Answers to Final Exam Physics 607 (due Dec. 14, 2001)

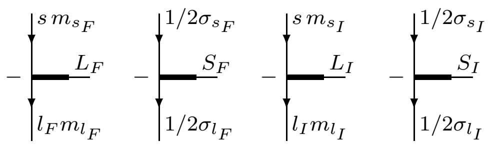
1. Consider a transition from the $(1s3d)\ {}^3D$ state to the $(1s2p)\ {}^3P$ state in a helium-like ion:

   (a) Show that, in the independent-particle approximation,

   $$\langle (1s2p)\ {}^3P||r||(1s3d)\ {}^3D\rangle = \langle 2p||r||3d\rangle$$

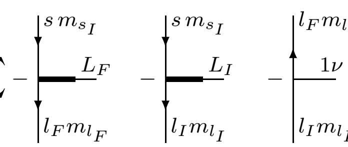
   We write

   $$\langle (1snl_F)\ {}^{2S_F+1}L_F|r_\nu|(1sml_I)\ {}^{2S_I+1}L_I\rangle$$

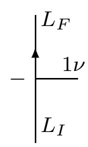
   $$= \sum_{m_k\ \sigma_k}$$ 

$\times$

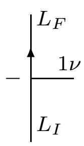
   $$\delta_{m_{s_F} m_{s_I}}\,\delta_{\sigma_{s_F}\sigma_{s_I}}\,\delta_{\sigma_{l_F}\sigma_{l_I}}\,\langle n l_F m_{l_F}|r_\nu|m l_I m_{l_I}\rangle$$

   $$= \sum_{m_k}$$ 

$\langle nl_F\|r\|ml_I\rangle\ \delta_{S_F S_I}$

   $$= (-1)^{l_I+L_F+1}\sqrt{[L_I][L_F]}\left\{\begin{array}{ccc} L_I & L_F & 1 \\ l_F & l_I & 0\end{array}\right\}\langle nl_F\|r\|ml_I\rangle$$ 

$\delta_{S_F S_I}$

   $$= \langle nl_F\|r\|ml_I\rangle$$ 

$\delta_{S_F S_I}.$

   From this, it follows that

   $$\langle (1snl_F)\ {}^{2S_F+1}L_F\|r\|(1sml_I)\ {}^{2S_I+1}L_I\rangle = \langle nl_F\|r\|ml_I\rangle\ \delta_{S_F S_I}.$$

   Therefore,

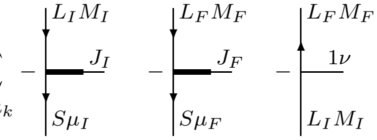
   $$\langle (1s2p)\ {}^3P\|r\|(1s3d)\ {}^3D\rangle = \langle 2p\|r\|3d\rangle\ .$$

   (b) Suppose that one can resolve the fine-structure of the initial and final states. Express the matrix elements $\langle (1s2p)\ {}^3P_{J_F}||r||(1s3d)\ {}^3D_{J_I}\rangle$ in terms of $\langle (1s2p)\ {}^3P||r||(1s3d)\ {}^3D\rangle$ or $\langle 2p||r||3d\rangle$.

We write

$$\left\langle {}^{2S+1}L_F \ J_F | r_\nu | {}^{2S+1}L_I \ J_I \right\rangle$$

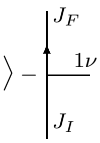
$$= \sum_{M_k \, \mu_k}$$



$$\left\langle {}^{2S+1}L_F \| r \| \ {}^{2S+1}L_I \right\rangle \delta_{\mu_I \mu_F}$$

$$= (-1)^{J_I + L_F + + S + 1} \sqrt{[J_I][J_F]} \left\{ \begin{array}{ccc} J_I & J_F & 1 \\ L_F & L_I & S \end{array} \right\} \times$$

$$\left\langle {}^{2S+1}L_F \| r \| \ {}^{2S+1}L_I \right\rangle -$$



From this, it follows

$$\left\langle {}^{2S+1}L_F \ J_F \| r \| {}^{2S+1}L_I \ J_I \right\rangle =$$
$$= (-1)^{J_I + L_F + + S + 1} \sqrt{[J_I][J_F]} \left\{ \begin{array}{ccc} J_I & J_F & 1 \\ L_F & L_I & S \end{array} \right\} \left\langle {}^{2S+1}L_F \| r \| \ {}^{2S+1}L_I \right\rangle .$$

Therefore,

$$\langle (1s2p) \ {}^3P_{J_F} || r || (1s3d) \ {}^3D_{J_I} \rangle$$
$$= (-1)^{J_I + 1} \sqrt{[J_I][J_F]} \left\{ \begin{array}{ccc} J_I & J_F & 1 \\ 1 & 2 & 1 \end{array} \right\} \langle 2p \| r \| 3d \rangle .$$

(c) The intensity of the lines from $|(1s3d) \ {}^3D_{J_I}\rangle$ to $|(1s2p) \ {}^3P_{J_F}\rangle$ is

$$A_{I \to F} \propto \frac{S_{FI}}{[J_I]} = \frac{|\langle (1s2p) \ {}^3\mathrm{P}_{J_F} || r || (1s3d) \ {}^3\mathrm{D}_{J_I} \rangle|^2}{[J_I]}.$$

By explicitly evaluating the relevant 6j symbols (using MAPLE, for example), show that the ratios of intensities for transitions $J_I \to J_F$:

$$1 \to 0 : 1 \to 1 : 2 \to 1 : 1 \to 2 : 2 \to 2 : 3 \to 2$$

are

$$20 : 15 : 27 : 1 : 9 : 36.$$

From the result of part (b) above, it follows

$$\frac{S_{FI}}{[J_I]} = [J_F] \left\{ \begin{array}{ccc} J_I & J_F & 1 \\ 1 & 2 & 1 \end{array} \right\}^2 \; | \langle 2p \| r \| 3d \rangle |^2 .$$

Setting $T(J_F, J_I) = S_{FI}/([J_I] \, | \langle 2p \| r \| 3d \rangle |^2)$, we find

$$\begin{aligned} T(0,1) = 1/9 &= 20/180 \\ T(1,1) = 1/12 &= 15/180 \\ T(1,2) = 3/20 &= 27/180 \\ T(2,1) = 1/180 &= 1/180 \\ T(2,2) = 1/20 &= 9/180 \\ T(2,3) = 1/5 &= 36/180 \end{aligned}$$

Multiplying the entries in this table by 180 leads to the desired result.

2. Suppose we choose to describe an atom in lowest order using a potential $U(r)$ other than the HF potential.

   (a) Show that the correction to the first-order energy from the single-particle part of the potential (V_1) for a one electron atom in a state v is

   $$E_v^{(1)} = \Delta_{vv},$$

   where $\Delta = V_{\rm HF} - U$.
   We use the fact that the contribution to the first-order energy from V_1 is

   $$\begin{aligned} E^{(1)} &= \langle \Psi_0 | V_1 | \Psi_0 \rangle \\ &= \sum_{ij} \Delta_{ij} \; \langle 0_c | a_v : a_i^\dagger a_j : a_v^\dagger | 0_c \rangle \\ &= \sum_{ij} \Delta_{ij} \; \delta_{iv} \, \delta_{jv} \\ &= \Delta_{vv}. \end{aligned}$$

   (b) Show that the corresponding second-order correction is

   $$E_v^{(2)} = \sum_{na} \frac{\Delta_{na} \tilde{g}_{avnv} + \tilde{g}_{nvnv} \Delta_{an}}{\epsilon_n - \epsilon_a} - \sum_{i \neq v} \frac{\Delta_{vi} \Delta_{iv}}{\epsilon_i - \epsilon_v}.$$

Here, i runs over a and n.

First, we note that if we add V_1 to the potential, then the expression for the correlation function becomes

$$\chi^{(1)} = \sum_{ma} \chi^{(1)}_{ma} a^\dagger_m a_a + \sum_{m} \chi^{(1)}_{mv} a_m a_v + \sum_{mnab} \chi^{(1)}_{mnab} a^\dagger_m a^\dagger_n a_b a_a + \sum_{mnb} \chi^{(1)}_{mnvb} a^\dagger_m a^\dagger_n a_b a_v,$$

where,

$$\begin{aligned}
\chi^{(1)}_{ma} &= -\frac{\Delta_{ma}}{\epsilon_m - \epsilon_a} \\
\chi^{(1)}_{va} &= -\frac{\Delta_{mv}}{\epsilon_m - \epsilon_v} \\
\chi^{(1)}_{mnab} &= -\frac{1}{2}\frac{g_{mnab}}{\epsilon_m + \epsilon_n - \epsilon_a - \epsilon_b} \\
\chi^{(1)}_{mnab} &= -\frac{1}{2}\frac{\tilde{g}_{mnvb}}{\epsilon_m + \epsilon_n - \epsilon_v - \epsilon_b}
\end{aligned}$$

The extra terms in the second-order energy from V_1 are

$$
\begin{aligned}
E^{(2)} &= \langle 0_c | a_v V_1 \left(\sum_{abmn} \chi^{(1)}_{mnab} a^\dagger_m a^\dagger_n a_b a_a + \sum_{mnb} \chi^{(1)}_{mnvb} a^\dagger_m a^\dagger_n a_b a_v \right) a^\dagger_v | 0_c \rangle \\
&+ \langle 0_c | a_v V_1 \left(\sum_{am} \chi^{(1)}_{ma} a^\dagger_m a_a + \sum_{m} \chi^{(1)}_{mv} a^\dagger_m a_v \right) a^\dagger_v | 0_c \rangle \\
&+ \langle 0_c | a_v V_2 \left(\sum_{am} \chi^{(1)}_{ma} a^\dagger_m a_a + \sum_{m} \chi^{(1)}_{mv} a^\dagger_m a_v \right) a^\dagger_v | 0_c \rangle \\
&= \sum_{ij} \Delta_{ij} \sum_{mnab} \chi^{(1)}_{mnab} \; \langle 0_c | a_v : a^\dagger_i a_j : a^\dagger_m a^\dagger_n a_b a_a a^\dagger_v | 0_c \rangle \\
&+ \sum_{ij} \Delta_{ij} \sum_{mnb} \chi^{(1)}_{mnvb} \; \langle 0_c | a_v : a^\dagger_i a_j : a^\dagger_m a^\dagger_n a_b | 0_c \rangle \\
&+ \sum_{ij} \Delta_{ij} \sum_{ma} \chi^{(1)}_{ma} \; \langle 0_c | a_v : a^\dagger_i a_j : a^\dagger_m a_a a^\dagger_v | 0_c \rangle \\
&+ \sum_{ij} \Delta_{ij} \sum_{m} \chi^{(1)}_{mv} \; \langle 0_c | a_v : a^\dagger_i a_j : a^\dagger_m | 0_c \rangle \\
&+ \frac{1}{2} \sum_{ijkl} g_{ijkl} \sum_{ma} \chi^{(1)}_{ma} \; \langle 0_c | a_v : a^\dagger_i a^\dagger_j a_l a_k : a^\dagger_m a_a a^\dagger_v | 0_c \rangle \\
&+ \frac{1}{2} \sum_{ijkl} g_{ijkl} \sum_{m} \chi^{(1)}_{mv} \; \langle 0_c | a_v : a^\dagger_i a^\dagger_j a_l a_k : a^\dagger_m | 0_c \rangle .
\end{aligned}
$$

The first and sixth terms above cannot contribute. The remaining terms give, in order,

$$
\begin{aligned}
E^{(2)} = &\sum_{bn} \Delta_{nb} \tilde{\chi}^{(1)}_{vnvb} \\
+ &\sum_{ma} \Delta_{am} \chi^{(1)}_{ma} - \sum_{a} \Delta_{av} \chi^{(1)}_{va} \\
+ &\sum_{m} \Delta_{vm} \chi^{(1)}_{mv} \\
+ &\sum_{ma} \tilde{g}_{vavm} \chi^{(1)}_{ma} .
\end{aligned}
$$

Substituting the values of the correlation coefficients, we find

$$E^{(2)} = -\sum_{bn} \frac{\Delta_{nb}\ \tilde{g}_{vnvb}}{\epsilon_n - \epsilon_b} - \sum_{ma} \frac{\Delta_{am}\Delta_{ma}}{\epsilon_m - \epsilon_a} + \sum_{a} \frac{\Delta_{av}\Delta_{va}}{\epsilon_v - \epsilon_a} - \sum_{m} \frac{\Delta_{vm}\Delta_{mv}}{\epsilon_m - \epsilon_v} - \sum_{ma} \frac{\tilde{g}_{vavm}\ \Delta_{ma}}{\epsilon_m - \epsilon_a}.$$

The second term, which is independent of v is the contribution of Δ to the core energy. The remaining terms are contributions to the valence energy. We therefore find

$$E_v^{(2)} = -\sum_{bn} \frac{\Delta_{nb}\ \tilde{g}_{vnvb} + \tilde{g}_{vbvn}\Delta_{nb}}{\epsilon_n - \epsilon_b} - \sum_{i\neq v} \frac{\Delta_{vi}\Delta_{iv}}{\epsilon_i - \epsilon_v}.$$

The first term has an unfortunate sign difference with the result given in the problem. The sign here is correct.