Answers to Problem Set 8 **Physics 607** **Nov. 16, 2001**

1. For later use, keep in mind the expansion of the gradient operator in a spherical basis $\boldsymbol{\nabla} = \sum_\mu (-1)^\mu \nabla_{-\mu}\, \xi_\mu$. Write the wave function for the state a as

$$\psi_a = \frac{P_a(r)}{r}\; Y_{l_a m_a}(\hat{r}).$$

One finds:

$$\begin{aligned}
\boldsymbol{\nabla}\,\psi_a &= \frac{d}{dr}\left(\frac{P_a(r)}{r}\right)\hat{\mathbf{r}}\,Y_{l_a m_a} + \frac{P_a(r)}{r}\,\boldsymbol{\nabla}\,Y_{l_a m_a} \\
&= \frac{1}{r}\left[\left(\frac{dP_a}{dr} - \frac{1}{r}\,P_a(r)\right)\mathbf{Y}^{(-1)}_{l_a m_a} + \frac{\sqrt{l_a(l_a+1)}}{r} P_a(r)\,\mathbf{Y}^{(1)}_{l_a m_a}\right] \\
&= \frac{1}{r}\left[\left(\frac{dP_a}{dr} - \frac{1}{r}\,P_a(r)\right)\left(\sqrt{\frac{l_a}{2l_a+1}}\mathbf{Y}_{l_a,l_a-1,m_a} - \sqrt{\frac{l_a+1}{2l_a+1}}\mathbf{Y}_{l_a,l_a+1,m_a}\right)\right. \\
&\quad\left. + \frac{\sqrt{l_a(l_a+1)}}{r}\,P_a(r)\left(\sqrt{\frac{l_a+1}{2l_a+1}}\mathbf{Y}_{l_a,l_a-1,m_a} + \sqrt{\frac{l_a}{2l_a+1}}\mathbf{Y}_{l_a,l_a+1,m_a}\right)\right] \\
&= \frac{1}{r}\;\left[\sqrt{\frac{l_a}{2l_a+1}}\left(\frac{dP_a}{dr} + \frac{l_a}{r}\,P_a(r)\right)\mathbf{Y}_{l_a,l_a-1,m_a}\right. \\
&\qquad\left. -\;\sqrt{\frac{l_a+1}{2l_a+1}}\left(\frac{dP_a}{dr} - \frac{l_a+1}{r}\,P_a(r)\right)\mathbf{Y}_{l_a,l_a+1,m_a}\right].
\end{aligned}$$

Extracting the coefficient of ξ_μ from the expressions for the vector spherical harmonics in the last lines of the above equation, it follows that

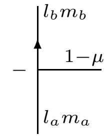
$$\begin{aligned}
&(-1)^\mu \nabla_{-\mu}|a\rangle = \\
&\frac{1}{r}\left[\sqrt{\frac{l_a}{2l_a+1}}\left(\frac{dP_a}{dr} + \frac{l_a}{r}\,P_a(r)\right)C(l_a-1,1,l_a;m_a-\mu,\mu,m_a)\,Y_{l_a-1,m_a-\mu}(\hat{r})\right. \\
&\left.-\sqrt{\frac{l_a+1}{2l_a+1}}\left(\frac{dP_a}{dr} - \frac{l_a+1}{r}\,P_a(r)\right)C(l_a+1,1,l_a;m_a-\mu,\mu,m_a)\,Y_{l_a+1,m_a-\mu}(\hat{r})\right]
\end{aligned}$$

From this, we find

$$\begin{aligned}
\langle b\,|\nabla_{-\mu}|\,a\rangle = (-1)^\mu &\left\{\sqrt{l_a}\int_0^\infty P_b(r)\left(\frac{dP_a}{dr} + \frac{l_a}{r}\,P_a(r)\right)dr\;\delta_{l_b,l_a-1}\right. \\
&\left.-\sqrt{l_a+1}\int_0^\infty P_b(r)\left(\frac{dP_a}{dr} - \frac{l_a+1}{r}\,P_a(r)\right)dr\;\delta_{l_b,l_a+1}\right\}\frac{C(l_b,1,l_a,m_b,\mu,m_a)}{\sqrt{2l_a+1}}\,.
\end{aligned}$$

One can easily verify that for $l_b = l_a \pm 1$,

$$\frac{C(l_b,1,l_a,m_b,\mu,m_a)}{\sqrt{2l_a+1}} = (-1)^{1-\mu}$$



Therefore,

$$\langle b \| \boldsymbol{\nabla} \| a\rangle = \Big\{ -\sqrt{l_a} \int_0^\infty P_b(r) \left(\frac{dP_a}{dr} + \frac{l_a}{r} P_a(r) \right) dr \ \delta_{l_b, l_a - 1}$$
$$+ \sqrt{l_a + 1} \int_0^\infty P_b(r) \left(\frac{dP_a}{dr} - \frac{l_a + 1}{r} P_a(r) \right) dr \ \delta_{l_b, l_a + 1} \Big\}$$

Now,

$$\langle l_b \| C_1 \| l_a \rangle = \begin{cases} -\sqrt{l_a} & \text{for} \quad l_b = l_a - 1 \\ \sqrt{l_a + 1} & \text{for} \quad l_b = l_a + 1 \end{cases}$$

Therefore, finally,

$$\langle b \| \boldsymbol{\nabla} \| a\rangle = \langle l_b \| C_1 \| l_a \rangle \ \Big\{ \int_0^\infty P_b(r) \left(\frac{dP_a}{dr} + \frac{l_a}{r} P_a(r) \right) dr \ \delta_{l_b, l_a - 1}$$
$$+ \int_0^\infty P_b(r) \left(\frac{dP_a}{dr} - \frac{l_a + 1}{r} P_a(r) \right) dr \ \delta_{l_b, l_a + 1} \Big\}$$

2. Let us first consider

$$\begin{aligned} \bar{f}_{kl \to l-1} &= \sum_{n\, m_n} \frac{2\omega_{nk}}{3} \ \langle k\, l\, m_k | \mathbf{r} | n\, l-1\, m_n \rangle \ \cdot \ \langle n\, l-1\, m_n | \mathbf{r} | k\, l\, m_k \rangle \\ &= -\frac{2}{3}\, i \sum_{n\, m_n} \langle k\, l\, m_k | \mathbf{r} | n\, l-1\, m_n \rangle \ \cdot \ \langle n\, l-1\, m_n | \mathbf{p} | k\, l\, m_k \rangle \\ &= -\frac{2}{3}\, i \sum_{n\, m_n \nu} (-1)^\nu \langle k\, l\, m_k | r_{-\nu} | n\, l-1\, m_n \rangle \ \langle n\, l-1\, m_n | p_\nu | k\, l\, m_k \rangle \\ &= -\frac{2}{3(2l+1)} \sum_n (-1)^1 \langle k\, l \, \| r \, \| n\, l-1 \rangle \ \langle n\, l-1 \| \boldsymbol{\nabla} \, \| k\, l \rangle \\ &= -\frac{2}{3(2l+1)} \ |\langle l \| C_1 \| l-1 \rangle|^2 \sum_n \int_0^\infty dr\, P_{kl}(r)\, r\, P_{nl-1}(r) \times \\ &\quad \int_0^\infty dr'\, P_{nl-1}(r') \left(\frac{dP_{kl}(r')}{dr'} + \frac{l}{r'} P_{kl}(r') \right) \end{aligned}$$

Now, we use completeness of the radial wave functions:

$$\sum_n P_{nl-1}(r) P_{nl-1}(r') = \delta(r - r')$$

to write the sum over n of the double integral on the last lines of the previous equation as

$$I = \int_0^\infty dr\, P_{kl}(r)\, r \left(\frac{dP_{kl}(r)}{dr} + \frac{l}{r} P_{kl}(r) \right).$$

Since $|\langle l\|C_1\|l-1\rangle|^2 = l$, we obtain

$$\begin{aligned}
\bar{f}_{kl\to l-1} &= -\frac{2l}{3(2l+1)}\int_0^\infty dr\, P_{kl}(r)\, r\left(\frac{dP_{kl}(r)}{dr} + \frac{l}{r}P_{kl}(r)\right)\\
&= -\frac{2l}{3(2l+1)}\int_0^\infty dr\left(\frac{1}{2}\frac{d(rP_{kl}^2)}{dr} + \frac{2l-1}{2}P_{kl}^2\right)\\
&= -\frac{2l}{3(2l+1)}\,\frac{2l-1}{2} = -\frac{l(2l-1)}{3(2l+1)}
\end{aligned}$$

Using $|\langle l\|C_1\|l+1\rangle|^2 = l+1$ and following the same argument for the case of intermediate $|n, l+1\rangle$ states, we find

$$\begin{aligned}
\bar{f}_{kl\to l+1} &= -\frac{2(l+1)}{3(2l+1)}\int_0^\infty dr\, P_{kl}(r)\, r\left(\frac{dP_{kl}(r)}{dr} - \frac{l+1}{r}P_{kl}(r)\right)\\
&= -\frac{2(l+1)}{3(2l+1)}\int_0^\infty dr\left(\frac{1}{2}\frac{d(rP_{kl}^2)}{dr} - \frac{2l+3}{2}P_{kl}^2\right)\\
&= \frac{2(l+1)}{3(2l+1)}\,\frac{2l+3}{2} = \frac{(l+1)(2l+3)}{3(2l+1)}
\end{aligned}$$

Note:

$$\bar{f}_{kl\to l-1} + \bar{f}_{kl\to l+1} = 1.$$

Note further: if $l = 0$, only $\bar{f}_{ks(l=0)\to 1}$ is possible and from the general result for $\bar{f}_{kl\to l+1}$ with $l = 0$,

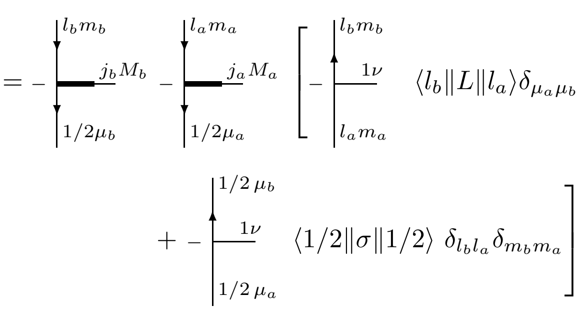
$$\bar{f}_{ks\to 1} = 1.$$

3. The Al ground state is a $3p$ doublet, the $3p_{3/2}$ state being above the $3p_{1/2}$ state by $\delta E = 112.061$ cm^{-1}. The $3p_{3/2} \to 3p_{1/2}$ transition wavelength is $\lambda = 10^8/\delta E = 892{,}371$ Å. The transition rate from $a = 3p_{3/2}$ to $b = 3p_{1/2}$ is

$$A_{a\to b} == \frac{2.69735\times 10^{13}}{\lambda^3}\,\frac{S_{\rm M1}}{g_a}\ \text{s}^{-1},$$

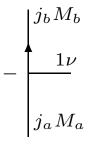
where $S_{\rm M1} = |\langle b||L+2S||a\rangle|^2$ and $g_a = 2j_a+1$. Now let us find the reduced matrix element:

$\langle j_b l_b M_b | L_\nu + 2S_\nu | j_a l_a M_a\rangle = -$



Carrying out the sums over magnetic quantum numbers, this reduces to

$$\langle j_b l_b M_b | L_\nu + 2S_\nu | j_a l_a M_a \rangle = -$$



$$\times$$

$$\sqrt{[j_b][j_a]}\left[(-1)^{j_a+l_b+3/2}\left\{\begin{array}{ccc} j_b & j_a & 1 \\ l_a & l_b & 1/2 \end{array}\right\}\langle l_b\|L\|l_a\rangle \right.$$
$$\left. +\,(-1)^{j_b+l_b+3/2}\left\{\begin{array}{ccc} j_b & j_a & 1 \\ 1/2 & 1/2 & l \end{array}\right\}\langle 1/2\|\sigma\|1/2\rangle\,\delta_{l_b l_a}\right].$$

From this, we can read off the reduced matrix element. Furthermore, $\langle l_b\|L\|l_a\rangle = \sqrt{l_a(l_a+1)(2l_a+1)}\,\delta_{bl_a}$ and $\langle 1/2\|\sigma\|1/2\rangle = \sqrt{6}$. Therefore, for the case $j_a = l+1/2$, $j_b = l-1/2$, and $l_a = l_b = l$,

$$\begin{aligned}
\langle b\|M\,\|a\rangle &= \sqrt{(2l)(2l+2)}\left[\sqrt{l(l+1)(2l+1)}\left\{\begin{array}{ccc} l-1/2 & l+1/2 & 1 \\ l & l & 1/2 \end{array}\right\}\right. \\
&\qquad\qquad \left. -\sqrt{6}\left\{\begin{array}{ccc} l-1/2 & l+1/2 & 1 \\ 1/2 & 1/2 & l \end{array}\right\}\right] \\
&= 2\sqrt{l(l+1)}\left[-\frac{1}{\sqrt{2(2l+1)}} + \frac{2}{\sqrt{2(2l+1)}}\right] \\
&= \sqrt{\frac{2l(l+1)}{2l+1}}\,.
\end{aligned}$$

It follows that for p states, where $l = 1$, the line strength is $S_{M1} = 4/3$ and $g_a = 2j_a + 1 = 4$. For the $3p$ doublet in Al, the transition rate is

$$\begin{aligned}
A_{3p_{3/2}\to 3p_{1/2}} &= \frac{2.69735\times 10^{13}\times(4/3)}{(10^8/112.061)^3\times 4} = 1.26526\,10^{-5}\ \mathrm{s}^{-1} \\
\tau(3p_{3/2}) &= \frac{1}{A} = 79035.18\ \mathrm{s} = 21\,\mathrm{h}\ 57\,\mathrm{m}\ 15\,\mathrm{s}
\end{aligned}$$

Relativistic Calculation: In a relativistic calculation, the reduced magnetic-dipole matrix element is given by

$$\begin{aligned}
\langle b\|M\|a\rangle &= 2c\,\langle b\|q_1^{(0)}\|a\rangle = 2c\,\langle b\|\frac{3}{k}t_1^{(0)}\|a\rangle \\
&= 2c\,\frac{\kappa_b+\kappa_a}{2}\,\langle -\kappa_b\|C_1\|\kappa_a\rangle\int_0^\infty dr\,\frac{3}{k}\,j_1(kr)\Big(P_bQ_a + P_aQ_b\Big)
\end{aligned}$$

We make two approximations: Firstly, $kr \approx 2\pi a_0/\lambda \approx 4\ 10^{-6} \ll 1$. This approximation permits us ignore higher-order terms in the expansion of the spherical Bessel function and approximate $3j_1(kr)/k$ by r. Secondly, we use the Pauli approximation for the atomic wave functions of the $3p$ states in Aluminum. This approximation, which is valid provided $(\alpha Z)^2 \approx$

$10^{-5} \ll 1$, permits us to approximate the small-component wave function by

$$\begin{aligned}
\int_0^\infty dr\, r \Big(P_b Q_a + P_a Q_b\Big) &\approx -\frac{1}{2c}\int_0^\infty dr\, r \left(P_b \left(\frac{dP_a}{dr} + \frac{\kappa_a}{r}P_a\right) + P_a \left(\frac{dP_b}{dr} + \frac{\kappa_b}{r}P_b\right)\right) \\
&= -\frac{1}{2c}\int_0^\infty dr\, r \left(\frac{d\,(P_b P_a)}{dr} + \frac{\kappa_a + \kappa_b}{r} P_b P_a\right) \\
&= -\frac{1}{2c}\int_0^\infty dr \left(\frac{d\,(r P_b P_a)}{dr} + (\kappa_a + \kappa_b - 1) P_b P_a\right) \\
&= -\frac{\kappa_a + \kappa_b - 1}{2c}\int_0^\infty dr P_b P_a = -\frac{\kappa_a + \kappa_b - 1}{2c}
\end{aligned}$$

where we have used the fact that, in the Pauli approximation, $P_b = P_a = P_{3p}$, where $P_{3p}(r)$ is the *nonrelativistic* $3p$ radial wave function. Therefore, in the Pauli approximation, the magnetic-dipole matrix element for transitions from states with $j_a = l + 1/2$, $\kappa_a = -l - 1$ to states with $j_b = l - 1/2$, $\kappa_b = l$ becomes:

$$\begin{aligned}
\langle b\|M\|a\rangle &= -2c\,\frac{\kappa_b + \kappa_a}{2}\,\frac{\kappa_a + \kappa_b - 1}{2c}\,\langle -\kappa_b\|C_1\|\kappa_a\rangle \\
&= -\frac{1}{2}(l - l - 1)(-l - 1 + l - 1)\,\langle -\kappa_b\|C_1\|\kappa_a\rangle \\
&= -\,\langle j_b = l - 1/2\|C_1\|j_a = l + 1/2\rangle \\
&= \sqrt{\frac{2l(l+1)}{2l+1}}\,.
\end{aligned}$$

Therefore, the relativistic matrix element, in the Pauli approximation, agrees precisely with the nonrelativistic matrix element.