Signal Detection:

virtual photons and coherent spontaneous emission

Stanislav Sýkora

www.ebyte.it/stan/Lecture_ISMRM_2010.html

Presented at the weekend Course *MRI Physics for Physicists*
at 18^{th} ISMRM, Stockholm (Sweden), May 1, 2010

First, an Apology

I consider *virtual photons* mathematical chimeras and I am quite convinced that MR *emissions* are neither *spontaneous*, nor [totally] *coherent*. Provided there *are* any *emissions* ?!

But the title of my talk was not to be discussed, so I just said: *Yes, Sir!*

In any case, *signal detection* is one solid point I am not going to deny! We *do* detect *something* – in many different ways - and it is quite useful.

A historic sketch of the topic

- 1897 P.Zeeman effect: quantum nature of angular momentum (understood later)
- 1925 G.Uhlenbeck – S.Goudsmit: discovery of electron spin
- 1926 O.Stern – W.Gerlach experiment: quantum nature of spin
- 1937 I.I.Rabi's molecular beams: gyrating magnetic fields (RF); ***resonance***
- 1939 I.I.Rabi et al: measurements of nuclear magnetic moments

---

- 1946 E.M.Purcell: CW NMR in MW cavities: ***spectroscopy***
- 1946 F.Bloch: CW NMR in coils: nuclear ***induction***
- 1950 E.L.Hahn: Pulsed NMR: first ***FID*** and ***echoes***

  Start of a controversy: What is FID? Is it a quantum phenomenon?
- 1954 R.H.Dicke: Coherence in Spontaneous Radiation Processes

  Rise of a Paradigm: FID as ***Coherent Spontaneous Emission*** (CSE)

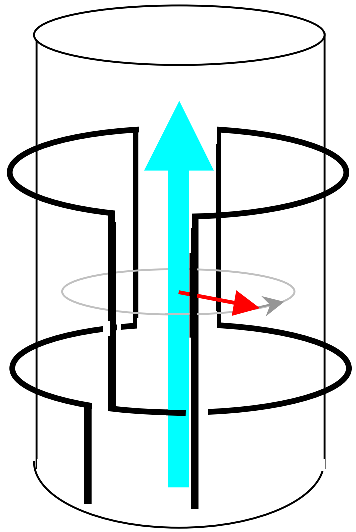
- 1989 D.I.Hoult et al: challenges of the Paradigm (from 1989 to today)
- 2002 J.Jeener, F.Henin: an attempt at full QED treatment
- 2008 L.G.Hanson: who says that quantum mechanics is really needed ☺

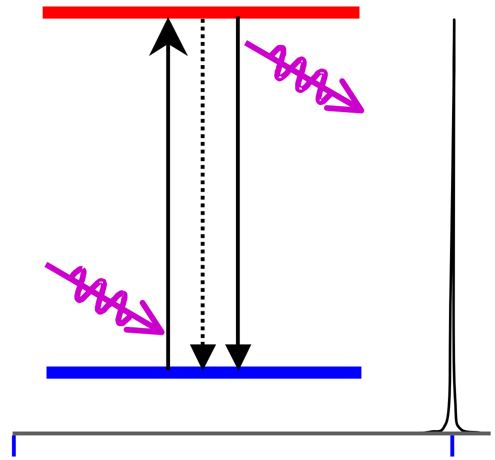
  So, does the Paradigm stink? **Yes, I think so**

  Do I have a better one: **No, I don't**

Do we truly understand Magnetic Resonance ?

$Q < 10^4$





$Q = \omega/\Delta\omega$
$\approx 10^{11}$

CLASSICAL

Engineering,
Bloch equations,
most of MRI,
…

HYBRID

QUANTUM

Sharp spectral lines,
Coupled spin systems,
Operator products,
…

Do we truly understand Magnetic Resonance ?

Not quite!

But to teach it, we select for any given situation the '*explanation*' which appears to suit it best.

Beware:

so far, nothing can replace experiments

CLASSICAL		**QUANTUM**
Engineering,	**HYBRID**	Sharp spectral lines,
Bloch equations,		Coupled spin systems,
most of MRI,		Operator products,
…		...

What is undoubtedly 'quantum' in MR

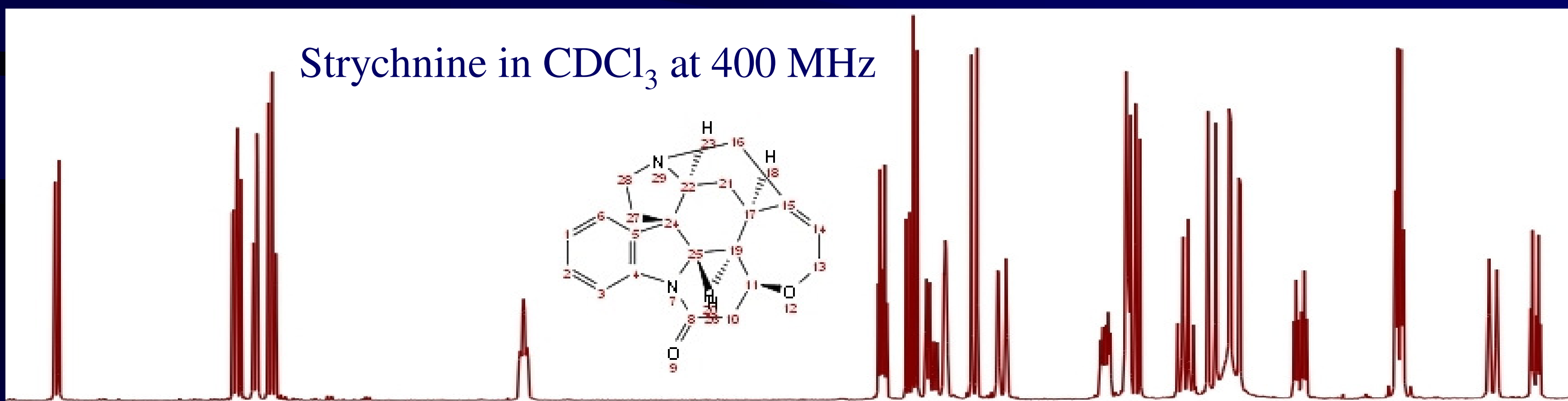
(1) The basic properties of spin (angular momentum)

(2) The existence of half-integer spins

(3) The constant value of magnetic moments

(4) The phenomena observed in single-spin experiments (MFM)

(5) The appearance of HR-NMR spectra of coupled spin systems



A spectroscopist is automatically driven to using terms like ***energy levels*****,** ***transitions*****, and** ***emission*****/absorption of** ***photons***

Quantum example: Simulation of HR-NMR spectra

One can simulate the spectrum of a spin system with its structure graph and its parameters δ_i , J_{ij} and D_{ij}

Quantum mechanical treatment is a must!

The Hamiltonian:

static, motionally averaged, isotropic

$$\mathbf{H} = \Sigma_i \, \delta_i \, \mathbf{I^z}_i + \Sigma_{ij} \, J_{ij} \, (\mathbf{I}_i \cdot \mathbf{I}_j) = \Sigma_i \, \delta_i \, \mathbf{I^z}_i + \Sigma_{ij} \, J_{ij} \, (\mathbf{I^z}_i \mathbf{I^z}_j) + \Sigma_{i<j} \, J_{ij} \, (\mathbf{I^+}_i \mathbf{I^-}_j + \mathbf{I^+}_j \mathbf{I^-}_i)$$

or axially oriented:

$$\mathbf{H} = \Sigma_i \, \delta_i \, \mathbf{I^z}_i + \Sigma_{ij} \, (J_{ij}+D_{ij}) \, (\mathbf{I^z}_i \mathbf{I^z}_j) + \Sigma_{i<j} \, (J_{ij}-2D_{ij}) \, (\mathbf{I^+}_i \mathbf{I^-}_j + \mathbf{I^+}_j \mathbf{I^-}_i)$$

Quantum example: Dimensions of the problem

for N nuclides with spin S = ½

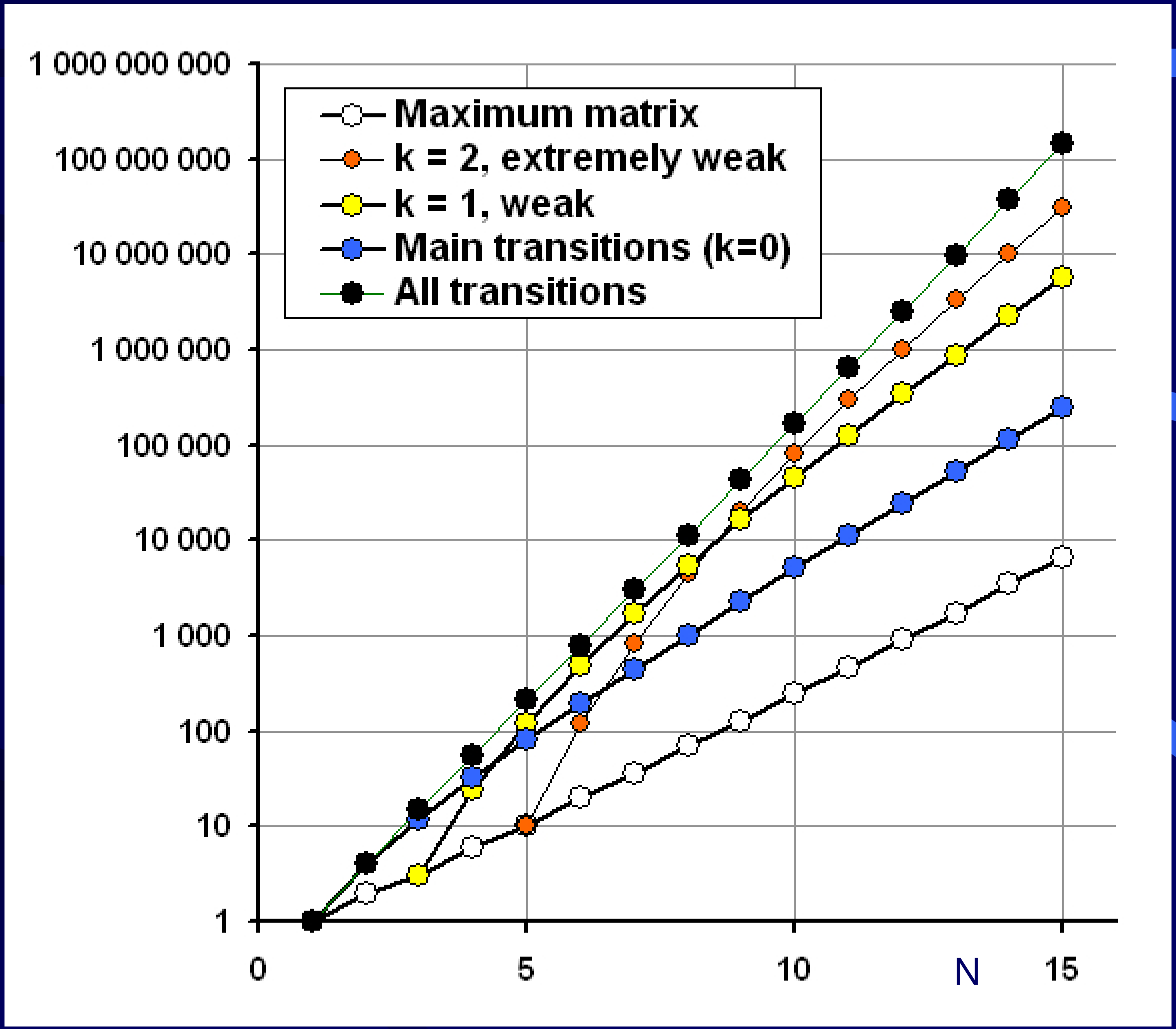
Maximum matrix …
the largest matrix to diagonalize

k …
the transition combination index:
one spin goes up, while k pair
of spins undergo exchange

Weak coupling limit:
transitions with k > 0
have zero intensity.

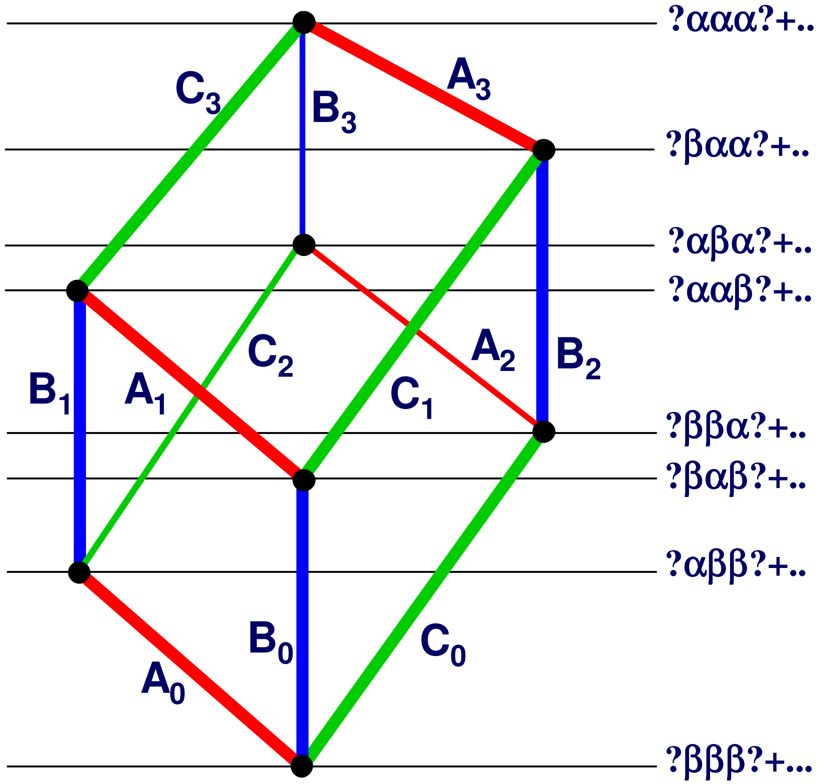
Strongly coupled systems:
transitions with k = 1
must be considered

<u>The numbers are HUGE !</u>



Quantum example: ABC Splitting Theorem

Level diagram and its consequences for an ABC subsystem



Constraints on the 12 main transitions:

$$A_1 - A_0 = B_1 - B_0$$
$$A_2 - A_0 = C_2 - C_0$$
$$A_3 - A_1 = C_3 - C_1$$
$$A_3 - A_2 = B_3 - B_2$$
$$B_2 - B_0 = C_1 - C_0$$
$$B_3 - B_1 = C_3 - C_2$$

These equalities hold no matter how strong are the couplings !!!

What is controversial in MR (1)

If the concept of *radiation emission* is so crucial,

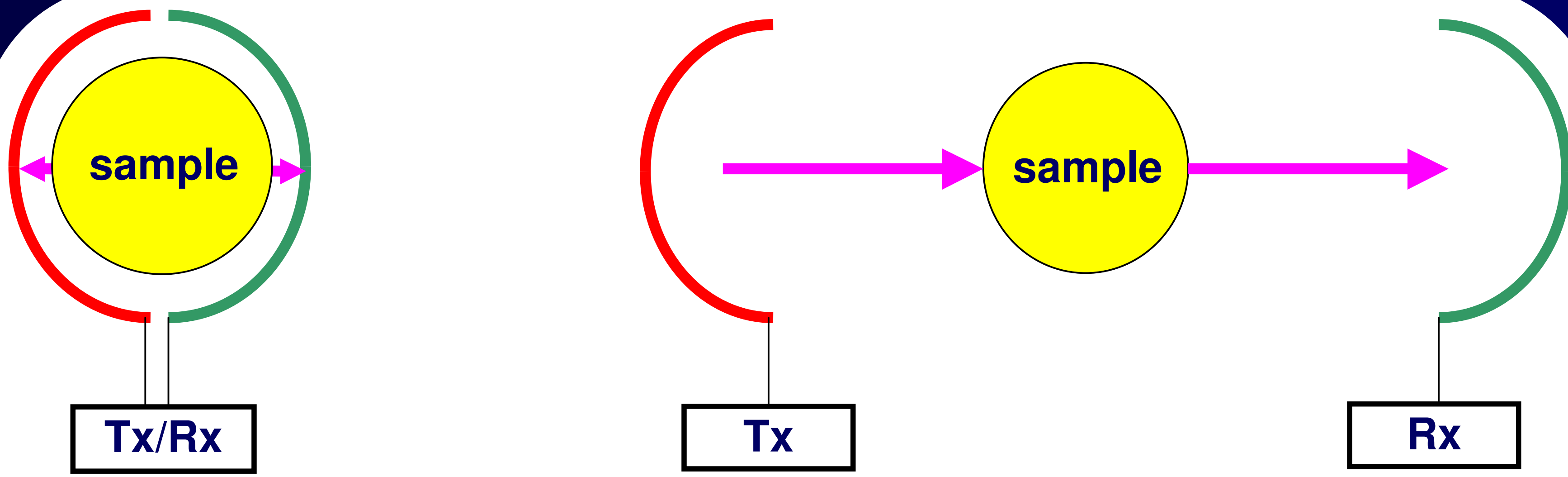
why don't we see any escaping out ?

There are three possibilities:

1) We are not looking carefully enough (unlikely, but possible)
2) There really is NO radiation (and spectroscopists are dumb)
3) It is <u>all</u> VIRTUAL (in which case I declare myself dumb)

What is controversial in MR (2)

Near versus **far** (**remote**) phenomena



NEAR

- $1/R^3$ distance dependences
- **Tx-sample-radiation-Rx** all interact
- Virtual or real photons ???
- QED creation/annihilation operators

REMOTE

- $1/R^2$ distance dependences
- **Sample-radiation** interaction only
- Photons are not virtual
- QED not necessary

Why all other spectroscopies but MR have a remote version ?
Why MW spectroscopy can be both near and remote and MR not ?

What is controversial in MR (3)

Is the phenomenon **stimulated** or **spontaneous** ?

It is not difficult to interpret the CW modality as stimulated.
But FID? The stimulation and detection are separated in time.
Hence the *'spontaneous'* in the **CSE** paradigm.

But spontaneous phenomena are typically incoherent and
in an ensemble cancel out! Hence the *'coherent'* in CSE.
So, is FID a self-stimulating collective phenomenon ?
Something like a maser ?

WAIT!!! I do not buy that at all !!!

All coherent collective phenomena are non-linear.
But MR is demonstrably linear to at least 6 digits.
The very quality of MRI depends on the linearity.

Moreover, coherent (collective) phenomena drive
most of the intensity into a single frequency band.
Hence: no spectra & no fancy MRI k-space data.

Moreover again, HR-NMR spectra are simulated
strictly on molecular basis – and it always works.
Each molecule acts on its own!

So, what coherence there is, it is just temporal,
not spatial (but is that possible?)

What is controversial in MR (4)

Single spin phenomena versus **ensemble** phenomena

- ✓ We need *mixed quantum states* (to explain transversal magnetization)
- ✓ But can a *single spin be in* or *give rise to* a mixed state? (no!)
- ✓ The path from eigenstates to mixed states (interactions needed!)

The *crucial role of relaxation*: without it there would be

- ✓ no Boltzman equilibrium and
- ✓ hence no thermal polarization and
- ✓ hence no signal !

Relaxation implies time-dependent interactions.
Fortunately, there are plenty of those – and very strong ones!
(But nobody seems to care ☹)

Some spherical cows of MR

(1) Single spin:

There is so far just MFM that can detect single spins. They have always seen them parallel or antiparallel to the field, never in a mixed state! A single-spin description in MR is like trying to describe water by considering a single H_2O molecule in deep space.

(2) Classical spontaneous emission estimates:

They invented QM because classical electric dipole (like H atom) would collapse. By definition, quantum eigenstates do NOT radiate!

(3) Discussing MR without considering relaxation:

Though the time dependent relaxation interactions average to zero, they are strong and at any moment interconnect the whole sample.

Alternative signal detection methods

and the lectures they teach us

- ✓ Magnetic Force Microscopy
  Confirms that single-spin detection picks-up only pure eigenstates

- ✓ Noise radiation (more precisely, *noise induction*)
  Shows that spins do not need to be excited: sponateous ‘emission’

- ✓ Electric detection (with S/N similar to induction detection)
  Shows that full-fledged electromagnetic waves are involved

- ✓ Waveguide between the sample and Tx/Rx assembly
  First step in the direction of ‘remote’ MR ?

- ✓ Optically detected magnetic resonance (ODMR)
  So far only with electron spin, but it might bring around a revolution

Central impass: the rise of transverse magnetization

So how do *I* think transverse magnetization arises ?

For nuclei with spin > ½

The transversal magnetization states already exist but cancel out because of incoherent phases.

The RF pulse causes transitions and introduces the phase coherence.

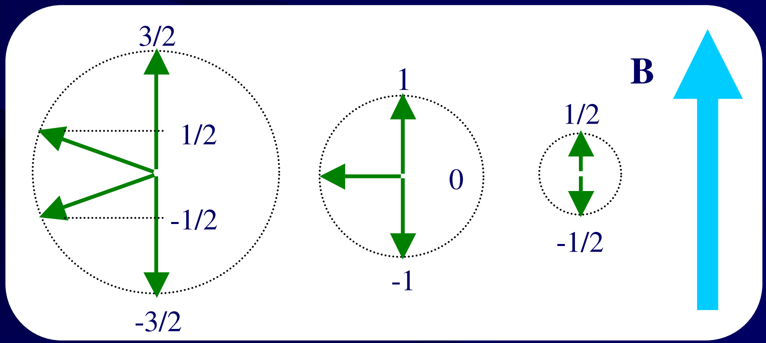
Even so, full explanation of spin > ½ MR still requires to take into account ensemble interactions.

For nuclei with spin ½

(definitely non-classical SO_3 rep.s)

There are no states with transversal magnetization to start with but, as simulations of MR spectra teach us, they immediately arise once we start combining the nuclei thanks to the ensemble interactions.

Talk about the AB => A_2 spin system



QED, virtual photons, etc. ?
Nice, but marginal

Single spin – coil interaction ?
Nice, but marginal

For any theory of MR to be acceptable

each of the many MR phenomena must exclaim

YES, Sir, that's correct!

We are still very far from that goal
and it would be irrational to pretend otherwise!

The Ontology of Photons

- ✓ How does an atomic-size system absorb/emit a 30m wave with a frequency precise to 1 part in 10^{11} and never miss a bit ?

  Scale the spin system to fit a 1m box (factor 10^{10}). Then the wavelength would be 2 au and the complete wave-packet would extend over 300000 light-years.

- ✓ What shape has a photon? Results of a poll of 30 physicists:

  1969: pointlike particle 16, infinite wave 9, wave-packet 3, f**k off 2
  2009: pointlike particle 2, infinite wave 3, wave-packet 9, f**k off 16

- ✓ Can an *indivisible quantum* have a shape and/or a duration ?

  A shape/duration implies component parts, but a quantum can't have any

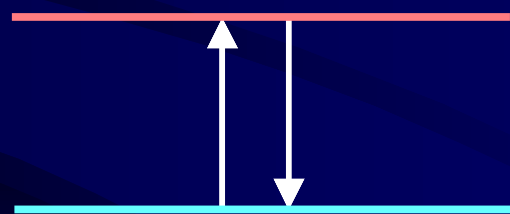
- ✓ Is photon just an *abstraction* of the constraints on energy and momentum exchange ? Max Planck would certainly approve this

What happens *during* a Quantum Transition ?

Quantum physics has NO theoretical apparatus
to answer this question.

By *convention*,

transitions are assumed to be instantaneous.



Can Magnetic Resonance help us to understand better Quantum Mechanics ?

It certainly looks so:

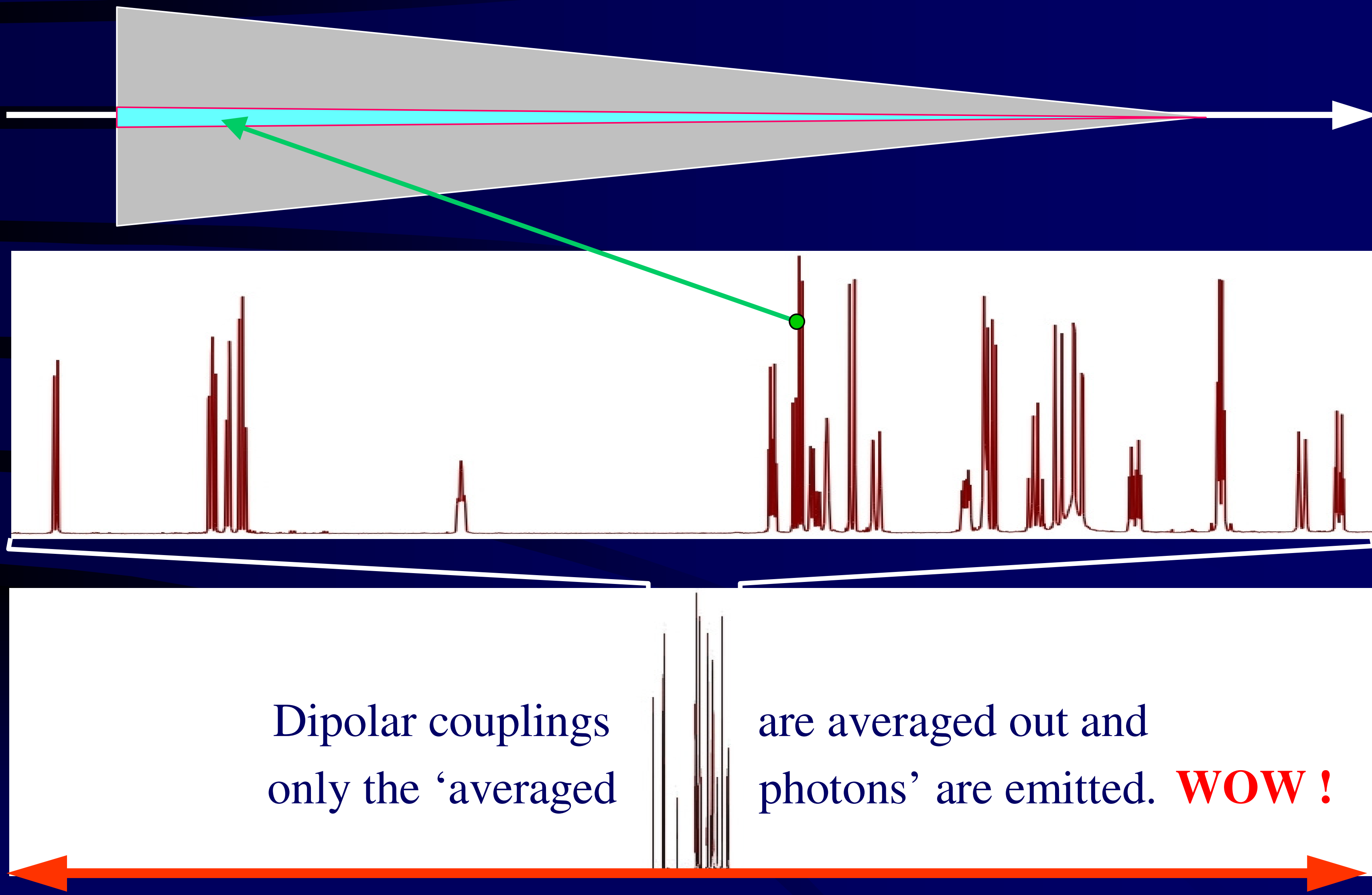
Ontology of Photons:

Among all spectroscopies, MR offers the *longest waves* and the *largest wavelength/linewidth ratios*!
This enhances the quantum physics paradoxes.

Duration of transitions:

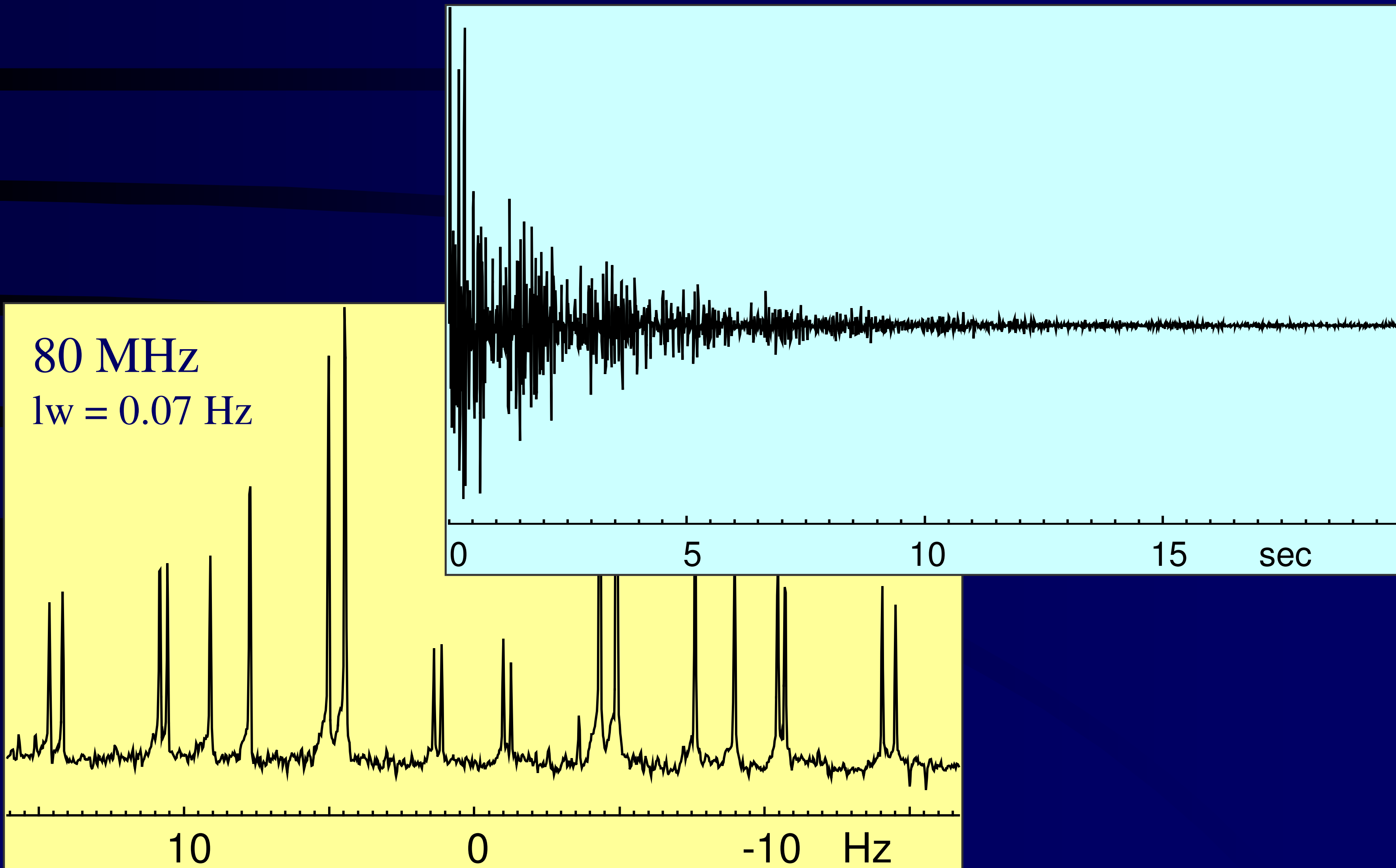
The lines in a HR-NMR spectrum match transitions of the *motionally averaged* spin-system Hamiltonian.
But the required averaging times equal the FID duration.

Might FID be a model of a quantum transition?



Come on, 15 seconds quantum transitions !?

Why not! Quantum physics can't contradict it



Why is MRI the *least controversial* of MR techniques

It is all in the eyes of the beholder ☺ meaning in the Hamiltonian:

$$\mathbf{H = H_Z + H_{SR} + H_C + H_{DD} + H_{DE} + H_F + H_J + H_Q}$$

Energy =	
Interaction with external field(s)	Z (Zeeman)
+ chemical shifts	C
+ indirect couplings	J
+ dipolar interactions with other nuclei	DD
+ dipolar interactions with elettrons	DE
+ contact interactions with electrons	F (Fermi)
+ spin-rotation interactions	SR
+ quadrupolar interactions	Q

MRI can afford to pay attention only to the Zeeman term and to cover all the others either phenomenologically (DD through $T_{1,2}$) or as a minor nuisance. Moreover, just spin ½ nuclides are normally observed!

The role of reciprocity principle

I have gratefully skipped this topic because
it will be covered in another lesson

Spins + Coil system

At this point I must be badly out of my time.
If so, sorry, next time.
If not, I will tell you briefly what I am up to.

Thank You for your Patience

All slides will appear on the web site www.ebyte.it