Some Thermodynamic and Quantum Aspects of NMR Signal Detection

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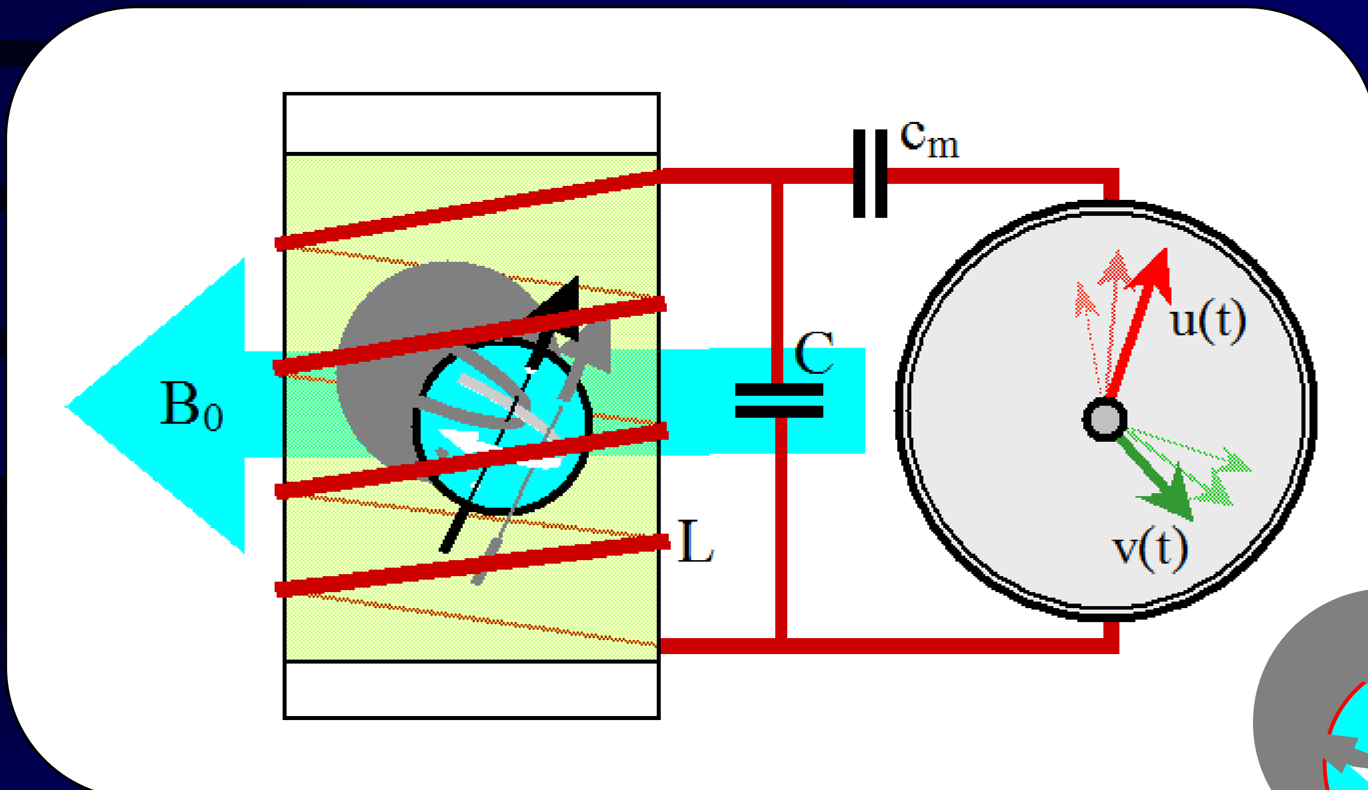
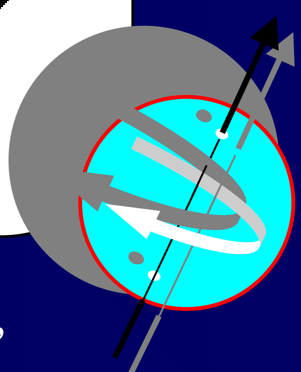




Presented at *6th BFF on Magnetic Resonance Microsystem*,
Saig/Titisee (Freiburg), Germany, 26-29 July 2011

Controversies about the nature of NMR signal and its most common modes of detection

There is a growing body of literature showing that the foundations of Magnetic Resonance are not as well understood as they should be

Principle articles:

Bloch F., *Nuclear Induction*, Phys.Rev. 70, 460-474 (1946).

Dicke R.H., *Coherence in Spontaneous Radiation Processes*, Phys.Rev. 93, 99-110 (1954).

Hoult D.I., Bhakar B., *NMR signal reception: Virtual photons and coherent spontaneous emission*, Concepts Magn. Reson. 9, 277-297 (1997).

Hoult D.I., Ginsberg N.S., *The quantum origins of the free induction decay and spin noise*, J.Magn.Reson. 148, 182-199 (2001).

Jeener J., Henin F., *A presentation of pulsed nuclear magnetic resonance with full quantization of the radio frequency magnetic field*, J.Chem.Phys. 116, 8036-8047 (2002).

Hoult D.I., *The origins and present status of the radio wave controversy in NMR*, Concepts in Magn.Reson. 34A, 193-216 (2009).

Controversies about the nature of NMR signal and its most common modes of detection

This author's presentations:

Magnetic Resonance in Astronomy: Feasibility Considerations, XXXVI GIDRM, 2006.

Perpectives of Passive and Active Magnetic Resonance in Astronomy, 22nd NMR Valtice 2007.

Spin Radiation, remote MR Spectroscopy, and MR Astronomy, 50th ENC, 2009.

Signal Detection: Virtual photons and coherent spontaneous emission, 18th ISMRM, 2010.

The Many Walks of Magnetic Resonance: Past, Present and Beyond, Uni Cantabria, Santander, 2010.

Do we really understand Magnetic Resonance?, MMCE, 2011.

Slides and more info: see

www.ebyte.it/stan/SS_Lectures.html

Questions, questions, questions …

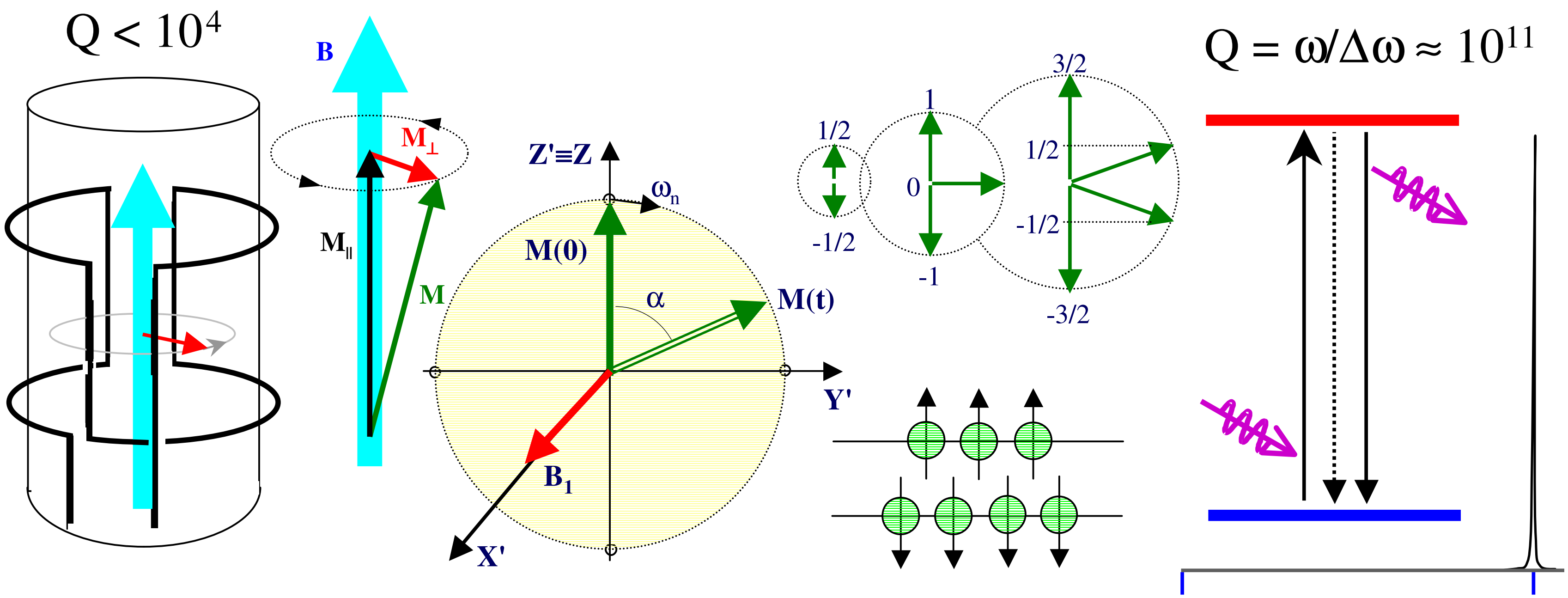
for which there *should* exist *simple* answers, but … do they?

(we have no time for these points now, but I have a handout and we can discuss them during the meeting)

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 descriptions* for *different MR phenomena* !



CLASSICAL	HYBRID	QUANTUM
Induction law,	Thermal equilibrium	Coupled spins spectroscopy,
Bloch equations,	Theory of CW-MR	Spin systems dynamics,
Reciprocity theorem,	Quantum coherences	Hilbert/Liouville QM,
Simplified MRI,	Operator products	Density matrix,…

The principle difficulty:

How to reconcile the manifestly quantum aspects of MR phenomena with the totally classical nature of the detection/excitation devices

Possible ways to tackle the problem

A. Rely on paradigms shared by both classical and quantum physics
Thermodynamics, Conservation Laws and (some) Statistical Physics
A problem: the approach provides good insights but remains incomplete

B. Approximate quantum spin systems in a classical way
A problem: arisal of a transversal magnetization from parallel spin eigenstates

C. Provide a quantum description of the detection/excitation devices
A problem: apparent complexity and necessity to conform to classical results
An extra task: how to couple the spin system to the detection/excitation device

The two parts of this talk:

A. **Part I: Classical paradigms shared also by quantum physics**
   Thermodynamics, Conservation Laws and (some) Statistical Physics

B. **Approximate quantum spin systems in a classical way**
   A problem: **everybody does this since 50 years, therefore I don't dig it**

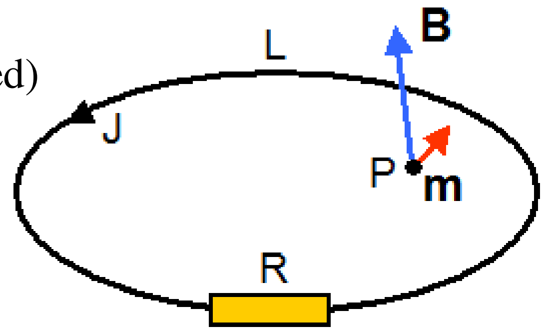
C. **Part II: Quantum description of the detection/excitation devices**
   An extra task: coupling the spin system to the detection/excitation device

Let us forget quantum physics for a while ☺

and remember just the conservation of energy (the first law of thermodynamics)

The physical system we will consider:

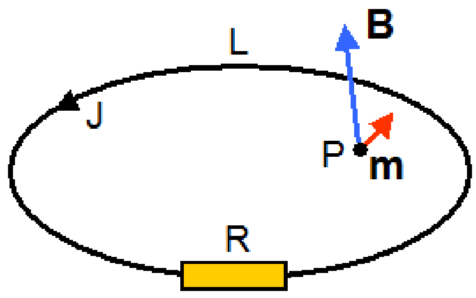
L	Loop and its Inductance
R	Resistance (may be distributed)
J	Electric current
P	just a Point
B	Magnetic Field
m	Magnetic Dipole



$\mathbf{B} = \mu\mathbf{H} = \mu\beta J\boldsymbol{\tau}_\beta$, where
μ is the permaebility, β a constant, and $\boldsymbol{\tau}_\beta$ a unit vector.
β and $\boldsymbol{\tau}_\beta$ depend only on the system's geometry.

$\mathbf{m} = m\boldsymbol{\tau}_m$, where $\boldsymbol{\tau}_m$ is a unit vector along $\mathbf{m}$

Setting up a master equation



Energy terms:

Inductive: $E_L = LJ^2/2$

Self-energy of **m**: $E_m = km^2/2$

Interaction: $E_i = -\mathbf{m}.\mathbf{B} = -\kappa mJ$,

where $\kappa = \mu\beta(\tau_\beta.\tau_m)$

Dissipation: $dE/dt = -J^2R$

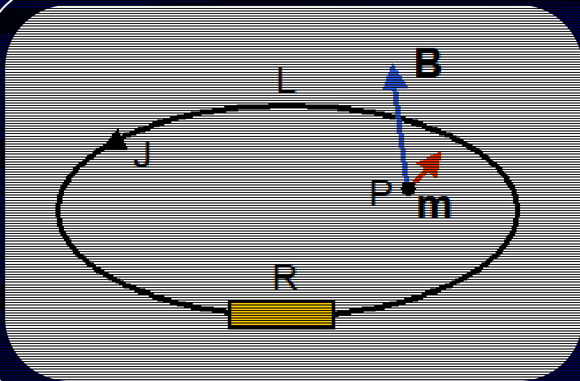
Since R is the only dissipative element in the circuit, the energy conservation law dictates

$$dE/dt = dE_L/dt + dE_i/dt + dE_m/dt = -J^2R$$

Hence, using the apostrophe to denote time derivatives,

$$\boxed{(LJ - \gamma m)J' - \kappa m'J + RJ^2 + kmm' = 0}$$

… a couple of useful notes …



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Dissipation: $dE/dt = -J^2R$

† Since $E_L = LJ^2/2$ and also $E_L = \int_V |B|^2 d\tau/2\mu = \mu J^2 \int_V \beta^2 d\tau/2$,

we have $L = \mu \int_V \beta^2\, d\tau = \mu \langle\beta^2\rangle V$

showing that, upon scaling, β correlates with $L^{1/2}$

The old terms *coil volume* and *filling factor* arise from here

† While β is positive by definition, $\kappa = \mu\beta\,(\tau_\beta.\tau_m)$

can be both positive or negative

(A,B) Special cases of the master equation

$$\boxed{(LJ - \gamma m)J' - \kappa m'J + RJ^2 + kmm' = 0}$$

A. When there is no magnetic dipole ($m = m' = 0$), we get

$$LJJ' + RJ^2 = 0 \;\Rightarrow\; LJ' + RJ = 0 \;\Rightarrow\; J = J_0\, e^{-(R/L)\,t}$$

This is the well-known equation of the LR-circuit.

B. The term kmm' is the power needed to *maintain* the dipole.

This is null in the case of *quantum particles*. It drops out also when the dipole is associated with a permanent magnet or when it is driven driven by an external device.

In such cases $k=0$ and we have a modified master equation:

$$\boxed{LJJ' - \kappa mJ' - \kappa m'J + J^2R = 0}$$

(C) Special cases of the modified master equation

$$\boxed{LJJ' - \kappa mJ' - \kappa m'J + J^2R = 0}$$

How must the dipole evolve to maintain a constant current?

$$J' = 0$$

The answer is that m must grow linearly with time at the rate

$$m' = JR/\kappa$$

One can *reverse the point of view* and say that this is *as though* the linearly increasing dipole generated in the circuit the emf

$$V_{emf} = JR = \kappa m' = \mu\beta(\tau_\beta.\tau_m)\ m'$$

which coincides *exactly* with the classical law of induction.

It is easy to show that this holds also when $J' \neq 0$, provided the induction law is properly extended ($LJ = \kappa m = -\Phi$).

(D-E) Oscillating magnetic dipoles

$$\boxed{LJJ' - \kappa m J' - \kappa m' J + J^2 R = 0}$$

D. What if the dipole is made to oscillate?

Let $m = m_0 \exp(i\omega t)$ and assume a solution of the type $J = J_0 \exp[i(\omega t+\varphi)]$.

Then the master equation gives $J_0 = 2\kappa\omega m_0/|R+i\omega L|$ and $\tan(\varphi) = R/\omega L$.

E. The amplitude of the detected current (signal)

is proportional to κ and therefore also to β. Since β describes the efficiency B/J of a current J to generate the field B at point P, this proves the **reciprocity theorem**:

The larger is the field B generated at a point P by a current J *in the loop, the stronger is the detected signal due to an oscillating dipole located at* P.

Hoult D.I., *The principle of reciprocity in signal strength calculations - a mathematical guide*, Concepts in Magn. Reson. 12, 173-187 (2000).

(F) Current detection of oscillating dipoles

$J_0 = 2\kappa\omega m_0/\lvert R+i\omega L\rvert$	Detected signal current
$J_{0,max} = 2\kappa m_0/L$	is attained for $R=0$
$N_J = [4kTB_w/R]^{½}$	Johnson noise current

$(S/N)_J = J_0/N_J = \omega\kappa m_0\,(kTB_w)^{-½}\,R^{½}/\lvert R+i\omega L\rvert$

$(S/N)_{J,max} = m_0\,\omega^{½}\,(2kTB_w)^{-½}\,\kappa L^{-½}$ is attained at $R=\omega L$

Comment:

While the maximum current is obtained for infinite-Q loops ($R=0$), the best S/N ratio is attained for the "matching" condition $R = \omega L$

(G) Voltage detection of oscillating dipoles

$V_0 = J_0 R = 2\omega\kappa m_0\, R/|R+i\omega L|$ Detected signal voltage

$V_{0,max} = 2\omega\kappa m_0$ is attained for $R=\infty$

$N_V = [4kTB_w R]^{1/2}$ Johnson noise voltage

$(S/N)_V = V_0/N_V = \omega\kappa m_0\,(kTB_w)^{-1/2} R^{1/2} / |R+i\omega L|$

$(S/N)_{V,max} = m_0\,\omega^{1/2}\,(2kTB_w)^{-1/2}\,\kappa L^{-1/2}$ is again attained at $R=\omega L$

Comment:

While the maximum voltage is obtained for open loops ($R = \infty$), the best S/N ratio is attained for the "matching" condition $R = \omega L$.

(H) Power detection of oscillating dipoles

$P_{eff} = ½ J_0^2 R = 2\omega^2\kappa^2 m_0^2\ R/[R^2+(\omega L)^2]$	Detected power
$P_{eff,max} = \omega\kappa^2 m_0^2/L$	is attained for $R=\omega L$
$N_P = 4kTB_w$	Johnson noise power
$(S/N)_P = P_0/N_0 = \omega^2\kappa^2 m_0^2\ (kTB_w)^{-1}\ R/[R^2+(\omega L)^2]^{½}$	
$(S/N)_{P,max} = m_0^2\ \omega\ (2kTB_w)^{-1}\ \kappa^2 L^{-1}$	attained at $R=\omega L$

Comment:

For signal power, the "matching" condition $R = \omega L$ gives both maximum signal and best S/N ratio.

(I) Comparing various detection modes

$$(S/N)_J = (S/N)_V = \sqrt{(S/N)_P} = \omega\kappa m_0 (kTB_w)^{-1/2} R^{1/2} / |R+i\omega L| = S/N$$

$(S/N)_{max} = m_0\, \omega^{1/2} (2kTB_w)^{-1/2} \kappa L^{-1/2}$ is ***always*** attained at $R=\omega L$

- ✓ S/N is independent of the detection mode, provided the matching condition $R=\omega L$ is satisfied.
- ✓ Since κ correlates with $L^{1/2}$, $(S/N)_{max}$ is little dependent on L (though there may be *some* dependence on coil geometry).
- ✓ $(S/N)_{max}$ is proportional to $\omega^{1/2}$ and to $(T_{loop})^{-1/2}$.
- ✓ In MR, under *thermal polarization*, m_0 is proportional to the Larmor frequency ($\approx \omega$) which makes $(S/N)_{MR}$ proportional to $\omega^{3/2}$. Geometric optimization factors can bring it to $\omega^{7/4}$.

Summing up what we did in Part I

Defined all **energy terms**

$\Downarrow$

Applied **thermodynamic laws** such as
energy conservation and thermal noise formulae

$\Downarrow$

and we have promptly obtained:

- Circuit equations
- Induction laws
- Reciprocity theorem
- Best signal detection conditions
- Expressions for S/N ratios
- Useful S/N rules
- … etc

Note: making the circuit more complicated (LC) is useful and may uncover some interesting engineering features, but nothing qualitatively new for the physicist

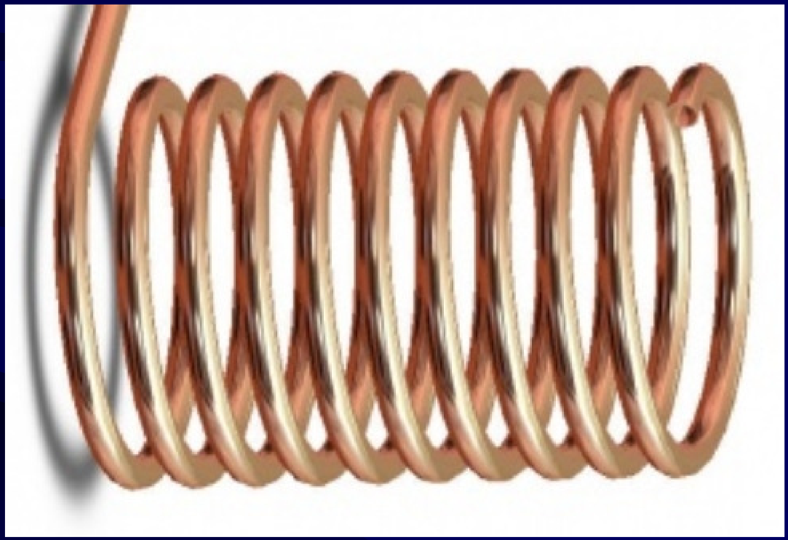
Part II – Quantization of the LC Circuit

Expressions for energy & thermodynamic principles are shared by classical and quantum physics.

Therefore,

casting Part I into quantum terms might work.

Note: this slide and the next one were parts of a single-slide animation!



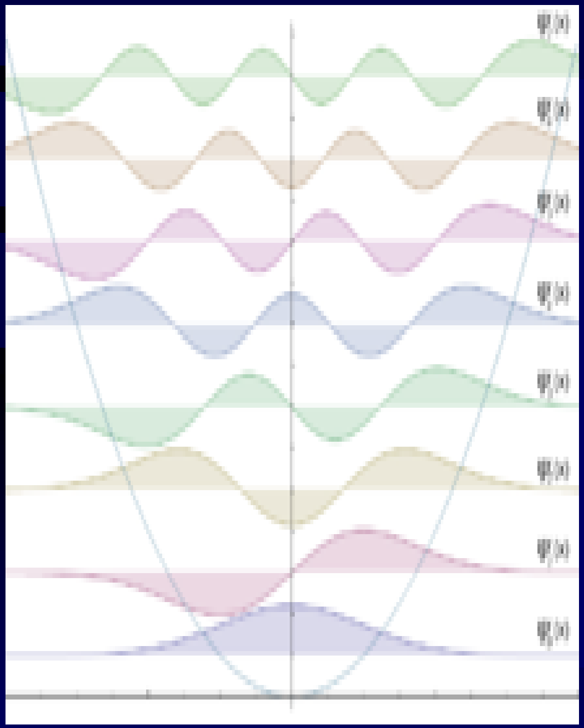
Part II – Quantization of the LC Circuit

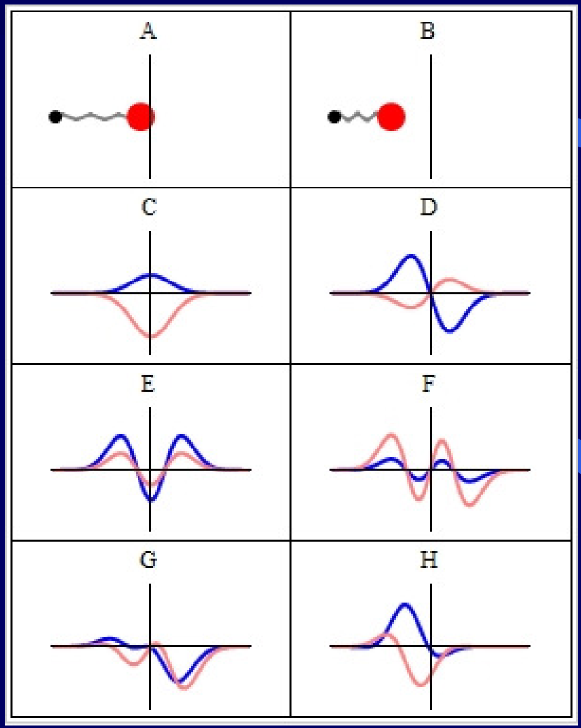
Expressions for energy & thermodynamic principles are <u>shared</u> by classical and quantum physics.

Therefore,

casting Part I into quantum terms might work.

After all, it did on other occasions, such as that of harmonic oscillator:





Classical Physics

A reminder of ye ol' school times when we were all young

The recipe (in Lagrange formalism)

1) Define a set of generalized coordinates $\mathbf{q}$
2) Define corresponding generalized velocities $\mathbf{v} = \mathrm{d}\mathbf{q}/\mathrm{d}t$
3) Define a "kinetic energy" $\mathcal{K} = \mathcal{K}(\mathbf{v})$
4) Define a "potential energy" $\mathcal{U} = \mathcal{U}(\mathbf{q})$
5) Form the Lagrangian $\mathcal{L}(\mathbf{q},\mathbf{v}) = \mathcal{K} - \mathcal{U}$
6) Define generalized momenta $\mathbf{p} = \partial\mathcal{L}/\partial\mathbf{v}$
7) Then the *differential* equations of motion are $\partial\mathcal{L}/\partial\mathbf{q} = \mathrm{d}\mathbf{p}/\mathrm{d}t$

That's all, folks, life was real simple back then!

Quantization of Classical Physics

This is where things started to get slightly weird

The recipe (in Schrödinger – de Broglie formalism)

Classical:

- $\mathbf{q}$
- $\mathbf{v} = d\mathbf{q}/dt$
- $\mathcal{K} = \mathcal{K}(\mathbf{v})$
- $\mathcal{U} = \mathcal{U}(\mathbf{q})$
- $\mathcal{L}(\mathbf{q},\mathbf{v}) = \mathcal{K} - \mathcal{U}$
- $\mathbf{p} = \partial\mathcal{L}/\partial\mathbf{v}$
- $d\mathbf{p}/dt = \partial\mathcal{L}/\partial\mathbf{q}$

Formal quantum transcription:

- Form the classical Hamiltonian $\mathcal{H}(\mathbf{q},\mathbf{v}) = \mathcal{K} + \mathcal{U}$
- Express it as a function of **q**,**p** $\mathcal{H} = \mathcal{H}(\mathbf{q},\mathbf{p})$
- Replace **q**'s with the operators $\mathbf{Q} \equiv \mathbf{q}$
- Replace **p**'s with the operators $\mathbf{P} \equiv -i\hbar\, \partial/\partial\mathbf{q}$
- Define a *state* function $\psi(\mathbf{q},t)$
- Evolution equation is $i\hbar\, d\, \psi(\mathbf{q},t)/dt = \mathcal{H}\,\psi(\mathbf{q},t)$
- … and now we are in the Hilbert-space QM track ☺

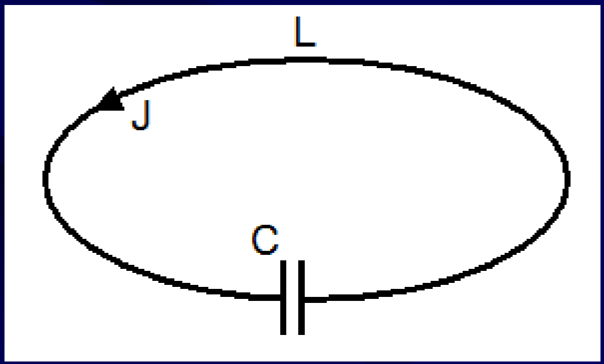
*Well, it's not **that** bad, after all, don't you think?*

Limitation to non-dispersive systems

The classical Lagrange (or Hamilton) formalism of classical physics and the corresponding formalism of quantum physics are **conservative**: they do not cover dispersive elements and phenomena.

In the case of electric circuits, this limits their applicability to nets composed only of **non-dispersive elements** such as inductors (L) and capacitors (C), the simplest of which is an LC loop.

A more general treatment including dispersive elements such as resistors (R) requires an extension of the formalisms to non-conservative phenomena.



Energy terms for an LC circuit

Magnetic energy: $E_L = Lj^2/2$

Electric energy: $E_C = Cv^2/2$

Faraday's induction law: $v = L(dj/dt)$

Hence $E_C = CL^2 (dj/dt)^2 /2$

Idea:

Consider the current j as a generalized variable!

Then, by analogy, we identify E_L with a 'potential' energy and E_C with a 'kinetic' energy and therefore identify the Lagrangian of an LC circuit with

$$\mathcal{L} = CL^2 (dj/dt)^2 /2 - Lj^2/2$$

Does it work in classical dressing?

Lagrange's recipe:	LC circuit correspondences (nDim=1):	
• $\mathbf{q}$	• j	generalized variable
• $\mathbf{v} = d\mathbf{q}/dt$	• $u = dj/dt$	generalized velocity
• $\mathcal{K} = \mathcal{K}(\mathbf{v})$	• $\mathcal{K} = CL^2\, u^2/2$	'kinetic' energy
• $\mathcal{U} = \mathcal{U}(\mathbf{q})$	• $\mathcal{U} = Lj^2/2$	'potential' energy
• $\mathcal{L}(\mathbf{q},\mathbf{v}) = \mathcal{K} - \mathcal{U}$	• $\mathcal{L} = CL^2\, u^2/2 - Lj^2/2$	Lagrangian
• $\mathbf{p} = \partial\mathcal{L}/\partial\mathbf{v}$	• $y = CL^2\, u \;\Rightarrow\; \mathcal{L} = (1/CL^2)\, y^2/2 - Lj^2/2$	
• Evolution:	• Evolution equation:	
$d\mathbf{p}/dt = \partial\mathcal{L}/\partial\mathbf{q}$	$dy/dt = -Lj \;\Rightarrow\; (LC)\, d^2j/dt^2 + j = 0$	

The ***'equation of motion'*** $(LC)\, d^2j/dt^2 + j = 0$ is satisfied by ***any harmonic function*** $j(t)$ having the frequency $\omega = 1/\sqrt{(LC)}$

Exactly as expected! **It works** ☺

LC circuit in quantum dressing

Classical LC circuit:

- ✓ j
- $u = dj/dt$
- $\mathcal{K} = CL^2\, u^2/2$
- $\mathcal{U} = Lj^2/2$
- $\mathcal{L} = CL^2\, u^2/2 - Lj^2/2$
- ✓ $y = CL^2\, u$
- $\mathcal{L} = (1/CL^2)\, y^2/2 - Lj^2/2$
- ✓ $\mathcal{H}(j,y) = (1/CL^2)\, y^2/2 + Lj^2/2$

Quantum LC circuit:

- ✓ j
- $y = -i\hbar\, \partial/\partial j$
- ✓ Hamiltonian:

  $\mathcal{H} = -[(\hbar\omega)^2/2L]\, \partial^2/\partial j^2 + (L/2)\, j^2$

  where $\omega = 1/\sqrt{(LC)}$
- ✓ Wavefunction: $\psi(j,t)$
- ✓ Evolution (Schrödinger) equation:

  $i\hbar\, d\psi(j,t)/dt = \mathcal{H}\, \psi(j,t)$

Expected stationary solutions:

$\psi(j,t) = \exp[\pm i(E/\hbar)t + i\varphi]\, \psi(j)$ where $\psi(j) = E\, \mathcal{H}\, \psi(j)$

Quantum LC Circuit and the Harmonic Oscillator

Quantum HO with frequency ω:

- x
- Hamiltonian:

  $\mathcal{H} = -[\hbar^2/2m]\,\partial^2/\partial x^2 + (m\omega^2/2)\,x^2$
- Wavefunction: $\psi(x,t)$
- Schrödinger equation:

  $i\hbar\, d\psi(x,t)/dt = \mathcal{H}\,\psi(x,t)$

Quantum LC with frequency ω:

- j
- Hamiltonian:

  $\mathcal{H} = -[(\hbar\omega)^2/2L]\,\partial^2/\partial j^2 + (L/2)\,j^2$
- Wavefunction: $\psi(j,t)$
- Schrödinger equation:

  $i\hbar\, d\psi(j,t)/dt = \mathcal{H}\,\psi(j,t)$

A perfect correspondence can be achieved by setting

$$m \approx CL^2 = L/\omega^2$$

saving a lot of work in finding the stationary solutions

Stationary solutions for the quantum LC

? Reflect !?

$$\psi_n(j,t) = exp\left(\pm i\frac{E_n}{\hbar}t + i\varphi\right)\psi_n(j) \text{ , with } E_n = \hbar\omega\left(n+\frac{1}{2}\right),$$

φ an arbitrary constant, and

$$\psi_n(j) = \sqrt{\frac{1}{2^n n!}}\left(\frac{L}{\pi\hbar\omega}\right)^{1/4} exp\left(-\frac{Lj^2}{2\hbar\omega}\right)H_n\left(j\sqrt{\frac{L}{\hbar\omega}}\right),$$

$$\psi_n(j) = \sqrt{\frac{\eta}{2^n n!\sqrt{\pi}}}\, exp\left(-\frac{1}{2}(\eta j)^2\right)H_n(\eta j), \text{ where } \eta = \sqrt{\frac{L}{\hbar\omega}},$$

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}(e^{-x^2}) \quad \text{are the Hermite functions.}$$

This might lead us to **new quantum features**/phenomena in molecular-size circuits as well as a better understanding of quantum **noise in conventional electronic circuits**

Hamiltonian of a Spin System with Coil (SSC)

$$\mathcal{H}_{SSC} = \mathcal{H}_S + \mathcal{H}_{LC} + \mathcal{H}_{SC}$$

$\mathcal{H}_S$ Spin system Hamiltonian associated with *spin degrees of freedom*. Once it *used to be a controversial concept* for a few years but it reaped such a success that today we rarely perceive it as an approximation. Well known (Zeeman, dipole-dipole, chemical shifts, scalar couplings, spin-rotation, etc …)

$\mathcal{H}_{LC}$ Hamiltonian of the receiver LC circuit (the Coil).

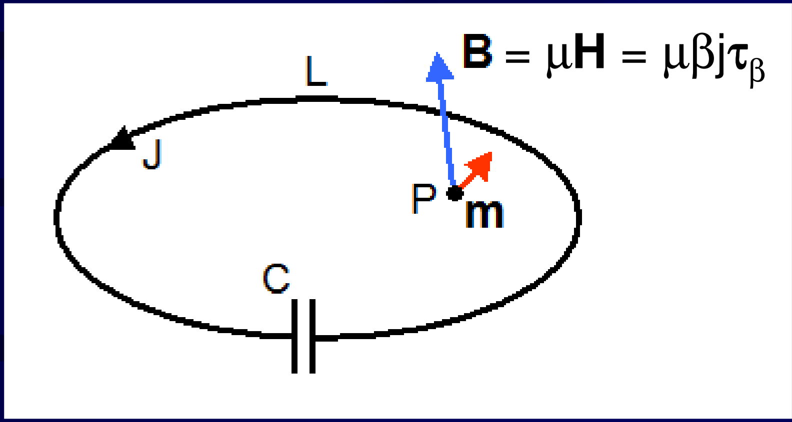
This is a new term, just derived in the previous part of this talk.

$\mathcal{H}_{SC}$ Spin-coil interaction term *without which we could see no signal*.

It is still to be defined!

My not-so-secret goal is to make the <u>coil current</u>
an integral part of the Spin System Hamiltonian

Interaction of a Spin with a Coil



Classical:

$E_i = -\,\mathbf{m}.\mathbf{B} = -\,\mu\beta j(\tau_\beta.\mathbf{m})$, where β and τ_β depend on system geometry

Quantum:

$$\mathcal{H}_{SC} = -\,\mu\beta\gamma j(\tau_\beta.\mathbf{S}) = \nu\gamma(\tau_\beta.\mathbf{S})\,j, \text{ where } \nu = -\,\mu\beta$$

Special case:

When the coil is aligned along the **X**-axis and the point **P** is at its center, then

$$\mathcal{H}_{SC} = \nu\gamma j S_x = \nu\gamma j(S^+ + S^-)/2$$

Full Hamiltonian of a Spin System and a Coil

$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_{LC} + \mathcal{H}_{SC}$	Total Hamiltonian
$\mathcal{H}_S = \mathcal{H}_L + \mathcal{H}_C + \mathcal{H}_{SS}$	Spin Hamiltonian
$\mathcal{H}_L = -\mathbf{B}_0 . \Sigma_k \gamma_k \mathbf{S}_k$	Larmor interaction
$\mathcal{H}_C = \Sigma_k \gamma_k (\mathbf{B}_0 . \mathbf{C}_k . \mathbf{S}_k)$	Chemical shift interactions
$\mathcal{H}_{SS} = \Sigma_{k,k'} \gamma_k \gamma_{k'} (\mathbf{S}_k . \mathbf{T}_{k,k'} . \mathbf{S}_{k'})$	Spin-spin interactions
$\mathcal{H}_{LC} = -[(\hbar\omega)^2/2L]\, \partial^2/\partial j^2 + (L/2)\, j^2$	LC coil Hamiltonian
$\mathcal{H}_{SC} = \nu\, (\boldsymbol{\tau}_\beta . \Sigma_k \gamma_k \mathbf{S}_k)\, j$	Spin-coil interactions

A single spin and a coil in lab coordinates

Z-axis along $\mathbf{B}_0$, X-axis along the coil

$\mathcal{H} = \mathcal{H}_L + \mathcal{H}_C + \mathcal{H}_{SC}$	Total Hamiltonian
$\mathcal{H}_L = -\gamma B S_z$	Larmor interaction
$\mathcal{H}_C = -[(\hbar\omega)^2/2L]\,\partial^2/\partial j^2 + (L/2)\,j^2$	Coil Hamiltonian
$\mathcal{H}_{SC} = \nu\gamma S_x j = \nu\gamma[(S^+ + S^-)/2]j$	Spin-coil interaction

B is the effective, chemically screened B_0

Heisenberg-form matrix elements

of a single spin + coil Hamiltonian; convention $\hbar \equiv 1$

Spin-space base functions	$|\sigma\rangle$, for $S = ½$, $\sigma = +½$, , $-½$
Coil current base functions	$|\psi_n(j)\rangle$
Full-system base functions	$|\Psi_n(\sigma, j)\rangle = |\sigma\rangle\, |\psi_n(j)\rangle$
Spin-Hamiltonian elements	$\mathcal{H}_L\, |\Psi_n(\sigma, j)\rangle = \sigma\, \Omega\, |\Psi_n(\sigma, j)\rangle$, $\Omega = \gamma B$ (Larmor)
Coil-Hamiltonian elements	$\mathcal{H}_C\, |\Psi_n(\sigma, j)\rangle = (n+½)\ \omega\, |\Psi_n(\sigma, j)\rangle$
Spin-coil interaction elements	$\mathcal{H}_{SC} |\Psi_n(\sigma, j)\rangle = \nu\, \gamma\, S_x\, j\ |\Psi_n(\sigma, j)\rangle$ = ???

Off-diagonal spin-coil interaction elements

of a single spin + coil Hamiltonian

Reminder: $\mathcal{H}_{SC}\,|\Psi_n(\sigma, j)\rangle = \nu\gamma S_x\, j\, |\Psi_n(\sigma, j)\rangle = ???$

Some mathematical tools:

$$j\psi_n(j) = \sqrt{\frac{\hbar\omega}{L}}\left[\sqrt{\frac{n+1}{2}}\psi_{n+1}(j) + \sqrt{\frac{n}{2}}\psi_{n-1}(j)\right]$$ see Hermite polynomials

$$\left\langle \psi_m(j)\,|\,j\,|\,\psi_n(j)\right\rangle = \left[\sqrt{\frac{m}{2}}\,\delta_{m,\,n+1} + \sqrt{\frac{n}{2}}\,\delta_{n,\,m+1}\right]\sqrt{\frac{\hbar\omega}{L}}$$

$$\left\langle \psi_n(j)\,|\,j\,|\,\psi_n(j)\right\rangle = 0$$

$$j^2\,\psi_n(j) = \frac{\hbar\omega}{2L}\left[\sqrt{(n+1)(n+2)}\,\psi_{n+2}(j) + (2n+1)\,\psi_n(j) + \sqrt{n(n-1)}\,\psi_{n-2}(j)\right]$$

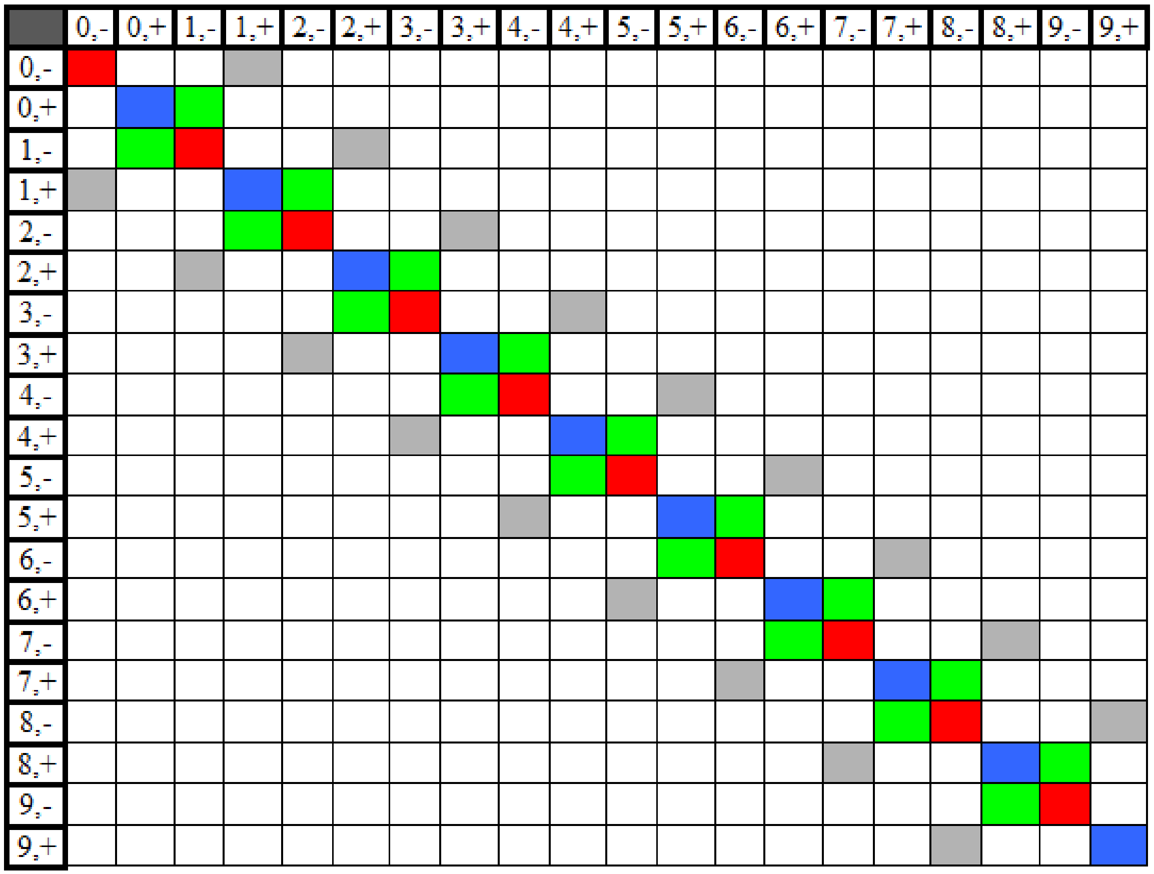
$$\left\langle \psi_n(j)\,|\,j^2\,|\,\psi_n(j)\right\rangle = \frac{\hbar\omega}{L}\left(n + \frac{1}{2}\right) = E_n/L$$ classical: $J_{eff}^2 = E/L$

For spins S = ½ : $S_x\left|\pm 1/2\right\rangle = (1/2)\left|\mp 1/2\right\rangle$

Full spin-coil Hamiltonian matrix

of a single spin S= ½ and a coupled LC circuit; convention $\hbar \equiv 1$

$$\langle \Psi_m(\sigma',j) \,|\, \nu\gamma S_x j \,|\, \Psi_n(\sigma,j)\rangle = \frac{\nu\gamma}{2}\sqrt{\frac{\omega}{L}}\left[\sqrt{\frac{m}{2}}\,\delta_{m,n+1} + \sqrt{\frac{n}{2}}\,\delta_{n,m+1}\right]\delta_{\sigma,-\sigma'}$$



Diagonal elements:

$\mathcal{H}_{n,-} = (n + ½)\ \omega - \Omega/2$

$\mathcal{H}_{n,+} = (n + ½)\ \omega + \Omega/2$

For green elements:

$\Delta_{diag} = \omega - \Omega$

Strong coupling for

$\omega = \Omega$

Resonance!

For gray elements:

$\Delta_{diag} = \omega + \Omega$

Weak coupling

Bloch-Siebert shifts

A detail of the spin-coil Hamiltonian

of a single spin S= ½ and a coupled LC circuit; convention ħ ≡ 1

	n, -	n, +	n+1, -	n+1, +
n, -	$\omega\left(n+\frac{1}{2}\right)-\frac{\Omega}{2}$	0	0	$\frac{\gamma\nu}{2}\sqrt{\frac{\omega(n+1)}{2L}}$
n, +	0	$\omega\left(n+\frac{1}{2}\right)+\frac{\Omega}{2}$	$\frac{\gamma\nu}{2}\sqrt{\frac{\omega(n+1)}{2L}}$	0
n+1, -	0	$\frac{\gamma\nu}{2}\sqrt{\frac{\omega(n+1)}{2L}}$	$\omega\left(n+\frac{3}{2}\right)-\frac{\Omega}{2}$	0
n+1, +	$\frac{\gamma\nu}{2}\sqrt{\frac{\omega(n+1)}{2L}}$	0	0	$\omega\left(n+\frac{3}{2}\right)+\frac{\Omega}{2}$

Diagonal elements grow with n
Off-diagonal elements grow with √n

Spin-coil Hamiltonian detail (2)

	n, -	n, +	n+1, -	n+1, +
n, -	$(E_n - \Omega/2)$	0	0	C
n, +	0	$(E_n + \Omega/2)$	C	0
n+1, -	0	C	$(E_n + \Omega/2) + (\omega - \Omega)$	0
n+1, +	C	0	0	$(E_n - \Omega/2) + (\omega + \Omega)$

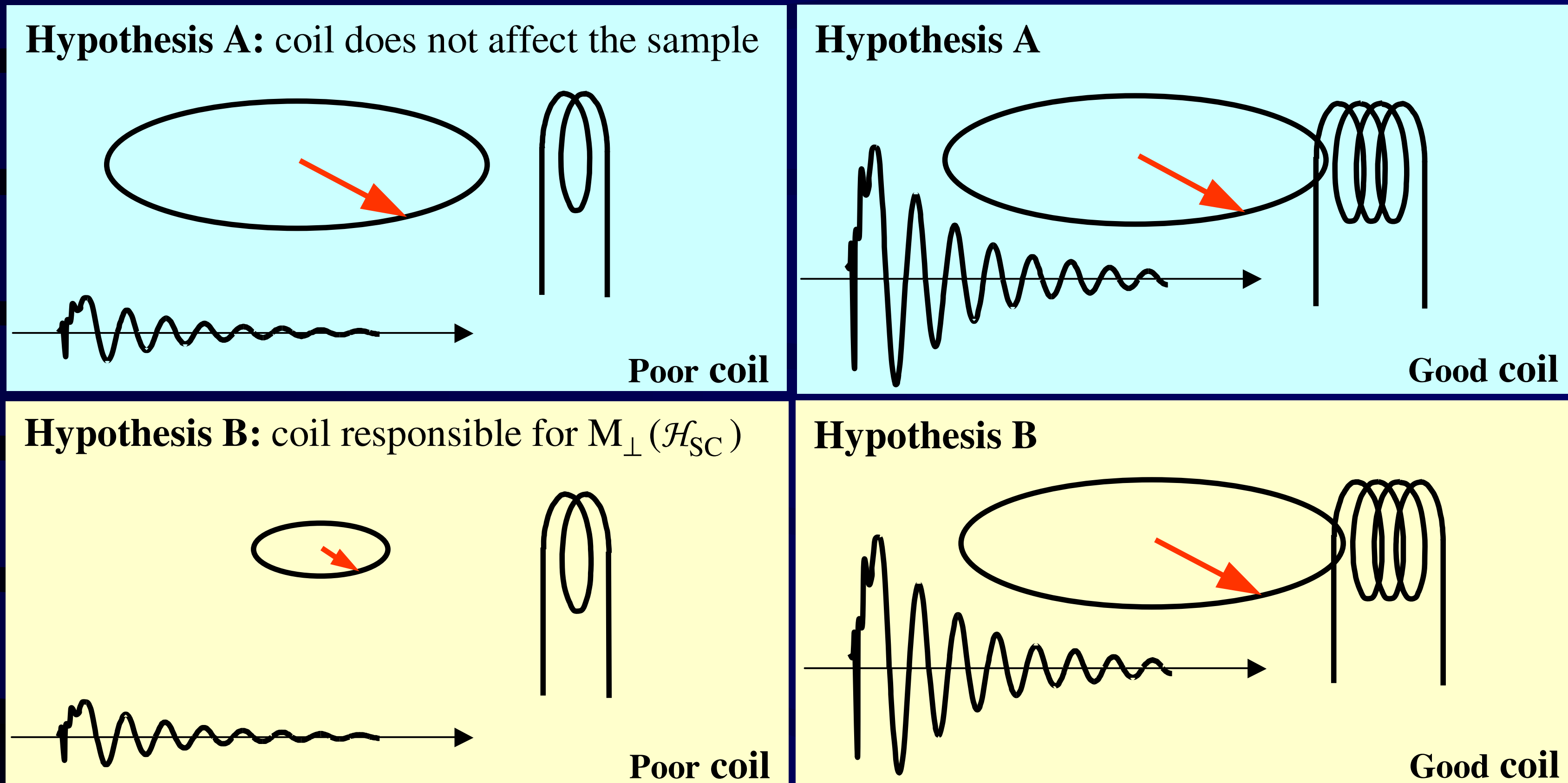
$$C = \gamma\nu\sqrt{\frac{\omega(n+1)}{2L}}$$

The gray off-diagonal elements may be neglected (?)

The green elements pair the eigenstates into 2x2 matrices which are easy to diagonalize explicitely

Work on spin_system – coil interaction is going on

What's going on during an FID when there is no coil?

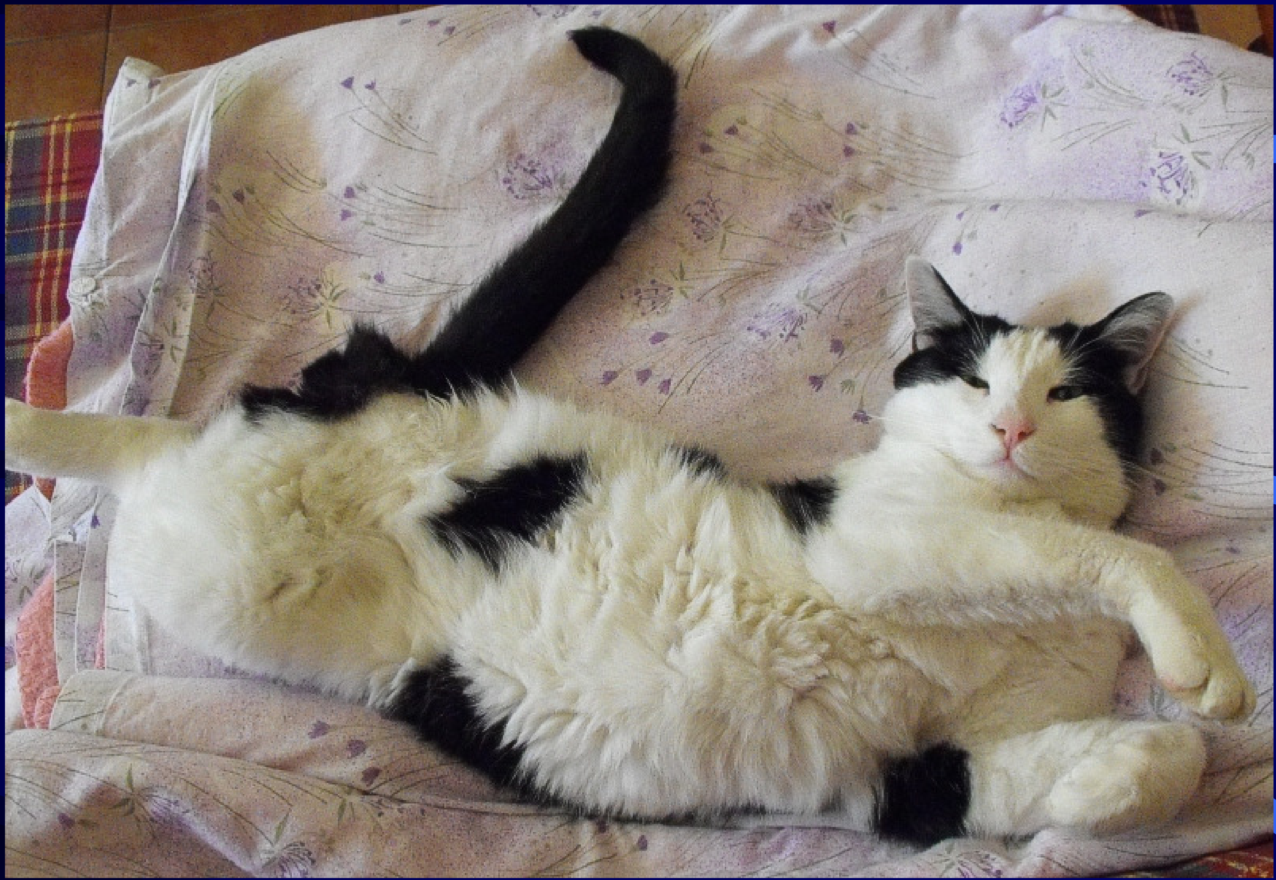


Hypothesis A: coil is just a detector (dependence on β: linear?)
Hypothesis B: coil is part of the $M_\perp$ generation (dependence on β: quadratic?)
Hypothesis C: no coil, no perpendicular magnetization !???
Sure! no coil, no signal? ☺ ? Theory works! But is it correct? ☹ ?

Limb lost, Wisdom gained

Erwin, a would be friend,
closed me in his Box; yet,
despite all odds, out I got
- and all on my own -
loosing just a limb in the
nasty quantum foam!

Most amazing things I saw,
states mixed and uncertain
Erwin could never imagine!
For the Box was Closed!
Inaccessible to **<u>his</u>** scrutiny
while I, **<u>I</u>** stayed Within.



Thank you – and let's discuss!