QM : APPROXIMATE METHODS

S.E. $H|\psi_i\rangle = E_i|\psi_i\rangle$

Variational Theorem:

$$E_0 \leq \langle\psi_T|H|\psi_T\rangle$$

Proof:
let $|\psi_T\rangle = \sum a_i|\psi_i\rangle$ where $H|\psi_i\rangle = E_i|\psi_i\rangle$

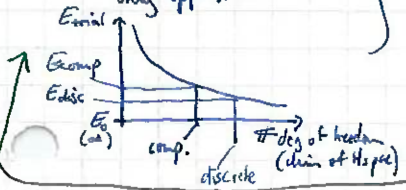
$\langle\psi_T|H|\psi_T\rangle = \sum_{ij} a_i a_j \langle\psi_i|H|\psi_j\rangle$ — $E_i\delta_{ij}$

$= \sum_i c_i^2 E_i \geq \sum_i c_i^2 E_0$, $\underbrace{\sum_i c_i^2}_{=1}$

Excited states:
$|\psi_T'\rangle = \sum a_i'|\psi_i\rangle$
$\Rightarrow \sum E_i a_i'^2 \geq E_1 \underbrace{\sum a_i'^2}_{1}$
only if $a_0' = 0$
only if ψ_T' is the exact G.S.!

Discrete systems: finite H-space
Cont. sys: infinite H-space
$\therefore$ can get exact
only approx

SYMMETRY:
variational parameters. use it for eg parity
$E_0^{even} \leq \langle\psi^T_{even}|H|\psi^T_{even}\rangle$
and $E_0^{odd} \leq \langle\psi^T_{odd}|H|\psi^T_{odd}\rangle$
or other symms.....



Time Independent Perturbation Theory (non-degenerate)

$H = H_0 + \lambda H_1$

$E_i = E_i^{(0)} + \lambda E_i^{(1)} + \lambda^2 E_i^{(2)} + \ldots$

$|\psi_i\rangle = \underbrace{c_i|\phi_i\rangle}_{|\psi_i^{(0)}\rangle} + \lambda \underbrace{\sum_{j\neq i} c_j'|\phi_j\rangle}_{|\psi_i^{(1)}\rangle} + \lambda^2 \underbrace{\sum_{j\neq i} c_j''|\phi_j\rangle}_{|\psi_i^{(2)}\rangle}$

normalisation: $\langle\psi_i^{(0)}|\psi_i\rangle = 1$ anything
$\Rightarrow \langle\psi_i^{(0)}|\psi_i^{(1)}\rangle = \langle\psi_i^{(0)}|\psi_i^{(2)}\rangle = 0$

1st order term: $H_0|\psi_i^{(1)}\rangle + H_1|\psi_i^{(0)}\rangle = E_i^{(0)}|\psi_i^{(1)}\rangle + E_i^{(1)}|\psi_i^{(0)}\rangle$

2nd order term: $H_0|\psi_i^{(2)}\rangle + H_1|\psi_i^{(1)}\rangle = E_i^{(0)}|\psi_i^{(2)}\rangle + E_i^{(1)}|\psi_i^{(1)}\rangle + E_i^{(2)}|\psi_i^{(0)}\rangle$

multiply 1st order term by $\langle\psi_i^{(0)}|$ and use orthog. property

$$E_i^{(1)} = \langle\psi_i^{(0)}|H_1|\psi_i^{(0)}\rangle$$

let $|\psi_i^{(1)}\rangle = \sum_{j\neq i} c_j|\psi_j^{(0)}\rangle$ and $c_j = \langle\psi_j^{(0)}|\psi_i^{(1)}\rangle$

multiply 1st order term by $\langle\psi_j^{(0)}|$ to find c_j

$$|\psi_i^{(1)}\rangle = \sum_{j\neq i} \frac{\langle\psi_j^{(0)}|H_1|\psi_i^{(0)}\rangle}{E_i^{(0)} - E_j^{(0)}}|\psi_j^{(0)}\rangle$$

$$E_i^{(2)} = \langle\psi_i^{(0)}|H_1|\psi_i^{(1)}\rangle = \sum_{j\neq i} \frac{|\langle\psi_j^{(0)}|H_1|\psi_i^{(0)}\rangle|^2}{E_i^{(0)} - E_j^{(0)}}$$

multiply 2nd order term by $\langle\psi_i^{(0)}|$
For G.S. 2nd order shift always $-$ve

Time Independent Perturbation Theory - Degenerate

$$E_{ni}^{(1)} = \langle\psi_{ni}^{(0)}|H_1|\psi_{ni}^{(0)}\rangle$$

$$\Rightarrow \sum_{deg.} c\left[\langle H_1\rangle - \delta_{ij}E^{(1)}\right] = 0$$

require W_{ij} diagonal
$W = H_1 = \begin{pmatrix} \ddots & 0 \\ 0 & \ddots \end{pmatrix}$
so $\sum_{j\neq i}$ has zero numerator $\therefore$ choose lin. comb such that H_1 is diagonalised.

Only requirement on $|\psi_{i\alpha}^{(0)}\rangle$ is that it gives $E_i\ \forall\alpha\ (1\ldots g)$
ie use e-states of H_1 and let H_0 be pert coz H_1 strong w.r.t. level spacing

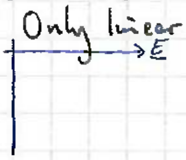
Numerical Methods

Let $\hat{O}$ be operator in question (eg $O = H_0 + \lambda H_1$)
then using any basis set, can find e-values and vecs of $\hat{O}$ on computer.... same comments about dimensionality of Hilbert space

Stark Effect:

shift in orb. energy with E.
Only linear in Hydrogen

For Hydrogen, ψ_{100} only shows quad. coz non-deg
ψ_2 has $l = 1, 0$ $m_l = -1, 0, 1$
$\therefore \exists$ deg's.



Treat as perturbation. Only for H-like atom have degenerate states. If nondeg, coz $H_1 = -eEr$ get no 1st order effect coz parity
If deg coz "states" (from before) are linear combs of even, odd... get 1st order effect

Time Dependent Perturbation Theory

$H_0|\phi_n\rangle = E_n|\phi_n\rangle$, let $H_1 \to H_1(t)$
and solve: $i\hbar\frac{d\psi}{dt} = (H_0 + H_1)\psi$ (S.E.)
let $\psi(t) = \sum_n c_n(t)e^{\frac{-iE_nt}{\hbar}}|\phi_n\rangle$ and sub
use orthogonality ie $\langle\phi_k|\ldots$ (TP1 eq'n 78)
get $\boxed{i\hbar\frac{dc_k}{dt} = \sum_n c_n(t)e^{i(E_k - E_n)t/\hbar}\langle\phi_k|H_1|\phi_n\rangle}$

low P.T.: let $c_i = c_i^{(0)} + \lambda c_i^{(1)} + \lambda^2 c_i^{(2)} + \ldots$
$H_1 \to \lambda H_1$ use zero order result: $c_i^{(0)}(t) = \delta_{im}$
first order term:
$\frac{dc_i^{(1)}}{dt}(t) = \frac{-i}{\hbar}H_{1im}e^{i\omega_{im}t}$ (system in state m at $t = 0$)

so $|c_k(t)|^2 = \frac{1}{\hbar^2}\left|\int_0^t dt' H_{km}(t')e^{i\omega_{km}t'}\right|^2$ ie $|c_{m}|^2$

$$\Gamma_{\substack{m\,n \\ \text{or } j\,k}} = \frac{2\pi}{\hbar}|V_{\substack{m n\\ k j}}|^2\delta(E_{\substack{n\\k}} - E_{\substack{m\\j}})$$

Switched-on Potential

let $H_1 = V(r)$ switched on at time $t = 0$

$\therefore P_{\substack{m n\\ j k}} = \frac{|V_{\substack{n m\\ k j}}|^2}{\hbar^2}\left(\frac{\sin\omega_{kj}t/2}{\omega_{kj}/2}\right)^2$

as $t \to \infty$ get delta f'n

Fermi's Golden rule

$$\Gamma = \frac{2\pi}{\hbar}\rho_f(E_m)|V_{\substack{nm\\kj}}|^2$$

$$\Gamma = \sum_n \Gamma_{mn} = \int \rho_f(E_n)dE_n\Gamma_{\substack{mn\\jk}}$$

Oscillatory Potential - eg incoming photon!

let $H_1 = V(r)e^{-i\omega t}$
subst and do S: $|c_k|^2 = \frac{4}{\hbar^2}|V_{kj}|^2\left(\frac{\sin\frac{1}{2}(\omega_{kj} - \omega)t}{\omega_{kj} - \omega}\right)^2$

$\Rightarrow$ $\boxed{\text{weight in final states oscillates if } \omega_{kj} \neq \omega \text{ but } \propto t^2 \text{ if } \omega_{kj} = \omega}$

so $\Gamma = \frac{dP}{dt}$ is $\propto t$) consider trans. to range $g(E_k)dE_k$

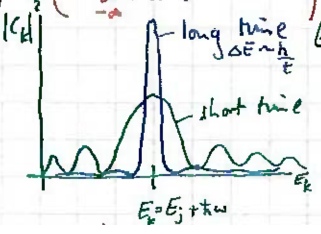
total prob $= \int_{-\infty}^{\infty}|c_k|^2 g(E_k)dE_k$

subst for u then say for long time, only consider narrow range of E around $E_j + \hbar\omega$.....

$\boxed{\text{In this range, } |V|^2 \text{ and } g \text{ are } \sim\text{const.}}$

$$\Rightarrow \frac{dP}{dt} = \Gamma_{jk} = \frac{2\pi}{\hbar}|V_{kj}|^2 g(E_j + \hbar\omega)$$

(as $\int_{-\infty}^{\infty}\left(\frac{\sin u}{u}\right)^2 du = \pi$)



Spontaneous Transitions

Thermal eq'm $\Rightarrow$ transition rates are equal
ie number in j $\times$ rate for one $=$ no. in k $\times$ rate for one
ie $n_j(\Gamma_{jk}^{spon} + \Gamma_{jk}^{stim}) = n_k\Gamma_{kj}^{stim}$ but $n_i \propto g(E_i)e^{-\frac{E_i}{kT}}$
For Γ^{stim} use Fermi's Golden Rule. $V = E_0(\omega_{jk})\cdot\underline{d}\cos(\omega_{jk}t) \times \frac{1}{2}$ — dipole trans operator
Average $|M|^2$ over all space $\to$ factor of $\frac{1}{3}$
Use energy density $\rho(\omega) = \frac{1}{2}\varepsilon_0|E_0(\omega)|^2 g(\omega)$ J m^{-3} ω^{-1}
$\to$ substitute then use BBR: $\rho(\omega) = \frac{\hbar\omega^3}{\pi^2c^3}\frac{1}{(e^{\frac{\hbar\omega_{kj}}{kT}} - 1)}$

Get $\boxed{\Gamma_{jk}^{spon} = \frac{\omega^3}{3\pi\varepsilon_0\hbar c^3}|\langle\phi_k|\underline{d}|\phi_j\rangle|^2 g(E_k)}$

Selection Rules

dipole transitions - need non-zero matrix element.
Dipole trans. operator $\underline{d} = -e\underline{r} = -er(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$
For m_l (z component of $\underline{L}$) (measuring mag. of dipole in x, y, z dirs)
$\langle\ \rangle$ means $\int$ over all angles. always get $\int_0^{2\pi} e^{im\phi}d\phi = \begin{bmatrix} 2\pi & \text{if } m_l = 0 \\ 0 & \text{if } m_l \neq 0 \end{bmatrix}$
So can get: $\Delta m_l = 0$ or ± 1
For l, consider $\hat{P}\langle\phi_k|\underline{d}|\phi_j\rangle$ - must be invariant under operation.
$\therefore \Delta l$ must be odd. By writing $\cos\theta Y_{lm_l} = \alpha Y_{l+1,m_l} + \beta Y_{l-1,m_l}$
use orthogonality and $\sin\theta e^{\pm i\phi}Y_{lm} = \gamma Y_{l+1,m_l\pm 1} + \delta Y_{l-1,m_l\pm 1}$
get $\Delta l = \pm 1$ as $\Delta j = \Delta l + \Delta m_s$ can write:
$\Delta l = \pm 1$
$\boxed{\Delta j = \pm 1 \text{ or } 0 \text{ but not } 0 \to 0}$

Q.M.: MOLECULAR STRUCTURE

Wavef'n for n electrons, N nuclei obeys S.E.:
$$i\hbar \frac{\partial}{\partial t}\Psi(\{\underline{r}_n\},\{\underline{r}_N\},t) = H\Psi$$

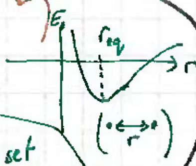
Exact Hamilton is $H = \sum_n \frac{p_n^2}{2m_e} + \sum_N \frac{p_N^2}{2m_N} + V(\ )$ (electrostatic)

Newton's 3rd law $\Rightarrow p_n\Psi \sim p_N\Psi$ which means nuclear motion term can be dropped ie to 1st approx, assume as ions move, electrons remain in their instantaneous eigenstates.

$\Rightarrow$ S.E.2: $\left[\sum_n \frac{-\hbar^2}{2m_e}\nabla_n^2 + V(\ )\right]u_k(\ ) = E_k(\{\underline{r}_N\}).\,u_k(\ )$

where $u_k(\ )$ are e-states for the electrons. **Born-Oppenheimer Approximation**

$\exists$ a complete set of $u_k(\ )$ for each pos'n of nuclei and so $\exists$ a set of energies for each pos'n of nuclei. As nuclei pos'ns vary, G.S. energy for e^- varies... follows the molecular potential energy curve see below!



There is a problem with using numerical methods near nuclei coz Coulomb potential diverges $\therefore$ need lots of pts in grid $\therefore$ slow convergence.

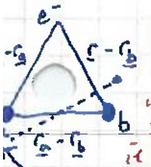
So – represent molecular wavef'ns as linear superpositions of atomic wavef'ns because they have correct form already. **L.C.A.O.**

Must remember that we are now using a non-orthog. basis $\therefore$ have overlap integral
$$\boxed{S = \int_{\text{all space}} \psi_a^*\psi_b\, d^3\underline{r}}$$

For proper results – use large no. of atomic wavef'ns (ie span the space....) but can get a good idea for GS by just taking G.S. wavef'ns for the superpositions as seen below (H_2^+)

H_2^+ Ion

Potential is $V(\underline{r},\underline{r}_a,\underline{r}_b) = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{|\underline{r}_a-\underline{r}_b|} - \frac{1}{|\underline{r}-\underline{r}_a|} - \frac{1}{|\underline{r}-\underline{r}_b|}\right)$



$\boxed{\text{L.C.A.O.: let } u(\underline{r},\underline{r}_a,\underline{r}_b) = \alpha\psi_a + \beta\psi_b}$

where ψ_a is G.S. wavef'n for proton a

ie $\boxed{\psi_a = \frac{1}{\sqrt{\pi a_0^3}}\exp\left[-\frac{|\underline{r}-\underline{r}_a|}{a_0}\right]}$

Standard Procedure: Use Variational Principle:
$$E_0 \le \frac{\langle u|H|u\rangle}{\langle u|u\rangle} = \frac{(\alpha^2+\beta^2)H_{aa} + 2\alpha\beta H_{ab}}{\alpha^2+\beta^2+2\alpha\beta S}$$

where: $H_{aa} = \int\psi_a H\psi_a\, d^3\underline{r}$ (on site) $\quad H_{ab} = \int\psi_a H\psi_b\, d^3\underline{r}$ (off site) and S....

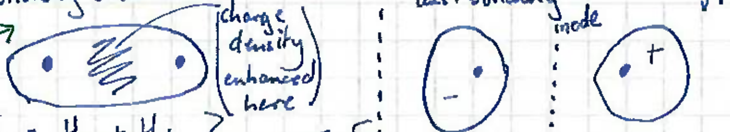
u must be symm or a/sym under mid pt inv... $\Longrightarrow \alpha = \pm\beta$, or 2 (always so)

(E_{min} at $\alpha=-\beta$ for $H_{aa} \le SH_{ab}$ and at $\alpha=+\beta$ for $\boxed{H_{ab} < SH_{aa}}$)

This is an inversion through nuclear midpt. – it interchanges ψ_a and ψ_b but is not a Parity inversion as origin is elsewhere – think......

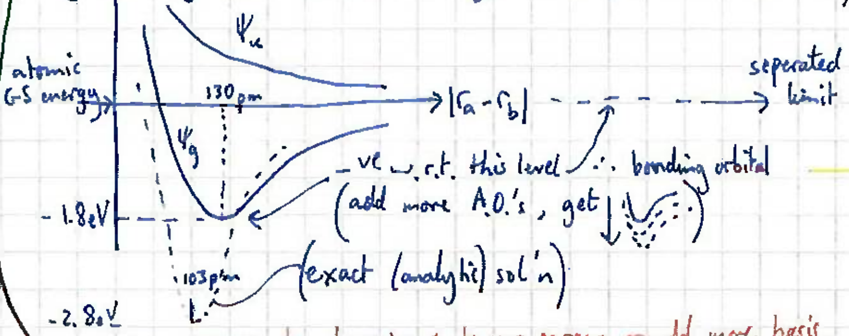
If $\alpha=\beta$ get $\psi_{gerade} = (\psi_a+\psi_b)\frac{1}{\sqrt{2+S}}$ "bonding orbital"

If $\alpha=-\beta$ get $\psi_{unger.} = \frac{\psi_a-\psi_b}{\sqrt{1+S}}$ "anti bonding"



$$E_g = \frac{H_{aa}+H_{ab}}{1+S} < E_u = \frac{H_{aa}-H_{ab}}{1-S}$$

(Note: ψ_g and ψ_u are orthogonal though ψ_a and ψ_b aren't)



–ve w.r.t. this level $\therefore$ bonding orbital

(add more A.O.'s, get ↓)

(exact (analytic) sol'n)

can improve by changing a_0 to var. param or add more basis states!

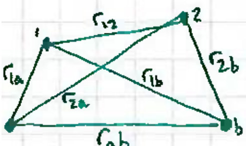
Total electronic ang mom not conserved – $[L^2,H]\neq 0$

But L_z does (z axis = mol. axis) so label states using **Notation**

atomic analogy: Z-comp. of e^- ang momentum $= 0\to\sigma,\ 1\to\pi,\ 2\to\delta$

H_2 Molecule

Potential is $V(\underline{r}_1,\underline{r}_2,\underline{r}_a,\underline{r}_b) = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{12}} + \frac{1}{r_{ab}} - \frac{1}{r_{1a}} - \frac{1}{r_{1b}} - \frac{1}{r_{2a}} - \frac{1}{r_{2b}}\right)$



$= \underbrace{V_1 + V_2}_{\text{(as for } H_2^+)} + \underbrace{\frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{12}} - \frac{1}{r_{ab}}\right)}_{\text{small coz they cancel}}$

$\boxed{\text{Ignore 3rd term,}}$ $\Longrightarrow \psi_g$ and ψ_u for each electron ie $\psi_g(\underline{r}_1)$ and $\psi_g(\underline{r}_2)$ and $\psi_u(\underline{r}_1)$ and $\psi_u(\underline{r}_2)$

$\exists$ 4 ways to combine these (ie 4 ways to put in 2 electrons....)

$\sigma_g(1)\sigma_g(2)$, $\sigma_u^*(1)\sigma_u^*(2)$, $\sigma_g(1)\sigma_u^*(2)$, $\sigma_u^*(1)\sigma_g(2)$.

So can make 6 states: Total wavef'n must be antisym

3 spatially sym combinations go with singlet spin wavef'n

ie ${}^1\Sigma_g$: $\sigma_g(1)\sigma_g(2)\chi_{0,0}$ $\quad |\chi_{0,0}\rangle = (|+-\rangle - |-+\rangle)\frac{1}{\sqrt{2}}$ (s,m_s)

G.S. wavef'n does not give good E_0 and r_0 coz $\sigma_g\sigma_g$ is not a good repres. of G.S. wavef'n

${}^1\Sigma_g$: $\sigma_u^*(1)\sigma_u^*(2)\chi_{0,0}$

${}^1\Sigma_u$: $\frac{(\sigma_g(1)\sigma_u^*(2) + \sigma_g(2)\sigma_u^*(1))}{\sqrt{2}}\chi_{0,0}$ ie Ignoring 3rd term is not so good after all....

and 3 spatially anti sym. combinations with triplet spin states:

${}^3\Sigma_u$: $(\sigma_g(1)\sigma_u^*(2) - \sigma_g(2)\sigma_u^*(1))\begin{Bmatrix}\chi_{1,-1}\\ \chi_{1,0}\\ \chi_{1,1}\end{Bmatrix}\cdot\frac{1}{\sqrt{2}}$

If we write $\sigma_g\sigma_g$ in terms of atomic wavef'ns $\psi_a(\underline{r}_1)$ $\psi_b(\underline{r}_1)$ etc....

get: $\sigma_g(1)\sigma_g(2) = \psi_g(\underline{r}_1)\psi_g(\underline{r}_2) \propto \underbrace{\left[\psi_a(\underline{r}_1)\psi_b(\underline{r}_2) + \psi_a(\underline{r}_2)\psi_b(\underline{r}_1)\right]}_{\text{COVALENT}} + \underbrace{\left[\psi_a(\underline{r}_1)\psi_a(\underline{r}_2) + \psi_b(\underline{r}_1)\psi_b(\underline{r}_2)\right]}_{\text{IONIC}}$

But are cov. and ionic really mixed in equal prop? NO

If try (cov + λ.ionic) get $\lambda \approx \frac{1}{6}$ $\therefore \frac{1}{36}\times 100$ % prob. of ionic.....!

(cannot write this as (separated) product of $f(\underline{r}_1)\times f(\underline{r}_2)$ because the electrons are correlated. If have M basis F'n per electron, need M^n for n e^-

Can write this as $\propto (1+\lambda)(1+S)\underbrace{\sigma_g(1)\sigma_g(2)}_{{}^1\Sigma_g} - (1-\lambda)(1-S)\underbrace{\sigma_u^*(1)\sigma_u^*(2)}_{{}^1\Sigma_g}$

ie it is a mixture of two ${}^1\Sigma_g$ states, but ionic and covalent configurations, called CONFIGURATION MIXING.

– ${}^1\Sigma_g$ have same symm $\therefore$ can mix.

At large internuc. distances according to this, $\exists$ separation into H and H or H^+ and H^- with weighting $\boxed{1^2 : \lambda^2}$

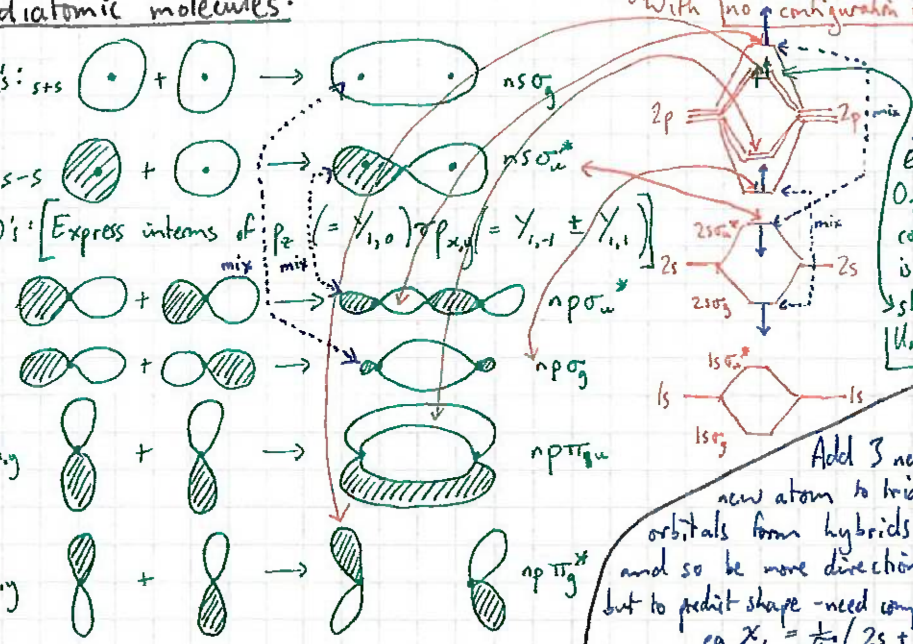
'small internuc. dist – no good coz A.O.'s are too spread

Q.M. : MOLECULAR STRUCTURE (CONTINUED)

L.C.A.O. for other diatomic molecules:

For ns AO's: s+s, $n \in \mathbb{Z}$

For np AO's: [Express in terms of $p_z (= Y_{1,0})$ & $p_{x,y} (= Y_{1,-1} \pm Y_{1,1})$]



The $2p\sigma_g$ is (usually) raised in energy, higher than $2p\pi_u$.
Examples: N_2 7 pairs − 3 bonds … no problem. O_2: 8 pairs − What is lowest energy (antibonding) configuration for the extra pair? In fact it is a spatially antisym triplet spin state as shown − each e^- in orthog. orbs (p_x and p_y). Unusual as non-zero spin … ∴ O_2 is paramag.

Polyatomic Molecules

Add 3 new degrees of freedom for nuc. pos'ns when add new atom to triatomic system. Shapes are wierd…. coz atomic orbitals form hybrids − can conc. charge in smaller region and so be more directional. If know shape, can infer hybridisation but to predict shape − need computer. Eg CH_4: different combs of $s, p_{x,y,z}$ eg $\chi_1 = \frac{1}{\sqrt{4}}(2s + 2p_x + 2p_y + 2p_z)$

QM : MOLECULAR TRANSITIONS

Radiative transitions ie absorption or emission of a photon − usually electronic transition induces nuclear motion. Strongest: E2 (single photon) $\Delta J = 0, \pm 1$ with further parity probs.

Overview

In gas or liq. get transitions due to molecular COLLISIONS − no selection rules here. If no radiation, get thermal distribution $n_i \propto g_i e^{-E_i/kT}$

Can get transitions due to Raman Scattering − incident photon scattered by molecule, gives or gets some energy.

Rate $\propto |V_{kj}|^2$ in normal (2nd order?) pert. theorem but now use:

$$\left(\langle \phi_k | V | \phi_j \rangle + \sum_{n \neq j,k} \frac{\langle \phi_k | V | \phi_n \rangle \langle \phi_n | V | \phi_j \rangle}{E_j - E_n} \right)$$

2nd term: $j \to n$ by photon abs. then $n \to k$ by emitting a photon. Energy is cons. ($E_j = E_k$) but $E_n \neq E_j$ ∴ intermed. state n is only occupied for $t \sim \hbar / |E_j - E_n|$ − it is a virtual state. $\Delta J = 0, \pm 1, \pm 2$ + par.

Electronic wavef'ns form a complete set so expand full wavef'n:
$\Psi(\{\underline{r}_n\}, \{\underline{r}_N\}) = \sum_k \phi_k(\{\underline{r}_N\}) u_k(\{\underline{r}_n\}, \{\underline{r}_N\})$, ϕ_k is weight of electronic state k at each set of nuclear positions, $\{\underline{r}_N\}$. Put into SE, 2:

$$\left[\sum_n \frac{p_n^2}{2m_e} + \sum_N \frac{P_N^2}{2m_N} + V(\ ) \right] \Psi(\ ) = E \Psi(\ )$$

this and this acting on $\phi_k u_k$ gives $E_k \phi_k u_k$ so SE becomes

Nuclear Motion (Born − Oppenheimer)

$$\sum_k \left[\sum_N \frac{P_N^2}{2m_N} + E_k \right] \phi_k u_k = \sum_k E \phi_k u_k$$

but dependence of u_k on $\{\underline{r}_N\}$ is weak compared with dep of ϕ_k on $\{\underline{r}_N\}$ so can say:

using B−O approx again ie $\longrightarrow \nabla_N^2 \phi_k u_k \simeq u_k \nabla^2 \phi_k$
can say; using orthogonality of $\langle u_k |$ to pick out, say, G.S.; (ϕ_0):

$$\left[\sum_N \frac{-\hbar^2 \nabla_N^2}{2m_N} + E_0(\{\underline{r}_N\}) \right] \phi_0 = E \phi_0 \quad \text{ie a regular SE}$$

but with $E_0(\{\underline{r}_N\})$ as the potential (the molecular P.E. curve or surface) ≡ saying e^- respond instantaneously to nuc. motion.

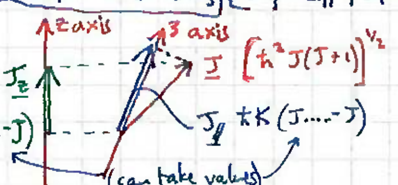
Rotation

From here, for each $|u\rangle$ there is a complete set of molecular energy levels ie nuc. pos'ns.

Simplest solutions of are translational states − continuum for free molecule or "particle in box" states.

Next simplest sol'ns: rotations about c.o.mass. $\hat{T}_r = \frac{\hat{J}_1^2}{2I_1} + \frac{\hat{J}_2^2}{2I_2} + \frac{\hat{J}_3^2}{2I_3}$ [For sym top molecule, $I_3 = I_{\parallel}$, $I_1 = I_2 = I_{\perp}$]

so $\hat{T}_r = \frac{\hat{J}^2}{2I_{\perp}} + \left(\frac{1}{2I_{\parallel}} - \frac{1}{2I_{\perp}} \right) \hat{J}_{\parallel}^2$



Energy does not dep on $\longrightarrow \hbar m_J$ (J…−J) so each J and K is deg set of (2J+1) states. (can take values)

Energy $\boxed{E_{JK} = \frac{\hbar^2}{2I_{\perp}} J(J+1) + \left(\frac{\hbar^2}{2I_{\parallel}} - \frac{\hbar^2}{2I_{\perp}} \right) K^2}$

If have linear molecule $I_{\parallel} = 0$ − can only make K=0 states. If have sph. symm $I_{\parallel} = I_{\perp}$ get $(2J+1)^2$ deg. (all K allowed but no effect on energy)

E_{JK} not dep on sign of K ∴ increase degeneracy (due to m_J) by factor of 2

Energies:

Rotational:	Electronic
$I \sim m_N a_0^2$	$p \sim \frac{\hbar}{a_0}$
$\Rightarrow E_{rot} \sim \frac{\hbar^2}{m_N a_0^2}$	$\Rightarrow E_{elec} \sim \frac{\hbar^2}{m_e a_0^2}$

$\Rightarrow E_{elec} \sim 10^4 . E_{rot}$.

For a radiative rot. trans, photon interacts with dipole moment of mol. Init and final electronic states are the same, so molecule must have a permanent dipole moment → Heteronuclear diatomics.

But a Raman scattering virtual state can have dip mom even in a Homonuclear diatomic

Selection rules for Rotational Transitions: Radiative

State with J, m_J has $|\phi\rangle \propto Y_{Jm_J}$ hence parity $(-1)^J$
Let $|u_k\rangle$ be an $\Lambda = 0$ state ie Σ (zero ang. mom) so even parity
E1 (dipole) ⇒ parity change so no $\Delta J = 0$. If non linear mol ∃ (K) but in a sym. top molecule, dipole is in 3 dir'n so $\Delta K = 0$

⟹ get $\boxed{\Delta J = \pm 1 \quad \Delta K = 0}$ (Radiative)

$\nu = \frac{E_{J+1,K}}{h} - \frac{E_{J,K}}{h} = B.2(J+1)$, $B = \frac{\hbar}{4\pi I_{\perp}}$ $(I_{\perp} = \mu R_{eq}^2)$

As molecule spins, $R_{eq} \uparrow$ so $I_{\perp} \uparrow$ so spacing changes (small effect 10^{-4})

Raman: $\Delta J = 0, \pm 1, \pm 2, \pm 3 \ldots$ and no parity change ∴ ΔJ is even

⟹ get $\boxed{\Delta J = 0, \pm 2, \ldots \quad \Delta K = 0}$ (Raman)

For $\Delta J = 2$ (Stokes) $\Delta \nu = -4B(J + \frac{3}{2})$
$\Delta J = -2$ (antistokes) $\Delta \nu = 4B(J - \frac{1}{2})$

Intensity Features:

Intensity dominated by no. in initial state. Due to collisions this is thermal $n_J \propto g_J \exp[-E_J/kT]$ so get

Raman − get alternation of intensity superposed, consequence of identical particle symmetry for like nuclei involved.

QM: MOLECULAR TRANSITIONS (CONTINUED)

Nuclear Statistics

Eg Hydrogen Molecule: Parity is same as interchanging nuclei but not spins.

nuclei are Fermions ∴ if J even, must have singlet state etc – hence alternating (para) line intensity in Raman spectrum.

Generalisation:

Let spin be $I_a = I_b \Rightarrow$ total $I = 2I_a \dots 0$.

$2I_a$ state is symm under spin exchange

$2I_a - 1$ antisym etc, alternating.

$\Rightarrow I = 0$ state is sym if I int or zero, antisym if I ½ integer.

For fermions, need overall antisym ∴ must pair $I=0$ with even J ..... Find that

$\boxed{\text{even } I \Rightarrow \text{even } J}$ $\boxed{\text{odd } I \Rightarrow \text{odd } J}$

Spin I state has spin deg. $(2I+1)$

$\Rightarrow$ Ratio of successive intensities is $I_a : 1$

Vibration

Expand molecular potential $E_0(R) = E_0(R_e) + \frac{1}{2}E_0''(R_e)\Delta R^2$

S.H.O. potential $\Rightarrow E = E_0(R_e) + (n+\frac{1}{2})\hbar\omega$ $[n = 1, 2, 3, \dots]$

Vibrational energies $\sim \sqrt{\frac{m_e}{m_N}}$ electronic energies (10μm – IR)

Selection rule:

Displacement $x = a - a^\dagger$ (ladder ops.) Radiative, $V \propto x$ so get $\langle \phi_{n'} | a - a^\dagger | \phi_n \rangle$ but $a|\phi_n\rangle \propto |\phi_{n-1}\rangle$, $a^\dagger|\phi_n\rangle \propto |\phi_{n+1}\rangle$

$\Longrightarrow \Delta n = \pm 1 \Rightarrow$ single freq in spectrum, ν corresponding to classical vib freq.

Anharmonicity $\Rightarrow$ higher levels are closer together. Also the wavef'ns are not precisely S.H.O. wavef'ns ∴ $\Delta n > 1$ can occur.

Rotation – Vibration

Simultaneous vib-rot transitions.

Eg $n \to n+1$, $\Delta J = 1 \Rightarrow \nu = \frac{(E_{n+1,J+1} - E_{nJ})}{h} = \nu_0 + 2B(J+1)$ $J = 0, 1, 2..$

called R branch

For $n \to n+1$, $\Delta J = -1 \Rightarrow \nu = (E_{n+1,J-1} - E_{nJ})\frac{1}{h} = \nu_0 - 2BJ$ $J = 0, 1, 2 \dots$

called P branch. Q branch for $\Delta J = 0$ but no – this is forbidden by the Parity selection rule – would need an electronic transition aswell.

Electronic Vibronic

When electronic trans. occurs, R_e changes. Assume it happens instantly, then it

Franck–Condon Principle. New energy $\sim \frac{1}{2}k(R_e - R_e')^2$, $\hbar\omega' = \sqrt{\frac{k}{\mu}}$ (new k)

Superposed on this, ∃ rotational bands P, Q, R (inc. freq)

$I_\perp$ and $I_\perp'$ may be substantially different.

If $I_\perp' < I_\perp$, P branch has a BAND HEAD

If $I_\perp' > I_\perp$, R " " " "

QM: EFFECTS OF MAGNETIC FIELDS

Particle In Uniform Field

Complication – velocity dependent potential/force $E = q(\underline{v} \times \underline{B})$

$\Rightarrow$ cannot write force/pot. as grad of scalar potential

– need vector pot: $\underline{B} = \underline{\nabla} \times \underline{A}$ let's use $\underline{A} = \frac{B}{2}(-y, x, 0)$

Ham: $H = \frac{1}{2m}(\underline{p} - q\underline{A})^2 = \frac{1}{2m}\left[(p_x + \frac{B}{2}qy)^2 + (p_y - \frac{B}{2}qx)^2 + p_z^2\right]$

$= \frac{p^2}{2m} - \frac{qB}{2m}(xp_y - yp_x) + \frac{q^2B^2}{8m}(x^2 + y^2)$

eq'ns of motion. see page 48...

Use $\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{O}]\rangle$ to check that it gives correct

$L = \underline{r} \times \underline{p}$ so $H = \frac{p^2}{2m} - \frac{qB}{2m}L_z + \frac{q^2B^2}{8m}(x^2 + y^2)$ (z field)

$= \frac{\hat{p}^2}{2m} - \boxed{\frac{q}{2m}\hat{\underline{B}}.\hat{\underline{L}}} + \frac{q^2}{8m}\left[\hat{B}^2\hat{r}^2 - (\hat{\underline{B}}.\hat{\underline{r}})^2\right]$ (any field) (in B dir')

This is interaction of B and $\underline{m}_L = -\mu_B\frac{\underline{L}}{\hbar}$, $\boxed{\mu_B = \frac{e\hbar}{2m}}$ (Bohr Magneton)

treat e^- as current loop, classically, get

Let $-\underline{m}_L . \underline{B}$ for e^- be: $m_L\mu_B B$ $m_L = L, \dots, -L$. (value of L_z)

so (neglect e^- spin for now) levels split in to $(2L+1)$

Can write: $H = \frac{p_z^2}{2m} + m_L\mu_B B + \left(\frac{p_x^2}{2m} + \frac{e^2B^2}{8m}x^2\right) + \left(\frac{p_y^2}{2m} + \frac{e^2B^2}{8m}y^2\right)$

Free particle in z direction. SHM in x, y dir'ns

freq: $\frac{1}{2}m\omega^2 = \frac{e^2B^2}{8m} \Rightarrow \omega = \frac{eB}{2m} = \frac{\mu_B B}{\hbar} \equiv \omega_L$

ω_L is the LARMOUR frequency. $E = \frac{p_z^2}{2m} + (m_L + n_x + n_y + 1)\hbar\omega_L$ (any value)

Let $2n = m_L + n_x + n_y$ then:

$\boxed{E = \frac{p_z^2}{2m} + (n + \frac{1}{2})2\hbar\omega_L}$ ← LANDAU LEVELS (levels are 2× classical, Larmour freq apart)

SPIN S-G expt and spectra of atoms in B $\Rightarrow$ that ∃ spin giving rise to mag. mom: $\underline{m}_S = -g_e\mu_B\frac{\underline{S}}{\hbar}$ ($g_e = 2$ from Dirac eq'n)

So spin is twice as effective at producing mag mom. (than orbital)

Put into Ham $(\underline{B}.(\underline{L} + 2\underline{S})) \longrightarrow$ get each level split. $n \to n + 2m_s$

where $m_s = \pm\frac{1}{2}$ (value of $S_z/\hbar$) If particle has internal structure eg proton, then gyromag. ratio $g_e \neq 1$ or 2. $g_e(\text{proton}) = 5.6 \Rightarrow$ ∃ quarks

Atom In Uniform Field

Scalar potential V(r) and spin orbit coupling are added:

$H = \frac{p^2}{2m} + \frac{e}{2m}\underline{B}.(\underline{L} + 2\underline{S}) + \frac{e^2}{8m}(B^2r^2 - (\underline{B}.\underline{r})^2) + V(r) + \frac{1}{2m_e^2c^2}\frac{1}{r}\frac{dV}{dr}\underline{L}.\underline{S}$

→ Diamagnetic term – corresponding to induced magnetic moment opposing field. $\underline{m} = \gamma\underline{B}$ has mag. energy $-\frac{1}{2}\gamma B^2$ so this term, averaging over all dir'n of r rel to B gives: $\gamma = -\frac{e^2}{6m}\langle r^2\rangle$

If $\langle r^2\rangle \sim a_0^2$, $\gamma B/\mu_B$ is approx: $10^{-6}B$ so NEGLECT this term

→ Paramagnetic term – splits levels into $2 \times (2L+1)$ (spin) (orbital) (in competition with)

Level spacing is $\mu_B B$

L precesses at ω_L, S at $2\omega_L$ → S and L decoupled

Spin-orbit term and paramagnetic term do not commute!

$[L_z + 2S_z, \underline{L}.\underline{S}] = i\hbar(L_x S_y - L_y S_x)$ so:

For weak field, this dominates, use e-states of the $\underline{L}.\underline{S}$ operator → J, m_J (and L and S) are good Q.no's.

For strong field, this dominates, use e-states of $L_z + 2S_z$ so L, m_L, S, m_s are good quantum numbers.

$$\boxed{|J, m_J\rangle = \sum_{m_L, m_s} C_{J,m_L,m_s}|L, S, m_L, m_s\rangle}$$

Lande g-factor

expectation value of magnetic moment along field dir'n:

$$\mu = -\mu_B\langle L_z + 2S_z\rangle = -\mu_B . g m_J$$

$$g = \sum_{m_L, m_s} |C_{J,m_L,m_s}|^2 \frac{m_L + 2m_s}{m_J}$$

$$= 1 + \sum_{m_L, m_s} |C_{J,m_L,m_s}|^2 \frac{m_s}{m_L + m_s}$$

$m_L + m_s = m_J$

Q.M. EFFECTS OF MAGNETIC FIELDS

Lande g-factor (continued)

Eg: Alkali atom: $S = \frac{1}{2}$, So $J = L \pm \frac{1}{2}$

top state: $m_L = L$, $m_S = +\frac{1}{2}$
$\therefore$ is e-state of $\underline{L}\cdot\underline{S}$ and L_z, S_z - special case.
$\Rightarrow \exists$ only one C-G coeff and it $= 1$ so:

$$|J = L+\tfrac{1}{2}, m_J = L+\tfrac{1}{2}\rangle = |L, \tfrac{1}{2}, m_L = L, m_S = \tfrac{1}{2}\rangle$$

Operate on this with J_- to get different m_J states (but still with same J) $(L_- + S_-)$

To get states of different J (same m_J) use orthogonality with this state.

So $g = 1 + \dfrac{\frac{1}{2}}{L+\frac{1}{2}} = 1 + \dfrac{1}{2J}$

Can use VECTOR MODEL: L, S precess around J which in turn precesses more slowly around field dir'n.
Rapid precession of L, S around J $\Rightarrow$ $\perp$ (to J) components average to zero.

$$\text{ie } \langle m_L + m_S\rangle = (\underline{L}\cdot\underline{n} + 2\underline{S}\cdot\underline{n})\,\underline{n}\,\frac{\mu_B}{\hbar}$$

in J dir

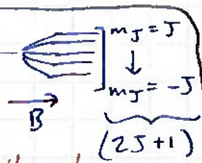
$$= g\mu_B \frac{J_z}{\hbar} \quad \text{by def'n}$$

$$\Rightarrow g = \frac{\underline{L}\cdot\underline{J} + 2\underline{S}\cdot\underline{J}}{|\underline{J}|^2} = 1 + \frac{\underline{J}\cdot\underline{S}}{|\underline{J}|^2}$$

$$\Rightarrow g = \frac{3}{2} - \frac{L(L+1) - S(S+1)}{J(J+1)}$$

Zeeman-Effect.

First order PT $\Rightarrow$ $\Delta E = g\mu_B B m_J$

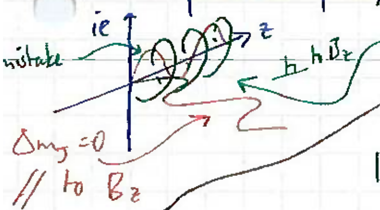
So J, m_J 

$m_J = J$ ... $m_J = -J$, $\vec{B}$, $\underbrace{\quad}_{(2J+1)}$

So spectral lines due to transition are also split, but not into $(2J+1)(2J'+1)$ - not all are allowed:
Photon has $1\hbar$ of ang mom $\therefore \Delta m_J = 0 \pm 1$ (for a start).

$\Delta m_J = 0 \longleftrightarrow$ z-dipole transition $\therefore$ see nothing in field dir

$\Delta m_J = \pm 1 \longleftrightarrow x \pm iy$ dipoles $\therefore$ circularly polarised light (when view along field direction)
polarised (plane) $\perp$ to B_z when viewed $\perp$ to B_z!



As B strength increases, decouples $\underline{L}$ and $\underline{S}$ so, best Q no's become m_L, m_S not J, m_J!

Paramagnetic Susceptability

In thermal eq: number with particular m_J in B_z is:

$$n(m_J) = \text{Const.}\; e^{-g\mu_B B m_J/kT}$$

All components $\perp$ to field direction have zero expectation values:

$$\Rightarrow |\langle m\rangle| = -\frac{\sum_{m_J} g\mu_B m_J e^{-g\mu_B B m_J/kT}}{\sum_{m_J} e^{-g\mu_B B m_J/kT}} \;(\text{ignore deg}) = -g\mu_B \frac{\sum_{m_J} m_J e^{-m_J x}}{\sum_{m_J} e^{-m_J x}} \quad \left(x = \frac{g\mu_B B}{kT}\right)$$

(magnetic moment per atom)

Can do sum but $x \ll 1$ if $B \ll T$ (Tesla) (Kelvin) so $e^{-m_J x} \simeq 1 - m_J x$

use $\underbrace{\sum_{m_J} 1 = 2J+1 \qquad \sum_{m_J} m_J = 0}_{\text{sum from } -J \to +J}$ $\qquad \sum_{m_J} m_J^2 = \frac{1}{3}J(J+1)(2J+1)$

$(-J + \dots + J$ cancels out$)$

$$\Rightarrow |\langle m\rangle| \simeq -g\mu_B \frac{\sum_{m_J} m_J - m_J^2 x}{\sum_{m_J} 1 - m_J x}$$

$$= \frac{1}{3} g\mu_B J(J+1)x$$

Magnetic Susceptability χ:

$$\chi = \frac{|\langle m\rangle|}{H} = \mu_0 \frac{g^2\mu_B^2}{3k} J(J+1) \cdot \frac{1}{T}$$

$$\text{So } \chi \propto \frac{1}{T} \quad (\text{Curie's Law})$$

T.S.P. : Model Systems :

Ideal Gas

Thermodynamics: How does energy flow
from : macro to microscopic length scales (and vice v.)
: one internal d.o.f. to another?
Statistical Mechanics: How is energy distributed among internal d.'s o. freedom?

Energy Storage: $U = \sum_{\text{particles}} \frac{1}{2} m v_i^2$ we know v_i from M-B.
so we can do the sum : $U = \frac{3}{2} N k_B T$.
by the way : $\boxed{S = S_0 - N k_B \ln p + C_p \ln T}$

Energy Flow :
macro → micro : Work, push piston, elastic collisions : $đW$
micro → micro : Heat, warm up walls, inelastic collisions : $đQ$
micro → micro : Particles μdN where $\boxed{\mu := \left.\frac{\partial U}{\partial N}\right|_{S,V}}$

Paramagnetic Salt in magnetic field.

Energy Storage $U \propto$ no. of up spins

$U = U_0 - \underline{M} \cdot \underline{B}$ (all non mag. energy)

$dU_0 = TdS + d\underline{M} \cdot \underline{B}$
ie when change internal mag'n, get heat flow | Adiab. de mag....

So, $\boxed{dU = dU_0 - \underline{M} \cdot d\underline{B}}$

$\left.\frac{\partial T}{\partial B}\right|_S = -\left.\frac{\partial T}{\partial S}\right|_B \left.\frac{\partial S}{\partial B}\right|_T = -\frac{T}{C_B}\left.\frac{\partial M}{\partial T}\right|_B$ want
$M = \chi(T) B$

Assembly of 1-D S.H.O.'s

Energy Storage : $U = \sum_{\text{osc.}} (n_i + \frac{1}{2}) \hbar \omega_0$

Energy Flow : macro → micro : change ω_0 ie shape of potential

Pure, Real Substances

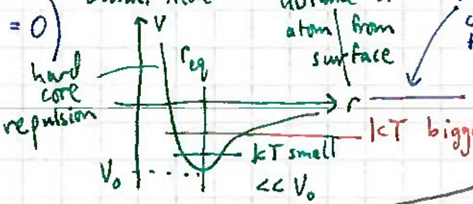
Behaviour of a J : Eq'n of state
$\Phi(p, V, T) = 0$ (eg $pV - NkT = 0$)

Often plot p as $f(V, T)$ → p-V-T surface

Van der Waals Gas :

$$\left(p + \frac{N^2 a}{V^2}\right)(V - Nb) = NkT$$

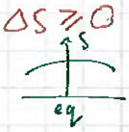
Latent Heat :



beyond, ∄ Latent heat - get second order phase transitions.

Equilibrium

$\Delta S \geq 0$ ⇒ equilibrium maximises entropy



Analytic Thermodynamics

Variables : "Thermodynamic"

ie averages over microscopic states/events
eg pressure...
Extrinsic : $\propto V, N$ ie size of system.
eg : V, C, S
Intrinsic : indep. of size of system.
eg. p, u, T, ρ
"Constraints" eg V "response" eg P
fix then NO WORK done
Functions of state : U (S)
but Q + W are not...

Potentials :

Property of system alone that corresponds to energy conservation for the system + reservoir (ie universe) } → and so coz $\Delta S = 0$ at equilib, appropriate potential is minimised at equilibrium.

flow processes = work done (rev)
eg  pg 28

thermally isolated	Internal Energy :		U
	Enthalpy :		$H = U + pV$
const. temp	Helmholtz free en. :		$F = U - TS$
	Gibbs free energy :		$G = F + pV$
	Grand potential :		$\Phi = F - \mu N$

Phase/chem equilibria
Pure substance $\boxed{G = \mu N}$
build up a system, const, T, p

$dG = -SdT + Vdp + \mu dN$
$= \mu dN$
$dN = ???$

Applications...

Relation between C_p and C_V

$T\left(\frac{dS}{dT}\right)_p = T\left.\frac{\partial S}{\partial T}\right|_V \left(\frac{dT}{dT}\right)_p + T\left.\frac{\partial S}{\partial V}\right|_T \left(\frac{dV}{dT}\right)_p$ → use ideal gas law

$\underbrace{}_{C_p}$ $\underbrace{}_{C_V}$ use Maxwell rel. $F = U - TS$

use reciprocity theorem

now, c_p (hard to measure) is a f'n of c_V + other easy " " things.
→ $c_p = c_V + Nk_B$

Entropy of ideal gas

$S(p, T)$ (as ∃ constraint $\Phi(p, V, T) = 0$)

$dS = \left.\frac{\partial S}{\partial p}\right|_T dp + \left.\frac{\partial S}{\partial T}\right|_p dT$ → $pV = nkT$

(Gibbs Maxwell) $= -\left.\frac{\partial V}{\partial T}\right|_p$; $\frac{C_p}{T}$

so $dS = -Nk\frac{dp}{p} + C_p \frac{dT}{T}$

$\boxed{S(p, T) = S_0 - Nk \ln p + C_p \ln T}$

or

$\boxed{S = S_0 - Nk \ln Nk + C_V \ln T + Nk \ln V}$
(as f'n of V, T)

Joule Expansion of real gas.

(free expansion into a vacuum)
- irrev. process (so can't rep. on p-V plane)
fns of state etc... ∴ invent reversible etc..
Write $T_f = T_i + \int_{V_i}^{V_f} \left.\frac{\partial T}{\partial V}\right|_U dV$ "Joule Coeff" use reciprocity, zero for ideal gas

but $\left.\frac{\partial T}{\partial V}\right|_U = -\left.\frac{\partial T}{\partial U}\right|_V \cdot \left.\frac{\partial U}{\partial V}\right|_T$; $\left.\frac{dU}{dV}\right|_T = T\left.\frac{dS}{dV}\right|_T - p\left.\frac{dV}{dV}\right|_T$

$\frac{1}{C_V}$; Maxwell

$\Rightarrow = -\frac{1}{C_V}\left(T\left.\frac{\partial p}{\partial T}\right|_V - p\right)$ now : $p = \frac{NkT}{(V - Nb)} - \frac{N^2 a}{V^2}$

$\left.\frac{\partial p}{\partial T}\right|_V = \frac{Nk}{V - Nb}$ → Joule coeff is $-\frac{1}{C_V}\left(-\frac{N^2 a^2}{V^2}\right)$

Black body radiation

$p = \frac{1}{3} n m c^2$; $\left.\frac{dE}{dV}\right|_T = T\left.\frac{dS}{dV}\right|_T - p\left.\frac{dV}{dV}\right|_T$
$\langle E \rangle$
but $n\langle E \rangle$ = energy density $\frac{E}{V}$ or $\left.\frac{dE}{dV}\right|_T$

use Maxwell $F = U - TS$

$\Rightarrow \frac{dp}{p} = 4\left.\frac{dT}{T}\right|_V$

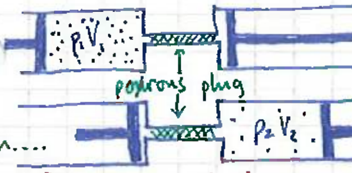
$\Rightarrow \boxed{p \propto T^4}$

So : Cooling comes from a ie interparticle attraction

} → ∃ increase in potential energy (lower pressure) - came from Kinetic Energy.

Applications Continued .... (T.S.P.)

Joule - Kelvin Expansion



Then....

No heat flow in or out of gas

$U_2 = U_1 + p_1V_1 - p_2V_2$

work done on gas; gas does work on piston

$\Rightarrow H_1 = H_2$ (isenthalpic)

$T_2 = T_1 + \int_{p_1}^{p_2} \frac{\partial T}{\partial p}\Big|_H dp$

Joule-Kelvin coeff.

follow method for J-coeff.

get: $-\frac{1}{C_p}\left(-T\frac{\partial V}{\partial T}\Big|_p + V\right)$

for vdW gas, $\propto -Nb + \frac{2Na}{kT}$

so "a" causes $T\downarrow$ as with

b: gas increases pressure - has greater effect on p_1V_1 side $\therefore$ do "extra" work, give gas energy.

(isenthalps)

inversion curve sep. two regions

EQUILIBRIUM IN OPEN SYSTEMS.

Availability.

Eq'm $\Leftrightarrow$ Entropy of universe is maximum

$dS_{tot} = dS_1 + dS_0 \geq 0$. $dU_0 = T_0dS_0 - p_0dV_0 + \mu_0dN_0$

(system) (res)

$\therefore T_0dS_{tot} = T_0dS_1 + dU_0 + p_0dV_0 - \mu_0dN_0$ ← Conservation Laws

$= T_0dS_1 - dU_1 - p_0dV_1 + \mu_0dN_1$

$= -dA$ where $\boxed{A = U - T_0S + p_0V - \mu_0N}$

use $dp_0 = 0$, $dT_0 = 0$, $d\mu_0 = 0$

A is prop of system

system properties

So $\boxed{\text{minimise } A \Leftrightarrow \text{maximise } S}$ the two important cases....

Eq'm at constant T and V :

ie $dT = dV = 0$ also let $dN = 0$

then $dA = dU - T_0dS = dF$!

So for isothermal, isochoric system, equilibrium $\Leftrightarrow$ minimise F

eg

$F = F_1 + F_2$ $dF = 0 \Rightarrow p_1 = p_2$. [F acts as potential energy]

Eq'm at constant T and P

$dA = 0 \Rightarrow G (= F + pV)$ is minimised.

Phase eq:

Calculate separate Gibbs' fns for liq and vap (say)

then $G = G_l + G_v \Rightarrow \boxed{dG_l = -dG_v}$

So $\mu_l dN_l = -\mu_v dN_v$

but $dN_l = -dN_v$ ⟶ Condition for phase eq'm is $\boxed{\mu_1 = \mu_2}$

From $d\mu = -sdT + vdp$ per particle

can see:

high T, phase with largest s has smallest $\mu \rightarrow$ stable.

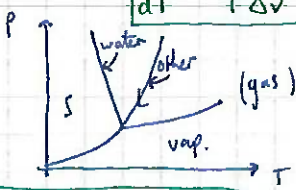
high p, phase with smallest v has smallest $\mu \rightarrow$ stable.

and...

Clausius - Clapeyron Equation

$d\mu_1 = -s_1dT + v_1dp$. Along coexistence line, $d\mu_1 = d\mu_2$

$\Rightarrow \boxed{\frac{dp}{dT} = \frac{T\Delta s}{T\Delta v} = \frac{L}{T\Delta v}}$ — latent heat per particle. (applies to first order phase trans.)



(liq → vap Δv is big and +ve)

Osmotic Pressure

Applications :

$\mu_s(T,p,1,0) + \int_p^{p+\pi} \frac{\partial\mu_{0s}(T,p)}{\partial p}\Big|_T dp$

= vol per particle, v_s, weak fn of p.

so get

pure solvent

$\mu_s(T, p+\pi, c_s, c_i) = \mu_s(T,p,1,0) + \pi v_s - kTc_i$

$\mu_s(T,p+\pi,c_s,c_i)$

$= \mu_s(T,p+\pi,1,0) + kT\ln c_s$ → $-kTc_i$ expanding...

$= \mu_s(T,p,1,0)$ for equilib. of particles

$\Rightarrow \boxed{\pi V = N_ikT}$ Osmotic pressure π

FINISH

START

$\frac{\partial\mu_{i,vap}}{\partial c_i}\Big|_{T,p} = \frac{\partial\mu_i^{vap}}{\partial p_i}\Big|_T \frac{\partial p_i}{\partial c_i}\Big|_{T,p}$

$= \frac{p_i}{c_i}$ (Henry's law) — coz $p_i \propto c_i$

$= \frac{v_ip_i}{c_i} = \frac{kT}{c_i}$ coz vapour phase

but for liq-vap equilib. $\mu_i^{vap} = \mu_i^{liq}$, so $\int$ to get:

$\boxed{\mu_i^{liq} = \mu_i^{liq}(\text{pure}) + kT\ln c_i}$

SYSTEMS WITH SEVERAL COMPONENTS

Entropy of mixing

{Ideal gas particles are non - interacting}

so can just add properties

eg $p = \sum_i p_i$ where $p_iV = N_ikT$

→ entropy : $S = \sum_i (S_{0i} + C_p\ln T - N_ik\ln p_i)$

$\Rightarrow \Delta S = \underbrace{S_{mixture} - S_{pure}}_{\text{same total } N} = -k_B\sum_i N_i\ln p_i + k_BN\ln p$

but $N = \sum_i N_i$

$\Rightarrow \boxed{\Delta S = -k_B\sum_i N_i\ln\left(\frac{p_i}{p}\right)}$ $\left(c_i = \frac{p_i}{p}\right)$

Chemical Pot'l change on mixing

Free energy $G = \sum_i G_i(p_i, T)$

Relate free energy of comp. i at p_i to that if in pure phase at total pressure p:

$G_i(p_i,T) = G_i(p,T) + \int_p^{p_i} \frac{dG_i}{dp}\Big|_{T,N} dp$

$= G_i(p,T) + N_ikT\ln(c_i)$ $V = \frac{N_ikT}{p_i}$

For ideal gases, $G_i = \mu_iN_i$ &

⟶ $\boxed{\mu_i(p_i,T) = \mu_i(\text{pure}) + k_BT\ln c_i}$

Different components: $\mu_i = \frac{\partial G}{\partial N_i}\Big|_{T,p}$

$\Rightarrow \frac{\partial\mu_i}{\partial N_j} = \frac{\partial\mu_j}{\partial N_i}\Big|_{T,p}$

Chemical Equilibrium of Ideal Gases

Minimise availability : $\Rightarrow dG = 0$ $G = \sum_i G_i \Rightarrow dG = \sum_i dG_i$

So $\underbrace{\sum_i \mu_i dN_i = 0}_{\text{eq.}}$ but $\underbrace{\sum_i \nu_i dN_i = 0}_{\text{cons of particles.}}$ $\Rightarrow \sum_i \mu_i\nu_i dN_i = 0$ ⟹ zero

ie $\boxed{\sum_i \mu_i\nu_i = 0}$

but using get

$\sum_i \nu_i\mu_i(\text{pure}) + kT\sum_i \nu_i\ln p_i - kT\sum_i \nu_i\ln p = 0$

$\therefore \sum_i \nu_i\mu_i(\text{pure}) + kT\ln\left(\prod_i p_i^{\nu_i}\right) = 0$

So: $\ln K_p = -\frac{1}{kT}\sum_i \nu_i\mu_{0i}(T)$ pure

where $K_p = \prod_i p_i^{\nu_i}$

T.S.P: STATISTICAL MECHANICS

(A note on rev/irrev mixing:)
mix 2 gases rev → no entropy change
mix 2 gases irrev → entropy change
What if make gas A same as B?
no entropy change → any two microstates which are perms of indistinguishable particles are the same microstate..... (Gibb's Paradox)

P.E.E.P. and its implications

all microstates are equally likely.
say have systems: 1 and 2 $(U_1)\,(U_2)$ with g_1, g_2
Prob of this $\propto g_1(U_1)\,g_2(U_2)$
let equilib. maximise P w.r.t. U_1 (or U_2)

$$0 = g_2\frac{\partial g_1}{\partial U_1} + g_1\frac{\partial g_2}{\partial U_1} \qquad (dU_1 = -dU_2)$$

$$\Rightarrow \boxed{\frac{\partial \ln g_1}{\partial U_1} = \frac{\partial \ln g_2}{\partial U_2}}$$

From thermodynamics, eq ⇒ $T_1 = T_2$ and $T^{-1} = \frac{\partial S}{\partial U}$

$$\Rightarrow \boxed{S_B = k_B \ln g}$$

Definitions of Entropy

1) Boltzman's def'n
2) Useful for fluctuations: $S = \sum_{\gamma=1}^{N} S_\gamma = \boxed{k_B \sum_{\gamma=1}^{N} \ln\left[g_{\frac{n}{N}}(U_\gamma)\right]}$
divide sys into N subsystems each with $\frac{n}{N}$ oscillators and energy U_γ.
Each subsys has diff. energy, entropy
must be big enough to have well defined U for timescale of measurement.
Infinite time average value of $U_\gamma = \frac{U}{N}$
then $g = \frac{\left(\frac{m+n}{N}\right)!}{\left(\frac{m}{N}\right)!\left(\frac{n}{N}\right)!}$ → leads to Boltzman def'n
3) Gibb's def'n: $S = -\sum_{\text{micro state } i} P_i \ln P_i$
Boltzman: $S = -k\ln\frac{1}{g} = -k\sum \frac{1}{g}\ln\frac{1}{g}$ — infinite time average.
good coz size no matter (if can find P_i....)

Applications: Thermally Isolated Systems

Find $S = k\ln g$ then $\frac{1}{T} = \frac{\partial \ln g}{\partial U}$
eg paramag. $g = \frac{N!}{N_\uparrow!\,N_\downarrow!}$ → $\frac{\langle m\rangle}{m} = \tanh\left(\frac{mB}{kT}\right)$

Constant temp. systems

$S = -k\sum_i P_i \ln P_i = -k\sum_i P_i\left(-\frac{E_i}{kT} - \ln Z\right)$
use $\sum_i P_i E_i = U$, $\sum_i P_i = 1$ and $F = U - TS$

$$\rightarrow \boxed{F = -kT\ln Z} \quad \text{and } S = -\frac{\partial F}{\partial T}\Big|_V \text{ etc....}$$

meaning of heat and work:
$TdS = -kT\sum_i (dP_i \ln P_i + dP_i)$ use Boltzman + $\sum_i dP_i = 0$
$\rightarrow = \underbrace{\sum_i E_i\,dP_i}_{\text{HEAT}}$ from $dU = TdS + dW$, $= d\sum_i E_i P_i$ get WORK

(empty space.....)

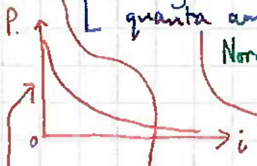
Assembly of 1-D S.H.O.'s

Macrostate: given U (thermodynamic variables)
Microstate: specific configuration

n oscillators, m quanta – so energy $U = m\hbar\omega$
number of possible configurations is: $g_n(U) = \frac{(m+n-1)!}{m!(n-1)!}$ think about $|\times\times|\times\times\times|\times$ etc
$g_n(U)$ rises very rapidly with U – use Stirling to calculate numbers

If all microstates are equally likely, $\boxed{\text{Prob} = \frac{1}{g_n(U)}}$ per microstate.

Prob (finding oscillator in ith excited state) $= \frac{1}{\ldots}\, g_{n-1}(U - i\hbar\omega)$ [ie ways of arranging remaining quanta amoung remaining s.h.o.'s] $(s=1)$ → When plot, get exp – more no.s better fit

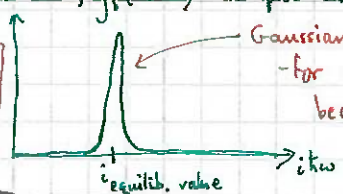


Normalisation:
$$K = \sum_{i=0}^{m} \underbrace{g_{n-s}(U - i\hbar\omega)}_{\text{ways of arranging "res"}}\,\underbrace{g_s(i\hbar\omega)}_{\text{ways of arranging "sys"}}$$
s = no. of oscillators in system. $(U = m\hbar\omega)$

So prob of (generalising) particular configuration (ie microstate) $= \frac{1}{K}\,g_{n-s}(U - i\hbar\omega)$

Prob of finding a particular macrostate eg S oscillators with i quanta
= Prob of each microstate × number of microstates
$= \frac{1}{K}\,g_{n-s}(U - i\hbar\omega)\,g_s(i\hbar\omega)$ If plot this, as f'n of (sub)system energy $i\hbar\omega$

So:
P(microstate) → Boltzman dist'n
P(macro) → equilib →



Gaussian shape – for realistic numbers, width becomes very small.

Microscopic problems

does small system have energy U? $\Delta E\Delta t \gtrsim \hbar$ ∴ must wait long time for ΔE to drop (>> age of univ.)
(ie for sys → eigenstate!)
→ $S = k\ln g$ → accessible states over finite energy range, ΔE
⇒ only meaningful for ∞ time average. [For subsystems, even worse ΔE (def'n ②)]

Ensembles: Microcanonical:

Infinite time average ≡ (∞) no. of copies of system. $p = \frac{\text{no. in state } i}{\text{total}}$
Collection of thermally isolated systems (use Boltzman entropy)

Canonical:

Collection of constant temperature systems – can exchange energy with reservoir
$S = k\ln g$ approach: Prob of find-ing subsystem with energy $E_i \propto g_{res}(U - E_i)\times \underset{\text{no of microstates}}{1}$ [res. is rest of sys]
$E_i \ll U$ so use Taylor
$P(E_i) = \exp\left[\ln g(U) - E_i\frac{\partial \ln g(U)}{\partial(U)}\right]$
$\propto e^{-E_i/kT}$ ← def'n of temp
BOLTZMAN DIST'N.

Grand Canonical:

Do same as here
use $\mu = -T\frac{\partial S}{\partial N}\Big|_U = -kT\frac{\partial \ln g}{\partial N}\Big|_U$
Normalisation: Grand Partition f'n, Ξ
$$\Xi = \sum_i \exp\frac{-(E_i - \mu N)}{kT} \quad \text{GIBB'S DIST'N}$$

Particle number changing:
$TS = -kT\sum_{\text{all microstates } N,i} p_{N,i}\ln p_{N,i}$ ← $p_{N,i} \propto e^{-(E_i - \mu N)/kT}$ $(E_i = E_i(N))$
$= U - \mu\langle N\rangle + kT\ln\Xi$
$\Rightarrow \boxed{\Phi = -kT\ln\Xi}$ ← {but $\Phi = F - \mu\langle N\rangle$ $= U - TS - \mu\langle N\rangle$

$$d\Phi = -SdT - pdV - Nd\mu$$

$$\Rightarrow S = -\frac{\partial\Phi}{\partial T}\Big|_{V,\mu} \text{ and } p = -\frac{\partial\Phi}{\partial V}\Big|_{T,\mu} \text{ and } N = -\frac{\partial\Phi}{\partial\mu}\Big|_{T,V}$$

T.S.P: STATISTICAL DESCRIPTION OF EQUILIBRIUM.

Fluctuations

Important coz: critical points
resistivity
⋮

If know energy eigenstates of system, can use Boltzman or Gibb's dist'n to calc $\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2 \ \forall x$.

Big if... even so, consider Paramagnet:

$\langle M \rangle = \frac{k_B T}{Z} \frac{\partial Z}{\partial B}\Big|_T$ (Boltzman dist'n)

$\langle M^2 \rangle = \frac{k_B T^2}{Z} \frac{\partial^2 Z}{\partial B^2}\Big|_T$ $\rightarrow \frac{\langle \Delta M^2 \rangle}{\langle M \rangle} \propto \frac{1}{\sqrt{N}}$

$\langle \Delta M^2 \rangle = kT \frac{\partial \langle M \rangle}{\partial B}\Big|_T$

ie fluctuation increases as system size decreases.

Also can do via Taylor series:

$$\mathrm{Prob}(N_\uparrow) \propto \underbrace{\frac{N!}{N_\uparrow! N_\downarrow!}}_{\text{degeneracy}} e^{mB(N_\uparrow - N_\downarrow)/kT}$$

very sharply peak at eq. value
∴ expand ln P.
get Gaussian, width ΔM.

Volume Fluctuation at constant T, p.

V can fluctuate as pressure caused by random collisions.

T_0

Proceed as here

$dA = dU - T_0 dS + p_0 dV$

$\frac{\partial A}{\partial V} = T\frac{\partial S}{\partial V} - p - T_0 \frac{\partial S}{\partial V} + p_0 \ (=0 \text{ at eq})$

$\Rightarrow \frac{\partial^2 A}{\partial V^2} = \underbrace{\frac{\partial T}{\partial V}\frac{\partial S}{\partial V}}_{=0?} + \cancel{(T - T_0)}\frac{\partial^2 S}{\partial V^2} - \frac{\partial p}{\partial V}$ 0

Slow fluctuations, isothermal, heat has enough time to pass from/to system from/to res.
Fast fluctuations, adiabatic.

Consider slow case: $\frac{\partial^2 A}{\partial V^2} = -\frac{\partial p}{\partial V}$

So at critical temperature, $\Delta V \rightarrow \infty$!

$\frac{\langle \Delta V^2 \rangle}{V} = \frac{\sqrt{kT\kappa}}{\sqrt{V}}$ where $\kappa = \frac{\partial \ln V}{\partial p}\Big|_T$

as usual

(isothermal compressibility)

Connection to Thermodynamics

Partition energy between subsystem + reservoir. Most probable partition is:

$P(U; U_s) \propto g_s(U_s)\, g_r(U - U_s)$

Using def'n ② of entropy $S = \sum_{\gamma=1}^{N} S_\gamma$, can rewrite as

$P(U; U_s) \propto e^{\ln g_s} e^{\ln g_r} = e^{S_s(U_s)/k} e^{S_r(U-U_s)/k}$ $(S = S_s + S_r)$

let $\Delta S = S(U; U_s) - S(U; \langle U_s \rangle)$

so then $e^{S(U;U_s)/k} = e^{(S(U;\bar{U}_s) + \Delta S)/k} = \exp\left[S(U; U_s)/k\right]$

but $T\Delta S = -\Delta A$

$\therefore P(U; U_s) \propto e^{S(U;\langle U_s \rangle)} e^{\frac{A(\langle U_s \rangle)}{kT}} e^{-\frac{A(U_s)}{kT}}$

$\propto e^{-A/kT}$ dropping constant factors

So for const T, V, $P \propto e^{-\frac{F}{kT}}$
and for const T, p, $P \propto e^{-G/kT}$

Fluctuations in U_s at const V, T_0, N

Expand A about $\langle A \rangle$:

$$e^{-A/kT} = \exp\left\{ -\frac{\langle A \rangle}{kT} - \frac{U - \langle U_s \rangle}{kT}\frac{\partial A}{\partial U}\Big|_{T,V} - \frac{(U_s - \langle U_s \rangle)^2}{2kT}\frac{\partial^2 A}{\partial U^2}\Big|_{T,V} \right\}$$

but $dV = 0 \therefore dA = dF$ $\quad \frac{\partial F}{\partial U} = 1 - \frac{T_0}{T}$ $(=0 \text{ at eq'm})$

$\Rightarrow \langle \Delta U_s^2 \rangle = kT^2 c_V$ $\quad \frac{\partial^2 F}{\partial U^2} = \frac{1}{T_0 C_V}$

Fluctuation in N at constant T, V, μ

eg small volume inside fluid.

system

T_0

Method 1 (Statistical Mechanics)

Calculate $\Delta N^2 = \langle N^2 \rangle - \langle N \rangle^2$ directly.

$\boxed{\frac{\partial \langle N \rangle}{\partial \mu}\Big|_{T,V} = \frac{\langle \Delta N^2 \rangle}{kT}}$ $\quad \left(\langle N \rangle = \frac{kT}{\Xi}\frac{\partial \Xi}{\partial \mu}\Big|_{T,V} \quad \langle N^2 \rangle = \frac{(kT)^2}{\Xi}\frac{\partial^2 \Xi}{\partial \mu^2}\Big|_{T,V} \right.$

$$\boxed{\langle \Delta N^2 \rangle = kT \frac{\partial N}{\partial \mu}\Big|_{T,V}}$$

Method 2 (Thermodynamics) $dA = dU - T_0 dS + p_0 dV - \mu_0 dN$

$\frac{\partial A}{\partial N}\Big|_{T,V} = (T - T_0)\frac{\partial S}{\partial N} + \mu - \mu_0 \ (=0 \text{ eq.})$ $\quad \frac{\partial^2 A}{\partial N^2}\Big|_{T,V} = \frac{\partial \mu}{\partial N}\Big|_{T,V}$

Note:

Thermodynamic variables are only precisely defined for infinitely big systems $\left(\frac{\langle \Delta N \rangle}{N} \propto \frac{1}{\sqrt{N}}\right)$ because they are all averages over microscopic events!

T.S.P. : IDEAL GASES

How to sum over eigenstates...

$\sum_{k} f(\varepsilon) \to \frac{\sigma V}{8\pi^3}\int_0^\infty f(\varepsilon)4\pi k^2 dk \equiv \int f(\varepsilon)\underbrace{D(\varepsilon)}d\varepsilon$ "Density of States"

could be Partition F'n averages...

$2s+1$; $\frac{1}{8}$ octant ; $\frac{V}{\Delta k_x \Delta k_y \Delta k_z}$; $k = \frac{n\pi}{L}$; density of k vectors in k space...

For particle in a box, dispersion relation is $\varepsilon = \frac{\hbar^2 k^2}{2m}$
$\to D(\varepsilon) \propto \varepsilon^{1/2}$

1 Particle in a box:

PARTITION F'N: $Z = \sum_k e^{-\beta\varepsilon_k}$

turn Σ into integral, $\varepsilon_k \to \varepsilon(k)$

get: $\boxed{Z = \sigma n_Q(T)V \quad n_Q = \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}}$

Quantum conc.

AVERAGE ENERGY $U = \frac{1}{Z}\sum \varepsilon_k e^{-\beta\varepsilon_k}$

$= k_BT^2\frac{\partial \ln Z}{\partial T}$

$\boxed{= \frac{3}{2}k_BT}$

ENTROPY $S = -\frac{\partial F}{\partial T}\Big|_V$

$= -\frac{\partial}{\partial T}\left(-k_BT\ln Z\right)$

$= \boxed{k_B \ln\left[\sigma V\left(\frac{em k_BT}{2\pi\hbar^2}\right)^{3/2}\right]}$

N-Particles in A Box

- have sorted out 1 particle in a box - can we just eg add entropies? ie $S_{tot} = NS$? (as with ideal gases classically...)

NO! [NS] is not EXTENSIVE ie if $N \to 2N$ and $V \to 2V$ then should get $S \to 2S$ but no...

What's wrong? We forgot about INDISTINGUISHABILITY

Consider $N=2$: and are the same state with symm wavefn's $\to \phi_a(r_1)\phi_b(r_2) \pm \phi_b(r_1)\phi_a(r_2)$ (B / F)

So, the states, g, (ie $S = k\ln g$) were over counted by $N!$. Use Stirling and correct [NS] formula to get the:

$$\boxed{\text{SACKUR-TETRODE ENTROPY:} \quad S = k_BN\ln\left[\frac{\sigma Ve}{N}\left(\frac{emk_BT}{2\pi\hbar^2}\right)^{3/2}\right]}$$

QM $\to$ classical crossover - further consequences of

Saying $S_{tot} = \sum_{(particles)} S_i$ counts states that are multiply occupied: This is FORBIDDEN for Fermions.

$\therefore$ Fermions (although don't interact via pot) cannot be treated as indep.

So: Don't treat Particles as independent systems $\longrightarrow$ treat Energy Levels as independent systems

not [res | sys] in real space but now [res | s] in energy level space

$\to$ now, N is not a "system constant" $\therefore$ use Grand Partition Function

The Picture: const T, μ ; n particles $U = n\varepsilon$

$\Xi = \sum_{N,E} \exp\left(-\beta[E(N) - N\mu]\right)$
$= \sum_n e^{-\beta(n\varepsilon - n\mu)}$

$n_{max} = \infty$ for Bosons.
$n_{max} = 2$ for Fermions.

$$\boxed{= \frac{1}{1 - e^{-\beta(\varepsilon-\mu)}}}$$ [Summing the G.P.]

Bose-Einstein Stats:

Ξ as on right

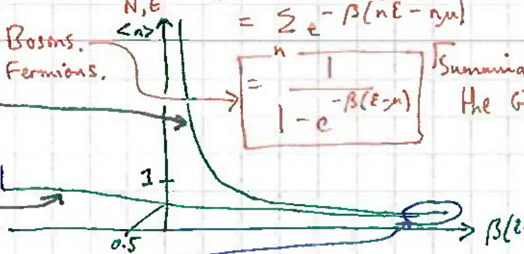
Average occupancy is $\langle n\rangle = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}$

Fermi-Dirac Stats:

Ξ is $\sum_{n=0}^{1}\left(e^{-\beta(\varepsilon-\mu)}\right)^n = 1 + e^{-\beta(\varepsilon-\mu)}$

$\Rightarrow \langle n\rangle = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}$

only diff.



Classical limit ie $e^{\beta(\varepsilon-\mu)} \gg 1$ ie $\langle n\rangle \ll 1$ - double occupancy never happens - so F or B - no matter!

Grand Partition F'n for Ideal Gas

Consider 2 levels + res: system $N = n_1 + n_2$, $E[N] = n_1\varepsilon_1 + n_2\varepsilon_2$

Grand Partition Function is $\sum_N \sum_{E[N]} \exp\left[-\beta(E[N] - N\mu)\right]$ sum over microstates.

$\sum_N\sum_{E[N]}$ specifies all microstates, as does $\sum_{n_1}\sum_{n_2}$ so use to get: $\Xi = \prod_k \Xi_k$ (kth level.)

So can generate all other therm. Potentials:

Grand Pot: $\Phi = \sum_k \Phi_k$ $\quad N = -\frac{\partial\Phi}{\partial\mu}\Big|_{T,V}$ $\quad S = -\frac{\partial\Phi}{\partial T}\Big|_{V,N}$ $\quad p = -\frac{\partial\Phi}{\partial V}\Big|_{T,N}$

and either $\langle n_k\rangle = \frac{1}{\Xi_k}\sum_n n\left(e^{-\beta(\varepsilon_k-\mu)}\right)^n$ (Gibbs Dist'n)

or $\langle n_k\rangle = -\frac{\partial\Phi_k}{\partial\mu}\Big|_{T,V}$

Classical Ideal Gases

Start with Partition F'n for an eigenstate of the gas: $\Xi_k = \sum_n\left(e^{-\beta(\varepsilon_k-\mu)}\right)^n$ (n = occupancy)

Prob. of $n \geq 2$ is negl. $\therefore \Xi_k \simeq 1 + e^{-\beta(\varepsilon_k-\mu)}$

$\Phi_k = -k_BT\ln\Xi_k = -k_BT\ln(1 + e^{-\beta(\ )}) \simeq -k_BTe^{-\beta(\varepsilon_k-\mu)}$

$\Rightarrow$ Distribution function is: $\langle n_k\rangle \approx e^{\beta\mu}e^{-\beta\varepsilon_k}$

So $\Phi\left(\equiv\sum_k\Phi_k\right) = \int_0^\infty D(\varepsilon)\Phi(\varepsilon_k)d\varepsilon = -kT\sigma Vn_Q(T)e^{\beta\mu}$

$N = \sigma Vn_Qe^{\beta\mu}$ if N const (eg atoms...) rearrange: $\mu = kT\ln\left(\frac{N}{\sigma Vn_Q}\right)$

Maxwell-Boltzman Distribution:

$n(\varepsilon)d\varepsilon$ = no. in each level $\times$ density of levels $d\varepsilon$
$= n_k \quad D(\varepsilon) \quad d\varepsilon$
$= e^{\beta\mu}e^{-\beta\varepsilon}D(\varepsilon)d\varepsilon$ and $D(\varepsilon) = \frac{\sigma V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\varepsilon}\,d\varepsilon$ and $\varepsilon = \frac{1}{2}mv^2$

$\Rightarrow$ Get: $\boxed{n(v)dv = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}e^{-\beta mv^2/2}4\pi v^2dv \quad \text{M-B dist'n!}}$ $\exists$ more direct ways though.....

REAL SPACE INTERPRETATION OF CLASSICAL LIMIT:
(k-space interpretation was prob $(n\geq 2) \sim 0$)

μ must be $-ve$ $\therefore \frac{N}{V} \ll n_Q$ ie classical conc $\ll$ quantum conc

$\to$ Subst for μ in $\Phi \to \Phi = -NkT$ (pV)

$p = -\frac{\partial\Phi}{\partial V}\Big|_{T,\mu} = -\frac{NkT}{V}$

ie IDEAL GAS LAW

Entropy: $S = -\frac{\partial\Phi}{\partial T}\Big|_{V,N}$ if subst for μ,

get Sackur-Tetrode formula
$S = k_BN\ln\left(\frac{e^{5/2}\sigma Vn_Q}{N}\right)$

ie S-T entropy is a Classical Expression.

Internal Degrees of Freedom + Ext Potentials

Let's assume that can write $\varepsilon = \varepsilon_k + \varepsilon_{int} + \varepsilon_{ext}$

eg for ideal gas diatomic molecule: $\varepsilon = \frac{\hbar^2k^2}{2m} + (n+\frac{1}{2})\hbar\omega + \frac{J(J+1)\hbar^2}{2I}$

Not always true that ε_{int} is indep of ε_{ext} - grav OK, mag field, not OK]

Eg classical gas at height h.....

$\Xi_k(h) = 1 + \sum_{int} e^{-\beta(\varepsilon_k + \varepsilon_{int} + \varepsilon_{ext} - \mu)}$

$= 1 + e^{-\beta(\varepsilon_k-\mu)}e^{-\beta\varepsilon_{ext}}Z_{int}$

So Grand Potential, Φ_k

$= -kT\ln\Xi_k \simeq -kTZ_{int}e^{-\beta\varepsilon_{ext}}e^{-\beta(\varepsilon_k-\mu)}$

So chemical Potential is then:

$\mu = kT\left(\ln\left(\frac{N}{\sigma Vn_Q}\right) - \ln Z_{int}\right) + \frac{Mgh}{kT}$ [Contribution from Gravity]

Equilibrium Constant.

From before, $\ln K_p(T) = \frac{-1}{kT}\sum_i \nu_i\mu_{0i}(T)$

ν_i = no of molecules of species i in reaction (eq'n)

μ_{0i} = "μ_i at 1 Atmosphere".

Using this can write

$\ln K_p(T) = \sum_i \nu_i\left[\ln\left(\frac{N}{\sigma Vn_Q}\right) - \ln Z^i_{int}\right]$

eg $He \to He^+ + e^-$, $Z^i_{int} = 1$ and all

T.S.P.: Quantum Gases

The Ideal Bose Gas.

Sackur-Tetrode entropy does not $=0$ for $T=0$ ie contradicts 3rd Law....

Einstein + Fermi both tried to overcome this, ∃ with ∞ occupation and Fermi with single occupation....

Begin with Grand Partition f'n for kth energy level:

$$\Xi_k = \sum_{n=0} \left(e^{-\beta(\varepsilon_k-\mu)}\right)^n$$

$\longrightarrow$ Grand Potential Φ_k

$\longrightarrow \langle \text{occupation} \rangle = -\left.\frac{\partial \Phi_k}{\partial \mu}\right|_{T,V}$

$$\boxed{\langle n_k \rangle = \frac{1}{e^{\beta(\varepsilon_k-\mu)}-1}}$$ BOSE-EINSTEIN DIST'N.

Eg Black body radiation

Photons: non interacting ∴ for thermal eq must interact with walls.

let μ = const. Const T, V ∴ equilib when $\left.\frac{\partial F}{\partial N}\right|_{T,V} = 0 \ (=\mu)$ so $\boxed{\mu = 0}$ B.B.R. as $\Phi = F - \mu N$, $(\Phi = F)$

$\Rightarrow \frac{1}{e^{\beta\varepsilon_k}-1}$ for B.B.R.

Phase space element

$$\frac{2 \cdot V}{8(2\pi)^3} 4\pi k^2 dk = \frac{V}{\pi^2 c^3}\omega^2 d\omega$$

$$\Rightarrow E_\omega d\omega = \frac{V}{\pi^2 c^3}\frac{\hbar\omega^3 d\omega}{\left(e^{\beta\hbar\omega}-1\right)}$$ $\int d\omega \longrightarrow E_{tot} \propto T^4 \longrightarrow C \propto T^3$

Low temperature limit of B-E gas:

For real gas, N fixed, μ changes. Determine N by $\int_0 D(\varepsilon) n(\varepsilon) d\varepsilon$

$$= \frac{\sigma V m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\underbrace{\int_0^\infty \frac{\sqrt{\varepsilon}\, d\varepsilon}{e^{\beta(\varepsilon_k-\mu)}-1}}_{\text{messy}}$$

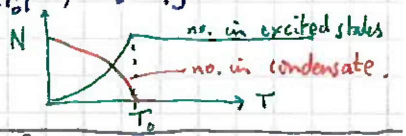
NB if $\mu \geq 0$, can have ∞ occupation at some energy, but even if $\mu \to 0_-$, N doesn't remain constant as $T \to 0$

problem? no. Atoms disappearing from under the integrand are macroscopically occupying the G.S.

$$\lim_{T\to 0} n\Big|_{\varepsilon=0} = \lim_{T\to 0}\left(\frac{1}{e^{-\beta\mu}-1}\right) = N \Rightarrow \mu \sim \frac{kT}{N}$$ (very small)

For excited states, set $\mu = 0$ (?) [still $T < T_0$]

$\rightarrow N_{G.S.} = N\left(1-\left(\frac{T}{T_0}\right)^{3/2}\right)$ $T_0 = $ eg ...



Energy and Specific heat of B-E condensed gas.

Standard way: $U = \int_0^\infty \frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}-1} D(\varepsilon)\, d\varepsilon$

For $T < T_0$, $\mu \simeq 0$ for excited states

then can evaluated, $U = \frac{1.005\sigma V}{\sqrt{2}} n_Q(T) kT$

So $C_V = \frac{5}{2}\frac{1.005\sigma V}{\sqrt{2}} n_Q(T)$ for $T > T_0$, class: $C = \frac{3}{2}Nk$

The Ideal Fermi Gas

Get $\langle n_k \rangle$ ie F-D distribution as above (or directly...!)

$$: \langle n_k \rangle = \frac{1}{e^{\beta(\varepsilon_k-\mu)}+1}$$ $T=0$: step f'n with $\varepsilon < \mu$ full and $\varepsilon > \mu$ empty. $\mu \equiv E_F$!

For $T > 0$, only electrons within kT of $\mu|_{T=0} = E_F$ are excited. E_F determined by $N \rightarrow k_F$ etc etc (S.S.)

Grand Potential: $\Phi = \sum_k \Phi_k = \int_0 D(\varepsilon)\Phi_k\, d\varepsilon$

Energy + Pressure

$\langle E \rangle = -\frac{3\Phi}{2}$ but $\Phi = -pV \rightarrow p = \frac{\sigma}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta\varepsilon}+1} d\varepsilon$

Exact equation of state for Ideal Fermi gas

Low temperature limit $\Phi(T) = \Phi(0) - \frac{\sigma V (kT)^2}{2}\left(\frac{2\varepsilon_F m^3}{6\hbar^3}\right)^{1/2}$

Entropy and Heat capacity at low temp:

$$S = -\left.\frac{\partial \Phi}{\partial T}\right|_{\mu,V} = \frac{\pi^2}{3}\varepsilon_F D(\varepsilon_F) k^2 T$$

$$\Longrightarrow C_V = T\left.\frac{\partial S}{\partial T}\right|_{V,\mu} \propto T$$

Chemical Potential of Fermi Gas:

$N = \int_0^\infty D(\varepsilon) n(\varepsilon) d\varepsilon$ = not nice.... as T changes, adjust μ s.t. N const

In high temp limit, $\Rightarrow \mu$ large and $-$ve and $\langle n_k \rangle \longrightarrow$ Maxwell-Boltzman result.

For $T \to 0$, $\mu \longrightarrow +^{ve}$ number!

Entropy per energy level (Gibbs:)

$S_G = \sum_k P_k \ln P_k$ so $\rightarrow S = -k_B \sum_k \left[\langle n_k \rangle \ln\langle n_k \rangle + (1-\langle n_k \rangle)\ln(1-\langle n_k \rangle)\right]$

either occupied (prob $\langle n_k \rangle$) or unoccupied (prob $1-\langle n \rangle$)

Phonons, Magnons, Electrons.

Break motion down into "Elementary excitations" ie normal modes. eg Phonons: get $\omega = v_s k$ for small k, flattening near BZ boundary.

$\Rightarrow$ same results as for photons eg $C \propto T^3$

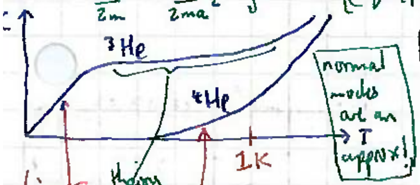
for spin waves in a ferromagnet (magnons) the disp rel is $\omega \propto k^2$ (same as ideal gas) $\rightarrow C \propto T^{3/2}$

for electrons, FD stats apply (BE for the above 2)

Quantum Liquids ^4He and ^3He

zero pt energy ~ binding energy of interatomic potential $\Rightarrow$ no solid phase

ie $\delta E \sim \frac{\Delta p^2}{2m} \approx \frac{\hbar^2}{2ma^2}$ get a from [(eq. sep)^3 - hard core]



Interacting Many Particle Systems

Classical Liquids.

Virial Expansion:

Virial: $\mathcal{V} = -\frac{1}{2}\sum \underline{F}_i \cdot \underline{r}_i$

$\langle \mathcal{V} \rangle$ = mean K.E. (Clausius V. theorem)

$\langle \mathcal{V} \rangle = \langle \mathcal{V} \rangle_{ext} + \langle \mathcal{V} \rangle_{int}$

$\frac{3}{2}pV$ $\qquad \frac{N}{2}\int_0 \frac{f(r)}{2} r n g(r) dV$ Monte-Carlo

$\frac{3}{2}kT$

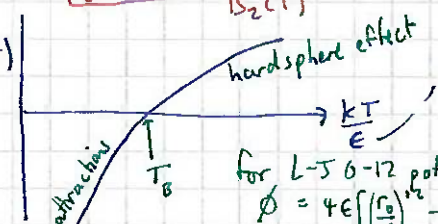
$$\Rightarrow p = nkT - \frac{n^2}{6}\int 4\pi r^3 f(r) g(r) dr$$

if $\mathcal{V} = 0$, ideal gas behaviour.

If density is so low that only 2 body correlations are important then $g(r) = e^{-\phi/kT}$ (ϕ is interat. pot)

$$\text{So } \frac{p}{kT} = n + \underbrace{\int_0^\infty 2\pi r^2\left(1-e^{-\phi/kT}\right)dr}_{B_2(T)} \cdot n^2 \text{ (parts)}$$

$\Rightarrow B_2(T)$



for L-J 6-12 potential: $\phi = 4\varepsilon\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^6\right]$

Virial Expansion: expand $g(r)$

$$g(r) = g_0(r) + g_1(r)n + g_2(r)n^2 + \ldots$$

$$\frac{p}{kT} = n + B_2(T)n^2 + \ldots$$ 2nd virial coeff.

Law of Corresponding States.

All substances have same reduced eq'n of state

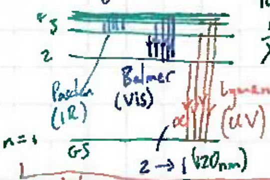
$\frac{p}{p_0} = f\left(\frac{n}{n_0}, \frac{T}{T_0}\right)$ $p_0 = \varepsilon r_0$, $n_0 = r_0^3$, $T_0 = \frac{\varepsilon}{k}$

Works well for spherical molecules but not for long ones or quantum gases or liquids

A.P.L.: Atoms

Basic Hydrogen Atom

elec. discharge through H gas produces spectrum (emitted)



Rydberg: $\frac{1}{\lambda} = R_H\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$

$E = hcR_H\left(\frac{1}{n^2}-\frac{1}{m^2}\right)$

ionisation $m \to n$: $0 \to \infty$

$2 \to 1$ (120nm)

determined experimentally so far...

Theory: SE: with ① Point charges! ② nuc. has ∞ mass! ③ no rel ie magnetism/spin!

$$\boxed{\left[\frac{-\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right]\psi = E\psi}$$

⇒ Seperable solutions $\psi_{nlm_l} = \underbrace{R_n(r)}_{} P_{lm_l}(\theta)\, e^{\pm im\phi}$ (actually $\cos\theta$)

where $n = 1, 2, 3 \ldots \infty$

$l = 0, 1, 2 \ldots (n-1)$

$m_l = -l \to +l$

energy part is $R_n(r)$

$E = -\alpha^2 m_e c^2 \left(\frac{Z}{2n^2}\right)$

hence Rydberg formula

Hydrogen atom Spectra

Transition strengths: E dipole, M dipole, E quad. ignore rest.

$\Delta m_l = 0$ or ± 1, $\Delta L = \pm 1$

(z dir'n; x or y dir'ns)

H-like atoms - examples:

"Rydberg" atoms: kick electron up to say $n = 400$ (in eg Ba) using lasers. $r_n = \frac{n^2}{2} a_0$ (Ba⁺ … 8μm … e⁻) so atom is quasimacroscopic

Highly ionised atoms found eg in x-ray astronomy. $R_{H(\text{eff})} \propto Z^2$

μ-onic atoms (replace one e⁻ by μ⁻) $m_\mu \sim 200 m_e$ and $a_0 \propto \frac{1}{\text{mass}}$ so μ⁻ penetrates close (short lived (10^{-6}s))

Better Hydrogen Atom.

Summary:

Correction	$E\sim$	name
Basic S.E.	α^2	–
Electrons are relativistic	α^4	Fine structure
Spin-orbit coupling	α^4	Fine structure
Quantise the E/M field	α^5	Lamb shift
Nuclear spin	$\frac{m_e}{m_p}\alpha^4$	Hyperfine structure

Use 1st order perturbation theory to calculate energy corrections $E_i^{(1)} = \langle\psi_i|W|\psi_i\rangle$

We used $T = \frac{p^2}{2m}$ (here) in this eq'ns so, $E_n^{(1)} \propto \langle p^4\rangle$ but $\frac{p^2}{2m_0} \equiv E_n - V$ → need $\langle V\rangle$ and $\langle V^2\rangle$

- we should use $T = (\gamma - 1)mc^2$
$= E - mc^2$
$= \sqrt{p^2c^2 - m^2c^4} - mc^2$
$= m_0c^2\sqrt{1 - \left(\frac{p}{m_0c}\right)^2}$
$\simeq \frac{p^2}{2m} - \underbrace{\frac{p^4}{8m_0^3c^2}}$ Relativistic correction

$$\boxed{\Delta E_{rel}^{(1)} = -\frac{\alpha^4 mc^2}{4n^4}\left[\frac{2n}{(l+\frac{1}{2})} - \frac{3}{2}\right]}$$

This is how α got it's name

Spin-Orbit Coupling: from e⁻ p.o.v. nucleus is current travels around it in a circle
⇒ $B = \frac{\mu_0 I}{2r}$, $I = \frac{e}{2\pi r/v} = \frac{ev}{2\pi r}$

but electron has spin ∴ mag. moment.
Energy of dipole in field $= -\underline{\mu}\cdot\underline{B}$
$= -\frac{e}{m}\underline{S}\cdot\frac{\mu_0 e}{4\pi m r^3}\underline{L} \propto \underline{L}\cdot\underline{S}$

also need $\langle\frac{1}{r^3}\rangle$ which is: $\frac{1}{l(l+\frac{1}{2})(l+1)n^3a_0^3}$

Write in terms of J^2, L^2, S^2 and use e-values. ⟶ $\Delta E_{S-O} = \alpha^4 mc^2 \frac{[j(j+1) - l(l+1) - \frac{3}{4}]}{4n^3 l(l+\frac{1}{2})(l+1)}$

If use fact that $j = l \pm \frac{1}{2}$ get $\boxed{\Delta E_{\text{fine structure}} = -\frac{\alpha^4 mc^2}{4n^4}\left[\frac{2n}{(j+\frac{1}{2})} - \frac{3}{2}\right]}$ compare

For H-like atom, $a_0 \propto \frac{1}{Z}$ ∴ $\Delta E \propto Z^4$ (strong!)
Thomas Precession gives factor of ½)

Q.E.D. predicts Lamb shift - seperates states of different L - ΔEs does only depend on j, not L. In particular, it splits the $^2S_{1/2}$ and $^2P_{1/2}$ states. See orange notes pg 13 for diag. of how to measure.

Hyperfine corrections: nucleus has spin mag mom
$\underline{\mu}_p = \gamma_p \frac{e}{m_p c}\underline{S}_p$ Need $\underline{F} = (\underline{L} + \underline{S}_e) + \underline{S}_p = \underline{J} + \underline{S}_p$

For $l = 0$, all effect is S_p, S_e coupling with $F = 1$ or 0 ($\frac{1}{2}\pm\frac{1}{2}$). This $E_{\text{triplet}} \to E_{\text{singlet}}$ gives the 21cm line in Radio Astronomy
For $l \neq 0$, all effect is S_p-O coupling from nucleus

Multi-Electron Atoms:

A simplified Hamiltonian: $H = \sum_{\text{elec's}}\left[\frac{-\hbar^2\nabla_i^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0 r_i}\right] + \underbrace{\sum_{i<j}^{N}\frac{e^2}{4\pi\varepsilon_0 r_{ij}}}_{\text{correlation problem}}$

because:
- nucleus has ∞ mass
- point like nucleus
- no rel/mag effects

this means cannot sep variables... $R_n Y_{lm}$

Central Field Approximation.

Consider one electron: $H = KE + \underset{(\text{nuc})}{PE} + \boxed{\underset{(\text{other elec's})}{PE}}$

let this = average field due to ther elec's, $V(r_i)$ so it only dep's on r_i ⇒ seperable, solvable eq'ns.

But what $V(r_i)$ to use?
large distances → $\frac{e^2}{4\pi\varepsilon_0 r_i}$
small distances → $\frac{Ze^2}{4\pi\varepsilon_0 r_i}$
Intermediate distances.... tricky: use Thomas-Fermi approch or Hartree-Fock method
iterate using Hydrogenic orbitals - gives ~10% error ∀ periodic table

Solve for each electron in CFA, get Energy dep on n, l. Get N indep. e⁻ wavef'ns. Combine in Slater determinant to satisfy Pauli exclusion and Fermion antisym requirements.

CFA. Periodic table...

Each pair of states with given n, l, m_l ≡ ORBITAL
Set of states with given n, l ≡ SUBSHELL
Set of states with given n ≡ SHELL
Degeneracy is $2(2l+1)$ from m_l, m_s so s states can fit 2 e⁻, p have 6, d have 10 etc etc.
Form of $E(n, l)$ ∂ s.t. energy ordering of orbs is:

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f 5g
etc

Term Symbols. $^{2S+1}L_J$

for L-S (Russ-Sanders) regime ie Correlation but no S-O coup. [splits J]

For eg: p^2 systems: find all possible m_L, m_S states:

	$m_s = -\frac{1}{2}$	$+\frac{1}{2}$
$m_l = -1$	·	·
0	·	·
1	·	·

(m_l small) For indiv. electrons!

∃ 15 states:

	$m_S = -1$	0	1
$m_L = 2$		×	
1	×	××	×
0	×	×××	×
-1	×	××	×
-2		×	

$^1S_0$, $^3P_{2,1,0}$, $^1D_2$

electrons in same l state → can't vectorially add the indiv. ang mom! - if add e⁻ to other (indep) subshell (eg p^2d^1) then use normal ang mom add.

Hund's Rules

1) Maximise $S = \sum s_i$
2) (Subject to 1,) max $L = \sum l_i$
3) Calc (2S+1) values of J; if shell < ½ full take $|L-S|$; if shell > ½ full take $L+S$
① Common Sense ② Pauli ③ L-S coupling

L-S vs j-j: The Angular Momentum Question!

Actually: $H_{\text{actual}} = H_{CFA} + H_{\text{correlations}} + H_{\text{spin-orbit coupling}}$

If can neglect S-O coupling eigenstates are those of $J^2, L^2, (L_z), S^2, (S_z)$ total atom - use L-S or Russell Sanders coupling:
In this regime, get term symbols, Hund's rules, splitting of states of different L and S - J is not a good quantum number for the system - ∃ degeneracy within J. Good for light atoms - e⁻ no more fast ∴ no big orb mag moment ≡ non rel!

Reality is somewhere in between!

If can neglect correlations w.r.t. spin-orbit coupling, then because of $[\hat{L}\cdot\hat{S}]$ term, e-states are now those of $\hat{J}^2, \hat{J}_z$ $\{\hat{j}_1, \hat{j}_2 \ldots \cancel{\hat{L}\,\&\,\hat{S}}\}$ - use j-j coupling. Term symbols no good now - states of different J have different energy - for heavy atoms.

$\cancel{|J, L, S\rangle = \sum|}$!?

$|J, m_J, j_i \ldots\rangle = \sum_{m_L}|J, L, m_L, S, m_S\rangle$

A.P.L. : Light

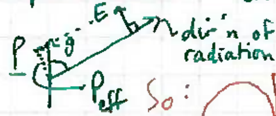
Classical Summary:

$E_x = E_0 \cos(kz - \omega t)$
H is $\perp$ to E and in phase

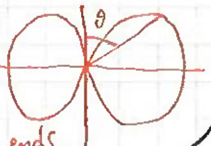
$\frac{E_x}{H_y} = \sqrt{\frac{\mu_0}{\varepsilon_0}} \simeq 377\,\Omega$ (free space)

Dipole emission: $P_{eff} = E \sin\theta$:

dir'n of radiation



So: $|E| \propto \sin\theta$

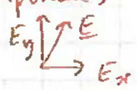


no radiation from ends.

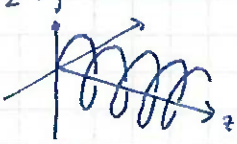
Polarisation

If $\boxed{\text{plane of } E \text{ is const}}$ for whole wave then: LINEAR POLARISATION

Any wave can be resolved into its 2 (linearly pol.) components

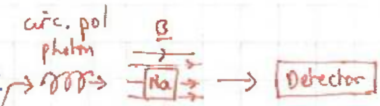


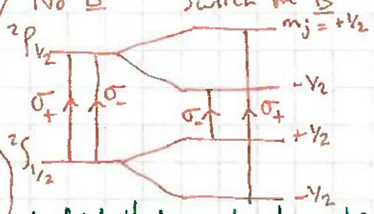
If $|E_x| = |E_y|$ but phase diff is $\frac{\pi}{2}$, get CIRCULAR POL'N.



ie Photons SPIN! they carry angular mom $\pm\hbar$

Evidence for photon spin: Sodium D one transition ie ${}^2P_{1/2} \to {}^2S_{1/2}$





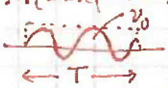
ie find that peak absorption energies of σ_+ photons and σ_- photons differ.

limited freq. accuracy

Uncertainty in energy related to uncertainty in time: $\Delta E \Delta t \geq \hbar$

$\Rightarrow \Delta\nu \Delta t \geq 1$

also, F.T. (wavepacket) ie FT of



is $T\,\text{sinc}(\pi(\nu-\nu_0)T)$

which has it's first zero at: $\nu - \nu_0 = \frac{1}{T}$

ie $\Delta\nu T = 1$

limited spatial accuracy

Fraunhofer diffraction:

$\Delta\theta \simeq \frac{\lambda}{a}$ from aperture width a

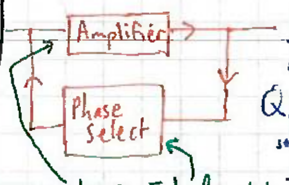
more generally.... $\Delta p_x . a \sim h$ $\quad (\Delta) p_z = \frac{h}{\lambda}$ (de Broglie)

$\Rightarrow$

$\boxed{\theta = \frac{\lambda}{a}}$

Light Sources: Signal Generator

feedback signal is in phase with original.

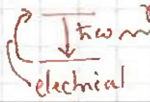


Stable amplitude if
- Gain = feedback loss

$Q_{\text{phase select}} = \frac{\nu_0}{\Delta\nu_{p.s.}} \ll \frac{\nu_0}{\Delta\nu_0}$ $\therefore$ good.

cf laser - atoms, Fab-Per etalon

Atomic Discharge Lamp



Spontaneous emission
an atom has a high $Q \sim 10^7$

Emitted light is non-coherent and unpolarisated - no connection between atoms.

Black Body Radiation

Energy density = (Freq) density of states (modes) × no. of photons in each mode × energy of each photon $\hbar\omega$

Particle in box argument Bose-Einstein dist'n

$\Longrightarrow \rho(\omega) \propto \frac{\omega^3}{e^{\beta\hbar\omega} - 1}$

Lineshapes/widths:

Doppler broadening

$\frac{\nu_{lab}}{\nu_0} = \sqrt{\frac{1 + \frac{v}{c}}{1 - \frac{v}{c}}} \simeq 1 + \frac{v}{c}$

observed

$\Rightarrow \frac{\Delta\nu}{\nu_0} = \frac{v}{c}$

prob of atom having KE $\propto \exp\left[-\frac{\frac{1}{2}mv^2}{kT}\right]$

so prob of observing particular freq is $\propto \exp\left[-\frac{mc^2 \Delta\nu^2}{2kT\nu_0^2}\right]$

GAUSSIAN

eg transition in O^{2+} emits light - shifted by equal + opp. amounts on each side of galaxy → calc speed of rotation

Lifetime Related

P(decay) per sec

$I(\omega) \propto \frac{1}{(\omega - \omega_0)^2 + \left(\frac{\gamma}{2}\right)^2}$

$|\psi|^2$ is prob of photon emission

also $= -\frac{dP}{dt} \propto e^{-\gamma t}$

$\psi(t) = A e^{-\gamma t/2} e^{-i\omega_0 t}$
so FT $\psi(t)$ gives $\psi(\omega)$

Prob that atom is in excited state at time $(t + dt)$,
$P(t+dt) = P(\text{in excited state at time } t) \times P(\text{has not decayed in } dt)$
$= P \times (1 - \gamma dt)$
$= P + \frac{dP}{dt} dt \rightarrow P = P_0 e^{-\gamma t}$ (P_0: P(0))

Kinetic theory: Collision freq $\gamma = n\sigma\sqrt{\frac{3kT}{m}}$ works ok...

$\frac{1}{\gamma}$ = natural lifetime or mean time between collisions

Polarisation and Coherence

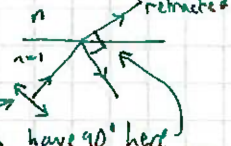
Random Light beams

Produce by:
1. BBR
2. Atomic lamp - each atom emits polarised wavetrain for $\sim 10^{-8}$s; diff transitions → diff wavelengths
3. Laser light + multiple scattering - Polarisation is randomised.

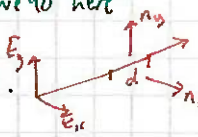
Producing Polarisation

Linear: Polaroid or Brewster angle reflection:
Hydrocarbon chains with Iodine.... Polarisation as $\perp$ light gets through. (or by scattering ....)

is not reflected when have 90° here
→ $n = \tan\theta_i$



Circular: Quarter wave plate: direction dependent n.



Correlation Functions

$\rightarrow G(T) = \int_{-\infty}^{\infty} f_1(t) f_2(t - T)\,dt$

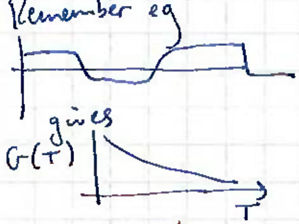
Normalisation $\longrightarrow \int_{-\infty}^{\infty} f_1(t) f_2(t)\,dt$

- measures how similar f_1 and f_2

Autocorrelation: $f_1 = f_2$:

$GT = \frac{\int f(t) f(t-T)\,dt}{\int f^2(t)\,dt}$

Remember eg



G measures the
INTERNAL PREDICTABILITY
of a function

First Order Coherence: Amplitude Correlation

between $E(r_1, t_1)$ and $E(r_2, t_2)$ — correlation function

$\Gamma_{12}(r_1, r_2, \tau) = \langle E(r_1, t+\tau) E^*(r_2, t) \rangle$

shift time origin at will coz stationary

normalise with $I_1 = |\Gamma_{11}(0)|^2$ and I_2

get: Complex degree of first order coherence

$\gamma_{12}^{(1)} = \frac{\Gamma_{12}(\tau)}{\sqrt{I_1 I_2}} \Rightarrow |\gamma_{12}^{(1)}|$ = degree of f.o.c.

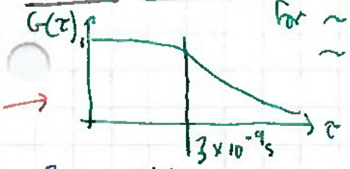
When $I_1 = I_2$, $|\gamma_{12}^{(1)}|$ is the visibility

incoherent $|\gamma| = 0$ coherent $|\gamma| = 1$ Partially coherent

A.P.L.: Polarisation and Coherence Continued

HeNe Laser
- Perfect sine wave for ~1 m, ~3×10^{-9} s

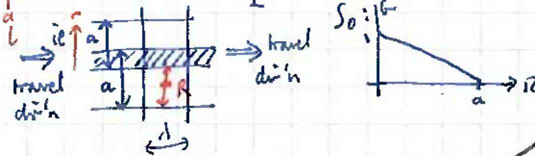
Temporal



Spatial

Beam width a

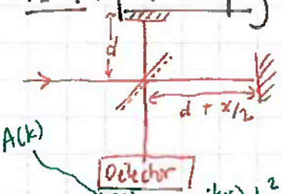
$\rightarrow G(R) = \frac{\langle E(r)E(r-R)\rangle}{I} = \frac{a-R}{a}$



Wiener - Kintchine theorem

$$\boxed{FT\left(\begin{array}{c}\text{autocorrelation}\\ \text{function}\end{array}\right) = \begin{array}{c}\text{Power}\\ \text{Spectrum}\end{array}}$$

F.T. Spectroscopy (With Michelson Spectral Interferometer)



$I_{det} = \left|\frac{A(k)}{2}(1+e^{ikx})\right|^2$

$\left(\propto \boxed{\cos^2\frac{kx}{2}}\right)$

let $A = \sum_k a_k e^{ikx}$ (x variable)

So $I(x) = \frac{1}{2}\int A(k)\,dk + \frac{1}{2}\mathrm{Re}(FT(A(k)))$

Visibility: $V(x) = \frac{I_{max} - I_{min}}{I_{max} + I_{min}}$

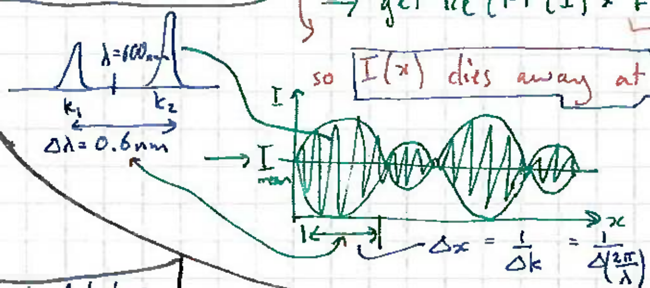
Eg Sodium D-lines

effect of linewidth: I(δf'n) is now I(δf'n) ∗ Gaussian (Narrow)

⟹ get $\mathrm{Re}(FT(I) \times FT(\text{Gaussian}))$ (wide)

so $I(x)$ dies away at edges

for Na, width δk $\therefore \delta x = \frac{1}{\delta k}$ big



$\Delta x = \frac{1}{\Delta k} = \frac{1}{\Delta\left(\frac{2\pi}{\lambda}\right)}$

Spectral Resolution.

Fabry Perot Etalon $\rightarrow \Delta\nu = \frac{c}{2d}$

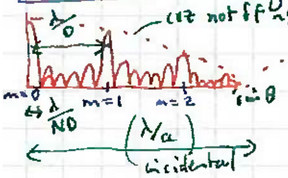
Standing wave condition

Beats at detector

$\Delta\nu$ must be s.t. $\frac{1}{\Delta\nu} \geq 10^{-9}$ s

Diffraction Grating

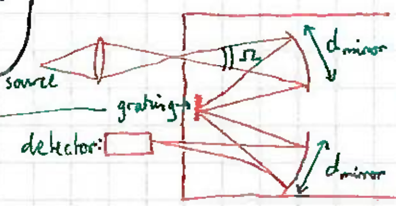
$\frac{\lambda}{ND} \leq \frac{\lambda_1}{D} - \frac{\lambda_2}{D}$



... m th order peak occurs at $\sin\theta = \frac{m\lambda}{D}$

width d

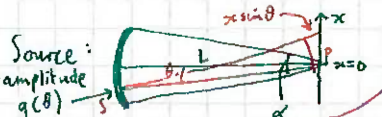
Classical Spectrometer compared with Fourier Spectrometer



	Classical	Fourier
Resolution $\Delta\left(\frac{1}{\lambda}\right) = \frac{1}{2d}$	d of grating	max. travel
Photon usage	Ω of slit turn grating	size of beam splitter
Scanning	- see one λ at a time	move mirror - see all photons all the time

So Fourier seems to win .... except have to take F.T. at the end. $\frac{\lambda}{d_{mirror}} < \frac{\lambda}{d}$ then OK - grating controls res.

van Cittert - Zernike Theorem



coz spherical waves

$f(0) = \frac{1}{L}\int g(\theta)\,e^{ik\overline{SP}}\,d\theta$ (source)

$f(x) = \frac{1}{L}\int g(\theta)\,e^{-ik(\overline{SP} + x\sin\theta)}\,d\theta$ (source)

Complex degree of first order spatial coherence,

$\gamma(x) = \frac{\langle f(0)f^*(x)\rangle_t}{|f(0)|^2}$ let $I(\theta) = g(\theta)g^*(\theta)$

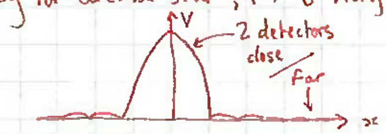
(f = amplitude of light)

$= \frac{\int_{-\infty}^{\infty} I(\theta)\,e^{ikx\theta}\,d\theta}{\int_{-\infty}^{\infty} I(\theta)\,d\theta}$ $\boxed{= \frac{F.T.\ I(\theta)}{\int I\,d\theta}}$

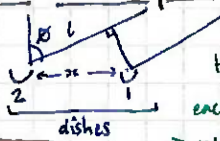
$I(\theta)$ is non-zero only for $|\theta| < \alpha$

and $|\gamma| = \text{Visibility}(x)$

eg for circular star, FT is Airy disc....



Radio Telescopes

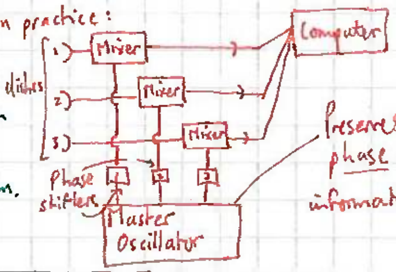


$\omega t_1 = \omega\frac{L}{c} = kx\sin\phi$

take signal from each dish and use v.C-Z theorem.

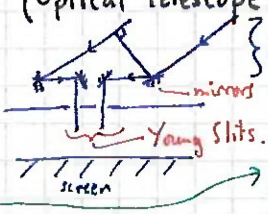
⟹ can get $I(\phi)$

In practice:



Preserves phase information

(Optical telescope:)



{same set up as above}

$V(x) = \frac{\int I(\phi)\cos(kx\phi)\,d\phi}{\int I\,d\phi}$

cf. v. C-Z theorem

Michelson Stellar Interferometer

Atmospheric Speckle

eg binary system in 2D: ∴

Take photo for 10 ms: get (.. ⁘ ⁘ ..)

take FT → from each

→ add many transforms then invert.... images constructively interfere but noise cancels out coz random.

Phase Closure

3 rays have phase shifts δ_1, δ_2 and δ_3 introduced by atmosphere. Measured phase of 2 compared to 1 is

$\phi_{21} = \phi_{21}^{actual} + \delta_2 - \delta_1$

$\rightarrow \sum \phi_{ij}\big|_{measured} = \sum \phi_{ij}\big|_{actual}$

Intensity Correlation: 2nd Order Coherence F'n

$\gamma_{12}^{(2)} = \frac{\langle I(r_1,t)\,I(r_2,t+\tau)\rangle}{\langle I(r_1)\rangle\langle I(r_2)\rangle}$

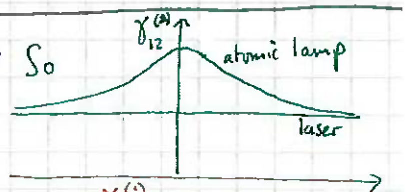
usually concerned with $r_1 = r_2 (\equiv r)$

write $I(t) = \langle I\rangle + \underbrace{\langle I\rangle\,\delta(t)}_{\text{fluctuation}}$

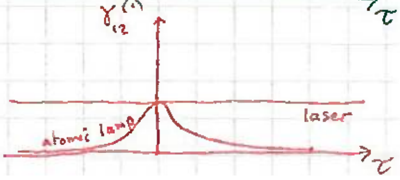
$\gamma_{12}^{(2)} = 1 + \langle\delta_1(t)\delta_2(t+\tau)\rangle \geq 1$

as $\langle\delta_1\rangle = \langle\delta_2\rangle = 0$ (fluctuations about mean)

So

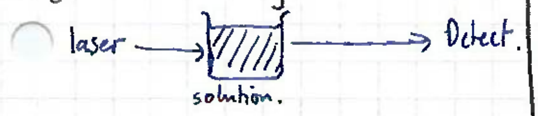


cf. 1st order coherence f'n:



A.P.L: Polarisation and Coherence Continued.

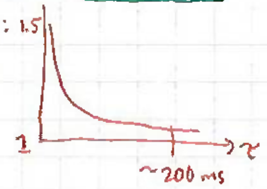
Light Scattering



Computer records : $n(1)$ $n(2)$ $n(3)$ $n(4)$....

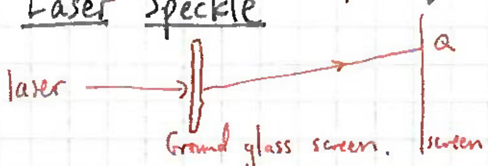
so eg. $\tau = 2$:

Compute $g_{12}^{(2)}$ get:



time delay corresponds to multiple scattering in solution.

Laser Speckle



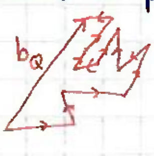
get speckled pattern ① not with atomic lamp pattern

② smaller laser spot → larger scale pattern

③ dark areas in pattern.

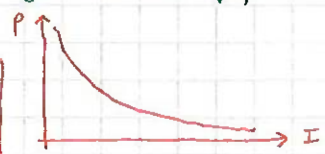
Model glass as array of scatterers. Each gives out light with random phase but (say) equal amplitude

So amplitude b at Q is random walk in phase space : $\Rightarrow P(b) \propto e^{-\frac{b^2}{s^2}}$ ($s \equiv$ no. of steps)



$\therefore P(I) \propto e^{-I/s^2}$

$\langle I \rangle = s^2 \Rightarrow \boxed{P = \frac{e^{-I/\langle I \rangle}}{\langle I \rangle}}$



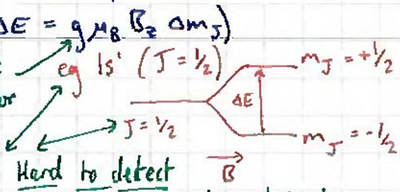
SPECTROSCOPY

Optical Pumping

Put atom in $\underline{B}$ → different m_J levels split (Zeeman Splitting)

$(\Delta E = g\mu_B B_z \Delta m_J)$

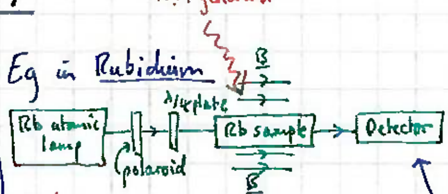
Lande g factor



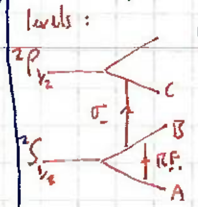
but Hard to detect as $\Delta E \ll kT$ ∴ get thermal background and coz relative occupancy is similar.

So: swamp with photon freq $\frac{\Delta E}{h}$ and observe secondary transition from upper state to a third level.

→ Eg in Rubidium

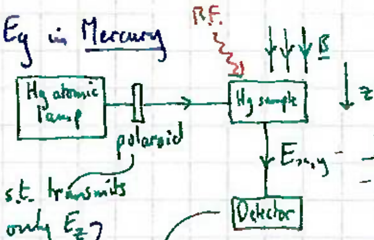


levels :



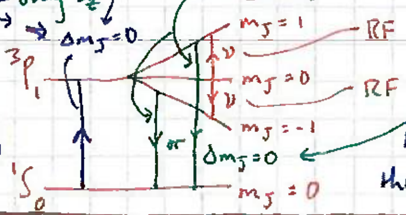
When RF. tuned s.t. B overpopulated, σ_- transition occurs so get drop in intensity at detector

Eg in Mercury



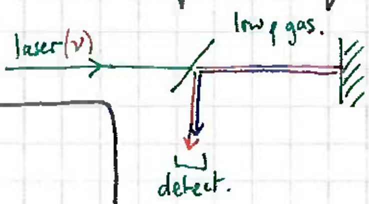
$E_{x,y}$ - ⊥ to z dir'n - in and out of page $\Rightarrow \Delta m_J = 0$

s.t. transmits only E_z $\Rightarrow \Delta m_J = 0$.



So: pump to $m_J = 0$, RF to $m_J = \pm 1$ then obs. green trans.

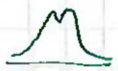
Lamb-dip technique



For atomic transition ν_0, will be excited in atom travelling at v by red stream if $\nu_{laser} = \nu_0(1+\frac{v}{c})$

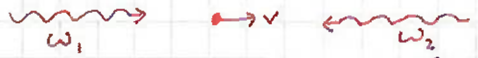
And blue beam will excite atoms travelling at $-v$: $\nu = \nu_0(1-\frac{v}{c})$

but for $v = 0$, ∃ only one set whereas for $v \neq 0$ ∃ two sets ∴ reduced ~~abs~~ absorption.

→  → Increased resolution.

2-photon Spectra

Another way to overcome Doppler problems.



atom sees energy $\hbar(\omega_1' + \omega_2') = \hbar\left[\omega_1\left(1-\frac{v}{c}\right) + \omega_2\left(1+\frac{v}{c}\right)\right]$

$= \hbar\left[(\omega_1+\omega_2) + \underbrace{(\omega_2-\omega_1)\frac{v}{c}}\right]$ (NB normal selection rules don't apply)

So make $\omega_1 = \omega_2$ so doppler cancels.

Rabi Oscillations

$n_a < n_b$ at thermal eq.

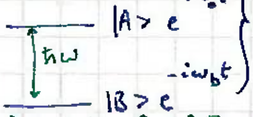
turn on laser at $\hbar\omega = E_a - E_b$

get $\underset{b}{\overset{a}{\uparrow\downarrow\uparrow\downarrow}}$ (abs then re-emitted)

get transient either $n_a > n_b$ or $n_a < n_b$ could occur

Collisions, spontaneous emissions return system to thermal equilibrium.

At time t :



where $|A\rangle, |B\rangle$ solve time indep S.E.

Perturbation $\hat{V} = \underline{p}.\underline{E}_0 \cos\omega t$

$(H_0 + V)(c_a|a\rangle + c_b|b\rangle) = i\hbar\frac{\partial}{\partial t}(c_a|a\rangle + c_b|b\rangle)$

If take $\langle a|$: $\langle a|V|a\rangle = 0$ coz parity

$\Rightarrow c_b\langle a|V|b\rangle = i\hbar\dot{c}_a$

If take $\langle b|$:

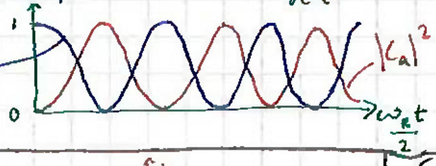
$\Rightarrow c_a\langle b|V|a\rangle = i\hbar\dot{c}_b$

$\langle B|\underline{p}.\underline{E}_0|A\rangle \frac{c_a}{2}\left[1 + \underbrace{e^{-2i\omega t}}\right] = i\hbar\dot{c}_b$ average over time → 0

same for $\langle A|\underline{p}.\underline{E}_0|B\rangle$

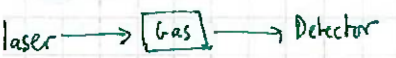
→ get SHM eq'ns for c_a and c_b with freq $\omega_R^2 = \left(\frac{|\langle A|\underline{p}.\underline{E}_0|B\rangle|}{\hbar}\right)^2$

Prob (finding e^- in state a or b) oscillates at ω_R.

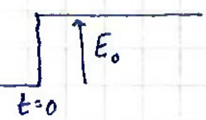


Symmetry between absorption and emission! ie absorb and emit: same way in presence of light field!

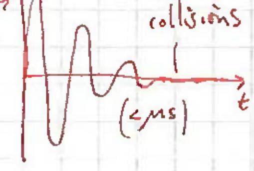
Transient Initial Absorption



Turn on electric field :



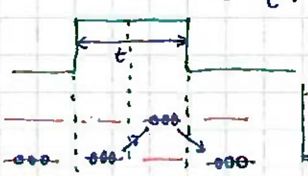
get :



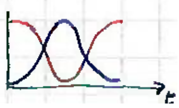
Self Induced transparency

light pulse:

t : $\omega_R t = 2\pi$



pump : bottom to top to bottom



A.P.L. Spectroscopy Continued.

Importance of Lasers in spectroscopy

(1) High spectral purity $\Delta\nu \sim 1\,MHz$

atomic lamp $\sim 1\,GHz$

(2) Highly collimated beam

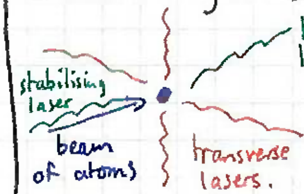
divergence $\sim 1/1000$ rad.

(atomic lamp $= 4\pi$ rad!)

(3) $E \sim 200\,V/m \Rightarrow \omega_R = 1\,MHz$

$\Rightarrow$ for $t < 10^{-6}s$ can create significant pop. inversion.

Laser cooling of atoms



a cool atom (~stat.) if absorbs photon will have photon

$\therefore \frac{(mv)^2}{2m} = \frac{3kT}{2}$

$\Rightarrow T \sim \mu K$

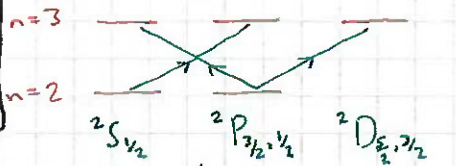
temperature measured using gravity trap: let atoms fall, measure arrival times.

Only atoms of certain speeds will be slowed but, for emergent beam $P(v) \propto v^3 e^{-v^2}$ (narrow...)

Precision Hydrogen Spectra

$E_n = -\frac{R}{n^2}$ measure $n=2 \rightarrow n=3$

- use Lamb dip for max resolution.



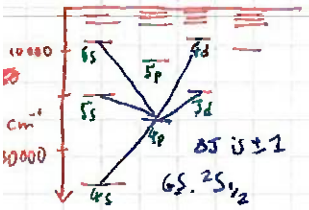
$\longrightarrow$ find that $J = 1/2, 3/2$ levels are seperate!

Lamb shift: In H, strongest for $n=2$ level: $^2S_{1/2}$ higher than $^2P_{1/2}$ by $\sim 9\,GHz$. - measure $n = 1 \rightarrow 2$ ($\lambda = 120\,nm$) and $n = 2 \rightarrow 4$ ($\lambda = 480\,nm$) using 2 photon spec.

Examples of Spectra

Alkali atoms: s^1 systems.

as $n\uparrow$, diff L states (s, p, d...) become more and more deg as pot approaches hydrogenic pot.



excited states: $^2P_{3/2,1/2}$ $^2D_{5/2,3/2}$

Nitrogen: p^3 system.

Ground state: $\uparrow\ \uparrow\ \uparrow$, $m_l = -1\ \ 0\ \ +1$

max spin $\rightarrow S = \frac{1}{2}+\frac{1}{2}+\frac{1}{2} = 3/2$ $\quad m_L = 0$

so GS: $^4S_{3/2}$

But if happen to get $\uparrow\ \uparrow\ \downarrow$

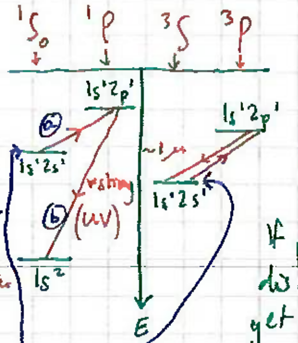
then GS is $^2S_{1/2}$

$\Rightarrow$ get 2 diff. sets of spectra (little changing between states) (L-S model good - N light!)

Helium

as with N, essentially 2 spectra - E1 cannot change spin so get $S=0$, $S=1$ sep. (In absence of spin-dep interactions...) For heavier atoms, L-S coupling is less good, $\Delta S = 0$ no longer true so see some triplet $\rightarrow$ singlet transitions.

Also, have metastable states



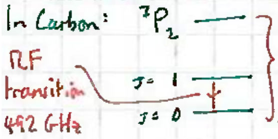
If put in (a) (IR ~2μm) get out (b).

If put He in elec. discharge, always get large proportion in metastable states.

(still lasers...) Methods of Operation

Fine Structure Transition.

$\Delta E_{\text{fine structure}}$ is a f'n of J



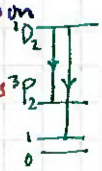
no parity change $\therefore$ mag dipole.

p^2 systems eg Carbon

$\exists$ $^1S_0$ $^1D_2$ $^3P_{210}$

plenty of strong trans'ns but $\exists$ weak ones: where $\Delta S \neq 0$!

$\Rightarrow$ $\boxed{\text{L-S model fails}}$

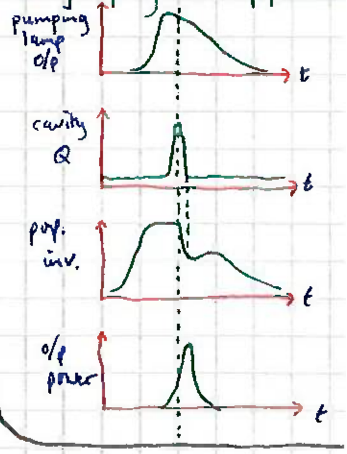


CW (Continuous Wave Laser o/p)

- Gaussian X-section (not plane wave!) E must reproduce itself.... Fraunhofer diffraction at each mirror = F.T. and FT (Gaussian) = Gaussian.
- balance pumping and o/p rates.

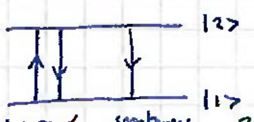
Q-Switched (pulse of power $\sim 10^8\,W$ for $\sim 50\,ns$) ~ 6 nuclear reactors.

- create v. large pop inversion with high loss cavity (so reducing stimulated emission) then suddenly increase Q of cavity...
- upper levels depopulate faster than pumping can repopulate.



LASERS

Einstein-Planck Analysis



stimulated emission and absorption (Rabi analysis)

For thermal eq., $\dot{N}_2 = -\dot{N}_1 = 0$.

Rate $1 \rightarrow 2$ (stim) is $\propto N_1 \rho(\omega) B_{12}$ (photon density)

Rate $2 \rightarrow 1$ (stim) $\propto N_2 \rho(\omega) B_{21}$

$\Rightarrow 0 = N_1 \rho B_{12} - N_2 \rho B_{21} - N_2 A$

Rate $2 \rightarrow$ (spon) $\propto N_2 A$

$\Rightarrow \rho(\omega) = \dfrac{A}{\frac{N_1}{N_2} B_{12} - B_{21}}$

but $\frac{N_2}{N_1} = \frac{g_2}{g_1} e^{-\hbar\omega/kT}$

compare $\rho(\omega)$ with B.B.R.

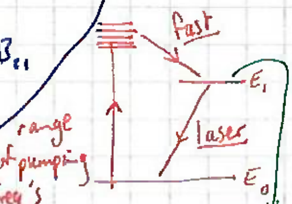
$\Rightarrow g_1 B_{12} = g_2 B_{21}$ and $\frac{A}{B} = \frac{\hbar\omega^3}{\pi^2 c^3}$ } Einstein Relations

Compare spon. rate / stim rate } for emission

find spon rate $\gg$ stim rate

Also, at room temp, $N_2 \ll N_1$

$\Rightarrow$ laser action not poss. if cavity in thermal eq. $\Rightarrow$ use PUMPING (optical i.e.



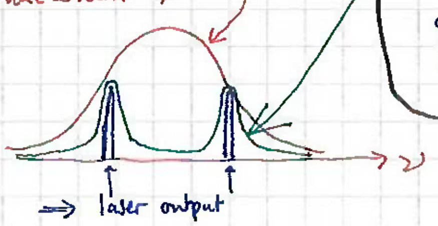
use feedback (F-P etalon) to give large power o/p

Beam Characteristics

Linewidth (axial modes)

Standing waves in F-P etalon produce $\nu_{cav.} = n\left(\frac{c}{2d}\right)$

but also $\exists$ atomic transition line width $\Rightarrow$



$\Delta\nu_{laser} \ll \Delta\nu_{cav}$ coz feed back! (Finesse!)

Homogenous limit: one frequency emitted (collision broadening)

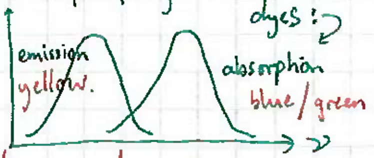
Inhomogeneous limit: > one frequency (mode) emitted (doppler broadening)

A.P.L. LASERS

Types of laser

Liquid dye lasers

use optical pumping: Characteristic of dyes:



liquid dyes good coz:
easy to make, homogeneous, density > gas, easily circulated thro' cav. for cooling
many levels ∴ can be tuned.

Doped-insulator lasers

eg YAG laser (Nd)
- energy levels that participate in lasing are due to Nd^{3+} ions.

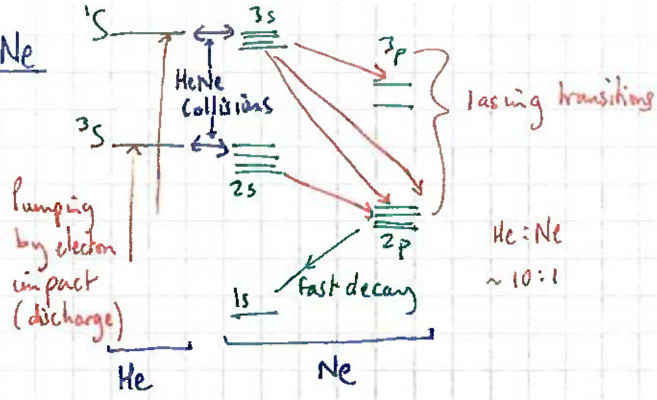
need to cool YAG rod with gas/water...

use optical pumping

Argon ion lasers

Argon atoms are ionised then pumped further....
$\lambda = 488nm$ and $514.5nm$.

HeNe

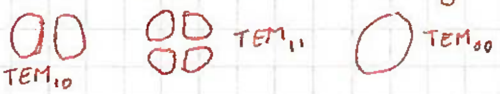


All 4 lasing transitions compete - select by mirrors reflect only one λ.

Semiconductor (Diode) laser

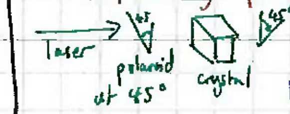
Transverse modes

F'n with FT = itself (as required by Fraun. diff) is product of Gaussian with Hermite polynomials. Modes labelled $TEM_{m,n}$
m, n vertical, horiz nodal lines. Eg:



Electro-optic modulation

- crystal whose ref. index changes anisotropically with applied $\underline{E}$ field → elliptically polarised light.



zero trans. when rel. phase change $= \pi$.

Acousto-optic modulation.

use Piezzo-Electric crystal to create pressure wave in another crystal which acts as a diffraction grating → Bragg condition.
(can think in terms of phonon - photon collisions: $\underbrace{\omega_i + \Omega = \omega_o}_{\text{energy}}$ $\underbrace{\underline{k_i} + \underline{k_\Omega} = \underline{k_o}}_{\text{crystal mom.}}$

⟹ Bragg condition.

Mode Locking

Diff. modes are usually out of phase. If all in phase, get pulses in time → mode locked.

$$E(t) = \sum_{n=1}^{N} E_o \exp i(\omega_n t + \delta_n) \longrightarrow \sum_n E_o e^{i(\omega_o t + n\Omega t)}$$

ω_n: nth mode; δ_n: random phase; where Ω = spacing between modes

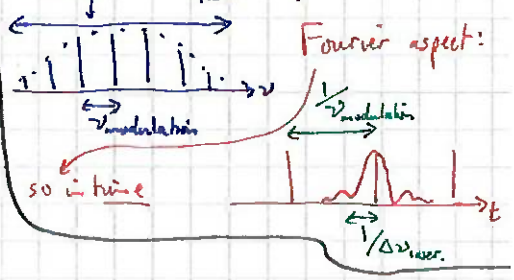
sum the GP

$$I \longrightarrow E_o^2 \frac{\sin^2(N\Omega t/2)}{\sin^2(\Omega t/2)}$$ system of pulses in time

When $\frac{\Omega t}{2} = p\pi$ $(p \in \mathbb{Z})$, $I = (E_o N)^2$ (peak height)

$\Omega = \omega_{modulation}$. $I = 0$ when $\frac{N\Omega t}{2} = \pi$ ie when $t = \frac{1}{N\nu_{modulation}}$

⟹ when $t = \frac{1}{\Delta\nu_{laser}}$ (ie bandwidth of laser)

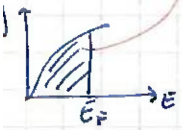


S.S: Free Electron Model

- valance electrons : Fermi Gas

$N = \int_0^\infty f(E)\, g(E)\, dE$

Particle in box gives $E^{1/2}$



$g(E) = \frac{3N}{2E_F}\left(\frac{E}{E_F}\right)^{1/2}$

Density of States

Fermi Wave vector

$k_F = \left(\frac{3\pi^2 N}{\Omega}\right)^{1/3}$

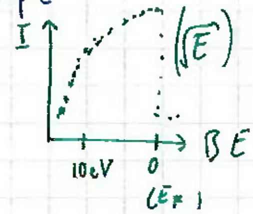
so $E_F = \frac{\hbar^2 k_F^2}{2m_e}$

Evidence for F.E.M.

XPS, UPS (X-ray / UV photoemission spectroscopy)

ie $\gamma \rightarrow$ sample $\rightarrow e^-$ KE of $e^- = \hbar\omega - \Phi$ - binding energy (w.r.t. Fermi level)

work f'n.



$\sqrt{E}$

Hall Effect

→ evidence for number of carriers per ion

Hall Coef $:= R_H = \frac{E_y}{j_x B_z} = \frac{1}{nq}$

Lorentz $F = q(E_y - v_x B)$

but prod. E field.

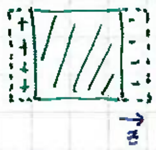
Steady state ⇒ $\boxed{F = 0}$

$(j_x = nqv_x)$

(small in metals (n large) big in semiconductors)

⇒ for some metals, no. of carriers $\underline{-ve}$ ∴ probs!

Energy loss Spectra (Plasmons)



$\omega_p^2 = \frac{ne^2}{\varepsilon_0 m}$

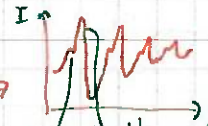
electron number density

from $E = \frac{ne}{\varepsilon_0}x$

⇒ SHM eq'n

Plasmons are actually quantised, $\boxed{E = n\hbar\omega_p}$

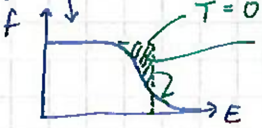
(fire) (put e^- through thin film)



surface plas. bulk e^- energy loss

Heat Capacity

$\langle E \rangle = \int_0^\infty f(E)\, g(E).E\, dE$ tricky so....



$T = 0$

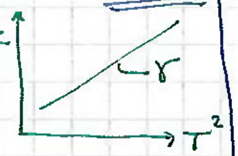
$E(T) \simeq E(0) + \underbrace{g(E_F)kT}_{\text{number with energy}} \times kT$

⇒ $C_e = \frac{\pi^2}{3} g(E_F) k^2 T$ (fancy prefactor)

re write with, get $C_e = \frac{\pi^2}{3} \frac{3Nk}{2} \underbrace{\frac{kT}{E_F}}_{\text{small}}$

expect from equipartition

$C_{tot} = \underbrace{\gamma T}_{e^-} + \underbrace{\alpha T^3}_{\text{phonons}}$ so $\frac{C}{T}$



(D.C.) Electrical Conductivity

Quick deriv: $j = n(-e)v$

In time τ, $v = \frac{-eE\tau}{m}$ ← N2L

QED

Mean free path for e^-

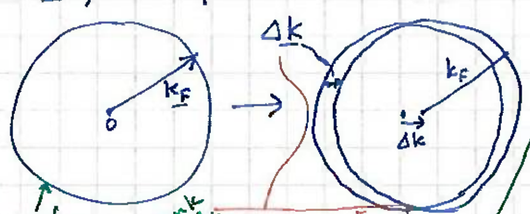
def'n: $\boxed{\lambda = v_F \tau}$

$\left[v_F = \frac{\hbar k_F}{m}\right]$

$$\boxed{j = \sigma E \quad \text{where } \sigma = \frac{1}{\rho} = \frac{ne^2\tau}{m}}$$

Relaxation time (prob of coll. $= \frac{1}{\tau}$)

In k-space: → no E, Fermi sphere : with E



Finite temp - surface is smeared out

meaning of wave packet

$\boxed{\Delta k = \frac{-eE\tau}{\hbar}}$

$\frac{d(\hbar k)}{dt} = -eE$

$\Delta v = \frac{\hbar \Delta k}{m} = \frac{-eE\tau}{m}$

so $j = n(-e)\Delta v$

Temperature Dependence of Elec. Conductivity

Assume e^-/phonon, e^-/defect collision rates are INDEPENDENT

⇒ $\frac{1}{\tau_{tot}} = \boxed{\frac{1}{\tau_{ph}}} + \frac{1}{\tau_{def}}$ ⇒ $\rho = \rho_{ph} + \rho_{def}$

temperature dependent

get linear

Wiedemann - Franz Ratio

$\frac{\text{Thermal Conductivity}}{\text{Electrical Conductivity}}$

Kinetic theory for gas of e^- ⇒ $K = \frac{1}{3}\lambda C_V v_F$

above $\sigma = \frac{ne^2\lambda}{mv_F}$

⇒ $\frac{K}{\sigma} = \underbrace{\frac{\pi^2 k_B^2}{3e^2}}_{\text{dependence on particular metal has cancelled.}} T$

is directly proportional to temperature (not at low temperatures though...)

SS: Nearly Free Electron Theorey.

S.E. with $\boxed{\text{periodic}}$ potential $V(\underline{r}+\underline{R}) = V(\underline{r})$

$\Rightarrow$ can expand as Fourier Series

$$\boxed{V(\underline{r}) = \sum_{\underline{G}} V(\underline{G}) e^{i\underline{G}\cdot\underline{r}}}$$

Primitive

$\underline{R} = n_1\underline{a}_1 + n_2\underline{a}_2 + n_3\underline{a}_3$

lattice translation vector

R.L. translation vectors:

$\underline{G} = m_1\underline{b}_1 + m_2\underline{b}_2 + m_3\underline{b}_3$

where $\underline{b}_1 = 2\pi \dfrac{\underline{a}_2 \times \underline{a}_3}{[\underline{a}_1, \underline{a}_2, \underline{a}_3]}$

Reciprocal Lattice

Why?

$\underline{G}\cdot\underline{R} = 2\pi n \quad \forall \underline{R}$

subst and find that these work.

$|\Phi(\underline{r}+\underline{R})|^2$ must $= |\Phi(\underline{r})|^2$ ie $\propto e^{if(\underline{R})}$

$f(\underline{R})$ is linear

Bloch's Theorem $\rightarrow$ $\boxed{\Phi(\underline{r}+\underline{R}) = e^{i\underline{k}\cdot\underline{R}}\,\Phi(\underline{r})}$

Change of Φ under trans $\leftrightarrow$ Wave vector of Φ

or

$\boxed{u_k(\underline{r}+\underline{R}) = u_k(\underline{r})}$ where $u_k = e^{-i\underline{k}\cdot\underline{r}}\,\Phi_k$

Φ_k is NOT an eigenstate of momentum $\boxed{\hbar\underline{k} \text{ is CRYSTAL MOMENTUM}}$

Eg

Nearly free electron model: Introduce $V = (\text{small})\, V_0 \cos\frac{2\pi x}{a}$ (1D)

V mixes free electron solutions. V weak $\therefore$ only similar energy wavef'ns also (Bloch) diff k states no mix so try as sol'n:

try $\Psi = Ae^{ikx} + Be^{-ikx}$ near degenerate points ie $\frac{\pi}{a}$

let $q = k - \frac{\pi}{a}$

solve, get deg. split $\rightarrow$ BAND GAPS

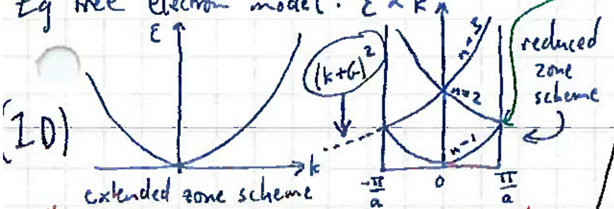
Band Structure: No difference if chose $\underline{k}$ or $\underline{k}+\underline{G}$ as $\underline{G}\cdot\underline{R} = 2\pi n$

So for each charge dist'n ($\underline{k}$) there are ∞ energies (?)

ie $\mathcal{E}(\underline{k})$ is cont. f'n of $\underline{k}$, $\exists\ \infty$ no. of states for each $\underline{k}$

$\Rightarrow$ state specified by n, k: $\Phi_{nk}(\underline{r})$

Eg free electron model: $\mathcal{E} \propto k^2$



Fill band $n=1$ means $2e^-$ per unit cell

" " $n=2$ " $4e^-$ " " "

etc

Filling the bands

(reciprocal space unit cell)

Volume of Brillouin Zone $\equiv [\underline{b}_1, \underline{b}_2, \underline{b}_3] = \dfrac{(2\pi)^3}{\Omega}$ see pg. 11

Pseudopotentials - need periodic V to be WEAK but it isn't near nuclei. Sol'n: write V for valence e^- only

then core electrons shield nuc. charge and weaken potential

Real: effective:

Conserving Energy and Crystal mom.

Momentum is conserved, by hard to calc

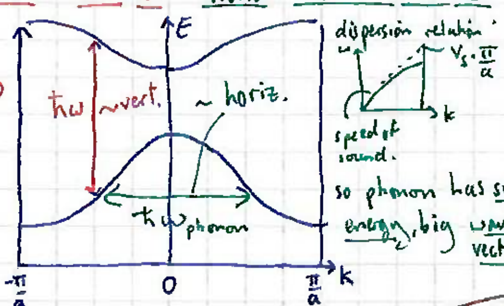
- use Chrystal mom of eg phonon or e^- state.

Conservation Law: $\sum_{\text{particle } i} \hbar \underline{k}_i = \sum_{\text{particle } f} \hbar \underline{k}_f + \hbar\underline{G}$

associated with periodic symmetry of Hamiltonian.

Photon collision with e^- Phonon collision with e^-

If have freq ω, $\rightarrow k = \frac{\omega}{c}$ $\therefore$ have small wavevector



so phonon has small energy, big wave vector

Electron Dynamics (now with periodic potential)

- effect of scattering from lattice is built into Bloch wavef'ns (const. interf.)

$\Rightarrow$ phonons / defects produces resistivity.

Current: think of wavepacket moving at group velocity v_{nk}

mean velocity of Bloch electron: $\boxed{v_{nk} = \dfrac{1}{\hbar}\dfrac{\partial \mathcal{E}_{nk}}{\partial \underline{k}}}$

eg Gaussian envelope

If $\Delta k \ll$ B.Z. in k space,

then $\Delta r \gg$ unit cell in real space

Semiclassical Model: external fields treated classically

internal field (ie effect of ions) is treated Q.M. (ie $\mathcal{E}_{nk}$, Ψ_{nk})

So $k(t)$, $r(t)$ given by: $\dot{\underline{r}} = \dfrac{1}{\hbar}\dfrac{\partial \mathcal{E}_{nk}}{\partial \underline{k}}$ and $\hbar\dfrac{d\underline{k}}{dt} = -e[\underline{E} + \underline{v}\times\underline{B}]$

$\Rightarrow \ddot{\underline{r}} = \underbrace{\dfrac{1}{\hbar^2}\dfrac{\partial^2 \mathcal{E}_{nk}}{\partial k^2}}_{\frac{1}{m^*}} \left(\hbar\dfrac{d\underline{k}}{dt}\right)$ force

acc'n. $\frac{1}{m^*}$ EFFECTIVE MASS

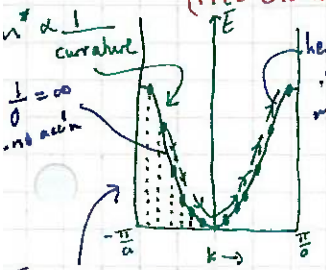
Electron feels ext force + force due to lattice. Latter is incorporated into the

Uniform Field

get:

$\hbar\dfrac{dk}{dt} = -eE \Rightarrow k(t) = k(0) - \dfrac{eEt}{\hbar}$

(Free Electron result)



here $m^* = -ve$ $\therefore$ electron moves back...

very hard to observe (need $T \sim 0$)

For insulator, e^- go out to right and re-enter from left - oscillate about fixed positions (Bloch-oscillations).

Holes Consider partially full band:

Current density: $\underline{j} = (-e)\,2\displaystyle\int_{\text{occupied states}} \underline{v}_k \frac{d\underline{k}}{(2\pi)^3}$ (2: spin degeneracy)

$= \underbrace{(-e)\,2\displaystyle\int_{\text{full band}} \underline{v}_k \frac{d\underline{k}}{(2\pi)^3}}\ -\ (-e)\,2\displaystyle\int_{\text{unoccupied states}} \underline{v}_k \frac{d\underline{k}}{(2\pi)^3}$ (holes)

gives zero as $\hbar k$, $-\hbar k$ have opposite group velocities.

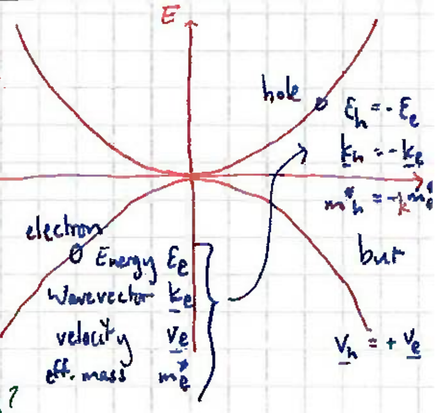
with effective charge $+e$

How do holes differ from electrons?

Eg: Charge: take e^- or add hole:

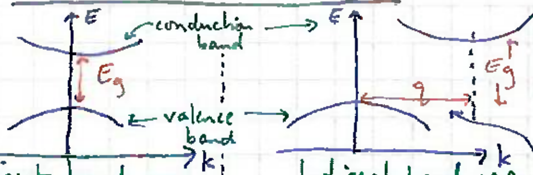
(full) $Q = \sum_{\text{full band}} -e - (-e)$ $\quad Q = \sum(-e) +$ hole charge

compare $\Rightarrow +e$



5.5 SEMICONDUCTORS

Basics

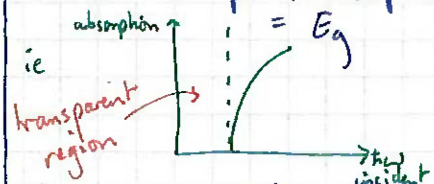


Direct band gap (eg GaAs)

Indirect band gap (eg Si)

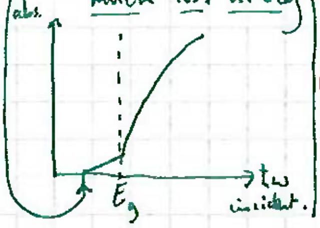
threshold for optical absorption: $\hbar\omega = E_g$

ie transparent region



$\hbar\omega = E_g - \hbar\omega_q$

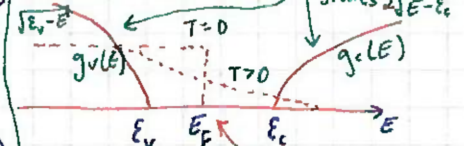
much less likely



Structure : Zinc Blende

: Tetrahedral

Thermal excitations



electrons in cond. band and holes in val " have effective masses m_e and m_h in density of states expression.

T > 0 : a few e^-, h are put into val, cond bands.

For non-doped semicond's : $\boxed{n = p}$ ⇒ determines E_F

$n = \int_{-\infty}^{\infty} g_c(E) f(E)\, dE$ approximate for $\boxed{E - E_F \gg kT}$

$= 2 n_Q^e e^{(E_F - E_c)/kT}$ with e^- eff mass

$p = \int g_v(E)(1 - f(E))\, dE$

$= 2 n_Q^h e^{(E_v - E_F)/kT}$

ie E_F is well away from band edges

⇒ E_F lies (T=0) in middle of band gap, E_g : write $n = p(E_g)$

$n = p = 2\left(\frac{kT}{2\pi\hbar^2}\right)^{3/2} (m_e m_h)^{3/4} e^{-E_g/kT}$

Intrinsic carrier concentration $n = p = \boxed{n_i}$

" non-degenerate semiconductor "

Doping

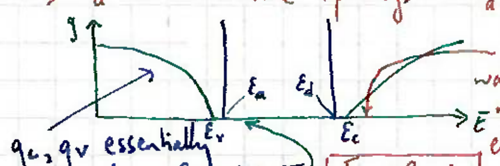
Donor : adds electron

Acceptor : adds hole

lowest energy level is that of swollen hydrogenic orbital (Coulomb pot. reduced by polarisation of lattice)

Bohr rad : $a_d = \frac{4\pi\varepsilon\varepsilon_0\hbar}{m_e e^2}$ $\boxed{\text{BOUND ORBIT!}}$ $m_e \sim 0.067\, m_{electron}$

⇒ $a_d \sim 20$ lattice spacings ⇒ E_d reduced.



If E_d here, wavef'n extended, not bound and electron can conduct.

g_c, g_v essentially unchanged as Group III, V atoms similar to Group IV

$\boxed{E_d = E_c - E_d}$ binding (ionisation) energy.

Occupancy of donor energy level : Grand canonical ensemble but let coulomb repulsion = ∞ to prevent double occupancy (so allowed numbers are 0, 1 spin up, 1 spin down)

$f_d = \frac{1}{\frac{1}{2} e^{(E_d - E_F)/kT} + 1}$

If conduction band edge is degenerate get $\frac{1}{2} \to \frac{1}{\text{deg.}}$

If this true then $np = n_i^2 = \text{const}$ as indep. of E_F ! (only f'n of E_g)

Impurities alter pos'n of Fermi level so this is invalid now (E_F is not in middle of b. g....)

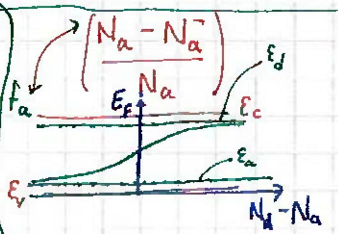
n and p are in chemical equilibrium (Law of mass action) so if n↑, p↓ etc.

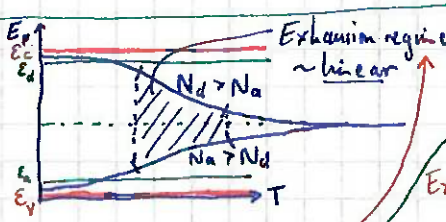
Add donors, increase (n+p) minimum at n=p (non doped) (decreasing n+p ≡ compensation)

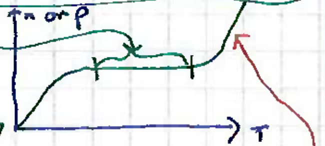
So where is Fermi level ? Can find from 5 sim eq'ns:

(1) $n(E_F)$ (2) $p(E_F)$ (3) f_d (4) f_a and (5) charge conservation

N_d donor atoms, N_d^+ are ionised. $N_d^+ - N_a^- + p - n = 0$







Excitation across main band gap (intrinsic)

$n_{intrinsic} \gg n_{impurities}$ so $\boxed{n_1 + n_2 \simeq n_1}$ (n_1) (n_2)

Exhaustion regime ~all donors ionised but prob of intrinsic excitation is small.

Let $N_d > N_a$. At T=0, N_a of the N_d donor electrons are in acceptor levels. E_F far below E_d (so $E_d - E_F \gg kT$)

so all available electrons in the donor levels are ionised.

⇒ $n = N_d - N_a$

⇒ $p = \frac{n_i^2}{N_d - N_a}$

(For $N_a > N_d$, $p = N_a - N_d$)

For $N_d \gg N_a$ $E_F = E_c - kT \ln\left(\frac{2 n_Q^e}{N_d}\right)$

For $N_a \gg N_d$ $E_F = E_v + kT \ln\left(\frac{2 n_Q^h}{N_a}\right)$

From ...

Carrier Dynamics In Semiconductors

Carrier Mobility

$\mu = \frac{|v|}{|E|}$ ← drift velocity for n type

$\mu_e \neq \mu_h$

σ varies like this...

Can write $\mu_e = \frac{e\tau_e}{m_e}$, $\mu_h = \frac{e\tau_h}{m_h}$ and $\boxed{\sigma = ne\mu_e + pe\mu_h}$

scattering times, τ_e, τ_h are f'n(T) $\frac{1}{\tau_{tot}} = \frac{1}{\tau_{ph}} + \frac{1}{\tau_i}$

how scatter? with Phonons + ionised impurities

Steady state ⇒ j = 0 and we know n, p because $E_c(r) = E_c - eV(r)$ and $E_v(r) = E_v - eV(r)$

Einstein Relations

If elec/hole conc's f(pos'n), get diffusion so:

$j_e = \underbrace{e\mu_e n(r) E(r)}_{\sigma} + \underbrace{eD_n \nabla n(r)}_{\text{diff. term}}$

and $j_h = e\mu_h p(r) - eD_p \nabla p(r)$

⇒ $\boxed{\mu_e = \frac{eD_n}{kT}}$

$\boxed{\mu_h = \frac{eD_p}{kT}}$

Carrier Generation and Recombination.

eg excite e^- across band gap with photon. (Hits a hole)

excess carrier conc = $n - n_{eq}$ (= $n - n_0$)

Simplest approx : $\frac{dn}{dt} = -\frac{(n - n_0)}{\tau_n}$ OK if $n \ll p$ so p const if no competing process.

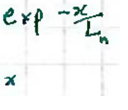
Another possibility : inject electrons into p-type where $j \simeq j_{diffusion}$

$\frac{d}{dt}\int_V n\, dV = \frac{1}{e}\int_S \underline{j} \cdot d\underline{S} - \int \frac{n - n_0}{\tau_n} dV$ ⇒ $\frac{\partial n}{\partial t} = D_n \nabla^2 n - \left(\frac{n - n_0}{\tau_n}\right)$

but $j = eD_n \nabla n$ ∴ use divergence theorem

solution in 1-D where $n - n_0 = C$ at $x = 0$, get $n - n_0 = C\exp\left(-\frac{x}{L_n}\right)$

$L_n = \sqrt{D_n \tau_n}$ (diff. length)

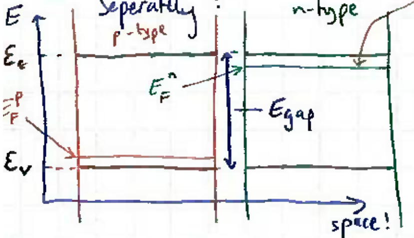


S.S.: DEVCIES!

p-n junction

Bring together p, n regions:

Separately:



for p > n, majority carrier conc's

electrons flow from n-type to p type to lower their energy

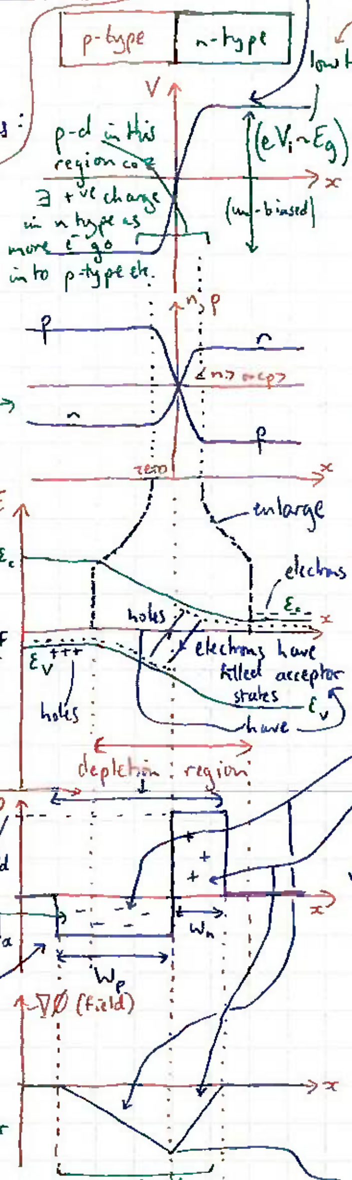
→ electrostatic dipole layer

→ potential difference

→ electric field pushing electrons back!

same for holes...

→ equalises Fermi level on the two sides



$W_p \neq W_n$ - depends on charge density in p, n regions so depletion region is now not centred on x = 0

e⁻ have hopped over from right

sharp edges: Depletion Approx

Linear dependence in the depletion region? to do with Fermi level:

Say $eV_i = E_F^n - E_F^p$

$= \varepsilon_c - kT\ln\left(\frac{2n_Q^e}{N_d}\right) - \varepsilon_v - kT\ln\left(\frac{2n_Q^h}{N_a}\right)$

Important eq'ns:
$n = 2n_Q^e e^{(E_F-\varepsilon_c)/kT}$
$p = 2n_Q^h e^{(\varepsilon_v - E_F)/kT}$

$$\boxed{= E_g - kT\ln\left(\frac{N_c P_v}{N_d N_a}\right)}$$

linear dep on T
$(N_c = 2n_Q^e,\ P_v = 2n_Q^h)$

Applying a Bias

Apply pot-diff across junction: (V)

$V_T = \phi(x=\infty) - \phi(x=-\infty) = V_i - V$ — so +ve V reduces V_T - forward bias; -ve V increases V_T - reverse bias.

Conductivity of depletion region is very low ⟹ ~all of V_T is across depletion region.

To get $\phi(x)$ from $\rho(x)$ (charge distribution) solve poisson's eq'n: $\boxed{\nabla^2\phi(x) = -\frac{\rho(x)}{\varepsilon\varepsilon_0}}$

$\phi(x) = \phi(x=-\infty)$ for $x < -W_p$

$= \phi(x=\infty)$ for $x > W_n$

$= \phi(x=-\infty) + \frac{eN_a}{2\varepsilon\varepsilon_0}(x+W_p)^2$ for $-W_p < x < 0$

$= \phi(x=+\infty) - \frac{eN_d}{2\varepsilon\varepsilon_0}(x-W_n)^2$ for $0 < x < W_n$

These determine widths W_p, W_n if use the: Charge Neutrality Condition $\boxed{N_a W_p = N_d W_n}$

→ $W_n = \sqrt{\frac{2\varepsilon\varepsilon_0 V_T}{e}\left(\frac{N_a}{N_d(N_d+N_a)}\right)}$ (swap $N_a \leftrightarrow N_d$ for W_p)

total width $= W_n + W_p$

Differential Capacitance $C = \frac{dQ}{dV_T} = \frac{d}{dV_T}\{eN_dW_n\}$ (or eN_aW_p) $= \sqrt{\frac{\varepsilon\varepsilon_0 e}{2V_T}\left(\frac{N_aN_d}{N_a+N_d}\right)}$ dep on V_i

Forward bias decreases magnitude of p-d

Reverse bias increases magnitude of pot-diff.

Current Flow:

p-n junction is potential barrier to the majority carriers but a potential door to the minority carriers!

In depletion approx ∃ no carriers in dep. region (ie low prob of recombination....)

high field so drift currents are saturated ~ indep of field ($v_d = \mu_e \frac{d\phi}{dx} \simeq$ const)

Current densities: sum of drift and diffusion terms:

$j_e(x) = -e\mu_e n\frac{d\phi}{dx} + eD_n\frac{dn}{dx} = 0$

$j_h(x) = -e\mu_h p\frac{d\phi}{dx} - eD_p\frac{dp}{dx} = 0$

for zero bias voltage

$\frac{dn}{dx}, \frac{dp}{dx}$ strongly dep on bias

$n(x) = 2n_Q^e e^{(E_F - \varepsilon_c + e\phi(x))/kT}$ $\quad p(x) = 2n_Q^h e^{(\varepsilon_v - e\phi(x) - E_F)/kT}$

not strictly valid when have bias.... only if $j_e = j_h$ and $j_e \simeq j_h$ only.

reverse arg for E-rels - requires $j_e = j_h$.

Now: $j_e(x) = eD_n\frac{d}{dx}\Delta n$ — Δn is excess carrier conc $= n(x) - n(-\infty)$, p-type

diffusion current due to excess electrons in p-type...

$= c.e^{(x+W_p)/L_n}$ (see prev. sheet)

But what is c? $c = n(-W_p) - n(-\infty)$

electrons injected into p-type from n-type

say $n(W_n) \simeq n(\infty)$

know $n(-W_p) = n(W_n)e^{-e(V_i-V)/kT}$

away from p-n junction n, p unaffected by bias ⟹ $\frac{n(\infty)}{n(-\infty)} = e^{eV_i/kT}$

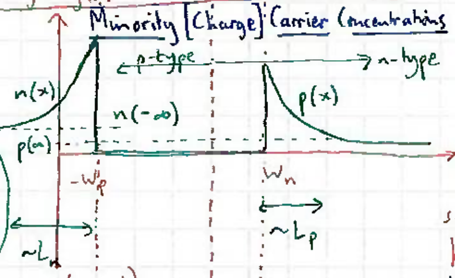
Reality: generation + recomb of holes, elec does happen in depletion region - often dominates in this region.

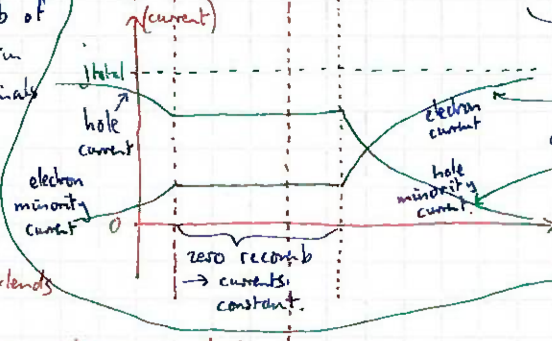
Breakdown: via

1) Zener: QM tunneling through barrier - not over.

2) Punch thro' - dep region extends to contacts

3) Avalanche: field so large in dep region that





$\Rightarrow j_e(x) = \frac{eD_n}{L_n}n(-\infty)\left(e^{eV/kT}-1\right)e^{(x+W_p)/L_n}$ (for $x < -W_p$)

and $j_h(x) = \frac{eD_p}{L_p}p(\infty)\left(e^{eV/kT}-1\right)e^{-(x-W_n)/L_p}$ (for $x > W_n$)

Total current $= j_e(-W_p) + j_h(W_n)$

$$\boxed{j_{tot} = \left(\frac{eD_n}{L_n}n(-\infty) + \frac{eD_p}{L_p}p(\infty)\right)\left(e^{\frac{eV}{kT}} - 1\right)}$$

dep on V, not x!

Nuclear Physics : Basic Nuclear Properties

mass $\sim 1000\, m_{e^-}$ size $\sim 1\,\text{fm}$ (at least $1000\, r_{e^-}$)

NUCLEUS

Proton mass $\times c^2 = 938$ MeV
Neutron mass $\times c^2 = 939.6$ MeV

$\boxed{\text{nuc mass} = Zm_p + Nm_n - B}$

lose energy on formation...

Binding Energy, B: Energy required to split nuc. up into its nucleons.

Measuring B:
① Mass spectrometer – know mass, get B
② Neutron capture on protons: $n + p \to d^* \to d + \gamma$ – measure γ energy, get B

$B_{\text{deuteron}} = 2.2$ MeV

SPIN (they have it)

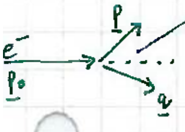
PARITY $PY_{lm} = (-1)^l Y_{lm}$

Stability: $Z \sim N$ – not as $Z\uparrow$ coz COULOMB.

Sizes / Shapes

Scatter electrons off nuclei (measure e^- energy + angle)

First Born approx
$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{Z^2 e^4 F^2(q^2)}{4p_0^2 \sin^4(\theta/2)}$$



$q = p_0 - p$

if include e^- spin, get extra $\cos^2\frac{\theta}{2}$ term.... Dirac...

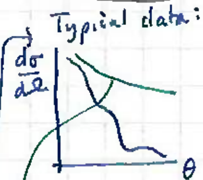
Form factor contains info about nuc. size
$$F(q^2) = \int_0^\infty \rho(r,\theta,\phi)\, e^{i\underline{q}\cdot\underline{r}}\, d^3\underline{r}$$

if nucleus spherically symmetric then
$$F(q^2) = \int_{\text{all space}} \rho(r) \frac{\sin qr}{qr}\, d^3\underline{r}$$
$$\Rightarrow \rho(r) = \frac{1}{2\pi^2}\int F \frac{\sin qr}{qr} q^2\, dq$$

so can get info about $\rho(r)$

(Sizes)

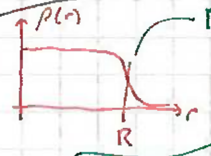
Typical data:



for point nuc, $F = 1$ – model fails.

1 parameter fit eg uniform, Gaussian also fails....

2 param. OK: eg $\rho(r) = \dfrac{\rho(0)}{1 + e^{(r-R)/a}}$



$R \sim 1.3 A^{1/3}$ fm

How to determine R:

Bring μ^- to rest in matter – captured into Bohr orbits, energy $\propto \frac{1}{n^2}$ → decay to lower energy levels, emitting X-rays → measure Xray energies, get R.

(Shapes)

Shape: contours of constant charge density

Parametrise shape with [elec] multipole expansion (compare G.F. expanded with axisym. gen. sol. of Laplace)

$E0 = \int \rho(\underline{r})\, d^3\underline{r}$ (charge, q)

$E1 = \int \rho(\underline{r})\, z\, d^3\underline{r}$ (dipole mom.)

$\boxed{\text{nuc}: E1 = 0}$

$= 0$ coz $\rho(\underline{r}) = |\psi|^2$ but $|\psi(\underline{r})|^2 = |\psi(-\underline{r})|^2$ (parity) ⇒ odd integrand ie no nucleus has a dipole moment.

$E2 = \frac{1}{e}\int \rho(\underline{r})(3z^2 - r^2)\, d^3\underline{r} = Q$ – quadrupole moment. (dimension = area)

Spherical symm ⇒ $Q = 0$

For spin zero nuclei, $\langle Q \rangle_t = 0$ but not Q inst.

Q +ve, prolate spheroid. Q −ve, oblate spheroid.

also use ellipticity, $\eta = \frac{b-a}{\frac{1}{2}(b+a)} \lesssim 10\%$, typically...)

Measuring Q:

Pot. energy of quadrupole $\Phi \propto Q \frac{\partial E}{\partial z} \left(= \frac{\partial^2 V}{\partial z^2}\right)$

apply $\underline{B}$ to molecule → Zeeman splitting $(2J+1)$ levels (J = nuc + elec.)

If due to e^- has big $\underline{V}$ at nuc ∴ $Q = 0$, levels equally split

$Q \neq 0$ levels unequally split. From splitting → Q.

Multipole expansion of $\underline{A}$ → Magnetic dipole moment: not get expected result ⇒ ∃ quarks and s–o coupling.... (more later)

related topic: N.M.R. need nuc with mag mom (ie no spin 0 nuclei eg ^{12}C)

dipole in steady $\underline{B}$ precesses at Larmour freq....

apply B_{rf} at right angles changing at ω_L → get peak absorption of energy coz resonance

Radioactivity

α decay: occurs for $A \geq 210$ tunnelling....

β decay: electron occurs $\forall Z$ cons. energy ⇒ ∃ neutrino!

γ decay: photon ~MeV transition, λ = pm cf atomic, 10eV, nm → μm

picometres

(more later.)

$N(t) = N(0)e^{-\lambda t}$ λ = prob per sec

$\lambda_{tot} = \lambda_1 + \lambda_2 ....$ for > 1 decay mode

or $\dfrac{1}{\tau_{tot}} = \dfrac{1}{\tau_1} + \dfrac{1}{\tau_2} + ...$

Measuring λ:

If $\frac{1}{\lambda} \sim$ mins / hours – count!

If $\frac{1}{\lambda}$ v. long use "specific activity" ie let rate $= N\lambda$, get N by mass spec or chemistry.

If $\frac{1}{\lambda} \sim$ secs, millisecs... use electronic counter – multichannel analyser.

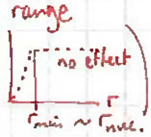
If $\frac{1}{\lambda} \sim 10^{-3} \to 10^{-11}$ s... use "delayed coincidence": start clock when form the nucleus then stop when detect the decay – do many times.

If $\lambda^{-1} \lesssim 10^{-11}$ s... measure widths of emission lines, use uncertainty principle.

The Nucleon-Nucleon Force

Tricky situation: strong ∴ cannot use P.T. Quarks don't behave as if independent or if bound to form protons etc } forget it at the quark level

and have very short range (from scattering data) but need to know more:



So to a 1st approx, say: nucleus is protons + neutrons
) nucleons are sometimes excited
) " " correlated
) force is dominated by π-meson exchange

Start with force between 2 nucleons: only stable combination is np, – The Deuteron. SE is
$$\left(\frac{-\hbar^2}{2\mu}\nabla^2 + V\right)\psi = E\psi \text{ in stationary state}$$

V must be deep (Binding energy = 2.2 MeV)

Geometric interpretation of a:
$$\lim_{k\to 0}(r\psi) = r - a$$

$\boxed{\begin{array}{l} -^{ve}\, a \Rightarrow \text{unbound state} \\ +^{ve}\, a \Rightarrow \text{bound state} \end{array}}$

Proof:

Neutron – Proton Scattering

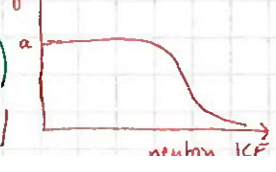
Slow neutrons (< 1eV) ∴ use Partial Wave analysis – s waves only ($l = 0$)
$$\Rightarrow \lim_{r\to\infty} \psi = e^{ikz} + f_0 \frac{e^{ikr}}{r}$$

where $f_0 = \dfrac{e^{i\delta_0}\sin\delta_0}{k}$ (scattering amplitude)

$\boxed{\lim_{k\to 0} f_0 = f_0 = a}$ Scattering Length

$\dfrac{d\sigma}{d\Omega} = |f_0|^2$ ∴ $\lim_{k\to 0} \sigma = 4\pi a^2$

Constant σ at low energy:

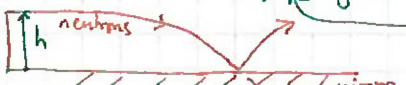


Nuclear Physics — Nucleon-Nucleon Force (Continued)

How measure scattering length (a)?

not liq. hydrogen coz a -ve – need TIR – fill up all space with liquid H etc!

Bounce neutrons off liquid hydrocarbon mirror. – coz surface imperfections in solid



For $h < h_0$, neutrons bounce off (Total External Reflection)

For $h > h_0$, some transmission occurs.

$$\boxed{h_0 = \frac{2\pi\hbar^2 Na}{gm^2}}$$

Grazing angle of incidence:

ϕ $(n=1)$ $\cos\phi = \sin\theta_c = n$

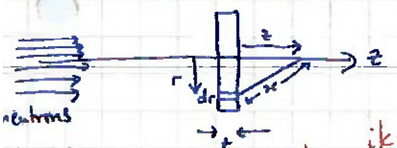
$n<1$

$\therefore \boxed{n \simeq 1 - \frac{\phi^2}{2}}$

and $\boxed{n - 1 = \frac{-2\pi Na}{k^2}}$ $\Rightarrow k\phi_0 = 2\sqrt{\pi Na}$

wiig: $p_\perp = \hbar k \phi_0$ (small angle) $= mv_\perp$

Place thin slab in slow neutron beam



(N nuclei per m³)

Amplitude at z, $A(z) = e^{ikz} - (Nt)a\int_{area} \frac{e^{ikx}}{x}\, d(\text{Area})$

$d(\text{Area}) = r\,dr\,d\theta$ but $r\,dr = x\,dx$ for given z

$$\Rightarrow \boxed{A(z) = e^{ikz}\left(1 - \frac{2\pi i a N t}{k}\right)}$$

Or: Say $A(z) = e^{ik(z-t)} \cdot e^{ik't}$ where $k' = \frac{\omega}{c'} = \frac{\omega}{c}\cdot\frac{c}{c'} = kn$

expand exponential for thin slab

$$\Rightarrow \boxed{A(z) = e^{ikz}\left(1 + ik(n-1)t\right)}$$

then equate A(z)

← here, have omitted **SPIN**:

deuteron can be in singlet or triplet state (giving scattering lengths: → a_s, a_t)

For coherent scattering off bound protons, $a = 2\left(\frac{a_s}{4} + \frac{3a_t}{4}\right)$

(coz protons no more)

(3 triplet states, 1 singlet state)

→ find $a = -4$ fm but separating a_s, a_t?

need neutrons with E low enough s.t. S-waves, but high enough for incoherent scattering so that $a^2 = \frac{a_s^2}{4} + \frac{3a_t^2}{4}$

→ $a_s \simeq -24$ fm, $a_t \simeq 5$ fm

almost (but not) bound — bound.

So: Nuclear force is spin dependent

Proton-Proton Elastic Scattering

Identical Particles ⇒ can only have ^1S, ^3P, ^1D, ^3F...

Find: $\boxed{a_s^{pp} = -17 \quad a_s^{np} = -24}$ } So: nuclear force is charge dependent

but we can understand this: p, n exchange pions.

eq'n of motion for pion is K-G eq'n. Solve in static limit, get Yukawa Potential $U(r) = g\frac{\exp[-r/\hbar m c]}{r}$ (coupling constant ↗ g)

look at spatial averages: $\frac{\langle U_{np}\rangle - \langle U_{pp}\rangle}{\frac{1}{2}(\langle U_{np}\rangle + \langle U_{pp}\rangle)} \simeq 2\%$

Difference comes from: ① n, p mass diff ② diff mag moments ③ pion mass differences

Charge Symmetry

ie is a_s^{nn} diff. from a_s^{pp}? (→ not very...)

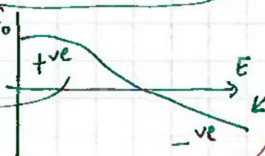
get $a_s^{nn} = -16$, $a_s^{pp} = -17$ } approximately coz a_s^{nn} hard to measure.

$\pi^- + d \to n + n + \gamma$ so whack d with π^- and measure γ spectrum.

Nucleon-Nucleon Potential

Large r: attractive Small r: repulsive

from δ_0 (phase shifts:)



long range attraction

One pion exchange pot. ↔ Yukawa

(As r↓, exchange more bosons) so pot gets complicated

Fit parameters to data → potentials:

eg Hamada-Johnson

- Hard core
- Deep
- narrow
- < 1 fm

∃ many problems with the "Potential" Idea:

- r not rel. invariant.
- spin dependence?
- spin-orbit force ⇒ vel. dep!

But at least the following features must be included:

Tensor Force:

non-central potential – would imply that $\mu_D \neq \mu_p + \mu_n$

and it's true! ∴ ∃ tensor force or $\mu_{p,n}$ change on binding.

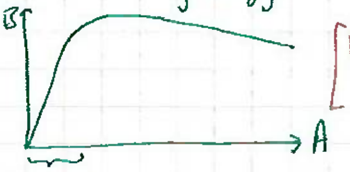
Relativistic Effects.

Nuclear Physics — Elementary Nuclear Models

Liquid Drop Model

Binding energy $B = \underbrace{Z m_p}_{\text{protons}} + \underbrace{N m_n}_{\text{neutrons}} - m(A,Z)$

Plot Binding energy:



$\exists$ peaks at $A = 4 \times$ integer (α particle)

[If nucleon binds to neighbour only, get $B \propto A$.]

$$B = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(N-Z)^2}{A} \pm \delta(A)$$

surface energy — not δ f'n!

Coulomb repulsion in sphere of radius $A^{1/3}$

assymetry term — nuclei with equal numbers of neutrons/p. are more stable.

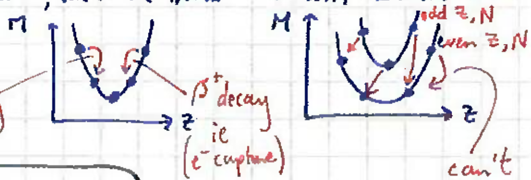
Pairing energy [only non-zero in [odd-odd / even-even] nuclei]

Predicts well:
- const density of nuclei.
- Binding energy
- limits on Z, N
- β decay!

$$M(Z,A) = ZM_H + m_n(A-Z) - a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_a \frac{(A-2Z)^2}{A} \pm \delta$$

(Semi-Empirical Mass Formula)

Plot as f'n of Z: Odd A, one stable isobar. Even A, >1 stable isobar



β^- decay; β^+ decay ie (e^- capture); can't happen!

Nuclear Shell Model

Problem with liq drop: cannot explain properties which dep on specific N and Z.

$\therefore$ Solve S.E. with central potential $\longrightarrow$ shells with Q.N. $\underline{L}$

As with atoms, $\exists$ magic numbers (closed shells)

Simple potentials don't give these $\Im$ … need SPIN-ORBIT COUPLING.

$\Rightarrow$ $j = l - \frac{1}{2}$, $j = l + \frac{1}{2}$ ($V_{central}$, V_{so}) $\longrightarrow$ gives magic numbers: 2, 8, 20, 28, 50, 82, 126.

$\Rightarrow$ even-even nuclei have $J^P = 0^+$

even-odd have that of odd nucleon.

Works O.K. except: away from closed shells when nucleus is deformed (non-central pot.)

Schmidt Limits (Magnetic moment of nucleus)

$\hat{\mu}_s$ (due to spin) $= g_s \hat{\underline{S}}$

$\hat{\mu}_L$ (due to orb.) $= g_L \hat{\underline{L}}$

$\hat{\mu}_{tot} = g \hat{\underline{J}}$ where $g = \left(g_L \underline{L}\cdot\underline{J} + g_s \underline{S}\cdot\underline{J}\right)\frac{\underline{J}}{|\underline{J}|}$ unit

take expectation values use $J = L \pm \frac{1}{2}$, get:

For $J = L + \frac{1}{2}$: $\boxed{g = g_L + \frac{g_s - g_L}{2L+1}}$ For $J = L - \frac{1}{2}$: $\boxed{g = g_L - \frac{g_s - g_L}{2L+1}}$

measured g falls between these limits.

problems: – have used free particle g_s, g_L
– no work away from closed shells.

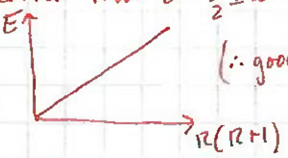
The Collective Rotational Model

As molecules have rot + elec states, nuc has rot + "intrinsic" states.

Firstly, even-even nuclei: $J = 0$ $\therefore$ spherical ie Quadrupole moment $= 0$ when at rest. Mom of inertia due to deformation; surface wave travelling around.

Say I = mom of inertia then $E = \frac{1}{2} I \omega^2 \Rightarrow E = \frac{\hbar^2 R(R+1)}{2I}$ (where R is e-value of $\hat{L}$)

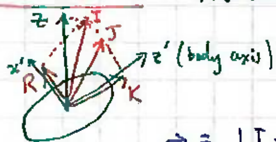
Observed eg Hf: ($\therefore$ good!)



Secondly, odd A nuclei:

Now, total angular momentum $= \underline{I} = \underline{J} + \underline{R}$

M is z axis proj of I



$R \perp$ to z' coz axisymm – only get phase change when rotate which is unobservable $\therefore R_{\parallel} = 0$.

$$H_{rot} = \frac{|R|^2}{2I_n} = \frac{|I - J|^2}{2I_n}, \quad |I-J|^2 = |I|^2 + |J|^2 - 2K^2 - (I'_+ J'_- + I'_- J'_+)$$

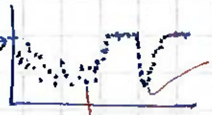
raising / lowering ops w.r.t. to body axes

these couple rot / intrinsic equiv to Born-Op approx – let $= 0$

Then $E_{rot} = \frac{\hbar^2}{2I_n}\left[I(I+1) + \underbrace{J(J+1)}_{} + K^2\right]$ constant for given intrinsic state.

$\rightarrow$ get graph like this

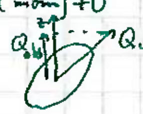
$\frac{E_2}{E_1}$ should $= 3\frac{1}{3}$: get



lead doubly magic – spher

126 – magic number

[For $J \neq 0$, Q (quad mom) $\neq 0$ but:



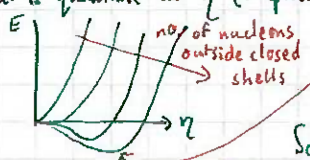
$Q_{obs} = F(J) Q_{int}$.]

More Sophisticated Models.

Problem: liq drop $\Rightarrow$ sphere is most stable, but $\exists$ nuc with non zero Q (quad. moment) ….? Solution:

Rainwater (1950): Combine Liquid Drop model with shell model to get:

Deformed Shell Model – Use ellipsoidal potential. get ΔE (from nuc.shell) that is quadratic in η (ellipticity)

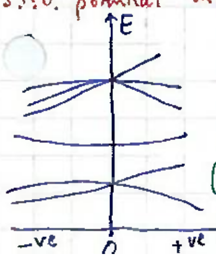


deformed ground state. Nucleons outside closed shells POLARISE THE CORE.

(But now predicted Q > expt (< expt before))

So: $\boxed{\text{Nilsson (1955)}}$

$\rightarrow$ S.H.O. potential deformed along one axis (+ spin orbit coupling) $\Rightarrow$ E is f'n of δ ($\sim\eta$)



For $\delta = 0$, get usual nuc. shell model levels. Levels split into $(2J+1)$ levels (each 2 fold deg in M_J.)

$\boxed{\text{Inglis (1956)}}$ Cranking Model: Calc nuc shell regime but in a rotating ellipsoidal pot.
– need to include nucleon-nucleon interactions (eg pairing)

Results:
- Density variations within nucleus
- Detailed description of rot. states
- Vibrational (dip, quad etc) states

But predictions not that good still.

Improvement from HARTREE-FOCK calculations….

Nuclear Physics — More Sophisticated Models

Hartree-Fock Calculations

- take best info on density distribution
- use it to calc potential at every point.
- Solve S.E. with this
- Use wavefunctions to get better

ITERATE → self consistency.

Excited States

involve mixtures of states... } messy
take nuc shell basis ψ_i and diagonalise $\langle \psi_i | H | \psi_j \rangle$ where

$H = H_0 + H_1$ ← residual pert.

H_0: nuc shell model + sph sym average of n-n force.

Isomorphic Shell Model (Anagnostatos 1985)

H-Fock ⇒ α particles important in dens. distributions. So: n, p hard spheres on vertices of rotating polyhedra, dim's related to classical orbits. Dist. particles among verts to minimise energy.
→ magic numbers without spin-orbit coupling! Maybe coincidence?!

Recent Evidence

Exotic Nuclei: Bash heavy ions into heavy nuc. Analyse shattered fragments → ^6He, ^{11}Li etc
→ Normal core + neutron "halo"

Super-Deformed Nuclei: repeat but off centre
→ high ang. mom states.
get bands based on stable configurations

cross over from low band

(axis ratios ~ 2:1:1)

Exotic Decay Modes. Emission of say ^{14}C nucleus or ^{24}Ne nuc ⇒ preformation plays large part in G.S.

NUCLEAR DECAY

Alpha Decay

$m(A,Z) = m(A-4, Z-2) + m_\alpha +$ Energy realese

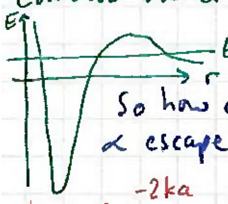
$m(A-4,Z-2)$: maybe G.S. if not, γ decay follows.

Energy realese: usually called $Q \simeq KE$ of α

Semi Emp. Mass Formula ⇒ $Q > 0$ only for $A \gtrsim 140$
expt: find stable nuclides upto $A = 210$
(also ∃ strong dep of τ on Q)

Answer:

Coulomb barrier:



So how does α escape?

→ Tunneling. Imagine α exists already
⇒ transmission coeff $= e^{-2G}$ where
G is Gamow Factor.

For deep tunneling (normal case)
$G \propto \frac{Z'}{Q^{1/2}}$ (Geiger-Nutall Law)

trans ∝ e^{-2ka}

$k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$; E: $-Q$, V: $-\frac{B}{r}$ (coulomb)

Integrate to get G.

Problems:
this is approx
need to ang mom eff. potential $\frac{l(l+1)\hbar^2}{2mr^2}$

Selection Rules In $X \to Y + \alpha$ ← $0^+ \therefore J = L$

$\therefore l = J_x + J_y \to |J_x - J_y|$

Parity conserved so if l even, X, Y have same parity, l odd, X, Y have diff.

Gamma Decay

like atomic transitions but: Higher energies
Collective motion of protons increases rate (and → higher multipoles...
(in atom, just one e^-)

λ (decay const - transitions per unit time) $= \frac{\omega^3}{3\pi\varepsilon_0\hbar c^3} |\langle \psi_f^* | W | \psi_i \rangle|^2$

W: Perturbing Ham. is Photon - has vector potential of plane wave

So $A = e^{-ik.r} = 1 - ik.r + -\frac{1}{2}(k.r)^2 + \ldots\ldots$
(monopole, dipole, quadrupole)

⇒ each one is reduced by $\sim kR \sim 10^{-3}$

∴ Prob: 1 ~10^{-3} ~10^{-6} etc →

E1	E2	E3
	M1	M2

For rough estimate, dipole, use $W_{ij} = eR$ (elec), μ_{nuc} (mag) $\left(\frac{e\hbar}{m_p c}\right)$

For odd electric, parity change
even electric, no parity change
odd magnetic, no p. change
even magnetic, parity change.
} → Selection rules

Angular momentum: E(L) or M(L) trans,
$|J_f - J_i| \le L \le |J_f + J_i|$ ΔJ = 0 forbidden if $J_i = J_f$?
can get ΔJ = 0 eg spin flip (M1) $\Delta M_J = 1$ think....

Internal Conversion

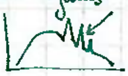
competes with γ decay: instead of emission of γ, a γ hits an electron
→ X-ray emission.

Define: Internal Conversion coeff:

$\alpha = \frac{Rate(A^* \to A + e^-)}{Rate(A^* \to A + \gamma)}$

dep on multipolarity

⇒ lines seen against β emission spectrum



Electron-Positron Pair emission

For $\Delta E > 2m_ec^2$, can get
$A^* \to A + e^+ + e^-$
but limited phase space
- can compete with, for $0^+ \to 0^+$
eg $^{16}O^* \to {}^{16}O + e^+ + e^-$ is this

Nuclear Isomerism

Usually, lifetimes short for γ decay
But if J very diff. from G.S. then high multipole required → slow rate.
States with $\tau > \sim 10^{-9}$s are called isomers.
also, this can occur if poss...

Angular Correlation

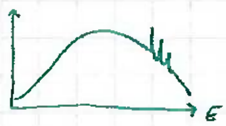
Consider decay to G.S. by 2 successive dipole trans (for example). After detect first spin axis probably ⊥ to plane of detector - but could be //. Define
$W(\theta) = \frac{Rate(\theta)}{Rate(90)}$ - use to investigate spins of excited levels, etc - all sorts...

The Mössbauer Effect

Nuclear Physics DECAY (continued)

Beta Decay

Get continuous spectrum of electrons



Half life is seconds → years.

FERMI THEORY:

Write down plane wavef'ns for e^-, $\bar{\nu}_e$ → $e^{i\underline{q}\cdot\underline{r}}$, $e^{i\underline{p}\cdot\underline{r}}$

∃ analogous diags for β^+ decay

Then expand in matrix element:

$e^{-i(\underline{p}+\underline{q})\cdot\underline{r}} = 1 - i(\underline{p}+\underline{q})\cdot\underline{r} + \ldots\ldots$

S, P, D etc

→ e^-, ν_e have one unit of orbital angular momentum. $\Delta L = 1$: (FIRST FORBIDDEN)

("SECOND FORBIDDEN")

For $\Delta L = n$ → nth forbidden

Parity changes for odd n.

e^-, $\bar{\nu}_e$ have no orbital angular momentum, ie $\Delta L = 0$ ∴ $\Delta J = \Delta L + \Delta S = \Delta S$ only.

(ALLOWED TRANSITION)

If $\Delta S = 0$, e, ν_e emitted in singlet state, called FERMI $J=0 \to J=0$ allowed. $\Delta J = 0$

If $\Delta S = 1$, e, $\bar{\nu}_e$ emitted in triplet state called GAMOW-TELLER $J=0 \to J=0$ not allowed. $\Delta J = 0$ or ± 1

In some decays, G-T or F can happen: only for $\Delta J = 0$.

eg
n → p + $\underline{e + \bar{\nu}_e}$
↑ → ↑ + ↑↓ F.
↑ → ↓ + ↑↑ G-T.

Mirror nuclei → "SUPER ALLOWED"
$\psi_f^* \simeq \psi_i$ ∴ large overlap. eg n → p

For Allowed transitions, matrix element is ~ same. Density of final states governs rate: Consider:

e^- $(E_e, \underline{p})$
ν_e $(E_\nu, \underline{q})$
nucleus recoiling $(T, \underline{P})$

$\boxed{\underline{P} + \underline{p} + \underline{q} = 0}$

$\cancel{T} + E_e + E_\nu = Q$
ignore.

$\Rightarrow Q = E_e + \underbrace{qc}_{(rel)}$

number of final states corresponding to electron mom p and neutrino mom q is

$dN = \underbrace{\frac{4\pi}{h^3} p^2 dp}_{\text{electron}} \cdot \underbrace{\frac{4\pi}{h^3} q^2 dq}_{\text{nutrino}}$

use to find $q\,dq$ at const E_e

$\Rightarrow \boxed{\frac{dN}{dQ} \propto p^2 (Q-E)^2}$ number of electrons of mom. p per unit interval of mom and ...

So: Plot $\sqrt{\frac{dN/dQ}{p^2}}$ vs Q and get straight line: Curie Plot.

If m_ν not zero, get estimate for mass.

For $Q \gg m_e c^2$ ie very relativistic, $E = pc$

So number of electrons emitted per sec is $\int_0^Q dp \propto Q^5$ SARGENT RULE

Comparative half life:

Violation of Parity Conservation.

If $\hat{O}$ is a pseudoscalar operator, changes sign on inversion of coords ie $PO = (-1)O$

$\langle O \rangle = 0$ as $\langle O \rangle = \langle OP^2 \rangle = -\langle POP \rangle$
these are same ∴ zero

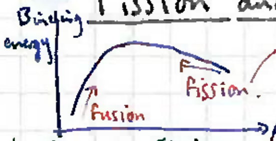
it was found that $\langle \underbrace{\underline{\sigma}\cdot\underline{p}}_{\text{pseudoscalar}} \rangle \neq 0$ by measureing angular correlation in γ decay after β decay in ^{60}Co.

(Sample spins polarised up and down - more β particles emitted opposite to pol. dir'n than along it)

Emitted electrons are in mixture of $l=0$ and 1 states - mixed parity!

Fermi theory matrix element changed but nuclear wavef'ns unaffected ∴ selection rules OK.)

Fission and Reactors

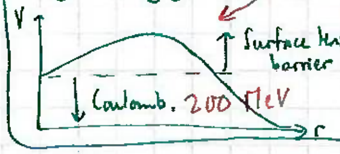


reduce Coulomb energy

Spontaneous Fission:

Stretch liquid drop:

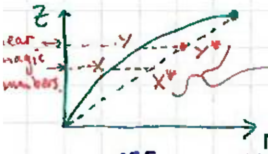
NOT TO SCALE!



apply α-decay theory ⇒ large fragment mass means rate $\sim 10^{-4} \times$ α decay.

not likely.

Induced Fission:

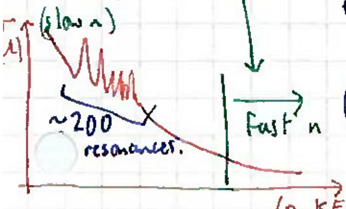


same $\frac{Z}{N}$ as U

eg $n + {}^{235}U \to {}^{236}U \to \underbrace{X^* + Y^*}_{\text{fission fragments}} \to X + Y + 2.6n$ on average.

→ (more fission)

Absorption of 2.6n:



⇒ want to change fast n into slow n so they are absorbed by ^{235}U again.

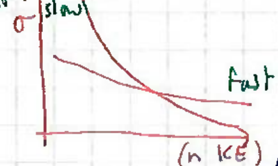
Solution: let neutrons lose energy by hitting light nuclei (^{12}C or water) moderator

Problem: $n + H \to D$ producing heavy water

∴ use heavy water!

Another problem. Natural U is > 99% ^{238}U which captures n.

but:

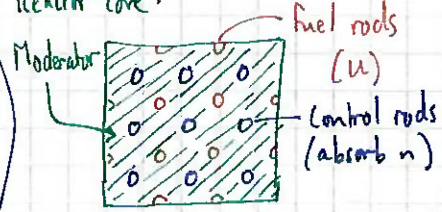


⇒ must slow down n away from U.

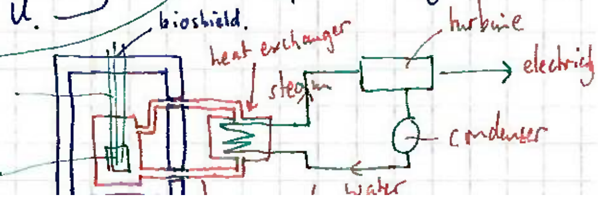
⇒ build reactor as follows:

fission → fast neutrons
↓
get them out of U
↓
(HEAT!) thermalise them)
↓
drift back into fuel

Reactor core:



Typical configuration.



Nuclear Physics — Reactors and Reactions

Reactor kinetics

$k = \dfrac{\text{number of neutrons in one generation}}{\text{number of neutrons in previous generation}}$

$k < 1$ subcritical
$k = 1$ critical
$k > 1$ supercritical

k dep. on:
- σ as f'n of energy
- average no. of neutrons prod'd.
- % of ^{235}U
- all sorts: geom, size of core ....

dn (change in neutron number in one cycle, dt) $= \tau_c$
$= n(k-1)$

$\dfrac{dn}{dt} = \dfrac{(k-1)n}{\tau_c} \Rightarrow n = n_0 e^{t/T}$ $\quad T = \dfrac{\tau_c}{k-1}$

$\tau_c = \dfrac{\lambda}{v}$ (mean free path) $\simeq \dfrac{2.8\,m}{2\,km/sec}$

$\therefore \tau_c \simeq \frac{5}{4}\,ms \Rightarrow$ n increases uncontrollably fast for say $k = 1.001$.

Solution: Delayed neutrons
ie neutrons emitted by fission products with $\tau_{1/2}$ of ~ 10 seconds
but only present in $< 1\%$ core.
$\longrightarrow$ average τ_c OK.

eg $^{87}Br \xrightarrow[\beta\text{ decay (slow)}]{} {}^{87}Kr \longrightarrow {}^{86}Kr + n$ (fast, 51 = magic + 1)

Breeder Reactors

$n + {}^{238}U$ yields ^{239}Pu
$^{239}Pu + n \longrightarrow 2.9n$ cf $2.6n$....
$\therefore$ for same power o/p don't need to thermalise $\Rightarrow$ small core
Use liquid Na coolant.

Reactions

Conservation Laws

b $\to$ bangs a emitting c leaving d
$\Updownarrow$
$a(b,c)d$.

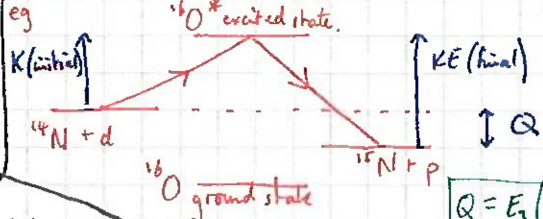
Conserved quantities in all nuclear reactions:
Charge, Baryon number, Parity (intrinsic $+(-1)^l$ (ang mom)), Momentum, Energy

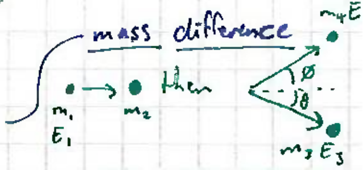
Q-Values

Q value is KE (final) − KE (initial) as measured in the centre of mass frame

elastic scattering: $Q = 0$

in C.M.F.: $x + X \to y + Y + Q$





$$\boxed{Q = E_3\left(1 + \frac{m_3}{m_4}\right) - E_1\left(1 - \frac{m_1}{m_4}\right) - \frac{2\sqrt{m_1 E_1 m_3 E_3}\cos\theta}{m_4}}$$

"Q-equation" (non relativistic).

Principle of Detailed Balance

Fermi's Golden rule for $\sigma_{a\to b}$ and $\sigma_{b\to a}$ in $1+2 \rightleftarrows 3+4$.

$\Gamma \propto |M|^2 \rho(E_f) \longrightarrow \propto p_f^2 \dfrac{dp_f}{dE_f} \times$ spin factor $(2J_{\text{each}}+1)$ $\Rightarrow \boxed{\dfrac{\sigma_a}{\sigma_b} = \dfrac{p_b^2}{p_a^2}\dfrac{g_b}{g_a}}$

$|M|$: same coz Hermitian

Breit-Wigner Formula

$\Gamma = \sum \Gamma_{\text{partial}}$ (decay modes)

$x + X \longrightarrow Z^* \longrightarrow y + Y$

$\sigma(x+X \to y+Y) = \sigma_{xy} = \sigma_x \dfrac{\Gamma_y}{\Gamma}$

Excited state Z^* is not a stationary state - has a natural lifetime $\Rightarrow$ not a single energy - smeared out into Lorentzian lineshape.

$P(t) \propto e^{-\gamma t}$ $\quad \gamma$ is rate $= \dfrac{\Gamma}{\hbar}$

$\therefore \psi = \psi(0)e^{-i\omega_0 t}e^{-\frac{i\Gamma t}{2\hbar}}$
$= \int f(\omega)e^{i\omega t}d\omega$ (superpos of stat. states)
$I = |f|^2$ is Lorentzian.

2nd order P.T. gives $M_{xy} = \sum_z \dfrac{M_{xz}M_{zy}}{E - E_z}$

$\dfrac{dp_y}{dE} = \dfrac{1}{v_y}$

Fermi's Golden rule $\Rightarrow$

$$\boxed{\sigma_{xy} = \frac{2\pi}{\hbar}|M_{xy}|^2 \frac{4\pi}{h^3}\frac{p_y^2\, g}{v_x v_y}}$$

$\sigma = \dfrac{\Gamma}{\text{flux}}$ (flux $= v_x/V$ (for $N=1$))

and, $\boxed{\dfrac{\Gamma_x}{\hbar} = \dfrac{2\pi}{\hbar}|M_{xz}|^2\dfrac{4\pi}{h^3}\dfrac{p_x^2}{v_x}}$ and same for Γ_y

g - spin statistics factor

$$\boxed{g = \frac{(2J_z+1)}{(2J_x+1)(2J_X+1)}}$$

but z-state has $E_z = E_0 + \dfrac{i\Gamma}{2}$

so $\boxed{|M_{xy}|^2 = \dfrac{|M_{xz}|^2|M_{zy}|^2}{(E-E_0)^2 + \frac{\Gamma^2}{4}}}$

Subst all of that $\longrightarrow$

get: $\boxed{\sigma = \pi\lambda\!\!\!^{-2} g \dfrac{\Gamma_x\Gamma_y}{(E-E_0)^2 + \frac{\Gamma^2}{4}}}$

Applications: Neutron Capture (resonance absorption)

ie (n,γ) reactions.
Slow neutrons $\to$ s waves only ($l=0$)
slow neutrons, heavy nuclei,
$\Gamma_\gamma + \Gamma_n \simeq \Gamma_\gamma$ $\Rightarrow$ at resonance

$$\boxed{\sigma(n,\gamma) = 4\pi\lambda\!\!\!^{-2} g\frac{\Gamma_n}{\Gamma_\gamma} \gg \pi R^2}$$

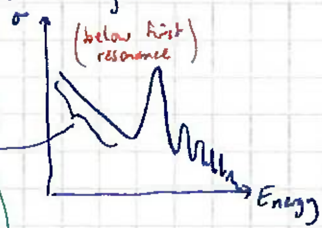
eg Xe $\quad \sigma \simeq 10^4\sigma_{\text{geometric}}$

$\frac{1}{v}$ Laws

For very slow neutrons...
Γ_n is dominated by density of states $\longrightarrow \propto v$
So (for $E_0 \gg E$)

$$\sigma = \underbrace{\lambda\!\!\!^{-2} v}_{\propto \frac{1}{v}} \underbrace{\left(\frac{\pi g \Gamma_\gamma}{E_0^2 + \frac{\Gamma^2}{4}}\right)}_{\text{const.}}$$

So on log scale:



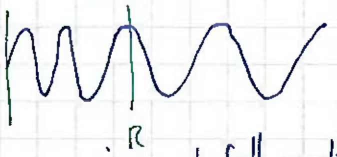
Resonance Scattering

$y + Y \to Z^* \to y + Y$

$\sigma_{max} = 4\pi\lambda\!\!\!^{-2} g\dfrac{\Gamma_n^2}{\Gamma^2}$

For "pure", $\Gamma_n = \Gamma$ (no other channels)

But sometimes $\cos k_i R = 0$ $\longrightarrow$ resonance $T = 1$

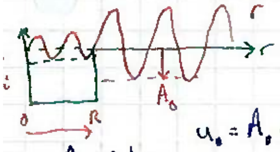


joins at full amplitude.

Elastic Potential Scattering

Consider S waves, spinless low energy neutrons scattering off a spherical square well....

let $u = \dfrac{\psi}{r}$ (radial wavef'n)



$u_i = A_i \sin k_i r$ $(r < R)$ $\quad u_0 = A_0\sin(k_0 r + \delta)$ $(r > R)$

match u and u'

get Transmission coeff $= \underbrace{\dfrac{v_i}{v_0}}_{\text{Flux Factor}}\dfrac{A_i^2}{A_0^2} = \dfrac{v_i}{v_0}\left(1 + \left(\dfrac{k_i^2}{k_0^2} - 1\right)\cos^2 k_i R\right)^{-1}$

So usually ($\cos^2 k_i R \neq 0$)
for $k_i \gg k_0$ (low energy incident part.)
get $\boxed{T \sim \dfrac{k_0^2}{k_i^2}}$

Fluids : Statics

Def'ns: Stress : τ_{ij} : i component of force per unit area in j dir'n

Pressure $p = -\frac{1}{3}(\tau_{11} + \tau_{22} + \tau_{33})$

Strain $e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$

volume strain $e_V = \frac{dV}{V} = -\frac{d\rho}{\rho} = \underline{\nabla} \cdot \underline{u}$

Shear modulus ; $\tau_{12} = 2G e_{12}$ etc

Bulk modulus : $-p = B e_V$

Shears

Pure shear : $\frac{\partial u_1}{\partial x_2}$ and $\frac{\partial u_2}{\partial x_1}$ in equal amounts

Simple shear : $\frac{\partial u_1}{\partial x_2}$ only

Simple shear = Pure shear + rotation

also, rotate pure shear (45°) and get extension + compression

Viscous Flow

volume flow rate : $Q = \int_{surf.} \underline{v} \cdot d\underline{S}$

Planar Poisseuille Flow

$v_1(x_2)$ $\quad dp = p(x_1 + dx_1) - p(x_1)$

$\tau_{12} = 2\eta \frac{de_{12}}{dt} = \eta\left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1}\right)$

$$\boxed{\eta \frac{\partial^2 v_1}{\partial x_2^2} = \frac{\partial p}{\partial x_1}}$$

balance viscous / press. forces

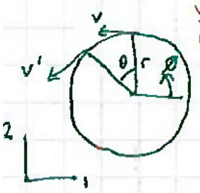
Poisseuille Flow in cylinder

$$\underbrace{\pi r^2}_{\text{area}} \underbrace{\frac{dp}{dz} dz}_{dp} = \underbrace{2\pi r dz}_{\text{area}} \cdot \underbrace{\eta \frac{dv_z}{dr}}_{\tau_{zr}}$$

b.c. no slip at surface.

$$\Rightarrow \boxed{v_z = -\frac{(a^2 - r^2)}{4\eta} \frac{dp}{dz}}$$

Couette Flow



$\tau_{\phi r} = \eta\left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1}\right)$ $\quad \frac{v \sin\theta}{r \sin\theta}$ as $\theta \to 0$ $\quad -\frac{dv}{dr}$

$= \eta\left(\frac{v}{r} - \frac{dv}{dr}\right)$

$$\therefore \boxed{\tau_{\phi r} = \eta r \frac{d\omega}{dr}}$$

Torque on cyl. shell :

$$T_z(r) = \underbrace{2\pi r L}_{\text{area}} \cdot \underbrace{\eta r \frac{d\omega}{dr}}_{F/A} \cdot \underbrace{r}_{\text{moment}}$$

$$= 2\pi L \eta \, r^3 \frac{d\omega}{dr}$$

Net torque $= \frac{d}{dt}$ (ang. mom of shell)

$$\Rightarrow \boxed{\eta \frac{d}{dr}\left(r^3 \frac{d\omega}{dr}\right) = \rho r^2 \frac{dv}{dt}}$$

a sol'n: $v = \frac{K}{2\pi r}\left(1 - e^{\frac{-r^2\rho}{4\eta t}}\right)$

short times: $v = \frac{K}{2\pi r}$ VORTEX

long times: body rotation: $v = r\omega$

can get from $\frac{d}{dt} = 0$ steady state sol'ns....

Vorticity

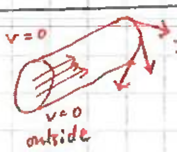
Def'n: $\underline{\Omega} = \underline{\nabla} \times \underline{v}$

$\langle \Omega \rangle = \frac{\int d\underline{A} \cdot \underline{\Omega}}{A}$

$= \oint_C d\underline{l} \cdot \underline{v}$ (STOKES LAW)

eg:

eg Submerged Jet of solenoid.



$v=0$ outside

Ω cylindrical shell of vorticity.

NB. : $\Omega_{\text{VORTEX}} = 0$ (Irrotational Flow)

$\Omega_{\text{BODY ROT.}} = 2\omega$

NAVIER – STOKE'S Equation

N2L for Incompressible Flow

Force (m^{-3}) $= \frac{\partial \tau_{11}}{\partial x_1} + \frac{\partial \tau_{12}}{\partial x_2} + \frac{\partial \tau_{13}}{\partial x_3}$ ordinary def'ns $\rightarrow -\frac{\partial p}{\partial x_1} - \frac{\eta}{\rho} \underline{\nabla} \times \underline{\nabla} \times \underline{v}$

use vector identity: $\underline{\nabla} \times \underline{\nabla} \times \underline{v} = \underline{\nabla}(\underline{\nabla} \cdot \underline{v}) - \nabla^2 \underline{v}$, $\underline{\nabla} \cdot \underline{v} = 0$

$\tau_{11} = -p - 2\eta\left(\frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3}\right)$

Incompressible $\therefore \underline{\nabla} \cdot \underline{v} = 0$

$$\boxed{\frac{\eta}{\rho} \nabla^2 \underline{v} - \underline{\nabla}\left(\frac{p}{\rho} + gh\right) = \frac{D\underline{v}}{Dt}}$$

acc'n as you follow the fluid $(\underline{v} \cdot \underline{\nabla})\underline{v} + \frac{\partial \underline{v}}{\partial t}$

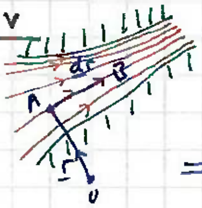
take curl and get and

$$\boxed{\dot{\underline{\Omega}} = \frac{\eta}{\rho} \nabla^2 \underline{\Omega}}$$

Diffusion Equation } ie vorticity diffuses out into regions that were $\underline{\Omega} = \underline{0}$.

Inertial term $(v \cdot \text{grad})v$

Consider convergent flow



$v_B > v_A$

but $v(\underline{r})$ const for given $\underline{r}$
ie $\exists$ accelerations but $\frac{\partial v}{\partial t}$ at each point $= 0$

$v(\underline{r} + d\underline{r}) - v(\underline{r})$ = convective acc.
$= dx_i \frac{\partial v}{\partial x_i}$ summation convention.

$\Rightarrow \frac{dv}{dt} = \frac{dx_i}{dt} \frac{\partial v}{\partial x_i}$ "

$$\Rightarrow \boxed{\text{acc'n} = (\underline{v} \cdot \underline{\nabla})v}$$

Reynold's number

ratio of $\frac{\text{inertial stresses}}{\text{viscous stresses}}$

$$\text{ie} \quad \boxed{R_e = \frac{\rho |(\underline{v} \cdot \underline{\nabla})\underline{v}|}{\eta \nabla^2 \underline{v}}}$$

pick characteristic length $L \sim \nabla$

then $\boxed{R_e = \frac{\rho L v}{\eta}}$

For $R_e \gg 1$ ignore viscosity, inertia important

For $R_e \ll 1$ ignore inertia, viscosity important

Fluids: Bernoulli's Theorem, Potential Flow

Inertial Effects

$\exists$ pressure variation in any non uniform velocity field.

locally - motion in a circle with rad of curv: R

ie

$$\boxed{\frac{dp}{dR} = \frac{\rho v^2}{R}}$$

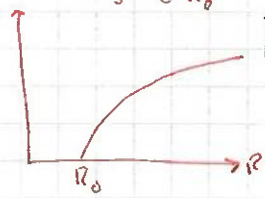
$$\boxed{\text{c.f. } \rho(\underline{v}\cdot\underline{\nabla})\underline{v} \text{ with } \nabla = \frac{1}{R}}$$ $\Rightarrow$ inertial effect.

eg body rotation $v = R\omega$

$p_{extra} = \rho g z$

eg vortex $v = \frac{K}{r}$

$$z = \frac{K^2}{g}\left(\frac{1}{R_0^2} - \frac{1}{R^2}\right)$$



$p_{out} > p_{inside}$ $\therefore$ force inwards balance centrip.

Bernoulli's Theorem

Force args then integrate: Pressure gradient + grav. force = conv. derivative

c.f. Navier Stokes $\equiv$ Newton's 2nd Law
integrate to get:
Bernoulli $\equiv$ Conservation of energy

ie Navier-Stokes $\Rightarrow \eta\nabla^2\underline{v} - \underline{\nabla}(p + \rho g h) = \underbrace{\rho(\underline{v}\cdot\underline{\nabla})\underline{v}}_{= \frac{1}{2}\rho\underline{\nabla}(v^2)} + \rho\frac{d\underline{v}}{dt}$

all along a ~~flow line~~ steady flow line ie a stream line!

set $\eta = 0$

steady state $\equiv$ energy cons.

get: $$\boxed{p + \rho g h + \frac{1}{2}\rho v^2 = \text{Const}}$$

so - valid for:
- negligable η effects
- steady state
- Incompressible flow

Generalised Bernoulli Theorem:

applies in a non steady state, $\frac{d\underline{v}}{dt} \neq 0$

$v_s = \frac{\partial\phi}{\partial t}$ $\therefore$ get $\frac{\partial\phi}{\partial t}$ term in here...

ie $\underline{v} = \underline{\nabla}\phi$

Potential Flow

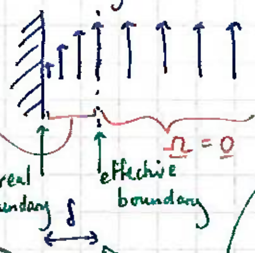
For ZERO VORTICITY: $\nabla\times\underline{v} = 0$
so there is a ϕ s.t. $\underline{v} = \underline{\nabla}\phi$

For incompressible fluid, $\underline{\nabla}\cdot\underline{v} = 0$

$$\Rightarrow \boxed{\nabla^2\phi = 0}$$

Boundary Conditions: $\boxed{\underline{V}_\perp = 0}$

$\Omega \neq 0$



useful solutions:

$\phi = v_0\cos\theta$ (uniform flow)

$\phi = \frac{p\cos\theta}{4\pi r^2}$ (dipole field)

$\phi = \frac{Q}{4\pi r}$ (monopole field - point source)

$\phi = \frac{K\theta}{2\pi}$ (vortex)

General solutions:
in plane (cylindrical) polars:
$\phi_n = \left(r^n + \frac{1}{r^n}\right)(a_n\cos n\theta + b_n\sin n\theta)$

spherical polars:
$\phi_n = \left(r^n + \frac{1}{r^{n+1}}\right)[P_n(\cos\theta)]$

note: diffusion of B-L $\propto\sqrt{\text{kinematic visc.} \times \text{time}}$

Kelvin Circulation Theorem.

$$\boxed{\frac{DK}{Dt} = 0}$$ $\Rightarrow$ vortex lines are embedded in fluid and are conserved in number.

$K = \oint\underline{v}\cdot d\underline{l}$ so $\frac{DK}{Dt} = \oint \frac{D\underline{v}}{Dt}\cdot d\underline{l} + \underline{v}\cdot\frac{D\,d\underline{l}}{Dt}$

$\frac{D\underline{v}}{Dt} = -\underline{\nabla}\left(\frac{p}{\rho} + gz\right) + \eta\nabla^2 v$ ($\eta \to 0$)

$= \underline{v}\cdot d\underline{v}$
$= \frac{1}{2}d(v^2)$

Stokes theorem
$\Rightarrow \oint = \int_{surf}\nabla\times\nabla(\;) = 0$

one complete passage around loop leaves v unchanged $\to = 0$

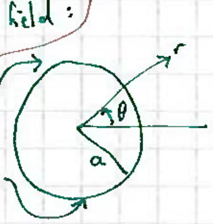
Magnus Effect

v^2 (net) $= V_0 \times K$

Rotating cylinder in uniform flow:
Solution: vortex + line dipole + uniform field:

$$\Phi = V_0\cos\theta\left(r + \frac{a^2}{r}\right) + \frac{K\theta}{2\pi}$$

$\Rightarrow V_\theta(r=a) = -2V_0\sin\theta + \frac{K}{2\pi a}$ So p here $>$ p here

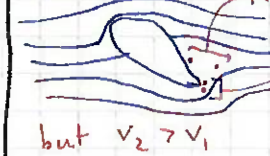


Magnetic Analogy

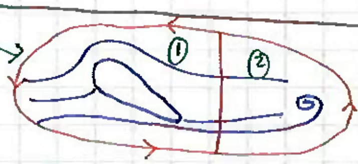
Fluids:	E/mag:
$\underline{v} = \underline{\nabla}\phi$	$\underline{H} = -\underline{\nabla}\phi_m$
(so $\underline{v} \equiv -\underline{H}$)	
$K = \oint\underline{v}\cdot d\underline{l}$	$I = \oint\underline{H}\cdot d\underline{l}$
$\frac{1}{2}\rho v^2$	$-\frac{1}{2}\mu_0 H^2$
$\rho\underline{v}_0\times\underline{K}$	$-\mu_0\underline{I}\times\underline{H}$ (Force)

Aerofoils

Basic idea: Bound vortex
so $\underline{F} = \rho(\underline{V}_0\times\underline{K})$
Start:



but $v_2 > v_1$
$\therefore p_1 > p_2$
$\therefore$ B.L. pushed off foil and off tip $\to$ vortex...



$\int_{① + ②}\underline{v}\cdot d\underline{l} = 0$ (Kelvin)

$\int_{②}\underline{v}\cdot d\underline{l} = K_{eddy} \Rightarrow \boxed{-K_{\text{vortex on wing}}}$

region of downward moving air

Fluids

Drag

Drag and Waves

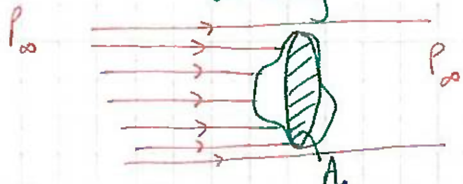
(rem. d'Alembert's Paradox - $p_{north} = p_{south} \to$ no drag)

Viscous drag

- pressure (pot flow) + viscous $\left(\eta \frac{dv_\theta}{dr}\right)$

$\underbrace{\qquad\qquad\qquad}$ stokes law
$F = 6\pi\eta a v_0$

Inertial drag: Ideal drag $\equiv$ if all flow stopped on body $\to$ Ideal drag force (from Bern.)



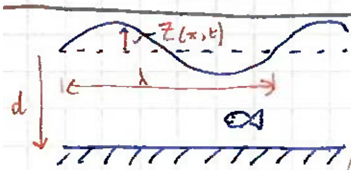
$F_{ideal} = \frac{1}{2}\rho v_0^2 A_p$

F_{actual} always $< F_{ideal}$.

Drag coeff $= \frac{F_{actual}}{\frac{1}{2}\rho v_0^2 A_p} \equiv \frac{A_{effective}}{A_p} = C_D$

Scaling: C_D is same f'n of Re for bodies of same shape.

WAVES



$\boxed{\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial z^2} = 0} \Rightarrow \boxed{\phi = \sum_k \left(a_k e^{kz} + b_k e^{-kz}\right) e^{ikx}}$

$\to$ contact with bottom $\boxed{\left.\frac{\partial\phi}{\partial z}\right|_{-d} = 0}$

Boundary Conditions: (i) (ii) $\frac{DZ}{Dt} = \left.\frac{\partial\phi}{\partial z}\right|_Z$ (iii) Gen. Bernoulli $\Rightarrow dp$ = surface t.

$\frac{\sigma}{\rho}\frac{\partial^2 Z}{\partial x^2} = gZ + \cancel{\frac{v^2}{2}} + \dot\phi(Z)$

Linearisation approximations: $(\underline{v}.\nabla\underline{v}) = 0$ and $\frac{v^2}{2} \ll gZ$

$\to \boxed{\frac{\partial Z}{\partial t} = \left.\frac{\partial\phi}{\partial z}\right|_Z}$

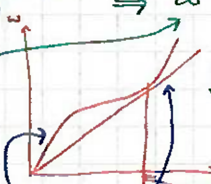
Deep Water

only take decaying part of ϕ (e^{kz})

$\Rightarrow \omega^2 = gk + \frac{\sigma k^3}{\rho}$

grav S.T.

equal when $k = \sqrt{\frac{\rho g}{\sigma}}$



limits: $\omega = \sqrt{gk}$ for big λ and $\omega = \sqrt{\frac{\sigma}{\rho}}\, k^{3/2}$ for small λ

$\frac{c_{ph}}{2} < c_g < \frac{3c_{ph}}{2}$

Liq - Liq interface:

ϕ_1, ρ_1, p_1

ϕ_2, ρ_2, p_2

$\phi_1 = A e^{-kz} e^{i(kx-\omega t)}$

$\phi_2 = A e^{kz} e^{i(kx-\omega t)}$

Just consider gravity case

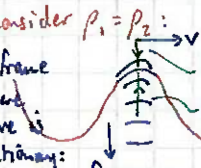
Gen Bernoulli: $p_1 = p_1 + \rho_1 g Z + \dot\phi_1(Z)$

$p_2 = p_2 + g Z \rho_2 + \dot\phi_2(Z)$

$\Rightarrow \boxed{\omega^2 = \left(\frac{\rho_1 + \rho_2}{\rho_1 - \rho_2}\right) gk}$

note if $\rho_1 = \rho_2$ $\to$ disaster!

Consider $\rho_1 = \rho_2$: Kelvin-Helmholtz Instability



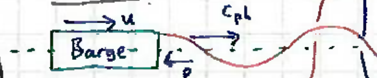
In frame where wave is stationary:

sheet of vorticity! [In stat frame, before wave, $\xleftarrow{v_1}$ $\xrightarrow{v_2}$]

$\to p_2 > p_1 \to$ feedback $\to$ instability.

For away, moves with speed $\underline{v} = \frac{v_2 - v_1}{2}$

Losses



Let $u > c_g$ $(= c_{ph}^{min})$

groups of grav. waves appear behind boat

groups of S.T. waves appear in front of boat.

If $u < c_g$ ie $u < c_{ph}^{min}$ then no waves - no losses.

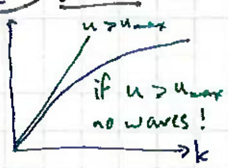
Finite Depth (Shallow)

need e^{-kz} as well!

get $\omega^2 = gk\tanh(kD)$

so non dispersive for $kD \ll 1$

Losses



Finite Amplitude Effects

Consider Shallow case so....

$\phi = A\cosh(k(z+D))\sin(kx-\omega t)$

ϕ indep of z $\therefore$ vertical slabs move...

Consider in moving frame s.t. pattern stationary.

ie let $x' = x + \frac{\omega}{k}t$

$\Rightarrow gZ = A\omega\cos(kx')$

$v_x = Ak\cos(kx')$

$v_x' = v_x - c_{ph}$

Apply continuity condition in the co-moving frame

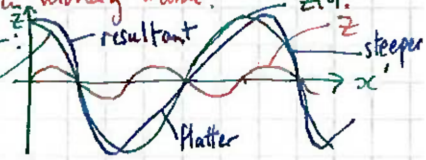
$\frac{\partial}{\partial x'}\underbrace{(v_x - c_p)}_{vel}\underbrace{(D+Z)}_{area} = \dot Z = \frac{\partial}{\partial x'}\left(\frac{A^2\omega k}{g}\cos^2 kx'\right)$

vol. flow rate

$= \frac{A^2\omega k^2}{g}\sin(2kx')$

$\Rightarrow \dot Z = 0$ to first order as it should in moving frame.

2nd order effect:



$\Rightarrow$ Waves break as $D \to 0$

Solitary Waves

Finite depth effect: $\to$ Dispersion $\Rightarrow$ wave packet spreads

Finite amplitude effect (Non-linear) $\Rightarrow$ wavepacket sharpens

Sol'ns of KdV eq'n: [suitable combination of these $\to$ pulse of unchanging form.

$\frac{dZ}{dt} = \pm\sqrt{gD}\,\frac{d}{dx}\left(Z + \frac{1}{6}D^2\frac{\partial^2 Z}{\partial x^2} + \frac{3}{4}\frac{Z^2}{D}\right)$

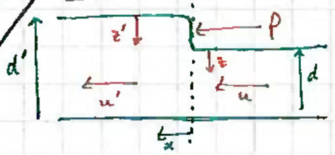
Sol'n: $Z = Z_0\,\mathrm{sech}^2\left[(x - ct)\sqrt{\frac{3Z_0}{4D^3}}\right]$

where $C = \sqrt{gD}\left(1 + \frac{Z_0}{2D}\right)$

note - Z_0, amplitude determines shape and speed.

- can pass through each other unchanging in amp. and shape but $\exists$ uncertainty in pos'n!

Bores



Continuity: $d'u' = du$

Force in x dir'n = $p(d'-d) - \int_0^{d'} dz'(p + \rho g z') + \int_0^d dz(p + \rho g z)$

$= -\frac{\rho g}{2}(d'^2 - d^2)$

Balance with change in mom flux = $\rho u'u'd' - \rho u u d$

$\Rightarrow u = \sqrt{\frac{gd'(d'+d)}{2d}}$

Small bores $u = \sqrt{gd}$

Big bores: get undulations

Bigger bores: front sharpens then breaks.

Rel + Electromag: Special Relativity

Evidence

- Particle speeds always $< c$
- Particle speeds in one reachins
  - no can add (even in 1D)
- Time dilation
- Michelson - Morely

Tests

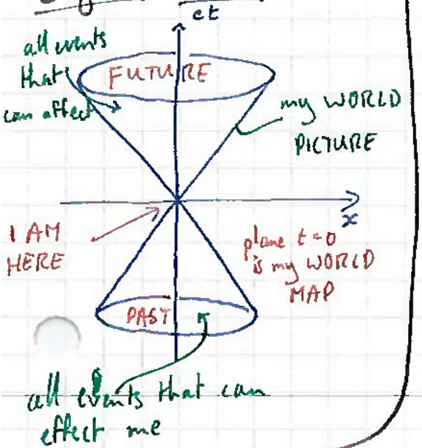
- speed of photons from π^0 decay
- Arrival times of x-rays from pulsars in binary star systems
- $\mu^{\pm}$ lifetimes in storage ring
- mag moment of e^-

Lorentz Transforms

$$x^{\mu'} = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} x^{\mu}$$

analogous to rotation in 3-D.

Light Cone



"Position" 4-vector $\underset{\sim}{r} = (ct, \underline{r})$

$d(ct, \underline{r})$ must be 4-vec

$d\tau$ is Lorentz inv. $\Rightarrow \underline{u} = \frac{d(ct, \underline{r})}{d\tau}$ is 4-vec

but $\tau = \frac{t}{\gamma}$

$\Rightarrow$

4-Velocity

$$\underset{\sim}{u} = (\gamma_u c, \gamma_u \underline{u})$$

Apply LT to $\underset{\sim}{u}$

$$\rightarrow \begin{bmatrix} \gamma_u' c = \gamma_v(\gamma_u c - \beta\gamma_u u_x) \\ \gamma_u' u_x' = \gamma_v(\gamma_u u_x - \beta\gamma_u c) \end{bmatrix}$$

$$\Downarrow$$

$$\frac{\gamma_u'}{\gamma_u \gamma_v} = \left(1 - \frac{V u_x}{c^2}\right)$$

Velocity Transformations

$$u_x' = \frac{u_x - V}{1 - \frac{V u_x}{c^2}}$$

etc

Require: if mom cons in one frame, it is in all inertial frames.

multiply $\underset{\sim}{u}$ by Lorentz invariant mass, m_0

$\rightarrow$ new mass $m = \gamma m_0$

Relativistic (total) Energy

$E = mc^2$
$= \gamma m_0 c^2$

4-Momentum

$$\underset{\sim}{p} = (mc, \underline{p}) = (\gamma m_0 c, \gamma m_0 \underline{u})$$

$$\boxed{\underset{\sim}{p} \cdot \underset{\sim}{p} = \frac{E^2}{c^2} - p^2 = m_0 c^2}$$

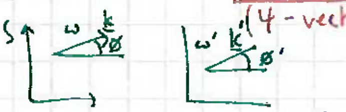
$\underset{\sim}{p_1} + \underset{\sim}{p_2} = \underset{\sim}{p_3} + \underset{\sim}{p_4}$

- cons mom
- cons energy (mass)
- valid in all in. frames

Plane Waves

$$\underset{\sim}{p} = \left(\frac{E}{c}, \underline{p}\right) = \hbar \underset{\sim}{k} \Rightarrow \boxed{\underset{\sim}{k} = \left(\frac{\omega}{c}, \underline{k}\right)}$$

(4-vector)



apply LT to $\underset{\sim}{k}$

$$\Rightarrow \begin{bmatrix} \frac{\omega'}{c} = \frac{\gamma\omega}{c} - \beta\gamma k\cos\phi \\ k'\cos\phi' = \gamma k\cos\phi - \beta\gamma\frac{\omega}{c} \end{bmatrix}$$

Aberration:

$$\tan\phi' = \frac{\sin\phi}{\gamma(\cos\phi - \beta)}$$

Doppler Effect

$$\omega' = \gamma\omega(1 - \beta\cos\phi)$$

Compton Scattering - see notes.

4-Acceleration

$$\underset{\sim}{a} = \gamma\frac{d}{dt}(\underset{\sim}{u})$$

In IRF $\boxed{\underset{\sim}{a} = (0, \underline{a})}$

$\Rightarrow$ In all frames $\boxed{\underset{\sim}{a} \cdot \underset{\sim}{a} = -a^2}$

$$\underset{\sim}{a} = \frac{d}{d\tau}\underset{\sim}{u} \quad (L \text{ inv})$$

$$= \left(c\gamma\frac{d\gamma}{dt}, \gamma^2\underline{a} + \gamma\frac{d\gamma}{dt}\underline{u}\right)$$

4-force

$$\underset{\sim}{f} = m_0 \underset{\sim}{a}$$

note! $\underset{\sim}{f} = \frac{d}{d\tau}(\underset{\sim}{p}) = \frac{d}{d\tau}(m_0 \underset{\sim}{u})$

$$= \gamma\frac{d}{dt}(\underbrace{\gamma m_0 c}_{\text{rate of change of } E/c}, \underbrace{\underline{p}}_{\text{of mom}})$$

ie power input

Transformation of 4-force

$$\underline{f} = \frac{d}{dt}(m\underline{u}) = m\underline{a} + \underline{u}\frac{dm}{dt}$$

$$= m\underline{a} + \left(\frac{\underline{f}\cdot\underline{u}}{c^2}\right)\underline{u}$$

3-acc'n $\underline{a}$ not parallel to 3-force $\underline{f}$ producing it

except:

$\underline{f}\cdot\underline{u} = fu$ $\rightarrow$ $\underline{f} // \underline{u} \longrightarrow \underline{f} = \gamma^3 m_0 \underline{a}$

$\underline{f}\cdot\underline{u} = 0$ $\rightarrow$ $\underline{f} \perp \underline{u} \longrightarrow \underline{f} = \gamma m_0 \underline{a}$

apply LT to $\underset{\sim}{f}$

$$\Rightarrow \left[\gamma_u' f_x' = \gamma_v\left(\gamma_u f_x - \frac{\beta\gamma_u}{c}\underline{f}\cdot\underline{u}\right)\right]$$

$$\rightarrow f_x' = \frac{f_x - \frac{\beta}{c}\underline{f}\cdot\underline{u}}{1 - \frac{\beta u_x}{c}}$$

$= f_x$ if $\underline{f}$ is along x axis.

[ACCELERATING FRAMES: $\underset{(\text{earth})}{dv} = \frac{1}{\gamma^2}dv'$ in I.R.F.]

Rel + Electromag : Electrodynamics

Vector Potential $\underline{B} = \nabla \times \underline{A}$

Does a vec. pot always exist?

$\underline{A} = \left(\int^z B_y\, dz,\ -\int^z B_x\, dz,\ 1 \right)$

Proof: $\underline{B} = \nabla \times \underline{A}$
(use $\nabla \cdot \underline{B} = 0$)

Non-Uniqueness

$\underline{A} \to \underline{A} + \nabla \phi$ (ϕ any scalar)
leaves $\underline{B}$ unchanged
[Gauge Invariance]

So can choose $\nabla \cdot \underline{A}$ } "Choosing a Gauge"

$\underline{A}$ for steady currents $\longrightarrow$ **Integral Solution** (G.F.)

$\Longrightarrow$ Poisson's Equation.

Maxwell $\Rightarrow \mu_0 \underline{j} = \nabla \times \underline{B}$
$= \nabla(\nabla \cdot \underline{A}) - \nabla^2 \underline{A}$

(choose) Coulomb Gauge : $\nabla \cdot \underline{A} = 0$

to get $\boxed{\nabla^2 \underline{A} = -\mu_0 \underline{j}}$

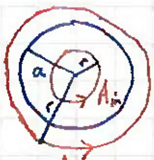
$$\underline{A} = \frac{\mu_0}{4\pi} \int \frac{\underline{j}(\underline{r}')\, d^3\underline{r}'}{|\underline{r} - \underline{r}'|}$$

Vector equation

If one current say wire
$(\underline{j}\, d^3 r = I\, d\underline{l})$ $\boxed{\underline{A} \parallel \underline{j}}$

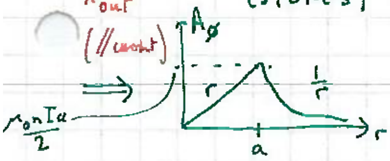
Examples - Finding $\underline{A}$

Long Solenoid :



$B_{inside} = \mu_0 n I$
$B_{outside} = 0$

$\int \underline{A} \cdot d\underline{l} = \int \underline{B} \cdot d\underline{S}$
(STOKES)



Straight Wire:

Either : use electrostat. analogy

Gauss: $E_r 2\pi r L = \frac{\rho L}{\varepsilon_0}$

$\Rightarrow \phi(r) = -\frac{q}{2\pi \varepsilon_0} \ln r$ + const.

So by analogy :

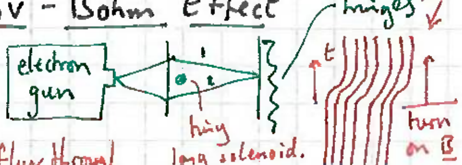
$$\boxed{A_z = -\frac{\mu_0 I}{2\pi} \ln r + \text{const}}$$

or: Stokes + Ampere

$2\pi r B_\phi = \mu_0 I$ $\to$ same answer, but not necessarily so!

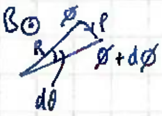
Aharanov - Bohm Effect

Detection of $\underline{A}$:



Phase diff between paths 1, 2 $= \frac{e}{\hbar} \times \Phi$ (Flux through solenoid / stokes)

because.... QM: $\psi = \psi(0) e^{\frac{-iEt}{\hbar}}$



so $d\phi = -\frac{E\, dt}{\hbar}$

$E = \frac{p^2}{2m}$ $\longleftarrow$ $\frac{mv^2}{r} = evB$

$$\Rightarrow \boxed{\phi = -\frac{e}{\hbar} \int_{path} \underline{A} \cdot d\underline{l}}$$

So phase diff $\phi_1 - \phi_2$
$= -\frac{e}{\hbar} \int_1 \underline{A} \cdot d\underline{l} + \frac{e}{\hbar} \int_2 \underline{A} \cdot d\underline{l}$
$= \frac{e}{\hbar} \oint_{loop\ 1,2} \underline{A} \cdot d\underline{l}$
$= \frac{e}{\hbar} \int \underline{B} \cdot d\underline{S}$

(ie phase shift $= \frac{e}{\hbar} \times$ total flux)

Rewriting Maxwell with $\underline{A}$, ϕ.

Maxwell : $\boxed{\nabla \cdot \underline{B} = 0} \Longrightarrow \boxed{\underline{B} = \nabla \times \underline{A}}$ $\quad \boxed{\nabla \times \underline{H} = \underline{j}_f + \frac{\partial \underline{D}}{\partial t}}$

Finding $\underline{E}$: $\boxed{\nabla \times \underline{E} = -\dot{\underline{B}}}$

$\Rightarrow \underline{E} = -\dot{\underline{A}} - \nabla \phi$

$\therefore \frac{1}{c^2} \ddot{\underline{A}} - \nabla^2 \underline{A} = \mu_0 \underline{j}_f - \nabla \underbrace{\left(\nabla \cdot \underline{A} + \frac{\dot{\phi}}{c^2} \right)}_{=0}$

$\boxed{\nabla \cdot \underline{D} = \rho_f}$

$\therefore -\nabla \cdot \dot{\underline{A}} - \nabla^2 \phi = \frac{\rho_f}{\varepsilon_0}$

use L.G. to get

$$\boxed{\begin{aligned} \nabla^2 \underline{A} - \frac{\ddot{\underline{A}}}{c^2} &= -\mu_0 \underline{j}_f \\ \nabla^2 \phi - \frac{\ddot{\phi}}{c^2} &= -\frac{\rho_f}{\varepsilon_0} \end{aligned}}$$

choosing Lorentz Gauge:

$$\boxed{\nabla \cdot \underline{A} + \frac{\dot{\phi}}{c^2} = 0}$$

Solutions of wave equations:

Retarded Potentials : $\underline{A}(\underline{r}, t) = \frac{\mu_0}{4\pi} \int \frac{\underline{j}\left(\underline{r}', t - \frac{|\underline{r} - \underline{r}'|}{c}\right)}{|\underline{r} - \underline{r}'|} dV$ $\quad (d^3 r')$

and $\phi(\underline{r}, t) = \frac{1}{4\pi \varepsilon_0} \int \frac{\rho\left(\underline{r}', t - \frac{|\underline{r} - \underline{r}'|}{c}\right)}{|\underline{r} - \underline{r}'|} d^3 \underline{r}'$ $\quad \left(t - \frac{r}{c}\right)$

ie $\underline{A}$ and ϕ now depends on ρ and $\underline{j}$ some time ago

note $\frac{\partial}{\partial t}[\rho] = [\dot{\rho}]$ and $\frac{\partial}{\partial r}[\rho] = -\frac{1}{c}[\dot{\rho}]$

Hertzian Dipole

Find $\underline{A}$ from retarded potentials $\Longrightarrow$ $\int \underline{j} \cdot dV = I\underline{L}$ $\quad \boxed{\underline{A} = \frac{\mu_0}{4\pi} \frac{[\dot{\underline{p}}]}{r}}$

Find $\underline{B}$ from $\underline{B} = \nabla \times \underline{A}$

To find $\underline{E}$: get ϕ from Lorentz Gauge
then use $\underline{E} = -\dot{\underline{A}} - \nabla \phi$ (all in sph. polars...)

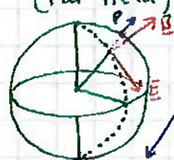
Summary: $A_\phi = 0$
$\underline{B}$ is in ϕ dir'n
$E_\phi = 0$

$\exists$ 3 types of field : $\begin{cases} \text{dipole} & \frac{[p]}{r^3} \\ \text{induction} & \frac{[\dot{p}]}{r^2} \\ \text{radiation} & \frac{[\ddot{p}]}{r} \end{cases}$

field equations

Radiation Properties :

(Far field)



$\underline{P} = \underline{E} \times \underline{H}$ radial. $\quad P = E_\theta \frac{B_\phi}{\mu_0} = \frac{\mu_0}{16\pi^2 c} \sin^2\theta \frac{[\ddot{p}]^2}{r^2}$

total radiated power

$W = \int_{sphere} \underline{P} \cdot d\underline{S} = \frac{\mu_0 [\ddot{p}]^2}{6\pi c}$ $\leftarrow$ indep of r

same across any sphere.

Power Gain $= \frac{\text{energy flux } (\theta, \phi)}{\text{average flux } (\theta, \phi)} = \frac{F(\theta, \phi)}{\frac{1}{4\pi} \int F(\theta, \phi)\, d\Omega}$

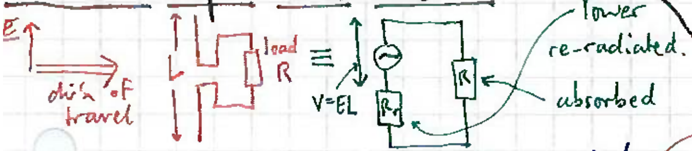
($\to$ indep!)

$= \frac{3}{2} \sin^2 \theta$ for H.D.

Radiation resistance
$= \frac{\langle W \rangle}{\langle I^2 \rangle}$ take $I = I_0 \cos \omega t$

$= \frac{2\pi}{3} Z_0 \left(\frac{L}{\lambda} \right)^2$ (for $L \ll \lambda$)

Hertzian Dipole as a Receiver



Current $I = \frac{EL}{R + R_r}$

so Power absorbed
$= \langle I^2 \rangle R = \frac{R \langle E^2 \rangle L^2}{(R + R_r)^2}$

max when matched
$R = R_r$

so $P = \frac{1}{4} \frac{3}{2\pi} \lambda^2 \frac{\langle E^2 \rangle}{Z_0}$ (incident energy flux ie $\text{J m}^{-2}\text{s}^{-1}$)

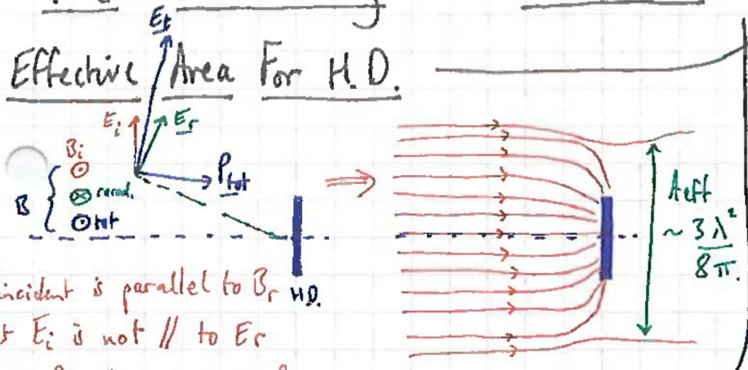
So effective area for HD $= A_{eff} = \frac{3\lambda^2}{8\pi}$ $\quad$ indep of L ($\ll \lambda$)

$(A_{eff} \gg L^2)$

Reradiated power
$= \langle I^2 \rangle R_r \neq \langle I^2 \rangle R$ in general.

Rel + Electromag: Radiation

Effective Area for H.D.

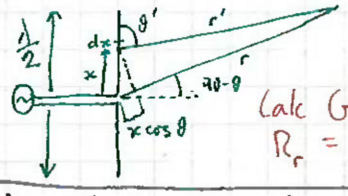


$B_{incident}$ is parallel to B_r but E_i is not // to E_r

$\Rightarrow P_{tot}$ is not // to P_{inc}.

Half Wave Dipole

unless $L = \frac{n\lambda}{2}$ get complex R_r → phaseshifts.

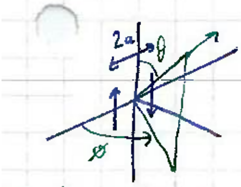


Current distribution in the dipole is $I(x,t) = I_0 \cos(kx)\sin(\omega t)$

Calc G → find ~ H.D.

$R_r = 73.1\,\Omega$ hence $75\,\Omega$ co-axial cable.

An Electric Quadrupole



out of phase, $a \ll \lambda$

Path differences w.r.t to origin $= \pm a\sin\theta\cos\phi$

$\Rightarrow$ Phase diff $= \pm\delta = \pm ka\sin\theta\cos\phi$

$\begin{pmatrix} + & - \\ - & + \end{pmatrix} \leftrightarrow \begin{pmatrix} - & + \\ + & - \end{pmatrix}$

Resultant mag. field

$B = \left(e^{i\delta} - e^{-i\delta}\right)\frac{\mu_0 [\dot{I}] L\sin\theta}{4\pi r c} = i2ka\frac{\mu_0[\dot{I}]L}{4\pi r c} \times \sin^2\theta\cos\phi$

π out of phase already

So $B_{quad} \simeq \underbrace{2ka}_{\frac{4\pi a}{\lambda}} B_{dipole}$

So $\frac{\text{Quad power}}{\text{Dip. power}} = \left(\frac{4\pi a}{\lambda}\right)^2$

Power $\propto \sin^4\theta$ ∴ more directional than dipole ($\sin^2$)

NOT cylindrically symmetric.

Electric vs Magnetic Dipoles

To get magnetic dipole from electric (or vice versa) replace:

$\left[\begin{array}{l} \underline{B} \text{ with } -\underline{E} \\ \underline{E} \text{ with } +\underline{B} \end{array}\right]$ sign change...

$[p]$ with $[m]$

$\frac{1}{\varepsilon_0}$ with μ_0

Relative strengths:

$$\frac{|\underline{P}|_{ED}}{|\underline{P}|_{MD}} = \frac{\left|\frac{\mu_0}{4\pi}\frac{[\ddot{p}]\sin\theta}{rc}\cdot\frac{1}{4\pi\varepsilon_0}\frac{[\ddot{p}]\sin\theta}{rc^2}\right|}{\left|\frac{\mu_0}{4\pi}\frac{[\ddot{m}]\sin\theta}{rc^2}\cdot\frac{-1}{4\pi\varepsilon_0}\frac{[\ddot{m}]\sin\theta}{rc^3}\right|}$$

$$= \frac{c^2[\ddot{p}]^2}{[\ddot{m}]^2} \simeq \frac{c^2(\omega^2 IL)^2}{(\omega^2 IL^2)^2} = \left(\frac{\lambda}{2\pi L}\right)^2 \gg 1$$

Thompson Scattering (from free electrons)

$\uparrow E \quad \uparrow z$

Eq'n of motion: $m_e\ddot{z} = -eE_0 e^{i\omega t} \Rightarrow \boxed{\sigma_T = \frac{\mu_0^2 e^4}{6\pi m_e^2}}$

$\ddot{p} = -e\ddot{z}$

indep of λ except at v. small λ when cannot ignore photon momentum] Compton effect.

Classical Electron radius, r_e

dist apart s.t. E is mc^2

ie $\frac{e^2}{4\pi\varepsilon_0 r_e} = m_e c^2 \Rightarrow \sigma_T \sim 10 r_e^2$

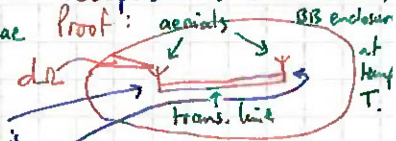
Scattering from pure crystals etc still happens, but it destructively interferes...

Relation to Power Gain:

Reciprocity theorem: Polar diagram of any antenna is same for reception as transmission.

$\boxed{A_{eff} = \left(\frac{\lambda^2}{4\pi}\right) G}$ ∀ antennae

Proof:



Power from Johnson noise in R is absorbed in R' and vice versa.

Detailed balance $\Rightarrow \langle I^2\rangle R = \langle I^2\rangle R'$

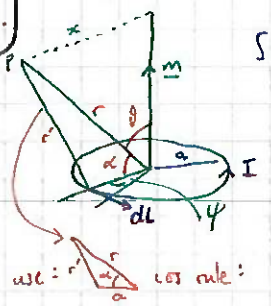
Thermal eq $\Rightarrow$ mean power sent into dΩ = that received

ie. $\langle I^2\rangle R.\frac{d\Omega}{4\pi} G = A_{eff}\, f(T)\, d\Omega$ (B.B. R. flux)

$\Rightarrow \boxed{\frac{A_{eff}}{G} = \frac{A_{eff}'}{G'} = k}$ $\left(k_{H.D.} = \frac{\lambda^2}{4\pi}\right)$

Magnetic Dipole

Retard pot: $\underline{A} \propto \int \frac{[\underline{j}]}{r} dV$



So $A_\phi = \frac{\mu_0}{4\pi}\int\frac{[I]\,dL}{r'}$

$= \int_0^{2\pi} \frac{a\,d\psi\cos\psi}{r'} I_0 e^{i\omega(t - \frac{r'}{c})} \cdot \frac{\mu_0}{4\pi}$

use: cos rule: $r' = r\left(1 - \frac{a}{r}\cos\alpha\right)$ and $\frac{1}{r'} = \frac{1}{r}\left(1 + \frac{a}{r}\cos\alpha\right)$

and $\underbrace{r a\cos\alpha}_{\underline{r}\cdot\underline{a}} = \begin{pmatrix} x \\ 0 \\ z \end{pmatrix}\cdot\begin{pmatrix} a\cos\psi \\ a\sin\psi \\ 0 \end{pmatrix} = x a\cos\psi$

and expand exponential $\rightarrow A_\phi = \frac{\mu_0}{4\pi}\left(\frac{[m]}{r^2} + \frac{[\dot{m}]}{cr}\right)\sin\theta$

$A_r = A_\theta = 0$

Then $\underline{B} = \underline{\nabla}\times\underline{A}$ gives B_r, B_θ, B_ϕ

and $\underline{\nabla}\cdot\underline{A} = 0 \Rightarrow \underbrace{\phi \text{ taken as } 0}_{\text{Lorentz Gauge}}$ so $\boxed{\underline{E} = -\dot{\underline{A}}}$ $(\Rightarrow E_r = E_\theta = 0)$

Scattering by Particles

E field incident on particle creates dipole which re-radiates: $W = \frac{\mu_0\langle\ddot{p}^2\rangle}{6\pi c}$

Cross section:

$\sigma = \frac{W}{\text{Incident flux}} = \frac{W}{\text{energy density} \times \text{speed}}$

usually $p \propto E_0$ so σ not a f'n of E_0!

Rayleigh Scattering (from neutral particles)

In general, $p = \alpha E \Rightarrow \sigma_R = \frac{\mu_0^2\omega^4\alpha^2}{6\pi} \propto \frac{1}{\lambda^4}$ (λ^4 law)

eg for dielectrics $\alpha = \varepsilon_0(\varepsilon - 1)a^3$ (sphere rad a)

conductors $\alpha = 4\pi\varepsilon_0 a^3$ (sphere rad. a)

Dependence on particle seperation d: $(L \gg d)$ (in volume $V = L^3$)

For $\lambda \ll d$, expect incoherent scattering for n particles, total power $\propto n$

For $\lambda \gg d$, expect coherent scattering - and get it! for n particles, total power is still $\propto n$! coz scattering occurs from fluctuations which are still random

Rel + Electromag. :

Evidence for charge invariance

Atoms are neutral in gas even when warmed or cooled !

Particle accelerators / mass spec etc use $\frac{e}{m}$. Variations with v totally explained by taking $m = \gamma m_0$

Relativistic Electrodynamics.

The 4 - Gradient

$\underset{\sim}{\square} = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\underline{\nabla}\right)$ is it a 4 vector?

Yes because its components transform according to the L.T.

In S' (IRF) $\forall$ derivatives...

$$\frac{\partial}{\partial t'} = \underbrace{\frac{\partial t}{\partial t'}}_{\gamma}\frac{\partial}{\partial t} + \underbrace{\frac{\partial x}{\partial t'}}_{\gamma V}\frac{\partial}{\partial x} + \underbrace{\frac{\partial y}{\partial t'}}_{0}\frac{\partial}{\partial y} + \underbrace{\frac{\partial z}{\partial t'}}_{0}\frac{\partial}{\partial z}$$

$$\therefore \frac{1}{c}\frac{\partial}{\partial t'} = \underbrace{\gamma\left[\left(\frac{1}{c}\frac{\partial}{\partial t}\right) - \frac{V}{c}\left(-\frac{\partial}{\partial x}\right)\right]}$$

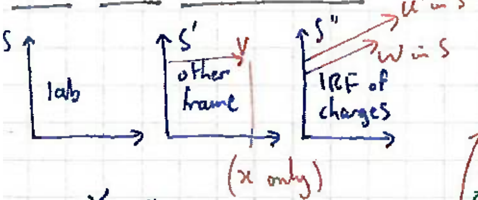
Lorentz Transform. same for $-\underline{\nabla}'$

$\Rightarrow \underset{\sim}{\square}\cdot\underset{\sim}{\square} = \square^2 = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 \equiv$ Wave operator is Lorentz invariant.

Aside : $i\hbar\underset{\sim}{\square} = \left(\frac{\hat{E}}{c}, \hat{\underline{p}}\right)$ in Q.M. and $\square^2$ gives the Klein - Gordan eq'n for spinless particle :

$$\boxed{\square^2\psi = m_0^2c^2\psi}$$

Charge Invariance and the 4 - Current



Transform charges and currents from S into S' via S''. vol. occupied is contracted

$$j_x = \overbrace{W_x\rho}^{\text{in S}} = W_x\overbrace{\gamma_w}\rho'' \leftarrow \text{can write in S' by } \rho' = \gamma_u'\rho''$$

{ordinary velocity transformation : W_x = etc.

Transform 4-vel 1st component to get

$$= \underbrace{\frac{u_x' + V}{1 + \frac{u_x'V}{c^2}}} \cdot \underbrace{\gamma_V\gamma_{u'}\left(1 + \frac{Vu_x'}{c^2}\right)} \cdot \frac{\rho'}{\gamma_u'} = \gamma_V(\underbrace{u_x'\rho'}_{j_x'} + V\rho')$$

ie in the form of Lorentz Trans! $(j_y = j_y')$

$\rho = \gamma_w\rho''$

$$= \gamma_V\gamma_{u'}\left(1 + \frac{V\overset{j_x'}{u_x'}}{c^2}\right)\frac{\rho'}{\gamma_u'}$$

$$= \underbrace{\gamma_V\left(\rho' + \frac{V}{c^2}j_x'\right)}_{\text{Lorentz transform!}}$$

$\Rightarrow \boxed{\underset{\sim}{j} \equiv (c\rho, \underline{j})}$ is a 4-vector $\boxed{\underset{\sim}{j}\cdot\underset{\sim}{j} = c^2\rho^2 - j^2 = c^2\rho_0^2}$ invariant

$S \to S'$ is independent of S'' so any superposition of currents / charges is OK.

cf. ρ multiplied by $\underset{\sim}{u} = (\gamma c, \gamma\underline{u})$!

The 4 - Potential

$\boxed{\underset{\sim}{A} = \left(\frac{\phi}{c}, \underline{A}\right)} \Rightarrow \boxed{\square^2\underset{\sim}{A} = \mu_0\underset{\sim}{j}}$ 1st component gives ϕ wave eq'n others give $\underline{A}$ eq'ns.

$\boxed{\underset{\sim}{\square}\cdot\underset{\sim}{A} = 0}$ is Lorentz Gauge (Scalar prod of 2 4-vecs) $\Rightarrow$ invariant

In IRF, $\to$ Coulomb gauge !

To allow for dielectric media, change $c = \frac{1}{\sqrt{\epsilon\epsilon_0\mu\mu_0}}$

Conservation of Charge

$\underset{\sim}{\square}\cdot\underset{\sim}{j}$ = Invariant = 0 ie $\boxed{\underset{\sim}{\square}\cdot\underset{\sim}{j} = 0}$

because:

$\hookrightarrow \frac{\partial\rho}{\partial t} + \underline{\nabla}\cdot\underline{j} = ?$

Maxwell. $\underbrace{\nabla\times\underline{B} = \mu_0\left(\epsilon_0\frac{\partial\underline{E}}{\partial t} + \underline{j_c}\right)}$

take divergence.... get = 0 ! use M1 !

Transforming E and B

$$\boxed{\begin{array}{ll} E_{\parallel}' = E_{\parallel} & B_{\parallel}' = B_{\parallel} \\ E_{\perp}' = \gamma(\underline{E} + \underline{V}\times\underline{B})_{\perp} & B_{\perp}' = \gamma\left(\underline{B} - \frac{1}{c^2}[\underline{V}\times\underline{E}]\right)_{\perp} \end{array}}$$

Prove by taking 1st Lorentz Transform of $\underset{\sim}{A}$ and $\underset{\sim}{\square}$ (to get derivatives)

then : calc $\underline{B} = \underline{\nabla}\times\underline{A}$

and $\underline{E} = -\underline{\nabla}\phi - \dot{\underline{A}}$

Transforming Maxwell's Equations : For example take

(Same Physics in all frames.....)

x component of $\left(\underline{\nabla}\times\underline{B} - \frac{1}{c^2}\frac{\partial\underline{E}}{\partial t} = \mu_0\underline{j}\right)$

$$\text{In S': } \left(\underline{\nabla}'\times\underline{B}' - \frac{1}{c^2}\frac{\partial\underline{E}'}{\partial t'}\right)_x = \frac{\partial B_z'}{\partial y'} - \frac{\partial B_y'}{\partial z'} - \frac{1}{c^2}\frac{\partial E_x'}{\partial t'}$$

$$= \frac{\partial}{\partial y}\gamma\left(B_z - \frac{VE_y}{c^2}\right) - \frac{\partial}{\partial z}\gamma\left(B_y + \frac{VE_z}{c^2}\right) - \frac{\gamma}{c^2}\left(\frac{\partial}{\partial t} + V\frac{\partial}{\partial x}\right)E_x$$

$$= \gamma\left[\left(\underline{\nabla}\times\underline{B} - \frac{1}{c^2}\frac{\partial\underline{E}}{\partial t}\right)_x - \frac{V}{c^2}\underline{\nabla}\cdot\underline{E}\right] = \gamma\left(\mu_0 j_x - \frac{V}{c^2}\frac{\rho}{\epsilon_0}\right)$$

$$= \mu_0 j_x' \text{ by L.T.}$$

Magnetism as a rel. effect

wire $\longrightarrow$ I In S (lab frame)

q (charge) $\longrightarrow$ vel V $\rho = 0$, $j_x = \frac{I}{\text{Area}}$

In S' (rest frame of charge), $j_x' = \gamma(j_x - V.0)$

$\exists$ charge density ! $\to \rho' = \gamma\left(0 - \frac{V}{c^2}j_x\right) = \frac{-\gamma VI}{c^2 A_r}$

So Gauss $\Rightarrow$ radial $\underline{E}$ field $= -\frac{\mu_0 I}{2\pi r}\gamma V$ $\Rightarrow$ So force on q $= \underbrace{-\frac{\mu_0 I}{2\pi r}}\gamma Vq \left(= \frac{dp_y'}{dt'}\right)$ ($\perp$ in V)

$\left.\begin{array}{l} p_y' = p_y \\ \frac{d}{dt'} = \gamma\frac{d}{dt} \end{array}\right\} \Rightarrow \frac{dp_y}{dt} = -qVB$ (Lorentz force)

ie electric force in one frame is mag force when measured in the other frame!

Magnitude of forces :

$$\frac{|\text{magnetic force}|}{|\text{electric force}|} = \frac{V^2}{c^2} \simeq 10^{-23} !$$

But OK. ie electro-static force doesn't swamp mag force because $\exists$ neutrality to better than 1 part in 10^{23} in universe!

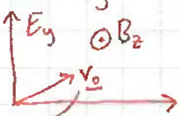
$\Rightarrow$ Mag forces are rel. effects with $\underline{V} \simeq 10^{-11}$

Rel + Electromag

Crossed $\underline{E}$ and $\underline{B}$ fields

N.B. if $\underline{E}$ and $\underline{B}$ $\perp$ in one frame they are $\perp$ in all frames

eg $\underline{E}$ in y dir'n, $\underline{B}$ in z dir'n:



In S' $E_y' = \gamma(E_y - VB_z)$

$B_z' = \gamma\left(B_z - \frac{V}{c^2}E_y\right)$

(the other components $= 0$)

speed of charged particle

(If $E_y < cB_z$) now choose V s.t. $V = \frac{E_y}{B_z}$

Then $E_y' = 0$ – only mag. field $\left(= \frac{B_z}{\gamma}\right)$ sol'n is circular motion – then transform back to S

If $E_y > cB_z$ choose $V = \frac{B_z c^2}{E_y}$ $(< c)$

then $B_z' = 0$

– get only Elec field $= \frac{E_y}{\gamma}$ etc...

Charge moving very fast.

For $\gamma \sim 1$ $\underline{E}$ is radial + isotropic, $\underline{B}$ azimuthal and small.

$\gamma \gg 1$: $\theta = 0$, $E_{\parallel}$ v. small $\left(\sim \frac{1}{\gamma^2}\right)$

$\theta = \frac{\pi}{2}$ $E_{\perp}$ v. larrge

So fields are flattened into plane $\perp$ to motion ie particle $\longrightarrow$ e/m wavepacket!

Radiation by accelerated charge

$\gamma \sim 1$ get dipole pattern

(p 955)

In IRF of charge, const field E_0 gives radiated power $W_0 = \sigma_T \cdot \underbrace{\tfrac{1}{2}\varepsilon_0 E_0^2}_{U_0} c \times 2$

$W_0 = -\frac{d\mathcal{E}_0}{d\tau}$ $\left.\begin{array}{l}\mathcal{E}_{lab} = \gamma\mathcal{E}_0 \\ dt_{lab} = \gamma d\tau\end{array}\right]$ cancel

$\Rightarrow$ $W_{lab} = W_0 = 2c\sigma_T U_0$

CHARGE IN MAGNETIC FIELD:

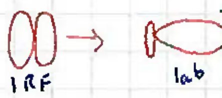
Circular orbit with $qVB = \dot{p} = \omega\gamma m_0 V$

where $\omega = \frac{\omega_g}{\gamma}$ $\left(\omega_g = \frac{qB}{m_0}\right)$

$\gamma \sim 1$

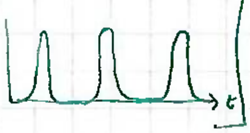
Distant observer sees two dipoles in quadrature freq $\sim \omega_g$] cyclotron

$\gamma \gg 1$



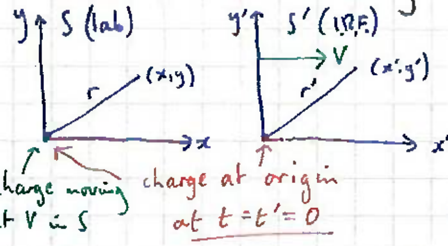
syncrotron radiation.

see:



Relativistic Electrodynamics

Fields due to Uniformly Moving Charge



Can write $\underline{E}'$ easily coz $\underline{A} = 0$ in IRF:

$\underline{E}' = \frac{q}{4\pi\varepsilon_0}\left(\frac{x'}{r'^3}, \frac{y'}{r'^3}, 0\right)$

then transform $\underline{E}' \longrightarrow \underline{E}$ $(E_x, E_y, 0)$ and use $x' = \gamma x$ and $y = y'$ (L.T.)

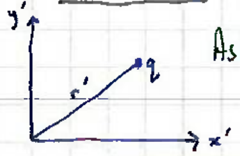
System has axial sym about x axis $\equiv$ polar axis with $x = r\cos\theta$, $y = r\sin\theta$

So $r'^2 = x'^2 + y'^2 = \gamma^2 r^2\left(1 - \frac{V^2}{c^2}\sin\theta\right)$

$\Rightarrow$ $E_{\parallel} = \frac{q\cos\theta}{4\pi\varepsilon_0\gamma^2 r^2\left(1 - \frac{V^2}{c^2}\sin\theta\right)^{3/2}}$ $\quad E_{\perp} = \frac{q\sin\theta}{4\pi\varepsilon_0\gamma^2 r^2\left(1 - \frac{V^2}{c^2}\sin\theta\right)^{3/2}}$

$\left(B_r = B_\theta = 0 \quad B_\phi = \frac{V}{c^2}E_{\perp}\right)$ ← Fields in frame where particle is moving at V

Lienard – Wiechart Potentials



Ask: what is potential at origin in S (frame where q is moving at V)?

In S', q at rest so $\underline{A}' = \left(\frac{\phi'}{c}, \underline{A}'\right)$ $= \left(\frac{q}{4\pi\varepsilon_0 r'c}, \underline{0}\right)$ earlier!

Transform → $\underline{A} = \left(\frac{\gamma q}{4\pi\varepsilon_0 cr'}, \frac{\beta\gamma q}{4\pi\varepsilon_0 cr'}, 0, 0\right)$

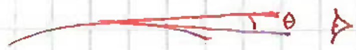
but what is r' in S? Effects travel at c so $r' = -ct'$

transform → $\left(t - \frac{V}{c^2}x\right)$

$\Rightarrow$ $r' = \gamma\left(r + \frac{\underline{V}\cdot\underline{r}}{c}\right)$ → L-W Potentials.

If charge accelerating, E points to where it would have been if it had carried on with const vel.

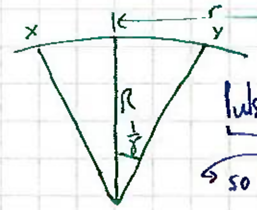
Synchrotron Radiation



From L-W (small θ, big γ approx's) or aberration results, get:

Pulse width $\sim \frac{2}{\gamma}$ (radians)

So might expect pulse of duration $\frac{2}{\omega\gamma}$ but no!



see leading edge at X, trailing edge at Y

Pulse duration: $\delta t = \underbrace{\frac{1}{c}\left(r - \frac{R}{\gamma}\right)}_{\text{light travel time}} + \underbrace{\frac{2R}{\gamma V}}_{\text{time } X\to Y} - \underbrace{\frac{1}{c}\left(r + \frac{R}{\gamma}\right)}_{\text{light travel time}}$

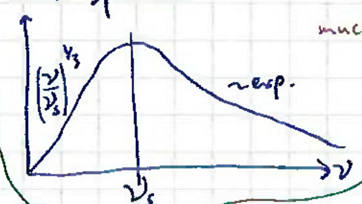
so $\delta t \sim \frac{1}{\gamma^3\omega}$

δt is shorter than might be expected by $\frac{1}{\gamma^2}$!

Observed spectrum contains signif. contributions at $2\pi\nu_s = \frac{1}{\delta t} = \gamma^2\omega_g$

much higher frequencies than ω_g!

Power spectrum:



$W_{lab} = 2c\sigma_T U_0$ → In IRF $E_0 = \gamma V B_{lab}$

$U_0^{elec} = \frac{\varepsilon_0 E_0^2}{2} = \beta^2\gamma^2\frac{B_{lab}^2}{2\mu_0}$ → U_{lab}^{mag}

– sets limit on energy attainable in circular particle accelerators

$\Rightarrow$ $\boxed{W_{lab} = 2c\sigma_T U_{lab}^{magnetic}(\beta\gamma)^2}$

TP2: BASIC LAGRANGIAN MECHANICS

Lagrange's Eq'ns of motion

$$\boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right) - \frac{\partial L}{\partial q_i} = 0}$$

Consider N particle system, in cartesian coords has pot $V(x_1 \dots x_n)$ $n = 3N$.

$p_i = m v_i = \frac{\partial T}{\partial v_i} = \frac{\partial L}{\partial \dot x_i}$ so eq'ns of motion obey Hamilton's Principle ....

$F_i = -\frac{\partial V}{\partial x_i} = \frac{\partial L}{\partial x_i}$

$\Rightarrow$ can use in any coord system, get

Hamilton's Principle:

System moves from $A \to B$ such that $\int_A^B L\,dt$ is minimum

The statement is indep of any particular coord. sys.

Symmetry and Conservation Laws

If system (L) is independent of a coordinate q_i then $L(q_i + \epsilon)\big|_{\substack{\text{const}\\ \text{else}}} = L(q_i) + \epsilon \frac{\partial L}{\partial q_i} = L(q_i)$

ie it is invariant under displacements of q_i (SYMMETRY)

then E-L $\Rightarrow \frac{\partial L}{\partial \dot q_i} = $ Const. (ie CONSERVATION LAW)

L indep of position $\Leftrightarrow$ total linear momentum conserved.

L indep of orientation $\Leftrightarrow$ total angular momentum conserved.

L independent of time (explicitly) $\Rightarrow 2T - T + V = T + V = E$ total energy.

(IF V is independent of velocity so that $\frac{\partial L}{\partial \dot q_i} = mv$)

E-L equation if L independent of time

$$\sum_i \dot q_i \frac{\partial L}{\partial \dot q_i} - L = C$$

Velocity Dependent Potentials

If can find V s.t. $F_i = -\frac{\partial V}{\partial q_i} + \frac{d}{dt}\left(\frac{\partial V}{\partial \dot q_i}\right)$

then E-L eq'ns still hold.

So $-\frac{\partial V}{\partial q_i} + \frac{d}{dt}\left(\frac{\partial V}{\partial \dot q_i}\right) = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right)$

$\Rightarrow$ new momentum

Hamilton's Equations

Define: "Generalised" or "Canonical" Momentum to be $p_i = \frac{\partial L}{\partial \dot q_i}$ then re-write eq'ns of motion as $f(p_i, q_i)$ and so get rid of velocity: $\dot q_i$.

$\delta L = \frac{\partial L}{\partial t}\delta t + \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot q_i}\delta \dot q_i$ but E-L $\Rightarrow \frac{\partial L}{\partial q_i} = \dot p_i$

$\Rightarrow \delta L = \frac{\partial L}{\partial t}\delta t + \dot p_i \delta q_i + p_i \delta \dot q_i$ so $\delta(L - p_i \dot q_i) = \frac{\partial L}{\partial t}\delta t + \dot p_i \delta q_i - \dot q_i \delta p_i$

$\Rightarrow \dot p_i = \frac{\partial H}{\partial q_i}\Big|_{\text{other } p_i, q_i, t}$ and $\dot q_i = -\frac{\partial H}{\partial p_i}\Big|_{\text{others}}$ where $H = p_i \dot q_i - L$

OK for $V(\dot q_i)$, can see symm $\Leftrightarrow$ cons laws easier, if $V = V(q_i)$ or linearly dep on $\dot q_i$ then $H = T + V$ eg mag.

Hamilton's Principle of Least Action.

For a system of FIXED ENERGY, system moves from $A \to B$ such that $\int_A^B p \cdot dq$ is minimum

$\delta S = \delta \int_A^B (p \cdot \dot q - H)\,dt = \delta \int p\,dq - E\,dt$

Also, can go from $q_1, t_1 \to q_2 - \delta q_2, t_2$ then ask what is variation due to extra time δt:

$\delta S = \int_{q_1, t_1}^{q_2 - \delta q_2, t_2} \delta L\,dt + L(q_2, \dot q_2, t_2)\delta t$

$\delta L = \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot q_i}\delta \dot q_i$

$= \left[\frac{\partial L}{\partial \dot q_i}\delta q_i\right]_{q_1, t_1}^{q_2 - \delta q_2, t_2} + \int \frac{\partial L}{\partial q_i}\delta q_i - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right)\delta q_i + L\delta t$

but $\delta q_i\big|_{q_1} = 0$ $\therefore -p_2 \cdot \delta q_2 + (p_2 \cdot \dot q_2 - H)\delta t$

$\Rightarrow \delta S = -E\delta t + \int\left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right)\right)\delta q_i\,dt$

0 by E-L compare

$\Rightarrow \delta \int \underbrace{p \cdot dq}_{\text{action}} = 0$ QED.

Classical Approximation to Quantum Mechanics

QM $\Rightarrow \frac{d\Psi}{dt} = \mathcal{O}\left(\frac{\partial}{\partial q_i}, q_i\right)\Psi$ Classical limit: λ much shorter than system (ie scale of var. of V) (energy (freq) very high) and small mom range where Ψ big (Ψ vs mom) then the QM waves are locally like plane waves

so $\Psi = \Psi_0(q, t) e^{i(k_i q_i - \omega t)}$

so $\frac{\partial \Psi}{\partial t} = \frac{\partial \Psi_0}{\partial t} e^{i(\ )} - i\omega\Psi$

$\simeq -i\omega\Psi$ if $\frac{\partial \Psi_0}{\partial t}$ small and $\frac{\partial \Psi}{\partial q_i} = ik_i\Psi + \frac{\partial \Psi_0}{\partial q_i} e^{i(\ )} \simeq ik_i \Psi$

QM condition: constructive interference, ie $\int k \cdot dq - \omega\,dt$ stationary

But $\omega = i\,\mathcal{O}(ik_i, q_j)$

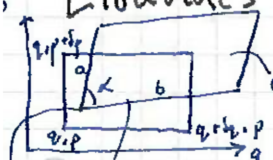
so $\delta \int k \cdot dq - i\,\mathcal{O}(ik_i, q_j)\,dt = 0$ compare to classical: $\delta \int \frac{p \cdot dq}{\hbar} - \frac{H\,dt}{\hbar} = 0$

So can get A Q.M. description of classical sys with $\mathcal{O}$ s.t. same function of $\frac{\partial}{\partial q_i}$ as p_i in H..... (?)

Not unique though eg electron spin (remember Hermiticity of Operators)

Liouville's Theorem:

Volume in phase space occupied by set of representative points is conserved. (for a non-dissipative system.)



area $= \frac{1}{2}ab\sin\alpha$

$\simeq$ horiz comp of b $\times$ vert comp of a.

$= (\dot q dt + \delta\dot q dt - \dot q dt + \delta q) \times (\dot p dt + \delta \dot p dt - \dot p dt + \delta p)$

$\delta \dot q = \frac{\partial \dot q}{\partial q}\delta q = \frac{\partial^2 H}{\partial q \partial p}\delta q$ $\left(-\frac{\partial^2 H}{\partial p \partial q}\delta p\right)$

after time dt this pt has moved $\dot q\,dt$ to right

so area $= \delta q \delta p \left(1 + \frac{\partial^2 H\,dt}{\partial q \partial p}\right)\left(1 - \frac{\partial^2 H}{\partial p \partial q}dt\right) = \delta q \delta p$ to 1st order in dt

Put together lots of such rectangles, get L.Th.

More formal proof: $\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + (\underline{v} \cdot \underline{\nabla})\rho$

$= -(\underline{\nabla} \cdot \rho \underline{v}) + (v \cdot \nabla \rho)$

$= -\rho(\underline{\nabla} \cdot \underline{v}) - \cancel{(\underline{v} \cdot \underline{\nabla})\rho} + \cancel{(v \cdot \nabla)\rho}$

but $\underline{\nabla} \cdot \underline{v} = \frac{\partial \dot p}{\partial p} + \frac{\partial \dot q}{\partial q} = 0$ as $\underline{v} = (\dot p, \dot q)$?

$\therefore \frac{D\rho}{Dt} = 0$ density constant.

Only for Conservative (non-diss.) systems.

TP2: Lagrangian Mechanics (Continued)

Charged Particle In E.M. field:

$\underline{F} = e(\underline{E} + \underline{v} \times \underline{B})$ $\therefore \underline{F} = e\left(-\nabla\phi - \frac{\partial \underline{A}}{\partial t} + \underline{v} \times \nabla \times \underline{A}\right)$ $\therefore F = e\left(-\nabla[\phi - (\underline{v}\cdot\underline{A})] - \frac{D\underline{A}}{Dt}\right)$

but $\underline{E} = -\nabla\phi - \frac{\partial \underline{A}}{\partial t}$ and $\underline{B} = \nabla \times \underline{A}$ $\quad [= \nabla(\underline{v}\cdot\underline{A}) - (\underline{v}\cdot\nabla)\underline{A}]$ ie let $V = e(\phi - \underline{v}\cdot\underline{A})$

So can write $\underline{F} = -\frac{\partial V}{\partial q_i} + \frac{d}{dt}\left(\frac{\partial V}{\partial \dot{q}_i}\right)$ so $L = \frac{1}{2}m\dot{q}_i^2 - e(\phi - \dot{q}_i A_i)$ and $p_i = m\dot{q}_i + eA_i$

Hamiltonian $H = p_i\dot{q}_i - L = \frac{1}{2}m\dot{x}^2 + e\phi$ (total energy) and $H = \frac{1}{2m}(p_i - eA_i)^2 + e\phi$

Relativistic Particle: (free)

Route 1: (to the Lagrangian)

Guess $\underline{p} = \frac{\partial L}{\partial \underline{v}} = \gamma(v) m_0 \underline{v}$ — expand in powers of v^2/c^2, get non-rel limit.

Integrate $\int d\underline{v} \Rightarrow \boxed{L(\underline{r},\underline{v}) = -\frac{m_0 c^2}{\gamma} - f(r)}$

where $f(\underline{r}) = V(\underline{r})$ by requiring that E-L gives correct eq'ns of motion.

So for free relativistic particle trajectory in space time from one event to another extremises the elapsed proper time

Route 2: Analyse in co-moving ish frame and find frame-invariant form: $S = \int L dt = \int \underline{p}\cdot d\underline{r} - H dt$

ie $S = -\int p_\mu dx^\mu$ (in four vectors)

[This is frame inv!] compare

In IRF $= m_0 c^2 d\tau$ In other frame $\therefore$ OK

$S = \int \frac{m_0 c^2}{\gamma} dt$

Always use $\frac{dt}{\gamma}$ for proper time. coz b.c's.....

Rel. particle in a potential field.

Four-potential contribution $-\int V dt - \underline{A}\cdot d\underline{r} = -\int A_\mu dx^\mu$

then get: $\boxed{S = -\int m_0 c^2 d\tau - \int q A_\mu dx^\mu}$

free particle + field interaction.

Mechanical Mom: $p^m = \gamma m_0 \underline{v}$

Canonical Mom: $p^c = \frac{\partial L}{\partial v} = \gamma m_0 \underline{v} + q\underline{A}$

from $\boxed{L = -\frac{m_0 c^2}{\gamma} - q(V - \underline{A}\cdot\underline{v})}$

So Action is $S = -\int p^c_\mu dx^\mu$ and $p^c_\mu = \gamma m_0 \frac{dx_\mu}{dt} + qA_\mu$

Note on Lagrange vs Hamilton

Hamiltonian and Lagrangian are not frame indep but Lag. Action S is

Basic Continuous Systems

Eg 1-D sound. $x \to x + u(x,t)$

dynamical variable is $\underline{u}$ not x. displacement u dep on x and time.

Lagrangian $L = T - V = \int \frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2 dx - \int \frac{1}{2}k\left(\frac{\partial u}{\partial x}\right)^2 dx$ (elastic P.E.)

So Lag. Action $S = \int L dt = \iint \mathcal{L}\, dx\, dt$ where $\mathcal{L}$ is the

Lagrangian density $\mathcal{L} = \frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2 - \frac{1}{2}k\left(\frac{\partial u}{\partial x}\right)^2$

$\Rightarrow$ E-L eq'ns are now: $\boxed{\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial t}\right)} + \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x}\right)}}$

(subject to: u or $\frac{\partial u}{\partial x}$ fixed at spatial boundaries, same for t)

In this case, get $0 = \frac{\partial}{\partial t}\rho\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}k\frac{\partial u}{\partial x}$ ie 1-D wave eq'n.

Canonical Momentum Density $\pi = \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial t}\right)}$ $\left(= \rho\frac{\partial u}{\partial t}\right.$ in this case ie normal mom density$\left.\right)$

Conservation law for $\frac{\partial \mathcal{L}}{\partial u} = 0$:

E-L $\Rightarrow \boxed{\frac{\partial \pi}{\partial t} + \frac{\partial}{\partial x} j = 0}$ so interpret $j = \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x}\right)}$ as current of can. mom

so can. mom overall is conserved

ie springs cause exchange of momentum as if $k = 0$, get $j = 0$

Continuous Systems in d-dimensions

keep $u(\underline{r},t)$ scalar: $S = \iint\ldots\int dt\,dx_1\ldots dx_d\, \mathcal{L}\left(u, \frac{\partial u}{\partial t}, \nabla u\right)$

E-L eq'ns for $\delta S = 0$ are:

$\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial t}\right)} + \frac{\partial}{\partial x_1}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x_1}\right)} + \ldots$ etc. $\to$ or can write more neatly as: $\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial t}\right)} + \nabla\cdot\frac{\partial \mathcal{L}}{\partial(\nabla u)}$

or more neatly still:

$\boxed{\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial}{\partial x^\mu}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x^\mu}\right)}}$ — have put t and r on same footing — x^μ looks like 4-vec but eq'ns not particular to Special Relativity

A More complicated Continuous System. 3D elasticity.

displacement field $\underline{u} = (u_1, u_2, u_3)$. Strain tensor $e_{ij} = \frac{\partial u_j}{\partial x_i} = \partial_i u_j$ (unsymmetrised)

Stress tensor $\sigma^{ij} = C^{ijkl}e_{kl} = C^{ijkl}\partial_k u_l$

C, the elasticity tensor is symm. wrt to interchanging: (k,j), (k,l), (ij,kl).

Stored elastic energy: $V = \frac{1}{2}e_{ij}\sigma^{ij} = \frac{1}{2}\partial_i u_j C^{ijkl}\partial_k u_l$ $\quad \frac{\partial V}{\partial(\partial_j u_i)} = C^{ijkl}\partial_k u_l$ use in E-L

Lagrangian density $\mathcal{L} = \frac{1}{2}\left(\rho\left(\frac{\partial u}{\partial t}\right)^2 - \partial_i u_j C^{ijkl}\partial_k u_l\right)$

E-L eq'ns $\Rightarrow$ $\boxed{0 = \underbrace{\frac{\partial}{\partial t}\rho\frac{\partial u_i}{\partial t}}_{\text{mass}\times\text{acc'n}} + \underbrace{\frac{\partial}{\partial x_j}\overbrace{C^{ijkl}\partial_k u_l}^{\sigma^{ij}}}_{\text{force}}}$ (general eq'n of sound)

The EM field itself

The free field: $F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha$ (antisym)

S is frame inv. scalar so $\mathcal{L}$ must be too with E-L eq'ns that are linear in $\underline{E}, \underline{B}$ $\therefore \mathcal{L}$ must be $\leq$ quadratic

try $\mathcal{L}_0 = aF_{\alpha\beta}F^{\alpha\beta}$ (a const)

Effect of currents on the field: $\mathcal{L}_1 = j^\mu A_\mu$

So we get: $\boxed{\mathcal{L} = aF_{\alpha\beta}F^{\alpha\beta} - j^\mu A_\mu}$

S but not $\mathcal{L}$ is gauge invariant if current is conserved and does not flow through boundaries.

But is it really electromagnetism?

Check: For $\delta S = 0$, E-L eq'ns are $\Rightarrow$

$\frac{\partial \mathcal{L}}{\partial A_\alpha} = \frac{\partial}{\partial x^\mu}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial A_\alpha}{\partial x^\mu}\right)}$ $\quad$ [LHS is $-j^\alpha$]

RHS: need $\frac{\partial}{\partial(\partial_\mu A_\alpha)} aF_{\delta\gamma}F^{\delta\gamma} = 4aF^{\mu\alpha}$

$j^\alpha + 4a\partial_\mu F^{\mu\alpha} = 0$

or $j^\alpha + 4a\left(\underbrace{\partial_\mu\partial^\mu}_{\Box^2} A^\alpha - \partial^\alpha\overbrace{\partial_\mu A^\mu}^{\text{Lorentz gauge},\ =0}\right) = 0$

$4a = -\mu_0$

ie Maxwell's Equations

Summary:

The action for e/m field and charged relativistic particles is:

$$S = \sum_{\text{particles}}\left[\underbrace{-\int m_0 c^2 d\tau}_{\text{free particles}} - \underbrace{\int q A_\mu dx^\mu(t)}_{\text{coupling to field}}\right] - \underbrace{\frac{\mu_0}{4}\iiiint F_{\alpha\beta}F^{\alpha\beta} d^4x}_{\text{free field}}$$

$\delta S = 0$ gives motion of particles in field and dynamics of field due to particles.

SYSTEMS: LINEAR, CONTINUOUS (ANALOGUE)

System

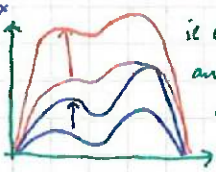
$u(t)$ input → system → $x(t)$ output

output is input convolved with point-spread f'n

ie $\boxed{x(t) = u(t) * h(t)}$

→ for multiple inputs/o/ps have a vector – matrix eq'n .... easy generalisation

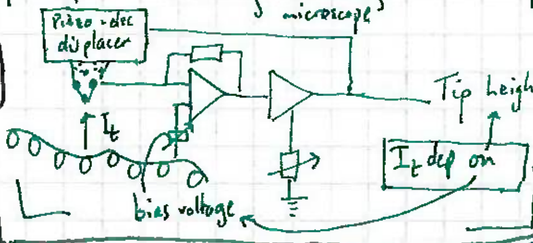
→ dynamics can be described by a linear differential eq'n.



ie double input at any time, double output.....

Linearity ⇒ Superposition

Example: Scanning tunnelling microscope



If input begins at $t=0$, causal system only has $x>0$ for $t>0$

Causality – restricts the possible forms of $H(s)$ [or $h(t)$]

Complex freq domain related to time domain by LAPLACE transform.

Convolution theorem ⇒ $H(s) = \dfrac{X(s)}{U(s)}$

Complex Methods ⟺ Complex freq $s = \sigma + j\omega$

Usually, H reduces output at high frequencies: → ω

Prob with F.T. – needs bounded f'n. L.T. overcomes this prob. Useful ones:

$\boxed{\frac{df}{dt} \to sF}$

$\boxed{\int_0^t f dt \to \frac{F}{s}}$

$\boxed{f(t+T) \to e^{sT}F}$

$\boxed{f(\alpha t) \to \frac{1}{\alpha}F\left(\frac{s}{\alpha}\right)}$

Differential eq'ns are transformed into ALGEBRAIC ones!

Inverse Laplace Transform

$$f(t) = \frac{1}{2\pi j}\int_{\sigma-j\infty}^{\sigma+j\infty} F(s)\,e^{st}\,ds$$ formal def'n

But usually: let $F(s) = \dfrac{A(s)}{B(s)}$ ← polynomials

then use Partial fractions: $F(s) = \dfrac{c_0}{s-p_0} + \dfrac{c_1}{s-p_1} + \dots \dfrac{c_n}{s-p_n}$ (H)

$\left[c_n = (s-p_n)F(s)\Big|_{s=p_n}\right]$

so (h) $\boxed{f(t) = c_0 e^{p_0 t} + \dots c_n e^{p_n t}}$

This only works if system can be described by finite order differential eq'n; more complex methods

Eg – no work for time delay ie simple loudspeaker – microphone feedback system.

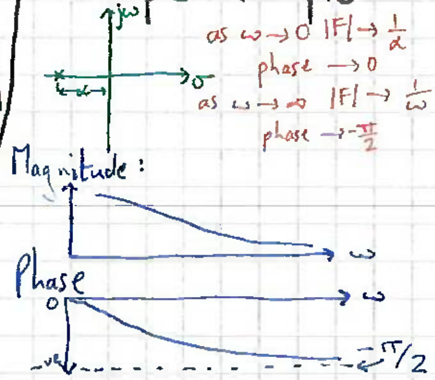
⇒ if p_n imag, get oscillation; real –ve get stability; real +ve get instab. complex, get

Poles and zeroes always come in c.c. pairs. See notes for examples

Simple example: $F(s) = \dfrac{1}{s+\alpha}$

as $\omega \to 0$ $|F| \to \frac{1}{\alpha}$, phase $\to 0$

as $\omega \to \infty$ $|F| \to \frac{1}{\omega}$, phase $\to -\frac{\pi}{2}$



Lecture 2

Stability

– Stable if $h(t) \to 0$ as $t \to \infty$

(– Stable if $H(s)$ has no poles in right half plane)

Routh-Hurwitz Criteria: (when know h(t) analytically) (large order systems get messy...)

2nd order: $B(s) = as^2 + bs + c$

⇒ $\boxed{a, b, c > 0}$

3rd order: $B(s) = as^3 + bs^2 + cs + d$

$\boxed{a, b, c, d > 0 \text{ and } bc > ad}$ $\begin{vmatrix} a & b \\ c & d \end{vmatrix} < 0$

In general, det|coeffs| < 0 ...?

→ Example: Op-Amp

Transfer f'n is approximately $A(s) = \dfrac{A_0}{(1+\tau_1 s)(1+\tau_2 s)(1+\tau_3 s)}$

$s = -\frac{1}{\tau_1}$: Introduced for stability (Internal freq. compensation)

$s = -\frac{1}{\tau_{2,3}}$ Inherent delays in system.

need: ① large A_0 ② stability in all feed-back configs.

Unity Gain buffer:

$x(t) = A(u(t) - x(t))$

use L.T., sub for $A(s)$

apply R-H criteria

→ get: $\tau_1 > \left(\dfrac{\tau_2\tau_3}{\tau_2+\tau_3}\right)A_0$

if $A_0 \gg 1$. $\tau_1 \gg \tau_2$ or τ_3

so get straight line

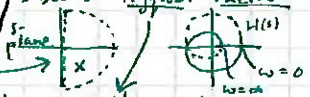
Nyquist Criterion: (when don't know h(t) analytically)

$\boxed{\text{Stability if loop gain does not encircle} \begin{pmatrix}-1\\0\end{pmatrix}}$

Used for feed back systems

$H(s) = \dfrac{A(s)}{1 + A(s)\beta(s)}$ ← loop gain.

Based on Nyquist theorem:

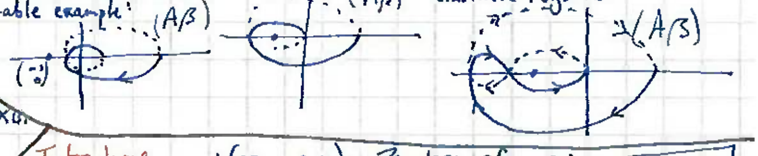


Locus of H encircles origin n times; n = no. of zeros – no. of poles encircled, in same dir'n, by D contour in s-plane."

Stable example:

Unstable example:

Stable, in principle, but inc A, expand contour, go through an unstable regime:



Diagramatic Representation – use building blocks

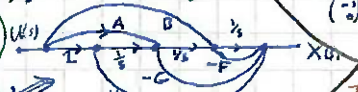
Integrator: $H(s) = -\dfrac{1}{RCs}$

Write as $\boxed{\frac{-1}{RCs}}$ or

virtual earth

$A = -\infty$

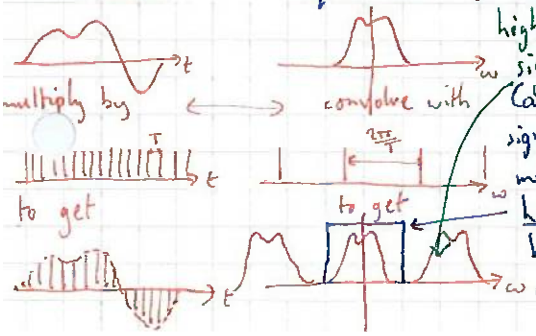
eg 3rd order system:



(Transfer f'n: $H(s) = \dfrac{1 + As + Bs^2}{s^3 + Fs^2 + Gs + H}$)

DISCRETE, SAMPLED (DIGITAL)

Time domain | Freq. domain



Aliasing

T too large, get overlap

so: effect is to create higher freq copies of signal.

→ (cannot reconstruct signal even with perfect window)

Can we get continuous signal back? Yes if multiply by top hat (Shannon window) but in reality – can't make perfect top hat

Shannon Sampling Theorem: A signal containing frequency components $\le \omega_0$ can be completely defined by sampling at a rate that is: $\ge 2\omega_0$

Z transforms:

(non-ex.) $F(s) = \int_0^\infty f(t)e^{-st}dt = f(0) + f(T)e^{-sT} + \dots = \boxed{\sum_{k=0}^{\infty} f_k z^{-k}}$ where $z = e^{sT}$

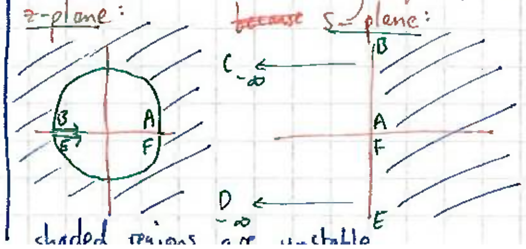
Eg. exp decay: $h_k = \{1, e^{-T/\tau}, \dots\}$

$H(z) = 1 + e^{-\frac{T}{\tau}}z^{-1} + e^{-\frac{2T}{\tau}}z^{-2} \dots = \dfrac{1}{1-\alpha z^{-1}} = \dfrac{z}{z-\alpha}$ $\alpha = e^{-\frac{T}{\tau}}$

Locus of true freq: $z = e^{sT}$ at $s = j\omega$ $z = e^{j\omega T}$

⇒ get unit circle. For stability, require poles in circle

z-plane: ~~because~~ s-plane:

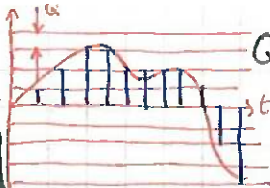


shaded regions are unstable

SYSTEMS

Discrete Systems Continued...

Quantised Sampling



Signal can only take discrete values ⇒ errors. assume uniform dist'n ie $\langle \varepsilon \rangle = 0$

⇒ errors:

$+Q/2$, $-Q/2$

⇒ Prob of $\varepsilon = 1/Q$

$\langle \varepsilon^2 \rangle = \int_{-Q/2}^{Q/2} \varepsilon^2 \frac{1}{Q} \, d\varepsilon$

Random noise (white). Have assumed uniform dist'n of levels ie Q const.

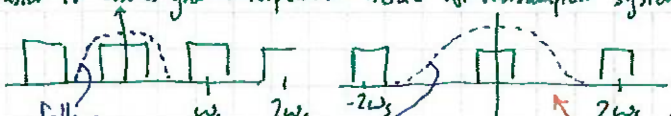
⇒ RMS error $= \frac{Q}{\sqrt{12}}$

To reduce noise and enhance ease of reconstruction of signal.... use **OVERSAMPLING.**

ie sample at $> 2\omega_{max}$ from Shannon theorem. "M times oversampling" – M times more measurements of signal, error on mean reduced by $\frac{1}{\sqrt{M}}$.

Dynamic range / bandwidth is increased.

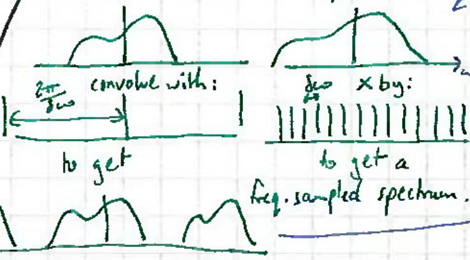
Easier to build good interpolation filters for oversampled systems:



Filter (not oversampled) ω_s $2\omega_s$ $-2\omega_s$ $2\omega_s$ wider filter (2× oversampled)

Compare impulse response of top hat and Gaussian

Frequency Sampling → Circular Convolution.



Time domain — convolve with: $\frac{2\pi}{\delta\omega}$ — to get

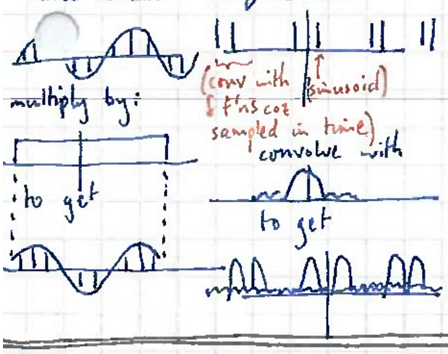
Freq. domain — $\delta\omega$ × by: — to get a freq. sampled spectrum.

continuous frequency variable ω – can ask what is f'n at any frequency. ← sample at discrete freq's

Periodicity ie Circular conv! How get rid of problem?

Finite Sequence → Leakage

eg sinusoid..



Time domain — multiply by: — to get

Freq domain — (conv with f'ns coz sampled in time) (sinusoid) — convolve with — to get

NON-LINEAR SYSTEMS

In general, differential eq'n can be split: $\dot{x}_1 = f_1(x_1, x_2 \ldots x_n)$, $\dot{x}_2 = f_2(\quad)$, ⋮ $\dot{x}_n = f_n(\quad)$ — 1st order non linear diff eq'ns.

Behaviour of system linked to dimensionality of problem. n variables → $\Leftrightarrow$ n dimensional problem.

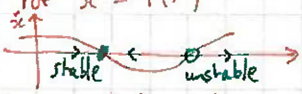
Eg $m\ddot{x} + b\dot{x} + kx = 0$ is same as $\boxed{\dot{x}_1 = x_2,\quad \dot{x}_2 = -\frac{k}{m}x_1 - \frac{b}{m}x_2}$

1-D

Heavy damping, $m\ddot{x} \sim 0$, get 1-D system where $\dot{x} = -\frac{k}{b}x$ (linear – not in general though)

get stable pt

In general for $\dot{x} = f(x)$ can get



stable, unstable

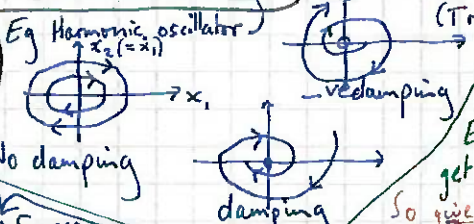
Also can get a half stable pt

No oscillations in 1-D system.

1-D (see lect. 6 btem pg. 4)

2-D

⇒ Can get LIMIT CYCLES (closed trajectories in pos'n-phase space) (Trajectories never cross)



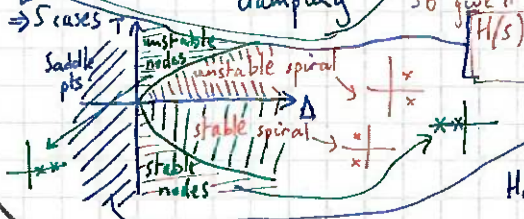
Eg Harmonic oscillator $x_2 (= \dot{x}_1)$, x_1 — No damping — damping — -ve damping

General 2-D Linear System. $\dot{\underline{x}} = \underline{A}\underline{x}$, $\underline{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, $\underline{A} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ Trace = T, det = Δ

Eliminate x_2, get $\ddot{x}_1 - T\dot{x}_1 + \Delta x_1 = 0$ this is o/p for no input

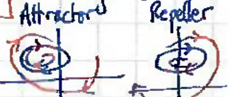
So give it i/p and LT ⇒ $\boxed{H(s) = \frac{1}{s^2 - Ts + \Delta}}$

⇒ 5 cases



T, Δ, Saddle pts, unstable nodes, unstable spiral, stable spiral, stable nodes

On the parabola – a limit cycle.



Attractor, Repeller

Half stable limit cycle:

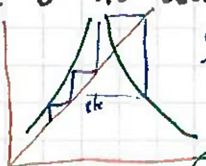
3-D

⇒ Can get Chaotic Behaviour. (sensitive to initial conditions)

Dissipative (vol of phase space occupied by trajectories decreases monotonically with time) implies that ∃ some kind of attractor. ⇒ If plot one coord as f(t) typically get aperiodic but non-divergent curve

STRANGE attractor has: zero volume (coz dissip.) and ⇒ fractal character. Infinite length line (coz aperiodic)

1-D Iterated Maps: Plot pos'ns of maxima, y_n

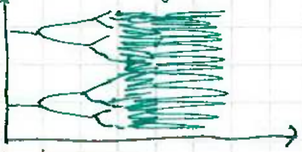


y_{n+1}

Simple example is the Logistic Map: $y_{n+1} = r y_n (1 - y_n)$

y_{n+1}, y_n

Plotting y_n as f(r) gives and orbit diagram

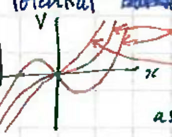


∃ regions when system emerges from chaotic regime, then goes back by "Period Doubling" $2 \to 4 \to 8 \to 16$

Stability: (one control parameter)

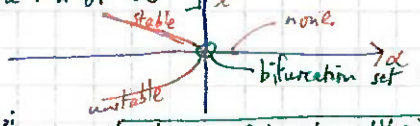
Limit Point Instability also called saddle node bifurcation or fold.

Potential: $x^3 + \alpha x$



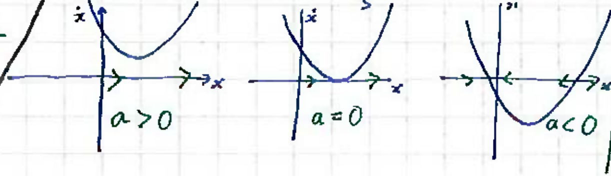
$\alpha < 0$ ∃ one stable equilibrium, one unstable equilibrium. $\alpha > 0$ ∃ no equilibrium. (use one dyn. variable with little l.o.g.)

Plot eq. points as a f'n of α ie in the control space



x^*, stable, none, unstable, α, bifurcation set (just a point...)

– Have already had this ex. $\dot{x} = x^2 + a \Rightarrow V = \frac{x^3}{3} + ax$



$a > 0$, $a = 0$, $a < 0$

Note on Potentials: $-\frac{dV}{dx}$ gives dir'n of motion, $\frac{dV}{dx} = 0$ is eq'm x^*. $\frac{d^2V}{dx^2}$ gives stability of point. Not always mechanical – often can get f'ns like V – decrease mono'lly along at traj – Liapanov functions

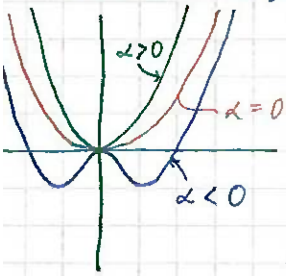
Systems: Stability of non-linear systems (cont'd)

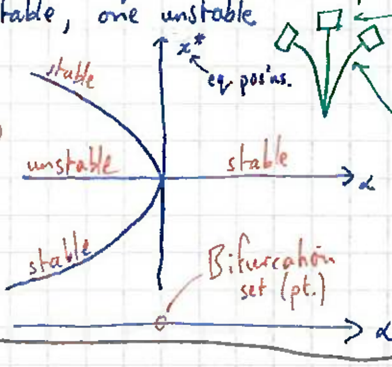
Stable symmetric transition. (or Pitchfork Bifurcation)

one control parameter.

Potential: $V(x) = \alpha x^2 \pm x^4$ — $-$ve sign – nothing new.

For $\alpha \geq 0$ one stable eq'm
$\alpha < 0$ two stable, one unstable





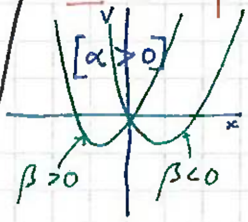
Example: Euler strut

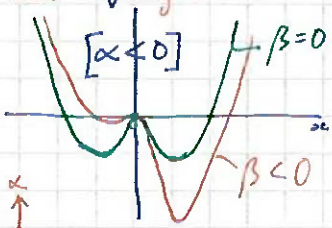
Stable pos'n is no longer stable – $\exists$ two symmetric stable pos'ns!

Cusp Catastrophe (or Imperfect Bifurcation)

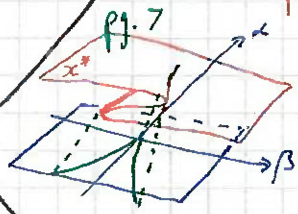
Potential: $V(x) = \alpha x^2 + x^4 + \beta x$

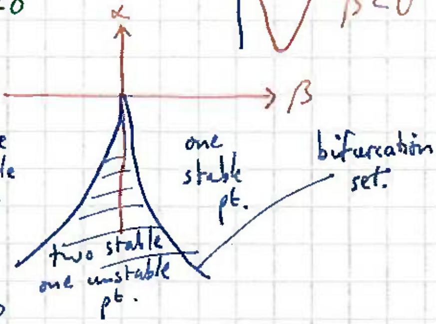
Two control parameters. asymmetric term.





In control space:





examples – see lecture 8