Do we *really* understand Magnetic Resonance?

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A Philosopher's answer would be

Of course we don't !

Science is not about ***understanding****, it is about* ***describing!***

But I am not a Philosopher. I am just a Physicist.

I try to do my job well, and I am *not* a total failure:

- I tell the engineer how to build an MR instrument.
- I simulate nD spectra of molecules for the chemist.
- I devise ways to produce MR images.

Yet I feel that do not *quite* comprehend my abilities.
If I understood them better, I might do a better job.

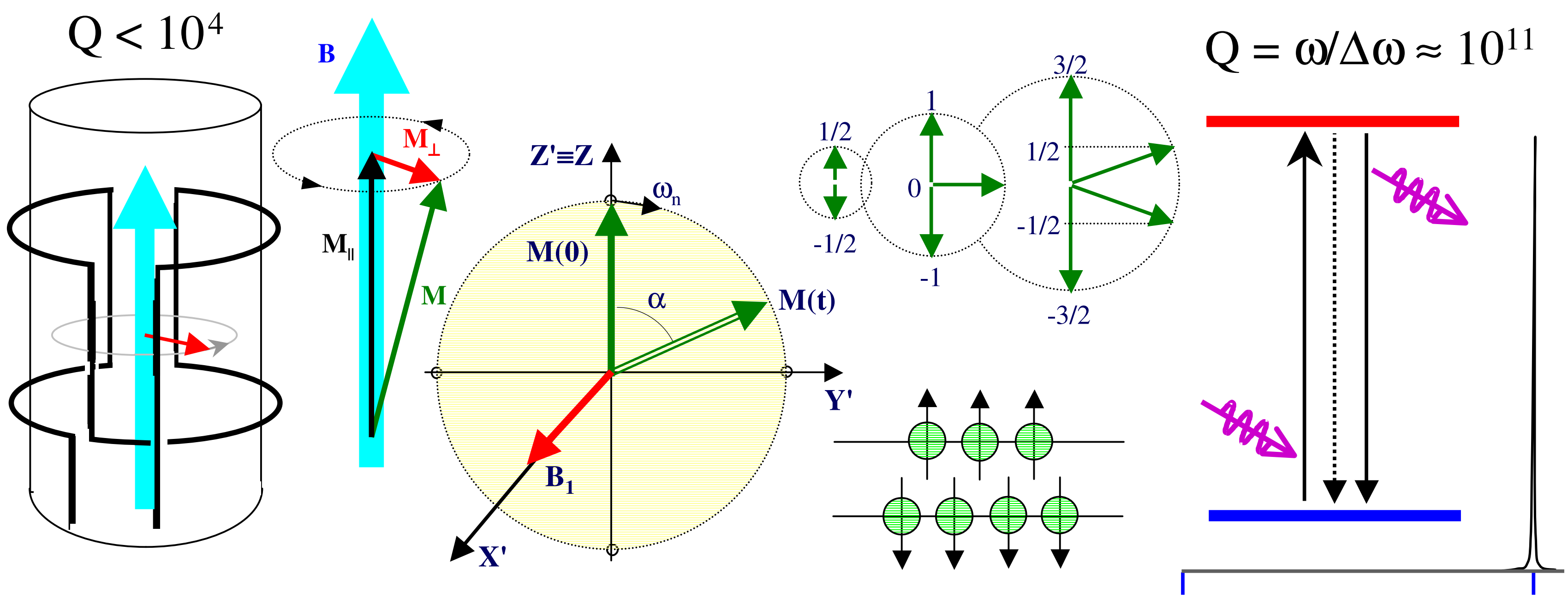
This talk, paradoxically, is about those aspects of MR which I do not *really* understand

Questions, questions, questions …
for which there *should* exist *simple* answers, but …

1) Why do we use different explanations for different aspects of MR ?
2) Which aspects of MR are undeniably quantum and cannot be described classically ?
3) Are Bloch equations classical? Is it *sensible* to try derive them from quantum theory ?
4) Is electromagnetic radiation involved in magnetic resonance? If so, is it true or virtual ?
5) Does spontaneous emission from spin systems occur? If so, what are its properties ?
6) Is MR a *near* or a *far* phenomenon? Is remote excitation and/or detection possible ?
7) Can an FID be described as *coherent spontaneous emission*? What about CW-NMR ?
8) How do the spins interact with nearby conductors, and with the coil ?
9) Which phenomena can be described considering an *isolated* spin, and which can't ?

a) What is the role of relaxation processes in all this? Are they essential or marginal ?
b) What is the role of time-averaged Hamiltonians in magnetic resonance ?
c) Can an FID be described as a sum of individual quantum transitions ?
d) Does all this uncover some gaping holes in quantum physics ?
e) Does all this tell us something about the ontology of photons ?
f) Can MR throw new light on basic aspects of physics ?

! We use *different explanations* for *different MR phenomena* !



CLASSICAL

Induction law,
Bloch equations,
Reciprocity theorem,
Simplified MRI,
…

HYBRID

Thermal equilibrium
Theory of CW-MR
Quantum coherences
Operator products
…

QUANTUM

Coupled spins spectroscopy,
Spin systems dynamics,
Hilbert/Liouville QM,
Density matrix,
…

?? Why is this so ??

We feel that a **Unified Magnetic Resonance Theory** *should* exist !

The reason why it does not *could* be plain laziness but, more likely,

we are still too ignorant to set it up!

A hint:

Some people desire most ardently a

Unified Theory of Everything

and yet it still does not exist!

Nagging doubt: Why should it exist at all?

Is it some separate Law of Nature?

The maze of Physics Paradigms

Basic Concepts:

Conservation principles CP, Interaction-at-distance ID, Potential field PF, Least action LA,
Quantization principle QP, Interference principle IP, Uncertainty priciple UP,
Wave-Particle duality WP, Lorentz invariance LI, Space-time curvature SC,
…

Basic types of Interactions:

- **Strong**
- **Weak**
- **Electromagnetic**
- **Gravitational**

Weak + Electromagnetic → Electro-Weak

Further unifications are pending

Note: this slide and the three following ones were part of a single animation

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…

Ensembles of bodies (particles)	**Classical mechanics** (Lagrange-Hamilton-…)	CM	Lagrange & Hamilton equations
		PS	Physics of phase space (concept?)
		SP	Statistical physics
		TD	Thermodynamics
		…	
	Special relativity (Lorentz-Einstein-…)	SR	Imposes Lorentz-invariance
		RP	Retarded potentials (concept?)
		…	
	Quantum theory (Planck-Einstein-…)	QP	Basic quantum physics
		QM	Quantum (wave) mechanics
		QT	Quantum theory in HL-spaces
		…	
	General relativity (Einstein-…)	GR	Imposes space-time curvature
		…	
	Relativistic Quantum	RQ	Relativistic QM (Dirac)

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…

Fields	**Classical** (Faraday-Maxwell-…)	EMF	Electro-magnetic field
		CWO	Classical wave optics
		CG	Classical gravity
		HD	Hydro-dynamics
		SSE	Solid-state elasticity
		…	
	Quantum-Relativistic (Feynman-…)	QED	Quantum electro-dynamics
		QWO	Quantum wave optics
		QCD	Quantum chromo-dynamics
		QG	Quantum gravity
		EW	Electro-weak theory
		…	
Strings		STR	A Googol of varieties
Etc …		…	Let all the flowers bloom

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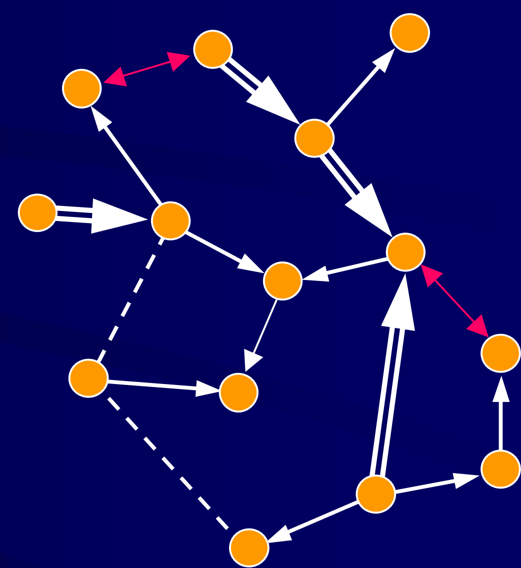
Hybrid aspects	**Wave aspects of particles**	- Schrödinger's wave function in QM - DeBroglie's particle waves (abandoned?)
	Particle aspects of fields	- Second quantization - Virtual particles
	Optics/Photons: a cross-discipline	- Classical wave optics - Classical particle optics - Radiative solutions to Maxwell equations - Quantum aspects of EMF (photons) - Coherence phenomena (laser, maser) - Spontaneus emission - Controversial aspects - Ontology of photon (a total mess)
	Spin physics & MR	- **Where does it fit?**

Physics paradigms are NOT a hierarchy!

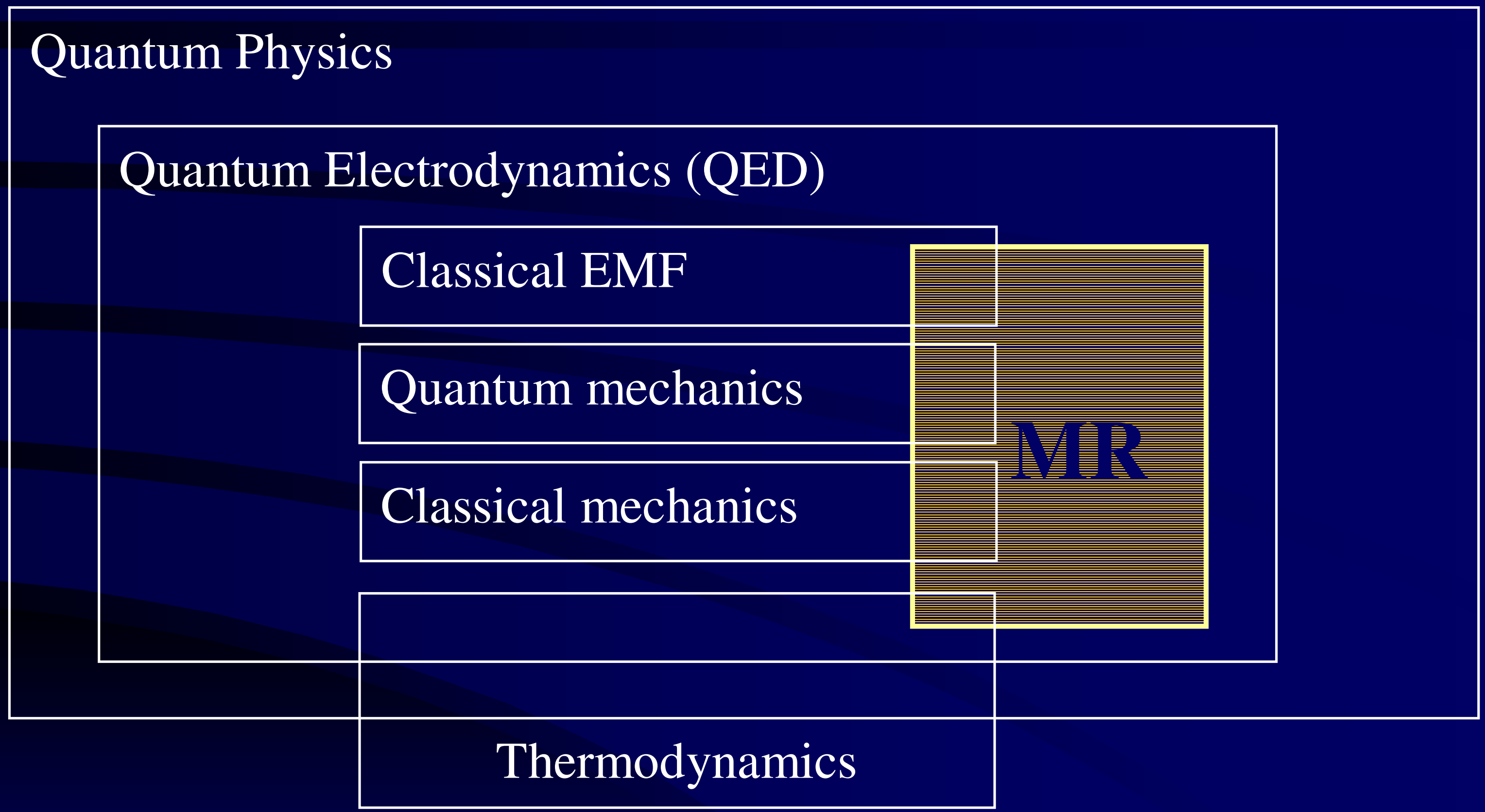
At best, there are very short hierarchic "threads"
interconnected by a maze of edges of different types

- ● Paradigm
- ⇒ is an approximation of …
- → follows from …
- ↔ conflict …
- - - - - some shared elements …



Idea: such a **Graph of Physics** with
vertices for theories and "colored" edges for relationships
could be itself the object of a scientific study

Physics Graph edges congruent to Magnetic Resonance

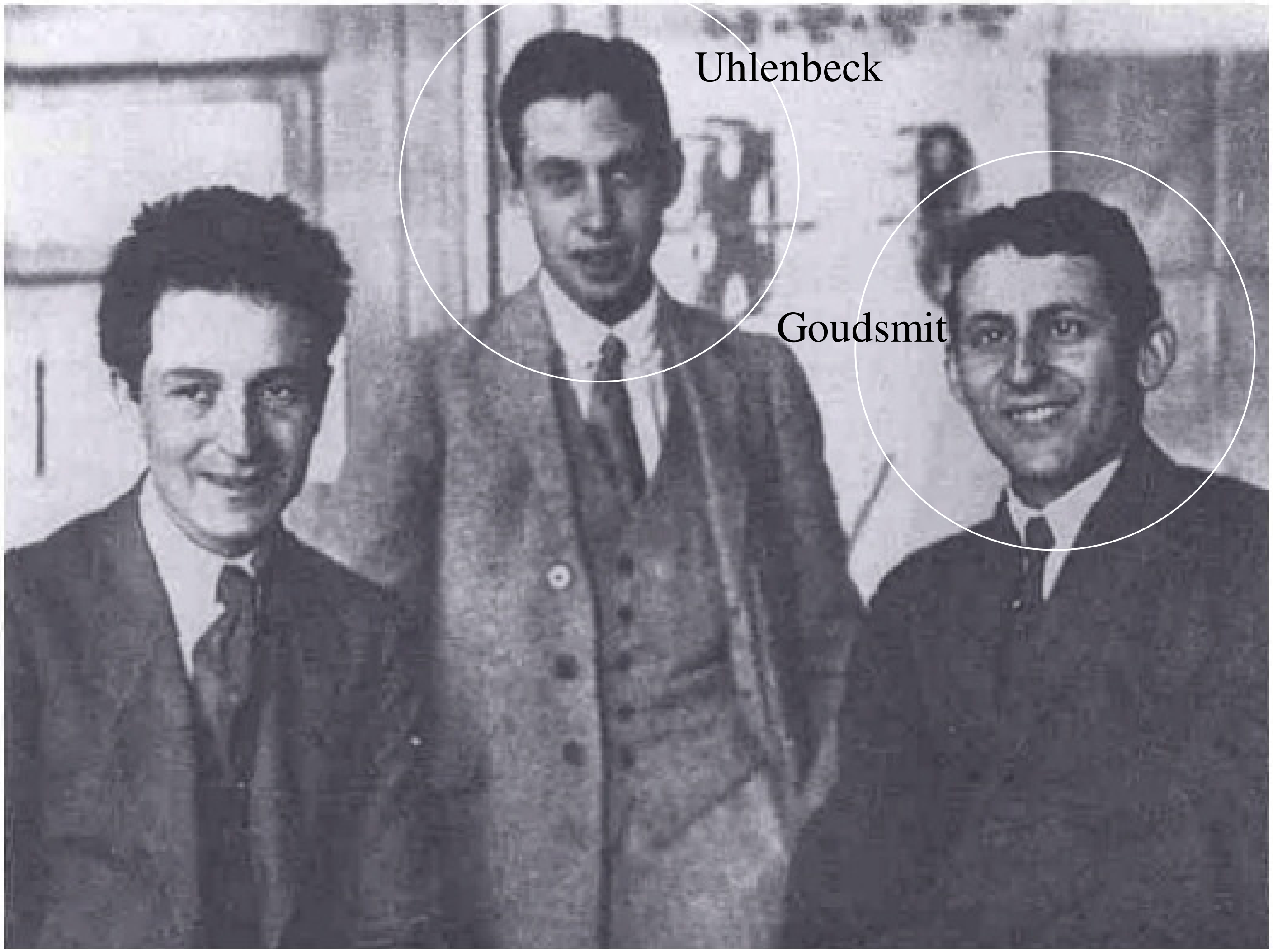


A mini-chronicle of electron spin

- 1897: Pieter Zeeman finds that magnetic field broadens spectral lines
- 1921: Arthur H.Compton advocates axial electrons to explain magnetism
- Atoms have nearly twice the expected number of spectral lines
- In the Wilson cloud chamber, electron trajectories have strange “kinks”
- 1925: Ralph Kronig suggests that electron has an angular momentum (spin)
- Wolfgang Pauli tells him it is a foolish idea and poor Ralph desists !
- Later in 1925: George E.Uhlenbeck & Samuel A.Goudsmit submit a paper to *Naturwissenshaften*, also claiming that electron has a spin
- They show it to the great Hendrik A.Lorentz who deems it impossible !
- They urge the Editor to *please* withdraw the paper, but it is too late !
- Fortunately, further investigations by many physicists prove them correct. The paper becomes a cornerstore of modern physics !
- 1927: a converted Wolfgang Pauli builds the best formal model of spin
- Later: Paul A.M.Dirac, the theoretician, says that *“… a particle with a spin of half a quantum is really simpler than a particle with no spin at all …”*
- In other words: ***what’s all the fuss about, isn’t it trivial to start with ?***

Note: Names in red indicate Nobel Prize winners

The pioneers (electron spin)



1926: Oscar Klein, George E.Uhlenbeck, and Samuel A.Goudsmit.
Courtesy of AIP Emilio Segré Visual Archives

Which aspects of MR are definitely quantum?

There are particles of many kinds

and *all* the particles of *each kind* are *exactly* alike,

and *some kinds* have a *permanent*

half-integer spin

and thus an *immutable*

angular momentum,

a *spinor*, associated with a

magnetic moment,

which is a vector.

$\mathbf{M} = \hbar\mathbf{S}$ $\quad \boldsymbol{\mu} = \gamma\mathbf{M}$ $\quad \hbar$ ... Planck constant, γ ... gyromagnetic ratio

Plus, all particles obey the *exclusion principle*!

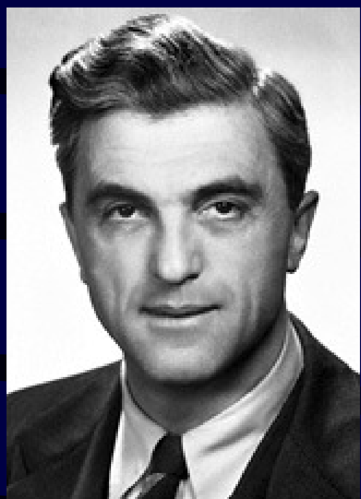
This much was clear already in 1938 and is still looks true today

Are Bloch equations classical?

There is no doubt about that, both historically and *de-facto*

They are classical, phenomenological, unpretentious

They just encapsulate BASIC observations



$$d\mathbf{M}/dt = (\mathbf{L}+\mathbf{R}) \cdot (\mathbf{M}-\mathbf{M}_\infty)$$

$$\mathbf{L} = \begin{Bmatrix} 0 & (\omega-\omega_r) & 0 \\ -(\omega-\omega_r) & 0 & 0 \\ 0 & 0 & 0 \end{Bmatrix}, \quad \mathbf{R} = \begin{Bmatrix} -R_2 & 0 & 0 \\ 0 & -R_2 & 0 \\ 0 & 0 & -R_1 \end{Bmatrix}$$

A problem is that they deal only with
the magnetization vector but not with the associated spin

This is convenient for the NMR or MRI engineer, but completely
useless for the NMR spectroscopist who deals with spin systems

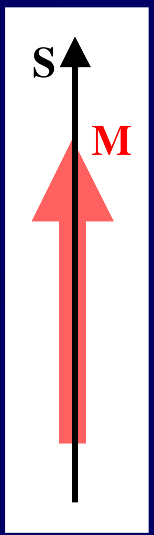
Does it make sense to derive Bloch equations from Quantum Physics?

Such derivations are a staple in courses for physicists, using widely varying assumptions. They invariably show that QM is *<u>not in conflict</u>* with Bloch equations, but they don't tackle the strong coupling between the spin and magnetization subspaces.

In principle we have:

Spin coordinates:	1	$\lvert\sigma\rangle$	discrete
Magnetic moment coordinates:	3	(x,y,z,t)	continuous

Hilbert spin space:	(2S+1) - dimensional
Hilbert space of magnetic moment:	$\propto$ - dimensional



The *non-quantized* magnetic moment **m** and the *quantized* spin **S** are tightly bundled at a sub-particle level: $\mathbf{m} = \gamma h \mathbf{S}$

The duality of Spin and Magnetic moment

The ***strong bundling*** between spin and magnetic moment makes it possible to limit oneself to just one of the two “spaces”, but only in special cases such as when studying the magnetization of an ensemble (engineering) or exploring the spin space of a coupled spin system (NMR spectroscopy).

- **The spin confers quantum properties of angular momentum to the magnetization**
- **The magnetization confers to the spin a way to manifest itself in ‘our’ space**

If we take care of one of these two aspects, the other *“will take care of itself”*
Unless we need to follow both simultaneously, we can get away with a partial description:

That is what Bloch equations are:
a partial description of reality based on the magnetization vector

The opposite case is represented by the whole of MR spectroscopy, where
the Hilbert/Liouville quantum set-ups use only spin spaces and Hamiltonians
Hilbert: $\mathbf{H}\,|\sigma\rangle = \lambda\,|\sigma\rangle$, $|\sigma\rangle = \Sigma_i\, c_i\, |\sigma_{Ai}\rangle\, |\sigma_{Bi}\rangle \ldots |\sigma_{Xi}\rangle$
Liouville: $\mathbf{L}$ … the space of all linear operators on $\mathbf{H}$

Hybrid/more complete descriptions:
- Product wave functions in atomic/molecular physics $|\Psi\rangle = |\sigma_{spin}\rangle\, |\psi(\mathbf{r},t)\rangle$
- Dirac’s equations for leptons and muons

The Hamiltonian of a spin system

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

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

This is just to say that even the partial descriptions do not need to be simple.
Historically, once the concept of a spin-system Hamiltonian arose,
it soon became sophisticated.

Further indications that there is more at stake

- ✓ **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 radiation might be involved
- ✓ **Magnetic Force Microscopy**
  Confirms that single-spin detection picks-up only pure eigenstates
- ✓ **Waveguide between the sample and Tx/Rx assembly**
  First step in the direction of ‘remote’ MR

The mysteries of an [isolated] spin S

$\langle S_z \rangle \neq 0$

$\langle S_x \rangle = \langle S_y \rangle = 0$

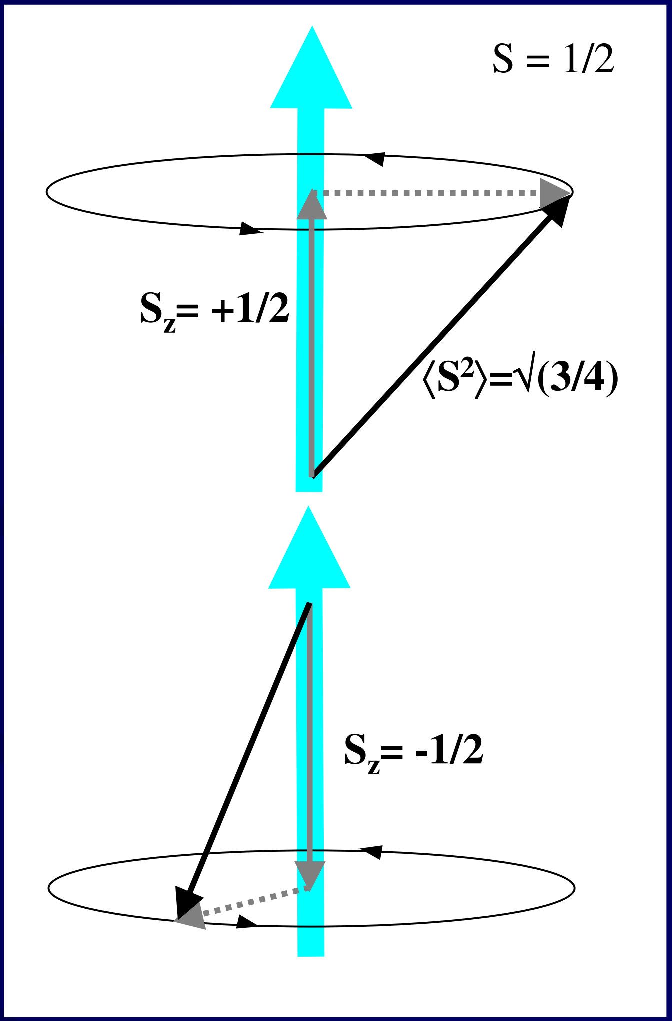
$\langle S_x^2 \rangle = \langle S_y^2 \rangle = \langle S_z^2 \rangle = \langle S^2 \rangle/3$

$\langle S_\perp^2 \rangle = 2\langle S^2 \rangle/3$

Precise value of S_z =>
undefined azimuth angle
(an uncertainty relation)

Vice versa:
nonzero $S_\perp$ => *fuzzy* S_z

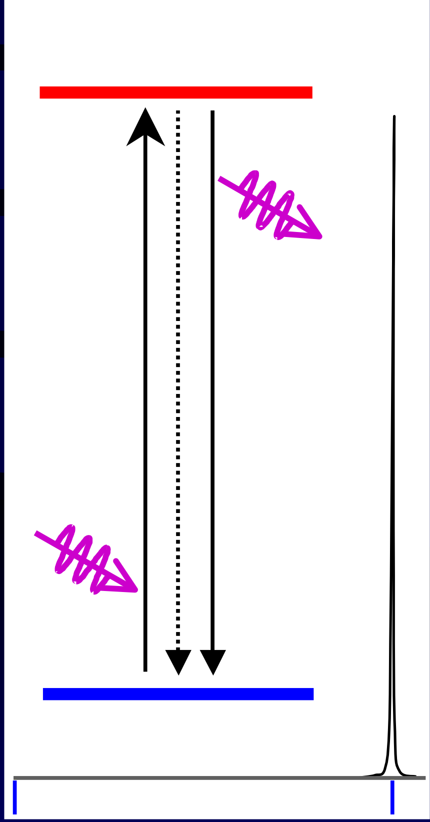
This happens only when S_z is not a true eigenstate, i.e. when S is NOT isolated

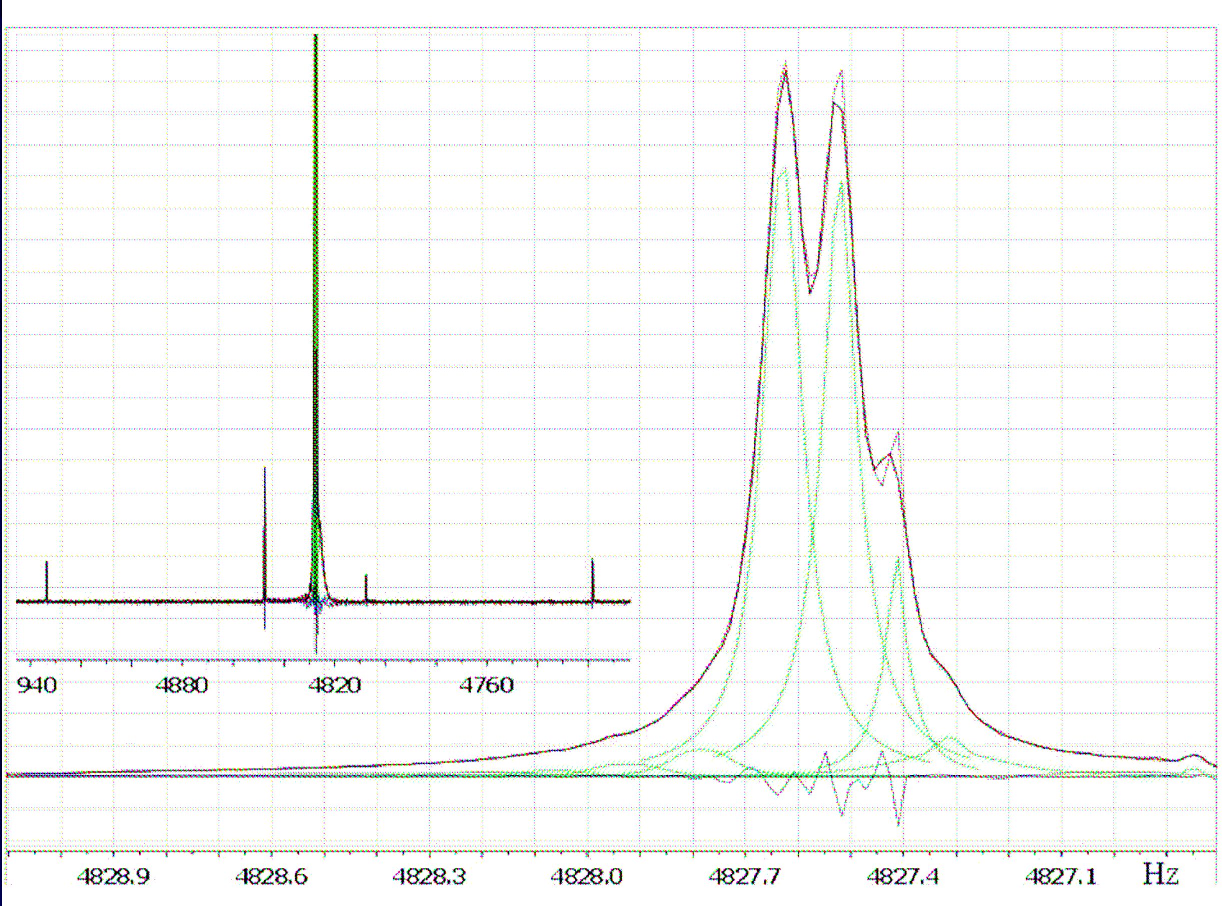


Is electromagnetic spin-radiation involved?

When we see sharp spectral lines and transitions between energy levels, we instinctively think about absorption and emission of photons.

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

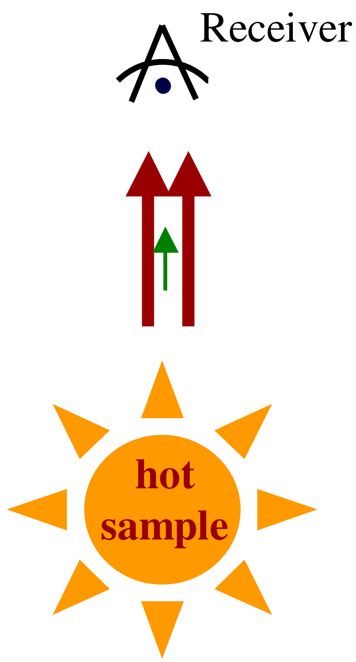




Ok, but then, why we never see it ?

Why can't we have a *remote* MR Spectroscopy ?

Passive emission

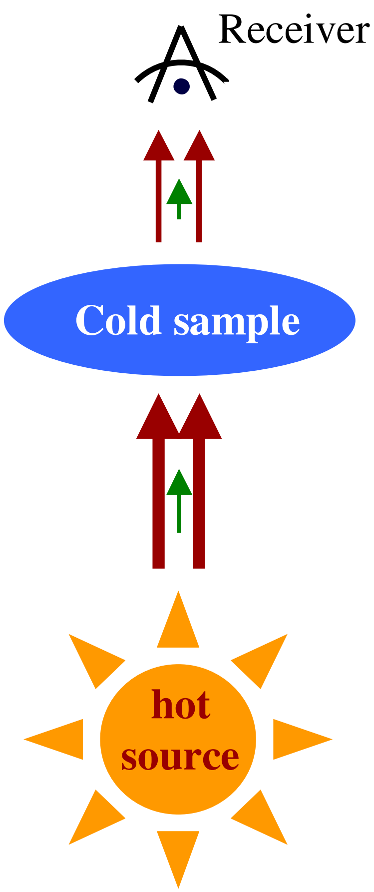


We must separate the desired signal from the bulk

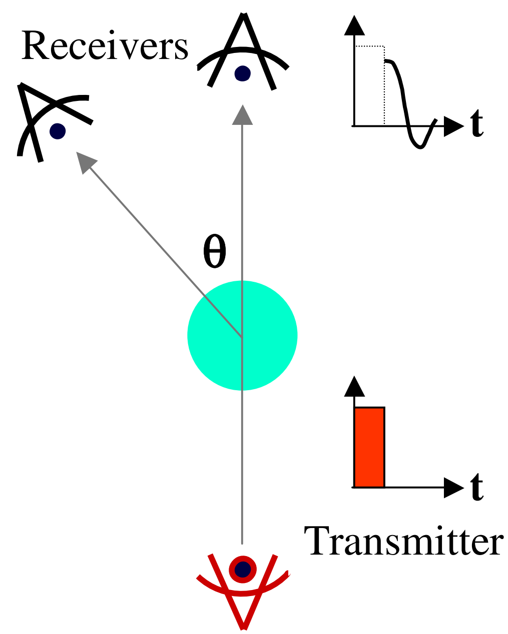
We need:

- Special signal features
- Sophisticated receiver

Passive absorbtion



Active absorbtion
Stimulated emission
Fluorescence



Here we have also θ and t to play with, but we need more hardware

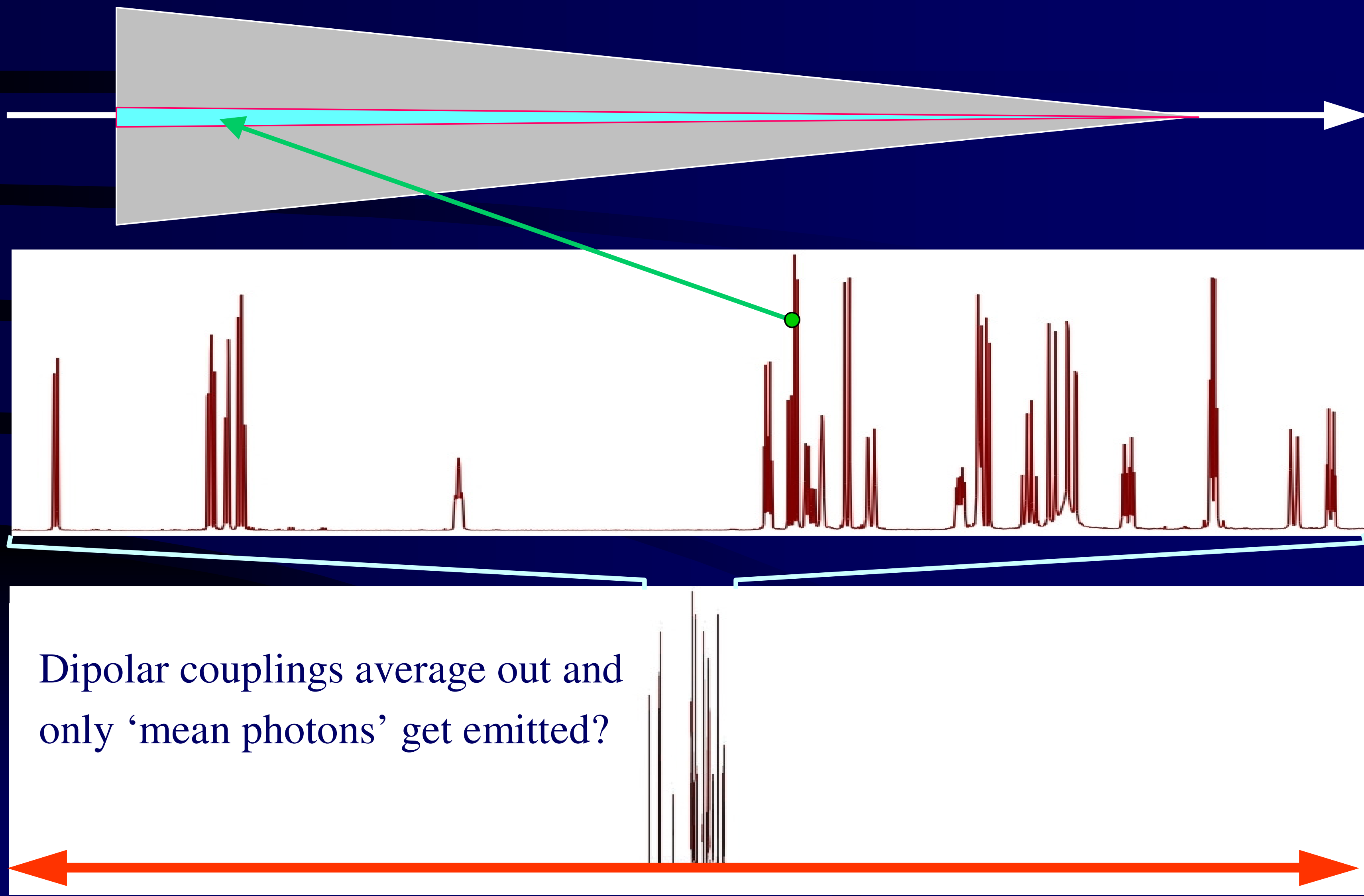
No radiation seems to escape the sample

Is it because it is there, but we do not look well enough?
In which case, what specific properties it might have?
Frequency, chirality, directionality

Is it because there is no radiation and our intuition is wrong?
In which case, how do the spins interact with the coil?
Magnetic coupling to electrons in the coil,
Field-theory with virtual photons,
Quantization of the coil current
($H = \gamma\, \mathbf{S.B} + \kappa\, \mathbf{S}.\boldsymbol{\tau}_{coil}\, j$)
?

FID's of time-averaged quantum systems

a mind-boggling puzzle



So what really is an FID?

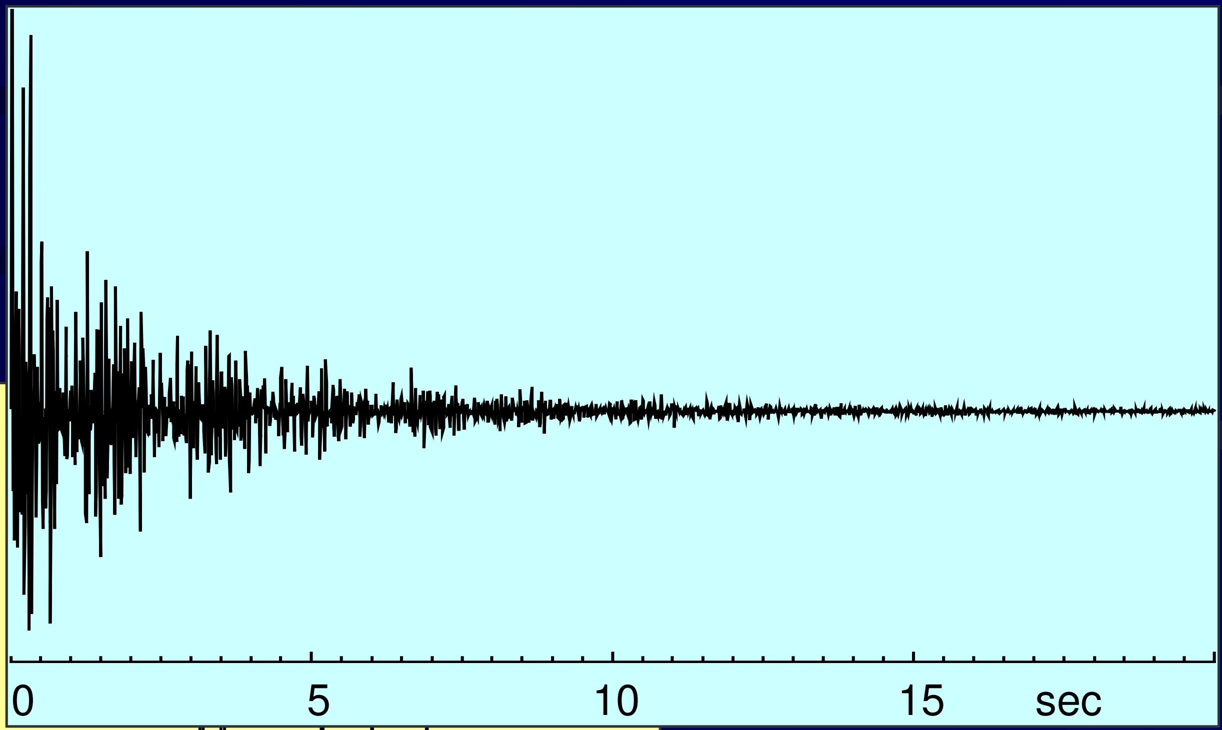
? *Coherent spontaneous emission (Dicke)*

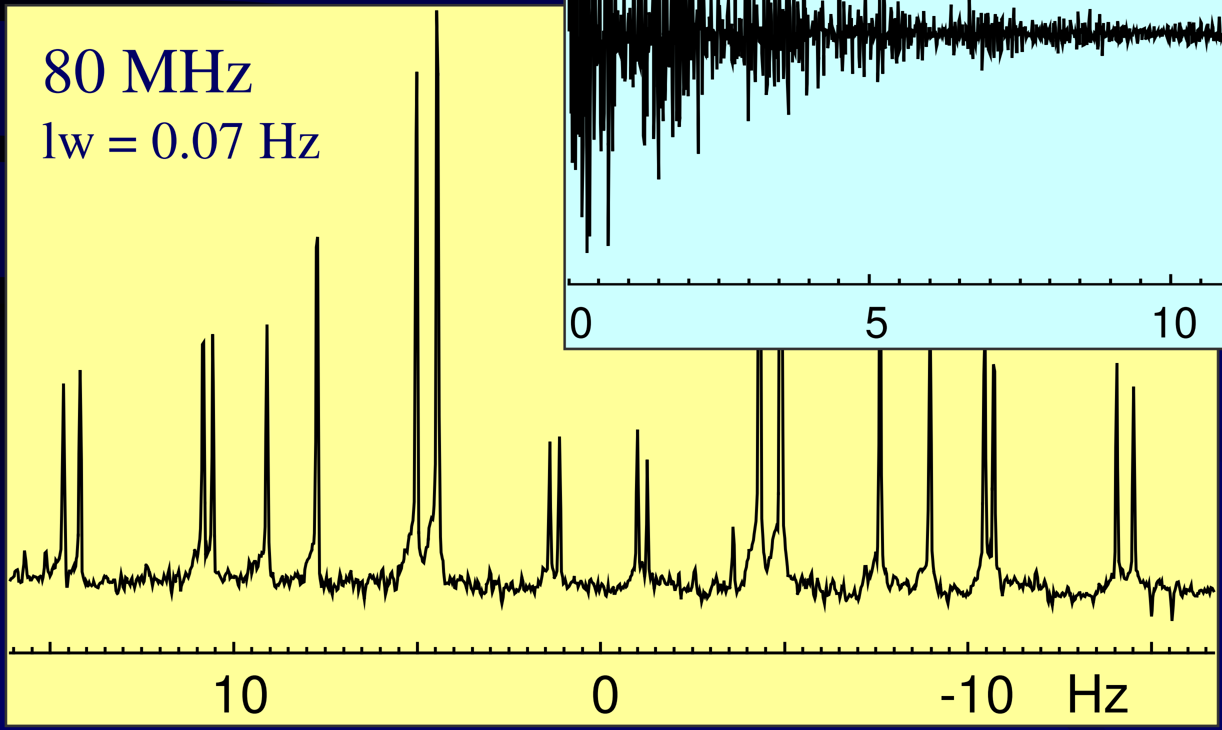
? A *swarm* of *brief, pulse-like transitions*

? A *superposition* of many *long transitions*

Quantum transitions lasting 15 seconds !?

Why not! Quantum Physics can't contradict it





Transitions in Quantum Physics?

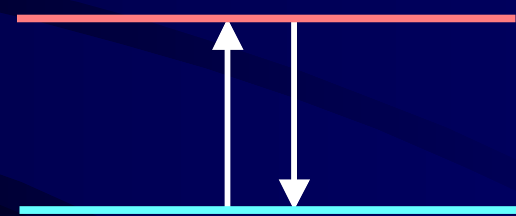
Consider just this:

Quantum Physics has NO *apparatus* to tell us

what happens *<u>during</u>* a Quantum Transition!

By *convention*, and *convention* only,

transitions are assumed to be instantaneous.



Another puzzle that I like: *Ontology* of *Photons*?

- ✓ **How does an atomic-size system absorb/emit a 3m wave with a frequency precise to 1 part in 10^{11} and never miss any bit of it ?**

  Scale the spin system to fit a 1m box (factor 10^{10}). Then the wavelength would be 0.2 au and the complete wave-packet would extend over 30000 light-years.

- ✓ **What is the shape of 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 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

MR is in pole position to help filling some Quantum Physics gaps

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.

Thank you for your patience

Please keep visiting

Stan's Hub*

and, should you have any novel idea

about any of the problems discussed,

let me know and alleviate my

IGNORANCE

* Google '*stan nmr*'