TSI CMMS Aug 2011: Lecture #16

Theory of Magnetic Resonance #2

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Part I: Two Level System; + A Random Perturbation

1) S.E. $\quad i\hbar \dfrac{\partial|\psi\rangle}{\partial t} = \mathcal{H}(t)|\psi(t)\rangle \quad$, $\mathcal{H}$ is Hermetian i.e $\mathcal{H}^{+}=\mathcal{H}$

for a spin $S=1/2 \quad |\psi\rangle = \begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix}$ & Hermetian $\mathcal{H} \Rightarrow$

$$\langle\psi(t)|\psi(t)\rangle = \left[\alpha^*(t), \beta^*(t)\right]\begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix} = 1$$

and the spin operators are

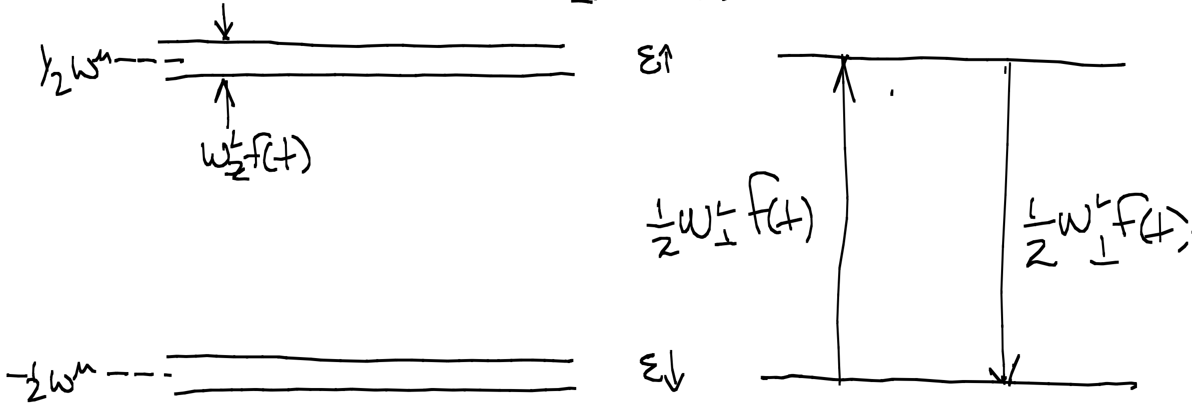
$$S_z = \begin{bmatrix}1/2 & \\ & -1/2\end{bmatrix},\quad S_x = \begin{bmatrix}0 & 1/2\\ 1/2 & 0\end{bmatrix},\quad S_y = \begin{bmatrix}0 & i/2\\ -i/2 & 0\end{bmatrix}$$

Assume $\mathcal{H}(t)$ is of the following form

$$\frac{1}{\hbar}\mathcal{H}(t) = \omega^{\mu} S_z + \vec{\omega}^{L}\cdot\vec{S} f(t), \text{ where } f(t) \text{ is random}$$

$$\Rightarrow \int f(t) = \phi,\ f(0)=1$$

a) $$= \frac{1}{2}\begin{bmatrix}\omega^{\mu}+\omega^{L}_{z}f(t) & 0\\ 0 & -\omega^{\mu}-\omega^{L}_{z}f(t)\end{bmatrix} + \frac{1}{2}\begin{bmatrix}0 & \omega^{L}_{\perp}e^{-i\varphi}\\ \omega^{L}_{\perp}e^{i\varphi} & 0\end{bmatrix} f(t)$$



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The SE (eqn 1) has the solution

2) $$|\psi(t)\rangle = \begin{bmatrix} \alpha(t)\, e^{-i\left(\frac{1}{2}\omega_\mu t + \int_0^t \frac{1}{2}\omega_z^L f(\tau)d\tau\right)} \\ \beta(t)\, e^{i\left(\frac{1}{2}\omega_\mu t - \int_0^t \frac{1}{2}\omega_z^L f(\tau)d\tau\right)} \end{bmatrix}$$

if the coefficients α, β statisfy the following

3) $$i\frac{d}{dt}\begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{2}f(t)\,\omega_\perp^L e^{-i\varphi} e^{-i\left(\omega_\mu t + \int_0^t \omega_z^L f(\tau)d\tau\right)} \\ \frac{1}{2}f(t)\,\omega_\perp^L e^{i\varphi} e^{i\left(\omega_\mu t + \int_0^t \omega_z^L f(\tau)d\tau\right)} & 0 \end{bmatrix}\begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix}.$$

or $$i\begin{bmatrix}\dot\alpha\\ \dot\beta\end{bmatrix} = \begin{bmatrix} 0 & g(t) \\ g^*(t) & 0\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix}$$

which has the formal solution

4) $$\begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix} = \exp\left\{ i\begin{bmatrix} 0 & G(t) \\ G^*(t) & 0\end{bmatrix}\right\}\begin{bmatrix}\alpha(t=0)\\ \beta(t=0)\end{bmatrix}. \quad , \; G(t) = \int_0^t g(\tau)\,d\tau = |G(t)|\,e^{i\xi(t)}$$

$$= \left\{\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\cos\left(|G(t)|\right) + i\begin{bmatrix} 0 & e^{i\xi} \\ e^{-i\xi} & 0\end{bmatrix}\sin\left(|G(t)|\right)\right\}\begin{bmatrix}\alpha_0\\ \beta_0\end{bmatrix}$$

(can the student prove this identity)?

Our problem is solved !!

$\Rightarrow$ Let us go & calculate the spin polarizations

Let us now calculate the polarization functions. In transverse field we want

5) $$S_x(t) = \langle \psi(t)_{TF} | S_x | \psi(t)_{TF} \rangle \quad , \; S_x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Now $\langle \psi_{TF}(t=0)| = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $\quad \therefore \langle \psi_{TF}(0) | S_x = \frac{1}{2} S_x$

i.e $\langle \psi_{TF}(0)|$ represents an initial pol^{n} along $\hat{x}$.

Rather than using $S_x(t)$ it is easier to calculate $S_+(t)$, where $S_+ = 2(S_x + iS_y) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

The real/complex parts are S_x/S_y, so we get both!

Using eq^n 2) one easily finds

6a) $$S_+(t) = \underbrace{\alpha^*_{TF}(t)\, \beta_{TF}(t)}_{\substack{\text{spin flips from } \omega_\perp \\ \text{or spin-lattice "}T_1\text{" processes}}} \underbrace{e^{i\omega_{\mu}t}}_{\text{ext field}} \underbrace{e^{i\int_0^t \omega_z^L f(\tau)d\tau}}_{\substack{\text{time dependence of local field comp} \\ \parallel \text{ to ext field}}}$$

time dependence comes from

In LF we need $\langle \psi_{LF}(t) | S_z | \psi_{LF}(t) \rangle$, $S_z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

6b) $$\Rightarrow S_z(t) = \alpha^*_{LF}(t)\alpha_{LF}(t) - \beta^*_{LF}(t)\beta_{LF}(t) \quad , \; \langle \psi_{LF}(0)| = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

However, a μSR experiment is carried out on an ensemble average ... whereas the preceeding calculation is done for a single "time evolution" $f(t)$ coupled with a specific initial amplitud & orientation of the local field $\vec{\omega}^L$. So let $\langle\langle\ \rangle\rangle \equiv$ integration over the initial distributions and the (independent) averaging over time evolutions.

7) $\therefore \quad \langle\langle S^+ \rangle\rangle = \langle\langle \alpha^*_{TF}(t)\, B_{TF}(t)\, e^{i\omega_\mu t} e^{i\int_0^t \omega_z^L f(\tau)d\tau} \rangle\rangle$

Now we could have put an independent $f(t)$ for both the ω_z^L & the $\omega_\perp^L$

$\therefore \quad \langle\langle S^+ \rangle\rangle = \langle\langle \alpha^*_{TF}(t)\, B_{TF}(t) \rangle\rangle \langle\langle e^{i\omega_\mu t} e^{i\int_0^t \omega_z^L f(\tau)d\tau} \rangle\rangle$

$$\langle\langle S_z(t) \rangle\rangle = \langle\langle \alpha^*_{LF}(t)\,\alpha_{LF}(t) - B^*_{LF}(t)\, B_{LF}(t) \rangle\rangle$$

and we now must calculate these ensemble averages.

AVERAGING FUNCTIONS OF A STOCHASTIC VARIABLE α

9) Example 1: $\langle\langle e^{\alpha}\rangle\rangle = e^{\langle\langle\alpha\rangle\rangle_c}$

$$\langle\langle\alpha\rangle\rangle_c = \ln\left(1+\sum_{n=1}^{\infty}\frac{1}{n!}\langle\langle\alpha^n\rangle\rangle\right)$$

$$= \sum_{n'=1}^{\infty}\frac{(-1)^{n'+1}}{n'}\left(\sum_{n=1}^{\infty}\frac{1}{n!}\langle\langle\alpha^n\rangle\rangle\right)^{n'}$$

10)

$$\left.\begin{aligned}
&= \langle\langle\alpha\rangle\rangle + \frac{1}{2}\left\{\langle\langle\alpha^2\rangle\rangle - \langle\langle\alpha\rangle\rangle^2\right\} \\
&+ \frac{1}{6}\left\{\langle\langle\alpha^3\rangle\rangle - 3\langle\langle\alpha^2\rangle\rangle\langle\langle\alpha\rangle\rangle + 2\langle\langle\alpha\rangle\rangle^3\right\} \\
&+ \frac{1}{24}\left\{\langle\langle\alpha^4\rangle\rangle - 4\langle\langle\alpha^3\rangle\rangle\langle\langle\alpha\rangle\rangle - 3\langle\langle\alpha^2\rangle\rangle^2 + 12\langle\langle\alpha^2\rangle\rangle\langle\langle\alpha\rangle\rangle^2 - 6\langle\langle\alpha\rangle\rangle^4\right\}
\end{aligned}\right\}$$

these are called cumulants

$$+ \;....$$

More Generally:

11) $\langle\langle f(\alpha)\rangle\rangle = \langle\langle f(\bar{\alpha}+\delta\alpha)\rangle\rangle$, $\delta\alpha = \alpha - \bar{\alpha}$

$$= f(\bar{\alpha}) + \langle\langle\delta\alpha\rangle\rangle \left.\frac{\partial f(\alpha)}{\partial\alpha}\right|_{\alpha=\bar{\alpha}}$$

$$\frac{\langle\langle\delta\alpha^2\rangle\rangle}{2}\left(\left.\frac{\partial^2}{\partial\alpha^2}f(\alpha)\right|_{\alpha=\bar{\alpha}}\right) + \sum_{n=3}^{\infty}\frac{\langle\langle\delta\alpha^n\rangle\rangle}{n!}\left(\left.\frac{\partial^n}{\partial\alpha^n}f(\alpha)\right|_{\alpha=\bar{\alpha}}\right)$$

which is an expansion of $\langle\langle f(\alpha)\rangle\rangle$ into the "moments" $\langle\langle \delta\alpha^n \rangle\rangle$ around some value average value $\bar{\alpha}$.

One can then pick an appropriate "characteristic" function $C(\langle\langle \alpha \rangle\rangle_c)$

and its "caverage" $\equiv \langle\langle \ \rangle\rangle_c$
so ~~that~~
$$\langle\langle f(\alpha)\rangle\rangle = C\left(\langle\langle \alpha \rangle\rangle_c^f\right)$$

$$\Rightarrow \langle\langle \alpha \rangle\rangle_c^f = C^{-1}\left(\langle\langle f(\alpha)\rangle\rangle\right)$$

12) which is eq$\underline{\text{n}}$ 9 if f and C are exponentials.
The choice of C is determined some physical insight into the problem, so ~~that~~ only one or two cumulants are sufficient to characterize the behaviour.

For example if α has a Gaussian distribution then $\langle\langle e^{\alpha} \rangle\rangle$ is best described by an exponential cumulant (i.e. eq$^{\underline{n}}$ 9) since all the cumulants above 2 vanish, and in this case the "truncated" cumulant expansion is exact!

Now, we can "evaluate" the pieces of the polarization functions

First look at $\left\langle\left\langle e^{i\omega_\mu t} e^{i\int_0^t \omega_z^L f(\tau)\,d\tau}\right\rangle\right\rangle$ &

assume: (i) the values of ω_z^L have a Gaussian distribution

and (ii) stochastic $f(\tau)$ is characterized (only) with an exponential memory.

13) i.e. $$P(\omega_z^L) = \frac{1}{\sqrt{2\pi}\,\omega_L} e^{-(\omega_z^L)^2/2\omega_L^2}$$;

initial value distribut^{n} $$\left\langle F(\omega_z^L)\right\rangle = \int_{-\infty}^{\infty} P(\omega_z^L)\, F(\omega_z^L)\, d\omega_z^L$$

14) ensemble average of the time correlation $$\overline{f(t)\,f(t-\tau)} = e^{-\nu|\tau|}$$

Now the ensemble average $\langle\langle\ \rangle\rangle$ can be carried out in two independent steps:

15) $\langle\langle\ \rangle\rangle = \overline{\langle\ \rangle}$

where $\overline{}$ is the average of time evolutions and $\langle\ \rangle$ the initial value average ω_z^L over the ensemble, therefor doing the cumulant expansion

16) $$\left\langle\left\langle e^{i\omega_\mu t}\, e^{i\int_0^t \omega_z^L f(\tau)\,d\tau}\right\rangle\right\rangle = e^{i\omega_\mu t}\, e^{i\left\langle\left\langle \int_0^t \omega_z^L f(\tau)\,d\tau\right\rangle\right\rangle_e}$$

$$= e^{i\omega_\mu t}\, e^{i\langle\cancel{\omega_z^L}\rangle \overline{\int_0^t \cancel{f(\tau)}\,d\tau}}$$

$$e^{-\frac{1}{2}\langle\omega_z^{L2}\rangle \overline{\int_0^t f(\tau)\,d\tau \int_0^t f(\tau')\,d\tau'}}$$

(all other cumulants of ω_z^L vanish!)

17) $$\overline{\int_0^t \int_0^t f(\tau) f(\tau')\,d\tau\, d\tau'} = 2\int_0^t \int_0^\tau e^{-\nu(\tau-\tau')}\,d\tau' d\tau$$

$$= 2\left[\frac{t}{\nu} + \frac{1}{\nu^2}\left(e^{-\nu t} - 1\right)\right]$$

17a)

∴

18) $$\langle\langle\ \ \rangle\rangle = e^{i\omega_\mu t}\, e^{-\langle\omega_z^{L2}\rangle\left[t/\nu + 1/\nu^2\left(e^{-\nu t}-1\right)\right]}$$

Spin Precession in $\vec{B}_0$

"Abragam" Relaxation Function

Note, that for $t \to 0$

19) $$e^{-\langle \omega_z^{L^2}\rangle[t/\nu + 1/\nu^2(e^{-\nu t}-1)]} \to e^{-\langle \omega_z^{L^2}\rangle t^2}$$

and for $t > 1/\nu_z \longrightarrow e^{-\langle \omega_z^{L^2}\rangle t/\nu_z}$

- Gaussian for short times
- Exponential for long times

Going back to eq$^{\underline{ns}}$ 6), 7) & 8)
what about the "spin-lattice"
$\langle\langle \alpha^*(t)\beta(t)\rangle\rangle$ contribut$^{\underline{n}}$ to TF relaxat$^{\underline{n}}$?

Using $|\psi(t=0)\rangle_{TF} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} = \begin{bmatrix}\alpha_0\\\beta_0\end{bmatrix}$

then eq$^{\underline{n}}$ 4) yields

20) $$\alpha(t) = \cos(|G(t)|) + i e^{i\xi}\sin(|G(t)|)$$
$$\beta(t) = \cos(|G(t)|) + i e^{-i\xi}\sin(|G(t)|)$$

21) $$\Rightarrow \alpha^*(t)\beta(t) = \cos^2(|G(t)|) - e^{2i\xi}\sin^2(|G(t)|)$$

Recall that $G(t) = \int_0^t f(\tau)\,\omega_\perp^L e^{-i\varphi} e^{-i\omega_\mu \tau} d\tau$

$\therefore$ ξ is a linear function of φ (angle of $\omega_\perp^L$), when we go to take the ensemble average of $\langle\langle \alpha^*(t)\,\beta(t)\rangle\rangle$ the average over φ will render the term $\propto \langle e^{-2i\xi}\rangle = 0$ which leaves us with

22) $$\langle\langle \alpha^*(t)\beta(t)\rangle\rangle_{TF} = \langle\langle \cos^2(|G(t)|)\rangle\rangle$$

what is "odd" about this result?

Similarily, expressing the LF relaxat$^{\underline{n}}$ function gives

$$S_Z(t) = \langle\langle \cos^2(|G(t)|) - \sin^2(|G(t)|)\rangle\rangle$$

23) $$= \langle\langle \cos(2|G(t)|)\rangle\rangle$$

Now to make further progress one must select how "to do" the ensemble average, i.e. what cumulant funct$^{\underline{n}}$ "C" appropriately reflects the behavior.

If one expects "exponential" relaxat^{n} of the form $e^{-\Lambda(t)}$ then the exponential cumulant could be used. Taking this approach, we calculate

24) $$\langle\langle \cos(2\alpha)\rangle\rangle = e^{\langle\langle 2\alpha\rangle\rangle_e^{\cos}},$$

$$\Rightarrow \langle\langle 2\alpha\rangle\rangle_e^{\cos} = \ln\left[1+\sum_{n=1}^{\infty}\frac{(-1)^n(2\alpha)^{2n}}{(2n)!}\right].$$

$$\Rightarrow \langle\langle \alpha\rangle\rangle_e^{\cos} = \sum_{n'=1}^{\infty}\frac{(-1)^{n'+1}}{n'}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(2n)!}(2\alpha)^{2n}\right)^{n'}$$

24a) $$= -2\langle\langle\alpha^2\rangle\rangle + 2\left\{\frac{\langle\langle\alpha^4\rangle\rangle}{3} - \frac{\langle\langle\alpha^2\rangle\rangle^2}{2}\right\} + \ldots$$

& Similarly:

25) $$\langle\langle \cos^2(\alpha)\rangle\rangle = e^{\langle\langle\alpha\rangle\rangle_e^{\cos^2}}$$

25a) $$\Rightarrow \langle\langle\alpha\rangle\rangle_e^{\cos^2} = -\langle\langle\alpha^2\rangle\rangle + \left\{\frac{\langle\langle\alpha^4\rangle\rangle}{3} - \frac{\langle\langle\alpha^2\rangle\rangle^2}{2}\right\} + \ldots$$

In our case $\alpha^2 \equiv G^*(t)\,G(t)$, using 3) & 4)

26) $$= \int_0^t \tfrac{1}{2} f_\perp(\tau)\,\omega_\perp^L e^{-i\varphi} e^{-i\omega_\mu\tau}\,d\tau \cdot \int_0^t \tfrac{1}{2} f_\perp(\tau)\,\omega_\perp^L e^{+i\varphi} e^{+i\omega_\mu\tau'}\,d\tau'$$

(ignoring the small value of $\omega_z^L \ll \omega_\mu$)

27) $$= \frac{1}{4}\omega_\perp^{L2}\int_0^t\int_0^t f_\perp(\tau)\,f_\perp(\tau')\,e^{-i\omega_\mu(\tau-\tau')}\,d\tau\,d\tau'$$

Taking the ensemble average is entirely similar to the process 16) → 18)

28) $$\langle\langle G^*(t)G(t)\rangle\rangle = \frac{1}{4}\langle\omega_\perp^{L2}\rangle 2\int_0^t\int_0^{\tau} e^{-\nu_\perp(\tau-\tau')}\cos\omega_\mu(\tau-\tau')\,d\tau\,d\tau'$$

The ∫ can be evaluated using the results of eq^n 17 & 17a by replacing $\nu \to \nu_\perp + i\omega$ and then taking the real part. However, before doing this note ~~that~~

the LF relaxat^n is governed by the Fourier Transform coefficient @ ω_μ of the ensemble time correlation function.

Proceeding:

$$\langle\langle G^*(t)G(t)\rangle\rangle = -\frac{\langle\omega_\perp^{L2}\rangle}{2}\,\mathrm{Re}\left[\frac{t}{\nu+i\omega_\mu} + \frac{e^{-(\nu+i\omega_\mu)t}-1}{(\nu+i\omega_\mu)^2}\right]_{\nu=\nu_\perp}$$

29) $$= -\underbrace{\frac{\langle\omega_\perp^{L2}\rangle}{2}\left[\underbrace{\frac{\nu t}{\nu^2+\omega_\mu^2}}_{\text{Standard perturbat}^n\text{ theory}} + \frac{(\omega_\mu^2-\nu^2)(1-e^{-\nu t}\cos\omega_\mu t) - 2\nu\omega_\mu e^{-\nu t}\sin(\omega_\mu t)}{(\nu^2+\omega_\mu^2)^2}\right]}_{\text{"KEREN" RELAXATION Funct}^n}$$

Journal of Physics: Condensed Matter, 16 (2004)

So, pulling all the results together for times $\nu_\perp t \gg 1$

30) $$\frac{\langle\langle S_z(t)\rangle\rangle}{\langle\langle S_z(0)\rangle\rangle_{LF}} \simeq e^{-\langle\omega_\perp^{L\,2}\rangle \frac{\nu_\perp t}{\nu_\perp^2+\omega_\mu^2}} = e^{-t/T_1}$$

"defines $1/T_1$" $= \langle\omega_\perp^{L\,2}\rangle \dfrac{\nu_\perp}{\nu_\perp^2+\omega_\mu^2}$

& $$\frac{\langle\langle S_x(t)\rangle\rangle}{\langle\langle S_x(0)\rangle\rangle_{TF}} =$$

31) $$\cos(\omega_\mu t)\, e^{-t/2T_1}\, e^{-\langle\omega_z^{L\,2}\rangle\left[t/\nu_z + 1/\nu_z^2\left(e^{-\nu_z t}-1\right)\right]}$$

and also for $\nu_z t \gg 1$

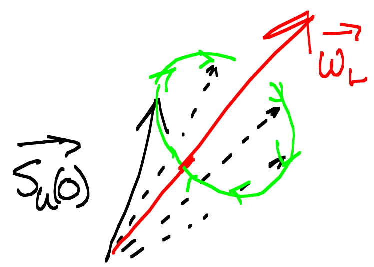
$$\simeq \cos(\omega_\mu t)\, e^{-t/2T_1}\, e^{-t/T_2}\,, \quad \frac{1}{T_2} = \frac{\langle\omega_z^{L\,2}\rangle}{\nu_z}$$

What does $\overline{f(t)\,f(t+\tau)} = e^{-\nu|\tau|}$ imply for a single "time evolution" of the ensemble?

32) ERGODIC PRINCIPLE $\Rightarrow \displaystyle\int_{-\infty}^{\infty} f(t)\,f(t+\tau)\,d\tau = \frac{1}{\nu}$

PART II: KUBO-TOYABE ZERO FIELD POL^{n}

Suppose now the external field is zero & one does not have the "luxury" of $\omega^L << \omega^{EXT}$.



33) Eq^n of motion

$$\frac{d}{dt}\vec{S}^\mu(t) = \vec{S}^\mu(t) \times \vec{\omega}_L(t)$$

$$, \vec{\omega}_L = \gamma_\mu \vec{B}_L(t)$$

Assuming $\vec{S}^\mu(0) = \hat{z}$ and a <u>fixed</u> local field

34) $$P_{\mu z}^{\mu}(t) = \cos\theta + \sin\theta \cos(\omega_L t)$$

where θ is the (invariant) angle between spin and field.

Assume now we have an ensemble which has a random orientation & has a Gaussian distribution along any fixed direction (of the static local field).

Using the isotropic probability distribut^n function:

$$D(\theta,\varphi,\omega_L) = D(\omega_L)\,\omega_L^2 \sin\theta\, d\theta\, d\varphi\, d\omega_L$$

35) Gives $\langle P_z^\mu(t)\rangle = \frac{1}{3} + \frac{2}{3}\int D(\omega_L)\,\omega_L^2 \cos(\omega_L t)\, d\omega_L$

for a Gaussian dist^n $D_G(\omega_L) = \left(\frac{1}{\sqrt{2\pi}\,\omega_G}\right)^3 e^{-\omega_L^2/2\omega_G^2}$

36) $\rightarrow \langle P_{z,G}^\mu(t)\rangle = \frac{1}{3} + \frac{2}{3}(1-\omega_G^2 t^2)\, e^{-\omega_G^2 t^2/2}$

Gaussian K-T function

and for an exponential dist^n $D_E(\omega_L) = \frac{1}{2\nu^3} e^{-\omega_L/\omega_E}$

37) $$\langle P_{z,E}^\mu(t)\rangle = \frac{1}{3} + \frac{2}{3}\,\frac{1-3(t\omega_E)^2}{\left[(t\omega_E)^2+1\right]^3}$$

DYNAMICS VIA STRONG COLLISSION

Focus on occupation of an initial state i) & the probability of a transition to the ensemble averge of the polarizat^n at a time τ. Assuming that the probability of remaing in $|i\rangle$ at t if $|i\rangle$ is occupied at $t=0$ is $e^{-\nu t}$, i.e a site occupancy correlation time of $1/\nu$, then one can write

38) $$\overline{P_i(t)} = \underbrace{P_i^{STAT}(t)}_{\text{static Pol}^n \text{ in } |i\rangle} \cdot \underbrace{e^{-\nu t}}_{\substack{\text{probability to remain in } |i\rangle \\ \text{to time } t \text{ if it started there} \\ \text{at time } 0.}} + \nu \int_0^t \underbrace{e^{-\nu\tau}}_{\substack{\text{probability remain in } |i\rangle \\ \text{only up to } \tau<t \\ \text{or} \\ e^{-\nu\tau}\nu \text{ is the jump rate at } \tau.}} P_i^{STAT}(\tau) \underbrace{\langle\langle P(t-\tau)\rangle\rangle}_{\substack{\text{jumps to ensemble} \\ \text{average at } \tau}} d\tau$$

39) $$\therefore \left\langle \overline{P_i(t)} \right\rangle = \left\langle P_i^{STAT}(t)\right\rangle \cdot e^{-\nu t} + \nu\int_0^t e^{-\nu\tau} \left\langle P_i^{STAT}(\tau)\right\rangle \langle\langle P(t-\tau)\rangle\rangle d\tau$$

But $\left\langle \overline{P_i(t)} \right\rangle = \langle\langle P(t)\rangle\rangle$, $\langle \ \rangle = \frac{1}{N_i}\sum_i$

40) $$\therefore \langle\langle P(t)\rangle\rangle = \left\langle P_i^{STAT}(t)\right\rangle \cdot e^{-\nu t} + \nu\int_0^t e^{-\nu\tau}\left\langle P_i^{STAT}(\tau)\right\rangle \langle\langle P(t-\tau)\rangle\rangle d\tau$$

Self consistent eq^n for the "Strong Collossion MODEL"

41) For those who have been introduced to the Laplace transform, $\mathcal{L}\{P(t)\} \equiv P(s)$

$$40) \rightarrow \quad P(s) = P^{STAT}(s+\nu) + \nu P^{STAT}(s+\nu) P(s)$$

$$\rightarrow P(s) = P^{STAT}(s+\nu) \big/ \left(1 - \nu P^{STAT}(s+\nu)\right)$$

PART III: SPIN-SPIN INTERACTIONS

42) **Zeeman Interaction** (review)

$$\mathcal{H}^i = -\vec{m}^i \cdot \vec{B}_{EXT}(t) \quad \Rightarrow \quad \vec{p}(t) = \vec{p}(t) \times \vec{\omega}(t)$$

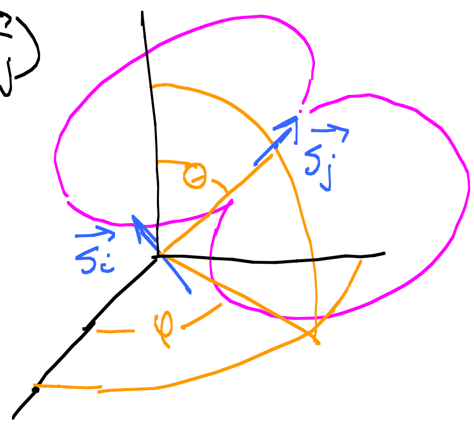
$\vec{p}(t) = \langle \psi(t) | \vec{S} | \psi(t) \rangle \equiv$ polarization, $\quad \vec{\omega}(t) = \vec{B}_{EXT}(t)/\gamma_i$

For a static field along the $\hat{z}$ direction

42a) $$\mathcal{H}_z^i = -\omega_{EXT}^i S_z^i \qquad (\hbar = 1)$$

Dipole-Dipole Interaction

Magnetic Field from $\vec{S}_j(\vec{r}_j)$



43) $$\vec{B}_j(\vec{r}_{ij}) = \frac{3\hat{r}_{ij}(\vec{m}_j \cdot \vec{r}_{ij}) - \vec{m}_j}{r_{ij}^3}$$

, where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ & $\vec{m}_j$ is the magnetic moment of $\vec{S}_j$

$\therefore$ The energy of interaction with the spin i is

$$\mathcal{H}_D = -\vec{m}_i \cdot \vec{B}_j(\vec{r}_{ij}) = \frac{\vec{m}_i \cdot \vec{m}_j - 3(\vec{m}_i \cdot \hat{r}_{ij} \; \vec{m}_j \cdot \hat{r}_{ij})}{r_{ij}^3}$$

The magnetic moment $\vec{m}_j \equiv \gamma_j \hbar \vec{S}_j$,

44) $$\mathcal{H}_D^{ij} = \frac{\gamma_i \gamma_j \hbar^2}{(r_{ij})^3}\left[\vec{S}_i \cdot \vec{S}_j - 3(\vec{S}_i \cdot \hat{r}_{ij})(\vec{S}_j \cdot \hat{r}_{ij})\right]$$

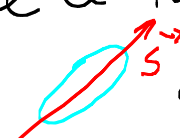
$\gamma_i \equiv$ gyromagnetic ratio

Hyperfine Interaction:

45) $$\mathcal{H}_{HYP} = \sum_i \{ A_i (\vec{S_i} \cdot \vec{S_e}) + D_i [\vec{S_i} \cdot \vec{S_e} - 3(\vec{S_i} \cdot \hat{n}_i)(\vec{S_e} \cdot \hat{n}_i)] \}$$

$\hat{n}_i$ is a principle axis of the Hyperfine Field created throug the contact interaction between a bound unpaired electron and a nucleus or muon. A is the isotropic part, & D the dipolar part.

Quadrupolar Interaction: (not a spin-spin interaction)

Nuclei with spin $> \frac{1}{2}$ have "nuclear shape" which in an electric field gradient have a potential energy & experience a torque. Since the shape of nuclei 

are related to the spin direction $\vec{S}$ (Wigner-Eckart Thm)

46) $$\mathcal{H}_Q^j = \frac{e^2 q Q_j}{4S^j(2S^j-1)} \left[(3 S_z^{j\,2} - S^{j2}) + \frac{1}{2}\eta (S_x^{j2} - S_y^{j2}) \right]$$

$eq = V_{zz}$, $\eta = (V_{xx} - V_{yy})/V_{zz}$

$V_{\alpha\alpha} \equiv$ electric field gradient principal values, $Q_j \equiv$ Quadrupole moment of nucleus

Interaction of Two $S=\frac{1}{2}$ "SPINS"

I) An initially polarized μ

+ II) an initially unpolarized Pseudo spin.

The μ & p spins have operators $\vec{S}^{\mu}$ & $\vec{S}^{p}$

47) $\vec{S} = \frac{1}{2}\vec{\sigma} = \sum_i \frac{1}{2}\sigma^i \hat{n}^i$ $\sigma^i \equiv$ Pauli spin ½ operators

48) $\sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, $\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

The generalized time independent interaction between these spins can be written:

49) $$\mathcal{H}^{2spin} = \vec{\omega}_{\mu}\cdot\vec{S}^{\mu} + \vec{\omega}_p\cdot\vec{S}^{p} + \vec{S}^{\mu}\cdot\overset{\Rightarrow}{I}\cdot\vec{S}^{p}$$

$\vec{S}^{\mu}\cdot\overset{\Rightarrow}{I}\cdot\vec{S}^{p}$ is a Hermetian, traceless 4x4 matrix since the state space is spanned by $|\psi\rangle = \alpha_{ij}|i\rangle_{\mu}|j\rangle_p$, with $|i\rangle_{\mu}$ & $|i\rangle_p$ eigenstates of $\vec{\omega}_{\mu}\cdot\vec{S}^{\mu}$ & $\vec{\omega}_p\cdot\vec{S}^{p}$ respectively (or $\hat{z}$ when the $\vec{\omega}\equiv 0$). For this example we assume that I is a isotropic scalar A.

50) i.e. $\mathcal{H}^{2spin}_{\mu p} = \vec{\omega}_\mu \cdot \vec{S}^\mu + \vec{\omega}_p \cdot \vec{S}^p + A\, \vec{S}^\mu \cdot \vec{S}^p$

Recall that $\vec{S}^\mu \cdot \vec{S}^p$ may be written as

51) $\vec{S}^\mu \cdot \vec{S}^p = S^\mu_z S^p_z + \frac{1}{2}\left(S^\mu_+ S^p_- + S^\mu_- S^p_+\right)$, $S_\pm = S_x \pm i S_y$

and the matrix representation of the Hamiltonian is, $|\uparrow\uparrow\rangle = |\uparrow_\mu \uparrow_p\rangle$ etc

52) $$\mathcal{H}^{2spin}_{\mu p} = \begin{array}{c|cccc} & |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ \hline \langle\uparrow\uparrow| & \frac{1}{2}(\omega_\mu+\omega_p)+\frac{1}{4}A & & & \\ \langle\uparrow\downarrow| & & \frac{1}{2}(\omega_\mu-\omega_p)-\frac{1}{4}A & \frac{1}{2}A & \\ \langle\downarrow\uparrow| & & \frac{1}{2}A & -\frac{1}{2}(\omega_\mu-\omega_p)-\frac{1}{4}A & \\ \langle\downarrow\downarrow| & & & & -\frac{1}{2}(\omega_\mu+\omega_p)+\frac{1}{4}A \end{array}$$

$= \mathcal{H}^{2\times 2}$

It is clear the $|\uparrow\uparrow\rangle$ & $|\downarrow\downarrow\rangle$ are eigenstates & the two states $|\uparrow\downarrow\rangle$ & $|\downarrow\uparrow\rangle$ with $\langle |S_z| \rangle = \langle |S^\mu_z + S^p_z| \rangle = 0$ interact through the "flip-flop" term.

The time evolution operator $e^{-i\mathcal{H}t}$ can be written as

53) $$e^{-i\mathcal{H}t} = |\uparrow\uparrow\rangle\langle\uparrow\uparrow|\, e^{-i\left(\frac{1}{2}(\omega_\mu+\omega_p)+\frac{1}{4}A\right)t} + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\, e^{i\left(\frac{1}{2}(\omega_\mu+\omega_p)-\frac{1}{4}A\right)t} + \left[|\uparrow\downarrow\rangle \;\; |\downarrow\uparrow\rangle\right] e^{-i\mathcal{H}^{2\times2}t} \begin{bmatrix} \langle\uparrow\downarrow| \\ \langle\downarrow\uparrow| \end{bmatrix}$$

"outer" product of $|ket\rangle\langle bra|$ containing $|\uparrow\downarrow\rangle\langle\uparrow\downarrow|$, $|\uparrow\downarrow\rangle\langle\downarrow\uparrow|$ etc

54) Defining $\omega_{eff} = \left|\sqrt{(\omega_\mu-\omega_p)^2+A^2}\right|$, $\sin\varphi = A/\omega_{eff}$, $\cos\varphi = \dfrac{\omega_\mu-\omega_p}{\omega_{eff}}$

(similar to identity of eq^n 4) show (via series expansion, or otherwise; $\partial^2/\partial t^2$), that

46) $$e^{-i\mathcal{H}^{2\times2}t} = e^{i\frac{A}{4}t}\left\{\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\cos\left(\frac{\omega_{eff}}{2}t\right) - i\begin{bmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{bmatrix}\sin\left(\frac{\omega_{eff}}{2}t\right)\right\}$$

This expansion of $e^{i\mathcal{H}^{2\times2}}$ is essentially a diagonalizat^n of the matrix. The eigenvalues are $\pm\,\omega_{eff}$, with corresponding eigenvectors

47) $\cos(\varphi/2)\langle\uparrow\downarrow| + \sin(\varphi/2)|\downarrow\uparrow\rangle$ & $-\sin(\varphi/2)\langle\uparrow\downarrow| + \cos(\varphi/2)\langle\downarrow\uparrow|$

Prove the above statement!

With $e^{-i\mathcal{H}t}$ now expressed in a convenient closed form we can calculate

$$Pol_z^{\mu}(t) = \langle \psi(t) | S_z^{\mu} | \psi(t) \rangle \Big/ \langle \psi(0) | S_z^{\mu} | \psi(0) \rangle$$

55) $$\& \; Pol_z^{p}(t) = \langle \psi(t) | S_z^{p} | \psi(t) \rangle \Big/ \langle \psi(0) | S_z^{\mu} | \psi(0) \rangle$$

Before doing this, there is the question of what is $|\psi(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}^{\mu} \begin{bmatrix} ? \\ ? \end{bmatrix}^{p}$, since we want the "p" spins to be unpolarized. Well in the formulation of 48) the best one can do is to assume the initial polarizt^{n} of the "p" spins is random ensemble average of $\psi^p(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}^{p}$ & $\begin{bmatrix} 0 \\ 1 \end{bmatrix}^{p}$, since $\psi^p(0)$ "must" have some initial state. However if one writes

56) $$\begin{aligned} \langle \psi(t) | S_z^{\mu} | \psi(t) \rangle &= \langle \psi^{\mu}(0) | e^{i\mathcal{H}t} S_z^{\mu} e^{-i\mathcal{H}t} | \psi^{\mu}(0) \rangle \\ &= Tr\left\{ e^{i\mathcal{H}t} S_z^{\mu} e^{-i\mathcal{H}t} |\psi^{\mu}(0)\rangle\langle\psi^{\mu}(0)| \right\} \\ &= Tr_{\text{"p"}} \langle \psi^{\mu}(0) | e^{i\mathcal{H}t} S_z^{\mu} e^{-i\mathcal{H}t} | \psi^{\mu}(0) \rangle \\ &= \langle \psi^{\mu}(0) | Tr_{\text{"p"}} \left\{ e^{i\mathcal{H}t} S_z^{\mu} e^{-i\mathcal{H}t} \right\} | \psi^{\mu}(0) \rangle \end{aligned}$$

57) $$\& \; \langle \psi(t) | S_z^{p}(t) | \psi(t) \rangle = \langle \psi^{\mu}(0) | Tr_{\text{"p"}} \left\{ e^{i\mathcal{H}t} S_z^{p} e^{-i\mathcal{H}t} \right\} | \psi^{\mu}(0) \rangle$$

Taking the $\mathrm{Tr}_{\text{"p"}}\{\ \}$ in 49) & 50) corresponds to projecting out the observed muon polarization from an eigenvector basis set ~~that~~ contains spins which are not observed.

Exercise for the students.

58 Prove $\mathrm{Tr}_{\text{"p"}}\left\{e^{i\mathcal{H}t} S_z^{\mu} e^{-i\mathcal{H}t}\right\} / \mathrm{Tr}_{\text{"p"}} \equiv S_z^{\mu}(t)$

58a) $= \frac{1}{2}\left(1+\cos^2\varphi + \sin^2\varphi \cos(\omega_{eff}\, t)\right) S_z^{\mu}$

58b) & $S_z^{p}(t) = \mathrm{Tr}_{\text{"p"}}\left\{e^{i\mathcal{H}t} S_z^{p} e^{-i\mathcal{H}t}\right\} / \mathrm{Tr}_{\text{"p"}} = S_z^{\mu} - S_z^{\mu}(t)$

58 a), b) $\Rightarrow$ when $\omega_\mu = \omega_p$, $\varphi = \pi/2$ & ½ the polarization oscillates at ω_{eff}. In this case $S_z^p(t)$ obtains the "lost" polarizat^n even though the "p" system was initially unpolarized. The μ & p systems have an equal energy splitting and the interaction term A serves to transfer energy

(which is conserved) back & forth between the systems. The fraction of polarization ~~that~~ is active is (in this 2 spin 1/2 model)

59) $$\frac{1}{2}\sin^2\varphi = \frac{1}{2}\frac{A^2}{(\omega_\mu-\omega_p)^2+A^2}$$

60) & the frequency is $w_{eff} = \left|\sqrt{(\omega_\mu-\omega_p)^2+A^2}\right|$

$\int\mu SR$ = Integral μSR

In an $\int\mu SR$ experiment one integrates the entire muon asymmetry as the beam continuosly enters the spectrometer.

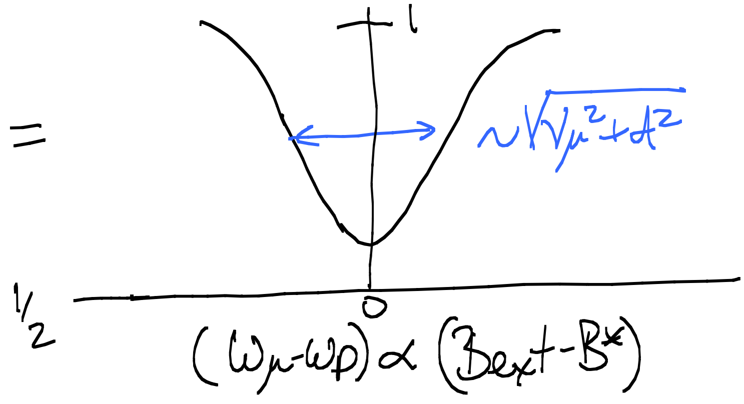
The instantaneous total detector rate for the forward (F) & backward (B) directions are

$$N_{F/B} = N^0_{F/B}\int_{-\infty}^{t}\gamma_\mu e^{-\gamma_\mu(t-\tau)}\left(1\mp A_{F/B}P(t-\tau)\right)d\tau, \quad \gamma_\mu = 1/2.2\mu s$$

Calculating $(N_F-N_B)/(N_F+N_B)$ using 51a) with $N_F^0 = N_B^0$ & $A_F = A_B$ (not realistic!)

61) gives: $$\frac{N_B-N_F}{N_B+N_F} = 1-\frac{1}{2}\frac{A^2}{\gamma_\mu^2+w_{eff}^2}$$

62) $$\frac{N_B - N_F}{N_B + N_F} =$$



An example for a liquid phase muonium radical coupled to a nucleus. Consider

63) $$\mathcal{H}_{HYP} = \omega_\mu S_z^\mu - \omega_e S_z^e + \omega_n S_z^N + A_\mu(\vec{S}^e \cdot \vec{S}^\mu) + A_N(\vec{S}^e \cdot \vec{S}^N)$$

Assume $\omega_e \gg \omega_\mu, \omega_N \quad \because \gamma_e \simeq 200\gamma_\mu \simeq 630\gamma_p$

64) & breakup
$$\left.\begin{aligned} \mathcal{H}_{HYP} = &-\omega_\mu S_z^\mu + \omega_e S_z^e - \omega_n S_z^N \\ &+ \tfrac{1}{2}|\uparrow^e\rangle\langle\uparrow^e|\left[A_\mu S_z^\mu + A_N S_z^N\right] \\ &- \tfrac{1}{2}|\downarrow^e\rangle\langle\downarrow^e|\left[A_\mu S_z^\mu + A_N S_z^N\right] \end{aligned}\right\} \mathcal{H}_0$$
$$\left.\begin{aligned} &+ \tfrac{1}{2} S_+^e\left(A_\mu S_-^\mu + A_N S_-^N\right) \\ &+ \tfrac{1}{2} S_-^e\left(A_\mu S_+^\mu + A_N S_+^N\right) \end{aligned}\right\} \mathcal{H}_1 \ll \mathcal{H}_0$$

It can be shown that in this limit one can reformulate the Hamiltonian as

65) $\mathcal{H}_{HYP} \equiv \mathcal{H}^{\uparrow} |\uparrow_e\rangle\langle\uparrow_e| + \mathcal{H}^{\downarrow} |\downarrow_e\rangle\langle\downarrow_e| = \mathcal{H}_{EF}$ (EF = Effective FIELD)

Hint: Find a unitary transformation $e^{-O} \ni e^{-O} \mathcal{H}_{HYP} e^{O} = \mathcal{H}_{EF}$

66a) $$\mathcal{H}_{EF} = |\uparrow_e\rangle\langle\uparrow_e| \Big\{ (\tfrac{1}{2}A_\mu - \omega_\mu) S_z^\mu + (\tfrac{1}{2}A_N - \omega_N) S_z^N + \omega_e \tfrac{1}{2} + \frac{1}{\omega_e 4}\Big[(A_\mu S_-^\mu + A_N S_-^N)(A_\mu^\mu S_+ + A_N S_+^N) \Big] \Big\}$$

66b) $$+ |\downarrow_e\rangle\langle\downarrow_e| \Big\{ (-\tfrac{1}{2}A_\mu - \omega_\mu) S_z^\mu - (\tfrac{1}{2}A_N + \omega_N) S_z^N - \omega_e \tfrac{1}{2} - \frac{1}{\omega_e}\Big[(A_\mu S_-^\mu + A_N S_-^N)(A_\mu^\mu S_+ + A_N S_+^N) \Big] \Big\}$$

In the $|\uparrow_e\rangle\langle\uparrow_e|$ manifold we see ~~that~~ the single particle Zeeman terms can become equal when $\tfrac{1}{2}A_\mu - \omega_\mu = \tfrac{1}{2}A_N - \omega_N$ & then the flip flop part $\frac{A_\mu A_N}{\omega_e}(S_+^\mu S_-^N + S_-^\mu S_+^N)$ will transfer polarization between $|\uparrow_e\rangle\langle\uparrow_e| S_z^\mu$ & $|\uparrow_e\rangle\langle\uparrow_e| S_z^n$

The analogy between eq$^{\underline{n}}$ 50) & eq^n 66a) lets us associate
$$\omega_\mu \longrightarrow \tfrac{1}{2}A_\mu - \omega_\mu$$
$$\omega_N \longrightarrow \tfrac{1}{2}A_N - \omega_N$$
$$A \longrightarrow A_\mu A_N / 2\omega_e$$

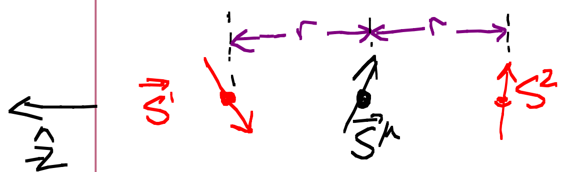
67) The "Level Crossing Resonance" will occur when $\frac{1}{2}A_\mu - \omega_\mu = \frac{1}{2}A_N - \omega_n$

and the shape of the $\int \mu SR$ line will be

68) $$\frac{N_B - N_F}{N_B + N_F} = 1 - \frac{1}{4}\,\frac{(A_\mu A_N/2\omega_e)^2}{\nu_\mu^2 + (\omega_\mu - \omega_n - \frac{1}{2}A_\mu - A_N)^2 + \left(\frac{A_\mu A_N}{2\omega_e}\right)^2}$$

factor of 1/4 occurs because 1/2 of 1/2 of the polarizat^n is active in the $|\uparrow^e\rangle\langle\uparrow^e|$ manifold.

The F-μ-F System:



Consider 3 collinear spin ½, with the $\vec{S}_\mu$ in the center. There is no external field & the spins are coupled via dipolar interactions to the muon.

$$\mathcal{H}^{F\mu F} = \omega_D \left[\vec{S}_\mu \cdot (\vec{S}_1 + \vec{S}_2) - 3 S^\mu_z (S^1_z + S^2_z) \right] \quad , \quad \omega_D = \frac{\gamma_\mu \gamma_F \hbar^2}{r^3}$$

$$= \omega_D \left[-2 S^\mu_z (S^1_z + S^2_z) + \frac{1}{2}\left(S^\mu_+ (S^1_- + S^2_-) + S^\mu_- (S^1_+ + S^2_+) \right) \right]$$

Note ~~that total~~ $S_z = S^\mu_z + S^1_z + S^2_z$ is conserved

$\mathcal{H}/\omega_D$	$\vert\uparrow\uparrow\uparrow\rangle$	$\vert\uparrow\rangle\frac{1}{\sqrt2}\vert\uparrow\downarrow-\downarrow\uparrow\rangle$	$\vert\uparrow\rangle\frac{1}{\sqrt2}\vert\uparrow\downarrow+\downarrow\uparrow\rangle$	$\vert\downarrow\rangle\vert\uparrow\uparrow\rangle$	$\vert\downarrow\rangle\frac{1}{\sqrt2}\vert\downarrow\uparrow+\uparrow\downarrow\rangle$	$\vert\uparrow\rangle\vert\downarrow\downarrow\rangle$	$\vert\downarrow\rangle\frac{1}{\sqrt2}\vert\uparrow\downarrow-\downarrow\uparrow\rangle$	$\vert\downarrow\downarrow\downarrow\rangle$
$\langle\uparrow\uparrow\uparrow\vert$	-1							
$\langle\uparrow\vert\frac{1}{\sqrt2}\langle\uparrow\downarrow-\downarrow\uparrow\vert$		0						
$\langle\uparrow\vert\frac{1}{\sqrt2}\langle\uparrow\downarrow+\downarrow\uparrow\vert$			0	$1/\sqrt2$				
$\langle\downarrow\uparrow\uparrow\vert$			$1/\sqrt2$	1				
$\langle\downarrow\vert\frac{1}{\sqrt2}\langle\downarrow\uparrow+\uparrow\downarrow\vert$					0	$1/\sqrt2$		
$\langle\uparrow\downarrow\downarrow\vert$					$1/\sqrt2$	1		
$\langle\downarrow\vert\frac{1}{\sqrt2}\langle\uparrow\downarrow-\downarrow\uparrow\vert$							0	
$\langle\downarrow\downarrow\downarrow\vert$								-1

STUDENT EXCERCISE:

i) From the techniques & 2×2 matrix "tricks" you have been introduced to in this document, diagonalize $\mathcal{H}^{F\mu F}$ and calculate $P_z^{\mu}(t)$; $|\psi(0)\rangle = |\uparrow\rangle^{\mu}$

ii) Do the same for $P_x^{\mu}(t)$; $|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle^{\mu} + |\downarrow\rangle^{\mu}\right)$

iii) Since the angle between the FμF bond & the initial direction of μ polarization is random, use i) & ii) to calculate the "powder average" of the μ polarization.

The answer should be

$$\langle P_z^{F\mu F}(t)\rangle = \frac{1}{2} + \frac{1}{6}\left[\cos\sqrt{3}\,\omega_D t + \left(1-\frac{1}{\sqrt{3}}\right)\cos\left(\frac{3-\sqrt{3}}{2}\right)\omega_D t + \left(1+\frac{1}{\sqrt{3}}\right)\cos\left(\frac{3+\sqrt{3}}{2}\right)\omega_D t\right]$$

THE END!