Evaluation of the full J-coupling exponential PhL 1.8.08

Evaluate: $\exp(-\alpha\, \mathbf{I_1}\bullet \mathbf{I_2})\ \mathbf{I_1}\ \exp(+\alpha\, \mathbf{I_1}\bullet \mathbf{I_2})$. To simplify, define L and S:

$\mathbf{I_1} = \mathbf{L}$ $\mathbf{I_2} = \mathbf{S}$ so evaluate $\exp(-\alpha\, \mathbf{L}\bullet \mathbf{S})\ \mathbf{L}\ \exp(+\alpha\, \mathbf{L}\bullet \mathbf{S})$

Let's try a **brute force application of Campbell-Hausdorff:**

$A = \alpha\, \mathbf{L}\bullet \mathbf{S} = \alpha\, L_i S_i = \alpha D$ $D = \mathbf{L}\bullet \mathbf{S}$

$B = L_k$

$C_0 = B = L_k$

$C_1 = [B,A] = [L_k\,,\, \alpha\, L_i S_i\,] = \alpha\, [\, L_k\,, L_i\,]\, S_i = i\alpha\, \varepsilon_{kis} L_s S_i$ // $[L_i, L_j] = i\, \varepsilon_{ijk} L_k$

$= [L_k\,,\, \alpha\, D\,] = \alpha\, [L_k\,,\, D] = -\, i\alpha \varepsilon_{ksi}\ L_s S_i = -i\alpha\, [\, \mathbf{L} \times \mathbf{S}]_k$

I have written out C_1 about every way I can think of. Now move on to the next one:

$C_2 = [\, C_1\,,\, A] = [\ -\, i\alpha \varepsilon_{ksi}\ L_s S_i\,,\, \alpha D] = -\, i\alpha^2\, \varepsilon_{ksi}\, [\ L_s S_i\,,\, D]$

At this point we digress to obtain a little theorem. First, quote this known theorem:

$[ab,cd] = a[b,c]d + ac[b,d] + [a,c]db + c[a,d]b$

Then apply as follows: [don't be confused by reuse of symbols]

$[\, L_a S_b,\, L_c S_d\,] = 0 + L_a L_c\, [\ S_b,\, S_d\,] + [\, L_a,\, L_c]\, S_d S_b + 0$

$= L_a L_c\, i\varepsilon_{bde} S_e + i\varepsilon_{acf} L_f\, S_d S_b$

Now suppose we have c = d and a summation on the resulting index. We then get:

$[\, L_a S_b,\, L_c S_c\,] = L_a L_c\, i\varepsilon_{bce} S_e + i\varepsilon_{acf}\, L_f\, S_c S_b = [L_a S_b\,,\, D\,]$

Now apply this to our case above to get

$[\, L_s S_i,\, L_c S_c\,] = L_s L_c\, i\varepsilon_{ice} S_e + i\varepsilon_{scf}\, L_f\, S_c S_i = [\, L_s S_i,\, D\,]$

Then we have $C_2 = i\alpha^2\, \varepsilon_{kis}\, [\, L_s S_i,\, D]$

$C_2 = i\alpha^2\, \varepsilon_{kis}\ [\, L_s S_i,\, L_j S_j\,] = i\alpha^2\, \varepsilon_{kis}\, \{\ L_s L_j\, i\varepsilon_{ije} S_e + i\varepsilon_{sjf}\, L_f\, S_j S_i\ \}$

But we then have

$\varepsilon_{kis}\,\varepsilon_{ije} = \varepsilon_{isk}\,\varepsilon_{ije} = \delta_{sj}\delta_{ke} - \delta_{se}\delta_{jk}$

$\varepsilon_{kis}\varepsilon_{sjf} = \varepsilon_{ski}\ \varepsilon_{sjf} = \delta_{kj}\delta_{if} - \delta_{kf}\delta_{ij}$

Therefore

$C_2 = (i\alpha)^2 \{ (\delta_{sj}\delta_{ke} - \delta_{se}\delta_{jk}) L_s L_j S_e + (\delta_{kj}\delta_{if} - \delta_{kf}\delta_{ij}) L_f S_j S_i \}$

$= (i\alpha)^2 \{ \ 0 \ - L_e L_k S_e + L_i S_k S_i - 0 \}$

$= - (i\alpha)^2 \{ L_e L_k S_e - L_i S_k S_i \} = - (i\alpha)^2 \{ L_e S_e L_k - L_i S_i S_k \}$

$= - (i\alpha)^2 \{ D L_k - D S_k \} = - (i\alpha)^2 D \{ L_k - S_k \}$ // $D = L_i S_i$

Summary to this point:

$C_0 = B = L_k$

$C_1 = \alpha [L_k , D] = - i\alpha\varepsilon_{ksi} L_s S_i = -i\alpha [\mathbf{L} \times S]_k$

$C_2 = - i\alpha^2 \varepsilon_{ksi} [L_s S_i , D] = - (i\alpha)^2 D \{ L_k - S_k \}$

Next we have

$C_3 = [C_2 , \alpha D] = [- (i\alpha)^2 D \{ L_k - S_k \} , \alpha D]$

$= -\alpha (i\alpha)^2 [D \{ L_k - S_k \}, D] = -\alpha (i\alpha) D [\{ L_k - S_k \}, D]$

where I used the rule [ab,a] = a[b,a] to pull out the D to the left.
Now we know that

$[L_k , D] = - i \varepsilon_{ksi} L_s S_i \ \Rightarrow \ [S_k , D] = - i \varepsilon_{ksi} L_i S_s$

where to get the second item we just switch $L \leftrightarrow S$. So we can say that

$C_3 = \alpha (i\alpha) D [\{ L_k - S_k \}, D] = - (i\alpha)^2 D \varepsilon_{ksi} \{ L_s S_i - L_i S_s\} = - (i\alpha)^2 2D \varepsilon_{ksi} L_s S_i$

$= (i\alpha) 2D\{ -i\alpha\varepsilon_{ksi} L_s S_i \} = (i\alpha) 2D C_1$

We are starting to see the recursion form. Let's go another step:

$C_4 = [C_3 , \alpha D] = [(i\alpha) 2D C_1 , \alpha D] = (i\alpha) 2 [D C_1 , \alpha D]$

But we again use our rule [ab,a] = a[b,a] to pull D out to the left to get

$C_4 = (i\alpha)\ 2D\ [C_1\ ,\ \alpha D]\ = (i\alpha)\ 2D\ C_2$

and we have yet another recursion. Lets try another term:

$C_5 = [C_4,\ \alpha D]\ = [(i\alpha)\ 2D\ C_2,\ \alpha D]\ = (i\alpha)\ 2\ [\ D\ C_2,\ \alpha D]$

and we again pull D out to the left using the same rule and we have

$C_5 = (i\alpha)\ 2D\ \ [\ C_2,\ \alpha D]\ = (i\alpha)\ 2D\ C_3$

I think I am now convinced of this fact:

$C_{n+2}\ =\ (i\alpha)\ 2D\ C_n$ starting with n = 1

So let's try to build up the result:

$C_1 =\ \ - i\alpha\varepsilon_{ksi}\ L_s\ S_i$

$C_3 =\ (i\alpha)\ 2D\ C_1 = (2i\alpha D)\ C_1$

$C_5 =\ (i\alpha)\ 2D\ C_3\ = (2i\alpha D)^2\ C_1$

$C_7 = (i\alpha)\ 2D\ C_5\ = (2i\alpha D)^3\ C_1$

So the sum of all the odd terms is going to be (include the factorials now)

odd terms $= C_1 + C_3/3!\ + C_5/5! + ...$

$= [\ 1\ + x/\ 3!\ \ + x^2/5!\ + x^3/7! + ...\ ]\ C_1$ $x = (2i\alpha D)$

Now the even look like this:

$C_0\ = B\ =\ L_k$

$C_2 =\ - (i\alpha)^2\ D\ \{\ L_k - S_k\ \}$

$C_4 = (i\alpha)\ 2D\ C_2\ = (2i\alpha D)\ C_2$

$C_6 = (2i\alpha D)\ C_4 =\ (2i\alpha D)^2\ C_2$

So ignoring the first term, we get

even terms $= C_2/2! + C_4/4!\ + C_6/6! + ...$

$= [\ 1/2!\ \ + x/4!\ + x^2/6! + ...]\ C_2$

So we can at this point state our answer as follows:

$\exp(-\alpha\ \mathbf{L}\bullet\mathbf{S})\ L_k \exp(+\alpha\ \mathbf{L}\bullet\mathbf{S}) = \exp(-\alpha D)\ L_k \exp(+\alpha D) =$

$L_k + [\ 1 + x/3! + x^2/5! + x^3/7! + \ldots\ldots\ ]\ \{ - i\alpha\varepsilon_{ksi}\ L_s S_i \}$

$+ [\ 1/2! + x/4! + x^2/6! + \ldots.]\ (\{ - (i\alpha)^2 D\ \{ L_k - S_k \})$

where $x = (2i\alpha D) = 2i\alpha\ \mathbf{L}\bullet\mathbf{S}$.

Now let $\alpha = i\beta$ or $-i\alpha = \beta$ so we have what we really want,

$\exp(-i\beta\ \mathbf{L}\bullet\mathbf{S})\ L_k \exp(+i\beta\ \mathbf{L}\bullet\mathbf{S}) = \exp(-i\beta D)\ L_k \exp(+i\beta D) =$

$L_k + [\ 1 + x/3! + x^2/5! + x^3/7! + \ldots\ldots\ ]\ \{\beta\ \varepsilon_{ksi}\ L_s S_i \}$

$+ [\ 1/2! + x/4! + x^2/6! + \ldots.]\ (\{ - \beta^2 D\ \{ L_k - S_k \})$

where $x = (-2\beta D) = -2\beta\ \mathbf{L}\bullet\mathbf{S}$. Now define $y = 2\beta D = -x$ so we get

$\exp(-i\beta\ \mathbf{L}\bullet\mathbf{S})\ L_k \exp(+i\beta\ \mathbf{L}\bullet\mathbf{S}) = \exp(-i\beta D)\ L_k \exp(+i\beta D) =$

$L_k + [\ 1 - y/3! + y^2/5! - y^3/7! + \ldots\ldots\ ]\ \{\beta\ \varepsilon_{ksi}\ L_s S_i \}$

$+ [\ 1/2! - y/4! + y^2/6! + \ldots.]\ (\{ - \beta^2 D\ \{ L_k - S_k \})$

Now consider the first bracket:

$[\ 1 - y/3! + y^2/5! - y^3/7! + \ldots\ldots\ ]$ // $y = 2\beta D$

Now define $y = z^2$ so we get

$= [\ 1 - z^2/3! + z^4/5! - z^6/7! + \ldots\ldots\ ]$

$= z^{-1} [\ z - z^3/3! + z^5/5! - z^7/7!\ ] = z^{-1} \sin(z)$ $z = \sqrt{2\beta D}$

Now consider the second bracket:

$[\ 1/2! - y/4! + y^2/6! + \ldots.] = [\ 1/2! - z^2/4! + z^4/6! + \ldots.]$

$= z^{-2} [\ z^2/2! - z^4/4! + z^6/6! + \ldots\ ]$

$= z^{-2} [\ 1 -1 + z^2/2! - z^4/4! + z^6/6! + \ldots\ ] = z^{-2} [\ 1 - \cos(z)\ ]$

So we arrive at our final result which is

$\exp(-i\beta\,\mathbf{L}\bullet\mathbf{S})\;\; L_k \exp(+i\beta\,\mathbf{L}\bullet\mathbf{S}) = \exp(-i\,\beta\,D)\;\; L_k \exp(+i\,\beta\,D) =$

$$L_k \;+\; \beta z^{-1} \sin(z)\,\{\beta\,\varepsilon_{ksi}\; L_s S_i\} \;+ z^{-2}\,[\,1-\cos(z)\,]\,(\{-\beta^2\,D\,\{L_k - S_k\}\})$$

$$= L_k \;+\; \beta\, z^{-1} \sin(z)\,\varepsilon_{ksi}\; L_s S_i \;-\; \beta^2\, z^{-2}\, D\,[\,1-\cos(z)\,]\,(L_k - S_k)$$

where $z = \sqrt{2\beta D}$. In vector notation we get

$\exp(-i\,\beta\,D)\;\; \mathbf{L}\; \exp(+i\,\beta\,D) =$

$$= \mathbf{L} \;+\; \beta\, z^{-1} \sin(z)\,\mathbf{L}\times\mathbf{S} \;-\; \beta^2\, z^{-2}\, D\,[\,1-\cos(z)\,]\,(\mathbf{L} - \mathbf{S})$$

where $D = \mathbf{L}\bullet\mathbf{S}$ and $z = \sqrt{2\beta D}$.

This is certainly an exceedingly obscure result. Notice that D and z are operators.

Let's restate this in Malcolm language

$\exp(-i\,\beta\,\mathbf{I_1}\bullet\mathbf{I_2})\;\; \mathbf{I_1}\; \exp(+i\,\beta\;\mathbf{I_1}\bullet\mathbf{I_2}) =$

$$= \mathbf{I_1} \;+\; \beta\, z^{-1} \sin(z)\,\mathbf{I_1}\times\mathbf{I_2} \;-\; \beta^2\, z^{-2}\, D\,[\,1-\cos(z)\,]\,(\mathbf{I_1} - \mathbf{I_2})$$

where $D = \mathbf{I_1}\bullet\mathbf{I_2}$ and $z = \sqrt{2\beta D}$.

So this is now a non-secular J-coupling Hamiltonian would transform one of the spins in Levitt.

If we were in the L-S coupling scheme where L^2 and S^2 and J^2 are good, we could say for matrix elements in $|JLS; m_\ell, m_s\rangle$ states that

$$D = \mathbf{L}\bullet\mathbf{S} = (1/2)[\,J(J+1) - L(L+1) - S(S+1)] = \text{a number}$$

and then things like sin(z) are more reasonable.