Solutions to Phys. 507 Hour Exam, 11 May 1971

5/9/71

(0) The solution here proceeds from the solution to problem (71). In $\vec{H}$ (to left of origin) the particle's eigenfcn is $\binom{1}{0}$. If $\vec{H} \to \vec{H}'$ "suddenly" (i.e. in a period of time short compare to Larmor precession period), then that eigenfcn (the one for (+)ve energy) becomes

$$\psi_+(\beta) = \begin{pmatrix} \cos(\beta/2) \\ e^{i\varphi}\sin(\beta/2) \end{pmatrix}, \text{ for } \vec{H}' \text{ oriented at } \measuredangle\text{s } \beta \;\&\; \varphi \text{ w.r.t. z-axis}$$

The spin flip probability will be $\left|\binom{0}{1}^\dagger \cdot \psi_+(\beta)\right|^2 = \sin^2\beta/2$.

(2) For two equivalent 2p electrons in Russell-Saunders coupling

total spin : $S = S_1+S_2, \ldots, |S_1 - S_2| = 1$ or 0 ⇒ triplets & singlets

total orbital ∢ mom : $L = L_1+L_2, \ldots, |L_1-L_2| = 2, 1, 0$ ⇒ D, P, S states

a) Possible states are : ${}^3D_{J=3,2,1}$, ${}^1D_2$, ${}^3P_{J=2,1,0}$, ${}^1P_1$, ${}^3S_1$, ${}^1S_0$.

b) Spin $\begin{matrix}\text{triplets}\\\text{singlets}\end{matrix}$ have $\begin{matrix}\text{even}\\\text{odd}\end{matrix}$ exchange symmetry.

Exchange symmetry (or parity) of state (L) is $(-1)^L$ ⇒ D & S states are even, P state is odd.

So ${}^3D_J$, ${}^1P_1$ and ${}^3S_1$ states have overall even exch. symm, which disallows them for a system of Fermions.

c) Remaining states are ${}^1D_2$, ${}^3P_{2,1,0}$, ${}^1S_0$. The triplet will lie lowest (since the P wavefcn is odd ⇒ e^-'s far apart → minimize electrostatic repulsion e^2/r_{12}). And the state of lowest J will lie lowest (since this minimizes spin-orbit energy). So gnd state is ${}^3P_0$.

3 $\mathcal{H} = \begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$, $E_2 > E_1$. Find eigenenergies $\mathcal{E}$ 1

$a \to V_{13}$, $b \to V_{23}$: levels 1 & 3 repel; so do 2 & 3.

$$\det(\mathcal{H} - \mathcal{E}\,\mathbb{I}) = \begin{vmatrix} E_1-\mathcal{E} & 0 & a \\ 0 & E_1-\mathcal{E} & b \\ a^* & b^* & E_2-\mathcal{E} \end{vmatrix} = 0 \text{ gives desired eigenenergies.}$$

i.e.// $(E_1-\mathcal{E})\left[(E_1-\mathcal{E})(E_2-\mathcal{E}) - (|a|^2+|b|^2)\right] = 0$

$\Rightarrow$ $\mathcal{E}_1 = E_1$, and $\mathcal{E} = \mathcal{E}_{2,3}$, which satisfy

$$(\mathcal{E}-E_1)(\mathcal{E}-E_2) - (|a|^2+|b|^2) = 0$$ 5

or// $\mathcal{E}^2 - (E_1+E_2)\mathcal{E} + \left(E_1E_2 - (|a|^2+|b|^2)\right) = 0$

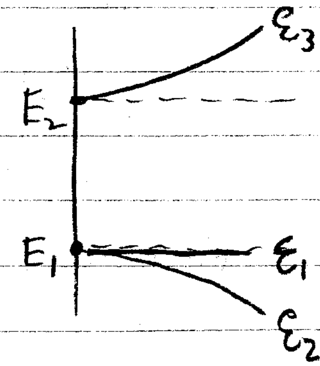
$$\Rightarrow \mathcal{E}_{2,3} = \frac{1}{2}\left[(E_1+E_2) \pm \sqrt{(E_1+E_2)^2 - 4\left(E_1E_2 - (|a|^2+|b|^2)\right)}\right]$$

$$= \frac{1}{2}\left[(E_1+E_2) \pm (E_1-E_2)\sqrt{1 + 4\frac{|a|^2+|b|^2}{(E_1-E_2)^2}}\right]$$

Assuming $|a|$ & $|b| = \alpha U$ & βU are small w.r.t. E_2-E_1, an expansion of this gives

upper sign: $\mathcal{E}_2 \simeq E_1 - \dfrac{(\alpha^2+\beta^2)U^2}{E_2-E_1}$

lower sign: $\mathcal{E}_3 \simeq E_2 + \dfrac{(\alpha^2+\beta^2)U^2}{E_2-E_1}$



4 $|\alpha\rangle = \sum_n c_n |n\rangle$, $c_n = c_n(t)$ in general.

a) Take exp. value of operator Q in state α

$$\langle Q\rangle = \langle\alpha|Q|\alpha\rangle = \sum_m c_m^* \langle m|\, Q \,|\cdot \sum_n c_n |n\rangle = \sum_m \sum_n c_m^* c_n \langle m|Q|n\rangle$$

Let $\langle m|Q|n\rangle = Q_{mn}$, and define $\rho_{nm} = c_n c_m^*$. Then

$$\langle Q\rangle = \sum_{m,n} \rho_{nm} Q_{mn} = \sum_n (\underset{\sim}{\rho}\, \underset{\sim}{Q})_{nn} \quad \left\{ \begin{array}{l} \underset{\sim}{Q} \text{ with entries } Q_{mn} \\ \underset{\sim}{\rho} \text{ with entries } \rho_{nm} \end{array} \right.$$

or, $\langle Q\rangle = \mathrm{Tr}(\underset{\sim}{\rho}\, \underset{\sim}{Q})$ as desired.

The density matrix $\underset{\sim}{\rho}$ has entries $\rho_{kl} = c_k c_l^*$.

Note: $\rho_{kk} = |c_k|^2$ = prob. of finding α in state $|k\rangle$.

The ρ_{kl}, $k \neq l$ have no direct interpretation -- they are related to $k \to l$ transition probabilities however.

b) $H|\alpha\rangle = i\hbar \frac{\partial}{\partial t}|\alpha\rangle \Rightarrow \sum_n c_n H|n\rangle = i\hbar \sum_n \dot{c}_n |n\rangle$

~~Here we have assumed all time dependence carried in the c_n.~~

Operate thru eqtn by $\langle m|$, use $\langle m|n\rangle = \delta_{mn}$ on RHS, to get

① $i\hbar \dot{c}_m = \sum_k c_k H_{mk}$, where $H_{mk} = \langle m|H|k\rangle$

② $-i\hbar \dot{c}_n^* = \sum_k c_k^* H_{nk}^*$, by complex conjugation

Multiply ① by c_n^*, ② by c_m, and set $H_{nk}^* = H_{kn}$. Then

①′ $i\hbar\, \dot{c}_m c_n^* = \sum_k c_k c_n^* H_{mk}$, ②′ $-i\hbar\, c_m \dot{c}_n^* = \sum_k c_m c_k^* H_{kn}$

Now subtract ②′ from ①′ to get

$$i\hbar(\dot{c}_m c_n^* + c_m \dot{c}_n^*) = \sum_k (H_{mk}\rho_{kn} - \rho_{mk}H_{kn})$$

or $$i\hbar \frac{d}{dt}\underbrace{(c_m c_n^*)}_{\rho_{mn}} = (\underset{\sim}{H}\,\underset{\sim}{\rho})_{mn} - (\underset{\sim}{\rho}\,\underset{\sim}{H})_{mn}$$

or $$i\hbar \frac{d}{dt}\underset{\sim}{\rho} = [\underset{\sim}{H}, \underset{\sim}{\rho}]$$ QED

c) Now $|\alpha\rangle = \sum_n c_n |n\rangle \Rightarrow c_n = \langle n|\alpha\rangle$.

So $\rho_{kl} = c_k c_l^* = \langle k|\alpha\rangle\langle l|\alpha\rangle^* = \langle k|\alpha\rangle\langle\alpha|l\rangle$

See that $\underset{\sim}{\rho}$ is just a matrix of the projection operator $\underset{\sim}{P_\alpha} = |\alpha\rangle\langle\alpha|$. In the $|n\rangle$ rep$^{\underline{n}}$ $\rho_{kl} = \langle k|P_\alpha|l\rangle$. In the x-rep$^{\underline{n}}$, $\underset{\sim}{\rho}$ would be a matrix of elements

$$\rho_{xx'} = \langle x|P_\alpha|x'\rangle = \langle x|\alpha\rangle\langle\alpha|x'\rangle = \langle x|\alpha\rangle\langle x'|\alpha\rangle^*$$

But $\langle x|\alpha\rangle = \psi_\alpha(x)$ is the cd. rep$^{\underline{n}}$ of state α. So

$$\rho_{xx'} = \psi_\alpha(x)\,\psi_\alpha^*(x')$$

The diagonal entries are $\rho_{xx} = |\psi_\alpha(x)|^2$, which is just the probability density of the state α.