Rabi Oscillations, the 2π Pulse, and γ

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The Standard Treatment from QM Class

Consider the Hamiltonian in the presence of both the DC field from the permanent magnet $\mathbf{H}_0 = B_Z \mu \sigma_z$, and an RF field perpendicular to that, $\mathbf{H}_1 = b_\perp(t)\mu\sigma_\perp$. Assume that the DC field is much larger than the RF field and points along $\hat{z}$: then you can treat $\mathbf{H}_1$ as a perturbation that causes transitions between the eigenstates $|+\rangle$ and $|-\rangle$ of $\mathbf{H}_0$. To be definite, suppose that $b_\perp(t) = 2b\cos\omega t$ in the $\hat{y}$ direction. Then, writing out the Pauli matrices in the Schroedinger representation,

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1 = -\frac{\hbar}{2}\gamma B_Z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \frac{\hbar}{2}\gamma b(e^{i\omega t} + e^{-i\omega t}) \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Assume that the wavefunction

$$\psi = C_+(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\omega_+ t} + C_-(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-i\omega_- t},$$

where $C_\pm(t)$ are the (time-dependent) amplitudes to be aligned/antialigned with B_Z. Then, putting this wavefunction into the Schroedinger equation with the Hamiltonian above, and keeping only the more slowly varying exponential piece, you should get:

$$\dot{C}_\pm \approx \pm\frac{\gamma b}{2} e^{\pm i(\omega_L - \omega)t} C_\mp,$$

with $\omega_L = \omega_+ - \omega_-$, the frequency difference between the aligned and antialigned states of $\mathbf{H}_0$. Differentiating with respect to time lets you uncouple these equations into:

$$\ddot{C}_\pm = \pm i(\omega_L - \omega)\dot{C}_\pm - \frac{\gamma^2 b^2}{4} C_\pm.$$

The frequency difference $\omega_L - \omega$ is how far-off of resonance the RF field is. Assuming an $e^{\Lambda t}$ time dependence and then solving for Λ, you find that $C_+(t)$ and $C_-(t)$ each break into two more pieces (because the quadratic in Λ in general will have two solutions):

$$C_+ = C_+^\pm e^{i\frac{\omega_L - \omega \pm \sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}}{2} t},$$

$$C_- = C_-^{\mp} e^{-i\frac{\omega_L - \omega \mp \sqrt{(\omega_L-\omega)^2+\gamma^2 b^2}}{2}t}.$$

(It may seem weird that C_+ and C_- are not monochromatic, but this just means that $|+\rangle$ and $|-\rangle$ are no longer energy eigenstates.) In your experiments, the initial condition of the nuclear spins is the thermal average of aligned/antialigned with B_Z. Hence, you get a mixture of initial conditions→solutions; but what matters for your signal is the net polarization, and it suffices to see what happens to a single polarized state. For example:

$$C_+(0) = 0 \to C_+^+(0) = -C_+^-(0)$$

$$\to C_+(t) = \frac{\gamma b}{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}} \sin\left(\frac{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}}{2} t\right) e^{i\frac{\omega_L - \omega}{2}t},$$

and

$$C_-(0) = 1 \to C_-^+(0) = 1 - C_-^-(0)$$

$$\to C_-(t) = e^{-i\frac{\omega_L-\omega}{2}t}\left(\cos\left(\frac{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}}{2} t\right) + i\frac{\omega_L - \omega}{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}} \sin\left(\frac{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}}{2} t\right)\right).$$

In the TF NMR experiment, once the pulse shuts off, the probe picks up the oscillations of the x and y components of the polarization $\vec{P}$. The signal from the coil will be proportional to the values $\langle P_x \rangle = 2\,\mathrm{Re}(C_+ C_-^* e^{-i\omega_L t})$ and $\langle P_y \rangle = -2\,\mathrm{Im}(C_+ C_-^* e^{-i\omega_L t})$. Near to resonance, this will be mostly

$$\langle P_x \rangle \approx \frac{\gamma b}{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}} \sin\left(\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t\right) \cos(\omega t),$$

$$\langle P_y \rangle \approx -\frac{\gamma b}{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}} \sin\left(\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t\right) \sin(\omega t).$$

The full expressions are

$$\langle P_x \rangle = \frac{\gamma b}{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}} \sin\left(\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t\right) \cos(\omega t)$$

$$-\frac{\gamma b(\omega_L - \omega)}{((\omega_L - \omega)^2 + \gamma^2 b^2)}\left(1 - \cos\left(\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t\right)\right) \sin(\omega t)$$

$$\langle P_y \rangle = -\frac{\gamma b}{\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}} \sin\left(\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t\right) \sin(\omega t)$$

$$+\frac{\gamma b(\omega_L - \omega)}{((\omega_L - \omega)^2 + \gamma^2 b^2)}\left(1 - \cos\left(\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t\right)\right) \cos(\omega t)$$

The length of the RF pulse and the RF frequency control the direction of $\vec{P}$. A pulse duration that generates an angle of $\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t = \pi$ is called a π pulse; one that generates an angle of $\pi/2$ is called a $\pi/2$ pulse. Consider a sample with $\vec{P} \parallel \hat{z}$. Sufficiently close to resonance, the signal after the π pulse will vanish, because there is no transverse component; on the other hand, the $\pi/2$ pulse maximizes the signal. In practice, it is easier to find the π pulse, and then find the $\pi/2$ pulse by cutting the duration in half. On-resonance, $\omega_L - \omega = 0$, so the π pulse has length $t = \pi/\gamma b$. As $|\omega - \omega_L|$ increases away from resonance, the Breit-Wigner-style resonance prefactors get smaller as $|\omega - \omega_L|$ increases; there will be admixture of the terms proportional to $\omega_L - \omega$; and the duration necessary to form a π pulse will shorten.

Mapping the Rabi Oscillation

In order for this to work well, the applied DC field should be as flat as possible. Otherwise you will not be able to establish a clear π pulse length, because there will be a wide distribution of ω_L's over the volume of the sample. So before embarking on this part of the experiment, you should have adjusted the shim coils so as to maximize the lifetime of the transient for pure water.

The Rabi theory predicts that for different RF pulse lengths, the FID signals should be the same shape, and differ only in their amplitudes, that is, on the angle through which the RF pulse tips the spins. So you may see the Rabi oscillation by plotting the size of the signal (at the same place on each trace) against the pulse length. Knowing the value of b (see below) and the Rabi period then tells you the size of γ.

An Experiment with 2π Pulses

Here is some data, taken with the TeachSpin apparatus.

The sample (water with some copper sulfate solute) was subjected to a 2π pulse on resonance ($\omega = \omega_L$). Then the RF frequency (ω) was adjusted away from ω_L. As the RF moved away from resonance in either direction, the signal amplitude increased–as one would expect. The pulse length was adjusted until the new signal came as close to zero as possible. This minimum indicated what ought to be the 2π pulse length ($t_{2\pi}$) for that particular ω. These steps were repeated over the range of RF in the figure.

The blue points show the putative 2π pulse length as a function of the RF (ω). This clearly peaks in a resonance-like behavior, just around ω_L. The red points show a naive fit to the Rabi formula for the 2π pulse as a function of detuning, $\omega - \omega_L$:

$$\sqrt{(\omega_L - \omega)^2 + \gamma^2 b^2}\, t_{2\pi} = 2\pi \rightarrow t_{2\pi} = \frac{1}{\sqrt{(\nu_L - \nu)^2 + (\gamma/2\pi)^2 b^2}}$$

(a ν is an $\omega/2\pi$). The fit assumes that the peak is at ν_L, and takes $t_{2\pi}$ at resonance to be $2\pi/\gamma b$. Then these parameters (ν_L, $\frac{2\pi}{\gamma b}$) from the peak are used to calculate the rest

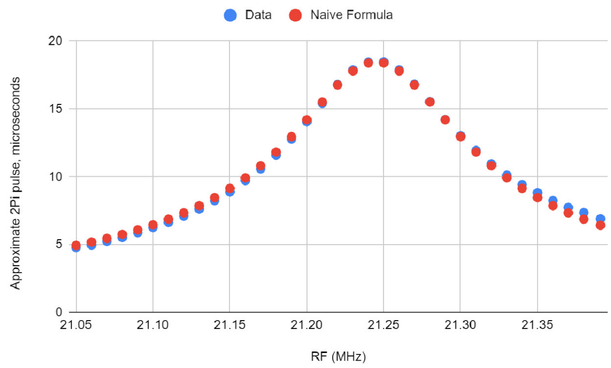

Figure 1: The length of the 2π pulse as a function of detuning from resonance.

of the points. The agreement is seemingly excellent!

Together with a direct measurement of b, a plot such as this will determine γ for the proton. Use the tuning loop tool to estimate b at the position of your sample via Faraday's Law. This requires as precise a measurement as you can manage of the loop's area and the voltage it produces during the RF pulse. The RF coil in the probe is only about $4cm$ long by $0.5cm$ diameter, so the field strength varies noticeably with position in the coil, and so you need to place your loop probe as close as you can to where your sample was. Recall that the derivation presented here begins with $b_y = 2b\cos\omega t$. There are two rectangular loops on the probe tool, with dimensions $L \times W$, and so on the trace from the loop tool, the peak to peak voltage is

$$V_{P-P} = 2 \times 2b\omega \times 2LW = 8b\omega LW.$$

You will notice that although the pulse from the RF synthesizer has a square wave envelope, the power provided to the sample does not. When the pulse turns on, the RF energy in the probe LCR circuit rises exponentially towards its maximum, and then when the pulse turns off, the RF energy decays away. Hence b is not really constant over the pulse, and for an accurate determination of γ you have to correct for this fact.

From the beginning of the pulse, b rises toward b_{Max} and then decays to zero after the driving voltage cuts out at the end of the pulse. On the other hand, the oscillation is coherent even as the size of b changes. This allows you to replace

$$\theta = \sqrt{(\omega_L - \omega)^2 + \gamma^2 b_{Max}^2 t}$$

(the angle that you would have for a constant b_{Max} over a square pulse) with

$$\theta = \int_0^t \sqrt{(\omega_L - \omega)^2 + \gamma^2 b_t^2} dt,$$

and on resonance,

$$\theta = \int_0^t \gamma b_t dt.$$

So you have

$$2\pi = \int_0^{t_{2\pi}} \gamma b_t dt \rightarrow \gamma = \frac{2\pi}{\int_0^t b_t dt}.$$

It is easy enough to get b_{Max} from the trace of a long enough pulse, and so you can figure out $\int_0^{t_{2\pi}} b_t dt$ numerically by comparing the trace of the pulse from the loop tool to the squared-off trace you would get for $b = b_{Max}$ with a duration of $t_{2\pi}$. The effect of this correction becomes less important as you move off of the resonance, because off-resonance, the γb term adds in quadrature with $\omega - \omega_L$.

Why do you not look at the same experiment using the π-pulse? The Rabi theory suggests that this might not work as well because the extra pieces proportional to $\omega - \omega_L$ that appear off-resonance are maximal for a π-pulse. The 2π-pulse however should still give a nice minimum.

Appendix: The Classical Picture

The Rabi formulas work wonderfully well, but it is also useful to imagine the expectation value that you measure as a classical magnetic moment. The classical picture is a good foundation of an intuitive understanding of the signal due to a pulse sequence. It's also a nice way to review some of the physics of spinning tops.

A magnetic field acting on a magnetic moment leads to a torque; and if the moment is proportional to an angular momentum (as it is for spin) then this leads to the equation of motion

$$\frac{d\vec{P}}{dt} = \gamma \vec{P} \times \vec{B}.$$

This is called the Bloch equation (with no relaxation). For a current loop composed of a single particle of charge q and mass m moving in a circle with angular momentum $\vec{J}$, $\gamma = \frac{q}{2m}$. This is a universal result for any classical particle. In the course of your experiments, you will find that this does not describe the proton.

From the cross product, the change in $\vec{P}$ is always perpendicular to $\vec{P}$. So in the absence (or benign neglect) of other processes[1], the tip of $\vec{P}$ always falls on a sphere of constant radius. This is called the Bloch Sphere.[2] To turn this classical picture into Quantum

[1] Like relaxation, which you will also investigate in another measurement

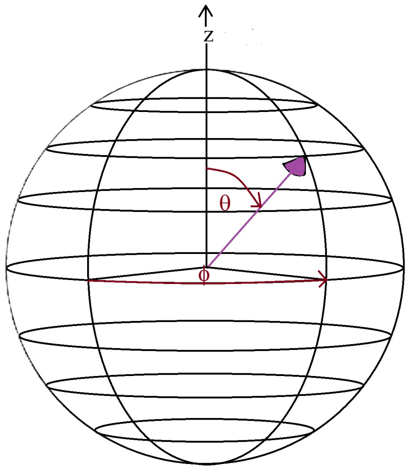

Figure 2: The Bloch sphere.

Mechanics, we could supplement the (θ, ϕ) coordinates on its surface with a rule that reproduces the QM probablities associated with a state $|\psi_{\theta,\phi}\rangle$.

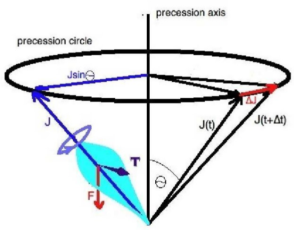

Figure 3: Precession in the DC field. The "spin" is a supported top with an angular momentum vector (purple J arrow) pointing along its axis. A force on the top creates a torque which causes the direction of the angular momentum to change. If only a DC force (the red arrow) is present, the spin precesses around a cone at a fixed opening angle θ (the red ΔJ_F indicates the increment of angular momentum due to the red F).

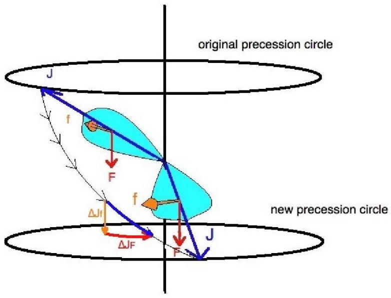

Figure 4: Steering the spin with a co-precessing perturbation field. The perturbing force (the orange f) makes a torque that increments the angular momentum (orange ΔJ_f) from one Bloch lattitude to another. At resonance, the force follows the spin around, always producing the same torque, and drives the spin efficiently from latitude to latitude around the Bloch sphere.

Classically, the "polarization" is a supported top with an angular momentum vector (purple J arrow) pointing along its axis. A force on the top creates a torque which causes the direction of the angular momentum to change. If only a DC force (the red arrow) is present, the polarization precesses around a cone at a fixed opening angle θ,

[2]Do something great, and you, too, can have a personalized version of a common geometric object!.

and its tip traces out a circle of constant latitude (the red ΔJ_F indicates the increment of angular momentum due to the red F). The perturbing force (the orange f) makes a torque that increments the angular momentum (orange ΔJ_f) from one lattitude to another. At resonance, the force follows the polarization around, always producing the same torque, with θ always increasing in the same sense.

In this apparatus, the torque is $\gamma \vec{P} \times 2b\hat{y} \cos \omega t$.[3] At resonance, the torque is proportional to

$$\cos \omega t \cos \omega_L t = \frac{1}{2} \cos(\omega - \omega_L)t + \frac{1}{2} \cos(\omega + \omega_L)t = \frac{1}{2} + \frac{1}{2} \cos(2\omega_L t).$$

You have to integrate this over time to see the change in latitude on the Bloch sphere, and the $\cos(2\omega_L t)$ term oscillates so quickly that it averages to zero. Only the first term survives, and is a constant: it is just like the orange $\vec{f}$ following the polarization around.

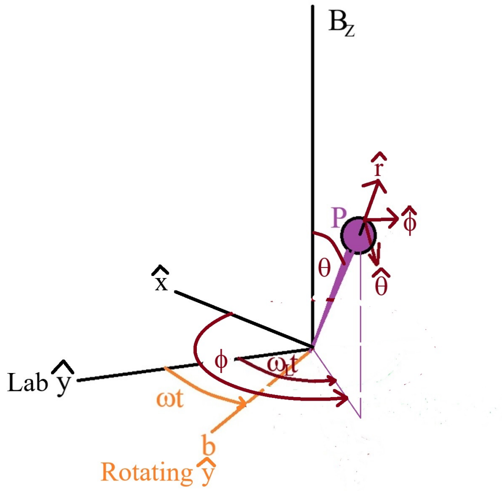

Figure 5: Setup for the calculation of the torque in the $\hat{\theta}$ direction.

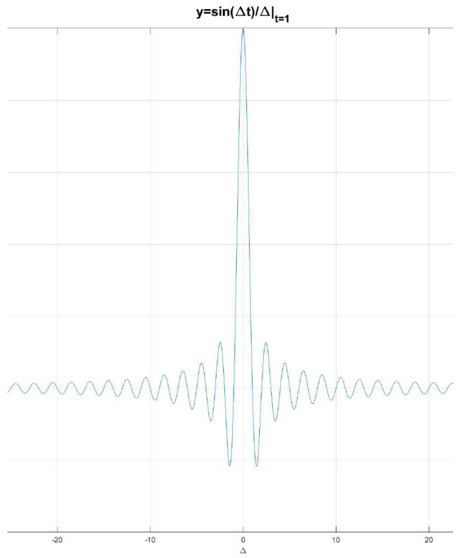

Figure 6: The sinc function. $\frac{\sin(\Delta t)}{\Delta}$ at $t = 1$ and a range of Δ. The larger the detuning (Δ), the smaller the amplitude of the θ oscillation.

When the RF is detuned from ω_L, the relative orientation of the rotating field and the polarization changes with time. Let us follow the motion. Suppose that the perturbing RF field starts out in the lab $\hat{y}$ direction and the initial polarization is along $\hat{z}$. The polarization tilts toward $-\hat{x}$ and proceeds to rotate around the big B_Z field at ω_L, but

[3] $b_y = 2b$ in order to be consistent with the QM calculation above. The frequency will be proportional to the total field, which is a bit larger than B_Z, but I assume that $2b \ll B_Z$, so the precession frequency $\approx \omega_L$. This is an approximation, as you'll see further on. I am also ignoring any relaxation, e.g. assuming that the pulse duration is small compared to the relaxation time.

the RF now varies at $\omega \neq \omega_L$. The unit vector $\hat{y} = \sin\theta\sin\phi\hat{r} + \cos\theta\sin\phi\hat{\theta} + \cos\phi\hat{\phi}$ and $\vec{P} = P\hat{r}$ so the $\hat{\theta}$ component of $\frac{d\vec{P}}{dt} = \gamma\vec{P}\times\vec{b}$ is

$$P\frac{d\theta}{dt} = P\gamma b\{\cos(\omega-\omega_L)t + \cos(\omega+\omega_L)t\}.$$

The low frequency term will have a much larger effect on the motion. The physical reason for this is that the $\cos(\omega-\omega_L)t$ term stays in-phase with $\vec{P}$ for longer, and so is still more effective at turning it in a consistent direction. So again, drop the high-frequency term. But now the orange $\vec{b}$ sweeps around at a different rate, and after some number of Larmor cycles, the low-frequency part falls out of phase with the polarization as well. If $|\omega-\omega_L|$ is large enough, the polarization won't reach $-\hat{z}$ before the rate of change of θ reverses toward $\hat{z}$. The larger $|\omega-\omega_L|$, the quicker this reversal happens. It occurs when the rotating field has fallen behind the polarization by another $\frac{\pi}{2}$, or $|\omega-\omega_L|t = \frac{\pi}{2}$. At that time, a polarization that started in the $\hat{z}$ direction will have descended by

$$\theta = \int_0^{\frac{\pi}{2|\omega-\omega_L|}} \gamma b\cos[(\omega-\omega_L)t]dt = \frac{\gamma b}{\omega-\omega_L}.$$

The indefinite integral is a sinc function (Figure 6):

$$\theta-\theta_0 = \gamma b\frac{\sin[(\omega-\omega_L)t]}{\omega-\omega_L}.$$

The time dependence (for fixed $|\omega-\omega_L| \neq 0$) is sinusoidal, with amplitude $\frac{\gamma b}{|\omega-\omega_L|}$.[4] Off-resonance, θ oscillates sinusoidally; exactly on-resonance, it grows linearly with time, and the polarization sweeps around and around, from pole to pole on the Bloch sphere. If we define the "classical linewidth" as the range of $|\omega-\omega_L|$ for which $|\theta|$ can equal π, then we get $|\omega-\omega_L| \leq \frac{\gamma b}{\pi}$ (absolute) or $\frac{|\omega-\omega_L|}{\omega_L} \leq \frac{\gamma b}{\pi\omega_L}$ (fractional).

The polarization always tries to precess around the field at a given instant, and when the field itself moves, its behavior becomes complicated. For example, a quick calculation shows that

$$\left[\frac{dP}{dt}\right]_{\hat{\phi}} = -\gamma bP\cos\theta\sin\phi \to \frac{d\phi}{dt} = -\gamma\cot\theta\sin\phi.$$

This implies that the polarization wobbles a bit in the $\hat{\phi}$ direction as well, and this rate depends on θ and ϕ in a seemingly involved way. A simplifying trick is to ride along with the rotating $\vec{b}$ in a **R**otating **R**eference **F**rame or RRF. Rotating along with $\vec{b}$ makes $B\hat{z}$ seem smaller (by ω/γ–see Figure 7) because the frame rotation catches up to the $\hat{\phi}$-ward precession. The combination of real and apparent fields $\vec{b} + (B_Z - \frac{\omega}{\gamma})\hat{z}$ in the rotating frame is static; and since the Bloch equations are linear in the fields, the motion in the

[4]It's instructive to see what happens if you don't drop the $\cos(\omega+\omega_L)t$ term. The same integration then yields two sinc functions, but the second one has $\omega+\omega_L$ in the denominator. The $\cos(\omega+\omega_L)t$ term is smaller for ω anywhere near resonance–which further justifies dropping it.

RRF is the same as if the spin were precessing about this static field, which is tilted at an angle

$$\alpha = \sin^{-1}\Big(\frac{\gamma b}{\sqrt{(\omega-\omega_L)^2+\gamma^2 b^2}}\Big)$$

from $\hat{z}$. The polarization describes a cone around the apparent field in the RRF, and the frequency of the conical precession is identical to the Rabi frequency derived via quantum mechanics. This motion is swept bodily around the Bloch sphere in the lab frame of reference. The compound motion of the tip of $\vec{P}$ is a spherical cycloid. The frequency of the conical precession is the classical analog to the Rabi frequency, while $P\sin\alpha$ is what the Rabi formula predicts for the size of $\langle P_x \rangle$ near resonance.

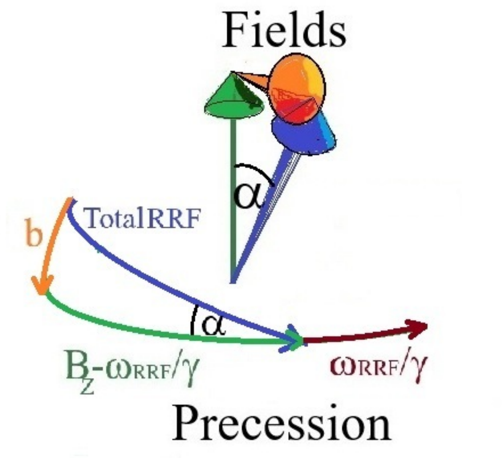

Figure 7: The effect of the RRF is to subtract some of the precession due to the DC field (the red arc indicates the subtracted part). When $\omega_{RRF} = \omega$ for b, the fields appear static in the RRF, and the motion is a cone centered on the effective static field (blue arrow) defined by $\vec{b}$ and the remaining part of the precession due to B_Z (the green arrow).