Sandwich Rules Page PhL 3.26.05

1. Sandwich Rules for a single J. The general rule for $R_{\hat{\mathbf{n}}}(\theta)\, J\, R_{\hat{\mathbf{n}}}(-\theta)$ is this: (see separate "evaluate n dot J rotation of J.doc")

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

Let's specialize to $\hat{n}=\hat{j}$, a unit vector in the j direction where j = x, y or z. Then we know that $n_k=\delta_{kj}$ and we get

$$\exp(-i\theta J_j)\;J_k\;\exp(+i\theta J_j) \;=J_k\cos\theta \;+\;\varepsilon_{kmj}J_m\sin\theta+\;\delta_{kj}J_j\,(1-\cos\theta) \qquad (2)$$

The non-trivial cases are those with $i\neq j$ for which we have

$$\exp(-i\theta J_j)\;J_k\;\exp(+i\theta J_j) \;=J_k\cos\theta \;+\;\varepsilon_{jkm}\;J_m\sin\theta \qquad i\neq j \qquad (3)$$

Now let's just for the moment further assume that j and k follow each other in forward cyclic order, so that the ordered set of indices is j,k,ℓ . In this case we get

$$\exp(-i\theta J_j)\;J_k\;\exp(+i\theta J_j) \;=J_k\cos\theta \;+\;J_\ell\;\sin\theta \qquad j,k,\ell \text{ cyclic}$$

Now suppose j,k are in reverse follow order. In this case we would say that j,k,ℓ was in anti-cyclic order and our second term changes sign due to $\varepsilon_{kjm}=-\;\varepsilon_{jkm}$. Then we have

$$\exp(-i\theta J_j)\;J_k\;\exp(+i\theta J_j) \;=J_k\cos\theta \;-\;J_\ell\;\sin\theta \qquad j,k,\ell \text{ anti-cyclic}$$

So let's group the above next to each other:

$$\begin{aligned}&\exp(-i\theta J_j)\;J_k\;\exp(+i\theta J_j) \;=J_k\cos\theta \;+\;J_\ell\;\sin\theta && j,k,\ell \text{ cyclic}\\ &\exp(-i\theta J_j)\;J_k\;\exp(+i\theta J_j) \;=J_k\cos\theta \;-\;J_\ell\;\sin\theta && j,k,\ell \text{ anti-cyclic}\end{aligned} \qquad (4)$$

We can now write down various special cases using either (4) or (5):

$$\begin{aligned}&\exp(-i\theta J_x)\;J_y\;\exp(+i\theta J_x) \;=J_y\cos\theta \;+\;J_z\;\sin\theta\\ &\exp(-i\theta J_x)\;J_z\;\exp(+i\theta J_x) \;=J_z\cos\theta \;-\;J_y\;\sin\theta\end{aligned}$$

So the rule is this: if you keep the same bread but change the filling, the sine term changes sign, and you set the J's to the obvious values on the right. Going back to (4) with j = y we get

$$\begin{aligned}&\exp(-i\theta J_y)\;J_z\;\exp(+i\theta J_y) \;=J_z\cos\theta \;+\;J_x\;\sin\theta\\ &\exp(-i\theta J_y)\;J_x\;\exp(+i\theta J_y\;) \;=J_x\cos\theta \;-\;J_z\;\sin\theta\end{aligned}$$

And finally we have

$$\exp(-i\theta J_z)\ J_x \exp(+i\theta J_z) = J_x \cos\theta + J_y \sin\theta$$
$$\exp(-i\theta J_z)\ J_y \exp(+i\theta J_z) = J_y \cos\theta - J_x \sin\theta$$

So let's put all these results together:

		special cases:	$\pi/2$	π	$-\pi/2$
$\exp(-i\theta J_x)\ J_y \exp(+i\theta J_x)$	$= J_y \cos\theta + J_z \sin\theta$		J_z	$-J_y$	$-J_z$
$\exp(-i\theta J_x)\ J_z \exp(+i\theta J_x)$	$= J_z \cos\theta - J_y \sin\theta$		$-J_y$	$-J_z$	J_y
$\exp(-i\theta J_y)\ J_z \exp(+i\theta J_y)$	$= J_z \cos\theta + J_x \sin\theta$		J_x	$-J_z$	$-J_x$
$\exp(-i\theta J_y)\ J_x \exp(+i\theta J_y)$	$= J_x \cos\theta - J_z \sin\theta$		$-J_z$	$-J_x$	J_z
$\exp(-i\theta J_z)\ J_x \exp(+i\theta J_z)$	$= J_x \cos\theta + J_y \sin\theta$		J_y	$-J_x$	$-J_y$
$\exp(-i\theta J_z)\ J_y \exp(+i\theta J_z)$	$= J_y \cos\theta - J_x \sin\theta$		$-J_x$	$-J_y$	J_x

(5)

3. Two subspaces J and j. Now suppose, in this last case, we has $\theta = j_n \phi$ where j_n is an angular momentum operator in some subspace different from the J_n. Since $[\mathbf{J},\mathbf{j}] = 0$, the results above all apply, except then each trig function is an operator mess, such as

$$\cos(j_n \phi) = \Sigma_{k=even}\ (-1)^{k/2} \quad (1/k!)\ j_n^k\ \phi^k$$

$$\sin(j_n \phi) = \Sigma_{k=odd}\ (-1)^{(k-1)/2}\ (1/k!)\ j_n^k\ \phi^k$$

3A. The case of j_n being spin-1/2. For j_n being spin-1/2, however, we know (see "rotation group generators.doc") that

$$(j_n)^k = (1/2)^k\ 1 \qquad k = \text{even}$$
$$(j_n)^k = (1/2)^{k-1}\ j_n \qquad k = \text{odd} \qquad // = (1/2)^k\ (1/2)^{-1}\ j_n = (1/2)^k\ 2j_n$$

so we can then write

$$\cos(j_n \phi) = \Sigma_{k=even}\ (-1)^{k/2} \quad (1/k!)\ (1/2)^k\ \phi^k = \cos(\phi/2) * 1$$

$$\sin(j_n \phi) = \Sigma_{k=odd}\ (-1)^{(k-1)/2}\ (1/k!)\ (1/2)^k\ \phi^k\ * 2\ j_n = \sin(\phi/2) * 2\ j_n$$

We can then go back to our general formula

$$\exp(-i\theta J_j)\ J_k \exp(+i\theta J_j) = J_k \cos\theta + \varepsilon_{jkm}\ J_m \sin\theta \qquad j \neq k \qquad [\ (3)\ ]$$

and replace $\theta = j_n \phi$ to get

$$\exp(-i\phi j_n J_j)\ J_k \exp(+i\phi j_n J_j) = J_k \cos(\phi/2) + \varepsilon_{jkm}\ 2j_n J_m \sin(\phi/2) \qquad j\neq k$$

but it now seems best to replace $\phi \to 2\phi$ and we get

$$\exp(-i\phi [2 j_n J_j])\ J_k \exp(+i\phi [2 j_n J_j]) = J_k \cos(\phi) + \varepsilon_{jkm}\ [2j_n J_m] \sin(\phi) \qquad j\neq k$$

where j_n goes along for the ride. Here are special cases:

$$\exp(-i\phi [2j_n J_j])\ J_k \exp(+i\phi [2j_n J_j]) = J_k \cos\phi + [2j_n J_\ell] \sin(\phi) \qquad j,k,\ell \text{ cyclic} \qquad j = 1/2$$
$$\exp(-i\phi [2j_n J_j])\ J_k \exp(+i\phi [2j_n J_j]) = J_k \cos\phi - [2j_n J_\ell] \sin(\phi) \qquad j,k,\ell \text{ anti-cyclic}$$

where we have $j_n = \sigma_n/2$ and σ_n are the Pauli matrices, so the generators are

$$j_x = (1/2)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad j_y = (1/2)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad j_z = (1/2)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad (6)$$

In Levitt's work on secular AX J-coupling, we use the above with n = z and j = z so we have:

$$\exp(-i\phi [2j_z J_z])\ J_x \exp(+i\phi [2j_z J_z]) = J_x \cos\phi + [2j_z J_y] \sin(\phi)$$
$$\exp(-i\phi [2j_z J_z])\ J_y \exp(+i\phi [2j_z J_z]) = J_y \cos\phi - [2j_z J_x] \sin(\phi)$$

where, in his application, $j = I_1$ and $J = I_2$ and vice versa. Write this out as

$$\exp(-i\phi [2 I_{1z} I_{2z}])\ I_{2x} \exp(+i\phi [2 I_{1z} I_{2z}]) = I_{2x} \cos\phi + [2 I_{1z} I_{2y}] \sin(\phi)$$
$$\exp(-i\phi [2 I_{1z} I_{2z}])\ I_{2y} \exp(+i\phi [2 I_{1z} I_{2z}]) = I_{2y} \cos\phi - [2 I_{1z} I_{2x}] \sin(\phi)$$

where usually $\phi = \pi J$.

3B. The case of j_n being spin-1. We repeat the above for the case j = 1. As before, we start with

$$\cos(j_n \phi) = \Sigma_{k=even}\ (-1)^{k/2} \qquad (1/k!)\ j_n^k\ \phi^k$$

$$\sin(j_n \phi) = \Sigma_{k=odd} \qquad (-1)^{(k-1)/2}\ (1/k!)\ j_n^k\ \phi^k$$

For j_n being spin-1, however, we know (see "rotation group generators.doc") that

$$j_n = j_n$$
$$(j_n)^2 = (j_n)^2$$
$$(j_n)^3 = j_n$$

$(j_n)^4 = (j_n)^2$

....

$(j_n)^k = (j_n)^2$ k = even

$(j_n)^k = j_n$ k = odd

so we then get:

$$\cos(j_n \phi) = \Sigma_{k=even} (-1)^{k/2} (1/k!) (j_n)^2 \phi^k = (j_n)^2 \cos(\phi)$$

$$\sin(j_n \phi) = \Sigma_{k=odd} (-1)^{(k-1)/2} (1/k!) j_n \phi^k = j_n \sin(\phi)$$

We can then go back to our general formula

$$\exp(-i\theta J_j) J_k \exp(+i\theta J_j) = J_k \cos\theta + \varepsilon_{jkm} J_m \sin\theta \qquad j \neq k \qquad [(3)]$$

and replace $\theta = j_n \phi$ to get

$$\exp(-i\phi j_n J_j) J_k \exp(+i\phi j_n J_j) = (j_n)^2 J_k \cos(\phi) + \varepsilon_{jkm} j_n J_m \sin(\phi) \qquad j \neq k$$

which we can write in the two cases: (for j = spin-1, J = any spin)

$$\exp(-i\phi j_n J_j) J_k \exp(+i\phi j_n J_j) = (j_n)^2 J_k \cos(\phi) + j_n J_\ell \sin(\phi) \qquad j,k,\ell \text{ cyclic} \qquad j = 1$$

$$\exp(-i\phi j_n J_j) J_k \exp(+i\phi j_n J_j) = (j_n)^2 J_k \cos(\phi) - j_n J_\ell \sin(\phi) \qquad j,k,\ell \text{ anti- cyclic}$$

where the generators are as follows:

$$J_x = (1/\sqrt{2}) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad J_y = (1/\sqrt{2}\, i) \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \qquad J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad (7)$$

3C. The case of j_n being spin-j for j>1 . For j > 1, I don't think there are any simple closed forms like this, see "rotation group generators.doc".

4. Rules applied to raise and lower operators.

Recall that $[J_\pm, J_z] = \mp J_\pm$ from our ang mom formulas sheet. Consider then this particular sandwich,

$$\exp(-i\theta J_z) J_\pm \exp(+i\theta J_z)$$

We could use our existing rules, or just run a fresh C-H on this, so let's do that:

$A = i\theta J_z \quad B = J_\pm : \quad C_0 = J_\pm \quad C_1 = [J_\pm,\ i\theta J_z] = \mp i\theta J_\pm \quad C_2 = [\mp i\theta J_\pm,\ i\theta J_z] = (i\theta)^2 J_\pm$

and so on with the $\mp$ appearing only in the odd terms. This as have

$= J_\pm [\ 1 \mp i\theta + (i\theta)^2/2! \mp (i\theta)^3/3! + \ldots.\ ] = J_\pm [\ 1 + (\mp i\theta) + (\mp i\theta)^2/2! + (\mp i\theta)^3/3! + \ldots]$

$= J_\pm \exp(\mp i\theta)$

So we get an interesting and very simple result which we add to our list of formulas:

$\exp(-\ i\ \theta\ J_z)\ J_\pm \exp(+\ i\ \theta\ J_z) = \exp(\mp i\theta)\ J_\pm$

This explains, for example, why a "+ coherence" propagates with a negative phase. We could derive other rules involving $J_\pm$ but let's wait until they are needed. // Well, they soon became "needed"!

$\exp(-\ i\ \theta\ J_x)\ J_\pm \exp(+\ i\ \theta\ J_x) = \exp(-\ i\ \theta\ J_x)\ [\ J_x \pm iJ_y]\ \exp(+\ i\ \theta\ J_x)$

$= J_x \pm i\ \exp(-\ i\ \theta\ J_x)\ J_y\ \exp(+\ i\ \theta\ J_x) = J_x \pm i\ [\ J_y \cos\theta + J_z \sin\theta]$

Special case of interest is $\theta = \pi$ in which case get $J_x \mp iJ_y = J_\mp$

Next:

$\exp(-\ i\ \theta\ J_y)\ J_\pm \exp(+\ i\ \theta\ J_y) = \exp(-\ i\ \theta\ J_y)\ [\ J_x \pm iJ_y]\ \exp(+\ i\ \theta\ J_y)$

$= \exp(-\ i\ \theta\ J_y)\ J_x\ \exp(+\ i\ \theta\ J_y) \pm i\ J_y = \pm i\ J_y + [\ J_x \cos\theta - J_z \sin\theta]$

Again, if $\theta = \pi$ we get $= \pm i\ J_y - J_x = - J_x \pm i\ J_y = -\ [\ J_x \mp i\ J_y\ ] = -\ J_\mp$

Now summarize all these last results:

$\exp(-\ i\ \theta\ J_x)\ J_\pm \exp(+\ i\ \theta\ J_x) = J_x \pm i\ [\ J_y \cos\theta + J_z \sin\theta]$ // $= J_\mp$ if $\theta = \pi$

$\exp(-\ i\ \theta\ J_y)\ J_\pm \exp(+\ i\ \theta\ J_y) = \pm i\ J_y + [\ J_x \cos\theta - J_z \sin\theta]$ // $= -\ J_\mp$ if $\theta = \pi$

$\exp(-\ i\ \theta\ J_z)\ J_\pm \exp(+\ i\ \theta\ J_z) = \exp(\mp i\theta)\ J_\pm$ // $= -\ J_\pm$ if $\theta = \pi$

Here are the special cases for $\theta = \pi/2$:

$\exp(-\ i\ \theta\ J_x)\ J_\pm \exp(+\ i\ \theta\ J_x) = J_x \pm i\ [\ J_y \cos\theta + J_z \sin\theta] = J_x \pm i\ J_z$

$\exp(-i\,\theta\,J_y)\;\; J_\pm \exp(+i\,\theta\,J_y) = \pm i\,J_y + [\,J_x \cos\theta - J_z \sin\theta] = \pm i\,J_y - J_z$

$\exp(-i\,\theta\,J_z)\;\; J_\pm \exp(+i\,\theta\,J_z) = \exp(\mp i\theta)\,J_\pm = \exp(\mp i\pi/2) = \mp i\,J_\pm$

$R_x(\pi/2)\,J_\pm\,R_x(-\pi/2) = J_x \pm i\,J_z$
$R_y(\pi/2)\,J_\pm\,R_y(-\pi/2) = \pm i\,J_y - J_z$
$R_z(\pi/2)\,J_\pm\,R_z(-\pi/2) = \mp i\,J_\pm$

$R_x(-\pi/2)\,J_\pm\,R_x(\pi/2) = J_x \mp i\,J_z$
$R_y(-\pi/2)\,J_\pm\,R_y(\pi/2) = \pm i\,J_y + J_z$
$R_z(-\pi/2)\,J_\pm\,R_z(\pi/2) = \pm i\,J_\pm$

$R_x(\pi)\,J_\pm\,R_x(-\pi) = J_\mp$
$R_y(\pi)\,J_\pm\,R_y(-\pi) = -J_\mp$
$R_z(\pi)\,J_\pm\,R_z(-\pi) = -J_\pm$