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Method to extract the water longitudinal relaxation time T_1

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Abstract

We present the method used to extract T_1 from the NMR sweeps performed with the water target.

1 Longitudinal Relaxation Time T_1 and Transverse Relaxation Time T_2

- **Longitudinal relaxation time T_1**

  During the NMR resonance, the protons of the water sample are excited from the low energy spin state to the high energy spin state. In the low energy state, their spin is aligned and parallel to the main holding field, along the z axis of the Hall A electron beam and pointing to the beam dump. In the high energy state, their spin is anti-aligned with the main holding field, still pointing downstream. The return from the excited state to the ground state along the holding field is characterized by the longitudinal (that is along the z axis) time constant T_1.

  If the net magnetization is placed along the $-z$ axis (high energy state), it will return naturally to its low energy equilibrium position M_{z0} along the $+z$ axis according to the following equation (refer to figures 1 and 2):

  $$M_z = M_{z0}(1 - 2e^{-t/T_1}) \tag{1}$$

  Therefore, T_1 represents the time to reduce the difference between the longitudinal magnetization M_z and its equilibrium value by a factor e.

- **Transverse relaxation time T_2**

  When rotating along the z axis, the net transverse magnetization located in the transverse plane starts to dephase, because each of the spin packets making it up is experiencing a slightly different magnetic field and rotates at its own Larmor frequency. Microscopically, the spins in the high and low energy state exchange energy. The longer the elapsed time, the greater the phase difference. This results macroscopically in a loss of transverse magnetization. The time constant describing the return to equilibrium, that is zero, of the transverse magnetization M_{xy} is called the spin-spin relation time T_2 or transverse relaxation time constant. The equation describing the behavior is (refer to figures 3 and 4):

  $$M_{xy} = M_{xy0}e^{-t/T_2} \tag{2}$$

  Then the spin-spin relaxation time is the time to reduce the transverse magnetization by a factor of e.

T_2 is always less than or equal to T_1. In summary, starting from the high energy spin state, the transverse component of the magnetization rotates about the applied holding field, dephases and goes to zero, with a rate determined by T_2. Simultaneously, T_1 governs the rate of recovery of the longitudinal magnetization until it reaches its equilibrium value along the z axis.

2 Extraction of the Relaxation Times T_1 and T_2

The Bloch equations describing the time evolution of the water sample depends on the longitudinal relaxation time T_1 and also on the transverse relaxation time T_2. Therefore, the shape of the water signal depends on the values of T_1 and T_2, and the functional form used to fit the water signal needs a numerical value for T_1 and T_2.

For the water sample, T_1 and T_2 are close to 2 s and smaller that the sweep duration, so the net magnetization of the sample is following closely the effective holding field. The numerical estimation of T_1 can be extracted from our water calibration data : the ratio of the up water signal amplitude to the down signal amplitude depends strongly on the value of T_1 and does not depend on the value of T_2. The smaller T_1 is, the closer to 1 the ratio is. Since T_2 is less than T_1, the height of the up signal and the height of the down signal are reduced by the same amount, and their ratio does not change.

The value of T_2 is known from the literature and can also be measured through specific pulsed NMR technics, which will not be described here.

3 Model of the Water NMR Signal

We have already defined the Bloch equations describing the time evolution of the water signal net polarization in [1]. They are written :

$$\begin{aligned}
\frac{dP_x}{dt}(t) &= -\frac{1}{T_2}P_x(t) + \gamma\alpha t P_y(t) + \frac{1}{T_2}\chi H_1 &(3)\\
\frac{dP_y}{dt}(t) &= -\gamma\alpha t P_x(t) - \frac{1}{T_2}P_y(t) + \gamma H_1 P_z(t) &(4)\\
\frac{dP_z}{dt}(t) &= -\gamma H_1 P_y(t) - \frac{1}{T_1}P_z(t) + \frac{1}{T_1}\chi(H_0+\alpha t) &(5)
\end{aligned}$$

If we assume $T_1 = T_2$, the net polarization can be described by the effective polarization P_{eff} :

$$P_{eff} = k\sqrt{P_x^2 + P_y^2 + P_z^2} \tag{6}$$

where $k = \pm 1$ and which time evolution is given by :

$$\frac{dP_{eff}}{dt}(t) = \frac{1}{T_1}[P_{eff}(t) - P_{eq}(t)] \tag{7}$$

where $P_{eq}(t)$ is defined by :

$$P_{eq}(t) = \chi\frac{H_1^2 + \alpha t(H_0+\alpha t)}{\sqrt{H_1^2 + \alpha^2 t^2}} \tag{8}$$

Parametrizing the ramp speed α (in Gs^{-1}) to describe the effective holding field evolution along the z axis during the sweep shown on figure 5 and according to :

- if $t \geq -\Delta t/2$ and $t < \Delta t/2$
$$\alpha = 1.2 \tag{9}$$
- if $t \geq \Delta t/2$ and $t < 3\Delta t/2$
$$\alpha = 0.6\Delta t/t \tag{10}$$
- if $t \geq 3\Delta t/2$ and $t < 5\Delta t/2$
$$\alpha = -1.2 + 2.4\Delta t/t \tag{11}$$
- if $t \geq 5\Delta t/2$ and $t < 7\Delta t/2$
$$\alpha = -0.6\Delta t/t \tag{12}$$

we can reproduce the water signal detected by the pick-up coils, as shown on figure 6. We have defined Δt as the ramp duration, that is $\Delta t = 7$ G / 1.2 Gs^{-1} = 5.83s. This model has been written using the Mathematica v3.0 software. From the solution of the differential equation, we obtain the ratio of the up signal to the down signal, as a function of $T_1 = T_2$, shown on figure 7. As expected, the ratio approaches 1 when $T_1 = T_2$ goes to zero.

The curve obtained assuming $T_1 = T_2$ can be parametrized with the following formula given by Mathematica :

$$Up/Down(T_1 = T_2) = a_0 + a_1 T_1 + a_2 T_1^2 + a_3 T_1^3 \tag{13}$$

where

- $a_0 = +0.9989378775132347$
- $a_1 = -0.1381862721576716$
- $a_2 = +0.0318150334184504$
- $a_3 = -0.0011210082249172$

The value of T_1 should then be extracted for each water calibration using this parametrization.

Now, if $T_1 \neq T_2$, we need to integrate numerically the whole set of Bloch equations. The dependence with T_2 for $T_1 = 1.5s$ is shown on figure 8 and the ratio for several values of T_1 is shown on figure 9. Clearly, the UP/DOWN ratio does not depend on the value of T_2, for T_1 fixed.

4 Effect of T_1 on the signal shape

We can study qualitatively the effect of the value of T_1 on the NMR signal as shown on figures 10 and 11, obtained for $T_1 = T_2$. Clearly, when T_1 increases, the NMR signal becomes completely symmetric (figure 10) and the signal keeps the same sign during the UP and DOWN ramp (figure 11). The higher T_1 is, the closer is the NMR signal shape to the square root of a Lorentzian, as obtained with the Helium target.

References

[1] S. Incerti and E. Lakuriqi, "Model of the water signal shape from the Bloch equations", E94-010 Technical Note 10, 11/4/98

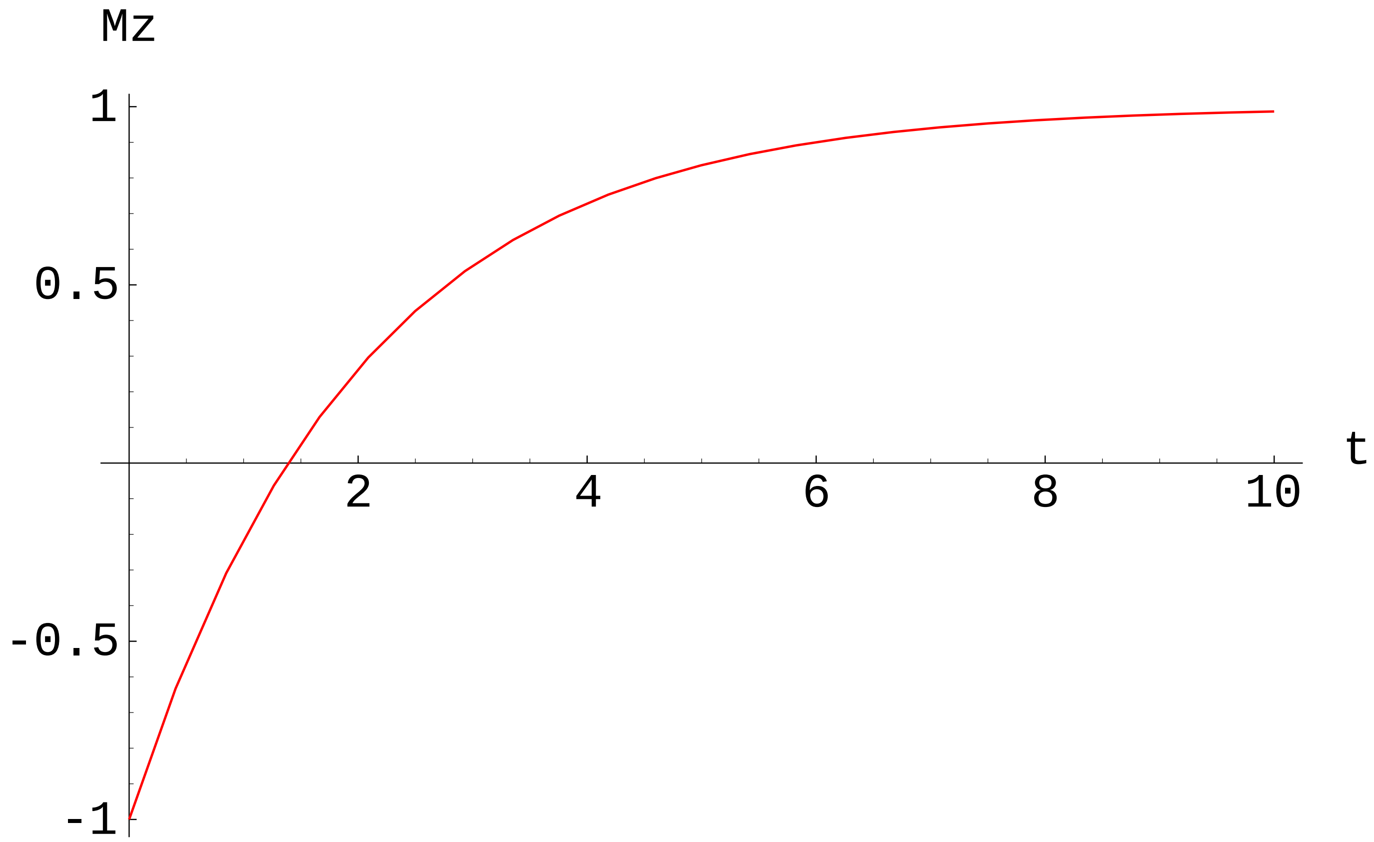

Figure 1: Longitudinal relaxation of the z component of the water net magnetization, from the high energy spin state, where M_z is anti-aligned with the effective holding field H_z along z. We have assumed T_1=2 s.

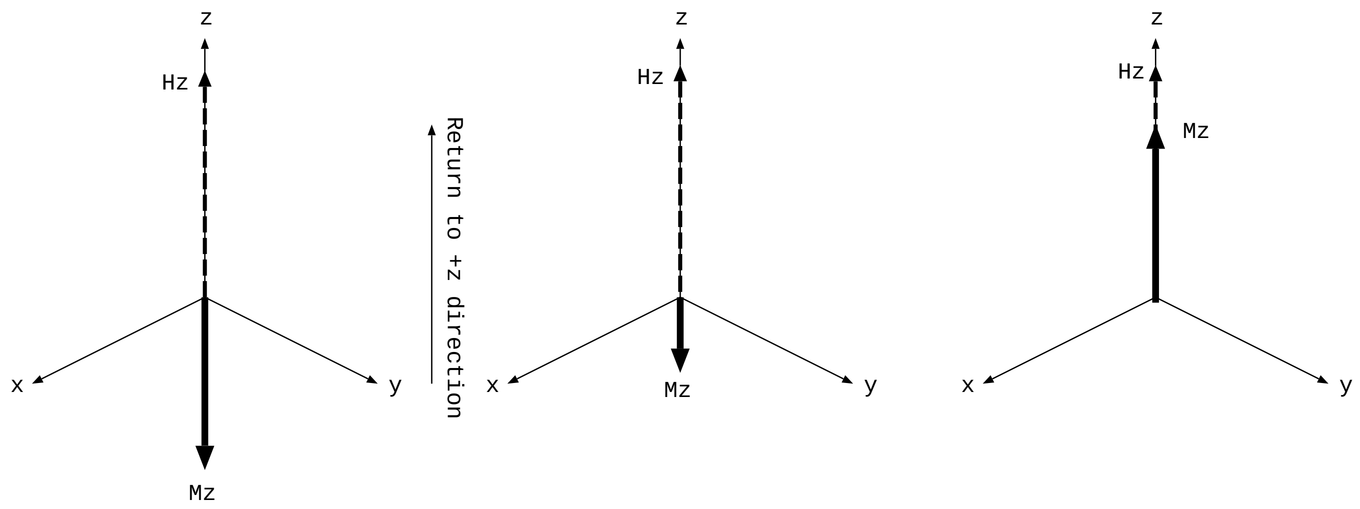

Figure 2: Representation of the longitudinal relaxation of M_z from the high energy spin state.

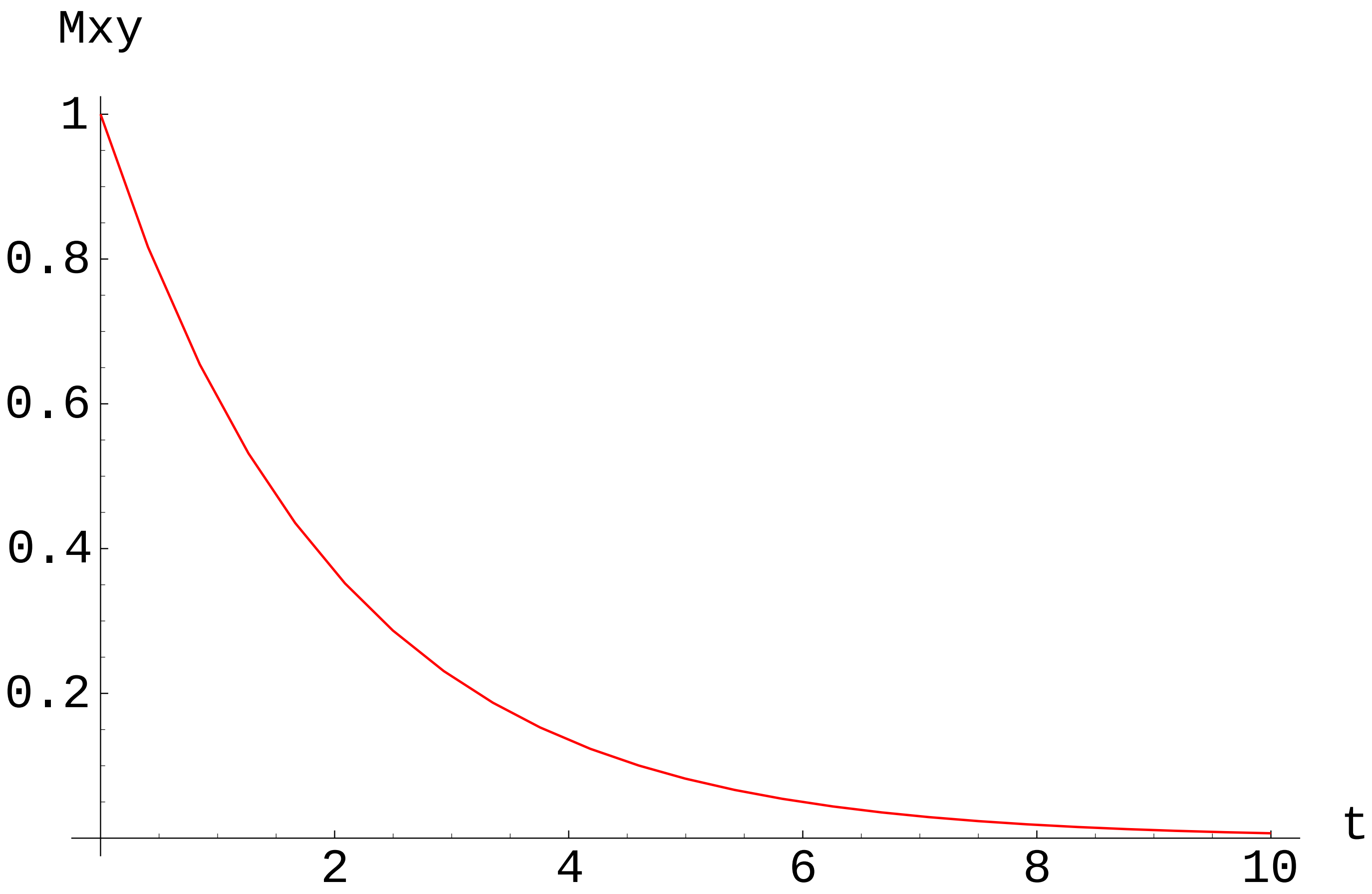

Figure 3: Relaxation of the transverse xy component of the water net magnetization. We have assumed T_2=2 s.

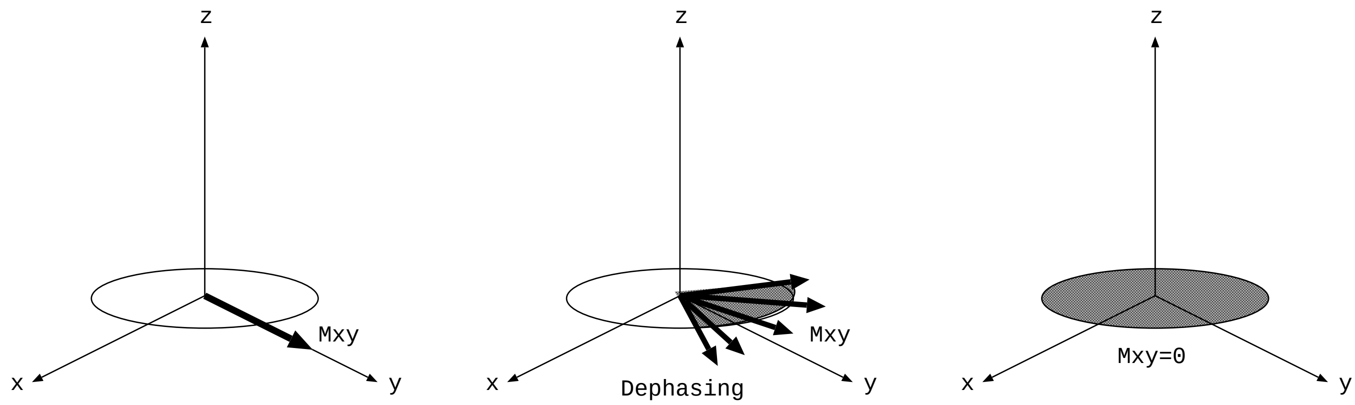

Figure 4: Representation of the transverse relaxation of M_{xy}. We have initially assumed that the transverse component of the magnetization is aligned with the y axis. While it rotates around the z axis at a frequency of 91 kHz, the spin packets dephase and the net transverse magnetization M_{xy} vanishes.

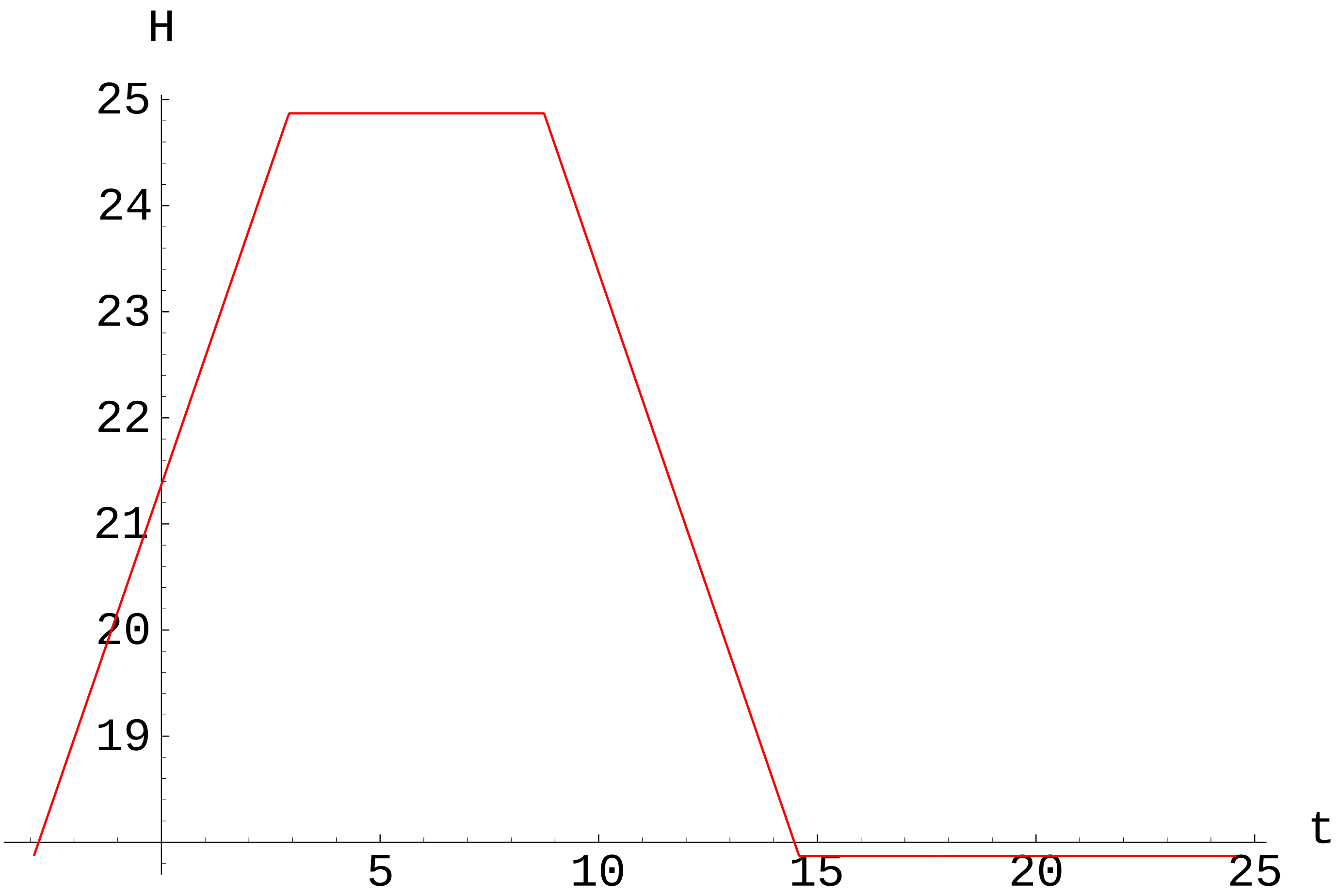

Figure 5: Time evolution of the effective holding field H along the z axis, during the UP and DOWN ramps. The sweep is performed at 1.2 G.s^{-1} and there is a plateau of 7 G / 1.2 G.s^{-1} = 5.83 s between the up ramp and the down ramp.

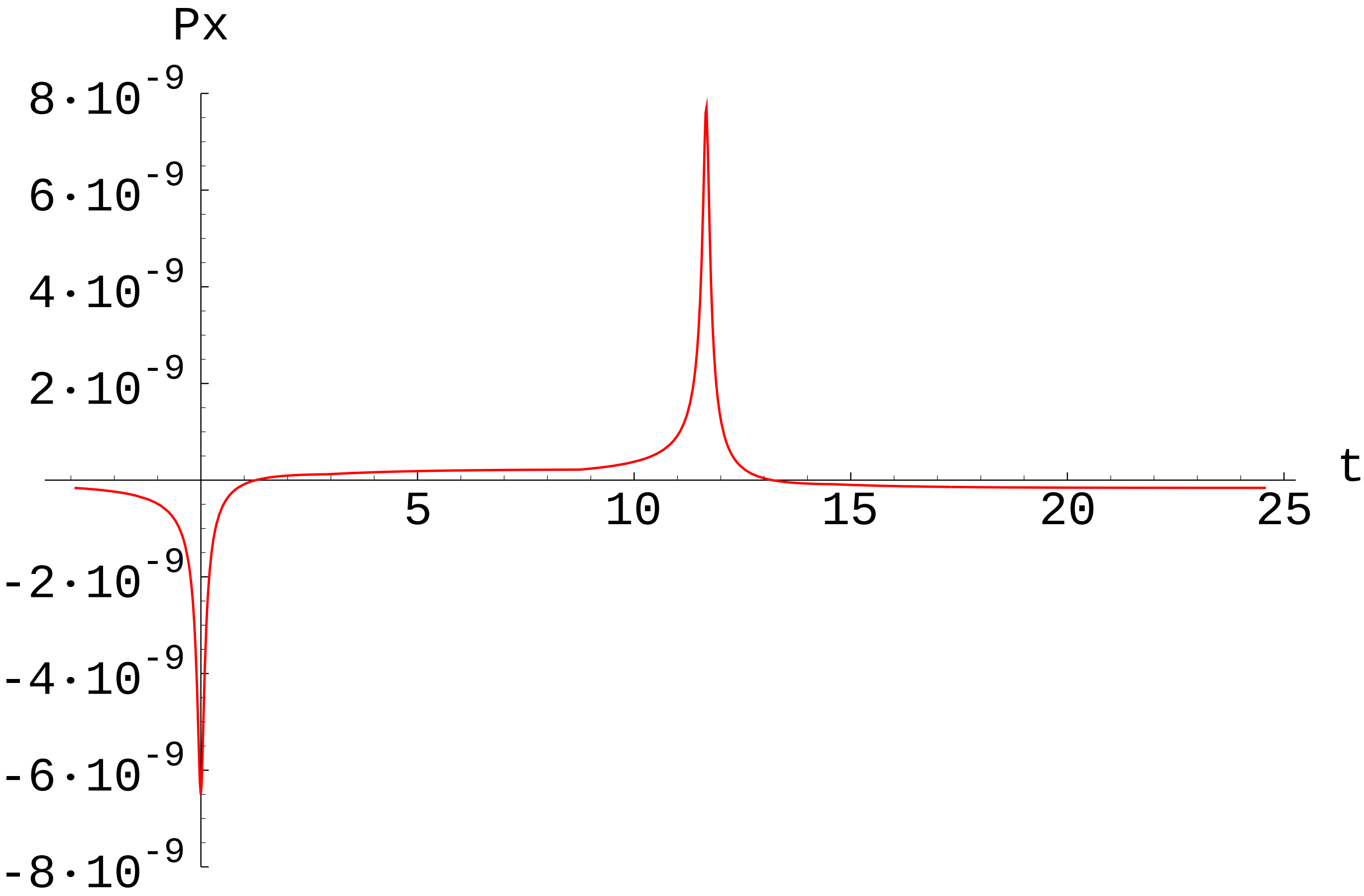

Figure 6: Model of the water signal detected by the pick-up coils during an NMR up and down sweep.

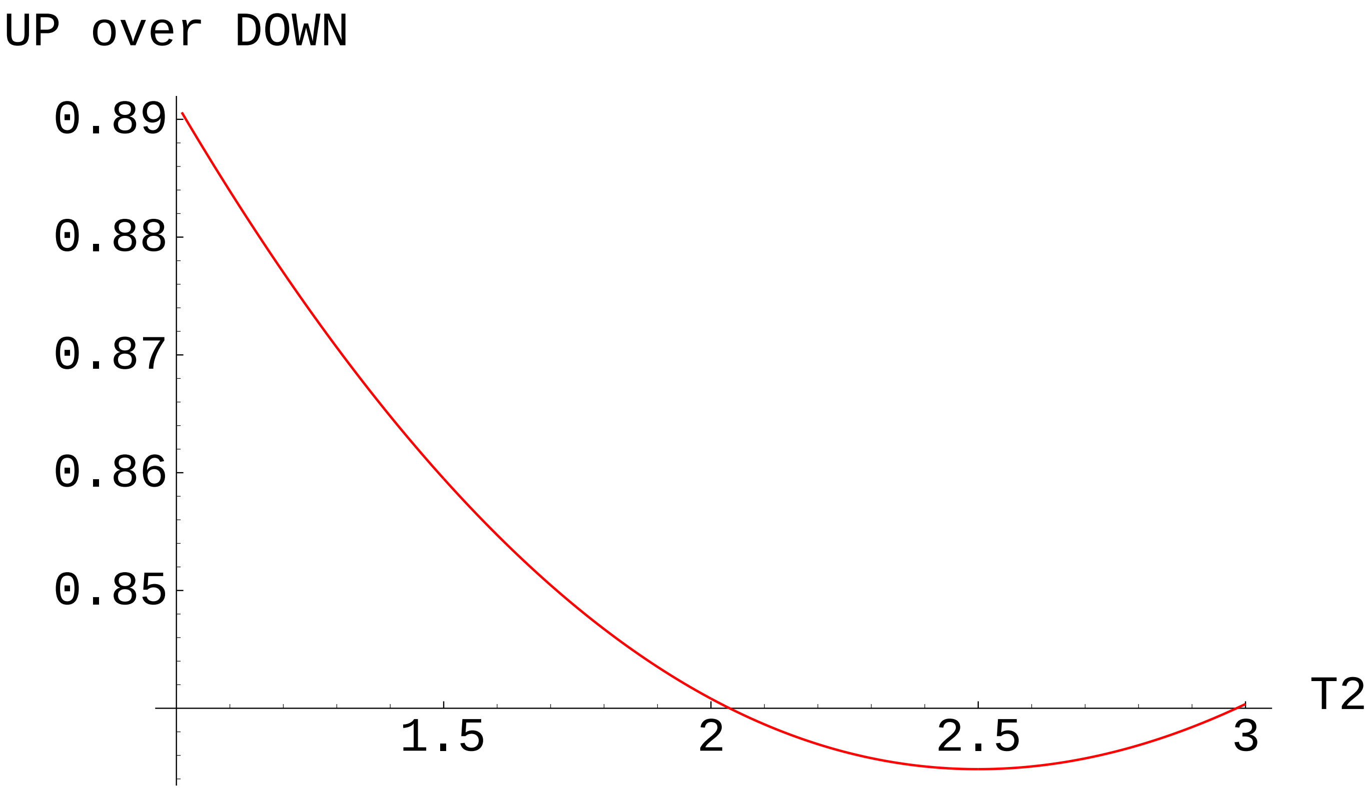

Figure 7: Parametrization of the ratio UP/DOWN water signal amplitude at resonance, as a function of T_2, for $T_1 = T_2$.

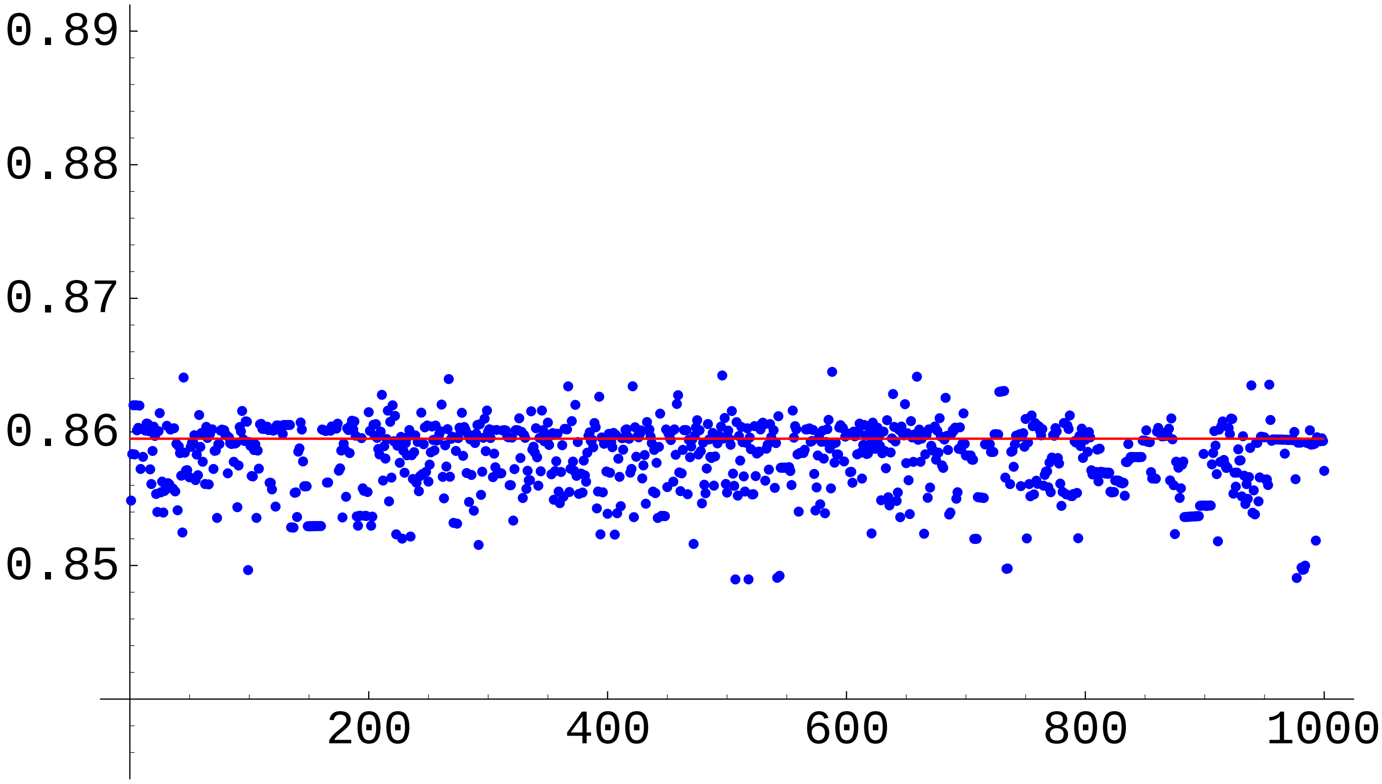

Figure 8: Ratio UP/DOWN water signal for $T_1 = 1.50s$ and 1000 values for T_2, ranging from 1 to 1.5, obtained with Mathematica. As expected, there is no obvious dependence of the ratio with T_2. The flat line represents the expected value of the ratio for $T_1 = T_2 = 1.50s$

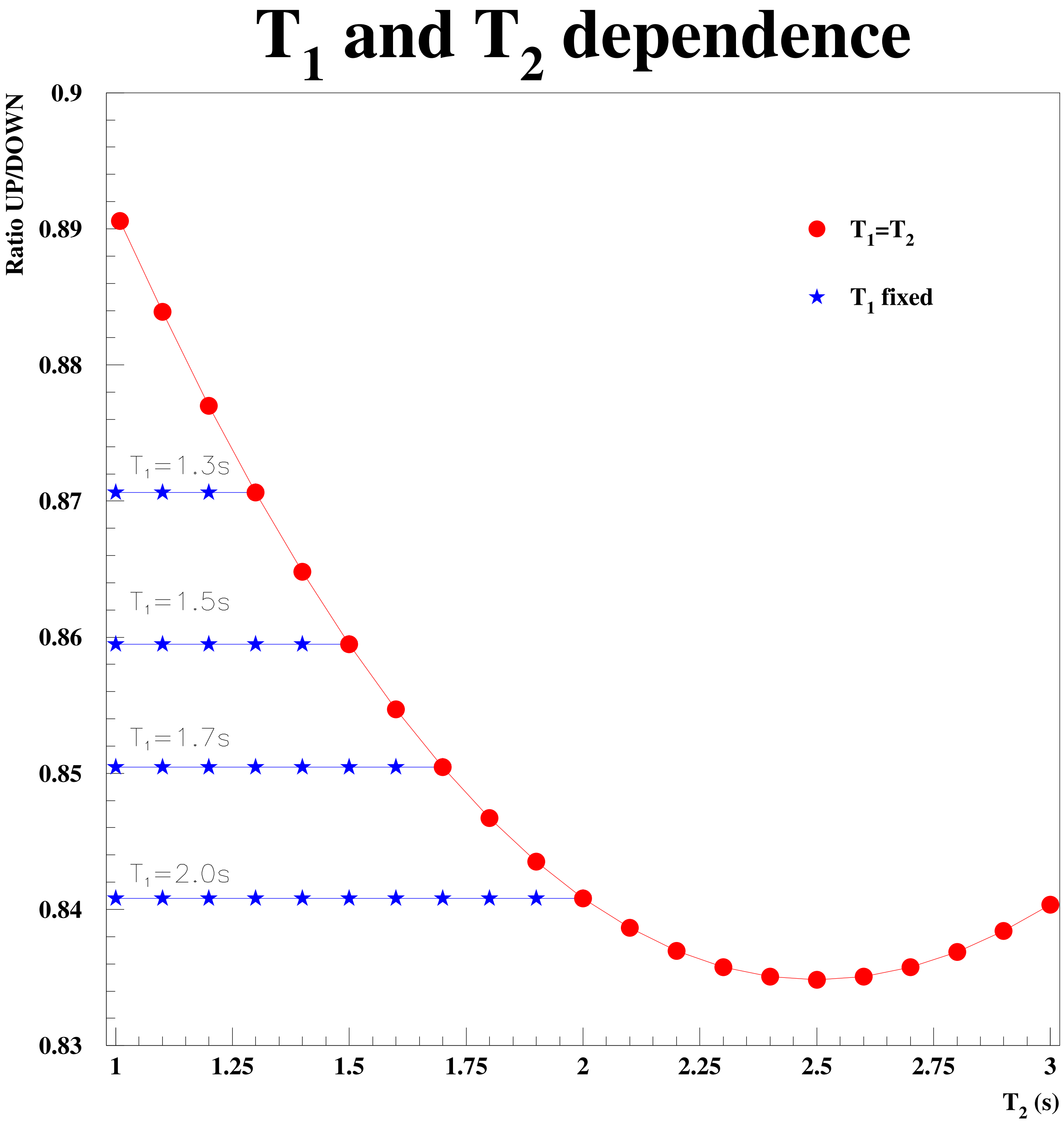

Figure 9: Ratio UP/DOWN water signal for $T_1 = T_2$ (plain circles) and T_1 fixed (plain stars), obtained using our Mathematica v3.0 code.

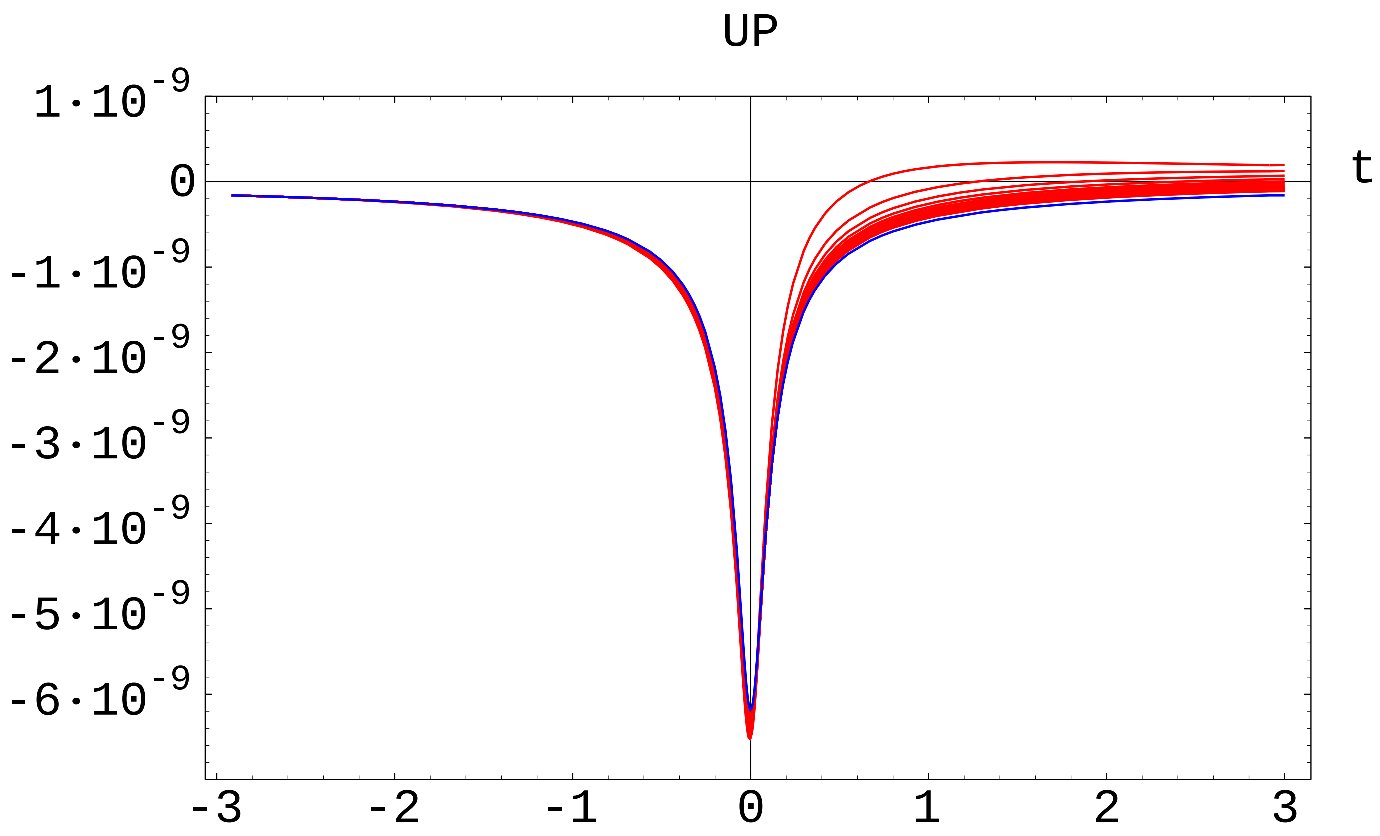

Figure 10: Water UP signal for several values of $T_1 = T_2$, ranging from 1 s to 20 s, as a function of time. The symmetric limit is plotted in blue, and is obtained for $T_1 = T_2 >> 1$ s.

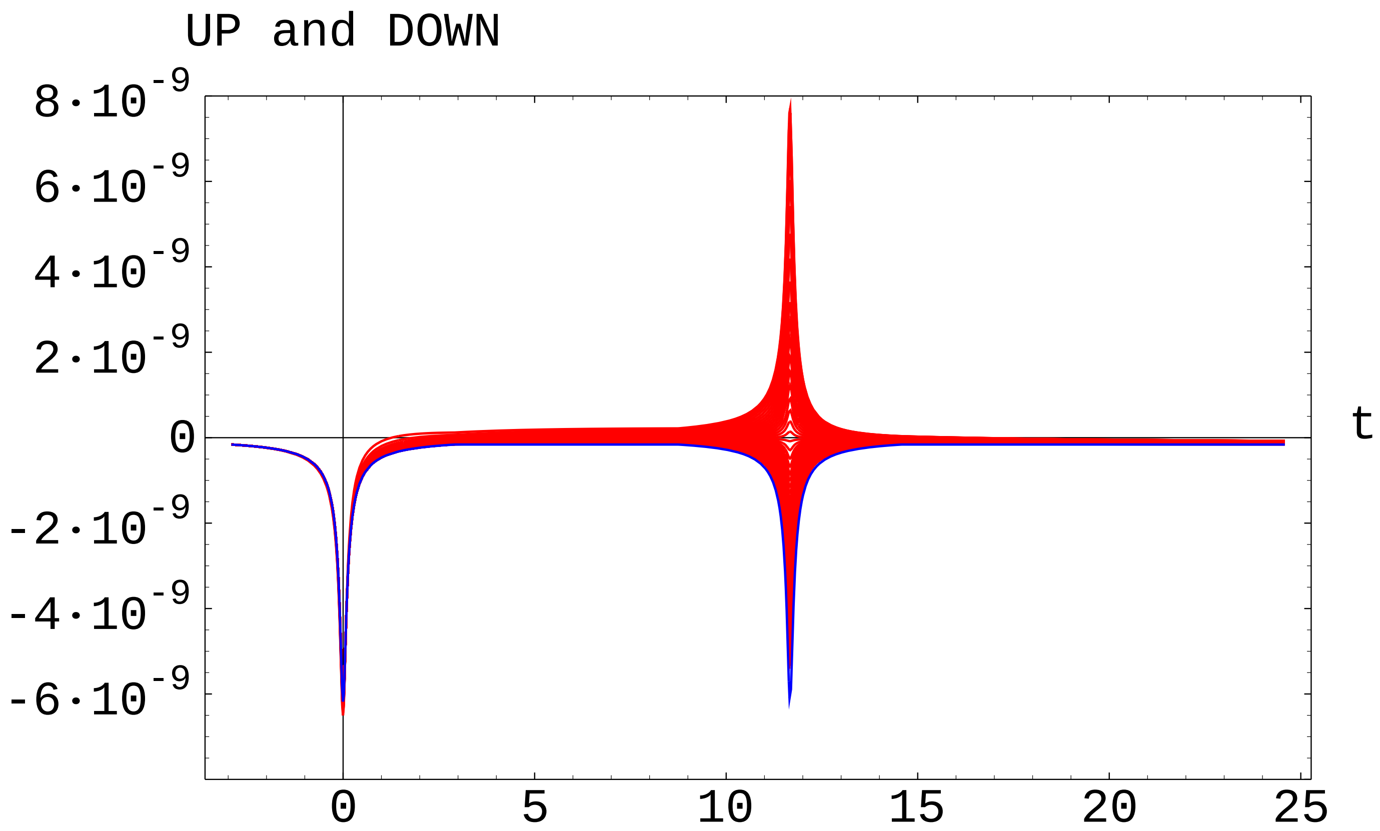

Figure 11: Water UP and DOWN signal for several values of $T_1 = T_2$, ranging from 2 s to 200 s, as a function of time. The "Heliun shape" in blue is obtained for $T_1 = T_2 >> 1$ s, when both UP and DOWN signals are negative and have approximately the same height.