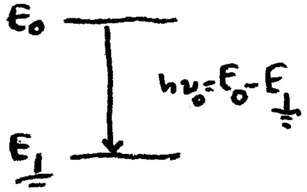
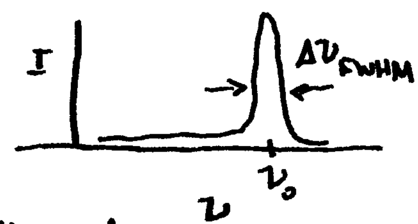
.... Mandl 7.3ff .....

Let's play with degenerate perturbation theory analytically and pictorally. First

#1 draw a very simple energy level diagram between a hypothetical ground state ($E_{\frac{1}{=}}$) and an excited state (E_0) which we will imagine is two fold degenerate.





There is also an intensity vs frequency graph to capture the 'spectral line'. Take a minute to draw in the 'lines' on both diagrams. What physical process gives rise to a finite thickness to the 'spectral line' on the right? Jot down an answer.

An ensemble of atoms in thermal equil. at temp T produces a 'Doppler-Broadened' line where the FULL WIDTH-HALF MAX (FWHM) is determined by T, $\Delta\nu_D = \nu_0 \sqrt{\frac{8RT\ln 2}{Mc^2}}$ ....†

#2 Imagine that the Hamiltonian, which gives the two fold degenerate energy eigenvalue E_0, may be represented as the matrix

$$\underline{\underline{H}}_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix},$$

and that there exists some 'small' perturbation, the matrix for which (in the basis in which the unperturbed Hamiltonian is diagonal) is shown below, <u>and</u> <u>added</u> to the unperturbed Hamiltonian, giving, to a first approximation, the complete Hamiltonian,

† the Sodium D line (1 of them! :-)) has a Doppler broading of 1.7 GHz at T = 500K... those sodium discharge lamps get HOT!

#2 $\underline{\underline{H}} = \underline{\underline{H}}_0 + \underline{\underline{V}}'$ $\quad \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} + \begin{pmatrix} V'_{11} & V'_{12} \\ V'_{21} & V_{22} \end{pmatrix} = \underline{\underline{H}}$

Try to find the new energy eigenvalues by diagonalizing the perturbation matrix (that is, by finding eigenvalues of the perturbation matrix). Find (or call them), assuming that $\underline{\underline{V}}'$ is hermitian,

(a)

$$\underline{\underline{V}}' = \begin{pmatrix} \bar{V} + \Delta E & 0 \\ 0 & \bar{V} - \Delta E \end{pmatrix}$$

in terms of the $\underline{\underline{V}}'$ matrix elements ... from $\underline{\underline{V}}' \cdot \underline{\chi}^\lambda = \lambda \underline{\chi}^\lambda \rightarrow \{\underline{\underline{V}}' - \lambda \underline{\underline{I}}\} \cdot \underline{\chi}^\lambda = 0$, we find the ev's of $\underline{\underline{V}}'$ from the determinant,

$$\det \begin{vmatrix} V'_{11} - \lambda & k \\ k & V'_{22} - \lambda \end{vmatrix} = 0 \quad \cdots (V'_{11} - \lambda)((V'_{22}) - \lambda) - k^2 = 0$$

$$V_{11}V'_{22} + \lambda^2 - \lambda(V'_{11} + V'_{22}) - k^2 = 0$$

$$\lambda^2 - \lambda(V'_{11} + V'_{22}) + (V'_{11})(V'_{22}) - k^2 = 0$$

$$\Rightarrow \lambda = \frac{V'_{11} + V'_{22}}{2} + \sqrt{\frac{(V'_{11} + V'_{22})^2}{4} - [V'_{11}V'_{22} - k^2]}$$

$\underline{\underline{V}}'$ must be hermitian, and for simplicity, let's take it to be real....

→ after a little algebra...

$\lambda = \bar{V} \pm \Delta E$

where $\bar{V}$ = 'level shift' $= \frac{V'_{11} + V'_{22}}{2}$ ← words!

$\Delta E = \sqrt{\left(\frac{V'_{11} - V'_{22}}{2}\right)^2 + k^2}$:-)

(b) The eigenstates of the perturbation then are linear combinations of the unperturbed eigenstates, say $\xi_1 = \sum_j c_j |\psi_j\rangle$, $\xi_2 = \sum d_j |\psi_j\rangle$ where $\hat{H}_0 |\psi_1\rangle = E_0 |\psi_1\rangle$ etc.

Q: is $\underline{\underline{H}}_0$ diagonal <u>in</u> <u>the</u> <u>new</u> <u>basis</u>? YES

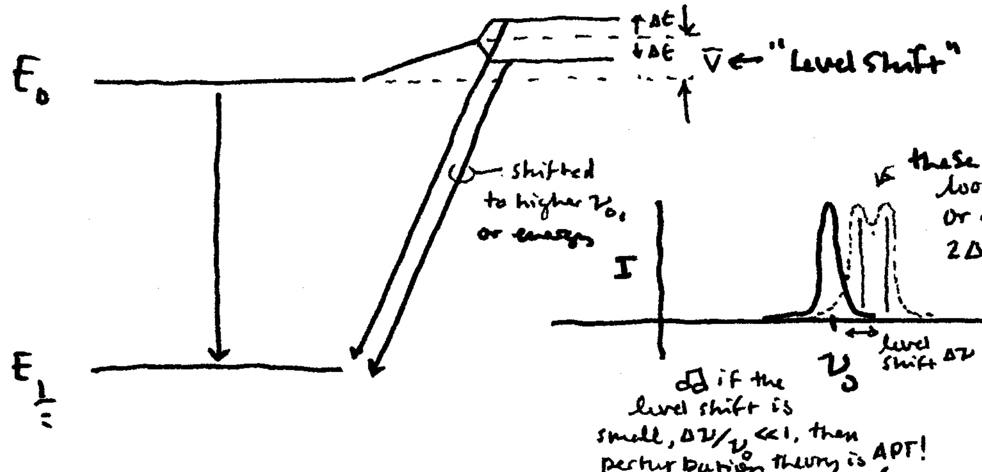
This follows from the original degeneracy $\hat{H}_0 \xi_1 = \sum_j c_j \hat{H}_0 |\psi_j\rangle = E_0 \sum_j c_j |\psi_j\rangle = E_0 \xi_1$ etc....

(c) -- just a comment. We expect that the <u>energy differences</u> will depend on quantum #'s somehow, which are associated with <u>operators that commute with $\underline{\underline{H}}$, that is, with both H_0 & $\underline{\underline{V}}'$</u>. These are called "GOOD QUANTUM #S"! Why are these quantum #s the 'good ones'?

because they are constants of the motion, which is to say, they have values that exist simultaneously with the energies (this has to be a good thing ...) The other day, by chance, I was reading the world's 2nd paper on Quantum Mechanics, and in it Born writes $\boxed{\begin{aligned} \dot{q} &= \tfrac{i}{\hbar}[H, q] \\ \dot{p} &= \tfrac{i}{\hbar}[H, p] \end{aligned}}$ which indicates that q & p are constants of the motion in they commute!

see Mandl Sec. 2.2

#3 Now let's picture our results, and construe, or consider the amplications. Go back to the 2 graphs, diagrams in part 1 and modify them in a way that make sense to you, but keep the 2 lines you drew .... use dashed lines or something for the new ones. What about your new picture expresses the truth that $V' \ll H_0$.



these two lines might look like a dimple on top or even just a blob if $2\Delta E \sim h\Delta\nu_D$!

of course it is really the dotted line that nature presents us in connection with the fine ~~structure~~ structure of H, which is part of the "spin-orbit" effect!

#4 Our first physical application is the 'SPIN-ORBIT' effect in which the electron experiences the electric field of the proton (think H), but which, relativistically, becomes a magnetic field in its own frame of rest. That there is a splitting indicates that an electron (in its own rest frame :) has its own magnetic moment $\vec{\mu}$ [the SG experiment was not understood, by them to prove this!! It's the Fine Structure that convinces physicists that the ~~the~~ 'intrinsic' magnetic moment exists! This is Sam Goudschmidt and George Uhlenbach! 'Discoverers of Spin' along with Pauli, who predicted/understood

L29

#4

its necessity in advance of the 'discovery' of Goudschmidt & Uhlen(bach). 1924 I think ....]

Anyway it turns out that → Uhlenbeck.

in '24 Pauli gets the 'two valued ness' of e^-, in 1925, Sept. ~~was when~~ Sam & George used spin to understand the fine structure.....

$$\hat{V}_{SO} = A\hat{L}\cdot\hat{S}$$

$\hat{S}$: $\propto \vec{\mu}_e$

$\hat{L}$: $\propto \vec{B}$ which arises by a relativistic transformation of the electric field experienced by an electron w. q#'s $n\ell$ in the H atom (or any atom....)

A depends on $\left\langle \frac{1}{r}\frac{dV}{dr} \right\rangle_{n\ell}$ ....
and can be gotten experimentally for precise comparison w. theory....

NB it's $\frac{A}{2}$!!

Mandl shows us that $\vec{J} = \vec{L} + \vec{S} \Rightarrow \vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

$\therefore\ \hat{V}_{SO} = \frac{A}{2}\left\{\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right\} \Rightarrow$ the good Q#s are J, L, & S (not! M!) so the kets $|JM\rangle$ are a natural basis for the spin-orbit effect, w. M suppressed and with L & S expressed in every ket, $|LSJ\rangle$....

Find $\underline{\underline{V}}_{SO}$ in the ^2P ket basis and read off the newe eigenvalues with the perturbation 'turned on'

* $L = 1, S = \frac{1}{2}$ for ^2P term.... $J = 3/2$, $3/2$

$\therefore\ \hat{L}\cdot\hat{S}\,|1\,\tfrac{1}{2}\,\tfrac{3}{2}\rangle = \hbar^2\left\{(\tfrac{3}{2})(\tfrac{3}{2}+1) - 1(1+1) - \tfrac{1}{2}(\tfrac{1}{2}+1)\right\}|1\,\tfrac{1}{2}\,\tfrac{3}{2}\rangle$

$= \hbar^2\left[\frac{15}{4} - \frac{8}{4} - \frac{3}{4}\right]$

$= \hbar^2\left[\frac{4}{4}\right]$

$2\Delta E = 4.6\times10^{-5}\,\text{eV}$

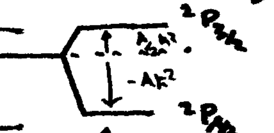
$\therefore\ \frac{3}{2}A\hbar^2 = 4.6\times10^{-5}\,\text{eV}$

$A = \frac{2}{3}\cdot\frac{4.6\times10^{-5}\,\text{eV}}{\hbar^2}$

$\underline{\underline{V}}_{SO} =$

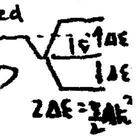
	$\lvert LS\,3/2\rangle$	$\lvert LS\,\frac{1}{2}\rangle$
$\langle LS\,3/2\rvert$	* $\frac{A\hbar^2}{2}$	0
$\langle LS\,\frac{1}{2}\rvert$	0	$-A\hbar^2$

NB $\langle L'S'J'|LSJ\rangle = ?$
$\delta_{L'L}\cdot\delta_{S'S}\cdot\delta_{J'J}$



how it's usually pictured

Show that there is a level shift of $-A/4$ and that $\Delta E = \pm 3A/4$. If the Gap is 4.6×10^{-5} eV, what is A?



So $\left.\begin{array}{l} +\frac{A}{2}\hbar^2 \\ \\ -A\hbar^2 \end{array}\right\}$ Gap energy $= \frac{3}{2}A\hbar^2 = 4.6\times10^{-5}\,\text{eV}$

$$\therefore A = \frac{2}{3}\cdot\frac{4.6\times10^{-5}\,\text{eV}}{\hbar^2} = \frac{2}{3}\cdot\frac{4.6\times10^{-5}\,\text{eV}}{\big(\underbrace{1.055\times10^{-34}\,\text{J}\cdot\text{s}}_{\hbar}\ \times\ \frac{1}{1.6\times10^{-19}}\frac{\text{eV}}{\text{J}}\big)^2}$$

$1\,\text{eV} = 1.6\times10^{-19}\,\text{J}$

$$= 7.06\times10^{25}\ \frac{1}{\text{eV}\cdot\text{s}^2}$$

crazy unit that!

$\hbar = \underline{\underline{6.59\times10^{-16}\,\text{eV}\cdot\text{s}}}$

but if $A\hbar^2 \cong 5\times10^{-5}\,\text{eV}$, $\hbar^2$ being fantastically small, A had better be fantastically big.....