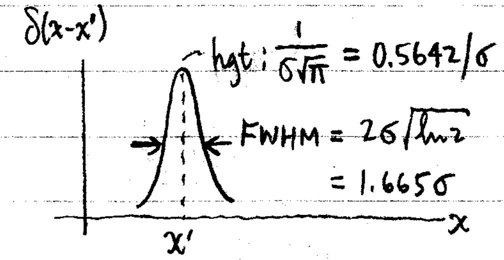
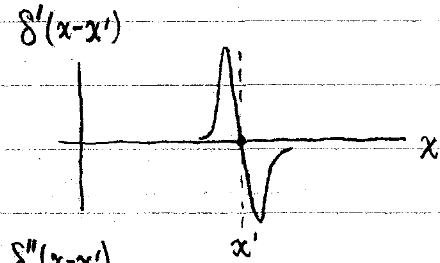
3/25/71 **2** a) The suitably normalized form is

$$\delta(x-x') = (1/\sigma\sqrt{\pi})\, e^{-(x-x')^2/\sigma^2}$$



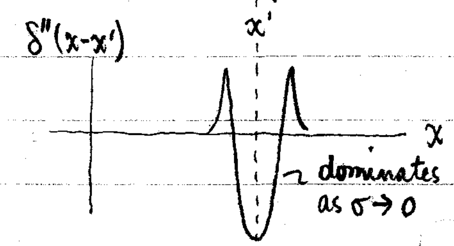
$$\hookrightarrow \int_{-\infty}^{+\infty} \delta(x-x')\,dx' \underset{\substack{\uparrow \\ u=\left(\frac{x'-x}{\sigma}\right)}}{=} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2}\,du = 1$$



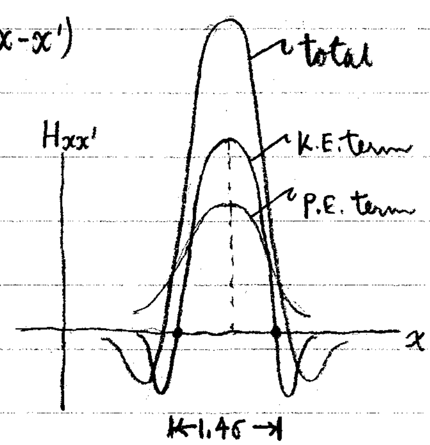
b) Calculate stfwdly...

$$\frac{d}{dx}\,\delta(x-x') = -\frac{2}{\sigma^2}(x-x')\,\delta(x-x')$$

$$\frac{d^2}{dx^2}\,\delta(x-x') = +\frac{2}{\sigma^2}\left[\frac{2}{\sigma^2}(x-x')^2 - 1\right]\delta(x-x')$$



$$\therefore\ H_{xx'} = \Big\{ \underbrace{\frac{\hbar^2}{m\sigma^2}\left[1 - \frac{2}{\sigma^2}(x-x')^2\right]}_{\text{K.E. term}} + \underbrace{V(x)}_{\text{P.E. term}} \Big\}\, \delta(x-x')$$



A rough sketch of $H_{xx'}$ vs x appears at right -- this is "looking along the diagonal" of the matrix $(H_{xx'})$. It is clear that this matrix is not diagonal -- it has non-zero elements ∞smally close to the main diagonal at $x' = x$ (see comment by Schiff, p. 158). It is interesting to note that as $\sigma \to 0$, the area under the $H_{xx'}$ curve blows up, as

$$\sum_{x'} H_{xx'} = \int_{-\infty}^{+\infty} dx'\, H_{xx'} = \frac{\hbar^2}{m\sigma^2} + V(x) \to \infty \quad \text{for } \sigma \to 0$$

What this means, we don't know. It is still true, however, that $\sum_{x'} H_{xx'}\psi_{x'}$ $= \int dx'\, H(x)\,\delta(x-x')\,\psi(x') = H(x)\,\psi(x)$ is finite.

4/9/71 (63) Bilinear form would be $f(A,B) = g_1 AB + g_2 BA$. Too simple!

Instead look at $C = f(A,B) = \sum_{\mu,\nu} g_{\mu\nu} A^\mu B^\nu$ (A1)

Denote the basis fcns ϕ_i by $|i\rangle$. Then have

$$\langle i|C|j\rangle = \langle i|\sum_{\mu,\nu} g_{\mu\nu} A^\mu B^\nu|j\rangle = \sum_{\mu,\nu} g_{\mu\nu} \langle i|A^\mu B^\nu|j\rangle$$

by linearity of the $\langle\,|\,\rangle$ operation. Now use compleatness of the ϕ_i, in the form $\sum_k |k\rangle\langle k| = 1$, to write

$$\langle i|C|j\rangle = \sum_{\mu,\nu} g_{\mu\nu} \sum_k \langle i|A^\mu|k\rangle\langle k|B^\nu|j\rangle$$

The LHS is just $\langle i|C|j\rangle = (\underset{\sim}{C})_{ij}$. On the RHS, we should show

$$\langle i|A^\mu|k\rangle = (\underset{\sim}{A}^\mu)_{ik}$$

Using compleatness, we can write LHS as

$$\langle i|A^\mu|k\rangle = \underbrace{\sum_{l,m,\ldots,n}}_{\mu-1 \text{ summands}} \langle i|A|l\rangle\langle l|A|m\rangle\langle m|\cdots A|n\rangle\langle n|A|k\rangle$$

or

$$(\underset{\sim}{A}^\mu)_{ik} = \sum_{l,m,n,\ldots} (\underset{\sim}{A})_{il} (\underset{\sim}{A})_{lm} (\underset{\sim}{A})_{mn} \cdots (\underset{\sim}{A})_{nk} = (\underset{\sim}{A}^\mu)_{ik}$$

So we have, as desired...

$$\langle i|A^\mu|k\rangle = (\underset{\sim}{A}^\mu)_{ik}, \quad \text{sim'ly } \langle k|B^\nu|j\rangle = (\underset{\sim}{B}^\nu)_{kj}$$

From the above, therefore

$$(\underset{\sim}{C})_{ij} = \sum_{\mu,\nu} g_{\mu\nu} \sum_k (\underset{\sim}{A}^\mu)_{ik} (\underset{\sim}{B}^\nu)_{kj} = \sum_{\mu,\nu} g_{\mu\nu} (\underset{\sim}{A}^\mu \underset{\sim}{B}^\nu)_{ij} = \Big(\sum_{\mu,\nu} g_{\mu\nu} \underset{\sim}{A}^\mu \underset{\sim}{B}^\nu\Big)_{ij}$$

$\therefore \underset{\sim}{C} = \sum_{\mu,\nu} g_{\mu\nu} \underset{\sim}{A}^{\mu} \underset{\sim}{B}^{\nu} = f(\underset{\sim}{A}, \underset{\sim}{B})$ QED

4/10/71 (4) $W_{k\lambda} = \int dx\, u_k^*(x) v_\lambda(x)$. Show $\underset{\sim}{W} = (W_{k\lambda})$ is unitary.

$$(\underset{\sim}{W}\underset{\sim}{W}^\dagger)_{k\ell} = \sum_\lambda W_{k\lambda} W^\dagger_{\lambda\ell} = \sum_\lambda W_{k\lambda} W^*_{\ell\lambda}$$

$$= \sum_\lambda \int dx\, u_k^*(x) v_\lambda(x) \int dx'\, u_\ell(x') v_\lambda^*(x')$$

$$= \int dx\, u_k^*(x) \int dx' \underbrace{\Big[\sum_\lambda v_\lambda(x) v_\lambda^*(x')\Big]}_{\delta(x-x')} u_\ell(x')$$

$$= \int dx\, u_k^*(x) u_\ell(x) = \delta_{k\ell}\text{, by orthonormality of } \{u_k(x)\}.$$

$\therefore \underset{\sim}{W}\underset{\sim}{W}^\dagger = \underset{\sim}{I}$. Simly $\underset{\sim}{W}^\dagger \underset{\sim}{W} = \underset{\sim}{I}$ QED

In v-rep^n, $\underset{\sim}{H}'' = (H_{\kappa\lambda} = \int dx\, v_\kappa^*(x) H(x) v_\lambda(x))$. Thus have

$$\underset{\sim}{H}' = \underset{\sim}{W}\,\underset{\sim}{H}''\,\underset{\sim}{W}^\dagger \Rightarrow H'_{k\ell} = \sum_{\kappa,\lambda} W_{k\kappa} H_{\kappa\lambda} \underbrace{W^\dagger_{\lambda\ell}}_{= W^*_{\ell\lambda}}$$

$$H'_{k\ell} = \sum_{\kappa,\lambda} \left(\int dx'\, u_k^*(x') v_\kappa(x')\right)\left(\int dx\, v_\kappa^*(x) H(x) v_\lambda(x)\right)\left(\int dx''\, u_\ell(x'') v_\lambda^*(x'')\right)$$

$$= \int dx'\, u_k^*(x') \int dx \underbrace{\Big[\sum_\kappa v_\kappa(x') v_\kappa^*(x)\Big]}_{\delta(x-x')} H(x) \int dx'' \underbrace{\Big[\sum_\lambda v_\lambda(x) v_\lambda^*(x'')\Big]}_{\delta(x''-x)} u_\ell(x'')$$

$$= \int dx'\, u_k^*(x') H(x') u_\ell(x')$$

But the $\{u_k(x)\}$ are eigenfons of H, i.e. $H(x')u_\ell(x') = E_\ell u_\ell(x')$.

$\therefore H'_{k\ell} = E_\ell \int dx'\, u_k^*(x')\, u_\ell(x') = E_k \delta_{k\ell}$, diagonal ... QED

$\underset{\sim}{H}'' \vec{a}_k = E_k \vec{a}_k$. Transform by $\underset{\sim}{W}$. Get

$$\underset{\sim}{H}' \vec{a}_k' = E_k \vec{a}_k' \quad \begin{cases} \underset{\sim}{H}' = \underset{\sim}{W}\,\underset{\sim}{H}''\,\underset{\sim}{W}^\dagger \\ \vec{a}_k' = \underset{\sim}{W}\, \vec{a}_k \end{cases}$$

Components of $\vec{a}_k'$ are

$$a'_{k\ell} = \sum_\mu W_{\ell\mu} a_{k\mu}, \quad \text{where } a_{k\mu} = \underbrace{W^*_{k\mu}}_{= \int dx\, v^*_\mu(x)\, u_k(x)} \text{ (see lecture (56), p. 237)}$$

$$= \sum_\mu W_{\ell\mu} W^*_{k\mu} = (\underset{\sim}{W}\,\underset{\sim}{W}^\dagger)_{\ell k} = \delta_{\ell k}$$

So the $\vec{a}_k'$ are single component unit vectors. QED

4/18/71 (57)

$$\mathcal{H}\psi = i\hbar \frac{\partial}{\partial t}\psi \quad \begin{cases} \mathcal{H}(x,p,t) = H(x,p) + V(x,t) \\ \psi = \psi(x,t) \end{cases}$$

Energy eigenfcns of H are $u_n(x)\, e^{-\frac{i}{\hbar}E_n t}$, $E_n = H$ eigenvalues. Expand ψ as the superposition...

$$\psi(x,t) = \sum_n a_n(t)\, u_n(x)$$

The a_n can be calculated in the usual way (since the u_n are orthonormal)

$$a_n(t) = \int dx\, u_n^*(x)\, \psi(x,t)$$

Putting ψ into the S. eqtn gives (assuming V not op$^{\underline{n}}$ly dep$^{\underline{t}}$ on t)

$$\sum_n a_n (H+V)\, u_n = i\hbar \sum_n \dot{a}_n u_n$$

But $H u_n = E_n u_n$. Operate from left with $\int dx\, u_m^*(x)$ to get

$$\sum_n a_n \int dx\, u_m^* (E_n + V) u_n = i\hbar \sum_n \dot{a}_n \int dx\, u_m^* u_n$$

or// (with $\int dx\, u_m^* u_n = \delta_{mn}$)...

$$i\hbar \dot{a}_m = E_m a_m + \sum_n V_{mn} a_n$$

where: $V_{mn}(t) = \int dx\, u_m^*(x) V(x,t) u_n(x)$

We can simplify this eqtn by defining new coefficients b_m as

$$b_m(t) = a_m(t) e^{+\frac{i}{\hbar}E_m t} \quad \left(\text{i.e. now } \psi(x,t) = \sum_n b_n(t) u_n(x) e^{-\frac{i}{\hbar}E_n t}\right)$$

$\hookrightarrow \therefore\ i\hbar \dot{a}_m = E_m a_m + i\hbar \dot{b}_m e^{-\frac{i}{\hbar}E_m t}$

$$\therefore\ i\hbar \dot{b}_m = \sum_n \mathcal{V}_{mn} b_n$$

where $\mathcal{V}_{mn}(t) = e^{\frac{i}{\hbar}(E_m - E_n)t} \int dx\, u_m^*(x) V(x,t) u_n(x)$ (21)

Let $\vec{b}(t)$ be a vector with comps. $b_m(t)$, and $\underset{m}{\mathcal{V}}(t)$ be a matrix with comps $\mathcal{V}_{mn}(t)$. Then this is the matrix eqtn

$$\boxed{i\hbar \frac{d}{dt}\vec{b}(t) = \underset{m}{\mathcal{V}}(t)\, \vec{b}(t)}$$

Now the matrix $\underset{m}{S}$ which diagonalizes $\underset{m}{\mathcal{V}}$ via a similarity transf$^{\underline{n}}$ ($\underset{m}{S}\,\underset{m}{\mathcal{V}}\,\underset{m}{S}^\dagger = \underset{m}{\mathcal{V}}'$, diag) must be time-dep$^{\underline{t}}$. Hence the transformed vector $\vec{b}' = \underset{m}{S}\,\vec{b}$ is manifestly time-dept. The best we can do is

$$i\hbar\, \underset{m}{S} \frac{d}{dt}\vec{b} = \underset{m}{\mathcal{V}}'\, \vec{b}' \quad \begin{cases} \underset{m}{\mathcal{V}}' = \underset{m}{S}\,\underset{m}{\mathcal{V}}\,\underset{m}{S}^\dagger \text{ diag.}, & \vec{b}' = \underset{m}{S}\,\vec{b} \\ (\mathrm{RHS})_k = \mathcal{V}_k'(t)\, b_k'(t), & \mathcal{V}_k' = \underset{m}{\mathcal{V}} \text{ eigenvalue} \end{cases}$$

or// $$i\hbar \frac{d}{dt}\vec{b}' = \underset{m}{\mathcal{V}}'\,\vec{b}' + (\dot{\underset{m}{S}}\,\underset{m}{S}^\dagger)\,\vec{b}'$$

this term is a messy sum!

4/14/71 (66) Work on the RHS of the eqtn. I.e. have

$$\sum_m \langle k|A|m\rangle\langle m|B|l\rangle = \sum_m \int dx\, u_k^*(x) A(x) u_m(x) \int dx'\, u_m^*(x') B(x') u_l(x')$$

$$= \int dx\, u_k^*(x) A(x) \int dx' \underbrace{\left(\sum_m u_m(x) u_m^*(x')\right)}_{= \delta(x-x'),\ \text{by compleatness of the } \{u_k\}} B(x') u_l(x')$$

Integrating over x', we get...

$$\sum_m \langle\ \rangle\langle\ \rangle = \int dx\, u_k^*(x) A(x) B(x) u_l(x) = \langle k|AB|l\rangle,\ \text{QED}$$

4/14/71 (67) $P_k = \prod_{j\neq k}\left(\frac{\Omega - \omega_j}{\omega_k - \omega_j}\right)$. Let a general state be $|\alpha\rangle = \sum_m |m\rangle\langle m|\alpha\rangle$

$\therefore P_k|\alpha\rangle = \sum_m \left(\prod_{j\neq k}\left(\frac{\Omega-\omega_j}{\omega_k-\omega_j}\right)|m\rangle\right)\langle m|\alpha\rangle$, where $|m\rangle$ are eigenfcns of Ω.

Since $\Omega|m\rangle = \omega_m|m\rangle$, get : $P_k|\alpha\rangle = \sum_m\left(\prod_{j\neq k}\left(\frac{\omega_m-\omega_j}{\omega_k-\omega_j}\right)\right)|m\rangle\langle m|\alpha\rangle$

For $m\neq k$, there is always some $j=m$ for which $\omega_m-\omega_j=0 \Rightarrow \prod = 0$.
For $m=k$, we have $\prod_{j\neq k}\left(\frac{\omega_k-\omega_j}{\omega_k-\omega_j}\right) = 1\times1\times1\cdots\times1\cdots = 1$, so that

$P_k|\alpha\rangle = |k\rangle\langle k|\alpha\rangle \Rightarrow P_k$ is <u>the</u> projection operator QED

Easiest way to show $\sum_k P_k = 1$, $P_k P_l = \delta_{kl} P_k$ is by using the compleatness of the $|m\rangle$'s -- the standard wheeze is in lecture (58), 4/9/71, p. 246

$P\psi(x) = \psi(-x)$. Show P is Hermitian

$$\langle\phi|P\psi\rangle = \int_{-\infty}^{+\infty} dx\, \phi^*(x)\, P\psi(+x) = \int_{-\infty}^{+\infty} dx\, \phi^*(x)\psi(-x)$$

Change variables, let $x = -\xi$. Then

$$\langle\phi|P\psi\rangle = -\int_{+\infty}^{-\infty} d\xi\, \phi^*(-\xi)\, \psi(\xi) = +\int_{-\infty}^{+\infty} d\xi \left(P\phi(\xi)\right)^* \psi(x) = \langle P\phi|\psi\rangle$$

$$= \langle\psi|P\phi\rangle^*$$

So $P_{\phi\psi} = P^*_{\psi\phi}$, and P is Hermitian.

Eigenvalues? $P u(x) = p u(x)$, w/ $u(-x) = p u(x)$. Operate thru with P again $\Rightarrow$ $P u(-x) = p\, P u(x)$, w/ $u(x) = p^2 u(x)$.
Clearly $p^2 = 1$ $\Rightarrow$ eigenvalues $p_1 = +1$, $p_2 = -1$.

From above, for just two states, projection operators will be

$$P_1 = \frac{P - p_2}{p_1 - p_2} = \frac{1}{2}(1 + P), \quad P_2 = \frac{P - p_1}{p_2 - p_1} = \frac{1}{2}(1 - P)$$

W.r.t. parity then, an arbitrary state $\psi(x)$ should be expansible as

$$\psi(x) = P_1 \psi(x) + P_2 \psi(x) = \frac{1}{2}(1+P)\psi(x) + \frac{1}{2}(1-P)\psi(x)$$

$$\text{or}\quad \psi(x) = \psi_+(x) + \psi_-(x) \quad \begin{cases} \psi_+(x) = \frac{1}{2}(1+P)\psi(x) = \frac{1}{2}\left(\psi(x) + \psi(-x)\right) \\ \psi_-(x) = \frac{1}{2}(1-P)\psi(x) = \frac{1}{2}\left(\psi(x) - \psi(-x)\right) \end{cases}$$

Clearly ψ_+ & ψ_- have, resp., even & odd parity.

4/14/71 — Prob. # 35 — ϕ507 (Mar. '92)

The bulk of this problem is done in lecture 59, 4/12/71, pp. 249-252.
The eigenenergies $\mathcal{E}_\mu$ are given by

$$\mathcal{E}_1 = E_1' + \Delta, \quad \mathcal{E}_2 = E_2' - \Delta \quad \begin{cases} E_k' = E_k + V_{kk}, \ \Delta = \frac{1}{2}(Q-1)(E_1' - E_2') \\ Q = \left[1 + \left(2|V_{12}|/(E_1' - E_2')\right)^2\right]^{\frac{1}{2}} \end{cases}$$

For V "small", $\Delta \simeq |V_{12}|^2/(E_1' - E_2')$, so the energies are obvious.
For V "large" on the other hand, we get...

$$Q \simeq \frac{2|V_{12}|}{E_1'-E_2'} \Rightarrow \Delta \simeq |V_{12}| \Rightarrow \begin{array}{l} \mathcal{E}_1 \simeq E_1 + V_{11} + |V_{12}| \\ \mathcal{E}_2 \simeq E_2 + V_{22} - |V_{12}| \end{array}$$

In case of degeneracy, $E_2 = E_1$, with $V_{kk} = 0$ but $|V_{12}| \neq 0$, we have (as above) the case where $|V_{12}| >> E_1'-E_2' = (E_1-E_2)+(V_{11}-V_{22}) = 0$. Then $\Delta \simeq |V_{12}|$ and $\mathcal{E}_1 \simeq E_1 + |V_{12}|$, $\mathcal{E}_2 \simeq E_1 - |V_{12}|$.

The small V result for the wfcns is written down on p. 252. V_{12} is called the "coupling term" because it mixes the original wfcns. In the case of degeneracy, we have $\Delta \simeq |V_{12}|$ as above, and from the exact forms of the $\vec{a}_\mu$ on p. 252, we get:

$$\vec{a}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\vartheta} \\ 1 \end{pmatrix}, \quad \vec{a}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ e^{-i\vartheta} \end{pmatrix}, \text{ where } V_{12} = |V_{12}|e^{i\vartheta}$$

4/18/71 (69) Prob. # ~~36~~ ~~ϕ507~~ (Mar. '92)

From prob 68, the energy levels are (exactly)

$$\mathcal{E}_1 = E_1 - \alpha U + \Delta, \quad \mathcal{E}_2 = E_2 + \beta U - \Delta$$

$\Delta E = E_1 - E_2$ is initial state separation

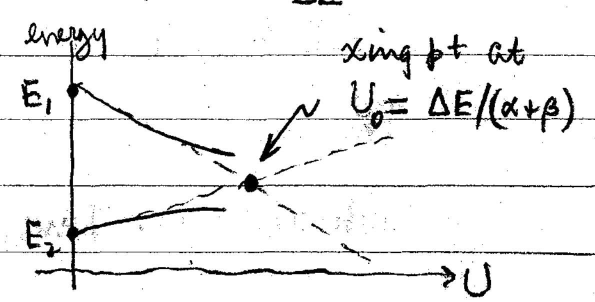
$$\text{where: } \Delta = \frac{1}{2}(Q-1)\Delta E' \begin{cases} \Delta E' = \Delta E - (\alpha+\beta)U \\ Q = \left[1 + (2\gamma U/\Delta E')^2\right]^{\frac{1}{2}} \end{cases}$$

$U << \Delta E \Rightarrow Q \simeq 1 + 2(\gamma U/\Delta E')^2 \simeq 1 + 2(\gamma U/\Delta E)^2$, to $O(U^2)$

$\therefore \Delta \simeq (\gamma U)^2/\Delta E$, and the levels are

$$\mathcal{E}_1 \simeq E_1 - \alpha U + \frac{(\gamma U)^2}{\Delta E}, \quad \mathcal{E}_2 \simeq E_2 + \beta U - \frac{(\gamma U)^2}{\Delta E}$$

So the levels start out as...



$\frac{\Delta E}{U_0} = \alpha + \beta$ **Done as prob. #36, ϕ 507 (Mar. 92)**

What happens at the xing pt. $U_0 = \Delta E/(\alpha+\beta)$? We note

$$Q \to \frac{2\gamma U_0}{\Delta E - (\alpha+\beta)U_0} \gg 1 \quad \text{and} \quad \Delta \to \gamma U_0$$

$$\therefore\ \mathcal{E}_1 \to E_1 - (\alpha-\gamma)U_0 = E_1 - \left(\frac{\alpha-\gamma}{\alpha+\beta}\right)\Delta E$$

$$\mathcal{E}_2 \to E_2 + (\beta-\gamma)U_0 = E_2 + \left(\frac{\beta-\gamma}{\alpha+\beta}\right)\Delta E$$

at xing pt

$$\Delta\mathcal{E} = \mathcal{E}_1 - \mathcal{E}_2 = \left(\frac{2\gamma}{\alpha+\beta}\right)\Delta E \quad > 0 \text{ at the xing pt.}$$

Does $\Delta\mathcal{E}$ ever $=0$, i.e. do the levels ever cross? We have

$$\Delta\mathcal{E} = \Delta E - (\alpha+\beta)U + 2\Delta = Q\left[\Delta E - (\alpha+\beta)U\right]$$

The only place where $\Delta\mathcal{E}$ could ever $=0$ is at the xing pt $U_0 = \Delta E/(\alpha+\beta)$, where -- as we have seen above -- ~~m~~ $\Delta\mathcal{E} = 2\gamma U_0 > 0$. So the levels never cross.

But something "funny" happens for $U > U_0$ ... the $\Delta\mathcal{E}$ defined above apparently goes $(-)$ve. This comes from the sign ambiguity in Q which may be written equivalently

$$Q = \left[1 + \left(\frac{2\gamma U}{\Delta E - (\alpha+\beta)U}\right)^2\right]^{\frac{1}{2}} = \left[1 + \left(\frac{2\gamma U}{(\alpha+\beta)U - \Delta E}\right)^2\right]^{\frac{1}{2}} \simeq \pm \frac{2\gamma U}{\Delta E - (\alpha+\beta)U}, \text{ as } U \to U_0$$

In order to keep $\Delta\mathcal{E}$ $(+)$ve always, we should define

$$\Delta\mathcal{E} = Q\left[(\alpha+\beta)U - \Delta E\right] \quad \text{for } U > U_0 = \Delta E/(\alpha+\beta)$$

This means that for $U > U_0$, the roles of $\mathcal{E}_1$ & $\mathcal{E}_2$ are interchanged. Thus, for $U \to \infty$, we get...

Done as prob # 36, ϕ507 (Mar '92)

$U >> \Delta E$

$$Q = \left[1 + \left(\frac{2\gamma/(\alpha+\beta)}{1-\epsilon}\right)^2\right]^{\frac{1}{2}}, \text{ where } \epsilon = \frac{\Delta E/U}{\alpha+\beta} << 1 \text{ for } U >> \Delta E$$

For $U \to \infty$, $Q \to Q_\infty = \left[1 + \left(\frac{2\gamma}{\alpha+\beta}\right)^2\right]^{\frac{1}{2}} = \text{cnst} > 1$. Expanding.

$$Q \simeq Q_\infty\left[1 + \left(\frac{Q_\infty^2 - 1}{Q_\infty^2}\right)\epsilon\right] = Q_\infty + \left(\frac{Q_\infty^2-1}{Q_\infty}\right)\epsilon, \text{ to } \theta(\epsilon)$$

After some algebra, we can write the original $\mathcal{E}_k$ exactly as

$$\mathcal{E}_1 = E_1 + \tfrac{1}{2}(Q-1)\Delta E - \tfrac{1}{2}U\left[(Q+1)\alpha + (Q-1)\beta\right] \leftarrow$$ for $U > U_0$ this is actually continuation of original $\mathcal{E}_2$

$$\mathcal{E}_2 = E_2 - \tfrac{1}{2}(Q-1)\Delta E + \tfrac{1}{2}U\left[(Q-1)\alpha + (Q+1)\beta\right] \leftarrow$$ for $U > U_0$, this is actually continuation of original $\mathcal{E}_1$

The terms here in [ ] are manifestly (+)ve, so indeed $\mathcal{E}_1$ & $\mathcal{E}_2$ switch roles, with $\mathcal{E}_1$ going (−)ve & $\mathcal{E}_2$ going (+)ve as $U \to \infty$. So if we define the new $\mathcal{E}_2' =$ old $\mathcal{E}_1$ and new $\mathcal{E}_1' =$ old $\mathcal{E}_2$, we have -- for $U >> U_0$, to $\theta(\epsilon = U/U_0)$...

$$\Delta = +\tfrac{1}{2}(\alpha+\beta)U(Q-1)(\epsilon-1) \simeq -\tfrac{1}{2}(Q_\infty - 1)\left[(\alpha+\beta)U + \frac{\Delta E}{Q_\infty}\right]$$

$$\therefore \mathcal{E}_1' = \mathcal{E}_2 = E_2 + \beta U - \Delta$$

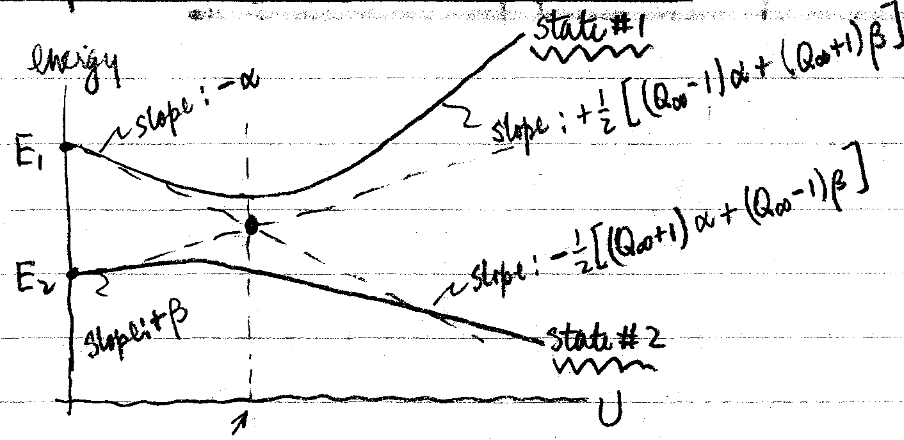
$$\simeq +\tfrac{1}{2}U\left[(Q_\infty - 1)\alpha + (Q_\infty+1)\beta\right] + \tfrac{1}{2}\left[\left(1-\tfrac{1}{Q_\infty}\right)E_1 + \left(1+\tfrac{1}{Q_\infty}\right)E_2\right]$$

$$\mathcal{E}_2' = \mathcal{E}_1 = E_1 - \alpha U + \Delta$$

$$\simeq -\tfrac{1}{2}U\left[(Q_\infty+1)\alpha + (Q_\infty - 1)\beta\right] + \tfrac{1}{2}\left[\left(1+\tfrac{1}{Q_\infty}\right)E_1 + \left(1-\tfrac{1}{Q_\infty}\right)E_2\right]$$

The high fld behaviour is thus linear with U. We have, altogether

Done as prob. # 36, ϕ 507 (Mar. '92)



xing pt at $U=U_0=\Delta E/(\alpha+\beta)$

Distance of closest approach is near U_0, where $\Delta\mathcal{E}\simeq 2\gamma U_0 = 2|V_{12}|_0$.

4/25/71 **70** Vector model $\Rightarrow$ average everything in direction of $\vec{J}$, e.g.

$$\underbrace{\langle\vec{\mu}_L+\vec{\mu}_S\rangle}_{\vec{\mu}_J} = \left[(\vec{\mu}_L+\vec{\mu}_S)\cdot\vec{J}/\vec{J}^2\right]\vec{J}$$

$$= -\mu_0\left[\left(g_L\vec{L}\cdot\vec{J}+g_S\vec{S}\cdot\vec{J}\right)/\vec{J}^2\right]\vec{J}$$

$$= -g_J\mu_0\vec{J}\text{, in exp. value sense}$$

where: $g_J = \left(\frac{\vec{L}\cdot\vec{J}}{\vec{J}^2}\right)g_L + \left(\frac{\vec{S}\cdot\vec{J}}{\vec{J}^2}\right)g_S$ } Landé g-factor

But: $\vec{L}\cdot\vec{J} = \vec{L}^2+\vec{L}\cdot\vec{S}$, $\vec{S}\cdot\vec{J} = \vec{S}^2+\vec{L}\cdot\vec{S}$

and $\vec{L}\cdot\vec{S} = \frac{1}{2}\left[\vec{J}^2-\vec{L}^2-\vec{S}^2\right]$

$$\therefore\ \vec{L}\cdot\vec{J} = \frac{1}{2}\left[\vec{J}^2+\vec{L}^2-\vec{S}^2\right] = \frac{1}{2}\left[j(j+1)+l(l+1)-s(s+1)\right]$$

$$\&\ \vec{S}\cdot\vec{J} = \frac{1}{2}\left[\vec{J}^2-\vec{L}^2+\vec{S}^2\right] = \frac{1}{2}\left[j(j+1)-l(l+1)+s(s+1)\right]$$

$$\Rightarrow g_J = \left[\frac{j(j+1)+l(l+1)-s(s+1)}{2j(j+1)}\right]g_L + \left[\frac{j(j+1)-l(l+1)+s(s+1)}{2j(j+1)}\right]g_S$$

$^2P_{J=3/2}$: $J=\frac{3}{2}$, $l=1$, $s=\frac{1}{2}$

$$g_J = \left[+\tfrac{2}{3}\right] g_L + \left[+\tfrac{1}{3}\right] g_S \simeq \frac{4}{3}$$

$$\text{Max}: \ \mu_J = \frac{4}{3}\mu_0 \frac{3}{2} = 2\mu_0$$

$^2P_{J=1/2}$: $J=\frac{1}{2}$, $l=1$, $s=\frac{1}{2}$

$$g_J = \left[+\tfrac{4}{3}\right] g_L + \left[-\tfrac{1}{3}\right] g_S \simeq \frac{2}{3}$$

$$\text{Max}: \ \mu_J = \frac{2}{3}\mu_0 \frac{1}{2} = \frac{1}{3}\mu_0$$

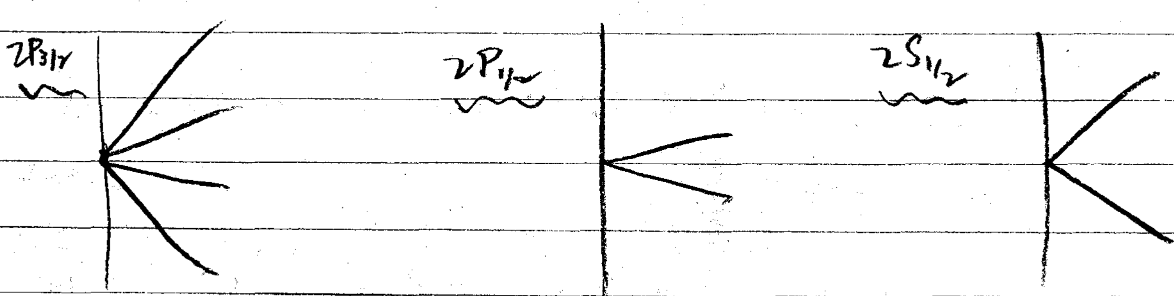
$^2S_{1/2}$: $J=\frac{1}{2}$, $l=0$, $s=\frac{1}{2}$

$$g_J = [0]\, g_L + [+1]\, g_S \simeq 2$$

$$\text{Max}: \ \mu_J = 2\mu_0 \frac{1}{2} = \mu_0$$

In external fld $\vec{H}$, get linear Zeeman effect...

$$\mathcal{E}_J = -\vec{\mu}_J \cdot \vec{H} = +g_J \mu_0 m_J H, \quad m_J = \vec{J} \text{ comp along } \vec{H}$$



4/30/71 (11) a) Std Pauli matrices $\binom{\text{Merz}}{\text{p.270}}$; $\vec{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)$

Ham^{n} is : $\mathcal{H} = -\vec{\mu} \cdot \vec{H} = +\mu_0 \vec{\sigma} \cdot \vec{H} = \mu_0 (\sigma_x H_x + \sigma_y H_y + \sigma_z H_z)$

n// $\underset{\sim}{\mathcal{H}} = \mu_0 \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix}$. Eigenvalue energies found from

$$\det(\underset{\sim}{\mathcal{H}} - E \underset{\sim}{I}) = \begin{vmatrix} \mu_0 H_z - E & \mu_0 (H_x - iH_y) \\ \mu_0 (H_x + iH_y) & -\mu_0 H - E \end{vmatrix} = 0$$

$$\therefore \quad (E - \mu_0 H_z)(E + \mu_0 H_z) + \mu_0^2 (H_x^2 + H_y^2) = 0$$

or// $E^2 = \mu_0^2 (H_x^2 + H_y^2 + H_z^2) = (\mu_0 H)^2 \Rightarrow E_\pm = \pm \mu_0 H$.

This is true no matter what the orientation of $\vec{H}$ is.

b) For $\vec{H}$ in spherical polars, the Ham^{t} is

$$\underset{\sim}{\mathcal{H}} = \mu_0 H \begin{pmatrix} +\cos\vartheta & e^{-i\varphi} \sin\vartheta \\ e^{+i\varphi} \sin\vartheta & -\cos\vartheta \end{pmatrix}$$

Find eigenspinors from $\underset{\sim}{\mathcal{H}} \begin{pmatrix} a \\ b \end{pmatrix} = E_\pm \begin{pmatrix} a \\ b \end{pmatrix}$, which gives...

$$\begin{pmatrix} \cos\vartheta \mp 1 & e^{-i\varphi} \sin\vartheta \\ e^{+i\varphi} \sin\vartheta & -\cos\vartheta \mp 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0 \Rightarrow a = \frac{e^{-i\varphi} \sin\vartheta}{-\cos\vartheta \pm 1} b$$

Should also impose norm, i.e. ; $|a|^2 + |b|^2 = 1$.

For E_+ Use: $-\cos\vartheta + 1 = 2\sin^2\frac{\vartheta}{2}$, $\sin\vartheta = 2\sin\frac{\vartheta}{2}\cos\frac{\vartheta}{2}$, so

$a = e^{-i\varphi} \left(\frac{\cos\frac{\vartheta}{2}}{\sin\frac{\vartheta}{2}} \right) b$

$|a|^2 + |b|^2 = 1 \Rightarrow |b|^2 = \sin^2\frac{\vartheta}{2}$

Can choose (up to phase) $\begin{pmatrix} a \\ b \end{pmatrix}_+ = \begin{pmatrix} \cos\frac{\vartheta}{2} \\ +e^{+i\varphi} \sin\frac{\vartheta}{2} \end{pmatrix}$

For E_- Use: $-\cos\vartheta - 1 = -2\cos^2\frac{\vartheta}{2}$, $\sin\vartheta = 2\sin\frac{\vartheta}{2}\cos\frac{\vartheta}{2}$, so

$$a = -e^{-i\varphi}\left(\frac{\sin\frac{\vartheta}{2}}{\cos\frac{\vartheta}{2}}\right) b$$

$$|a|^2 + |b|^2 = 1 \Rightarrow |b|^2 = \cos^2\frac{\vartheta}{2}$$

Can choose (up to phase)

$$\begin{pmatrix} a \\ b \end{pmatrix}_- = \begin{pmatrix} -e^{-i\varphi}\sin\frac{\vartheta}{2} \\ \cos\frac{\vartheta}{2} \end{pmatrix}$$

Note: $\begin{pmatrix} a \\ b \end{pmatrix}_+^\dagger \begin{pmatrix} a \\ b \end{pmatrix}_- = \left(c \;\; e^{-i\varphi}s\right)\begin{pmatrix} -e^{-i\varphi}s \\ c \end{pmatrix} = 0$, as should be.

If $\vec{H}$ along z-axis, $\vartheta = \varphi = 0$, then: $\begin{pmatrix} a \\ b \end{pmatrix}_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} a \\ b \end{pmatrix}_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

4/30/71 **17** We flailed around with this problem in WKBK # 18, p.93 (1/18/63). Referring to that work, we shall let α & β be the spin-up & spin-down eigenfcns as noted, and we will define

$$|n;\ell,s,j,m_j\rangle = \psi_j^{m_j}, \quad |n;\ell,m_\ell\rangle = \phi_\ell^{m_\ell}$$

Start at the top of the ladder, noting

$$\psi_{j=\ell+\frac{1}{2}}^{m_j=j} = \phi_\ell^{+\ell}\alpha, \text{ only} \qquad (1)$$

Apply step-down operator $J^{(-)} = L^{(-)} + S^{(-)}$, where generally

$$J^{(-)}|j,m_j\rangle = \sqrt{j(j+1) - m_j(m_j-1)}\;|j,m_j-1\rangle$$

Applying this to (1), get

$$J^{(-)}\psi_{j=\ell+\frac{1}{2}}^{m_j=j} = \sqrt{2j}\;\psi_{j=\ell+\frac{1}{2}}^{m_j=j-1}$$

Note: $S^{(-)}\alpha = \beta$

$$\left(L^{(-)} + S^{(-)}\right)\phi_\ell^{+\ell}\alpha = \sqrt{2\ell}\;\phi_\ell^{\ell-1}\alpha + \phi_\ell^{\ell}\beta$$

$$\therefore \psi_{j=\ell+\frac{1}{2}}^{m_j=j-1} = \sqrt{\frac{2\ell}{2\ell+1}}\;\phi_\ell^{\ell-1}\alpha + \sqrt{\frac{1}{2\ell+1}}\;\phi_\ell^{\ell}\beta \quad \leftarrow J^{(-)} \text{ applied } \underline{\text{once}}. \qquad (2)$$

Operating again with $J^{(-)}$ on (2), we get

$$J^{(-)}\psi^{m_j=j-1}_{j=l+\frac12} = \sqrt{\frac{2l}{2l+1}}\left[\left(L^{(-)}\phi_l^{l-1}\right)\alpha + \phi_l^{l-1}\beta\right] + \sqrt{\frac{1}{2l+1}}\left[\left(L^{(-)}\phi_l^{l}\right)\beta\right]$$

$$\sqrt{2(2j-1)}\,\psi^{m_j=j-2}_{j=l+\frac12} = \sqrt{\frac{2l}{2l+1}}\sqrt{2(2l-1)}\,\phi_l^{l-2}\alpha + 2\sqrt{\frac{2l}{2l+1}}\,\phi_l^{l-1}\beta$$

or, simplifying...

$$\psi^{m_j=j-2}_{j=l+\frac12} = \sqrt{\frac{2l-1}{2l+1}}\,\phi_l^{l-2}\alpha + \sqrt{\frac{2}{2l+1}}\,\phi_l^{l-1}\beta \leftarrow J^{(-)} \text{ applied } \underline{\text{twice}} \qquad (3)$$

Another application of $J^{(-)}$ to (3) gives...

$$\psi^{m_j=j-3}_{j=l+\frac12} = \sqrt{\frac{2l-2}{2l+1}}\,\phi_l^{l-3}\alpha + \sqrt{\frac{3}{2l+1}}\,\phi_l^{l-2}\beta \leftarrow J^{(-)} \text{ applied } \underline{\text{thrice}} \qquad (4)$$

Comparing (2), (3), (4), we see the obvious generalization

$$\psi^{m_j=j-k}_{j=l+\frac12} = \sqrt{\frac{2l-k+1}{2l+1}}\,\phi_l^{l-k}\alpha + \sqrt{\frac{k}{2l+1}}\,\phi_l^{l-k+1} \leftarrow J^{(-)}\ k \text{ times} \qquad (5)$$

But $m_j = j-k \Rightarrow k = l+\frac12 - m_j$. So we can write...

$$\psi^{m_j}_{j=l+\frac12} = \left(\sqrt{\frac{l+\frac12+m_j}{2l+1}}\right)\phi_l^{m_j-\frac12}\,\alpha + \left(\sqrt{\frac{l+\frac12-m_j}{2l+1}}\right)\phi_l^{m_j+\frac12}\,\beta \qquad (6)$$

These are desired $C_{1,2}(j=l+\frac12)$

To get the $\psi^{m_j}_{j=l-\frac12}$, we need only construct them $\perp$ $\psi^{m_j}_{j=l+\frac12}$, and impose normalization. Thus we must have

$$\left.\begin{aligned} &C_1(j=l-\tfrac12)\left(\sqrt{\frac{l+\frac12+m_j}{2l+1}}\right) + C_2(j=l-\tfrac12)\left(\sqrt{\frac{l+\frac12-m_j}{2l+1}}\right) = 0 \\ &\text{and } \left|C_1(j=l-\tfrac12)\right|^2 + \left|C_2(j=l-\tfrac12)\right|^2 = 1 \end{aligned}\right\} \quad (7)$$

These conditions are satisfied by

$$C_1(j=l-\tfrac{1}{2}) = \sqrt{\frac{l+\frac{1}{2}-m_l}{2l+1}}\ , \quad C_2(j=l-\tfrac{1}{2}) = (-)\sqrt{\frac{l+\frac{1}{2}+m_j}{2l+1}} \tag{8}$$

Thus the desired $j=l-\frac{1}{2}$ eigenfcns are ...

$$\psi^{m_j}_{j=l-\frac{1}{2}} = \left(\sqrt{\frac{l+\frac{1}{2}-m_j}{2l+1}}\right)\phi_l^{m_j-\frac{1}{2}}\alpha - \left(\sqrt{\frac{l+\frac{1}{2}+m_j}{2l+1}}\right)\phi_l^{m_j+\frac{1}{2}}\beta \tag{9}$$

Eqs (6) & (9) agree with the results of eqs.(22), p.98, WKBK #18, and (apparently) also with Condon & Shortley, eq. (8b), p.123.

For $2^2P_{3/2}$ state, $l=1$ & $j=3/2$. The four coupled eigenfcns are

$$\left.\begin{aligned}
m_j &= +3/2 : && \phi_1^{+1}\alpha\text{, only}\\
m_j &= +1/2 : && \sqrt{\tfrac{2}{3}}\,\phi_1^{0}\alpha + \sqrt{\tfrac{1}{3}}\,\phi_1^{+1}\beta\\
m_j &= -1/2 : && \sqrt{\tfrac{1}{3}}\,\phi_1^{-1}\alpha + \sqrt{\tfrac{2}{3}}\,\phi_1^{0}\beta\\
m_j &= -3/2 : && \phi_1^{-1}\beta\text{, only}
\end{aligned}\right\} \tag{10}$$

For $2^2P_{1/2}$ state, $l=1$ & $j=1/2$. The two coupled eigenfcns are

$$\left.\begin{aligned}
m_j &= +1/2 : && \sqrt{\tfrac{1}{3}}\,\phi_1^{0}\alpha - \sqrt{\tfrac{2}{3}}\,\phi_1^{+1}\beta\\
m_j &= -1/2 : && \sqrt{\tfrac{2}{3}}\,\phi_1^{-1}\alpha - \sqrt{\tfrac{1}{3}}\,\phi_1^{0}\beta
\end{aligned}\right\} \tag{11}$$

By inspection, all these eigenfcns are orthonormal. This can be shown quite generally for the general eigenfcns of eqs (6) & (9).