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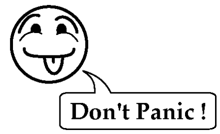

Quantum Mechanics II
1st Midterm Exam

27th February '98.
Solutions (T. Hübsch)

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The completeness and detail presented herein were by no means expected in the Student's solutions for full credit. The additional information given here is solely for the Student's convenience and education.

1. Let's abbreviate:

$$|\pm\rangle \stackrel{\rm def}{=} \psi_\pm(r,\theta,\phi) = \begin{pmatrix}\psi^\pm_\uparrow\\ \psi^\pm_\downarrow\end{pmatrix}\ , \qquad \begin{cases} \psi^\pm_\uparrow = F_l(r)\sqrt{\frac{l+\frac12\pm m_j}{2l+1}}\ Y_l^{m_j\mp\frac12}(\theta,\phi)\ ,\\ \psi^\pm_\downarrow = \mp F_l(r)\sqrt{\frac{l+\frac12\mp m_j}{2l+1}}\ Y_l^{m_j\pm\frac12}(\theta,\phi)\ , \end{cases}$$

where it is understood that $Y_l^\mu\equiv 0$ if $l<|\mu|$. With these an expectation value can be written as follows

$$\begin{aligned} \langle\hat O\rangle &= \langle+|\,\hat O\,|+\rangle + \langle-|\,\hat O\,|-\rangle\ ,\\ &= \int {\rm d}^3\vec r\ \Big[(\psi^+_\uparrow)^*\hat O\,\psi^+_\uparrow\ +\ (\psi^+_\downarrow)^*\hat O\,\psi^+_\downarrow\ +\ (\psi^-_\uparrow)^*\hat O\,\psi^-_\uparrow\ +\ (\psi^-_\downarrow)^*\hat O\,\psi^-_\downarrow\Big]\ , \qquad (1)\\ &= \int {\rm d}^3\vec r\ \Big[\big|\psi^+_\uparrow\big|^2\hat O\ +\ \big|\psi^+_\downarrow\big|^2\hat O\ +\ \big|\psi^-_\uparrow\big|^2\hat O\ +\ \big|\psi^-_\downarrow\big|^2\hat O\Big]\ . \end{aligned}$$

It should now be clear that the ϕ-dependence of the integrand stemms solely from $\hat O$. Now we need

$$z = r\cos(\theta)\ , \qquad z^2 = r^2\cos^2(\theta)\ .$$

Neither of these depending on ϕ, for both parts a. and b., the ϕ-integration in $\int {\rm d}^3\vec r = \int_0^\infty r^2{\rm d}r\int_0^\pi \sin\theta{\rm d}\theta\int_0^{2\pi}{\rm d}\phi$ merely produces an overall factor of 2π.

a. Now, when $l{=}0$, then for $|+\rangle$ we have that $m{=}0$, so $j{=}l{+}s{=}\frac12$ and $m_j{=}\pm\frac12$, and

$$|+\rangle = \left\{\begin{pmatrix}\psi^+_\uparrow\\ 0\end{pmatrix}\ ,\begin{pmatrix}0\\ \psi^+_\downarrow\end{pmatrix}\right\} \qquad \psi^+_\uparrow = -\psi^+_\downarrow = F_0(r)Y_0^0(\theta,\phi) = F_0(r)\frac{1}{\sqrt{4\pi}}\ .$$

while $|-\rangle\equiv 0$ ($j{=}l{-}s$ would be negative). Thus, (summing Eq. (1) over all allowed m_j)

$$\langle z\rangle = \int {\rm d}^3\vec r\ \Big[\big|\psi^+_\uparrow\big|^2 z + 0 + 0 + \big|\psi^-_\downarrow\big|^2 z\Big] = \frac{\langle r\rangle}{4\pi}\,2{\cdot}2\pi\int_0^\pi \sin(\theta){\rm d}\theta\ \cos(\theta) =\ 0\ ,$$

because of the θ-integration.

b. On the other hand, for $l{=}1$, $j=\frac32$ or $\frac12$. For the former, $m_j=\frac32,\frac12,-\frac12-\frac32$:

$$\frac{|+\rangle}{F_1(r)} = \left\{\begin{pmatrix}Y_1^1\\ 0\end{pmatrix}\ ,\ \begin{pmatrix}\sqrt{\frac23}Y_1^0\\ -\sqrt{\frac13}Y_1^1\end{pmatrix}\ ,\ \begin{pmatrix}\sqrt{\frac13}Y_1^{-1}\\ -\sqrt{\frac23}Y_1^0\end{pmatrix}\ ,\ \begin{pmatrix}0\\ -Y_1^{-1}\end{pmatrix}\right\}\ .$$

For $j=\frac{1}{2}$, $m_j=\frac{1}{2}$:

$$\frac{|-\rangle}{F_1(r)} = \left\{ \begin{pmatrix} \sqrt{\frac{1}{3}}Y_1^0 \\ \sqrt{\frac{2}{3}}Y_1^1 \end{pmatrix} , \quad \begin{pmatrix} \sqrt{\frac{2}{3}}Y_1^{-1} \\ \sqrt{\frac{1}{3}}Y_1^0 \end{pmatrix} \right\} .$$

(Have you noticed that the square-root coefficients are in fact Clebsch-Gordan coefficients?)

Now we sum Eq. (1), with $z^2 = r^2\cos^2\theta$, over all allowed m_j:

$$\begin{aligned} \langle z^2\rangle &= \langle r^2\rangle \int \mathrm{d}\Omega \Big[\big|Y_1^1\big|^2 + 0 + \tfrac{2}{3}\big|Y_1^0\big|^2 + \tfrac{1}{3}\big|Y_1^1\big|^2 + \tfrac{1}{3}\big|Y_1^{-1}\big|^2 + \tfrac{2}{3}\big|Y_1^0\big|^2 + 0 + \big|Y_1^{-1}\big|^2 \\ &\qquad + \tfrac{1}{3}\big|Y_1^0\big|^2 + \tfrac{2}{3}\big|Y_1^1\big|^2 + \tfrac{2}{3}\big|Y_1^{-1}\big|^2 + \tfrac{1}{3}\big|Y_1^0\big|^2 \Big] \cos^2\theta , \qquad (2a) \\ &= \langle r^2\rangle 2 \int \mathrm{d}\Omega \Big[\big|Y_1^1\big|^2 + \big|Y_1^0\big|^2 + \big|Y_1^{-1}\big|^2 \Big] \cos^2\theta , \qquad (2b) \\ &= \langle r^2\rangle 2 \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \Big[\tfrac{3}{8\pi}\sin^2\theta + \tfrac{3}{4\pi}\cos^2\theta + \tfrac{3}{8\pi}\sin^2\theta \Big] \cos^2\theta , \qquad (2c) \\ &= \langle r^2\rangle 2{\cdot}2\pi \int_{-1}^1 \mathrm{d}u \Big[\tfrac{3}{4\pi}\Big] u^2 \;=\; \langle r^2\rangle 3 \Big[\frac{u^3}{3}\Big]_{-1}^1 = 2\langle r^2\rangle . \qquad (2d) \end{aligned}$$

In the last line, we used the $u=\cos\theta$ change of variables. Note that the contribution in the square brackets in $(2a)$–$(2c)$ yields $\frac{3}{4\pi}$. Since $\int \mathrm{d}\Omega = 4\pi$, this factor by itself would after angular integrations produce 3—the degeneracy of P-state(s). The extra factor of 2 in $(2b)$ stemms from the spin-degeneracy. Indeed, one could have derived Eq. $(2b)$ using the product basis, $\Psi = \psi\chi$, where ψ is spin-independent. Since the operator z^2 is also spin-independent, $\langle\Psi|z^2|\Psi\rangle = \langle\psi|z^2|\psi\rangle\langle\chi|\chi\rangle$, and the latter factor would produce the multiplicity 2—owing to a sum over the two possible spin projections, $\pm\frac{1}{2}$. The three terms in the square brackets then simply stand for $\sum_{m=-l}^{l}|Y_l^m|^2$, for $l=1$: as the statement of the problem implied, all possible projections m contribute, we only require $l=1$.

There was also an easy argument for $\langle z\rangle = 0$: by definition, $\langle z\rangle = \langle\psi|z|\psi\rangle$ is an expectation value and so quadratic in the wave-function of the state $|\psi\rangle$. As long as the state has a definite parity (with respect to reflection: $\theta\to\theta{+}\pi$ and $\phi\to\phi{+}\pi$, the integrand will be odd and the integral (in symmetric limits) will vanish.

2.a. As suggested in the note, we use Cartesian basis for the electron in the 3-dimensional box:

$$\psi = \left(\tfrac{2}{L}\right)^{\frac{3}{2}} \sin\Big(n_x\pi\frac{x}{L}\Big) \sin\Big(n_y\pi\frac{y}{L}\Big) \sin\Big(n_z\pi\frac{z}{L}\Big) , \qquad n_x, n_y, x_z = 1,2,3,\ldots$$

b. In determining the lifetime $\tau = (A_{a\to b})^{-1}$, where $A_{a\to b}$ is the Einstein coefficient. For 'a first excited state' we are free to choose amongst $|2,1,1\rangle$, $|1,2,1\rangle$ and $|1,1,2\rangle$;

either of these could only decay into the ground state $|1,1,1\rangle$. As in Eq. (11.21), we have $A_{a\to b} = \frac{4e'^2\omega^3}{3\hbar c^3}\big|\langle b|\vec{r}|a\rangle\big|^2$. So, for example

$$
\begin{aligned}
A_{|1,1,2\rangle\to|1,1,1\rangle} &= \frac{4e'^2\omega^3}{3\hbar c^3}\big|\langle 1,1,1|\vec{r}|1,1,2\rangle\big|^2 = \frac{4e'^2\omega^3}{3\hbar c^3}\big|\langle 1,1,1|z|1,1,2\rangle\big|^2 \;, \\
&= \frac{4e'^2\omega^3}{3\hbar c^3}\left|\frac{2}{L}\int_0^L \mathrm{d}z\,\sin^2\Big(n_z\pi\frac{z}{L}\Big)\,z\right|^2 = \frac{4e'^2\omega^3}{3\hbar c^3}\left|\frac{2}{L}\frac{L^2}{4}\right|^2 = \frac{L^2e'^2\omega^3}{3\hbar c^3}
\end{aligned}
$$

where the second equality in the first line follows since $\langle 1,1,1|x|1,1,2\rangle \propto \langle 1|x|1\rangle = 0$ and similarly for y. The integral is easily done by using $\sin^2\alpha = \frac{1}{2}[1-\cos(2\alpha)]$ and integration by parts. Thus, $\tau = \frac{3\hbar c^3}{L^2e'^2\omega^3}$.

c. From, e.g., Eq. (11.19), we see that only $\langle 1,1,1|\hat{e}\cdot\vec{r}|2,1,1\rangle = \langle 1,1,1|x|2,1,1\rangle$ having been non-zero, the polarization vector $\hat{e}$ must have been in the x-direction. This then is the polarization of the photon's vector potential, in Eq. (11.12) and is referred to as the photon's polarization.

3. The composite wave-function for the three electrons must be antisymmetrized with respect to teh exchange of any two.

a. The lowest possible (ground) state will be obtained by choosing the lowest possible n,l,m's. As there are only two spin states available ($m_2{=}\pm\frac{1}{2}$), at least one of the electrons will have to have have a higher choice of n,l,m than the other two. Thus, two electrons (with opposite spins) will be in the $1S$-state, while the third will have to be in the $2S$-state, its spin arbitrary. Having fixed that $l=0=m$ for all electrons, we'll omit these and write $|nm_s\rangle$ for $|n,0,0;m_s\rangle$; also, we abbreviate $m_s{=}\pm\frac{1}{2}$ into $\pm$. Finally, we write $|n_1m_{s1};n_2m_{s2};n_3m_{s3}\rangle$ for the composite wave-function:

$$
\begin{aligned}
\Psi_g^{\pm} = \tfrac{1}{\sqrt{6}}\Big[\,&|1+;1-;2\pm\rangle - |1+;2\pm;1-\rangle + |2\pm;1+;1-\rangle \\
&- |2\pm;1-;1+\rangle + |1-;2\pm;1+\rangle - |1-;1+;2\pm\rangle\Big]\;.
\end{aligned}
\tag{3}
$$

b. As should be clear from (3), there is only the spin-projection of the $2S$ electron which has two possible values — hence a twofold degeneracy of $\Psi_g^{\pm}$: the ground state of Lithium is a doublet.

4. The electrons are free inside the line of length L and so may be considered as particles in a 1-dimensional box. The stationary wave-functions are $|n\rangle = \sqrt{\frac{2}{L}}\sin(n\frac{\pi x}{L})$. Their energy is

$$
E \;=\; \frac{\pi^2\hbar^2}{2mL^2}\,n^2\;, \qquad n = 1,2,\cdots
$$

whereupon $n = \frac{L}{\pi\hbar}\sqrt{2mE}$.

a. Within n and $n+\mathrm{d}n$, there are $\mathrm{d}N = 2\mathrm{d}n$ states; the factor 2 stems from two spin projections. Since

$$\mathrm{d}E \;=\; \frac{\pi^2\hbar^2}{2mL^2}\,2n\mathrm{d}n\;,$$

we obtain the energy distribution:

$$\rho(E) \stackrel{\text{def}}{=} \frac{\mathrm{d}N}{\mathrm{d}E} \;=\; \frac{L}{\pi\hbar}\sqrt{\frac{2m}{E}}\;.$$

b. The density of electrons is total number of electrons divided by the length:

$$\nu \stackrel{\text{def}}{=} \frac{N}{L} \;=\; \frac{1}{L}\int_0^{E_F}\mathrm{d}N \;=\; \frac{1}{L}\int_0^{E_F}\mathrm{d}E\;\frac{L}{\pi\hbar}\sqrt{\frac{2m}{E}} \;=\; \frac{\sqrt{8mE_F}}{\pi\hbar}\;.$$

Thus, $E_F = \frac{\pi^2\hbar^2}{8m}\nu^2$.

c. The average energy is ($N = \nu L = \frac{L}{\pi\hbar}\sqrt{8mE_F}$)

$$\overline{E} \stackrel{\text{def}}{=} \frac{\int_0^{E_F}\mathrm{d}N\,E}{N} \;=\; \frac{\pi\hbar}{L\sqrt{8mE_F}}\int_0^{E_F}\mathrm{d}E\;\frac{L}{\pi\hbar}\sqrt{\frac{2m}{E}}\,E \;=\; \tfrac{1}{3}E_F\;.$$

d. Pressure is, as always, defined in terms of infinitesimal work done to produce an isobaric expansion: $\mathrm{d}W = p\mathrm{d}V$. Since we are dealing with a line, $\mathrm{d}V = S\mathrm{d}L$, where S is the thickness of the line of length L. Since the work done increases the total energy, so $\mathrm{d}W = -\mathrm{d}U$. Now, we have that:

$$U = \overline{E}\,N = \frac{1}{3}E_F\,N = \frac{1}{3}\frac{\pi^2\hbar^2}{8m}\nu^2\,N = \frac{\pi^2\hbar^2}{24m}\frac{N^3}{L}\;.$$

Then

$$p = \frac{\mathrm{d}W}{\mathrm{d}V} = -\frac{1}{S}\frac{\mathrm{d}U}{\mathrm{d}L} = \frac{1}{S}\frac{E_F N}{3} = \frac{L}{3S}\nu E_F\;.$$

Note that the pressure blows up in the ideal limit, when the cross-section area, S, is much smaller than the length, L. That is as expected, since $\mathrm{d}W = F\mathrm{d}L$ is the work done by the force F acting to change the length of the system. Then $p = F/S$, and $\lim_{S\to 0} p \to \infty$.