}x) = \hat{H}\psi(x + \mathrm{d}x) = \hat{H}\hat{D}\psi(x) \Rightarrow [\hat{D}, \hat{H}] = 0$.

• $\psi(x + \mathrm{d}x) = \psi(x) + \frac{\partial\psi}{\partial x}\mathrm{d}x = \psi(x) + i\mathrm{d}x\hat{p}\psi(x) \Rightarrow \hat{D} = 1 + i\mathrm{d}x\hat{p} \Rightarrow [\hat{p}, \hat{H}] = 0 \Rightarrow$ conservation of linear momentum.

(3) *Rotation in space*. Total angular momentum $\hat{J} = \hat{L} + \hat{S}$, $\hat{J}^2\psi(x) = j(j + 1)\psi(x)$, $\hat{J}_z\psi(x) = m_j\psi(x)$. $[\hat{J}, \hat{H}] = 0, [\hat{J}_z, \hat{H}] = 0$.

• Composite systems: the spin of the bound system $\mathbf{S}_B = \mathbf{J}_{\text{constituents}}$.

(4) *Parity*. $x \xrightarrow{P} x' = -x$. $\hat{P}\psi_a(x) = P_a\psi(x)$, $P_a = \pm 1$. $[\hat{P}, \hat{H}] = 0$ for strong and EM interactions.

• Dirac eq. $\Rightarrow P_f P_{\bar{f}} = -1$. Convention: $P_f = +1$, $P_{\bar{f}} = -1$. Maxwell's equations $\Rightarrow P_\gamma = -1$. Bound system $P_B = \left(\prod_i^N P_i\right)(-1)^L$.

• Parity of mesons $P = P_a P_{\bar{b}}(-1)^L = (-1)^{L+1}$. Parity of baryons $P = P_a P_b P_c(-1)^L = (-1)^L$. $L = 0 \Rightarrow P = 1$ for baryons.

(5) *Charge conjugation*: $\hat{C}\psi_a(x) = \psi_{\bar{a}}(x)$. For $\gamma, \pi_0$, $\hat{C}\psi_a(x) = C_a\psi_a(x)$, $C_a = \pm 1$. $[\hat{C}, \hat{H}] = 0$ for strong and EM interactions.

• Maxwell's equations $\Rightarrow C_\gamma = -1$. $\hat{C}\psi_{f\bar{f}}(x) = C_{f\bar{f}}\psi_{f\bar{f}}(x)$, $C_{f\bar{f}} = (-1)^{L+S}$.

(6) *Hadrons*. *Mesons*: $q\bar{q}$. *Baryons* $qqq$. *Anti-baryons*: $\bar{q}\bar{q}\bar{q}$. Hadrons are color singlet objects.

• Charge $Q_{\text{hadron}} = \sum_i q_i$. *Baryon number* $B = \frac{1}{3}[N_q - N_{\bar{q}}]$. *Strangeness*: $S = -[N_s - N_{\bar{s}}]$. *Charmness*: $C = [N_c - N_{\bar{c}}]$. *Bottomness*: $\widetilde{B} = -[N_b - N_{\bar{b}}]$. *Topness*: $T = [N_t - N_{\bar{t}}]$.

(7) Spin of hadrons $\mathbf{S}_{\text{hadron}} = \mathbf{J}_{\text{constituents}} = (\mathbf{L} + \mathbf{S})_{\text{constituents}}$. The lowest energy states have $L = 0$.

• Allowed values of $\mathbf{S}_{\text{constituents}}$: $S_1 + S_2, S_1 + S_2 - 1, \cdots, |S_1 - S_2|$. Allowed values of $\mathbf{J}$: $L + S, L + S - 1, \cdots, |L - S|$.

(8) Spins of mesons $\mathbf{S}_M = \mathbf{S}_q + \mathbf{S}_{\bar{q}} \Rightarrow S = 0, 1$.

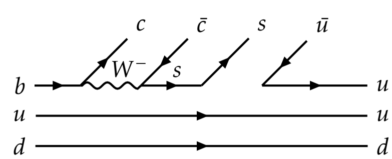
• If $L = 0$, then $J = 0, 1 \Rightarrow$ two states $^{2s+1}L_J = {}^1S_0$ and ${}^3S_1$.

• If $L = 1$, then $J = 1[S = 0]$, $J = 2, 1, 0[S = 1] \Rightarrow$ four states ${}^1P_1, {}^3P_2, {}^3P_1, {}^3P_0$.

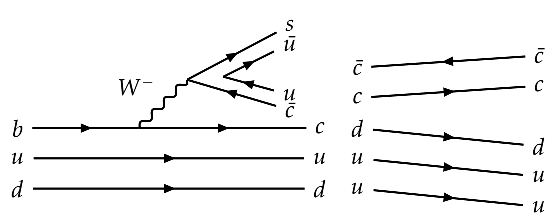
| | Quantum number | Photon | Bound state |
|---|---|---|---|
| Parity | Relativity $\Rightarrow P_f P_{\bar{f}} = -1$, $P_f = 1$, $P_{\bar{f}} = -1$ | $P_\gamma = -1$ | $P_B = \left(\prod_i^N P_i\right)(-1)^L$ |
| Charge conjugation | No distinct antiparticle: $C = \pm 1$. | $C_\gamma = -1$ | $C_{f\bar{f}} = (-1)^{L+S}$, $C_B = \left(\prod_i^N C_i\right)(-1)^{L+S}$ |
| Spin | integer/half-integer for bosons/fermions | $S_\gamma = \pm 1$ | $\mathbf{S}_{\text{hadron}} = \mathbf{J}_{\text{const.}} = (\mathbf{L} + \mathbf{S})_{\text{const.}}$ |

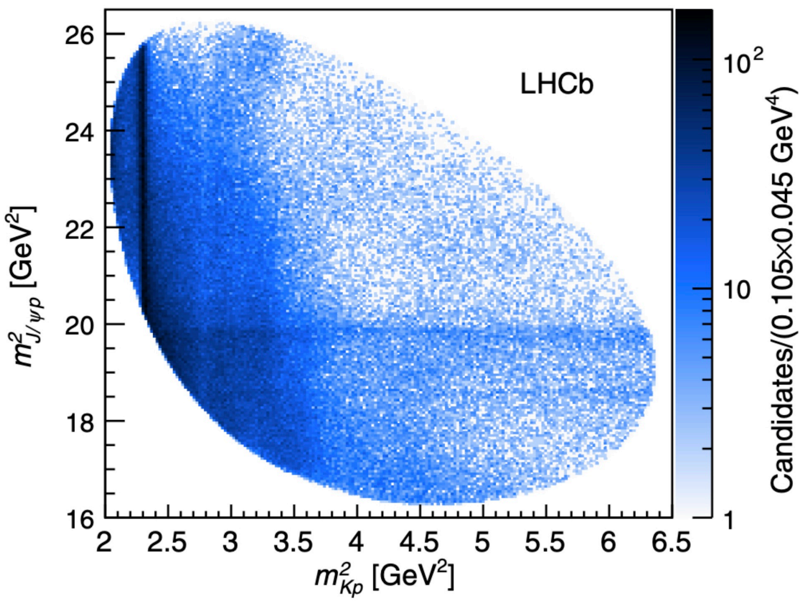
(10) *Exotic Hadrons*: Tetraquarks: $q\bar{q}q\bar{q}$ and pentaquarks $qqqq\bar{q}$.

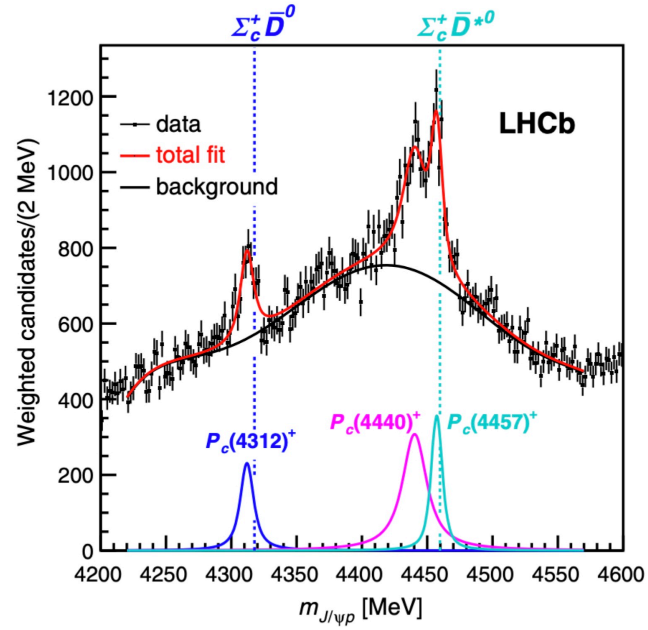
• Pentaquark search at LHCb. Consider $\Lambda_b^0 \to J/\psi + p + K^-$, $\Lambda_b^0 = udb$, $K^- = s\bar{u}$, $J/\psi = c\bar{c}$. Standard decays: $\Lambda_b^0 \to \Lambda^* J/\psi$, $\Lambda^* \to pK^- \Rightarrow$ Expect peak in the $m_{Kp}$ spectrum. The Dalitz plot indicates there are particles produced that decays to $J/\psi p$. The *Pentaquark explanation:* $\Lambda_b^0 \to K^- P_c^+$, $P_c^+ \to J/\psi p$.




The $P_c^+$ state consists of $uudc\bar{c}$. $\left(B, Q, S, C, \widetilde{B}\right) = (1, 1, 0, 0, 0)$ (same as proton). Ideal exotic has quantum numbers that are not possible for baryons and mesons. eg: $cccc\bar{s}$ with $\left(B, Q, S, C, \widetilde{B}\right) = (1, 7/3, 1, 4, 0)$. Alternative explanation for $uudc\bar{c}$: $\Sigma_c^+(udc) + \overline{D}^*(u\bar{c}) \Rightarrow$ particles need to not be decaying quickly for the bound state to form. $\Sigma_c^+ + \overline{D}^*$ is feasible since they are both narrow resonances (small width).






• 2-body threshold: energy needed to produce $\Sigma_c^+\overline{D}^*$ and the binding energy of the molecule system. For a strongly bound system like pentaquark system more of the mass will be used up and will be far away from the 2-body threshold.

### VI. Hadron spectroscopy

(1) Consider a family of particles with same $B, S, C, \widetilde{B}$ and $J^P$. Each particle in the family has the same *Hypercharge* $Y = B + S + C + \widetilde{B}$. Define the *third component of isospin* $I_3 = Q - \frac{Y}{2}$ and *Isospin* $I = (I_3)_{\text{max in family}}$.

• *Isospin multiplet*: family of particles with same $B, S, C, \widetilde{B}$ (same hypercharge $Y$) and $J^P$ but different $Q$ ($\Rightarrow$ different $I_3$).

• Isospin is a symmetry related to up and down quarks. Antiquarks have opposite $I_3$ to quarks.

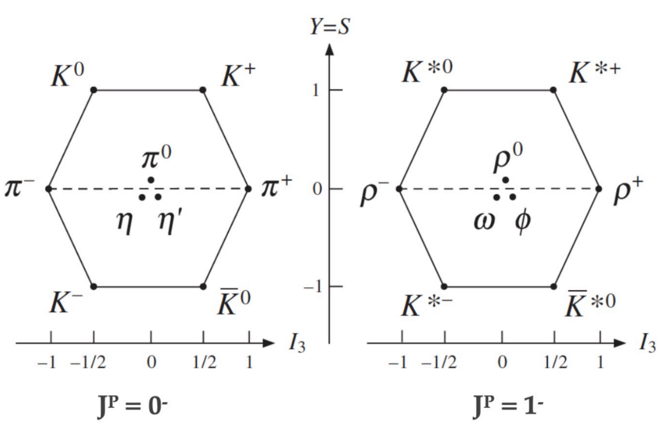
• Quark-based $I_3$ definition: $I_3 = \frac{1}{2}[(N_u - N_{\bar{u}}) - (N_d - N_{\bar{d}})]$. Addition of isospin: $\mathbf{I} = \mathbf{I}_a + \mathbf{I}_b$ has allowed values $I_a + I_b, \cdots, |I_a - I_b|$. $I_3 = I_3^a + I_3^b$.

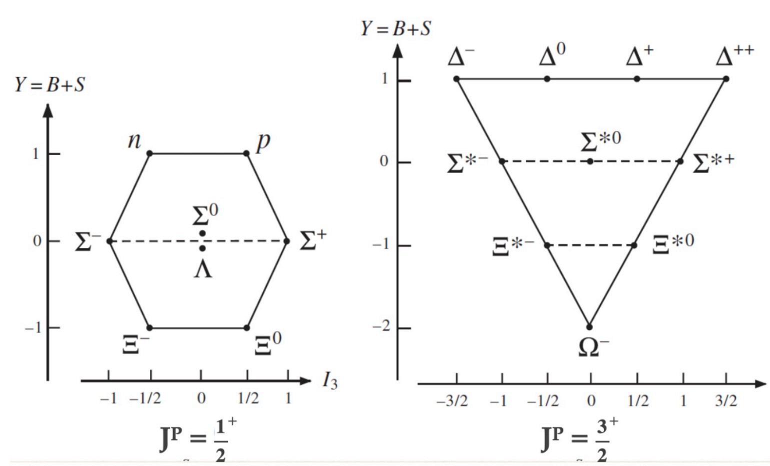
(2) *Supermultiplets*: particles with same $B$ and $J^P$. Consider light hadrons with $C = \widetilde{B} = 0$ $(u, d, s)$ and $L = 0$, $Y = B + S$.

$\Longrightarrow$ Particles can be described in $Y - I_3$ plane.

(3) *Ground-state meson nonets*: $u\bar{u}, u\bar{d}, u\bar{s}, d\bar{u}, d\bar{d}, d\bar{s}, s\bar{u}, s\bar{d}, s\bar{s} \Rightarrow$ defines $Y$ and $I_3$. For $L = 0$, $S_m = S_q + S_{\bar{q}} \Rightarrow 0, 1$.

$P_m = P_a P_b (-1)^L = -1 \Longrightarrow$ 9 states with $J^P = 0^-$, 9 states with $J^P = 1^-$. 3 states at $(Y, I_3) = (0, 0) \Rightarrow u\bar{u}, d\bar{d}, s\bar{s}$ conbinations.




(4) *Baryon supermultiplets*. Ten $q_a q_b q_c$ configurations: $uuu, uud, uus, ddu, dds, ddd, ssu, ssd, sss, uds \Rightarrow$ defines $Y$ and $I_3$.

• Pauli exclusion: hadron wave function must be antisymmetric under exchange of identical quarks. $\Phi_B = \Psi(x)\chi_s\chi_c$.

$\chi_c$ is antisymmetric, $\Psi(x)$ is symmetric $(L = 0) \Rightarrow \Psi(x)\chi_s$ must be symmetric $\Rightarrow$ spin of identical quarks are parallel.

| Baryon | Spin states | $J^P$ |
|---|---|---|
| $q_a q_b q_c$ $(uds)$ | $S_{ab} = 0, 1 \Rightarrow S_{abc} = \frac{1}{2}, \frac{1}{2}, \frac{3}{2}$ | $\frac{1}{2}^+(2)$, $\frac{3}{2}^+(1)$ |
| $q_a q_a q_a$ $(uuu)$ | $S = \frac{3}{2}$ (all spins are parallel) | $\frac{3}{2}^+(3)$ |
| $q_a q_a q_b$ $(uud)$ | $S_{aa} = 1 \Rightarrow S_{aab} = \frac{1}{2}, \frac{3}{2}$ | $\frac{1}{2}^+(6)$ $\frac{3}{2}^+(6)$ |

$\Longrightarrow$ 10 baryons with $\frac{3}{2}^+$, 8 baryons with $\frac{1}{2}^+$.
At $(Y, I_3) = (0, 0)$, 2 baryons $(uds)$ with $\frac{1}{2}^+$. $\Delta^{+++} = uuu$ is an evidence of color (colors of $uuu$ should be distinct).

(5) Hadron decays. If a hadron can decay via the strong interaction then its lifetime will be very short, $O(10^{-23})$ s.

• Electromagnetic decay suppression. Rough rule: $\frac{\alpha_{em}}{\alpha_s} \sim \sqrt{\frac{\tau_s}{\tau_{em}}}$. $\alpha_s \sim 1$ for low mass hadron decays $\Rightarrow \frac{\tau_{em}}{\tau_s} \sim 10^4$.

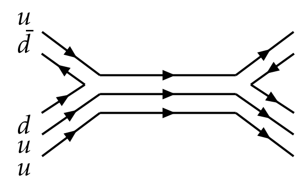
• Weak decay suppression: $\mathcal{M}_{fi} \sim -\frac{g_W^2}{m_W^2}$. This is equivalent to a suppression of $\alpha_W$ by a factor of $m_W^4$.

• eg: $n \to p e^- \overline{\nu}_e$: $\Delta E \sim 0.8$ MeV $\ll m_W$. Rough rule: $\frac{\alpha_w}{\alpha_s} = 10^{-7}$.

(7) Conservation laws:

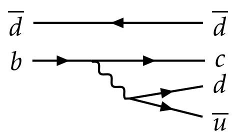
| Interaction | $B$ | $Q$ | $S$ | $C$ | $\widetilde{B}$ | $L_e$ | $L_\mu$ | $L_\tau$ | $J^{PC}$ |
|---|---|---|---|---|---|---|---|---|---|
| Strong | ✓ | ✓ | ✓ | ✓ | ✓ | — | — | — | ✓ |
| Electromagnetic | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| Weak | ✓ | ✓ | × | × | × | ✓ | ✓ | ✓ | only $J$ |

(8) Quark diagrams ($\pi^+ p \to \Lambda^{++} \to \pi^+ p$):




(9) Forbidden interactions: Consider $\pi^0 \to \gamma\gamma\gamma$. $S_{\pi^0} = J_{\gamma\gamma\gamma} = 0$, $C_{\pi^0} = (-1)^{L+S} = 1$, $C_{\gamma\gamma\gamma} = -1 \Rightarrow$ Forbidden.

(10) Hadronic weak decays. Example: $B^0 \to D^{*+}\pi^-$:




. $S, C, \widetilde{B}$ are all violated in weak interactions.

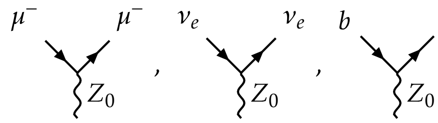
• In strong and EM interactions, quark flavour has to be conserved. In weak decay, the quarks can decay to lighter ones.

| Particle | Mass | Constituents | $B$ | $S$ | $C$ | $\widetilde{B}$ | $Y$ | $Q$ | $I_3$ | $I$ | $J^{PC}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $d$ | 4.7 MeV | | 1/3 | 0 | 0 | 0 | 1/3 | −1/3 | −1/2 | 1/2 | 1/2$^+$ |
| $u$ | 2.2 MeV | | 1/3 | 0 | 0 | 0 | 1/3 | 2/3 | 1/2 | 1/2 | 1/2$^+$ |
| $s$ | 96 MeV | | 1/3 | −1 | 0 | 0 | −2/3 | −1/3 | 0 | 0 | 1/2$^+$ |
| $c$ | 1.3 GeV | | 1/3 | 0 | 1 | 0 | 4/3 | 2/3 | 0 | 0 | 1/2$^+$ |
| $b$ | 4 GeV | | 1/3 | 0 | 0 | −1 | −2/3 | −1/3 | 0 | 0 | 1/2$^+$ |
| $t$ | 172 GeV | | 1/3 | 0 | 0 | 0 | 4/3 | 2/3 | 0 | 0 | 1/2$^+$ |
| $\pi^+, \pi^0, \pi^-$ | 140, 135 MeV | $u\overline{d}, (u\overline{u}, d\overline{d}), d\overline{u}$ | 0 | 0 | 0 | 0 | 0 | 1,0,-1 | 1,0,-1 | 1 | $0^-, 0^{-+}$ |
| $\eta, \eta'$ | 548, 978 MeV | $u\overline{u}, d\overline{d}, s\overline{s}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $0^{-+}$ |
| $K^+, K^0$ | 494, 498 MeV | $u\overline{s}, d\overline{s}$ | 0 | 1 | 0 | 0 | 1 | 1,0 | ±1/2 | 1/2 | $0^-$ |
| $K^-, \overline{K}^0$ | 494, 498 MeV | $\overline{u}s, \overline{d}s$ | 0 | −1 | 0 | 0 | −1 | −1,0 | ∓1/2 | 1/2 | $0^-$ |
| $\rho^+, \rho^0, \rho^-$ | 775 MeV | $u\overline{d}, (u\overline{u}, d\overline{d}), d\overline{u}$ | 0 | 0 | 0 | 0 | 0 | 1, 0, −1 | 1, 0, −1 | 1 | $1^{--}$ |
| $\phi$ | 1020 MeV | $s\overline{s}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $1^{--}$ |
| $\omega$ | 782 MeV | $u\overline{u}, d\overline{d}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $1^{--}$ |
| $D^+, D^0$ | 1.8 GeV | $c\overline{d}, c\overline{u}$ | 0 | 0 | 1 | 0 | 1 | 1,0 | 1/2, −1/2 | 1/2 | $0^-$ |
| $p, n$ | 938, 940 MeV | $uud$ | 1 | 0 | 0 | 0 | 1 | 1,0 | ±1/2 | 1/2 | 1/2$^+$ |
| $\Lambda$ | 1.1 GeV | $uds$ | 1 | −1 | 0 | 0 | 0 | 0 | 0 | 0 | 1/2$^+$ |
| $\Sigma^+, \Sigma^0, \Sigma^-$ | 1.2 GeV | $uus, uds, dds$ | 1 | −1 | 0 | 0 | 0 | 1, 0, −1 | 1, 0, −1 | 1 | 1/2$^+$ |
| $\Xi^0, \Xi^-$ | 1.3 GeV | $dss, uss$ | 1 | −2 | 0 | 0 | −1 | 0, −1 | ±1/2 | 1/2 | 1/2$^+$ |
| $\Delta^{++}, \Delta^+, \Delta^0, \Delta^-$ | 1.2 GeV | $uuu, uud, udd, ddd$ | 1 | 0 | 0 | 0 | 1 | 2, 1, 0, −1 | ±3/2, ±1/2 | 3/2 | 3/2$^+$ |
| $\Omega^-$ | 1.7 GeV | $sss$ | 1 | −3 | 0 | 0 | −2 | −1 | 0 | 0 | 3/2$^+$ |

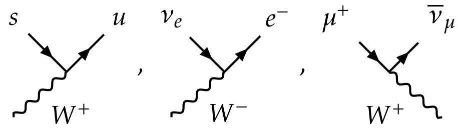
• Other mesons: $B^+$, $B^0$, $B_s^0$, $B_c^+$: $u\overline{b}$, $d\overline{b}$, $s\overline{b}$, $c\overline{b}$. $D^+$, $D^0$, $D_s$: $c\overline{d}$, $c\overline{u}$, $c\overline{s}$.

**VI. Electroweak interaction**

(1) *All leptons and quarks* experience the weak interaction. Exchange particles: $W, Z$. $m_W = 80.4$ GeV, $m_Z = 91.2$ GeV.

(2) *Neutral current*: 

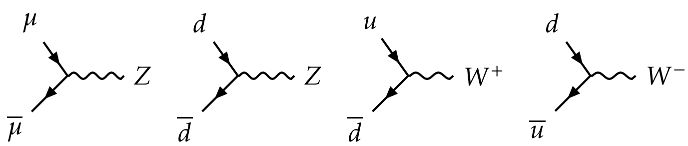
. $Q, L$ and quark flavour are conserved.

(3) *Charged current*: 

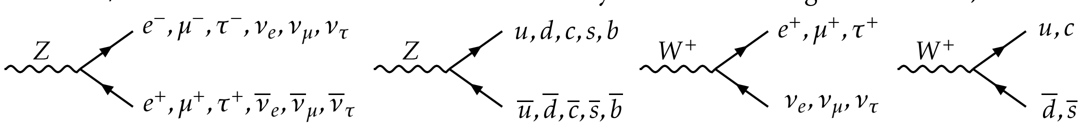
. The quark flavour is not conserved.

(4) *Discovery of the W and Z bosons.*

> The $W$ and $Z$ were discovered at the $Sp\bar{p}S$ (Super-Proton-Antiproton-Synchrotron). Collided $p\bar{p}$ have $\sqrt{s} \sim 540$ GeV, which is much higher than $m_W/m_Z$ as the quarks that are colliding carry only a fraction of the proton energy.
> The signature of a $W$ or $Z$ boson is an object with high transverse momentum, where the background is from the break-up of colliding protons which tend to travel in the longitudinal direction. When a new heavy particle is produced, it will typically be at rest and therefore the decay products travel at a large angle to the beam (back-to-back for 2 two decay products).

- Production: 


- The $W/Z$ boson has lifetime $\sim 10^{-25}$s and decays before reaching the detector, so we can only detect decay products.



(leptonic and hadronic).

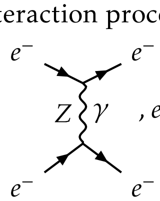
- Experimental signature of the $Z$.

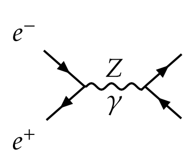
| Process | Signature | Comment |
|---|---|---|
| $Z \to \nu\overline{\nu}$ | Invisible | Impossible |
| $W/Z \to q\overline{q}$ | Two back-to-back jets | Hard because of hadronic backgrounds |
| $Z \to e^+e^-$ | Two showers in the ECAL + tracks | Best channel |
| $Z \to \mu^+\mu^-$ | Muon detector + tracks | Best channel |
| $Z \to \tau^+\tau^-$ | $\tau$ decays before reaching the detector | Very difficult |
| $W \to l\nu_l (\text{not } \tau)$ | High $p_T$ lepton and missing transverse momentum | Best channel |

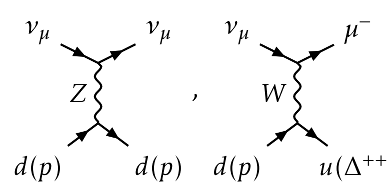
- It is difficult to measure the $W$ boson mass since the longitudinal momentum cannot be measured.
- $m_W^2 = \left(E_{T,l} + E_T^{\text{miss}}\right)^2 - \left(\mathbf{p}_{T,l} + \mathbf{p}_T^{\text{miss}}\right)^2 \overset{m_l \ll E_l}{=\!=} 2E_{T,l}E_T^{\text{miss}} - 2\mathbf{p}_{T,l} \cdot \mathbf{p}_T^{\text{miss}} = 2E_{T,l}E_T^{\text{miss}}(1 - \cos\phi_{l,\text{miss}})$.

(5) *Breit-Wigner function*: $\sigma \propto \frac{1}{(E-M_z)^2 + \Gamma^2/4}$, where the denominator contains the resonance term and the damping term.

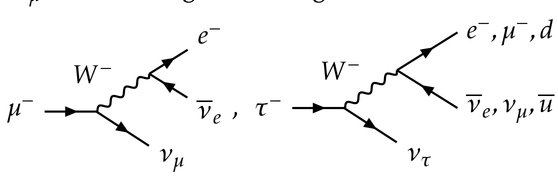
(6) Common weak interaction process.

- Electron scattering: 

, $e^+e^-$ annihilation: 

. Neutrino scattering: 


- Charged pion decay: $\pi^+ \to \mu^+\nu_\mu$. $\pi^+$ is the lightest charged meson $\Rightarrow$ cannot decay via the strong force.

- $\mu/\tau$ lifetimes: 2.2 $\mu$s/290 fs. 

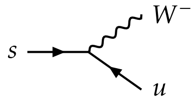
(1-prong). $\tau \to \nu_\tau + \pi^- + \pi^+ + \pi^-$ (3-prong).

(7) *Lepton universality*: The coupling strength of $W/Z$ to a lepton is independent of the lepton flavour.

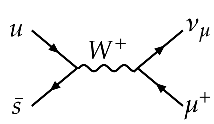
- $W^- \to e^-\overline{\nu}_e$, $W^- \to \mu^-\overline{\nu}_\mu$, $W^- \to \tau^-\overline{\nu}_\tau$ have the same coupling strength.

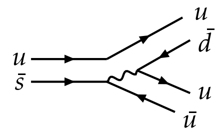
(8) *Lepton-quark symmetry*: The coupling strength of a $W$ to quarks is the same as the coupling strength of $W$ to a lepton.
$\Longrightarrow$ Hadronic decays $W^- \to \overline{u}d$, $W^- \to \overline{c}s$ have 3 times higher probability than leptonic decays (color factor).

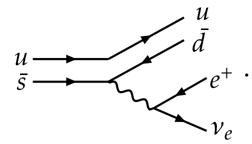
• Estimated $\tau$ decay branching ratios: $e^-\overline{\nu}_e$, $\mu^-\overline{\nu}_\mu$, hadrons have $1:1:3$.
• Estimated $W$ decay branching ratios: $e^-\overline{\nu}_e$, $\mu^-\overline{\nu}_\mu$, $\tau\overline{\nu}_\tau$, $d\overline{u}$, $s\overline{c}$ have $1:1:1:3:3$.
(9) *Decay rate* $\Gamma = 2\Delta E = \frac{\hbar}{\tau} = \frac{1}{\tau}$ in natural units. *Partial decay width* $\Gamma(X \to Y) = \Gamma_{\text{tot}}(X)\cdot B(X \to Y)$.
(10) The matrix element $[\mathcal{M}] = [E]^{-2}$, $[\Gamma] = [K][\mathcal{M}^2] = [K][E]^{-4} \Rightarrow [K] = [E]^5 \Rightarrow K \propto m_l^5 \Rightarrow \Gamma(\mu) \propto m_\mu^5, \Gamma(\tau) \propto m_\tau^5$.
• $\tau_\tau = \frac{1}{\Gamma_{\text{tot}}(\tau)} = \frac{B(\tau^-\to e\bar{\nu}_e\nu_\tau)}{\Gamma(\tau^-\to e\bar{\nu}_e\nu_\tau)} \propto \frac{B(\tau^-\to e\bar{\nu}_e\nu_\tau)}{m_\tau^5}, \tau_\mu = \frac{1}{\Gamma_{\text{tot}}(\mu)} = \frac{B(\mu^-\to e\bar{\nu}_e\nu_\mu)}{\Gamma(\mu^-\to e\bar{\nu}_e\nu_\mu)} \propto \frac{B(\mu^-\to e\bar{\nu}_e\nu_\mu)}{m_\mu^5} \Rightarrow \frac{\tau_\tau}{\tau_\mu} = \frac{B(\tau^-\to e\bar{\nu}_e\nu_\tau)}{B(\mu^-\to e\bar{\nu}_e\nu_\mu)}\frac{m_\mu^5}{m_\tau^5} = 1.328\times 10^{-7}$.
• Lepton universality: $\Gamma(Z\to\mu^+\mu^-)/\Gamma(Z\to e^+e^-) \approx 1$, $\Gamma(Z\to\tau^+\tau^-)/\Gamma(Z\to e^+e^-)\approx 1$.

(10) Decays of strange particles: 

. Typical strong, weak process lifetime: $O(10^{-23})$, $O(10^{-10})$.

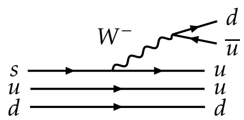
• $K^+(u\bar{s})$ lifetime $1.24\times 10^{-8}$s $\Rightarrow$ weak decay. 

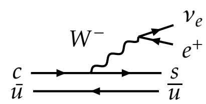
, 

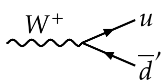
, 

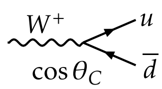
.

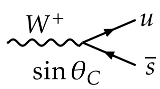
Branching ratios: $K^+\to\mu^+\nu_\mu$ (63.55%), $K^+\to\pi^+\pi^0$ (20.66%), $K^+\to\pi^0e^+\nu_e$ (5.07%).

• $\begin{bmatrix}\Lambda^0(uds)\\ 2.63\times10^{-10}\text{s}\\ 1115.7\text{ MeV}\end{bmatrix}$ 

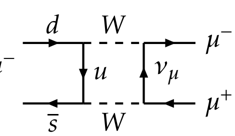
, $\begin{bmatrix}B(\Lambda^0\to p\pi^-) = 64\%\\ B(\Lambda^0\to n\pi^0) = 36\%\end{bmatrix}$. $\begin{bmatrix}D^0(c\overline{u})\\ 4.1\times10^{-13}\text{s}\\ 1864.8\text{ MeV}\end{bmatrix}$ 

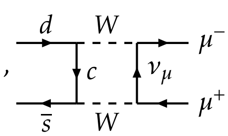
, $B(D^0\to K^-e^+\nu_e)\approx 3.5\%$.
(11) *Cabibbo mixing*. Nicola Cabibbo attempted to explain two observations: (i) The strong force cannot change the quark flavour. (ii) The weak charged current can change the quark flavour.
• Cabibbo's model: the strong interaction couples to the $d,u,s,c$ quarks, whereas the $W$ couples to a different set of quark eigenstates $\begin{pmatrix}u\\d'\end{pmatrix}$ and $\begin{pmatrix}c\\s'\end{pmatrix}$, where $\begin{pmatrix}d'\\s'\end{pmatrix} = \begin{pmatrix}\cos\theta_C & \sin\theta_C\\ -\sin\theta_C & \sin\theta_C\end{pmatrix}\begin{pmatrix}d\\s\end{pmatrix}$. $\begin{pmatrix}u\\d'\end{pmatrix} = \begin{pmatrix}u\\ d\cos\theta_C + s\sin\theta_C\end{pmatrix}$, $\begin{pmatrix}c\\s'\end{pmatrix} = \begin{pmatrix}c\\ s\cos\theta_C - d\sin\theta_C\end{pmatrix}$.
• 

$\Rightarrow$ 

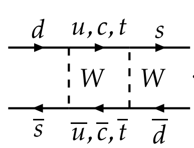
$+$ 

. Experimentally $\cos^2\theta_C = 0.949$, $\sin^2\theta_C = 0.051$, $\theta_C = 13.1°$.
• Similarly, $W^+\to c\bar{s}'$ contains $W^+\to c\bar{d}$ with an amplitude factor of $-\sin\theta_C$.
• Measurement of $\theta_C$. $\frac{\Gamma[K^-(s\bar{u})\to\mu^-\bar{\nu}_\mu]\propto\sin^2\theta_C}{\Gamma[\pi^-(d\bar{u})\to\mu^-\bar{\nu}_\mu]\propto\cos^2\theta_C} \propto \tan^2\theta_C$.

(12) *Flavour changing neutral current* $K^0\to\mu^+\mu^-$ 

, 

. The total amplitude is $\cos\theta_C\sin\theta_C - \cos\theta_C\sin\theta_C = 0$ is called the *GIM mechanism*.

(13) *Kaon mixing*. 

. $K^0$ and $\overline{K}^0$ can transform into each other. $\hat{C}\left|K^0\right\rangle = -\left|\overline{K}^0\right\rangle$, $\hat{C}\left|\overline{K}^0\right\rangle = -\left|K^0\right\rangle$. $\hat{P}\left|K^0\right\rangle = -\left|K^0\right\rangle$, $\hat{P}\left|\overline{K}^0\right\rangle = -\left|\overline{K}^0\right\rangle \Rightarrow \hat{C}\hat{P}\left|K^0\right\rangle = \left|\overline{K}^0\right\rangle$, $\hat{C}\hat{P}\left|\overline{K}^0\right\rangle = \left|K^0\right\rangle \Rightarrow$ Eigenstates $|K_1\rangle = \frac{1}{\sqrt{2}}\left[\left|K^0\right\rangle + \left|\overline{K}^0\right\rangle\right]$, $|K_2\rangle = \frac{1}{\sqrt{2}}\left[\left|K^0\right\rangle - \left|\overline{K}^0\right\rangle\right]$.
• A neutral kaon can decay to $\pi^+\pi^-$, $\pi^0\pi^0$, $\pi^0\pi^+\pi^-$, $\pi^0\pi^0\pi^0$ (lightest hadrons). The kaon has spin 0.
• $\pi^0\pi^0$. $J^P: 0^-\to 0^- + 0^- \Rightarrow L = 0$. $P = P_\pi^2(-1)^L = 1$, $C = C_\pi^2 = 1 \Rightarrow CP(\pi^0\pi^0) = +1$.
• $\pi^+\pi^-$. $L = 0$. $P = P_\pi^2(-1)^L = 1$. $C(\pi^+\pi^-) = P(\pi^+\pi^-) = (-1)^L = 1$. Here $\hat{C},\hat{P}$ have the same effect $\Rightarrow CP(\pi^+\pi^-) = +1$
• $\pi^0\pi^0\pi^0$. Define $\mathbf{L}_{12}$ to be the angular momentum of $\pi^0\pi^0$ and $\mathbf{L}_3$ the angular momentum of $\pi^0$ about the c.o.m. of $\pi^0\pi^0 \Rightarrow \mathbf{L}_{12} + \mathbf{L}_3 = \mathbf{0} \Rightarrow L_{12} = L_3$. $P = P_\pi^3(-1)^{L_{12}}(-1)^{L_3} = -1$. $C = C_{\pi^0}^3 = 1 \Rightarrow CP(\pi^0\pi^0\pi^0) = -1$.
• $\pi^+\pi^-\pi^0$. $P = -1$. $C = C(\pi^0)C(\pi^+\pi^-) = P(\pi^+\pi^-) = (-1)^{L_{12}} = 1$ (experimentally determined $L_{12} = 0$). $CP(\pi^+\pi^-\pi^0) = -1$.
• $K_1$ decays into two-pion final states, large mass difference $\Rightarrow$ big phase space $\Rightarrow$ short lifetime $\Rightarrow$ $K$–short ($K_S$).
• In the $K_2$ decays, there is much less phase space available $\Rightarrow$ long life time $\Rightarrow$ $K$–long ($K_L$).

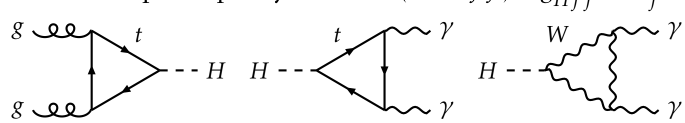
(14) The *CKM matrix* $\begin{pmatrix}d'\\s'\\b'\end{pmatrix} = \begin{pmatrix}V_{ud} & V_{us} & V_{ub}\\ V_{cd} & V_{cs} & V_{cb}\\ V_{td} & V_{ts} & V_{tb}\end{pmatrix}\begin{pmatrix}d\\s\\b\end{pmatrix} \approx \begin{pmatrix}\cos\theta_C & \sin\theta_C & 0\\ -\sin\theta_C & \cos\theta_C & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}d\\s\\b\end{pmatrix}$. $|V_{ub}|^2 \approx 2\times10^{-5}$, $|V_{cb}|^2\approx 2\times 10^{-3}$.
• The vertex $b\to uW^-$ gains a vertex amplitude of $V_{ub}$. The probability of this process is proportional to $|V_{ub}|^2$.

• Any decay of a $b$ quark is suppressed and the lifetime of $b$ is long $\Rightarrow$ A meson containing $b$ will travel a few millimetres before decaying $\Rightarrow$ secondary vertex.
(15) The $t$ quark being heavy $\Rightarrow$ short lifetime $\Rightarrow$ cannot hadronize.

## 7.5 Neutrinos

(1) Neutrinos are the second most abundant particle in the universe. $\gamma$: 400 cm$^{-3}$, $\nu$: 300 cm$^{-3}$, $p$: 0.5 cm$^{-3}$.
(2) Interaction with matter: $d(n)+\nu_e \to u(p)+e^-$, with cross section $10^{-43}$ cm$^2$.
(3) The interaction rate $W = Jn\sigma$, where $J$ is the particle flux, $n$ the number of target particles, $\sigma$ the cross section.
• The SNO detector contains 1000 t $D_2O$. $\sigma_{\nu_e D} = 0.4\times10^{-42}$ cm$^2$ for 1 MeV $\nu_e$. $J = 4.94\times10^6$ cm$^{-2}$s$^{-1}$ (from sun) $\Rightarrow$ $W = 1.18\times10^{-4}$ s$^{-1}$ $\Rightarrow$ 3736 interactions per year.
(4) *Additional neutrinos*. The width of the $Z$ boson depends on the number of decay modes. The more decay modes, the shorter the lifetime and therefore larger width. $\Gamma_Z = \Gamma_{ee}+\Gamma_{\mu\mu}+\Gamma_{\tau\tau}+\Gamma_{\text{had}}+N_\nu\Gamma_{\nu\nu}$.
(5) *Helicity*. If the spin and the direction of motion align/anti-align, then it's right/left–handed.
• Neutrinos can only be left–handed, and antineutrinos can only be right–handed.
(6) The weak interaction preferentially couples to left–handed particles and right–handed antiparticles. The chance of the weak interaction coupling to either a right–handed particle or a left–handed particle $\propto m^2$.
• Consider charged pion decay. $\overline{\nu}_l \longleftarrow \pi^- \longrightarrow l^-$. Pion spin is 0, $\overline{\nu}_l$ must be right–handed $\Rightarrow$ lepton must be right–handed to conserve angular momentum. $\frac{\mathcal{BR}(\pi^-\to e^-\overline{\nu}_l)}{\mathcal{BR}(\pi^-\to\mu^-\overline{\nu}_\mu)} = \frac{m_e^2}{m_\mu^2}\left(\frac{m_\pi^2-m_e^2}{m_\pi^2-m_\mu^2}\right)^2 = 1.3\times10^{-4}$.
(7) Cosmic rays interact with the upper atomsphere, producing showers of hadrons $\pi^+ \to \nu_\mu+\mu^+ \to \nu_\mu+e^++\nu_e+\overline{\nu}_\mu$ $\Longrightarrow$ Flavour ratio $2:1$ of $\nu_\mu:\nu_e$. Neutrinos that have traveled the full diameter of the earth have ratio $1:1 \Rightarrow$ Oscillations.
• A massless neutrino would be infinitely time-dilated $\Rightarrow$ could not change. Neutrino oscillation $\Rightarrow$ neutrinos have mass.

## 7.6 Misc

(1) $\alpha_{\text{em}} = 7.3\times10^{-3}$, $\alpha_{\text{w}} = 4.2\times10^{-3} \Rightarrow$ comparable. At high energies strength of EM and weak unify.
(2) GSW unify the electroweak interaction by introducing a *weak isospin* $T$.
• left–handed doublets $\begin{pmatrix} T=1/2, T_3=1/2 \\ T=1/2, T_3=-1/2\end{pmatrix}$: $\begin{pmatrix}\nu_{eL}\\ e_L\end{pmatrix}, \begin{pmatrix}\nu_{\mu L}\\ \mu_L\end{pmatrix}, \begin{pmatrix}\nu_{\tau L}\\ \tau_L\end{pmatrix}, \begin{pmatrix}u_L, c_L, t_L\\ d_L, s_L, b_L\end{pmatrix}$. Right-handed particles form $T=0$ singlets.
• $W$ boson has $T=1$. $T_3(W^-)=-1$, $T_3(W^+)=+1$. GSW predicted the existence of $W^0$ with $T_3=0$ ($Z_0$).
• Charged current weak interactions raise or lower $T_3$ by 1. $e^- \to \nu_e W^-$, $-\frac{1}{2} \to +\frac{1}{2}, -1$.
(3) *Unification condition*. $\frac{e}{2\sqrt{2\varepsilon_0}} = g_W\sin\theta_W = g_Z\cos\theta_W$, $\cos\theta_W = \frac{M_W}{M_Z}$. Measurements: $\frac{g_Z^2}{g_W^2} = \frac{G_Z}{G_F} = \tan^2\theta_W$, $\theta_W \sim 30°$.
(4) The Higgs mechanism states that the Higgs field permeates all space and gives masses to particles.
• Coupling strength between a fermion and the Higgs field $g_{Hff} = \sqrt{2}g_W\frac{m_f}{M_W}$.
(5) The Higgs boson was predicted to have spin 0, parity +1 and $\Gamma(H\to f\overline{f}) \propto g_{Hff}^2 \propto m_f^2$.
(6) Higgs production and decay 

. Massless particles don't couple directly to the Higgs and go through a virtual loop. The top quark is heavy and couples to the Higgs strongly.

| Channels | Comment | Channels | Comment |
|---|---|---|---|
| $H\to b\overline{b}$ | Hadronic background | $H\to\gamma\gamma$ | Although the branching ratio is small, the backgrounds are low and is a clean channel |
| $H\to gg$ | Hadronic background | $H\to ZZ$ | $H\to ZZ\to l^+l^-l^+l^-$. The channel is useful when both $Z$ decay to leptons since high $p_T$ leptons are hard to produce through a background process |
| $H\to\tau^+\tau^-$ | $\tau$ leptons decay before reaching the detector | $H\to WW$ | If $W$ decays to quarks $\Rightarrow$ Hadronic background. If $W$ decays to leptons $\Rightarrow$ Invisible neutrinos. |

(7) The coupling strength of the electroweak and strong interactions meet at $10^{15}$ GeV $\Rightarrow$ *Grand Unification*.
(8) The $W$ and $Z$ bosons have masses close to the energy at which the unification occurs (90 GeV) and the bosons are able to change particle types within doublets ($\nu_e$, $e^-$) and $(u,d)$. The GUT predicts the $X$ and $Y$ bosons.
• $X, Y$ have charge $-\frac{4}{3}$ and $-\frac{1}{3}$ and can change particle types within triplets $\begin{pmatrix}d\\ e^+\\ \nu_e\end{pmatrix}$: $d\to e^+X$, $d\to\nu_e e^- Y$, $X\to\bar{u}\bar{u}$, $X\to d\bar{e}^-$.
• Search for $X$ boson: $p\to e^+\pi^0$ $(u+u+d \xrightarrow{X} e^+ + \overline{u}+u)$.

(9) Less than $10^{-35}$ s after the Big Bang, the energy was greater than $10^{15}$ GeV. The following process can happen with CP violation: $X \to \overline{qq} < \overline{X} \to qq$, $X \to ql > \overline{X} \to \overline{q}\overline{l}$. The $q\bar{q}$ and $l\bar{l}$ pairs annihilate and result in matter-antimatter asymmetry.
(10) *Sakharov conditions* for matter-antimatter asymmetry.
- Baryon number violation, $C$–violation and $CP$–violation, Interactions out of thermal equilibrium ($\overline{X} \to qq, qq \to \overline{X}$).
- In the universe today $\frac{N_{\text{baryons}}}{N_{\text{photons}}} \sim 10^{-9}$.

## 7.7 Natural units

(1) Planck constant in SI units: $\hbar = 1.054 \times 10^{-34}$ J $\cdot$ s $= 6.582 \times 10^{-16}$ eV $\cdot$ s. $\hbar c \approx 197$ MeV $\cdot$ fm.
(2) Natural units: $c = \hbar = 1$, $1\text{s} = 3 \times 10^8$ m.
(3) $1 \text{ J} = 1 \text{ kg} \cdot \frac{\text{m}^2}{\text{s}^2} \xlongequal{\text{natural}} 1 \text{ kg} \cdot \frac{\text{m}^2}{(3\times 10^8 \text{m})^2} = \frac{1}{9\times 10^{16}} \text{ kg} \Rightarrow 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J} = 1.78 \times 10^{-36} \text{ kg}$.
(4) $\hbar c \approx 0.197 \text{ GeV} \cdot \text{fm} \xlongequal{\text{natural}} 1 \Rightarrow 1 \text{ fm} = 5.08 \text{ GeV}^{-1}$.