# Xe129 - Rb87 Spin Exchange Optical Pumping dynamics

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## 1 Bloch equations

The Block equation for the Xe spin are

$$\frac{d\mathbf{K}}{dt} = -\left[\gamma_{Xe}\left(\mathbf{B}_0 + \mathbf{B}_d\cos\left(\omega_{rf}t\right)\right) + b_{KS}\mathbf{S}\right]\times\mathbf{K} + \Gamma_{se}\left(\mathbf{S}-\mathbf{K}\right) - \Gamma_2\hat{x}\left(\hat{x}\cdot\mathbf{K}\right) - \Gamma_2\hat{y}\left(\hat{y}\cdot\mathbf{K}\right) - \Gamma_1\hat{z}\left(\hat{z}\cdot\mathbf{K}\right) \tag{1}$$

Let us assume that $b_{KS}\mathbf{S}$ is part of the DC field $\mathbf{B}_0 = B_0\hat{z}$, that $\Gamma_{se}\left(\mathbf{S}-\mathbf{K}\right) = \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix}$ and that the drive is

$$\mathbf{B}_d\cos\left(\omega_{rf}t\right) = B_d\cos\left(\omega_{rf}t\right)\hat{x}$$

.

Thus, we end up with the next Bloch equation

$$\begin{aligned}
\frac{d\mathbf{K}}{dt} &= -\left[\gamma_{Xe}\left(B_0\hat{z} + B_d\cos\left(\omega_{rf}t\right)\hat{x}\right)\right]\times\mathbf{K} + R_{se}\hat{z} - \Gamma_2\hat{x}\left(\hat{x}\cdot\mathbf{K}\right) - \Gamma_2\hat{y}\left(\hat{y}\cdot\mathbf{K}\right) - \Gamma_1\hat{z}\left(\hat{z}\cdot\mathbf{K}\right) && (2)\\
&= -\gamma_{Xe}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ B_d\cos\left(\omega_{rf}t\right) & 0 & B_0 \\ K_x & K_y & K_z \end{vmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} - \begin{pmatrix} \Gamma_2 & 0 & 0 \\ 0 & \Gamma_2 & 0 \\ 0 & 0 & \Gamma_1 \end{pmatrix}\cdot\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} && (3)\\
&= -\gamma_{Xe}\begin{pmatrix} -B_0K_y \\ B_0K_x - B_d\cos\left(\omega_{rf}t\right)K_z \\ B_d\cos\left(\omega_{rf}t\right)K_y \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} - \begin{pmatrix} \Gamma_2 & 0 & 0 \\ 0 & \Gamma_2 & 0 \\ 0 & 0 & \Gamma_1 \end{pmatrix}\cdot\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} && (4)\\
&= \begin{pmatrix} -\Gamma_2 & \gamma_{Xe}B_0 & 0 \\ -\gamma_{Xe}B_0 & -\Gamma_2 & \gamma_{Xe}B_d\cos\left(\omega_{rf}t\right) \\ 0 & -\gamma_{Xe}B_d\cos\left(\omega_{rf}t\right) & -\Gamma_1 \end{pmatrix}\cdot\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} && (5)\\
&= \begin{pmatrix} -\Gamma_2 & \omega_0 & 0 \\ -\omega_0 & -\Gamma_2 & \Omega_d\cos\left(\omega_{rf}t\right) \\ 0 & -\Omega_d\cos\left(\omega_{rf}t\right) & -\Gamma_1 \end{pmatrix}\cdot\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} && (6)
\end{aligned}$$

Finally, the Xe NMR dynamics can be described by the next Bloch equations

$$\begin{pmatrix} \dot{K}_x \\ \dot{K}_y \\ \dot{K}_z \end{pmatrix} = \begin{pmatrix} -\Gamma_2 & \omega_0 & 0 \\ -\omega_0 & -\Gamma_2 & \Omega_d\cos\left(\omega_{rf}t\right) \\ 0 & -\Omega_d\cos\left(\omega_{rf}t\right) & -\Gamma_1 \end{pmatrix}\cdot\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{7}$$

Now, let us move to the rotating frame (frame of Xe) using the next transformation

$$\begin{aligned}
\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} &= \begin{pmatrix} \cos(\omega_0t) & -\sin(\omega_0t) & 0 \\ \sin(\omega_0t) & \cos(\omega_0t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} && (8)\\
\begin{pmatrix} K_x \\ K_y \\ K_z \end{pmatrix} &= \begin{pmatrix} \cos(\omega_0t) & \sin(\omega_0t) & 0 \\ -\sin(\omega_0t) & \cos(\omega_0t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} && (9)
\end{aligned}$$

Also, the derivative with respect to time of the transformation is

$$\begin{pmatrix} \dot{K}_x \\ \dot{K}_y \\ \dot{K}_z \end{pmatrix} = \frac{d}{dt}\left[\begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix}\right] \tag{10}$$

$$= \frac{d}{dt}\begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\frac{d}{dt}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} \tag{11}$$

$$= \omega_0\begin{pmatrix} -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ -\cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\frac{d}{dt}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} \tag{12}$$

The Bloch equations transform as follows

$$\omega_0\begin{pmatrix} -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ -\cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\frac{d}{dt}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \tag{13}$$

$$\begin{pmatrix} -\Gamma_2 & \omega_0 & 0 \\ -\omega_0 & -\Gamma_2 & \Omega_d\cos(\omega_{rf} t) \\ 0 & -\Omega_d\cos(\omega_{rf} t) & -\Gamma_1 \end{pmatrix}\cdot\begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{14}$$

$$\omega_0\begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ \sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ -\cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \frac{d}{dt}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \tag{15}$$

$$\begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ \sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -\Gamma_2 & \omega_0 & 0 \\ -\omega_0 & -\Gamma_2 & \Omega_d\cos(\omega_{rf} t) \\ 0 & -\Omega_d\cos(\omega_{rf} t) & -\Gamma_1 \end{pmatrix}\begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{16}$$

Let us compute it separately term by term

$$\omega_0\begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ \sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ -\cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \omega_0\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} \tag{17}$$

$$= \omega_0\begin{pmatrix} \tilde{K}_y \\ -\tilde{K}_x \\ 0 \end{pmatrix} \tag{18}$$

Also,

$$\begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ \sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -\Gamma_2 & \omega_0 & 0 \\ -\omega_0 & -\Gamma_2 & \Omega_d \cos(\omega_{rf} t) \\ 0 & -\Omega_d \cos(\omega_{rf} t) & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix} = \tag{19}$$

$$\begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) & 0 \\ \sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -\Gamma_2 \cos(\omega_0 t) - \omega_0 \sin(\omega_0 t) & -\Gamma_2 \sin(\omega_0 t) + \omega_0 \cos(\omega_0 t) & 0 \\ -\omega_0 \cos(\omega_0 t) + \Gamma_2 \sin(\omega_0 t) & -\omega_0 \sin(\omega_0 t) - \Gamma_2 \cos(\omega_0 t) & \Omega_d \cos(\omega_{rf} t) \\ \Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) & -\Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) & -\Gamma_1 \end{pmatrix} = \tag{20}$$

$$\begin{pmatrix} -\Gamma_2 & \omega_0 & -\Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) \\ -\omega_0 & -\Gamma_2 & \Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) \\ \Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) & -\Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) & -\Gamma_1 \end{pmatrix} \tag{21}$$

combining the terms together we get

$$\omega_0 \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \frac{d}{dt} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \tag{22}$$

$$\begin{pmatrix} -\Gamma_2 & \omega_0 & -\Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) \\ -\omega_0 & -\Gamma_2 & \Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) \\ \Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) & -\Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{23}$$

$$\frac{d}{dt} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \tag{24}$$

$$\begin{pmatrix} -\Gamma_2 & \omega_0 & -\Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) \\ -\omega_0 & -\Gamma_2 & \Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) \\ \Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) & -\Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 & -\omega_0 & 0 \\ \omega_0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} \tag{25}$$

$$+ \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{26}$$

so finally

$$\frac{d}{dt} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \begin{pmatrix} -\Gamma_2 & 0 & -\Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) \\ 0 & -\Gamma_2 & \Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) \\ \Omega_d \cos(\omega_{rf} t) \sin(\omega_0 t) & -\Omega_d \cos(\omega_{rf} t) \cos(\omega_0 t) & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{27}$$

$$\tag{28}$$

Notice that in the case where we transfer to a different rotating frame of reference which rotates at some frequency $\omega_1$, then the Bloch equations would be a bit different after the transformation

$$\frac{d}{dt} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \begin{pmatrix} -\Gamma_2 & \omega_0 - \omega_1 & -\Omega_d \cos(\omega_{rf} t) \sin(\omega_1 t) \\ -(\omega_0 - \omega_1) & -\Gamma_2 & \Omega_d \cos(\omega_{rf} t) \cos(\omega_1 t) \\ \Omega_d \cos(\omega_{rf} t) \sin(\omega_1 t) & -\Omega_d \cos(\omega_{rf} t) \cos(\omega_1 t) & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{29}$$

$$\tag{30}$$

Using trigonometric identities we can simplify the drive terms in the Bloch matrix

$$\Omega_d \cos(\omega_{rf} t) \sin(\omega_1 t) = \frac{\Omega_d}{2} \left( \sin((\omega_{rf} + \omega_1) t) + \sin((\omega_{rf} - \omega_1) t) \right) \tag{31}$$
$$\Omega_d \cos(\omega_{rf} t) \cos(\omega_1 t) = \frac{\Omega_d}{2} \left( \cos((\omega_{rf} - \omega_1) t) + \cos((\omega_{rf} + \omega_1) t) \right) \tag{32}$$
$$\tag{33}$$

assuming that $\omega_{rf} - \omega_1 \ll 1$, then we can use the RWA which states that fast oscillations average out to zero

$$\Omega_d \cos(\omega_{rf} t) \sin(\omega_1 t) = \frac{\Omega_d}{2} \sin(2\omega_{rf} t) = 0 \tag{34}$$
$$\Omega_d \cos(\omega_{rf} t) \cos(\omega_1 t) = \frac{\Omega_d}{2} \left(1 + \cos(2\omega_{rf} t)\right) = \frac{\Omega_d}{2} \tag{35}$$
$$\tag{36}$$

Then, the Bloch equations with the RWA are

$$\frac{d}{dt} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \begin{pmatrix} -\Gamma_2 & \omega_0 - \omega_{rf} & 0 \\ -(\omega_0 - \omega_{rf}) & -\Gamma_2 & \frac{\Omega_d}{2} \\ 0 & -\frac{\Omega_d}{2} & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{37}$$

Next, we add to our model The effective magnetic field the Xe particles fill which produced by the alkali atoms, $b_{KS}\mathbf{S} = b_{KS} S_z \hat{z}$ and also some world rotation $\omega_{\mathbf{r}} = \omega_r \hat{z}$.

The modified equations are

$$\boxed{\frac{d}{dt} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \begin{pmatrix} -\Gamma_2 & M_{12} & 0 \\ M_{21} & -\Gamma_2 & \frac{\Omega_d}{2} \\ 0 & -\frac{\Omega_d}{2} & -\Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix}} \tag{38}$$

where $M_{21} = -M_{12}$ and

$$M_{12} = \omega_0 + \gamma_{Xe} b_{KS} S_z + \omega_r - \omega_{rf} \tag{39}$$
$$= \gamma_{Xe} B_0 + \gamma_{Xe} b_{KS} S_z + \omega_r - \omega_{rf} \tag{40}$$
$$\tag{41}$$

Next, let us find the steady state solution of the Bloch equations in the rotating frame with drive in $\hat{x}$ with the RWA

$$\begin{pmatrix} \Gamma_2 & -M_{12} & 0 \\ M_{12} & \Gamma_2 & -\frac{\Omega_d}{2} \\ 0 & \frac{\Omega_d}{2} & \Gamma_1 \end{pmatrix} \begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{42}$$

$$\begin{pmatrix} \Gamma_2 \tilde{K}_x - M_{12} \tilde{K}_y \\ M_{12} \tilde{K}_x + \Gamma_2 \tilde{K}_y - \frac{\Omega_d}{2} \tilde{K}_z \\ \frac{\Omega_d}{2} \tilde{K}_y + \Gamma_1 \tilde{K}_z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ R_{se} \end{pmatrix} \tag{43}$$

$$\tilde{K}_x = \frac{M_{12}}{\Gamma_2} \tilde{K}_y \tag{44}$$
$$\tag{45}$$

$$\begin{pmatrix} \frac{M_{12}^2+\Gamma_2^2}{\Gamma_2}\tilde{K}_y - \frac{\Omega_d}{2}\tilde{K}_z \\ \frac{\Omega_d}{2}\tilde{K}_y + \Gamma_1\tilde{K}_z \end{pmatrix} = \begin{pmatrix} 0 \\ R_{se} \end{pmatrix} \tag{46}$$

$$\begin{pmatrix} \left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2\tilde{K}_y - \frac{\Omega_d}{2}\tilde{K}_z \\ \frac{\Omega_d}{2}\tilde{K}_y + \Gamma_1\tilde{K}_z \end{pmatrix} = \begin{pmatrix} 0 \\ R_{se} \end{pmatrix} \tag{47}$$

$$\left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2\tilde{K}_y = \frac{\Omega_d}{2}\tilde{K}_z \tag{48}$$

$$\tilde{K}_y = \frac{\frac{\Omega_d}{2}}{\left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2}\tilde{K}_z \tag{49}$$

$$\tag{50}$$

$$\frac{\Omega_d}{2}\tilde{K}_y + \Gamma_1\tilde{K}_z = R_{se} \tag{51}$$

$$\frac{\Omega_d}{2}\frac{\frac{\Omega_d}{2}}{\left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2}\tilde{K}_z + \Gamma_1\tilde{K}_z = R_{se} \tag{52}$$

$$\frac{\frac{\Omega_d^2}{4} + \left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2\Gamma_1}{\left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2}\tilde{K}_z = R_{se} \tag{53}$$

$$\frac{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1} + \left(1+(M_{12}/\Gamma_2)^2\right)}{\left(1+(M_{12}/\Gamma_2)^2\right)/\Gamma_1}\tilde{K}_z = R_{se} \tag{54}$$

$$\tilde{K}_z = \frac{R_{se}}{\Gamma_1}\frac{\left(1+(M_{12}/\Gamma_2)^2\right)}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1} + \left(1+(M_{12}/\Gamma_2)^2\right)} \tag{55}$$

$$\tilde{K}_y = \frac{\Omega_d}{2\Gamma_2}\frac{R_{se}}{\Gamma_1}\frac{1}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1} + \left(1+(M_{12}/\Gamma_2)^2\right)} \tag{56}$$

$$\tilde{K}_x = \frac{M_{12}}{\Gamma_2}\frac{\Omega_d}{2\Gamma_2}\frac{R_{se}}{\Gamma_1}\frac{1}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1} + \left(1+(M_{12}/\Gamma_2)^2\right)} \tag{57}$$

Finally, the solution to the Bloch equation (eq.(38)) is

$$\boxed{\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \frac{\frac{R_{se}}{\Gamma_1}}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1} + \left(1+(M_{12}/\Gamma_2)^2\right)}\begin{pmatrix} \frac{M_{12}}{\Gamma_2}\frac{\Omega_d}{2\Gamma_2} \\ \frac{\Omega_d}{2\Gamma_2} \\ \left(1+(M_{12}/\Gamma_2)^2\right) \end{pmatrix}} \tag{58}$$

In the case where $M_{12} = 0$ we get

$$\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \frac{\frac{R_{se}}{\Gamma_1}}{1+\frac{\Omega_d^2}{4\Gamma_2\Gamma_1}}\begin{pmatrix} 0 \\ \frac{\Omega_d}{2\Gamma_2} \\ 1 \end{pmatrix} \tag{59}$$

Recall that we measure the transverse spin polarization. Let us compute the optimal drive amplitude for maximal $\tilde{K}_y$ polarization

$$\frac{d\tilde{K}_y}{d\Omega_d} = \frac{R_{se}}{2\Gamma_2\Gamma_1}\frac{1}{1+\frac{\Omega_d^2}{4\Gamma_2\Gamma_1}} - \frac{R_{se}}{2\Gamma_2\Gamma_1}\frac{\Omega_d^2}{\Gamma_2\Gamma_1}\frac{1}{\left(1+\frac{\Omega_d^2}{4\Gamma_2\Gamma_1}\right)^2} = 0 \tag{60}$$

we get the next optimal drive amplitude

$$\Omega_d^{\text{optimal}} = \sqrt{\frac{4\Gamma_2\Gamma_1}{3}}$$

for the optimal drive, the $\hat{z}$ polarization would be

$$\tilde{K}_z = \frac{3R_{se}}{4\Gamma_1}$$

We can make the same calculation in the case where $M_{12} \neq 0$

$$\frac{d\tilde{K}_y}{d\Omega_d} = \frac{R_{se}}{2\Gamma_2\Gamma_1}\frac{1}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1}+\left(1+(M_{12}/\Gamma_2)^2\right)} - \frac{R_{se}}{2\Gamma_2\Gamma_1}\frac{\Omega_d^2}{\Gamma_2\Gamma_1}\frac{1}{\left(\frac{\Omega_d^2}{4\Gamma_2\Gamma_1}+\left(1+(M_{12}/\Gamma_2)^2\right)\right)^2} = 0 \tag{61}$$

in that case the optimal drive amplitude is

$$\Omega_d^{\text{optimal}} = \sqrt{\frac{4\Gamma_2\Gamma_1}{3}}\sqrt{1+(M_{12}/\Gamma_2)^2} \tag{62}$$

Just for sports we can also solve the case of drive in $\hat{y}$, the Bloch equations in that case are

$$\boxed{\frac{d}{dt}\begin{pmatrix}\tilde{K}_x\\ \tilde{K}_y\\ \tilde{K}_z\end{pmatrix} = \begin{pmatrix}-\Gamma_2 & M_{12} & -\frac{\Omega_d}{2}\\ M_{21} & -\Gamma_2 & 0\\ \frac{\Omega_d}{2} & 0 & -\Gamma_1\end{pmatrix}\begin{pmatrix}\tilde{K}_x\\ \tilde{K}_y\\ \tilde{K}_z\end{pmatrix} + \begin{pmatrix}0\\ 0\\ R_{se}\end{pmatrix}} \tag{63}$$

then the steady state solution would be

$$\begin{pmatrix}\Gamma_2\tilde{K}_x - M_{12}\tilde{K}_y + \frac{\Omega_d}{2}\tilde{K}_z\\ M_{12}\tilde{K}_x + \Gamma_2\tilde{K}_y\\ -\frac{\Omega_d}{2}\tilde{K}_x + \Gamma_1\tilde{K}_z\end{pmatrix} = \begin{pmatrix}0\\ 0\\ R_{se}\end{pmatrix} \tag{64}$$

$$\tilde{K}_y = -\frac{M_{12}}{\Gamma_2}\tilde{K}_x$$

$$\begin{pmatrix}\frac{\Gamma_2^2+M_{12}^2}{\Gamma_2}\tilde{K}_x + \frac{\Omega_d}{2}\tilde{K}_z\\ -\frac{\Omega_d}{2}\tilde{K}_x + \Gamma_1\tilde{K}_z\end{pmatrix} = \begin{pmatrix}0\\ R_{se}\end{pmatrix} \tag{65}$$

$$\begin{pmatrix}\left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2\tilde{K}_x + \frac{\Omega_d}{2}\tilde{K}_z\\ -\frac{\Omega_d}{2}\tilde{K}_x + \Gamma_1\tilde{K}_z\end{pmatrix} = \begin{pmatrix}0\\ R_{se}\end{pmatrix} \tag{66}$$

$$\tilde{K}_x = -\frac{\Omega_d}{2}\frac{1}{\left(1+(M_{12}/\Gamma_2)^2\right)\Gamma_2}\tilde{K}_z$$

$$\tilde{K}_z = \frac{R_{se}}{\Gamma_1}\frac{\left(1+(M_{12}/\Gamma_2)^2\right)}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1}+\left(1+(M_{12}/\Gamma_2)^2\right)}$$

so finally,

$$\boxed{\begin{pmatrix} \tilde{K}_x \\ \tilde{K}_y \\ \tilde{K}_z \end{pmatrix} = \frac{\frac{R_{se}}{\Gamma_1}}{\frac{\Omega_d^2}{4\Gamma_2\Gamma_1} + \left(1 + (M_{12}/\Gamma_2)^2\right)} \begin{pmatrix} -\frac{\Omega_d}{2\Gamma_2} \\ \frac{M_{12}}{\Gamma_2}\frac{\Omega_d}{2\Gamma_2} \\ \left(1 + (M_{12}/\Gamma_2)^2\right) \end{pmatrix}} \tag{67}$$

# 2 NMR Gyroscope (NMRG)

Using the Xenon NMR model (the Bloch equations) we can implement a gyroscope which measures rotation along the primary axis of the system (in the case above: $\hat{z}$). Following Walker's notation in [WL16], we break the spin dynamics into two components, parallel and perpendicular to the primary axis $\hat{z}$

$$\mathbf{K} = K_z\hat{z} + \mathbf{K}_\perp$$

describing $\mathbf{K}_\perp$ using a phasor notation

$$K_+ = K_x + iK_y = K_\perp e^{-i\phi}$$

where

$$K_\perp = \sqrt{K_x^2 + K_y^2} \quad , \quad \phi = \arctan\left(\frac{K_y}{K_x}\right)$$

Now, if we solve for $\phi$ in the rotating frame of the drive, from eq.(67) we get

$$\phi = \arctan\left(\frac{\tilde{K}_y}{\tilde{K}_x}\right) = \arctan\left(-\frac{M_{12}}{\Gamma_2}\right) \tag{68}$$

for small phase, where $M_{12} \ll 1$ the phase can be approximated with its zeroth order Taylor expansion

$$\phi = -\frac{M_{12}}{\Gamma_2}$$

unfolding $M_{12}$ we get

$$\phi = -\frac{\gamma_{Xe}B_0}{\Gamma_2} - \frac{\gamma_{Xe}b_{KS}S_z}{\Gamma_2} - \frac{\omega_r}{\Gamma_2} + \frac{\omega_{rf}}{\Gamma_2}$$

In a real life NMR system we would also have some magnetic noise in the primary axis $\gamma_{Xe}B_{noise}$, so the phase would be

$$\phi = -\frac{\gamma_{Xe}B_0}{\Gamma_2} - \frac{\gamma_{Xe}B_{noise}}{\Gamma_2} - \frac{\gamma_{Xe}b_{KS}S_z}{\Gamma_2} - \frac{\omega_r}{\Gamma_2} + \frac{\omega_{rf}}{\Gamma_2}$$

all these parameters could in general be time dependent. Notice that in the phase equation we have two unknown parameters: fluctuations of the magnetic field $B_{noise}$ and the world rotation $\omega_r$. In order two extract the world rotation from the phase measurements we need to introduce another specie.

## 2.1 Dual species open-loop NMRG scheme

Having system with two species, Xe129 and Xe131, we can compute the world rotation as follows

$$\phi_{129} = -\frac{\gamma_{Xe}^{129}B_0}{\Gamma_2^{129}} - \frac{\gamma_{Xe}^{129}B_{noise}}{\Gamma_2^{129}} - \frac{\gamma_{Xe}^{129}b_{KS}S_z}{\Gamma_2^{129}} - \frac{\omega_r}{\Gamma_2^{129}} + \frac{\omega_{rf}^{129}}{\Gamma_2^{129}} \tag{69}$$

$$\phi_{131} = -\frac{\gamma_{Xe}^{131}B_0}{\Gamma_2^{131}} - \frac{\gamma_{Xe}^{131}B_{noise}}{\Gamma_2^{131}} - \frac{\gamma_{Xe}^{131}b_{KS}S_z}{\Gamma_2^{131}} - \frac{\omega_r}{\Gamma_2^{131}} + \frac{\omega_{rf}^{131}}{\Gamma_2^{131}} \tag{70}$$

Then, subtracting the two equations we get

$$\frac{1}{\gamma_{Xe}^{129}}\left(\phi_{129}\Gamma_2^{129}-\omega_{rf}^{129}\right)-\frac{1}{\gamma_{Xe}^{131}}\left(\phi_{131}\Gamma_2^{131}-\omega_{rf}^{131}\right)=\omega_r\left(\frac{1}{\gamma_{Xe}^{131}}-\frac{1}{\gamma_{Xe}^{129}}\right) \tag{71}$$

and finally the world rotation in an open-loop setting is given by

$$\omega_r=\left[\frac{\gamma_{Xe}^{129}\gamma_{Xe}^{131}}{\gamma_{Xe}^{129}-\gamma_{Xe}^{131}}\right]\left[\frac{1}{\gamma_{Xe}^{129}}\left(\phi_{129}\Gamma_2^{129}-\omega_{rf}^{129}\right)-\frac{1}{\gamma_{Xe}^{131}}\left(\phi_{131}\Gamma_2^{131}-\omega_{rf}^{131}\right)\right] \tag{72}$$

### 2.2 Dual species closed-loop NMRG scheme

In a Closed-Loop scheme we keep the phase of the spins with respect to the drive constant. To be partially-consistent with Walker in [WL16], we define the constant phase difference as $\beta$. Then, $\phi-\beta$ would be the actual accumulated phase of the drive. But, different from Walker we will solve the dynamics in the rotating frame. This means that in our case $\phi$ stands for the phase accumulated between the drive and the spins in the rotating frame of reference of the spins, so in resonance it is meant to be small, $\phi\approx 0$. Walker solve the dynamics in the lab frame of reference so there, $\phi\approx\frac{\pi}{2}$ for optimal drive (explained in sine driven dumped harmonic oscillator). Also, where Walker uses $\Omega_z$ we substitute $M_{12}=\Omega_z-\Omega_d$.

Finally, Walker define a constant phase difference (in the lab frame) $\phi-\beta\approx\frac{\pi}{2}$ so he multiply the drive with $\sin(\phi-\beta)\approx 1$. In our case (in the rotating frame) $\phi-\beta\approx 0$ so we need to multiply the drive with $\cos(\phi-\beta)\approx 1$.

Therefore, the previous solution to $\phi$ does not hold anymore so we need to solve the Closed-Loop NMRG dynamics in a formal way from the top. Then, in the rotating frame (from eq.(63, we drop the tilde sign for convenience) )

$$\frac{dK_+}{dt}=\frac{dK_x}{dt}+i\frac{dK_y}{dt} \tag{73}$$

$$\frac{d}{dt}\left(K_\perp e^{-i\phi}\right)=-\Gamma_2K_x+M_{12}K_y-\frac{\Omega_d}{2}\cos(\phi-\beta)K_z+iM_{21}K_x-i\Gamma_2K_y \tag{74}$$

$$e^{-i\phi}\frac{dK_\perp}{dt}+K_\perp\frac{d}{dt}e^{-i\phi}=-\left(\Gamma_2+iM_{12}\right)K_x-i\left(\Gamma_2+iM_{12}\right)K_y-\frac{\Omega_d}{2}\cos(\phi-\beta)K_z \tag{75}$$

$$\left(\frac{dK_\perp}{dt}-iK_\perp\frac{d\phi}{dt}\right)e^{-i\phi}=-\left(\Gamma_2+iM_{12}\right)\left(K_x+iK_y\right)-\frac{\Omega_d}{2}\cos(\phi-\beta)K_z \tag{76}$$

$$\left(\frac{dK_\perp}{dt}-iK_\perp\frac{d\phi}{dt}\right)e^{-i\phi}=-\left(\Gamma_2+iM_{12}\right)K_\perp e^{-i\phi}-\frac{\Omega_d}{2}\cos(\phi-\beta)K_z \tag{77}$$

$$\frac{dK_\perp}{dt}-iK_\perp\frac{d\phi}{dt}=-\left(\Gamma_2+iM_{12}\right)K_\perp-\frac{\Omega_d}{2}\cos(\phi-\beta)K_ze^{i\phi} \tag{78}$$

$$\tag{79}$$

Now we break the equation into real and imaginary parts such that

$$K_\perp\frac{d\phi}{dt}=M_{12}K_\perp+\frac{\Omega_d}{2}K_z\cos(\phi-\beta)\sin(\phi) \tag{80}$$

$$\frac{dK_\perp}{dt}=-\Gamma_2K_\perp-\frac{\Omega_d}{2}K_z\cos(\phi-\beta)\cos(\phi) \tag{81}$$

arranging the terms, we get

$$\frac{d\phi}{dt}=M_{12}+\frac{\Omega_d}{2}\frac{K_z}{K_\perp}\cos(\phi-\beta)\sin(\phi) \tag{82}$$

$$\frac{dK_\perp}{dt}=-\Gamma_2K_\perp-\frac{\Omega_d}{2}K_z\cos(\phi-\beta)\cos(\phi) \tag{83}$$

recall

$$\cos(\phi-\beta)\sin(\phi) = \frac{1}{2}\sin(2\phi-\beta) - \frac{1}{2}\sin(-\beta) = \frac{1}{2}\sin(\beta) \tag{84}$$

$$\cos(\phi-\beta)\cos(\phi) = \frac{1}{2}\cos(-\beta) - \frac{1}{2}\cos(2\phi-\beta) = \frac{1}{2}\cos(\beta) \tag{85}$$

where twice the phase oscillations, $2\phi$, quickly average to zero over time so we end up with

$$\frac{d\phi}{dt} = M_{12} + \frac{\Omega_d}{4}\frac{K_z}{K_\perp}\sin(\beta) \tag{86}$$

$$\frac{dK_\perp}{dt} = -\Gamma_2 K_\perp - \frac{\Omega_d}{4}K_z\cos(\beta) \tag{87}$$

Therefore, solving for steady state transverse polarization

$$\boxed{K_\perp = -\frac{\Omega_d}{4\Gamma_2}K_z\cos(\beta)} \tag{88}$$

such that

$$\boxed{\frac{d\phi}{dt} = M_{12} - \Gamma_2\tan(\beta)} \tag{89}$$

while, the longitudinal steady state polarization is given by

$$0 = \frac{dK_z}{dt} = -\frac{\Omega_d}{2}\cos(\phi-\beta)K_x - \Gamma_1 K_z + R_{se} \tag{90}$$

$$0 = -\frac{\Omega_d}{2}\cos(\phi-\beta)\sqrt{K_\perp^2 - K_y^2} - \Gamma_1 K_z + R_{se} \tag{91}$$

$$0 = -\frac{\Omega_d}{2}\cos(\phi-\beta)\sqrt{\frac{\Omega_d^2}{16\Gamma_2^2}K_z^2\cos^2(\beta) - K_y^2} - \Gamma_1 K_z + R_{se} \tag{92}$$

$$0 = -\frac{\Omega_d^2\cos(\beta)\cos(\phi-\beta)}{8\Gamma_2}\sqrt{1-\left(\frac{4\Gamma_1}{\Omega_d\cos(\beta)}\right)^2\left(\frac{K_y}{K_z}\right)^2}K_z - \Gamma_1 K_z + R_{se} \tag{93}$$

$$0 = -\frac{\Omega_d^2\cos(\beta)}{16\Gamma_2}\sqrt{1-\left(\frac{4\Gamma_1}{\Omega_d\cos(\beta)}\right)^2\left(\frac{K_y}{K_z}\right)^2}K_z - \Gamma_1 K_z + R_{se} \tag{94}$$

$$K_z = \frac{R_{se}}{\Gamma_1 + \frac{\Omega_d^2\cos^2(\beta)}{16\Gamma_2}\sqrt{1-\left(\frac{4\Gamma_1}{\Omega_d\cos(\beta)}\right)^2\left(\frac{K_y}{K_z}\right)^2}} \tag{95}$$

recall that we define the drive to be in the $\hat{y}$ direction so we maximize the $K_x$ polarization and minimize $K_y$ so in the case of optimal drive (eq.(62)) and small $\beta$ we get that

$$\boxed{K_z \approx \frac{R_{se}}{\Gamma_1 + \frac{\Omega_d^2\cos^2(\beta)}{16\Gamma_2}}} \tag{96}$$

### 2.3 Closing the Loop

## References

[WL16] Thad G Walker and Michael S Larsen. Spin-exchange-pumped nmr gyros. *Advances in atomic, molecular, and optical physics*, 65:373–401, 2016.