GRADUATE QUANTUM MECHANICS: 502 Spring 2002

Solutions to Take-home final.

1. If the electron were a $j = 3/2$ particle, then each hydrogenic orbital would acquire a $2j + 1 = 4$ fold spin degeneracy, so that a state with orbital angular momentum l could hold up to $4(2l + 1)$ electrons, thus an 1s or 2s -state could hold up to 4 electrons, and a 2p-state, could hold up to $4 \times (5) = 20$ electrons. The sequence of shell structure would be $1s^4 2s^4 2p^{20} 3s^4 \ldots$ and clearly, the periodic table would be dramatically different.

   (a) The configuration of a hypothetical Ne (Z=10) atom made up of such "electrons" would be

   $$1s^4 2s^4 2p^2$$

   Notice that the filled shell configuration $1s^4 2s^4$ is singly degenerate, the configuration $1s^4 2s^4 2p^1$ will have a degeneracy of $4 \times 3 = 12$, and the configuration $1s^4 2s^4 2p^2$ will be highly degenerate, with a $12 \times 11/2 = 66$ -fold degeneracy.

   The exclusion principle restricts the possible spin and angular momentum configurations, so that the spin wavefunction and the spatial wavefunction have opposite parity under particle exchange. The possible states are then

   $$\begin{aligned} |S, L\rangle &= |3, 1\rangle && \text{(21 states)} \\ &= |2, 2\rangle && \text{(25 states)} \\ &= |2, 0\rangle && \text{(5 states)} \\ &= |1, 1\rangle && \text{(9 states)} \\ &= |0, 2\rangle && \text{(5 states)} \\ &= |0, 0\rangle && \text{(1 state)} \end{aligned} \tag{1}$$

   making a total of 66.

   (b) The state with the maximum spin, i.e $S = 3$ will have the lowest Coulomb energy, which selects the first of these possibilities, with $\underline{S = 3, L = 1}$. Spin -orbit interactions will align the spin and orbital angular momenta in opposite directions, producing a state with $\underline{J = 2}$. In spectroscopic notation, the ground-state is thus $\underline{{}^{2S+1}L_J = {}^7P_2}$.

2. If a particle moving in 1D is subjected to a pulse travelling at speed c, represented by a time-dependent potential,

   $$V(t) = A\delta(x - ct),$$

   then, in the interaction representation, the state after time t is given by $|\psi\rangle = \sum_j a_j(t)|j\rangle$. If, at time $t = -\infty$, $|\psi\rangle = |i\rangle$, then in the distant future, to first order in A, the amplitudes a_j $(j \neq i)$ are given by

   $$\begin{aligned} a_j &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' \langle j|V|i\rangle e^{i\omega_{ji}t'} \\ &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' dx u_j^*(x) u_i(x) A\delta(x - ct') e^{\frac{i}{\hbar}(E_j - E_i)t'} \\ &= -\frac{iA}{\hbar c}\int_{-\infty}^{\infty} dx u_j^*(x) u_i(x) e^{\frac{i}{\hbar c}(E_j - E_i)x} \end{aligned} \tag{2}$$

   (a) The probability to be in state $j \neq i$ is thus

   $$p_j(t = +\infty) = |a_j|^2 = \frac{A^2}{(\hbar c)^2}\left|\int_{-\infty}^{\infty} dx u_j^*(x) u_i(x) e^{\frac{i}{\hbar c}(E_j - E_i)x}\right|^2$$

   (b) The first thing to note, is that energy is conserved in this transition process. On short-time scales, energy conservation does not hold, because the perturbation is time dependent, but on long time-scales, the energy-time uncertainty relation $\Delta E \Delta t \sim 1$ allows for the energy of the final state to be defined with arbitrary accuracy. The difference in energy

$$E_j - E_i = \hbar\omega$$

is provided by the absorption of a quantum of energy from the delta function pulse.
The delta-function perturbation can be regarded as a superposition of plane waves, with an infinitely broad frequency spectrum. We may write

$$V = \frac{1}{2\pi c}\int_{-\infty}^{\infty} d\omega A(\omega) e^{i\omega[(x/c)-t]} \tag{3}$$

$A(\omega) = A$ is independent of frequency. Had we written the potential in the above form, then the integral over time would have given

$$\int dt' e^{i(\omega_{ji}-\omega)t'} = 2\pi\delta(\omega - \omega_{ji})$$

In other words, if we are considering transitions from state i to state j only the component of the wave with a frequency that matches the the excitation energy

$$\omega = \frac{E_j - E_i}{\hbar}$$

will cause transitions. The transition probability from state i to state j is

$$p_{i\to j} = \frac{A(\omega_{ji})^2}{(\hbar c)^2}\left|\int_{-\infty}^{\infty} dx u_j^*(x) u_i(x) e^{\frac{i}{\hbar c}(E_j - E_i)x}\right|^2.$$

and it depends only on the intensity of radiation at frequency $\omega = \omega_{ji}$.
Finally, notice that if $\tilde{u}_j(p) = \langle p|j\rangle$ is the momentum-space wavefunction, then $u_j(x) = \int \frac{dp}{\sqrt{2\pi}} e^{ipx}\tilde{u}(p)$ then the transition probability becomes

$$p_{i\to j} = \frac{A(\omega_{ji})^2}{(\hbar c)^2}\left|\int_{-\infty}^{\infty} dx \tilde{u}_j^*(p + \omega_{ji}/c)\tilde{u}_i(p)\right|^2$$

In other words, the perturbation at frequency $\omega = \omega_{ji}$ also imparts a momentum impulse $p = \omega_{ji}/c$ to the state.

3. If the Hamiltonian of the rotator is

$$H = A\mathbf{L}^2 + \overbrace{B\hbar^2\cos 2\phi}^{V} \tag{4}$$

with $A >> B$, then we may regard the second term in the Hamiltonian as a perturbation. However, since a state of definite l is $2l+1$ fold degenerate, we must use <u>degenerate perturbation theory</u> to calculate the shift in the energy levels. In the manifold of states of definite l and m, $|l, m\rangle$, the Hamiltonian can be written

$$\langle l, m|H|l, m'\rangle = A\hbar^2 l(l+1)\delta_{m.m'} + \overbrace{B\hbar^2\langle l, m|\cos 2\phi|l, m'\rangle}^{V_{m,m'}} \tag{5}$$

The trick is to evaluate, and diagonalize the perturbation $V_{mm'}$. The eigenvectors of $V^l_{m',m}$ determine the energy eigenkets in leading order degenerate perturbation theory. Formally, the perturbation matrix is given by

$$V^l_{m,m'} = \int d\phi d\cos\theta ()Y^l_m(\phi,\theta))^* \cos 2\phi Y^l_m(\phi,\theta)$$

Now since $\cos 2\phi = \frac{1}{2}(e^{2i\phi} + e^{-2i\phi})$, and since $Y_m^l(\phi,\theta)^* Y_{m'}^l(\phi,\theta) \propto e^{i(m'-m)\phi}$, the integral over ϕ selects out terms where $m = m' \pm 2$, i.e

$$V_{m',m}^l = (\delta_{m',m+2} + \delta_{m',m-2})V_{m',m}^l$$

For the case $l = 0$, clearly, the above selection rule guarantees that $V_{m',m}^{l=0} = 0$, so the ground-state energy is a non-degenerate state with

$$E_{l=0} = 0, \qquad |\psi_g\rangle = |0,0\rangle$$

Evaluating $V_{m',m}^l$ for the case $l = 1$, we obtain

$$V_{1,-1}^1 = V_{-1,1}^1 = \int d\Omega Y_{11}^* \frac{1}{2} e^{2i\phi} Y_{1,-1} = -\pi \int_{-1}^1 dc \frac{3}{8\pi} s^2 = -\frac{1}{2}, \qquad (c \equiv \cos\theta, s \equiv \sin\theta)$$

so that

$$V_{m',m}^1 = B\hbar^2 \begin{bmatrix} 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 \end{bmatrix} \tag{6}$$

and the energies and corresponding energy eigenstates are given by

$$E^{l=1} = 2A\hbar^2 + B\hbar^2 \times \begin{cases} 0, & |1,0\rangle \\ \pm\frac{1}{2}, & \frac{1}{\sqrt{2}}(|1,1\rangle \mp |1,-1\rangle) \end{cases} \tag{7}$$

For the case $l = 2$, we obtain

$$\begin{aligned} V_{2,0}^2 &= V_{0,-2}^2 = V_{-2,0}^2 = V_{0,-2}^2 \\ V_{2,0}^2/(B\hbar^2) &= \int d\Omega Y_{22}^* \frac{1}{2} e^{2i\phi} Y_{2,0} = \pi \int_{-1}^1 dc \frac{1}{4}\sqrt{\frac{15}{2\pi}} s^2 \frac{1}{4}\sqrt{\frac{5}{\pi}}(3c^2-1) = -\frac{1}{2\sqrt{6}} \\ V_{1,-1}^2/(B\hbar^2) &= V_{-1,1}^2/(B\hbar^2) = \int d\Omega Y_{21}^* \frac{1}{2} e^{2i\phi} Y_{2,-1} = -2\pi \int_{-1}^1 dc \frac{1}{2}\left(\frac{15}{8\pi}\right) c^2 s^2 = -\frac{1}{2} \end{aligned} \tag{8}$$

$$V_{m',m}^2 = B\hbar^2 \begin{bmatrix} 0 & 0 & -\frac{1}{2\sqrt{6}} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{2\sqrt{6}} & 0 & 0 & 0 & -\frac{1}{2\sqrt{6}} \\ 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2\sqrt{6}} & 0 & 0 \end{bmatrix} \tag{9}$$

so that the energies and eigenstates are given by

$$E^{l=2} = 6A\hbar^2 + B\hbar^2 \times \begin{cases} 0, & \frac{1}{\sqrt{2}}(|2,2\rangle - |2,-2\rangle) \\ \mp\frac{1}{2}, & \frac{1}{\sqrt{2}}(|2,1\rangle \pm |2,-1\rangle) \\ \mp\frac{1}{\sqrt{12}}, & \frac{1}{2}(|2,2\rangle + |2,-2\rangle \pm \sqrt{2}|20\rangle) \end{cases} \tag{10}$$

4. (a) For a free particle, the solutions to the Schrödinger equation in spherical co-ordinates take the separable form

$$u(r,\theta,\phi) = \frac{u_l(r)}{r} Y_{lm}(\theta,\phi)$$

where the radial function $u_l(r)$ satisfies the radial wave-equation

$$(k^2 u_l - u_l''(r)) = l(l+1)u_l(r).$$

The case

$$u(r,\theta) = \frac{1}{r}\left(1+\frac{i}{kr}\right)e^{ikr}\cos\theta \tag{11}$$

takes the form

$$u(r,\theta,\phi) = \sqrt{\frac{4\pi}{3}}\frac{u_l(r)}{r}Y_{10}(\theta,\phi)$$

where $u_l(r) = (1+\frac{i}{kr})e^{ikr}$. The angular dependence is that of a p-wave with azimuthal quantum number $m_l = 0$. The exponential factor

$$e^{ikr}$$

describes an outgoing wave, but we must also verify that the detailed radial dependence is correct. By differentiating u_l we obtain

$$u_l'' = \left[-\left(1+\frac{i}{kr}\right)+\frac{2}{r^2}+\frac{2i}{kr^3}\right]e^{ikr},$$

so that

$$-\frac{u_l''}{2m}+l(l+1)\frac{u_l}{2mr^2} = \frac{k^2}{2m}\left(1+\frac{i}{kr}\right)e^{ikr} = \frac{k^2}{2m}u_l(r)$$

(where $l=1$), in other words, u_l satisfies the raidal wave equation for $l=1$

$$-\frac{u_l''}{2m}+l(l+1)\frac{u_l}{2mr^2} = \frac{k^2}{2m}u_l(r)$$

proving that we are dealing with with an outgoing p-wave with $l=1, m=0$.

(b) Since the low energy scattering phase shift $\delta_l(k)$ is proportional to to $(ka)^{2l+1}$, where a is the scattering length, we need only keep the scattering phase shift from channels with the lowest angular momenta. To obtain the scattering cross-section accurate to order $(ka)^2$ we need only to consider the s and p channels. The general radial wavefunction has the form

$$\psi_l(r) = \cos(\delta_l)j_l(kr) - \sin(\delta_l)\eta_l(kr)$$

For $l=0$, this simplifies to the form

$$\psi_{l=0}(r) = \cos(\delta_0)\frac{\sin(kr)}{kr}+\sin(\delta_0)\frac{\cos(kr)}{kr}$$

The condition $\psi_l(r=a)=0$, implies that $\tan(ka+\delta_{l=0})=0$, so that $\delta_0=-ka$. For $l=1$, the radial wave-equation can be written in the form

$$\psi_{l=1}(r) = \frac{1}{r}\left[e^{2i\delta_1}(1+\frac{i}{kr})e^{ikr}+(1-\frac{i}{kr})e^{-ikr}\right]$$

so the condition $\psi_{l=1}(r=a)=0$ implies that

$$e^{2i\delta_1}(1+\frac{i}{ka}) = -(1-\frac{i}{ka})e^{-ika}$$

so that

$$\delta_1 = -ka+\frac{1}{2i}\ln\left(\frac{1+ika}{1-ika}\right)$$

Expanding this for small ka, we obtain $\delta_1 = -\frac{(ka)^3}{3}$.
Now the scattering amplitude is given by

$$f(\theta) = \frac{1}{k}\sum_l(2l+1)e^{i\delta_l}\sin\delta_l$$

which for our case simplifies to

$$f(\theta) = \frac{e^{i\delta_o}\sin\delta_0}{k} + \frac{3e^{i\delta_1}\sin\delta_1}{k}\cos\theta + \ldots$$

For small scattering phase shifts, we can expand this as

$$\frac{1}{k}\left[(\delta_0 - \frac{2}{3}\delta_0^2 + i\delta_0^2) + 3\delta_1\cos\theta\right]$$

So the differential scattering cross-section is then

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= |f(\theta)|^2 \approx \frac{\delta_0^2}{k^2}\left[1 - \frac{1}{3}\delta_0^2 + 6\left(\frac{\delta_1}{\delta_0}\right)\cos\theta\right] \\ &= a^2[1 + (ka)^2(2\cos\theta - \frac{1}{3})]. \end{aligned} \tag{12}$$

5. If we seek solutions to the Dirac equation in the form

$$\psi(t) = \Psi e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} = \begin{pmatrix}\chi \\ \phi\end{pmatrix} e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}$$

then the Dirac equation takes the form

$$E\Psi = \left[c\vec{\alpha}\cdot\vec{p} + \beta mc^2\right]\Psi$$

where $\vec{p}$ is the momentum operator. Written out more explicitly gives

$$\begin{aligned}(E - mc^2)\chi - \vec{\sigma}\cdot\vec{p}\phi &= 0 \\ (E + mc^2)\phi - \vec{\sigma}\cdot\vec{p}\chi &= 0.\end{aligned} \tag{13}$$

From the second of these equations we obtain

$$\phi = \frac{\vec{\sigma}\cdot\vec{p}}{E + mc^2}\chi$$

and substituting into the first equation, we obtain

$$(E^2 - m^2c^4 - p^2c^2)\chi = 0$$

so that $E = \pm E(p)$, where $E(p) = \sqrt{m^2c^4 + p^2c^2}$.

(a) Now for a spin-up solution, we take $\chi = \begin{pmatrix}1 \\ 0\end{pmatrix}$, so that if $\vec{p} = (0, 0, p)$ and we take the positive energy solution, $E = E(p)$, then

$$\phi = \begin{pmatrix}\frac{cp}{E+mc^2} \\ 0\end{pmatrix}$$

so the wave-function takes the form

$$\begin{aligned}\Psi_{1p} &= \frac{\mathcal{N}}{L^{\frac{3}{2}}}\begin{pmatrix}1 \\ 0 \\ \frac{cp}{E_p+mc^2} \\ 0\end{pmatrix} e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} \\ &= \frac{1}{L^{\frac{3}{2}}}\sqrt{\frac{E_p + mc^2}{2E_p}}\begin{pmatrix}1 \\ 0 \\ \frac{cp}{E_p+mc^2} \\ 0\end{pmatrix} e^{i(\vec{p}\cdot\vec{x} - E_p t)/\hbar}\end{aligned} \tag{14}$$

where the normalization constant is chosen to give $\psi^\dagger\psi = 1/L^3$.

To obtain the negative energy solution, we repeat the above process, choosing $E = -E(p)$, and writing $\chi = \vec{\sigma}\cdot\vec{p}/(E - mc^2)\phi$, so that now with $\phi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, we obtain

$$\begin{aligned}
\Psi_{2p} &= \frac{\mathcal{N}}{L^{\frac{3}{2}}} \begin{pmatrix} \frac{cp}{-E_p - mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{i(\vec{p}\cdot\vec{x}+E_p t)/\hbar} \\
&= \frac{1}{L^{\frac{3}{2}}} \sqrt{\frac{E_p + mc^2}{2E_p}} \begin{pmatrix} -\frac{cp}{E_p + mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{i(\vec{p}\cdot\vec{x}+E_p t)/\hbar} \qquad (15)
\end{aligned}$$

(b) If

$$\psi(\vec{x}, 0) = \frac{1}{L^{3/2}} \begin{pmatrix} \alpha \\ 0 \\ \beta \\ 0 \end{pmatrix} e^{i\vec{p}\cdot\vec{x}/\hbar}$$

then the overlaps with the positive and negative energy solutions are respectively,

$$\begin{aligned}
\langle p^+|\psi\rangle &= \Psi_{1p}^\dagger \psi|_{t=0} = \left(\frac{E_p + mc^2}{2E_p}\right)^{\frac{1}{2}} \left(\alpha + \beta\frac{cp}{E_p + mc^2}\right) \\
\langle p^-|\psi\rangle &= \Psi_{2p}^\dagger \psi|_{t=0} = \left(\frac{E_p + mc^2}{2E_p}\right)^{\frac{1}{2}} \left(\beta - \alpha\frac{cp}{E_p + mc^2}\right) \qquad (16)
\end{aligned}$$

so that the wavefunction at later times is given by

$$|\psi(t)\rangle = |p^+\rangle\langle p^+|\psi\rangle e^{-iE_p t/\hbar r} + |p^-\rangle\langle p^-|\psi\rangle e^{iE_p t/\hbar r}$$

or

$$|\psi(t)\rangle = \frac{E_p + mc^2}{2E_p L^{\frac{3}{2}}} e^{ipz/\hbar} \left[\left(\alpha + \beta\frac{cp}{E_p + mc^2}\right) \begin{pmatrix} 1 \\ 0 \\ \frac{cp}{E_p + mc^2} \\ 0 \end{pmatrix} e^{-iE_p t/\hbar} + \left(\beta - \alpha\frac{cp}{E_p + mc^2}\right) \begin{pmatrix} -\frac{cp}{E_p + mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{iE_p t/\hbar} \right] \qquad (17)$$

The probabilities to be in the positive and negative energy states are given by

$$\begin{aligned}
p^+ &= \left(\frac{E_p + mc^2}{2E_p}\right) \left|\alpha + \beta\frac{cp}{E_p + mc^2}\right|^2 \\
p^- &= \left(\frac{E_p + mc^2}{2E_p}\right) \left|\beta - \alpha\frac{cp}{E_p + mc^2}\right|^2 \qquad (18)
\end{aligned}$$