Nuclear magnetization evolution in time-variable magnetic fields

Theory and exploitation

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www.ebyte.it/stan/Talk_FFC_2009.html

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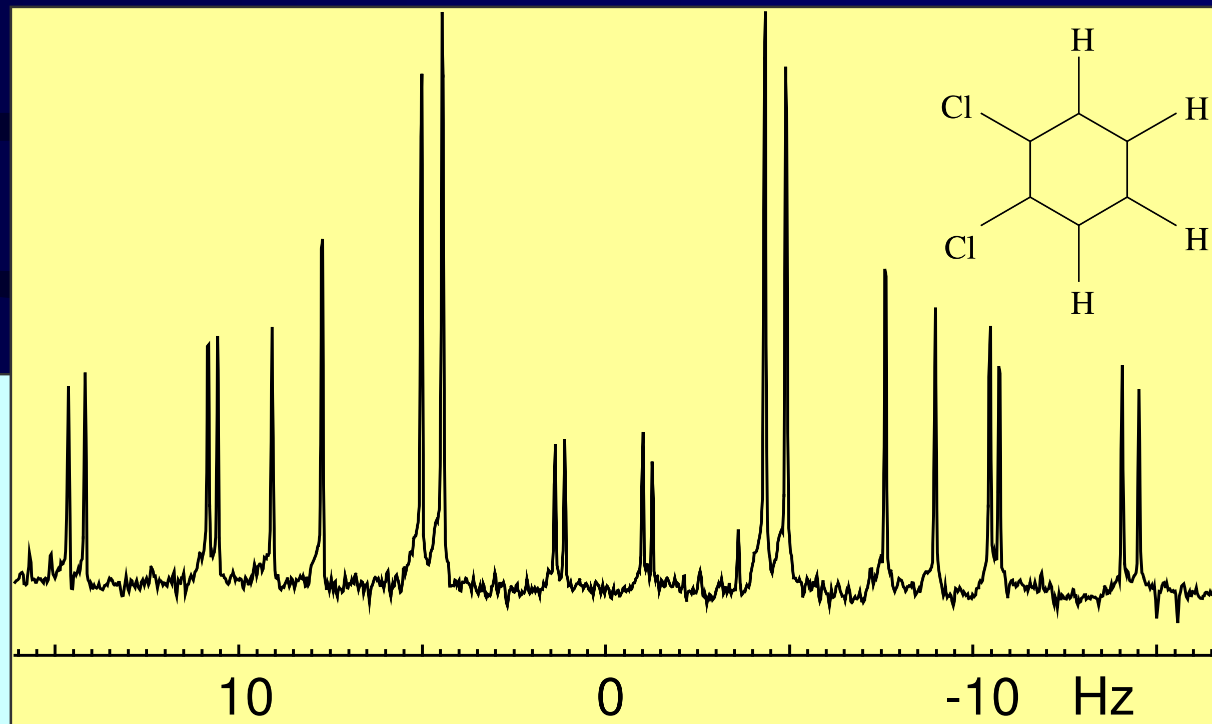
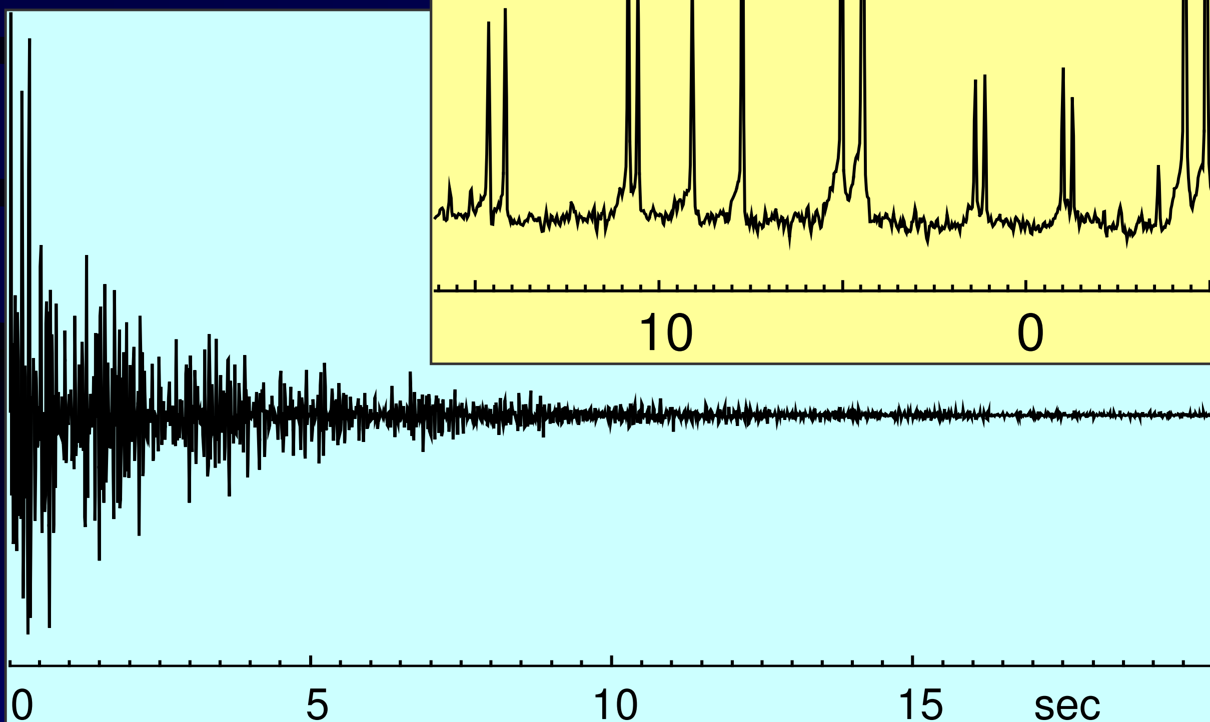
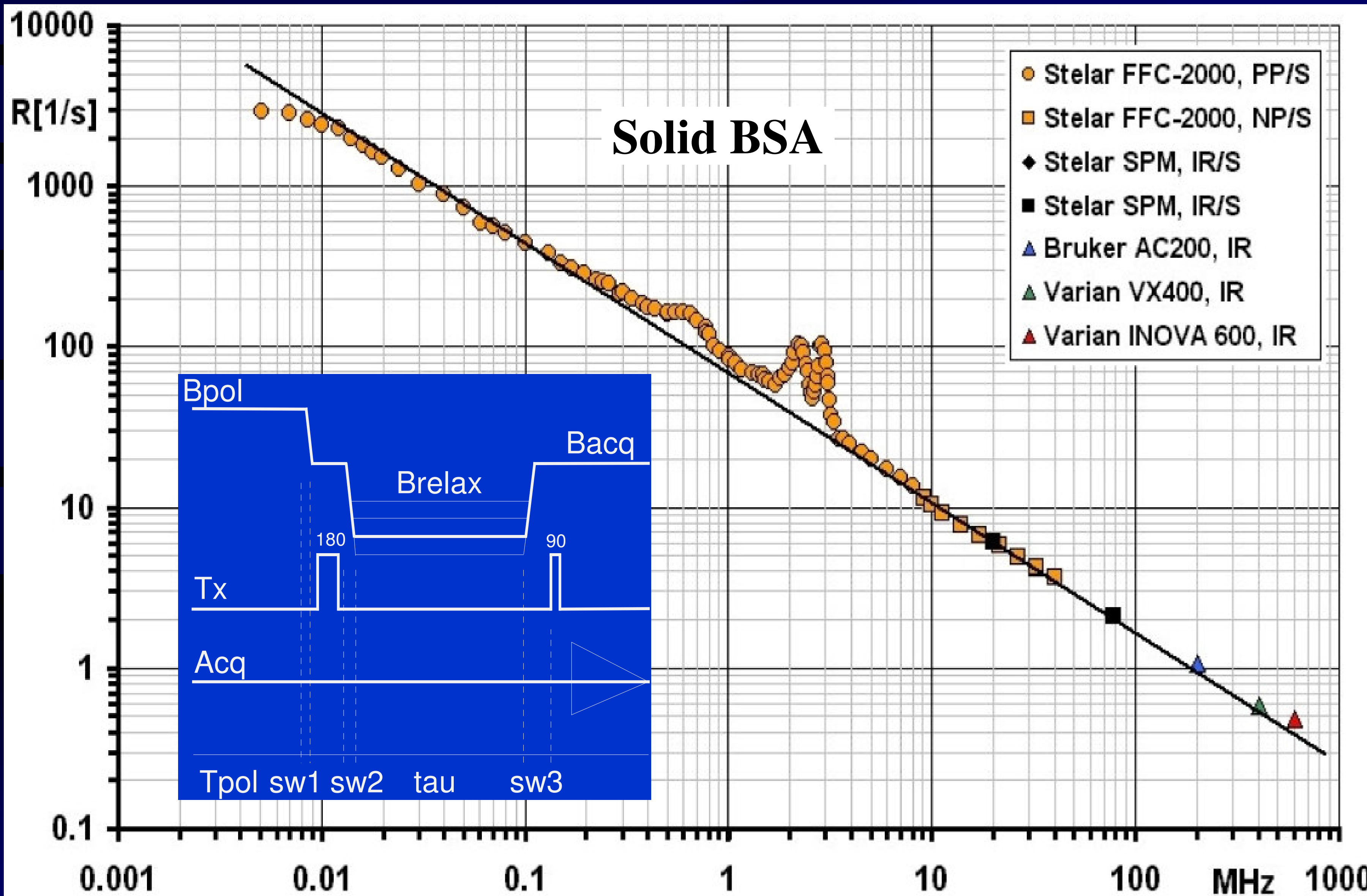
Fixed magnetic field B_0 can be useful …

0.07 Hz
resolution
and stability





… but so can be a variable field

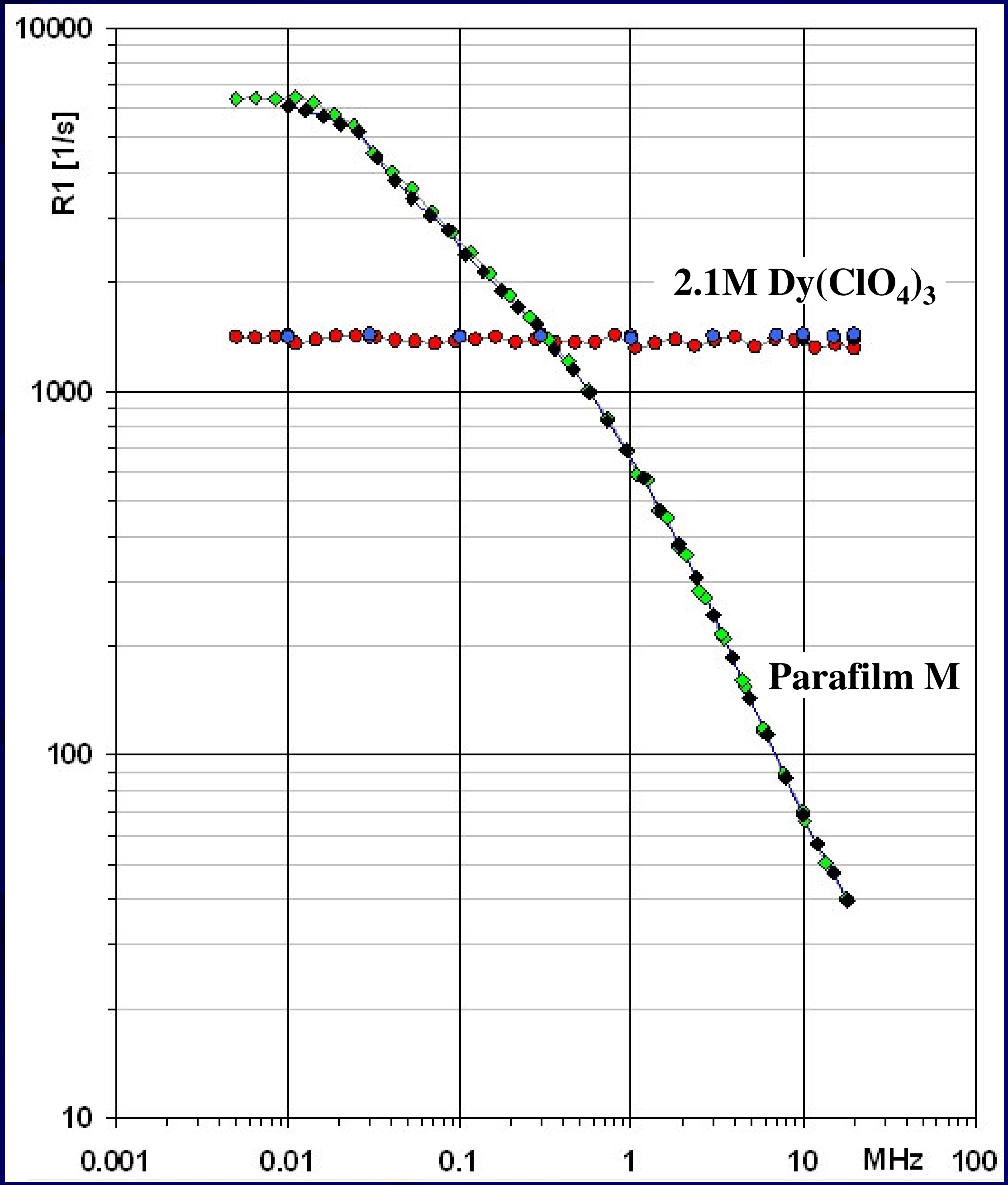


A mystery :

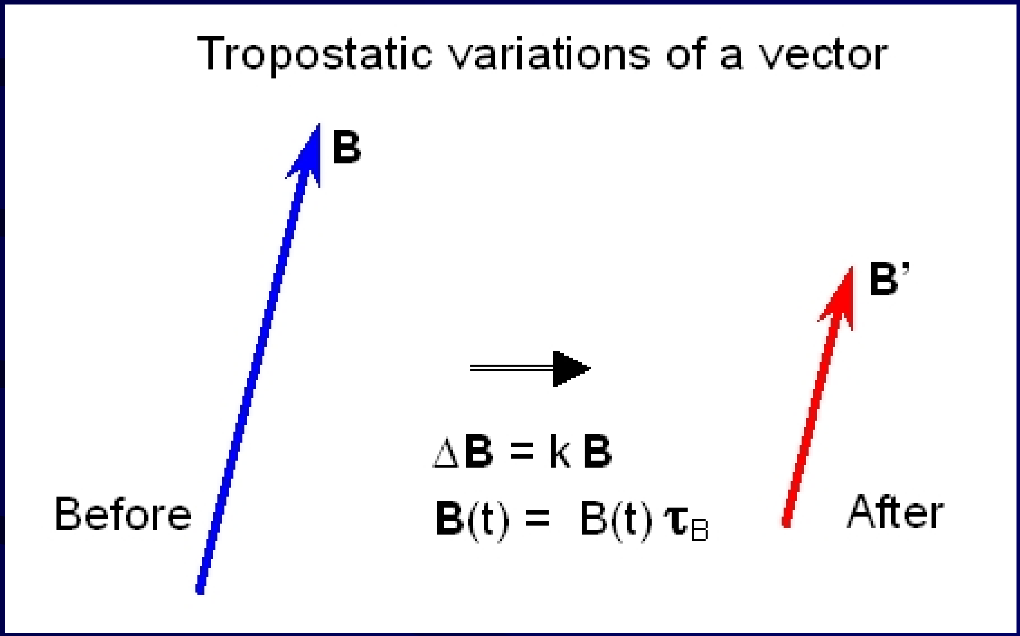
I have found that it was possible to measure low-field relaxation times of 0.15 ms using a switching time of 1 ms or more.

How comes that an appreciable amount of magnetization has managed to survive the switching-down period

??????????????????



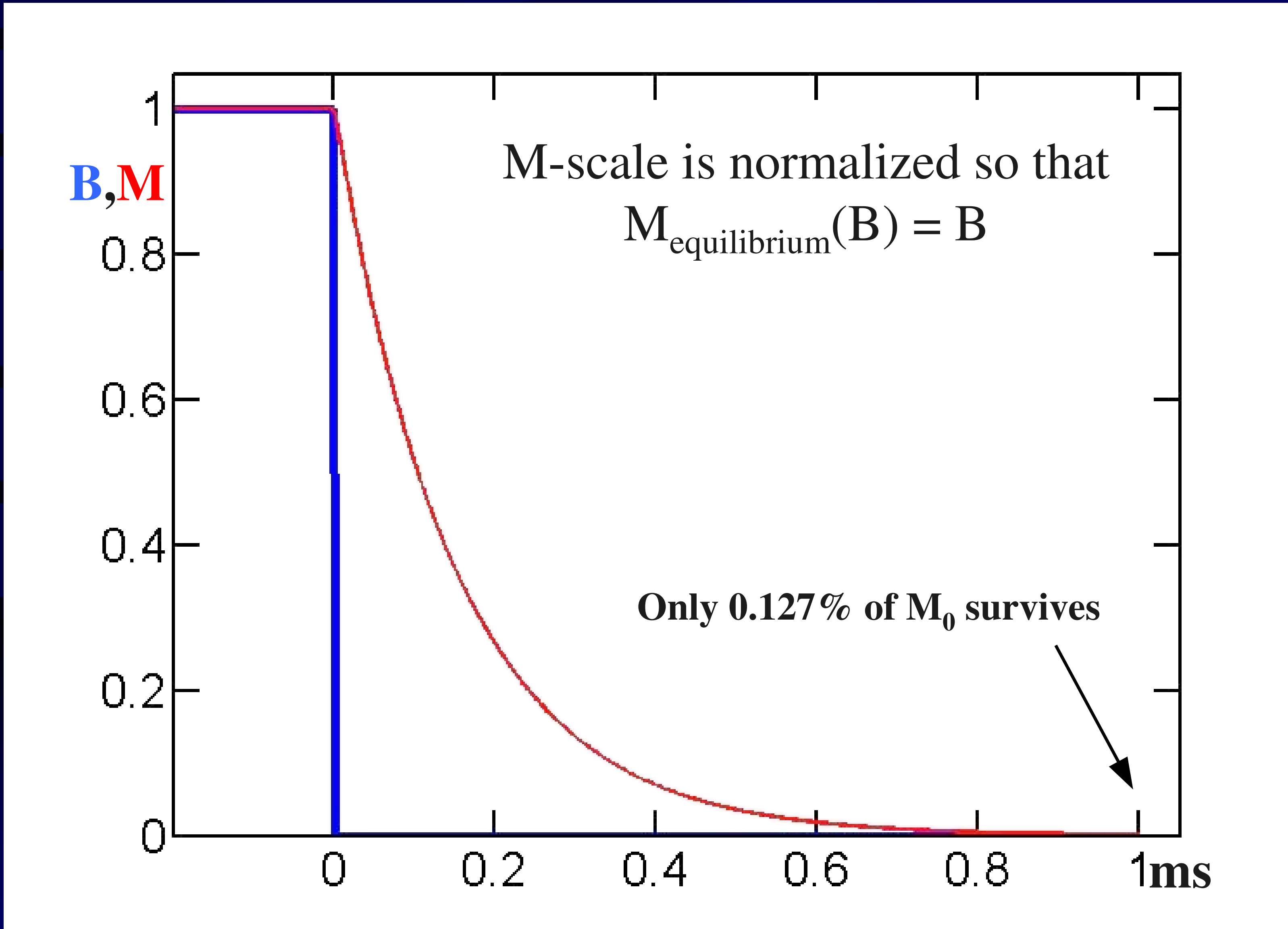
What happens to nuclear magnetization during tropostatic field variations ?



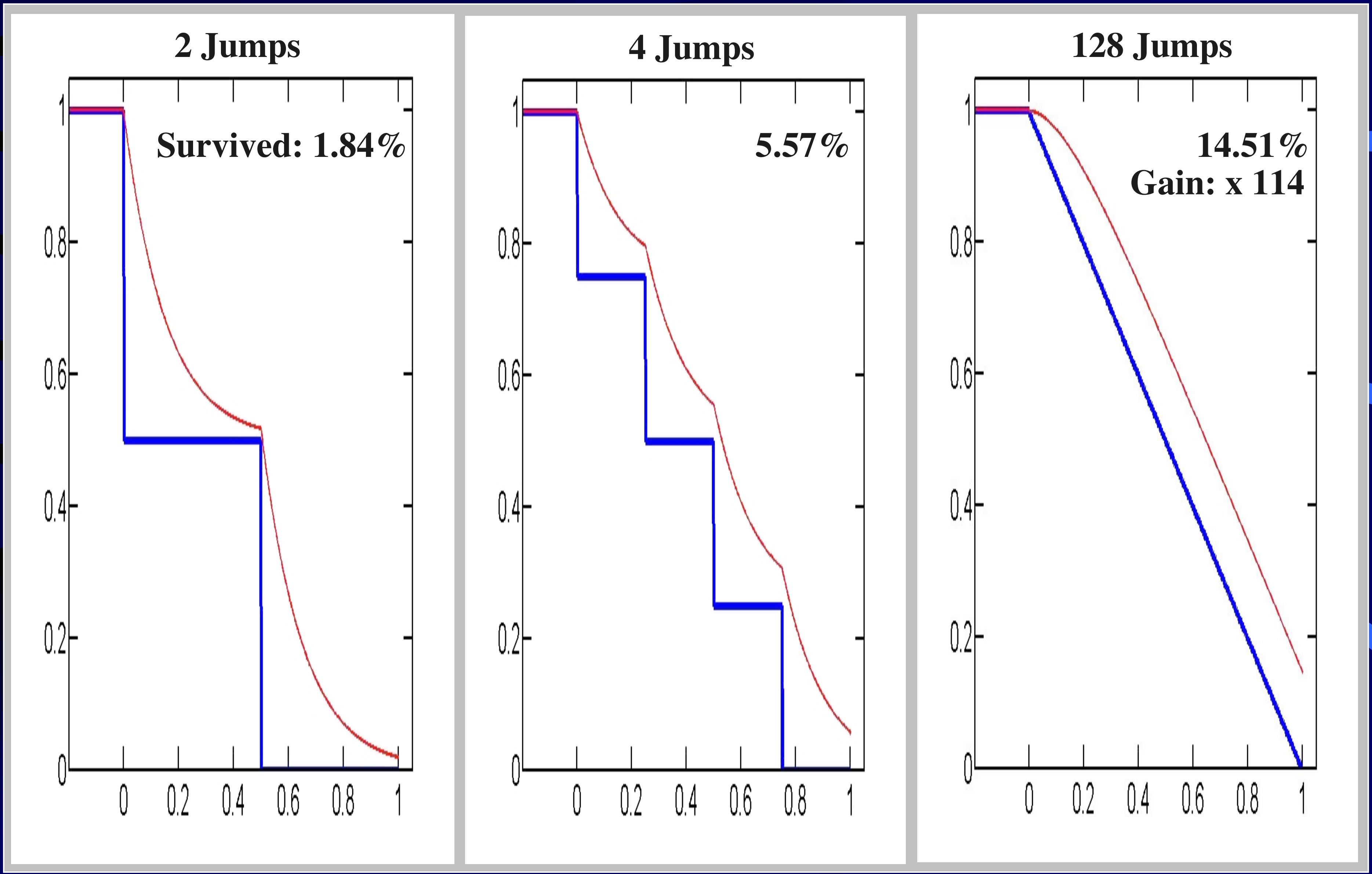
During tropostatic variations, the parallel and perpendicual components of nuclear magnetization still evolve apparently independently.

We will now limit the discussion to the parallel component and, for a moment, we will also assume that R_1 is field-independent.

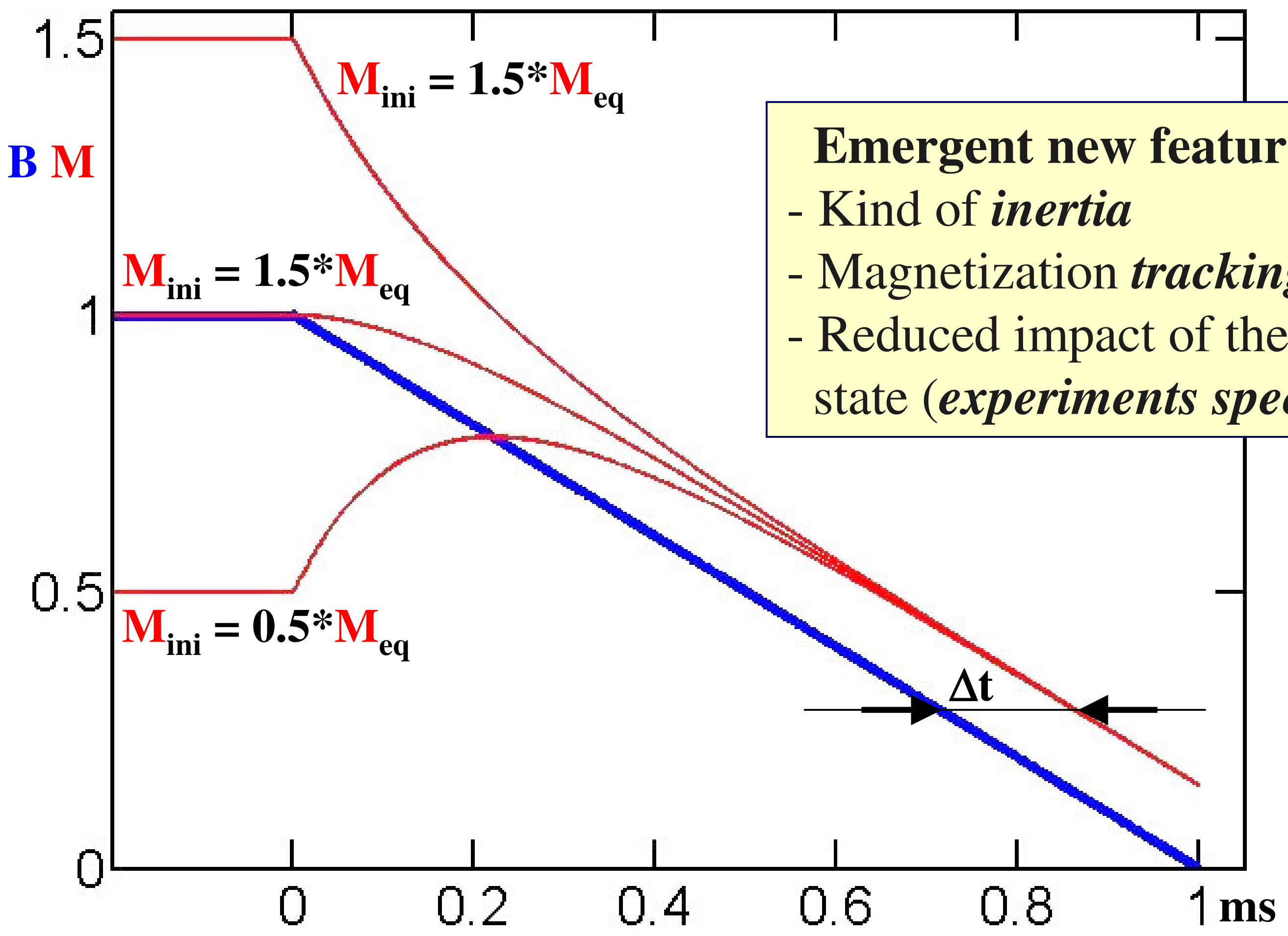
Instantaneous jump



A series of instantaneous jumps



A linear ramp as a limit case



Emergent new features:
- Kind of ***inertia***
- Magnetization ***tracking delay***
- Reduced impact of the initial state (***experiments speed-up***)

Numeric simulations

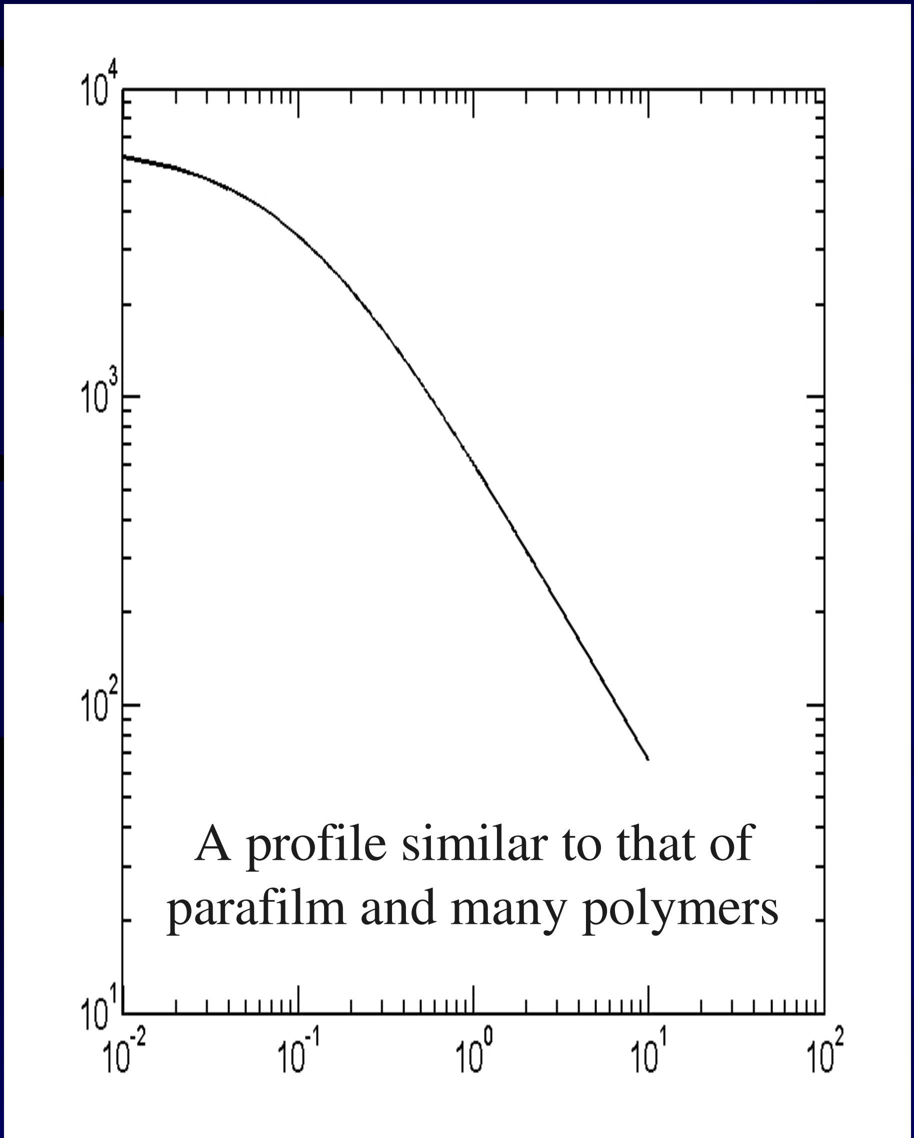
Numeric simulations of the magnetization evolution by concatenation of infinitesimal magnetic-fileld jumps are very easy even in the case of arbitrary switching waveforms and field-dependent relaxation (just a few lines of Matlab code)

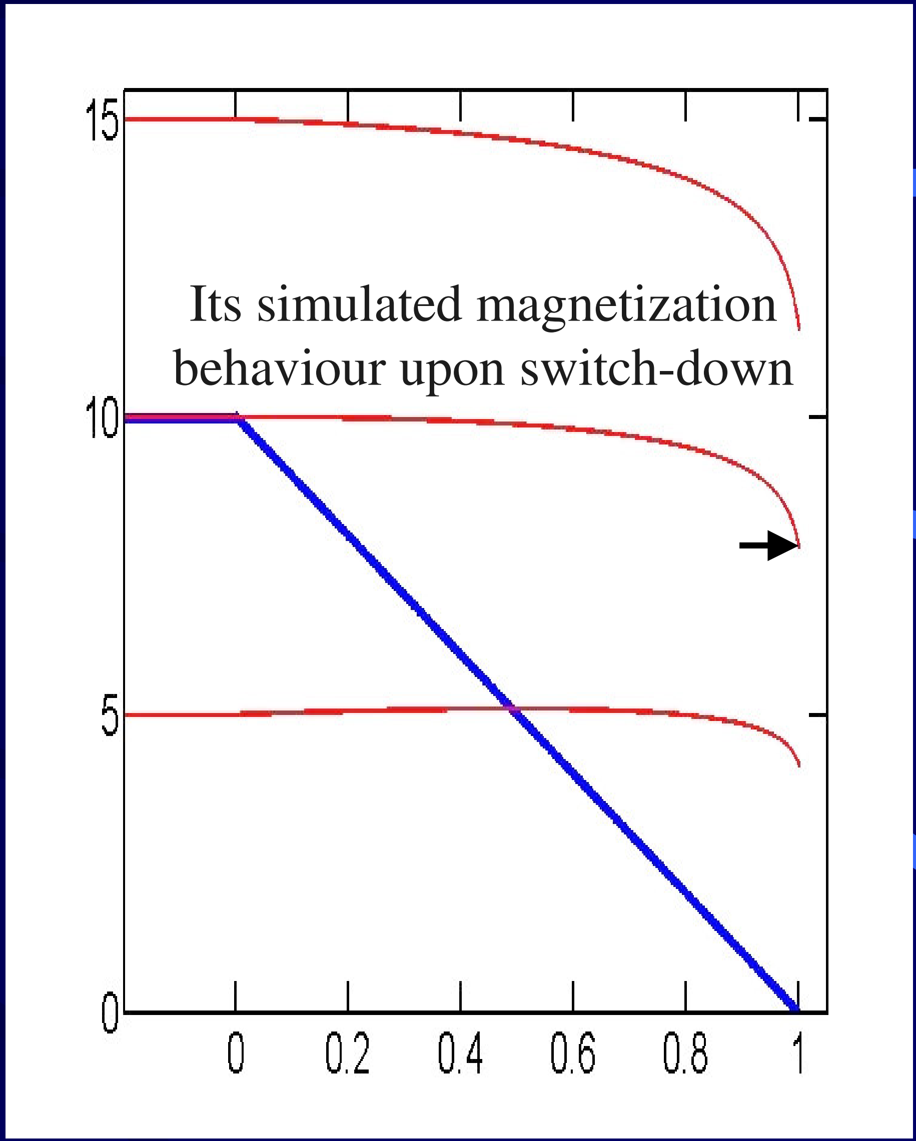
In each tiny step, we have a duration Δt, a final field value B_f, a relaxation rate $R(B_f)$ and an initial magnetization M_i.

From here, one calculates the final magnetization M_f, which then becomes the starting magnetization for the next step:

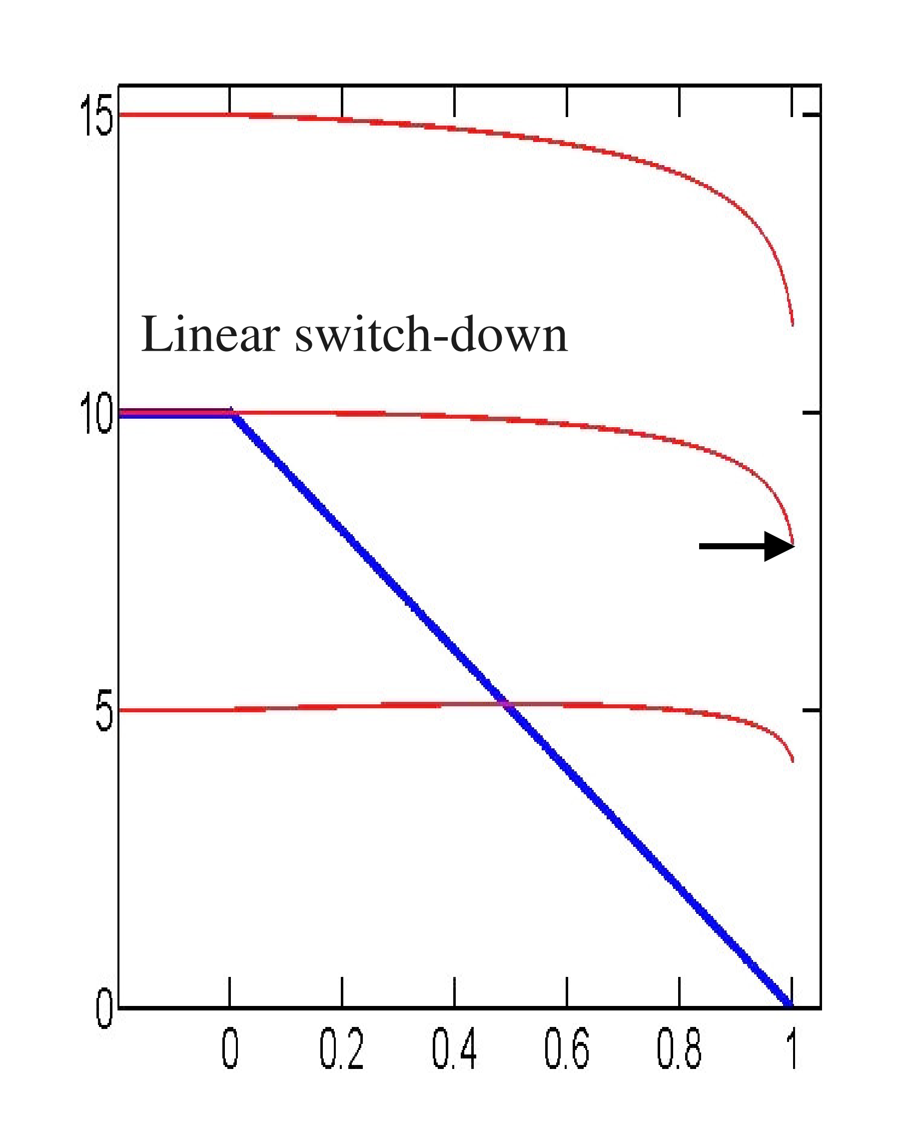
$$Mf = M_i * \kappa + B_f * (1-\kappa), \quad \text{where } \kappa = \exp[-R(B_f) * \Delta t]$$

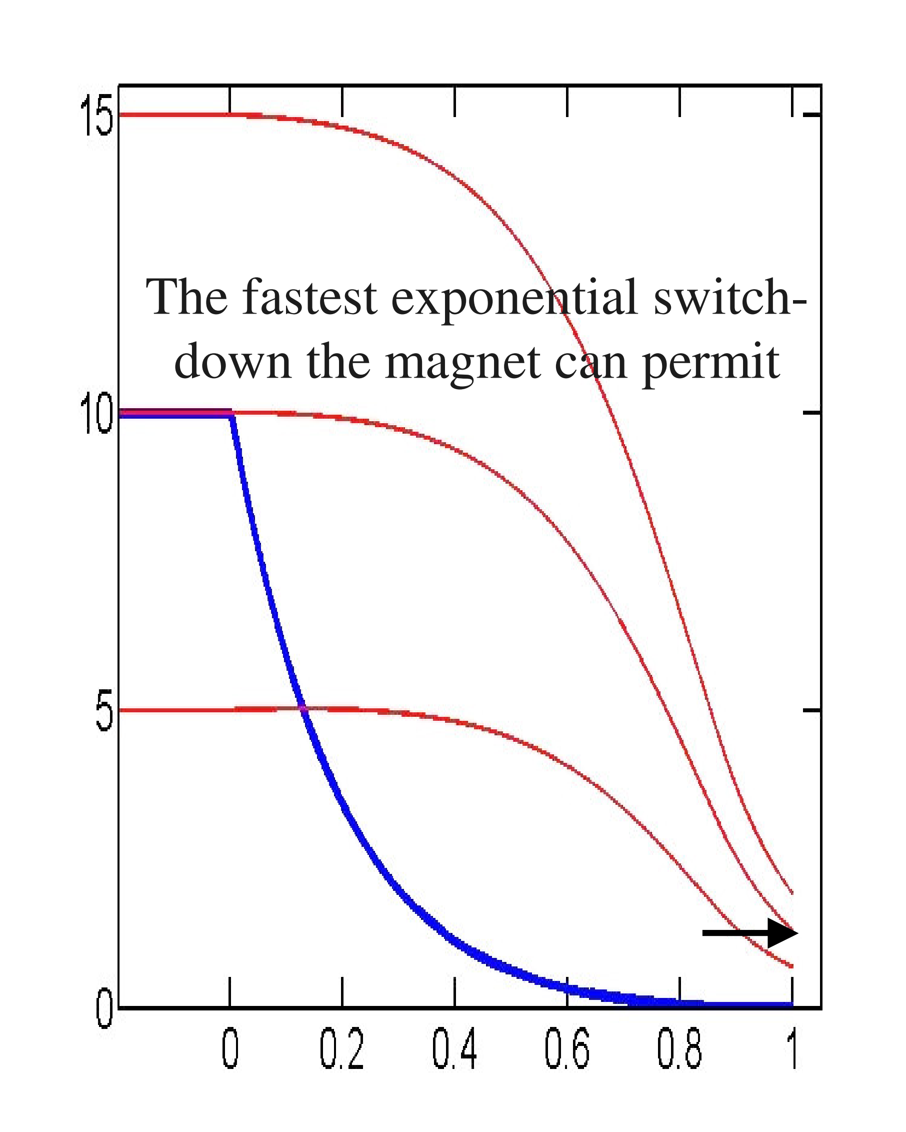
Example of a simulation: a parafilm-type profile





Example of a simulations continued





Explicit solution of the tropostatic case

Since the phenomenological evolution of the parallel magnetization component is described by a first-order differential equation, an "*explicit*" general solution is easily derived.

However, in the case of field-dependent R_1, it anyway requires numeric integration and therefore presents no special advantage over the brute-force numeric method.

But it does permit the clarification of some theoretical aspects and to address questions regarding optimal switching waveforms.

Optimal switching waveforms

I do not want to address this problem here
(for a talk, the formulas are too many and apparently too bulky)

The main conclusions of the variational analysis are:

- There is a large difference between the absolutely fastest field-switching the hardware will permit, and the fastest linear-ramp switching, which is always in favour of the latter.
- The gains from fine-tuning the switching waveform beyond the linear ramp are modest. Since the fastest linear ramp is the only sample-independent waveform, it is best to stick with it.

Generic field variations

We should now consider magnetic field variations which are not tropostatic and thus involve temporal variations of both the amplitude and the direction of a vector.

The most important special case of these are rotations.

The *adiabatic* field-rotation phenomenon …

In Magnetic Resonance, field rotations lead to a quite special phenomenon known as **adiabatic field [direction] switching**. The term is somewhat inappropriate, but it is now too late to try and correct it.

The phenomenon consists in a kind of locking of the nuclear magnetization *direction* to the *direction* of the magnetic field whenever the latter changes sufficiently slowly (in terms of angular velocity) compared with the [amplitude-dependent] Larmor frequency.

… and some of its uses

✓ Transport of polarization from one environment to another:

- Transport of prepolarized gases like ^{129}Xe can be done leisurely (1-3 hours) by any means in weakly magnetized containers.

- The presence of a weak magnetic field is sufficient (and essential) for a successful transfer of polarized substances from an external DNP system (or a para-hydrogen reaction chamber) into an NMR instrument.

✓ MRI in Earth magnetic field [very homogeneous] can be done after prepolarization in a system whose orientation does not need to have anything in common with the direction of the Earth field.

✓ My own interest: what does spin magnetization do in the atmospheres of pulsars (100 MT, *presumably rotating* at 100 Hz).

Why we care about it in FC-NMR

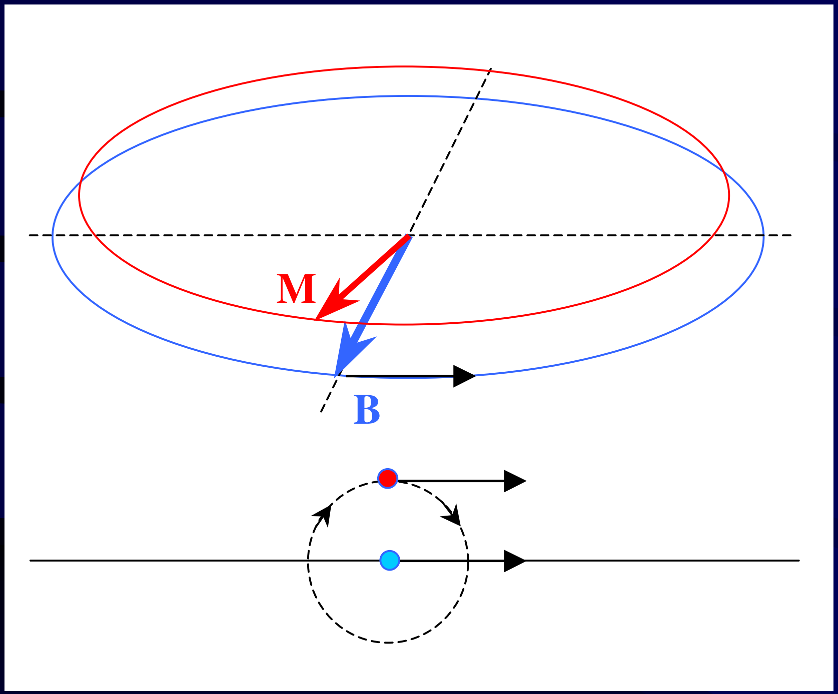
✓ When we switch the main field down to very low values, local fields ("*Earth*" field or whatever) can become appreciable in comparison and change the direction and magnitude of the effectively perceived field and, above all, the direction of the spin polarization generated earlier.

✓ In addition, when the sample is solid or nearly solid, its internal local magnetic fields (dipolar and other) may cause a similar kind of effects, except that now the re-orientations are appqrently random (they can be even dynamic).

✓ We might wish to impose small, perpendicular external magnetic fields which are under our control in order to investigate and maybe exploit what in the above two points appears as a complication.

✓ Controlled zero-crossing FFC techniques (to be developed).

Dynamic stationary-state of the magnetization when locked in a rotating magnetic field



$M_{\perp}\omega_L / M_{\parallel} = \omega_B$

$\tan(\alpha) = M_{\perp}/M_{\parallel} = \omega_B / \omega_L = \beta$,

where:

ω_B is the angular velocity of **B**

ω_L is the Larmor frequency in $|B|$

Additional condition:

$M_{\parallel}$ must be in equilibrium with $|B|$

Capture range, settling time and stability of the adiabatic magnetization lock

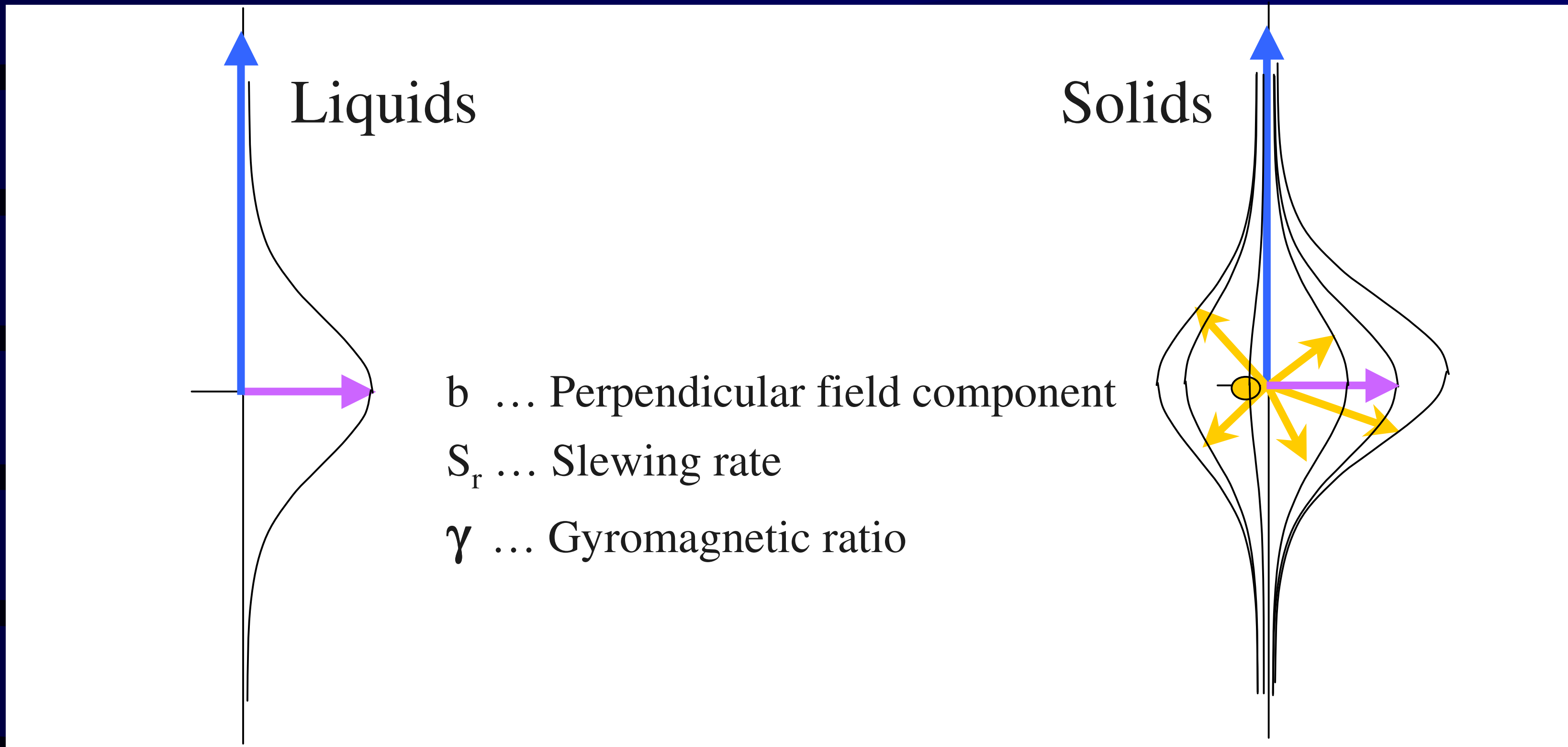
These properties are mathematically rather difficult to handle.

They are higher-order effects in terms of the solutions of Bloch equations in with time-variable magnetic field.

Empirically, adiabatic lock is very efficient whenever $\beta < 1$.

Numeric solutions, though possible, are much “heavier” than in the tropostatic case.

Types of adiabatic locking in FC-NMR



Approximate maximum angular velocity of B: $\omega_B = (S_r/b)/4$

Approximate Larmor frequency in that region: $\omega_L = \gamma b$

Approximate $\beta = S_r/(4\gamma b^2)$

S_r **= 200 T/s (8 MHz/ms),** b **= 50 μT,** ω_B **= 1 MHz,** ω_L **= 2 kHz,** β **= 500**

Unfortunately …

… there is no time left to finish this topic.

But a full-scale paper is coming

Thank you for your attention

and the organizers for giving me the opportunity to talk

Please, visit **www.ebyte.it**
for further details and work-in-progress along these lines.

I am preparing a major review of the topic.