Evaluation of the secular exponential PhL 1.8.08

Note added: A generalized version of this sandwich rule is given as equation (6) in document "sandwich rules page". There instead of having $I_{1z}I_{2z}$, we have the more general $I_{1n}I_{2j}$, and both are spin-1/2 I's.

Evaluate: $\exp(-i\beta I_{1z}I_{2z})\ \mathbf{I_1}\ \exp(+i\beta I_{1z}I_{2z})$. To simplify, define **L** and **S**:

$\mathbf{I_1} = \mathbf{L}$ $\mathbf{I_2} = \mathbf{S}$ so evaluate $\exp(-i\beta L_zS_z)\ \mathbf{L}\ \exp(+i\beta L_zS_z)$

In this particular problem, I think we can treat $I_{2z} = S_z$ as a constant (albeit a constant operator) because it commutes with *everything else in the expression*! We could not do this when we had $\mathbf{I_1 \bullet I_2 = L \bullet S}$ the exponential because in that case the components of $\mathbf{I_2}$ don't commute with each other so we cannot make the simplification. So consider then:

$\exp(-i\beta L_zS_z)\ \mathbf{L}\ \exp(+i\beta L_zS_z)$

and look at our general result

$$Q_k = \exp(-i\theta\,\hat{\mathbf{n}}\bullet\mathbf{J})\ J_k\ \exp(+i\theta\,\hat{\mathbf{n}}\bullet\mathbf{J}) = J_k\cos\theta + \varepsilon_{kms}J_m n_s\sin\theta + n_k(\hat{\mathbf{n}}\bullet\mathbf{J})(1-\cos\theta)$$

So, set $\hat{\mathbf{n}} = \hat{\mathbf{z}}$ and set $\mathbf{J} = \mathbf{L}$ and set $\theta = \beta S_z$ (which is an operator).

$$Q_k = \exp(-i\theta L_z)\ J_k\ \exp(+i\theta L_z) = L_k\cos\theta + \varepsilon_{kms}L_m n_s\sin\theta + n_k L_z(1-\cos\theta)$$

$$= L_k\cos\theta + \varepsilon_{kms}L_m\delta_{sz}\sin\theta + \delta_{kz}L_z(1-\cos\theta)$$

$$= L_k\cos\theta + \varepsilon_{kmz}L_m\sin\theta + \delta_{kz}L_z(1-\cos\theta)$$

In particular, we have

$$Q_x = L_x\cos\theta + \varepsilon_{xyz}L_y\sin\theta = L_x\cos\theta + L_y\sin\theta$$

$$Q_y = L_y\cos\theta + \varepsilon_{yxz}L_x\sin\theta = L_y\cos\theta - L_x\sin\theta$$

$$Q_z = L_z$$

In fact, we can treat our exponential operator as $R_z(\theta)$ and instantly write the above result.

Now, <u>there may be one more simplification we can do</u>. Consider that

$$\sin\theta = \theta - \theta^3/3! + \theta^5/5! - \ldots$$

We know that in the spin-1/2 representation we have $S_z^2 = 1/4$. Thus we have

$$\theta = \beta S_z = \beta\ S_z\ /\ 2^0$$

$\theta^3 = (\beta S_z)^3 = \beta^3 S_z (1/4) = \beta^3 S_z / 2^2$
$\theta^5 = (\beta S_z)^5 = \beta^5 S_z (1/4)^2 = \beta^5 S_z / 2^4$

$2\theta^n = (\beta/2)^n$

So consider:

$$(1/2)\sin\theta = (1/2)[\theta - \theta^3/3! + \theta^5/5! - ...]$$

$$= \beta S_z / 2^1 - \beta^3 S_z / 2^3 3! + \beta^5 S_z / 2^5 5!$$

$$= S_z [(\beta/2) - (\beta/2)^3/3! + (\beta/2)^5/5! - ...]$$

$$= S_z \sin(\beta/2)$$

Similarly,

$\theta^2 = (\beta S_z)^2 = \beta^2/4 = (\beta/2)^2$
$\theta^4 = (\beta S_z)^4 = \beta^4/4^2 = (\beta/2)^4$

so

$\cos\theta = [1 - \theta^2/2! + \theta^4/4! - ...] = [1 - (\beta/2)^2/2! + (\beta/2)^4/4! - ...]$
$= \cos(\beta/2)$

So our result now simplifies to become

$$Q_k = \exp(-i\beta L_z S_z) L_k \exp(+i\beta L_z S_z)$$

$$= L_k \cos\theta + \varepsilon_{kmz} L_m \sin\theta + \delta_{kz} L_z (1 - \cos\theta)$$

$$= L_k \cos(\beta/2) + \varepsilon_{kmz} L_m 2S_z \sin(\beta/2) + \delta_{kz} L_z (1 - \cos(\beta/2))$$

So finally I am seeing where the "factor of two" comes in that Levitt uses everywhere. Suppose we change things so that $\phi = \beta/2$. Then we get

$$\exp(-i\phi\, 2L_zS_z) L_k \exp(+i\phi\, 2L_zS_z)$$

$$= L_k \cos\phi + \varepsilon_{kmz} 2L_mS_z \sin\phi + \delta_{kz} L_z (1 - \cos\phi))$$

Another way to look at this is that we expect to find that

$$[2L_zS_z , L_k] = i\varepsilon_{zkm} 2L_mS_z$$

or

a b c

$[\ 2L_zS_z\ ,\ L_x\ ] = i\varepsilon_{zxm}\ 2L_mS_z\ = i\varepsilon_{zxy}\ 2L_yS_z\ = i\ 2L_yS_z$

The question is: does this form a *cyclic* set of operators with the same relationship? Let's look at the other two cases:

$[\ L_x\ ,\ 2L_yS_z\ ] = i\ 2L_zS_z\ \ ?$ lhs $= 2S_z\ i\ \varepsilon_{xyz}L_z\ = i\ 2\ L_z\ S_z$

$[\ 2L_yS_z,\ 2L_zS_z\ ] = i\ L_x\ \ ?$ lhs $= 4\ S_z^2\ i\ L_x\ = iL_x$ yes

So we see that it is <u>essential to have the factor of 2</u> if you want to have the operators a,b,c form a cyclic set! **This is how we get those Levitt pictures on page 377.**

So one more time for our final result:

$$\exp(-\ i\ \phi\ 2L_zS_z)\ \ L_k\ \exp(+\ i\ \phi\ 2L_zS_z\ )\ \ \ = L_k\ \cos\phi\ \ +\ \varepsilon_{kmz}\ 2L_mS_z\ \ \sin\phi\ +\ \delta_{kz}\ L_z\ (1\ -\ \cos\phi)$$

How do we write the above as a vector equation? Think of $\delta_{kz} = \hat{\mathbf{z}}_k$ then write

$$\exp(-\ i\ \phi\ 2L_zS_z)\ \ \mathbf{L}\ \exp(+\ i\ \phi\ 2L_zS_z\ )\ \ \ = \mathbf{L}\ \cos\phi\ \ +\ 2\ \mathbf{L}\ \mathrm{x}\ \mathbf{S}\ \ \sin\phi\ +\ \hat{\mathbf{z}}\ (\ \mathbf{L}\bullet\hat{\mathbf{z}}\ )(1\ -\ \cos\phi)$$