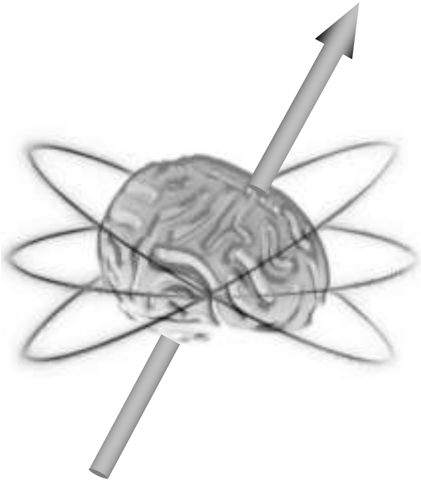


Az NMR és a bizonytalansági elv rejtélyes találkozása

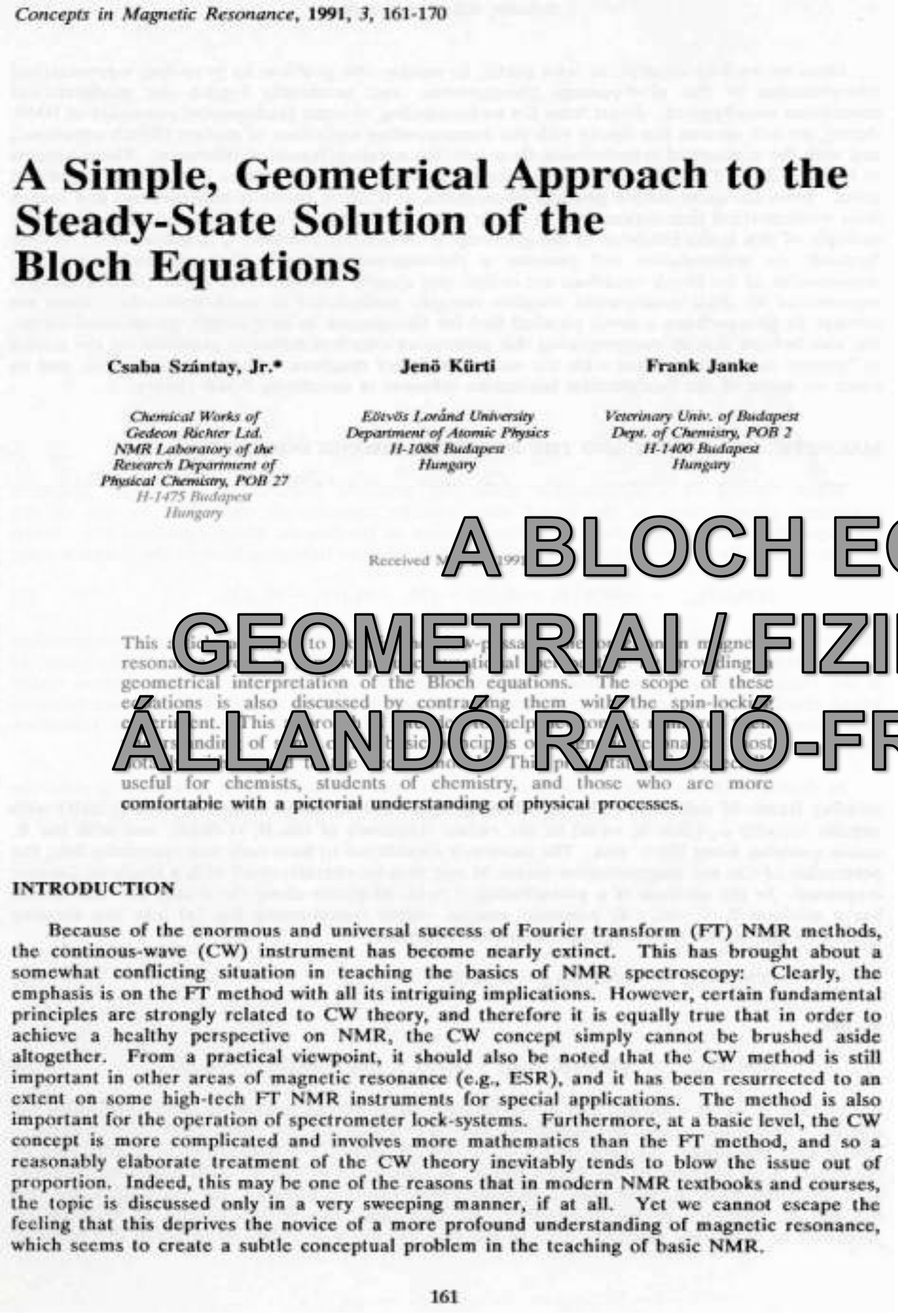
ifj. Szántay Csaba

MTA

Kémiai Tudományok Osztálya

2012. február 21.

A BLOCH EGYENLETEK GEOMETRIAI / FIZIKAI ÉRTELMEZÉSE ÁLLANDÓ RÁDIÓ-FREKVENCIÁS TÉRBEN



Concepts in Magnetic Resonance, 1991, 3, 161-170

A Simple, Geometrical Approach to the Steady-State Solution of the Bloch Equations

Csaba Szántay, Jr.* **Jenö Kürti** **Frank Janke**

Chemical Works of Gedeon Richter Ltd. NMR Laboratory of the Research Department of Physical Chemistry, POB 27 H-1475 Budapest Hungary

Eötvös Loránd University Department of Atomic Physics H-1088 Budapest Hungary

Veterinary Univ. of Budapest Dept. of Chemistry, POB 2 H-1400 Budapest Hungary

Received M[illegible] 1991

This a[illegible] to [illegible]w-passa[illegible] in magne[illegible] resona[illegible]tional [illegible] providing a geometrical interpretation of the Bloch equations. The scope of these equations is also discussed by contrasting them with the spin-locking experiment. This [illegible] helpful [illegible] understanding of [illegible] basic principles of magnetic resonance [illegible] most notably [illegible]. This presentation [illegible] useful for chemists, students of chemistry, and those who are more comfortable with a pictorial understanding of physical processes.

INTRODUCTION

Because of the enormous and universal success of Fourier transform (FT) NMR methods, the continous-wave (CW) instrument has become nearly extinct. This has brought about a somewhat conflicting situation in teaching the basics of NMR spectroscopy: Clearly, the emphasis is on the FT method with all its intriguing implications. However, certain fundamental principles are strongly related to CW theory, and therefore it is equally true that in order to achieve a healthy perspective on NMR, the CW concept simply cannot be brushed aside altogether. From a practical viewpoint, it should also be noted that the CW method is still important in other areas of magnetic resonance (e.g., ESR), and it has been resurrected to an extent on some high-tech FT NMR instruments for special applications. The method is also important for the operation of spectrometer lock-systems. Furthermore, at a basic level, the CW concept is more complicated and involves more mathematics than the FT method, and so a reasonably elaborate treatment of the CW theory inevitably tends to blow the issue out of proportion. Indeed, this may be one of the reasons that in modern NMR textbooks and courses, the topic is discussed only in a very sweeping manner, if at all. Yet we cannot escape the feeling that this deprives the novice of a more profound understanding of magnetic resonance, which seems to create a subtle conceptual problem in the teaching of basic NMR.

161

Szántay, Kürti, and Janke

Figure [illegible] Representation of [illegible] acting on M at an arbitrary point on the [illegible] curve.

respect to $\Sigma\mathbf{R}$. However, this results in a decreased **T** torque because of the shortened $\mathbf{B}_{eff}$. However, the [illegible] of the **R** vectors, which [illegible] of the bigger θ, requ[illegible] an inc[illegible] in order for this t[illegible]d, [illegible]se δ... etc. [illegible] this l[illegible] of thought, the reason for [illegible] **M** [illegible] explained.

At the resonance point, $\omega_1 = \omega_0$ and $\mathbf{B}_{eff} = \mathbf{B}_1$. Therefore, **M** has to assume a δ phase-delay of π/2 [illegible] At [illegible] further [illegible] the y' [illegible] **M** [illegible] drop back even farther in phase, as $\mathbf{B}_{eff}$ aligns along the −z direction [illegible], M arrives back at the z axis.

It is interesting to examine how the magnitude of $\mathbf{B}_1$ influences this picture. When $\mathbf{B}_1$ is increased, saturation becomes more significant. (In the vector model, the degree of saturation corresponds with the shortening of the **M** vector with respect to its original length, M_0). Figure 6 shows computer simulated resonance circles that were calculated by implementing the corresponding solutions of the Bloch equations for three different, increasingly higher $\mathbf{B}_1$ values, with all other parameters being unchanged. For simplicity, T_1 was taken to be equal to T_2. Each circle is positioned on the surface of the same sphere, which possesses the characteristic parameters depicted in Fig. 6a (it is a sphere only if $T_1 = T_2$). The projections of these circles onto the y' and x' axes, represented as a function of ω_1, afford the familiar absorption and dispersion resonance signals, respectively. The surface of this sphere represents the equilibrium of the absorption and relaxation rates, but now also as a function of the amplitude of $\mathbf{B}_1$. As $\mathbf{B}_1$ is increased, the plane of the circles tilts downward, and the net magnetization tends to disappear while moving on the surface of the sphere. The reason for this becomes clear from the following argument: Let us be exactly on resonance, with **M** lying within the zy' plane. The definition of the $\mathbf{R}_1$ and $\mathbf{R}_2$ vectors tells us that if $T_1 = T_2$, then $\Sigma\mathbf{R}$ always points toward the tip of the $\mathbf{M}_0$ vector. If, for simplicity, we take both T_1 and T_2 to be unity (e.g., 1 s), then $\Sigma\mathbf{R} = \mathbf{M}_0 - \mathbf{M}$ (Fig. 7). Since **T** is necessarily perpendicular to **M**, the $\mathbf{T} + \Sigma\mathbf{R} = 0$ equation ensures that $\Sigma\mathbf{R}$ is also perpendicular to **M**. Thus, when we force **M** to take up greater θ values by slowly increasing $\mathbf{B}_1$ (and thus **T**), **M** necessarily has to move along a *Thales circle*, and therefore its length decreases monotonically, as shown in Fig. 7. Evidently, **M** can never reach the y' axis, because at this point, **T** would have no $\mathbf{T}_{y'}$ component to counterbalance the influence of transverse relaxation, and the macroscopic net magnetization would be completely eliminated.

166

A GYENGE SUGÁRZÁSI CSILLAPÍTÁS DIAGNOSZTIKÁJA ÉS FIZIKÁJA

RADIATION DAMPING DIAGNOSTICS 123

Radiation Damping Diagnostics

CSABA SZÁNTAY, JR.,* ÁDÁM DEMETER

Gedeon Richter Ltd., Spectroscopic Research Division, H-1475 Budapest, 10, P.O.B. 27, Hungary

ABSTRACT: With the trend of designing supersensitive probes and very-high-fie magnets, the phenomenon of radiation damping is increasingly being perceived as startir to invade the realm of normal nuclear magnetic resonance. This article explores the scop and limitations of the various spectral tools available to diagnose the presence of radiatic damping. It is shown that the recovery rate of the M_z magnetization is the most sensitiv parameter to indicate weak damping. This effect can be measured by using suitable gradie techniques. © 1999 John Wiley & Sons, Inc. Concepts Magn Reson 11: 121–145, 1999

KEY W spectroscopy (RADDSY); transition-band signals.

INTRODUCTION

A substantial part of nuclear magnetic resonance (NMR) theory is based on the well-known linear differential equations of Felix Bloch (1). This delightfully linear world of NMR is occasionally disturbed by some rogue nonlinear phenomena, probably the most important of which is radiation damping. The phenomenon of radiation damping involves the coupling of the magnetic spin system with the radiofrequency (rf) coil used for signal reception. Following a perturbation, this interaction forcibly drives spins toward thermal equilibrium in a nonlinear process, which gives rise to some unorthodox spectral effects.

The magnitude of the spin–coil interaction increases with the length of the net magnetization vector involved and the sensitivity of the coil (related to the so-called Q factor). The moder-

ately high external magnetic fields probes that were in general use for an interaction so small as to be safel most applications as well as througho retical development of spin physics following its first description in 195 bergen and Pound (2), radiation mained an exotic phenomenon tradit ciated only with very intense resonar originating from a solvent signal o highly concentrated samples.

With the advent of high fields high-Q probes, radiation damping is perceived as potentially infiltrating typical, everyday samples, and has t come a renewed focus of NMR resea

The presence of radiation damp detected in several ways, provided th is sufficiently strong. However, we damping is less readily detected, alth appreciably influence the thermalizat This article gives a review of the va tion-damping markers by pointing ou and limitations in terms of evaluatin to which the studied system is affect ing. A unique radiation-damping tes

axis so that the angle θ shrinks from its initial value θ_0 to 0. Assuming that normal relaxation processes can be ignored, i.e., $\mathbf{M}_0$ does not change its length, this nutation is decribed by the following differential equation:

$$\frac{d\theta}{dt} = \gamma B_{rd}(\theta) = -\frac{\sin\theta}{T_{rd}^0} \qquad [1]$$

where T_{rd}^0 is the characteristic radiation-damping time constant (17). (Note that here we use "T_{rd}^0" instead of the generally used notation "T_{rd}" for reasons that will become clear shortly). The process is self-destructive in the sense that as $\mathbf{M}_0$ approaches z, the B_{rd}-initiating component $M_{y'}$ tends toward zero [Fig. 1(b,c)].

By a simple rearrangement of the equations given by Abragam (17), we can express the relation between $M_{y'}$ and B_{rd} for a tuned coil as

where

$$\frac{1}{T_{rd}^0 M_0} \qquad [3]$$

The effects of radiation damping are treated by the Bloch equations extended with the radiation-damping terms (18,19) (note again that the driving B_1 field of ω_1 angular frequency is along the rotating frame $+x'$ axis):

$$\frac{dM_{x'}}{dt} = -(\omega_1 - \omega_0)M_{y'} - \frac{M_{x'}}{T_2^*} - \mathscr{R}M_{x'}M_z$$

$$\frac{dM_{y'}}{dt} = (\omega_1 - \omega_0)M_{x'} + \gamma B_1 M_z - \frac{M_{y'}}{T_2^*}$$

$$-\mathscr{R}M_{y'}M_z \qquad [4]$$

$$\frac{dM_z}{dt} = -\gamma B_1 M_{y'} - \frac{M_z - M_0}{T_1} + \mathscr{R}(M_{x'}^2 + M_{y'}^2)$$

where T_1 and T_2^* are the longitudinal and transverse (instrumental) relaxation times, respectively.

Analytical solutions for Eqs. [4] can be obtained only if either radiation damping or relaxation can be ignored (19,20). Therefore, to keep our treatment of the effects of radiation damping general, we resort to the numerical integration of Eqs. [4] using the Runge–Kutta method (21).

At this point, it becomes useful to linger shortly on the meaning of $\mathscr{R}$ and T_{rd}^0. The strength of radiation damping is exclusively determined by the value of $\mathscr{R}$ which links, as noted above, $M_{y'}$ and B_{rd}. Assuming that the sample completely fills the tuned coil, the value of $\mathscr{R}$ is specifically characteristic of the probe, i.e., it depends only on the Q factor and γ. By diluting a sample to, say, half of its original concentration, M_0 will also be halved, but since $\mathscr{R}$ remains the same in a given probe, the value of T_{rd}^0 is doubled. Furthermore, if the influence of normal relaxation processes on the length of the net magnetization vector $\mathbf{M}$ cannot be ignored during radiation damping, at any given instant the torque $\mathbf{K}_{rd}$ will act on $\mathbf{M}$ [where $M = (M_{x'}^2 + M_{y'}^2 + M_z^2)^{1/2}$] and not, of course, on $\mathbf{M}_0$. Consequently, in Eq. [1], T_{rd}^0 must be replaced with T_{rd} to reflect the fact that the radiation-damping time constant actually changes d the process. This is a period for weak measurements (see below). Thus, Eq. [3] can be written in the most general form:

$$\mathscr{R} = \frac{1}{T_{rd}^0 M_0} = \frac{1}{T_{rd} M} \qquad [5]$$

It is now clear that we use the notations T_{rd}^0 and T_{rd} to stress whether the radiation-damping time constant is pertinent to the thermal-equilibrium net magnetization M_0 or a changing net magnetization M. Obviously, with a given probe (i.e., a given $\mathscr{R}$ value), the amount of radiation damping experienced by a system can usefully be characterized only in terms of T_{rd}^0—which is what is meant by the radiation-damping time constant of the system, although it is denoted as T_{rd} in the literature.

In this article, we will be comparing systems experiencing different degrees of radiation damping, and to this end we have two options. (a) We can envisage a given sample (i.e., a given M_0) being investigated on various probes with various $\mathscr{R}$, and consequently different T_{rd}^0, values. (b) We may use the same probe (i.e., a given $\mathscr{R}$) and imagine the concentration (i.e., M_0) of our sample being varied to obtain different T_{rd}^0 values. Although scenario (b) is more applicable to a real-life situation, it has the disadvantage that M_0 and T_{rd}^0 both change, which is inconvenient for the purpose of an intuitively well-accessible comparison of different systems as well as in the

Received 6 August 1998; revised 5 November 1998; accepted 5 November 1998

*Correspondence to: Cs. Szántay, E-mail: cs.szantay@richter.hu, fax: 36-1-260-5118.

Concepts in Magnetic Resonance, Vol. 11(3) 121–145 (1999)
© 1999 John Wiley & Sons, Inc. CCC 1043-7347/99/030121-25

121

A “REJTETT CSEREPARTNER” JELENSÉGE, KINETIKÁJA, ÉS ALKALMAZOTT NMR SPEKTROSZKÓPIAI HATÁSAI

JOURNAL OF MAGNETIC RESONANCE, Series A 115, 94–105 (1995)

The “Hidden” Exchange Partner in NMR Spectroscopy. Kinetic Properties and Implications in NOE Analysis

CSABA SZÁNTAY, JR.,* AND ÁDÁM DEMETER

Spectroscopic Research Centre, Chemical Works of Gedeon Richter Ltd., H-1475 Budapest 10, P.O. Box 27, Hungary

Received September 19, 1994; revised January 24, 1995

The presence of hidden exchange partners is a possible but not generally recognized source of negative effects in the $^1H\{^1H\}$ NOE difference spectra of molecules that fall in the extreme narrowing region. The true origin of these negative signals is not easily identified and this can lead to erroneous molecular structural conclusions. By introducing into the modified Bloch equations an extra term for transition probabilities induced by continuous selective RF irradiation, it is shown that in a two-site problem the “saturability” of the minor signal can be much lower than that of the major signal; [illegible] bility [illegible] interpretation in NOE difference experiments. The [illegible] such a hidden partner in ^1H spectroscopy is limited [illegible] narrow range [illegible] characteristic dynamical parameters (exchange rates, population ratios, relaxation times, and chemical-shift differences). Diagrams are provided for the [illegible] ratios determ[illegible] from [illegible] difference experiments. © 1995 [illegible]

INTRODUCTIO

In systems that exchange moderate[illegible] on the [illegible] frequency time scale, and the interconverting species have unequal populations (i.e., unequal lifetimes), the exchange contribution to line broadening is different for the exchanging entities. For very unequal populations, strong signals with long residence times can show marginal exchange broadening, while weak signals with short residence times may be broadened beyond detection. This latter phenomenon, known as the “hidden” exchange partner, is not uncommon, and has been the subject of various studies (*1–3*). To illustrate the problem, we take an uncoupled two-site exchange system in which the minor (m) and major (M) species interconvert with the respective forward and backward first-order rate constants k_m and k_M,

$$m \underset{k_M}{\overset{k_m}{\rightleftharpoons}} M$$

The fractional populations are p_m and p_M wi
1, and there is a frequency difference $\Delta\nu = |\nu_m$
the nonexchanging sites. The equilibrium ne
tions are M_{m0} and M_{M0} such that $M_{m0}k_m = M$

Figure 1 shows the behavior of this system
from slow exchange ($k_M, k_m \ll \Delta\nu$) through m
exchange ($k_M, k_m < \Delta\nu$) toward coalescence fo
populations $p_m \ll p_M$ as well as for $p_m = p_M$
from McConnell's solution of the modified B
(*4–6*) [illegible]
cha[illegible]
the ma[illegible]
large frequency range, which subsequently di
[illegible]escence is approached. The[illegible]
[illegible]ch the [illegible]nal becomes hidden while
[illegible]

[illegible]
partner” can pose regarding $^1H\{^1H\}$ NOE
[illegible]
particularly in relation to ^1H spectroscopy. T
the system to selective RF saturation is also e

RESULTS AND DISCUSSION

General Remarks Regarding “Exchange Win

We assume that a hidden exchange partner
because of two features: (i) The minor comp
tically invisible in the ^1H spectrum because o
onance and small signal height H_m relative to th
H_M (in practice the half-height linewidth $\Delta\nu_{1/2}$
greater than ≈30 Hz, and H_M/H_m must be at
(ii) Exchange broadening of the major reson
nonconspicuous or may be attributed to *other*
as field inhomogeneity or small unresolved sca
the main signal therefore does not reveal the
silent partner *per se*.

For slow exchange ($k_M, k_m \ll \Delta\nu$), the exc
bution to line broadening is independent of

---

* To whom correspondence should be addressed.

1064-1858/95 $12.00

minor signal. In effect, the major signal acts as a reservoir that drains the minor site of its saturated magnetization while feeding back less saturated magnetization, thereby making saturation of the minor signal M_m^* inefficient. Thus, in a difference experiment, irradiation of the minor signal will give a hardly detectable effect on the minor resonance itself, but the saturation transferred to the main site where spins “accumulate” gives a signal of greater intensity. It is therefore actually easier to saturate the minor signal by irradiating its major partner than by irradiating the minor signal itself. Any impurity (not involved in chemical exchange) which is nearly coincident with the minor signal will be more effectively saturated by irradiation than the minor signal (Fig. 3C). Originally hidden or hardly detected small impurities may thus be made visible in the difference spectrum, as exemplified in Fig. 3.

The above behavior of very biased exchange systems can also be rationalized as follows. When transitions are induced by a continuous irradiation, the time dependence of the net lon[illegible] by [illegible] where the transition pro[illegible] the [illegible] the ap[illegible] [illegible] tions, assuming equal relaxation rates $R_1 = 1/T_1$ for the minor and major isomers, are

[illegible]

$$\frac{dM_M}{dt} = R_1(M_{M0} - M_M) - k_M M_M + k_m M_m. \quad [5]$$

The effect of selectively irradiating the minor partner can be introduced by incorporating Eq. [3] into Eq. [4] which then gives the coupled differential equations

$$\frac{dM_m^*}{dt} = R_1(M_{m0} - M_m^*) - k_m M_m^* + k_M M_M - 2WM_m^* \quad [6]$$

$$\frac{dM_M}{dt} = R_1(M_{M0} - M_M) - k_M M_M + k_m M_m^*. \quad [7]$$

Some algebraic manipulation of Eqs. [6] and [7] leads to the steady-state normalized minor signal M_m^*/M_{m0}:

$$\frac{M_m^*}{M_{m0}} = \frac{R_1 + k_m + k_M}{R_1 + 2W + k_m + k_M[1 + (2W/R_1)]}. \quad [8]$$

In analogy to this, on irradiating the major partner introduction of the term $-2WM_M^*$ into Eq. [5] gives for the major signal M_M^*/M_{M0}

$$\frac{M_M^*}{M_{M0}} = \frac{R_1 + k_m + k_M}{R_1 + 2W + k_M + k_m[1 + (2W/R_1)]}. \quad [9]$$

The magnetizations M_m^*/M_{m0} (Eq. [8]) and M_M^*/M_{M0} (Eq. [9]) as a function of W for different values of k_m and k_M and calculated for $R_1 = 1\ s^{-1}$ are shown in Fig. 5. It is readily seen that the more biased the exchange system, the greater the difference in the saturabilities between the minor and major signals. At a population ratio of 1:15 ($k_m = 150\ s^{-1}$ and $k_M = 10\ s^{-1}$), the major signal saturates practically as if it were not involved in the exchange process. However, the minor signal is highly unresponsive to saturation, especially at the beginning of the W scale which corresponds to the low continuous-irradiation power levels normally employed to ensure adequate selectivity.

[illegible] radiation of the narrow major peak perturbs a large number of spins in the major site. The ensuing difference in transition [illegible] difference in saturabilities.

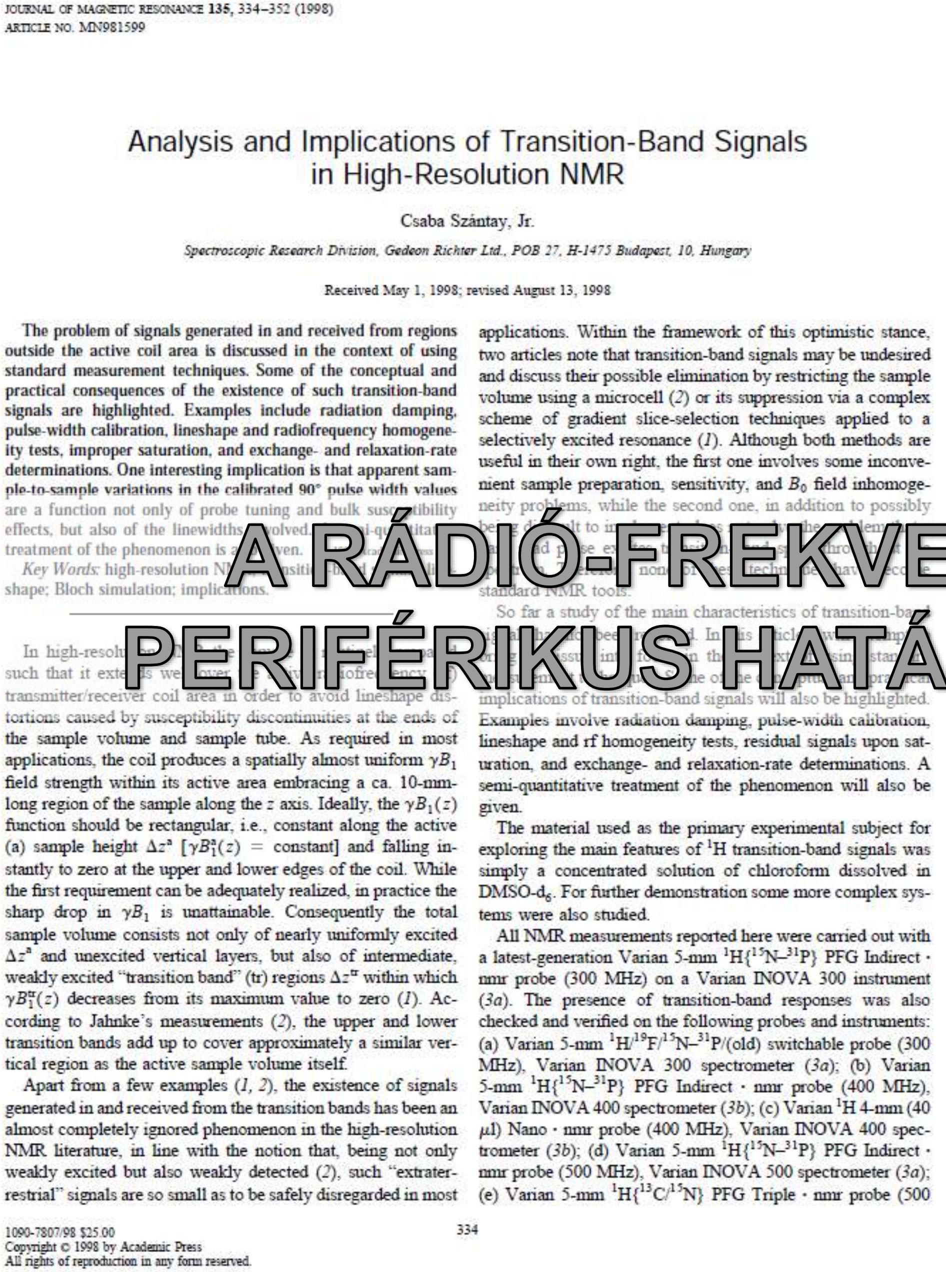
[illegible] the minor [illegible] coupling to the lattice allows less recovery for the spins while they visit the major site. Consequently, the longer the relaxation time[illegible] nced the difference between sensitivity [illegible] or signals to saturation (Fig. 6). Thus, [illegible] ent, the irradiated minor signal should be more easily detected in very small molecules and/or for highly isolated protons and is more likely to remain invisible in bigger molecules with shorter relaxation times.

These results accord with the above discussed and experimentally observed behavior of the system, and therefore our premise regarding the treatment of the problem in terms of the slow exchange approximation seems well founded.

Dynamical Properties of the System

A molecule undergoing a highly biased two-site exchange exhibits a set of $^1H_m \rightleftharpoons {}^1H_M$ proton pairs, each of which may potentially be in slow or fast exchange, or close to coalescence, depending on the specific $\Delta\nu = |\nu_m - \nu_M|$ values at the given exchange rates. Those main resonances that are close to coalescence (i.e., to maximal broadening) will be potentially the most indicative of the otherwise concealed exchange process. We therefore examine systems which show no obvious sign of the ongoing exchange process even if *some* of the $^1H_m \rightleftharpoons {}^1H_M$ pairs among the total set are near coalescence (both molecules **1** and **2** satisfy this condition). That is, in addition to our two preconditions regarding ex-

A RÁDIÓ-FREKVENCIÁS TEKERCS PERIFÉRIKUS HATÁSAINAK ELEMZÉSE



JOURNAL OF MAGNETIC RESONANCE **135**, 334–352 (1998)
ARTICLE NO. MN981599

Analysis and Implications of Transition-Band Signals in High-Resolution NMR

Csaba Szántay, Jr.

Spectroscopic Research Division, Gedeon Richter Ltd., POB 27, H-1475 Budapest, 10, Hungary

Received May 1, 1998; revised August 13, 1998

The problem of signals generated in and received from regions outside the active coil area is discussed in the context of using standard measurement techniques. Some of the conceptual and practical consequences of the existence of such transition-band signals are highlighted. Examples include radiation damping, pulse-width calibration, lineshape and radiofrequency homogeneity tests, improper saturation, and exchange- and relaxation-rate determinations. One interesting implication is that apparent sample-to-sample variations in the calibrated 90° pulse width values are a function not only of probe tuning and bulk susceptibility effects, but also of the linewidths involved. [illegible]-quantitative treatment of the phenomenon is a[illegible]ven.

Key Words: high-resolution N[illegible]nsiti[illegible] shape; Bloch simulation; implications.

In high-resolu[illegible] such that it exte[illegible]s we[illegible]over [illegible]ofrequency [illegible] transmitter/receiver coil area in order to avoid lineshape distortions caused by susceptibility discontinuities at the ends of the sample volume and sample tube. As required in most applications, the coil produces a spatially almost uniform γB_1 field strength within its active area embracing a ca. 10-mm-long region of the sample along the z axis. Ideally, the $\gamma B_1(z)$ function should be rectangular, i.e., constant along the active (a) sample height Δz^a [$\gamma B_1^a(z) = \text{constant}$] and falling instantly to zero at the upper and lower edges of the coil. While the first requirement can be adequately realized, in practice the sharp drop in γB_1 is unattainable. Consequently the total sample volume consists not only of nearly uniformly excited Δz^a and unexcited vertical layers, but also of intermediate, weakly excited "transition band" (tr) regions Δz^{tr} within which $\gamma B_1^{tr}(z)$ decreases from its maximum value to zero (*1*). According to Jahnke's measurements (*2*), the upper and lower transition bands add up to cover approximately a similar vertical region as the active sample volume itself.

Apart from a few examples (*1, 2*), the existence of signals generated in and received from the transition bands has been an almost completely ignored phenomenon in the high-resolution NMR literature, in line with the notion that, being not only weakly excited but also weakly detected (*2*), such "extraterrestrial" signals are so small as to be safely disregarded in most applications. Within the framework of this optimistic stance, two articles note that transition-band signals may be undesired and discuss their possible elimination by restricting the sample volume using a microcell (*2*) or its suppression via a complex scheme of gradient slice-selection techniques applied to a selectively excited resonance (*1*). Although both methods are useful in their own right, the first one involves some inconvenient sample preparation, sensitivity, and B_0 field inhomogeneity problems, while the second one, in addition to possibly bein[illegible] di[illegible]lt to i[illegible] [illegible]d p[illegible]se ex[illegible] [illegible] none [illegible] techn[illegible] hav[illegible] standard NMR tools.

So far a study of the main characteristics of transition-band signal[illegible] been [illegible]d. In [illegible]is article [illegible] [illegible] issu[illegible] in [illegible] the [illegible] [illegible]sing stan[illegible] [illegible]e of the [illegible] and practical implications of transition-band signals will also be highlighted. Examples involve radiation damping, pulse-width calibration, lineshape and rf homogeneity tests, residual signals upon saturation, and exchange- and relaxation-rate determinations. A semi-quantitative treatment of the phenomenon will also be given.

The material used as the primary experimental subject for exploring the main features of ^{1}H transition-band signals was simply a concentrated solution of chloroform dissolved in DMSO-d_6. For further demonstration some more complex systems were also studied.

All NMR measurements reported here were carried out with a latest-generation Varian 5-mm ^{1}H{^{15}N–^{31}P} PFG Indirect · nmr probe (300 MHz) on a Varian INOVA 300 instrument (*3a*). The presence of transition-band responses was also checked and verified on the following probes and instruments: (a) Varian 5-mm ^{1}H/^{19}F/^{15}N–^{31}P/(old) switchable probe (300 MHz), Varian INOVA 300 spectrometer (*3a*); (b) Varian 5-mm ^{1}H{^{15}N–^{31}P} PFG Indirect · nmr probe (400 MHz), Varian INOVA 400 spectrometer (*3b*); (c) Varian ^{1}H 4-mm (40 μl) Nano · nmr probe (400 MHz), Varian INOVA 400 spectrometer (*3b*); (d) Varian 5-mm ^{1}H{^{15}N–^{31}P} PFG Indirect · nmr probe (500 MHz), Varian INOVA 500 spectrometer (*3a*); (e) Varian 5-mm ^{1}H{^{13}C/^{15}N} PFG Triple · nmr probe (500

1090-7807/98 $25.00

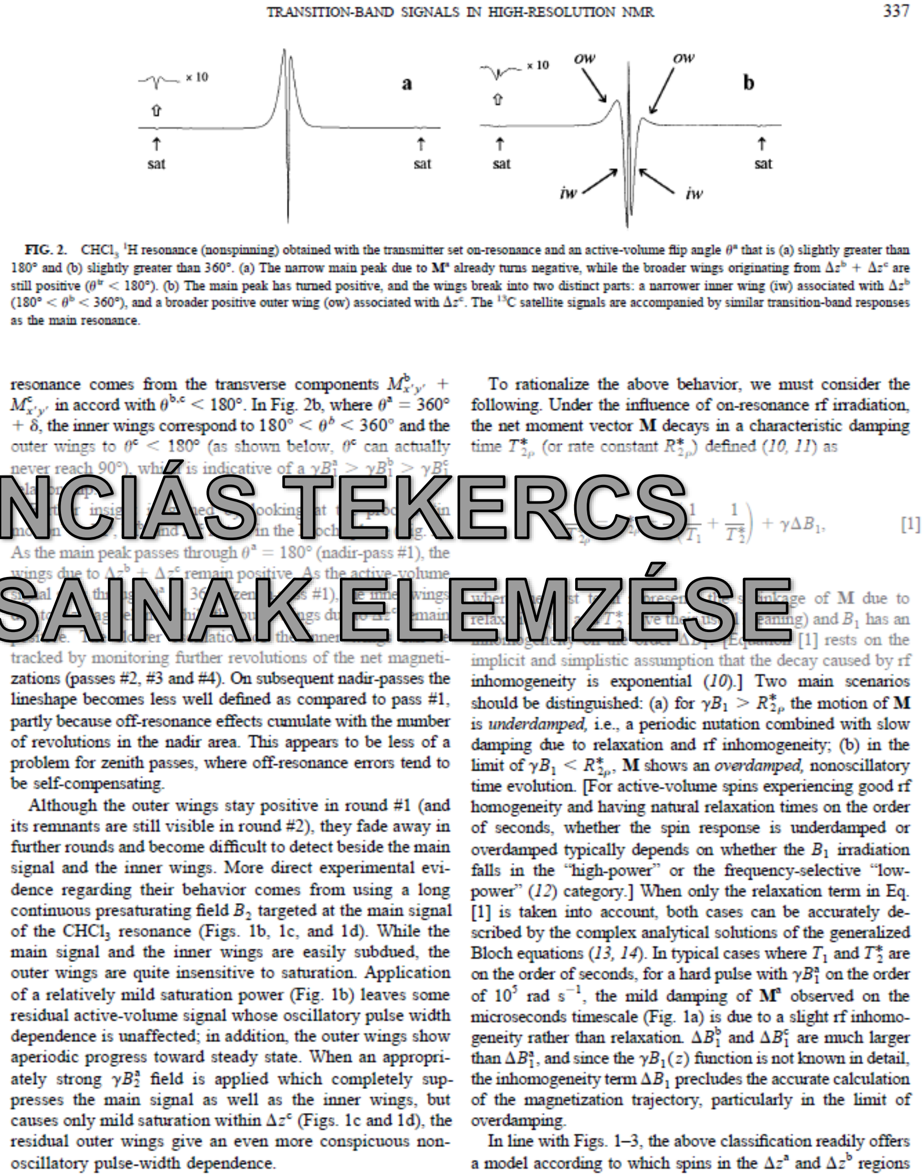


FIG. 2. CHCl$_3$ ^{1}H resonance (nonspinning) obtained with the transmitter set on-resonance and an active-volume flip angle θ^a that is (a) slightly greater than 180° and (b) slightly greater than 360°. (a) The narrow main peak due to M^a already turns negative, while the broader wings originating from $\Delta z^b + \Delta z^c$ are still positive ($\theta^{tr} < 180°$). (b) The main peak has turned positive, and the wings break into two distinct parts: a narrower inner wing (iw) associated with Δz^b ($180° < \theta^b < 360°$), and a broader positive outer wing (ow) associated with Δz^c. The ^{13}C satellite signals are accompanied by similar transition-band responses as the main resonance.

resonance comes from the transverse components $M^b_{x'y'} + M^c_{x'y'}$ in accord with $\theta^{b,c} < 180°$. In Fig. 2b, where $\theta^a = 360° + \delta$, the inner wings correspond to $180° < \theta^b < 360°$ and the outer wings to $\theta^c < 180°$ (as shown below, θ^c can actually never reach 90°), whi[illegible] is indicative of a $\gamma B_1^a > \gamma B_1^b > \gamma B_1^c$ [illegible]ation[illegible] [illegible] insig[illegible] [illegible]ed [illegible] looking at t[illegible] [illegible] in mo[illegible] [illegible] and [illegible] in the Bloch [illegible]. As the main peak passes through $\theta^a = 180°$ (nadir-pass #1), the wings due to $\Delta z^b + \Delta z^c$ remain positive. As the active-volume signal [illegible] through θ^a [illegible] 360 [illegible] zen[illegible] #1), the inner wings [illegible] [illegible]ings due to Δz^c remain positive. [illegible] [illegible] of the inner [illegible] tracked by monitoring further revolutions of the net magnetizations (passes #2, #3 and #4). On subsequent nadir-passes the lineshape becomes less well defined as compared to pass #1, partly because off-resonance effects cumulate with the number of revolutions in the nadir area. This appears to be less of a problem for zenith passes, where off-resonance errors tend to be self-compensating.

Although the outer wings stay positive in round #1 (and its remnants are still visible in round #2), they fade away in further rounds and become difficult to detect beside the main signal and the inner wings. More direct experimental evidence regarding their behavior comes from using a long continuous presaturating field B_2 targeted at the main signal of the CHCl$_3$ resonance (Figs. 1b, 1c, and 1d). While the main signal and the inner wings are easily subdued, the outer wings are quite insensitive to saturation. Application of a relatively mild saturation power (Fig. 1b) leaves some residual active-volume signal whose oscillatory pulse width dependence is unaffected; in addition, the outer wings show aperiodic progress toward steady state. When an appropriately strong γB_2^a field is applied which completely suppresses the main signal as well as the inner wings, but causes only mild saturation within Δz^c (Figs. 1c and 1d), the residual outer wings give an even more conspicuous nonoscillatory pulse-width dependence.

To rationalize the above behavior, we must consider the following. Under the influence of on-resonance rf irradiation, the net moment vector **M** decays in a characteristic damping time $T^*_{2\rho}$ (or rate constant $R^*_{2\rho}$) defined (*10, 11*) as

$$[illegible] \left(\frac{1}{T_1} + \frac{1}{T_2^*}\right) + \gamma\Delta B_1, \qquad [1]$$

where [illegible] [illegible] the s[illegible]nkage of **M** due to relax[illegible] T_2^* [illegible]ve their us[illegible]eaning) and B_1 has an inhomogeneity on the order ΔB_1. [Equation [1] rests on the implicit and simplistic assumption that the decay caused by rf inhomogeneity is exponential (*10*).] Two main scenarios should be distinguished: (a) for $\gamma B_1 > R^*_{2\rho}$, the motion of **M** is *underdamped*, i.e., a periodic nutation combined with slow damping due to relaxation and rf inhomogeneity; (b) in the limit of $\gamma B_1 < R^*_{2\rho}$, **M** shows an *overdamped*, nonoscillatory time evolution. [For active-volume spins experiencing good rf homogeneity and having natural relaxation times on the order of seconds, whether the spin response is underdamped or overdamped typically depends on whether the B_1 irradiation falls in the "high-power" or the frequency-selective "low-power" (*12*) category.] When only the relaxation term in Eq. [1] is taken into account, both cases can be accurately described by the complex analytical solutions of the generalized Bloch equations (*13, 14*). In typical cases where T_1 and T_2^* are on the order of seconds, for a hard pulse with γB_1^a on the order of 10^5 rad s^{-1}, the mild damping of M^a observed on the microseconds timescale (Fig. 1a) is due to a slight rf inhomogeneity rather than relaxation. ΔB_1^b and ΔB_1^c are much larger than ΔB_1^a, and since the $\gamma B_1(z)$ function is not known in detail, the inhomogeneity term ΔB_1 precludes the accurate calculation of the magnetization trajectory, particularly in the limit of overdamping.

In line with Figs. 1–3, the above classification readily offers a model according to which spins in the Δz^a and Δz^b regions

A MÁGNESEZETTSÉGI VEKTOR VISELKEDÉSE INHOMOGÉN GERJESZTŐ TÉRBEN

Evolution of Magnetization in a B_1 Field. I. The Impact of B_0/B_1 Inhomogeneity and Fast Chemical Exchange in High-Resolution NMR

CSABA SZÁNTAY, Jr.
Gedeon Richter Ltd., Spectroscopic Research Division, H-1[illegible] Budapest, 10, POB 27, Hungary;
Email: cs.szantay@richter.hu

ABSTRACT: Since the classical treatment by Torrey in 1949 of the problem of how magnetization evolves in [illegible] subsequent [illegible] received relatively little atte[illegible] importance [illegible] focuses on the behavior of the [illegible] constituents in both 'hard' and 'soft' resonant B_1 fields by examining the effects of B_0 and B_1 inhomogeneities and moderately fast chemical exchange. Discussion embraces the out-of-coil regions where spins experience large B_1 [illegible] and give, under suitable conditions, well-detected signals. It is shown [illegible] formally similar to increased transverse decay an[illegible] in a [illegible]neous B_1 field, and can lead to two different t[illegible] isochromatic net magnetizations, which in turn give different macroscopic behaviors. Some practical implications relating to these considerations are also noted. © 1999 John Wiley & Sons, Inc. Concepts Magn Reson 11: 343–362, 1999

KEY WORDS: High-resolution NMR; B_1 inhomogeneity; nutation; underdamping; overdamping; phase randomization of the first and second kind; transition-band signals; Bloch simulations

Received 8 February 1999; revised and accepted 22 March 1999.
Concepts in Magnetic Resonance, Vol. 11(6) 343–362 (1999)

positive absorption-mode resonance, while if $M_{y'}^{t=0} = -M_{y'}, M_{x'}^{t=0} = 0$, we obtain a pure negative absorption-mode signal. In this system, the time dependence of **M** is governed by the Bloch equations (*9*), which in this case take the following simple vectorial form:

$$\frac{d\mathbf{M}}{dt} = \gamma[\mathbf{M} \otimes \mathbf{B}_1] - \lambda_2\mathbf{M}_{y'} + \lambda_1(\mathbf{M}^0 - \mathbf{M}_z) \quad [1]$$

The term $\gamma\mathbf{M} \otimes \mathbf{B}_1$ represents the torque $\mathbf{K} = d\mathbf{M}/dt = \gamma\mathbf{M} \otimes \mathbf{B}_1$, which causes the net moment vector **M** to circulate (nutate) in the zy' plane with an angular frequency γB_1. [To conform to our previous discussion of related topics [illegible] M [illegible] B_1 [illegible] M [illegible] nutation.] The terms $\lambda_2\mathbf{M}_{y'}$ and $\lambda_1(\mathbf{M}^0 - \mathbf{M}_z)$, on the other hand, describe the fact that this [illegible] λ_2 [illegible] λ_1 simply correspond to the transverse and longitudinal relaxation rates, $\lambda_2 = 1/T_2$ and $\lambda_1 = 1/T_1$. The [illegible] nutation [illegible] Torrey (*2*), [illegible] ized at resonance by a damping time constant T_0 (or rate constant R_0) defined as

$$R_0 = \frac{1}{T_0} = \frac{1}{2}\left(\frac{1}{T_1} + \frac{1}{T_2}\right) = \frac{1}{2}(\lambda_1 + \lambda_2) \quad [2]$$

The time Γ_0 needed to (nearly) reach the steady-state condition $\mathbf{M}^{ss}$ in a B_1 field requires in practice a period $> 5T_0$.

By calculating the vector product in Eq. [1], we obtain the familiar equations

$$\frac{dM_{x'}}{dt} = -\lambda_2 M_{x'} \quad [3a]$$

$$\frac{dM_{y'}}{dt} = +\gamma B_1 M_z - \lambda_2 M_{y'} \quad [3b]$$

$$\frac{dM_z}{dt} = -\gamma B_1 M_{y'} + \lambda_1(M^0 - M_z) \quad [3c]$$

The steady-state solutions corresponding to the condition $d\mathbf{M}/dt = 0$ are easily obtained from Eqs. [3] to give:

$$M_{x'}^{ss} = 0 \quad [4a]$$

$$M_{y'}^{ss} = \frac{\gamma B_1 \lambda_1 M_0}{\lambda_1\lambda_2 + (\gamma B_1)^2} \quad [4b]$$

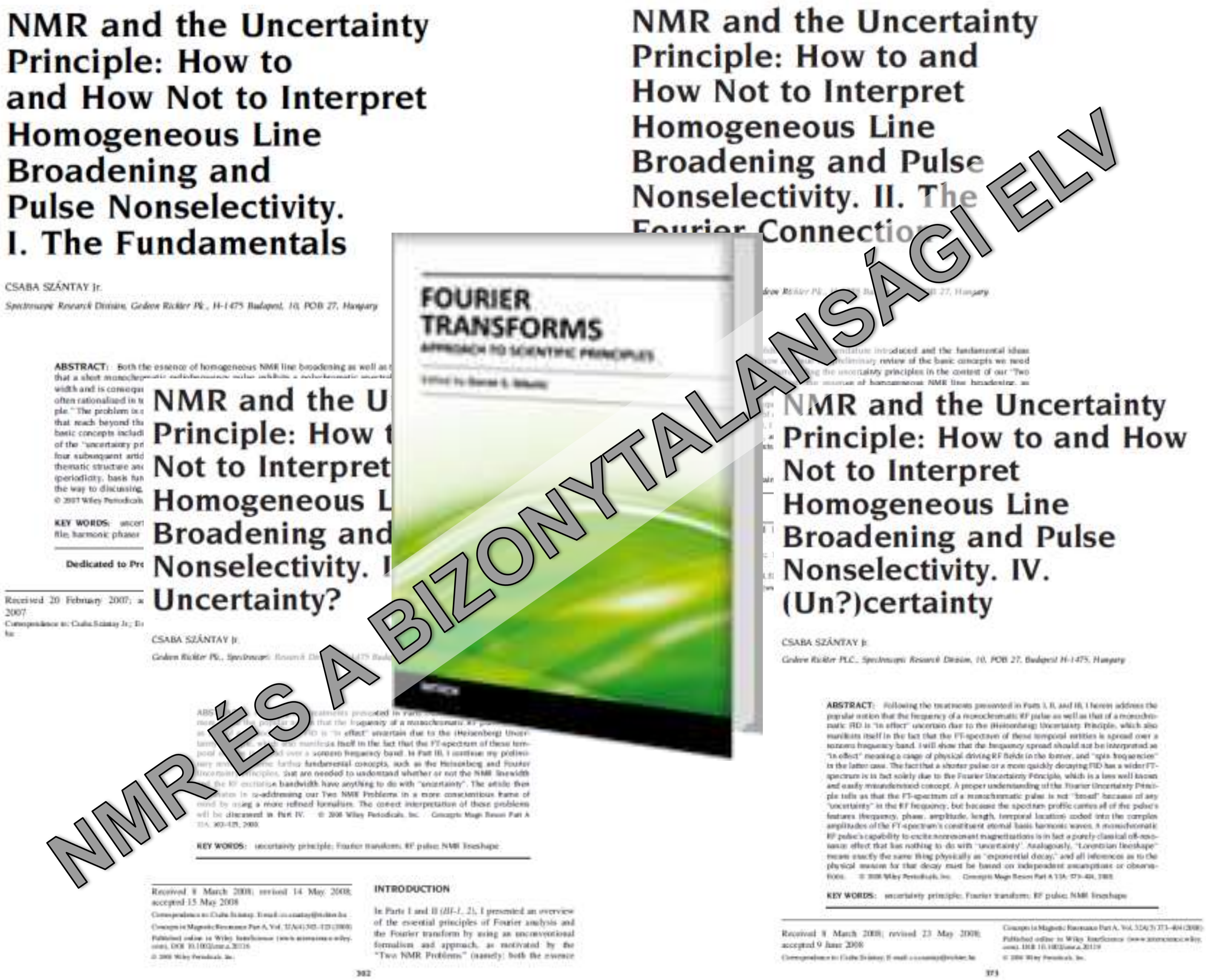
$$M_z^{ss} = \frac{\lambda_1\lambda_2 M_0}{\lambda_1\lambda_2 + (\gamma B_1)^2} \quad [4c]$$

A special but instructive case of this steady-state condition is represented in Fig. 1. $\mathbf{R}_1 = \lambda_1(\mathbf{M}^0 - \mathbf{M}_z)$ and $\mathbf{R}_2 = -\lambda_2\mathbf{M}_{y'}$ denote the *relaxation vectors* (*10*) which drive $\mathbf{M}_z$ toward $\mathbf{M}^0$ and $\mathbf{M}_{y'}$ toward 0, and are depicted here with the proportionality constants chosen to be unity so that $R_1 = M^0 - M_z$ and $R_2 = -M_{y'}$ and $\gamma B_1 = 1$. The equilibrium point is, of course, character[illegible] $+ \mathbf{K} = \mathbf{0}$, i.e., $\mathbf{R}_1 = -\mathbf{K}_z$, $\mathbf{R}$[illegible] $K_{y'} = \gamma M_z B_1$ (cf. Eq. [3b]) be[illegible] B_1 acting on M_z. In a way, the system "balances" the $\mathbf{R}_2$ and $\mathbf{K}_{y'}$ vec[illegible] by varying $K_{y'}$ through the proper "adjust[illegible] Conversely, $K_z = \gamma M_{y'} B_1$ (cf. Eq. [illegible]nting the fact that K_z is generated [illegible] on $M_{y'}$. Thus, a change in K_z is tied to a change in $M_{y'}$ to eventually give $\mathbf{R}_1 = -\mathbf{K}_z$.

From hereon it will prove useful to refer to the four quadrants (Q) of the zy' plane as QI–QIV (cf. Fig. 2). It can be shown (*10*) that when γB_1 is increased from a small value to a high-power irradiation, the steady-state point given by $\mathbf{M}^{ss}$ moves clockwise, with an increasing steady-state angle Θ^{ss}, along a Thales semicircle in QI (Fig.

Figure 1 The steady-state condition, represented for the special case when $\lambda_1 = \lambda_2 = \gamma B_1 = 1$ and the on-resonance $\mathbf{B}_1$ field is aligned along the $+x'$ axis of the rotating frame. The equilibrium point is characterized by the condition $\mathbf{R} + \mathbf{K} = \mathbf{0}$; i.e., the net relaxation vector **R** balances the torque $\mathbf{K} = \gamma\mathbf{M} \otimes \mathbf{B}_1$ (see text). By varying the γB_1 value, **M** moves along the depicted Thales circle but always remains in quadrant I (cf. Fig. 2).

NMR ÉS A BIZONYTALANSÁGI ELV



NMR and the Uncertainty Principle: How to and How Not to Interpret Homogeneous Line Broadening and Pulse Nonselectivity. I. The Fundamentals

CSABA SZÁNTAY Jr.

Spectroscopic Research Division, Gedeon Richter Plc., H-1475 Budapest, 10, POB 27, Hungary

NMR and the Uncertainty Principle: How to and How Not to Interpret Homogeneous Line Broadening and Pulse Nonselectivity. II. The Fourier Connection

NMR and the U Principle: How t Not to Interpret Homogeneous L Broadening and Nonselectivity. I Uncertainty?

CSABA SZÁNTAY Jr.

NMR and the Uncertainty Principle: How to and How Not to Interpret Homogeneous Line Broadening and Pulse Nonselectivity. IV. (Un?)certainty

CSABA SZÁNTAY Jr.

Gedeon Richter PLC., Spectroscopic Research Division, 10, POB 27, Budapest H-1475, Hungary

FOURIER TRANSFORMS

matematika

fizika

filozófia

pszichológia

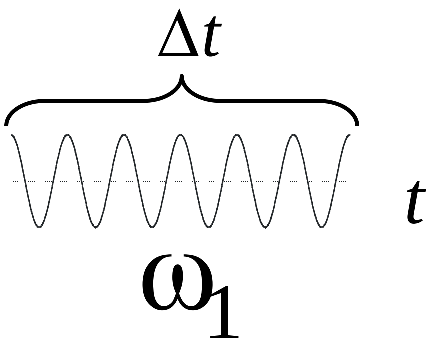
a magspínek pulzus-gerjesztésének értelmezési paradigmája

GLOBÁLISAN ELTERJEDT MAGYARÁZAT:

$\cos(\omega_1 \cdot t)$ alakú
rádió-frekvenciás
elektromágneses
pulzus

PFT NMR

FT



Heisenberg B. E.
$\Delta t \cdot \Delta\omega \geq$ konst.

$\Delta\omega_0$

Larmor frekvencia
rezonancia tartomány

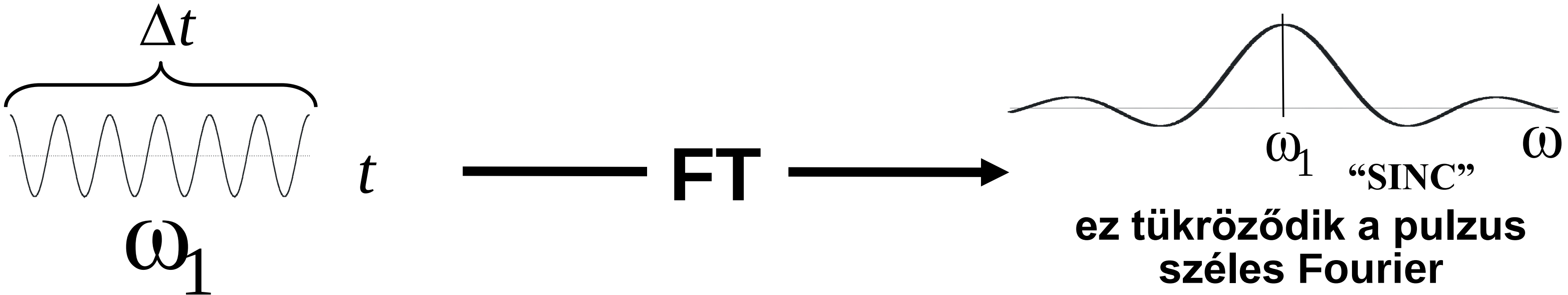
Δt ismert és véges $\rightarrow \Delta\omega_1 > 0$
(a hullám idejének
korlátozása a frekvenciát
<u>bizonytalanná</u> teszi)

a magspínek pulzus-gerjesztésének értelmezési paradigmája

GLOBÁLISAN ELTERJEDT MAGYARÁZAT:

$\cos(\omega_1 \cdot t)$ alakú rádió-frekvenciás elektromágneses pulzus

PFT NMR



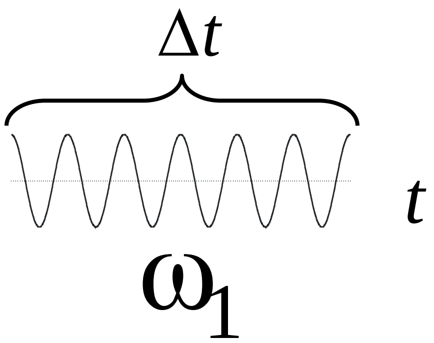
ez tükröződik a pulzus széles Fourier spektrumában is

a magspínek pulzus-gerjesztésének értelmezési paradigmája

GLOBÁLISAN ELTERJEDT MAGYARÁZAT:

cos($\omega_1 \cdot t$) alakú rádió-frekvenciás elektromágneses pulzus

PFT NMR



Heisenberg B. E.

$\Delta t \cdot \Delta\omega \geq$ konst.

FT

$\Delta\omega_0$

Larmor frekvencia rezonancia tartomány

NOMINÁLISAN MONOKROMATIKUS (ω_1) RF PULZUS

EFFEKTÍVE POLIKROMATIKUS ($\Delta\omega_1$)

⇓

ezért a Larmor frekvenciák széles tartományát képes gerjeszteni

“As the Uncertainty Principle indicates, a pulse of carrier frequency ω_1 will contain, in effect, a range of frequencies centred on ω_1. The distribution of RF magnetic field amplitudes takes the form sin(x)/x which is the frequency-domain equivalent of a short pulse in the time domain. The two domains are connected by the Fourier transform ”

“Although the applied excitation may be precizely centred at a frequency ω_1, our act of turning the excitation power on at time zero and off at time Δt effectively broadens the spectral range of the excitation to a bandwidth of ~$1/\Delta t$.”

“… the RF source is monochromatic, so we have to work out a way of using a single frequency to excite multiple frequencies. If the irradiation is applied for a time Δt, then, due to the Uncertainty Principle, the nominally monochromatic irradiation is uncertain in frequency by about $1/\Delta t$.”

“…if the pulse is made shorter, we will no longer have a truly monochromatic frequency spectrum even though the source is still monochromatic”.

“A pulse of monochromatic RF can be described in the frequency domain as a band of frequencies. The Heisenberg principle states that there is a minimum uncertainty in the simultaneous specification of the frequency and the duration of the measurement. This means that, as the pulse length decreases, irradiation is spread over a wider frequency band. The sinc Fourier spectrum of a rectangular RF pulse shows that a shorter pulse gives a wider sinc band.”

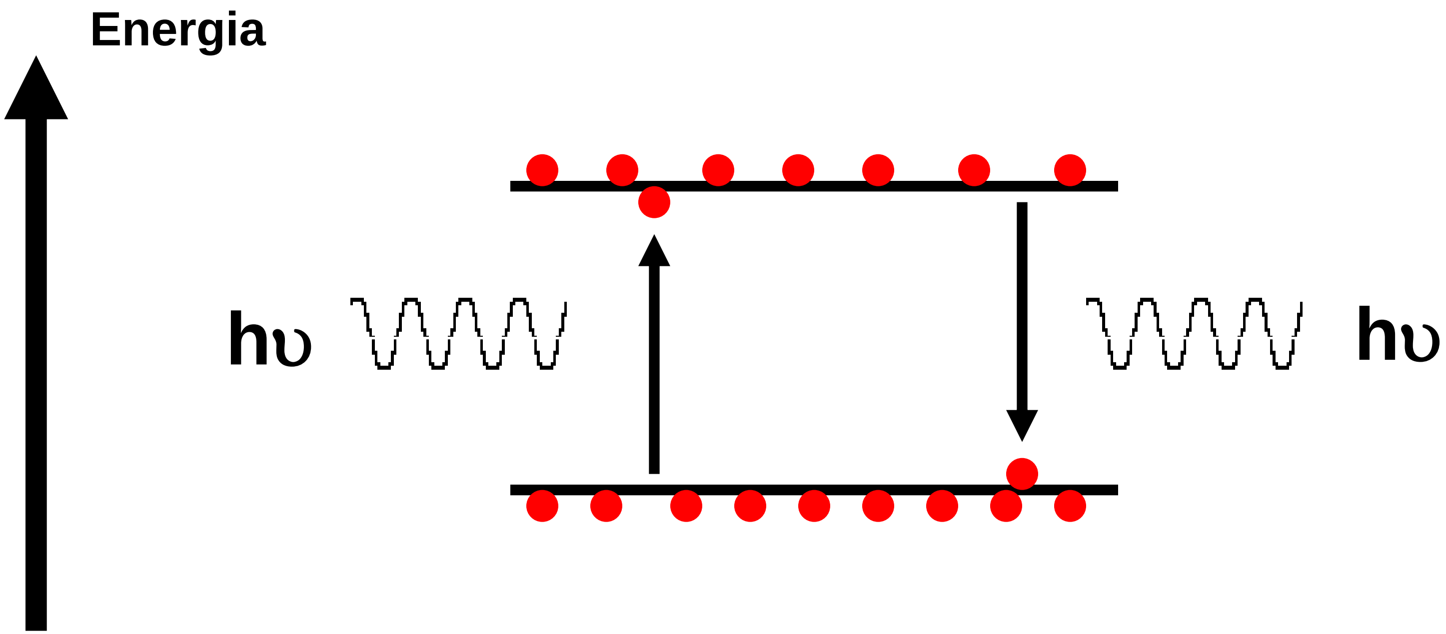
MILYEN (PRE)KONCEPCIÓK VEZETNEK EHHEZ A MAGYARÁZATHOZ?

#1

NMR = kvantummechanikai jelenség

⇓

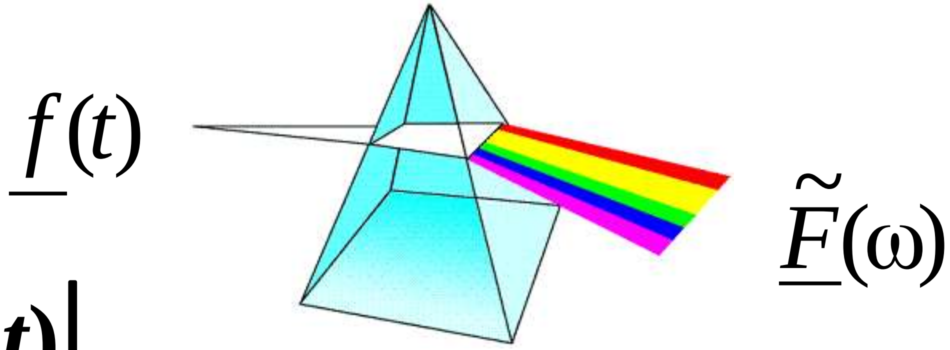
Heisenberg B.E. alkalmazható



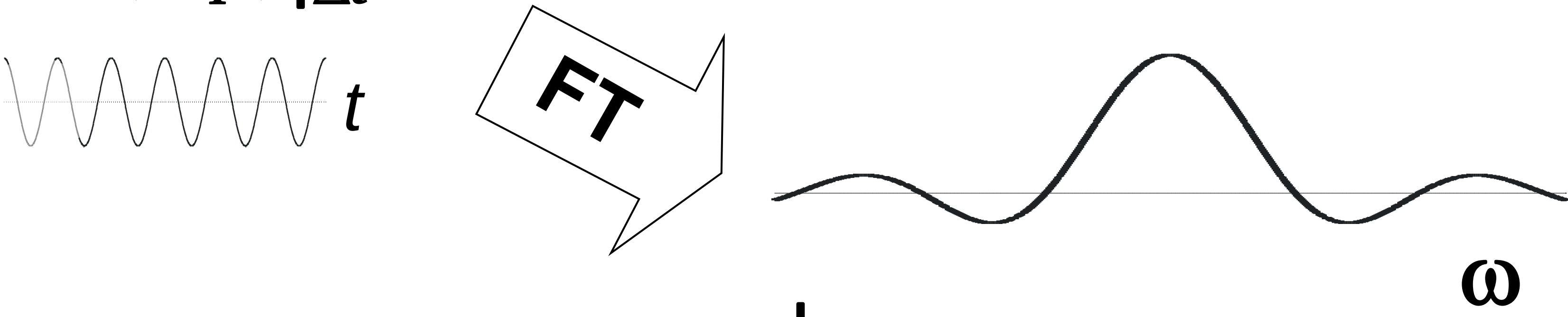
pulzus = kvantummechanikai “entitás”

#2

Fourier transzformáció = időbeli jel felbontása frekvencia komponenseire



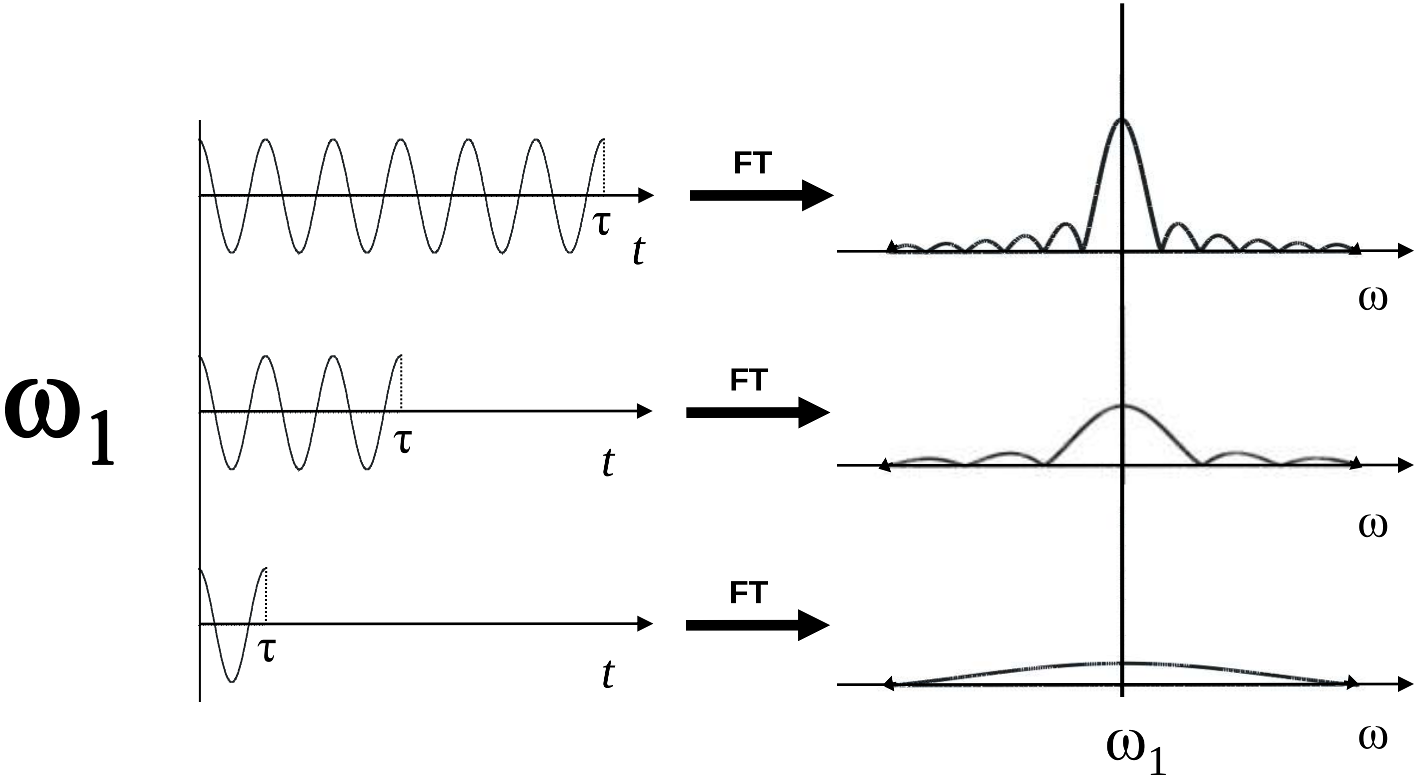
$$\cos(\omega_1 t)\big|_{\Delta t}$$



$\cos(\omega_1 t)\big|_{\Delta t}$ **spektruma =**

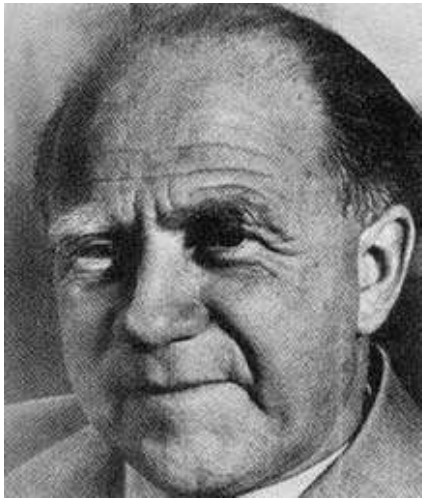
$\cos(\omega_1 t)\big|_{\Delta t}$ **“frekvencia komponensei”**

#3 a kvantummechanikai és klasszikus leírás korrelációja: a Heisenberg B.E. a FT területén is érvényesül:



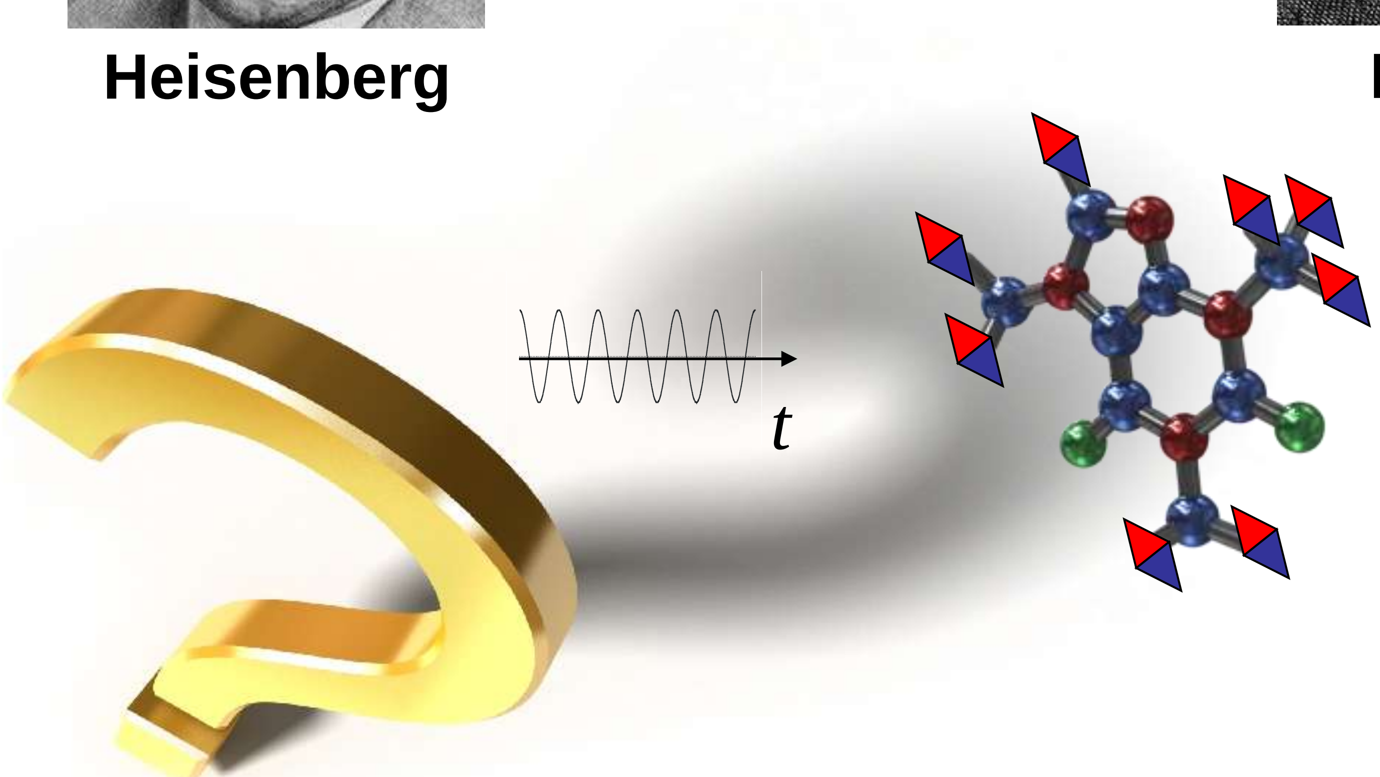
$$\Delta t \cdot \Delta\omega \geq \text{konst.}$$

a magyarázat helyesnek tűnik



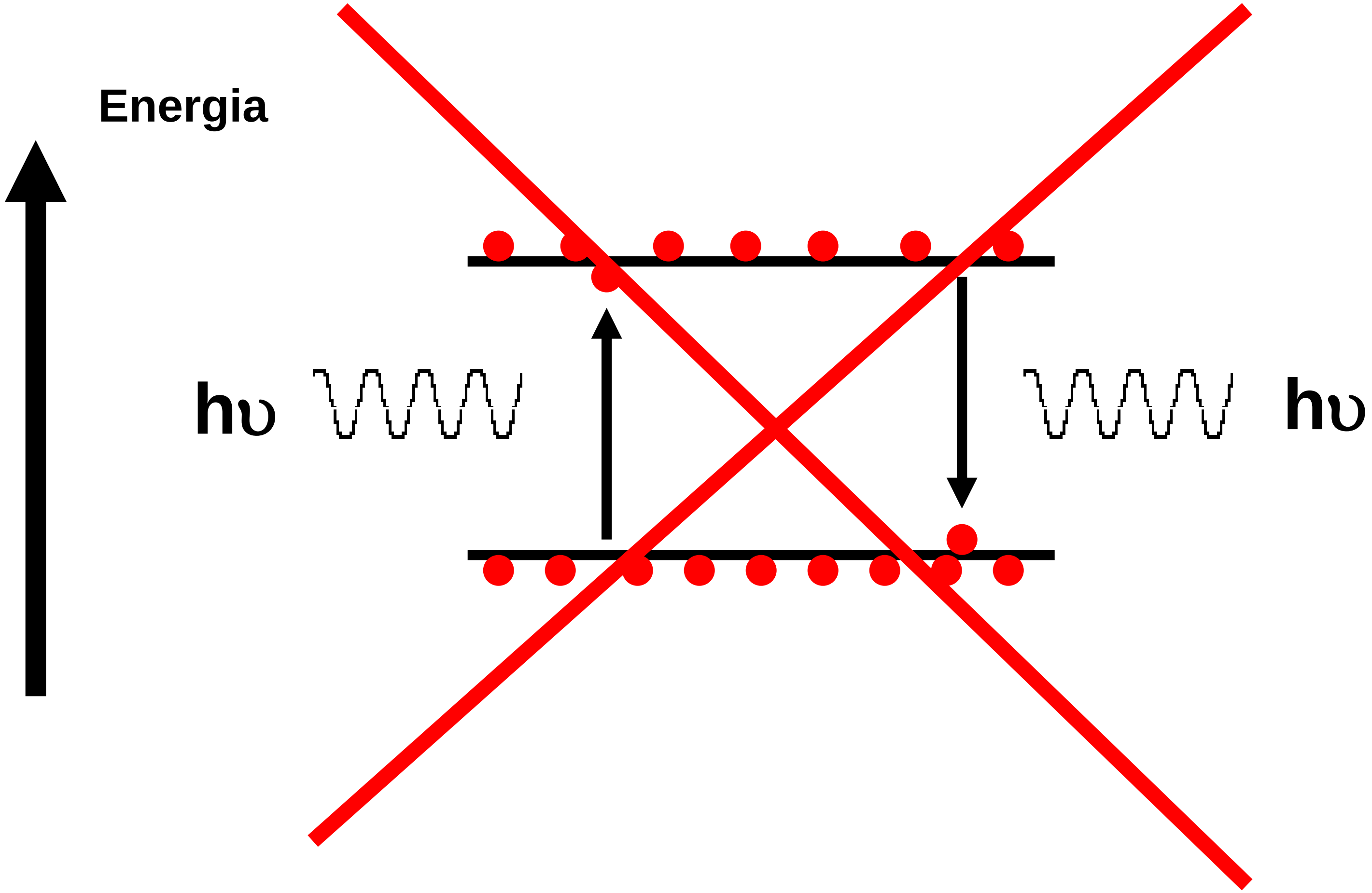
Heisenberg

Fourier



mi ezzel a probléma?

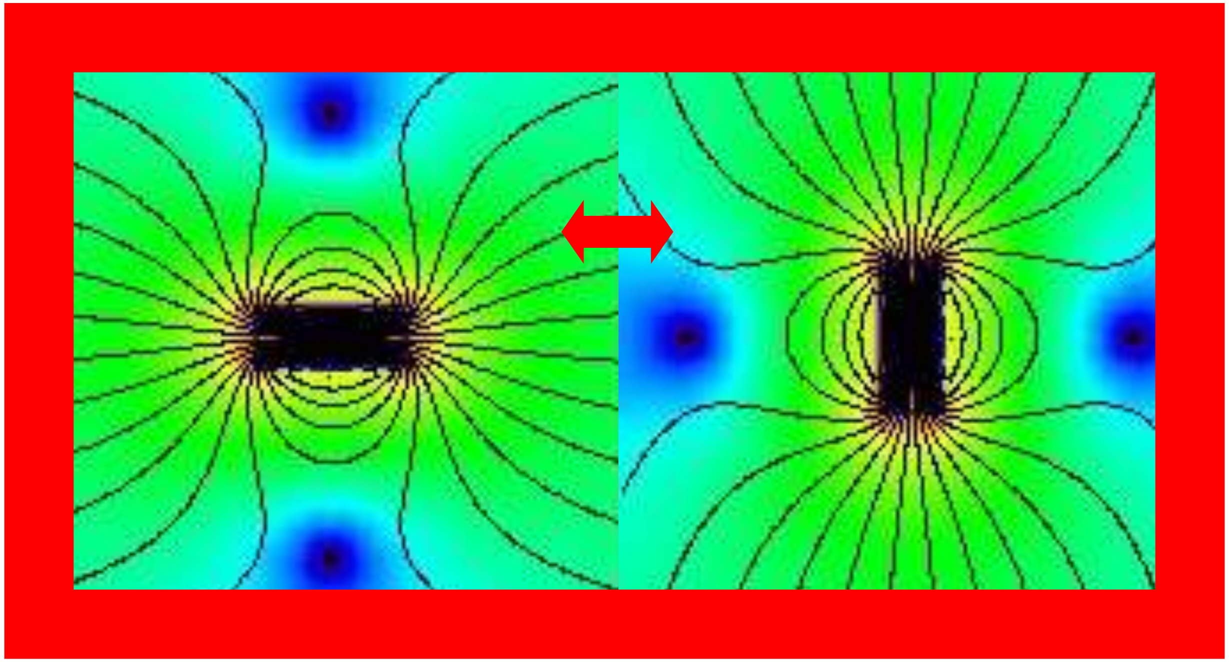
A mágneses rezonancia *NEM* rádió hullámok (fotonok) abszorpciója / emissziója!

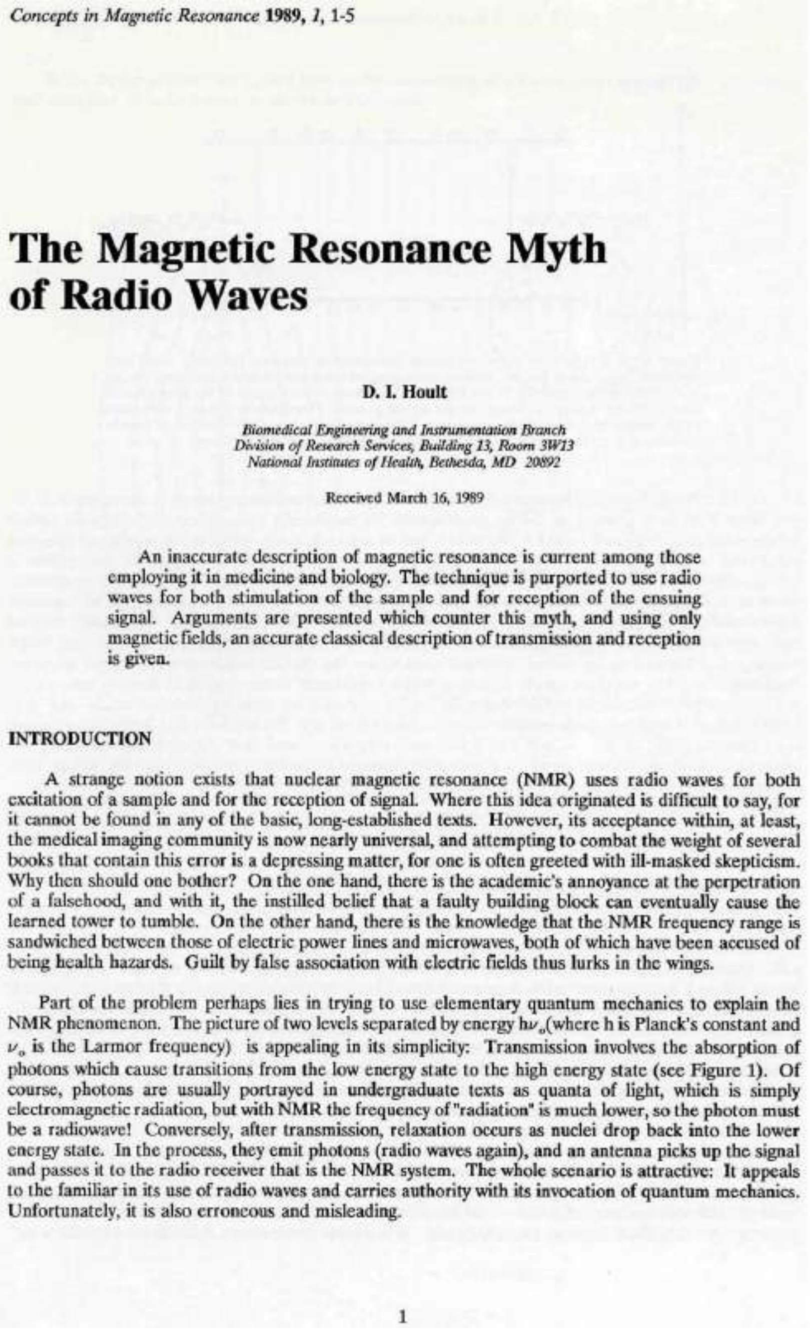


Valójában:
(makroszkópikus) mágneses rezonancia = klasszikus, determinisztikus jelenség (mágneses terek klasszikusan leírható kölcsönhatása)!

az RF hullám mágneses komponense

a minta mágnesezettsége





Concepts in Magnetic Resonance **1989,** *1,* 1-5

The Magnetic Resonance Myth of Radio Waves

D. I. Hoult

Biomedical Engineering and Instrumentation Branch
Division of Research Services, Building 13, Room 3W13
National Institutes of Health, Bethesda, MD 20892

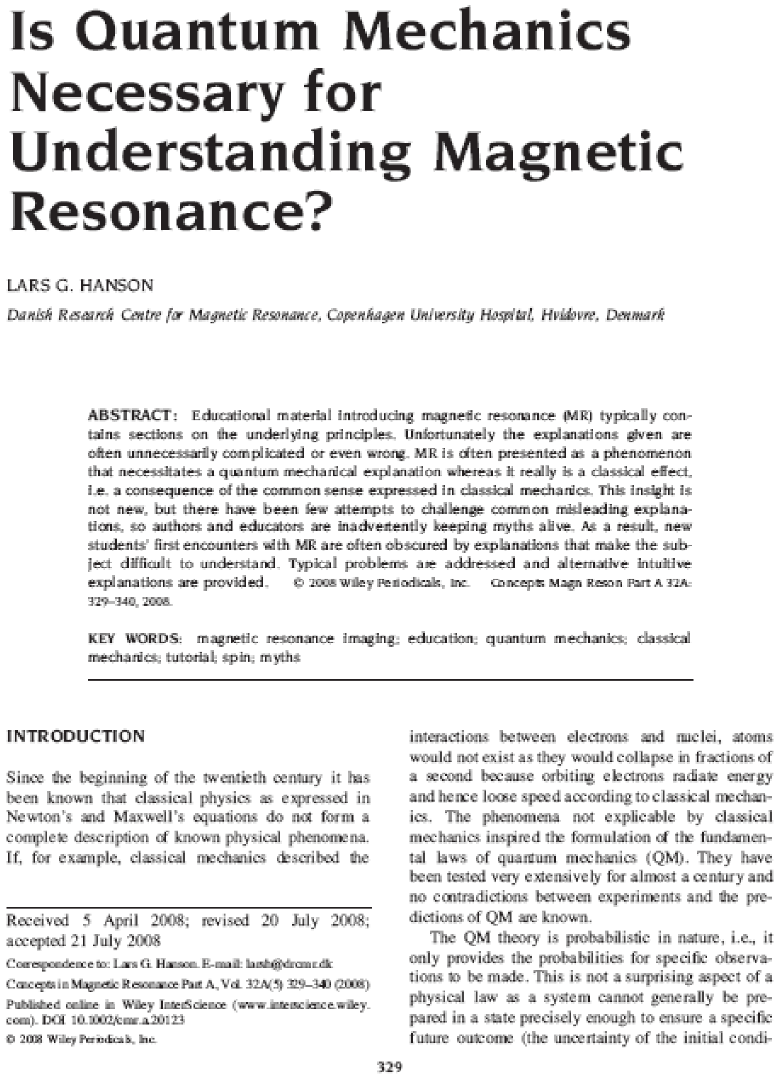
Received March 16, 1989

An inaccurate description of magnetic resonance is current among those employing it in medicine and biology. The technique is purported to use radio waves for both stimulation of the sample and for reception of the ensuing signal. Arguments are presented which counter this myth, and using only magnetic fields, an accurate classical description of transmission and reception is given.

INTRODUCTION

A strange notion exists that nuclear magnetic resonance (NMR) uses radio waves for both excitation of a sample and for the reception of signal. Where this idea originated is difficult to say, for it cannot be found in any of the basic, long-established texts. However, its acceptance within, at least, the medical imaging community is now nearly universal, and attempting to combat the weight of several books that contain this error is a depressing matter, for one is often greeted with ill-masked skepticism. Why then should one bother? On the one hand, there is the academic's annoyance at the perpetration of a falsehood, and with it, the instilled belief that a faulty building block can eventually cause the learned tower to tumble. On the other hand, there is the knowledge that the NMR frequency range is sandwiched between those of electric power lines and microwaves, both of which have been accused of being health hazards. Guilt by false association with electric fields thus lurks in the wings.

Part of the problem perhaps lies in trying to use elementary quantum mechanics to explain the NMR phenomenon. The picture of two levels separated by energy $h\nu_o$(where h is Planck's constant and ν_o is the Larmor frequency) is appealing in its simplicity: Transmission involves the absorption of photons which cause transitions from the low energy state to the high energy state (see Figure 1). Of course, photons are usually portrayed in undergraduate texts as quanta of light, which is simply electromagnetic radiation, but with NMR the frequency of "radiation" is much lower, so the photon must be a radiowave! Conversely, after transmission, relaxation occurs as nuclei drop back into the lower energy state. In the process, they emit photons (radio waves again), and an antenna picks up the signal and passes it to the radio receiver that is the NMR system. The whole scenario is attractive: It appeals to the familiar in its use of radio waves and carries authority with its invocation of quantum mechanics. Unfortunately, it is also erroneous and misleading.



Is Quantum Mechanics Necessary for Understanding Magnetic Resonance?

LARS G. HANSON

Danish Research Centre for Magnetic Resonance, Copenhagen University Hospital, Hvidovre, Denmark

ABSTRACT: Educational material introducing magnetic resonance (MR) typically contains sections on the underlying principles. Unfortunately the explanations given are often unnecessarily complicated or even wrong. MR is often presented as a phenomenon that necessitates a quantum mechanical explanation whereas it really is a classical effect, i.e. a consequence of the common sense expressed in classical mechanics. This insight is not new, but there have been few attempts to challenge common misleading explanations, so authors and educators are inadvertently keeping myths alive. As a result, new students' first encounters with MR are often obscured by explanations that make the subject difficult to understand. Typical problems are addressed and alternative intuitive explanations are provided. Concepts Magn Reson Part A 32A: 329–340, 2008.

KEY WORDS: magnetic resonance imaging; education; quantum mechanics; classical mechanics; tutorial; spin; myths

INTRODUCTION

Since the beginning of the twentieth century it has been known that classical physics as expressed in Newton's and Maxwell's equations do not form a complete description of known physical phenomena. If, for example, classical mechanics described the interactions between electrons and nuclei, atoms would not exist as they would collapse in fractions of a second because orbiting electrons radiate energy and hence loose speed according to classical mechanics. The phenomena not explicable by classical mechanics inspired the formulation of the fundamental laws of quantum mechanics (QM). They have been tested very extensively for almost a century and no contradictions between experiments and the predictions of QM are known.

The QM theory is probabilistic in nature, i.e., it only provides the probabilities for specific observations to be made. This is not a surprising aspect of a physical law as a system cannot generally be prepared in a state precisely enough to ensure a specific future outcome (the uncertainty of the initial condi-

---

Received 5 April 2008; revised 20 July 2008; accepted 21 July 2008

Correspondence to: Lars G. Hanson. E-mail: larsh@drcmr.dk

Concepts in Magnetic Resonance Part A, Vol. 32A(5) 329–340 (2008)

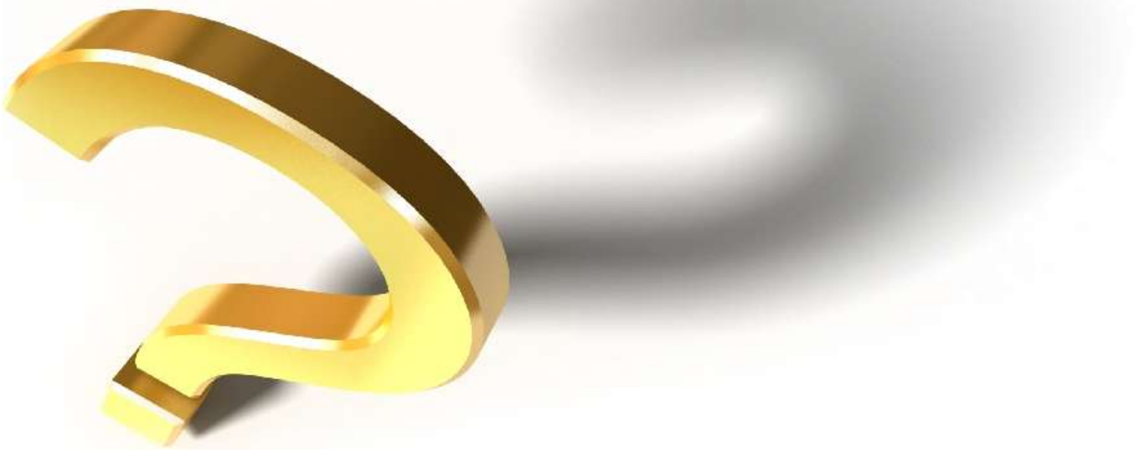
DOI 10.1002/cmr.a.20123

Mi köze van tehát mindehhez Heisenbergnek?

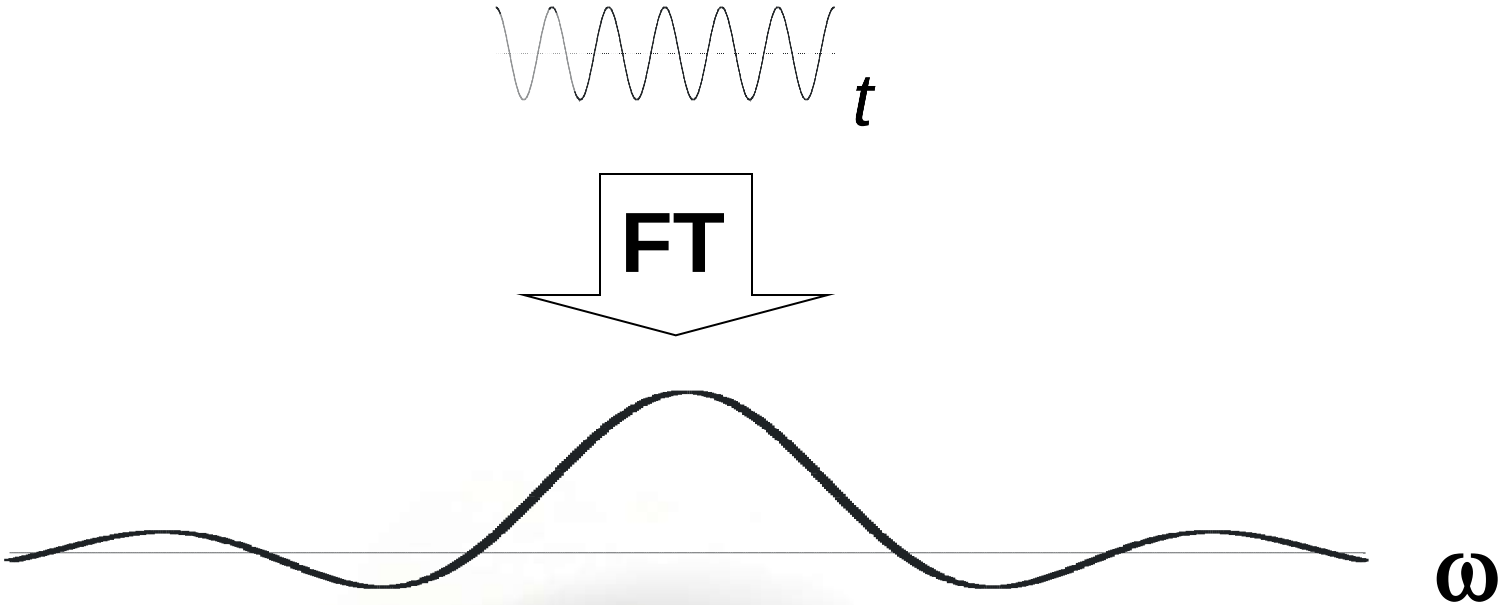
$$\Delta t \cdot \Delta\omega \geq \textbf{konst.}$$

kvantummechanikai + valószínűségi állítás!

RF pulzus = oszcilláló mágneses tér



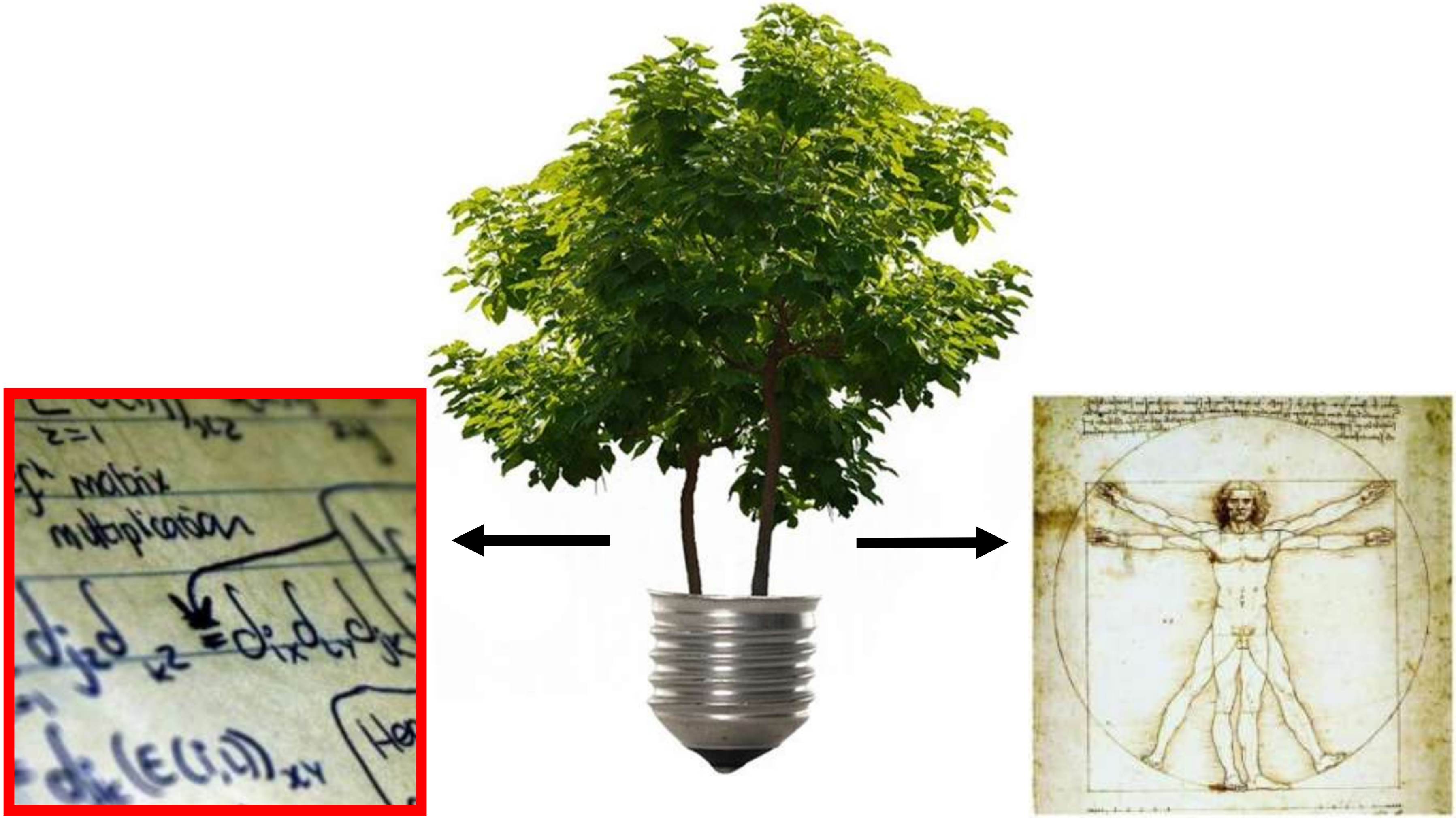
$$\cos(\omega_1 t)\big|_{\Delta t}$$



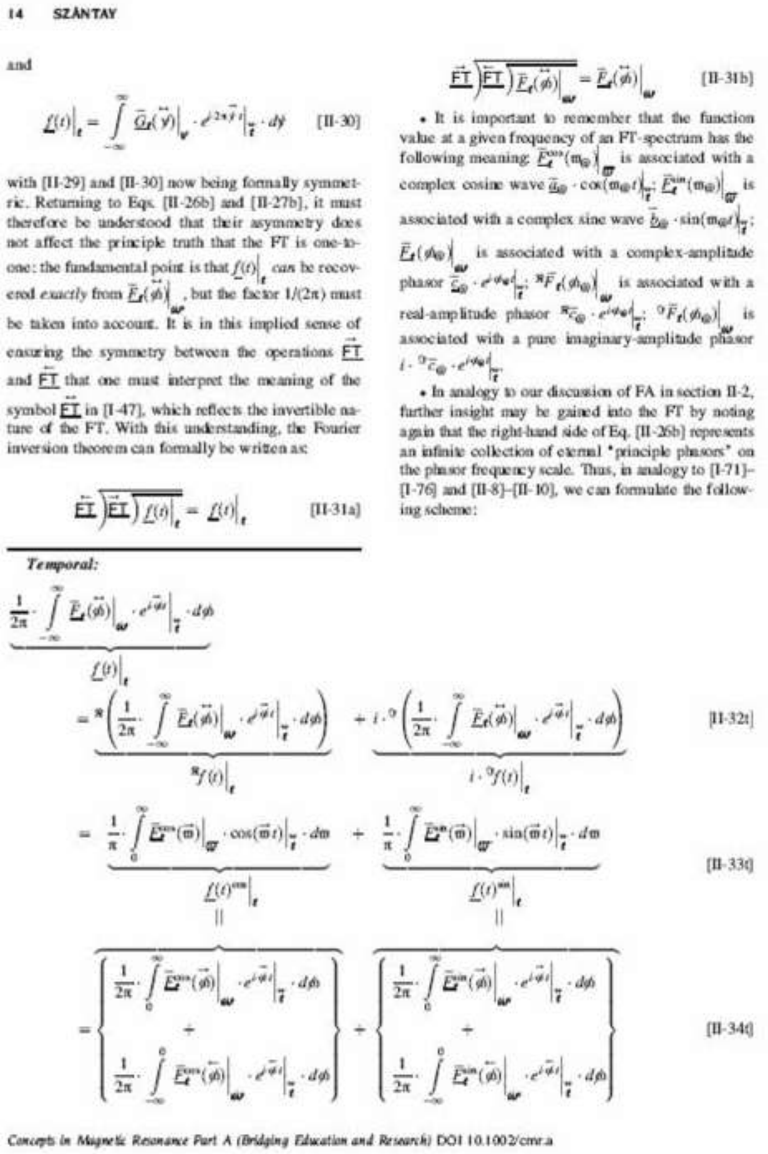
ω_1 az idő-dimenzióban pontosan definiált a frekvencia dimenzióban pedig NEM?

“NOMINÁLISAN” monokromatikus = “EFFEKTÍVE” polikromatikus???

A MEGOLDÁS



A LÉNYEG



and

$$\underline{f}(t)\Big|_{t} = \int_{-\infty}^{\infty} \underline{\bar{G}}_t(\overleftrightarrow{\nu})\Big|_{\nu} \cdot e^{i2\pi\vec{\nu}t}\Big|_{\bar{t}} \cdot d\nu \tag{II-30}$$

with [II-29] and [II-30] now being formally symmetric. Returning to Eqs. [II-26b] and [II-27b], it must therefore be understood that their asymmetry does not affect the principle truth that the FT is one-to-one: the fundamental point is that $\underline{f}(t)\big|_{t}$ *can* be recovered *exactly* from $\underline{\bar{F}}_t(\overleftrightarrow{\phi})\big|_{\omega}$, but the factor $1/(2\pi)$ must be taken into account. It is in this implied sense of ensuring the symmetry between the operations $\overrightarrow{\underline{\mathrm{FT}}}$ and $\overleftarrow{\underline{\mathrm{FT}}}$ that one must interpret the meaning of the symbol $\overleftrightarrow{\underline{\mathrm{FT}}}$ in [I-47], which reflects the invertible nature of the FT. With this understanding, the Fourier inversion theorem can formally be written as:

$$\overleftarrow{\underline{\mathrm{FT}}}\Big)\overline{\overrightarrow{\underline{\mathrm{FT}}}\Big)\overline{\underline{f}(t)\big|_{t}}} = \underline{f}(t)\Big|_{t} \tag{II-31a}$$

$$\overrightarrow{\underline{\mathrm{FT}}}\Big)\overline{\overleftarrow{\underline{\mathrm{FT}}}\Big)\overline{\underline{\bar{F}}_t(\overleftrightarrow{\phi})\big|_{\omega}}} = \underline{\bar{F}}_t(\overleftrightarrow{\phi})\Big|_{\omega} \tag{II-31b}$$

- It is important to remember that the function value at a given frequency of an FT-spectrum has the following meaning: $\underline{\bar{F}}_t^{\cos}(\varpi_{\circledcirc})\big|_{\varpi}$ is associated with a complex cosine wave $\underline{\bar{a}}_{\circledcirc}\cdot\cos(\varpi_{\circledcirc}t)\big|_{\bar{t}}$; $\underline{\bar{F}}_t^{\sin}(\varpi_{\circledcirc})\big|_{\varpi}$ is associated with a complex sine wave $\underline{\bar{b}}_{\circledcirc}\cdot\sin(\varpi_{\circledcirc}t)\big|_{\bar{t}}$; $\underline{\bar{F}}_t(\phi_{\circledcirc})\big|_{\omega}$ is associated with a complex-amplitude phasor $\underline{\bar{c}}_{\circledcirc}\cdot e^{i\phi_{\circledcirc}t}\big|_{\bar{t}}$; ${}^{\Re}\bar{F}_t(\phi_{\circledcirc})\big|_{\omega}$ is associated with a real-amplitude phasor ${}^{\Re}\bar{c}_{\circledcirc}\cdot e^{i\phi_{\circledcirc}t}\big|_{\bar{t}}$; ${}^{\Im}\bar{F}_t(\phi_{\circledcirc})\big|_{\omega}$ is associated with a pure imaginary-amplitude phasor $i\cdot{}^{\Im}\bar{c}_{\circledcirc}\cdot e^{i\phi_{\circledcirc}t}\big|_{\bar{t}}$.
- In analogy to our discussion of FA in section II-2, further insight may be gained into the FT by noting again that the right-hand side of Eq. [II-26b] represents an infinite collection of eternal "principle phasors" on the phasor frequency scale. Thus, in analogy to [I-71]–[I-76] and [II-8]–[II-10], we can formulate the following scheme:

Temporal:

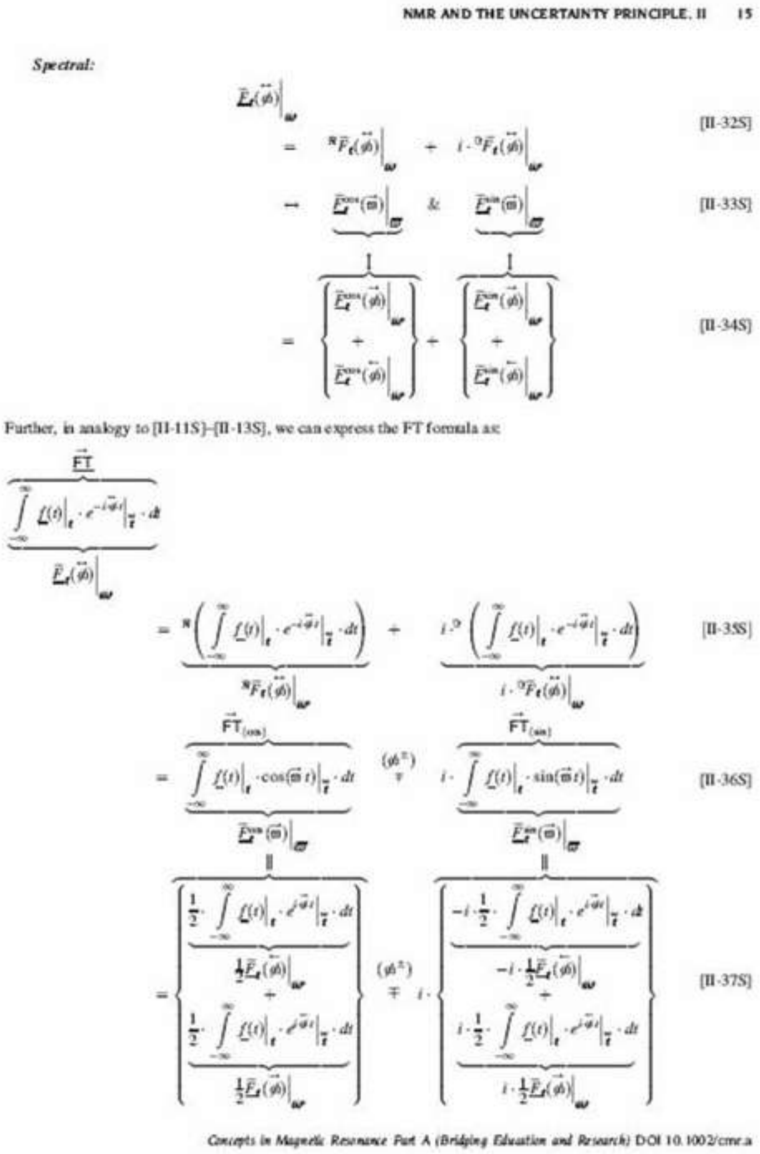
$$\underbrace{\frac{1}{2\pi}\cdot\int_{-\infty}^{\infty}\underline{\bar{F}}_t(\overleftrightarrow{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi}_{\underline{f}(t)|_{t}}$$

$$= \underbrace{{}^{\Re}\left(\frac{1}{2\pi}\cdot\int_{-\infty}^{\infty}\underline{\bar{F}}_t(\overleftrightarrow{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi\right)}_{{}^{\Re}f(t)|_{t}} + \underbrace{i\cdot{}^{\Im}\left(\frac{1}{2\pi}\cdot\int_{-\infty}^{\infty}\underline{\bar{F}}_t(\overleftrightarrow{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi\right)}_{i\cdot{}^{\Im}f(t)|_{t}} \tag{II-32t}$$

$$= \underbrace{\frac{1}{\pi}\cdot\int_{0}^{\infty}\underline{\bar{F}}_t^{\cos}(\vec{\varpi})\Big|_{\varpi}\cdot\cos(\vec{\varpi}t)\Big|_{\bar{t}}\cdot d\varpi}_{\underline{f}(t)^{\cos}|_{t}} + \underbrace{\frac{1}{\pi}\cdot\int_{0}^{\infty}\underline{\bar{F}}_t^{\sin}(\vec{\varpi})\Big|_{\varpi}\cdot\sin(\vec{\varpi}t)\Big|_{\bar{t}}\cdot d\varpi}_{\underline{f}(t)^{\sin}|_{t}} \tag{II-33t}$$

$$\Vert \qquad\qquad\qquad\qquad \Vert$$

$$= \overbrace{\left\{\begin{matrix}\frac{1}{2\pi}\cdot\int_{0}^{\infty}\underline{\bar{F}}_t^{\cos}(\vec{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi\\ +\\ \frac{1}{2\pi}\cdot\int_{-\infty}^{0}\underline{\bar{F}}_t^{\cos}(\overleftarrow{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi\end{matrix}\right\}} + \overbrace{\left\{\begin{matrix}\frac{1}{2\pi}\cdot\int_{0}^{\infty}\underline{\bar{F}}_t^{\sin}(\vec{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi\\ +\\ \frac{1}{2\pi}\cdot\int_{-\infty}^{0}\underline{\bar{F}}_t^{\sin}(\overleftarrow{\phi})\Big|_{\omega}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot d\phi\end{matrix}\right\}} \tag{II-34t}$$



Spectral:

$$\underline{\bar{F}}_t(\overleftrightarrow{\phi})\Big|_{\omega}$$

$$= {}^{\Re}\bar{F}_t(\overleftrightarrow{\phi})\Big|_{\omega} + i\cdot{}^{\Im}\bar{F}_t(\overleftrightarrow{\phi})\Big|_{\omega} \tag{II-32S}$$

$$\leftrightarrow \underbrace{\underline{\bar{F}}_t^{\cos}(\vec{\varpi})\Big|_{\varpi}} \;\&\; \underbrace{\underline{\bar{F}}_t^{\sin}(\vec{\varpi})\Big|_{\varpi}} \tag{II-33S}$$

$$\updownarrow \qquad\qquad\qquad \updownarrow$$

$$= \overbrace{\left\{\begin{matrix}\underline{\bar{F}}_t^{\cos}(\vec{\phi})\Big|_{\omega}\\ +\\ \underline{\bar{F}}_t^{\cos}(\overleftarrow{\phi})\Big|_{\omega}\end{matrix}\right\}} + \overbrace{\left\{\begin{matrix}\underline{\bar{F}}_t^{\sin}(\vec{\phi})\Big|_{\omega}\\ +\\ \underline{\bar{F}}_t^{\sin}(\overleftarrow{\phi})\Big|_{\omega}\end{matrix}\right\}} \tag{II-34S}$$

Further, in analogy to [II-11S]–[II-13S], we can express the FT formula as:

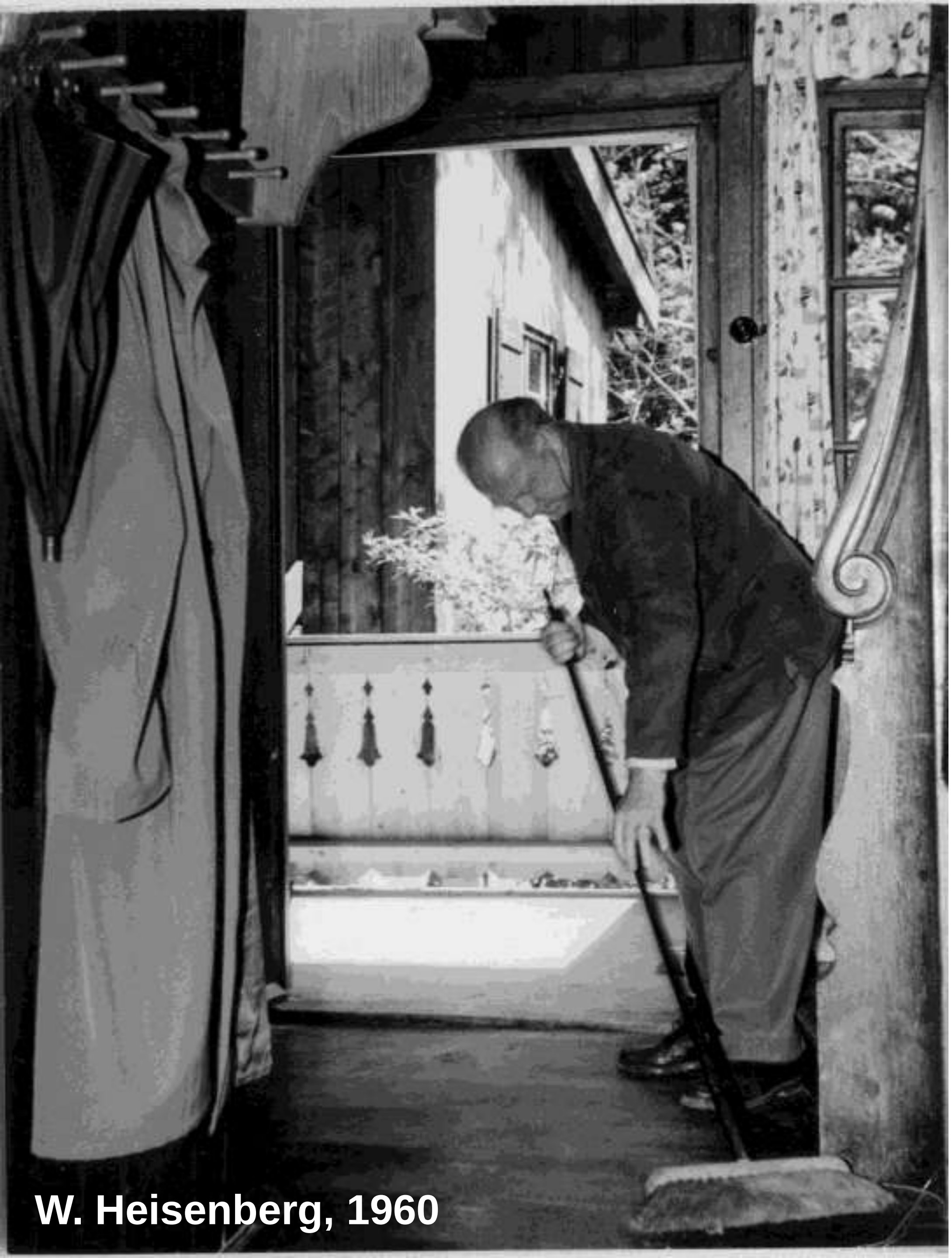
$$\underbrace{\overbrace{\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{-i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt}^{\overrightarrow{\underline{\mathrm{FT}}}}}_{\underline{\bar{F}}_t(\overleftrightarrow{\phi})|_{\omega}}$$

$$= \underbrace{{}^{\Re}\left(\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{-i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt\right)}_{{}^{\Re}\bar{F}_t(\overleftrightarrow{\phi})|_{\omega}} + \underbrace{i\cdot{}^{\Im}\left(\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{-i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt\right)}_{i\cdot{}^{\Im}\bar{F}_t(\overleftrightarrow{\phi})|_{\omega}} \tag{II-35S}$$

$$= \underbrace{\overbrace{\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot\cos(\vec{\varpi}t)\Big|_{\bar{t}}\cdot dt}^{\overrightarrow{\mathrm{FT}}_{(\cos)}}}_{\underline{\bar{F}}_t^{\cos}(\vec{\varpi})|_{\varpi}} \overset{(\phi^{\pm})}{\mp} \underbrace{\overbrace{i\cdot\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot\sin(\vec{\varpi}t)\Big|_{\bar{t}}\cdot dt}^{\overrightarrow{\mathrm{FT}}_{(\sin)}}}_{\underline{\bar{F}}_t^{\sin}(\vec{\varpi})|_{\varpi}} \tag{II-36S}$$

$$\Vert \qquad\qquad\qquad\qquad \Vert$$

$$= \overbrace{\left\{\begin{matrix}\underbrace{\frac{1}{2}\cdot\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt}_{\frac{1}{2}\underline{\bar{F}}_t(\overleftarrow{\phi})|_{\omega}}\\ +\\ \underbrace{\frac{1}{2}\cdot\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt}_{\frac{1}{2}\underline{\bar{F}}_t(\vec{\phi})|_{\omega}}\end{matrix}\right\}} \overset{(\phi^{\pm})}{\mp} i\cdot\overbrace{\left\{\begin{matrix}\underbrace{-i\cdot\frac{1}{2}\cdot\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt}_{-i\cdot\frac{1}{2}\underline{\bar{F}}_t(\overleftarrow{\phi})|_{\omega}}\\ +\\ \underbrace{i\cdot\frac{1}{2}\cdot\int_{-\infty}^{\infty}\underline{f}(t)\Big|_{t}\cdot e^{i\vec{\phi}t}\Big|_{\bar{t}}\cdot dt}_{i\cdot\frac{1}{2}\underline{\bar{F}}_t(\vec{\phi})|_{\omega}}\end{matrix}\right\}} \tag{II-37S}$$


W. Heisenberg, 1960

Heisenbergnek

SEMMI köze

az ÜGYHÖZ!

Két fajta Bizonytalansági Elv létezik!

IDŐ-FREKVENCIA
ANALÍZIS

Heisenberg
B. E.:
$\Delta t \cdot \Delta\omega \geq$ konst.

valószínűségi
állítás

**VALÓJÁBAN
EZZEL VAN
DOLGUNK!**

Fourier
B. E.:
$\Delta t \cdot \Delta\omega \geq$ konst.

determinisztikus
állítás

A név a formális alaki hasonlóságból ered!

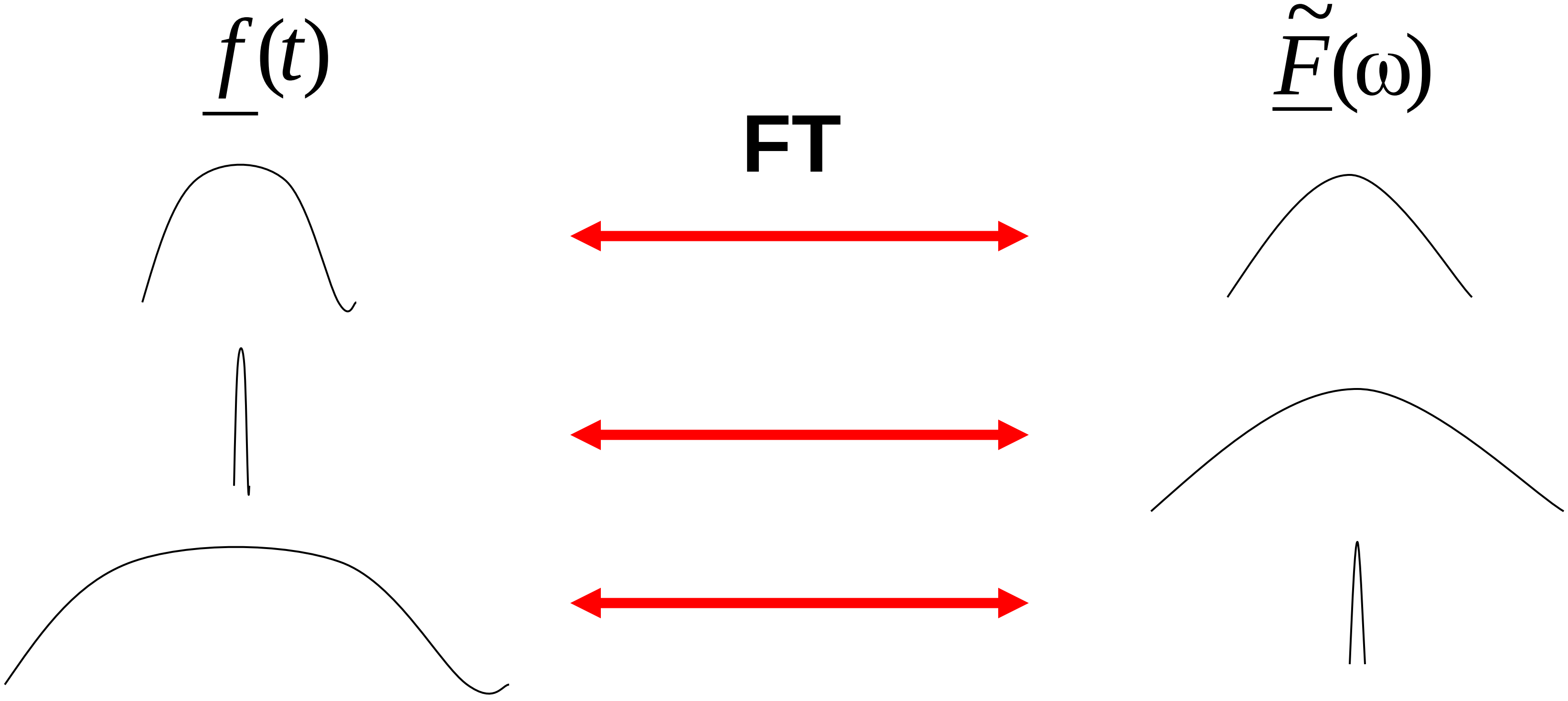
**Formális (matematikai) hasonlóság,
de különböző fizikai jelentés!**

A Fourier “Bizonytalansági” Elv állítása:

$f(t)$ “keskeny” $\rightarrow$ $F(\omega)$ “széles”

$f(t)$ “széles” $\rightarrow$ $F(\omega)$ “keskeny”

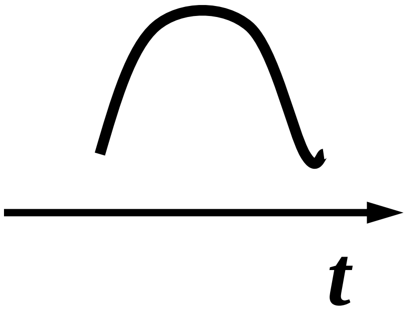
(SEMMI “BIZONYTALANSÁG”!)



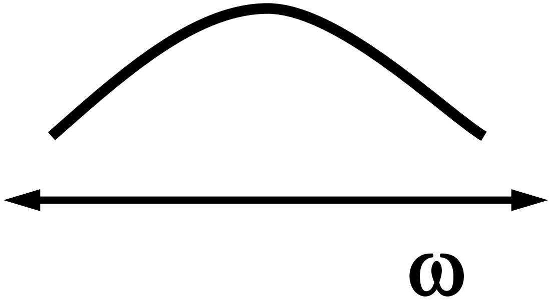
Mindkét dimenzióhoz azonos fizikai értelmezést kell rendelnünk!

A “KONJUGÁLT FIZIKAI EKVIVALENCIA” TÖRVÉNYE

natív dimenzió



transzformált dimenzió



$$\underline{f}(t)\quad \begin{matrix} \xrightarrow{\underline{\tilde{F}}(\omega)=\int\limits_{-\infty}^{\infty}\underline{f}(t)e^{-i\omega t}\mathrm{d}t} \\ \xleftarrow{\underline{f}(t)=\frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\underline{\tilde{F}}(\omega)e^{i\omega t}\mathrm{d}\omega} \end{matrix}\quad \underline{\tilde{F}}(\omega)$$

…mit “csinál” a Fourier transzformáció…

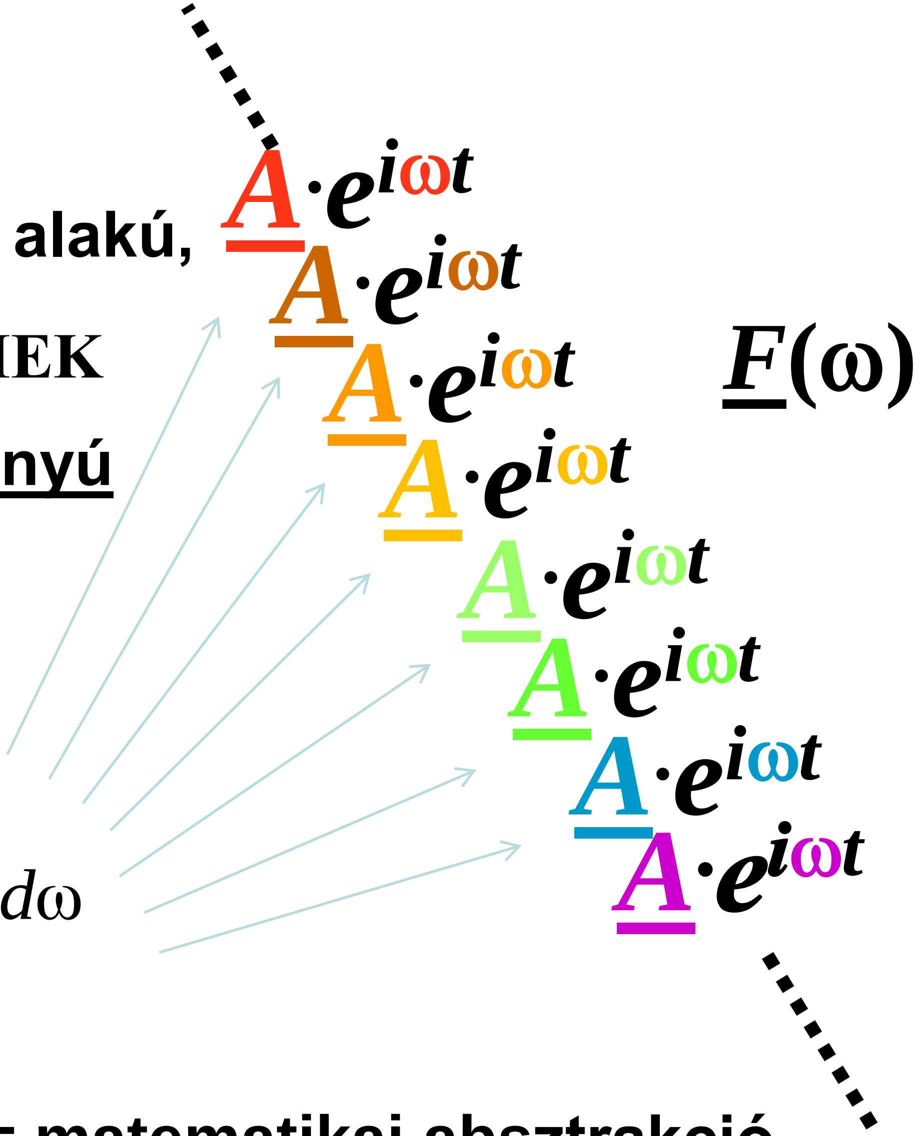
…mi a “spektrum” jelentése…?

$$\underline{\tilde{F}}(\omega) = \int_{-\infty}^{\infty} \underline{f}(t)\cdot \boxed{e^{-i\omega t}} \cdot \mathrm{d}t$$

A FT lényege:

$f(t)$ dekompozíciója $\underline{A}\cdot e^{i\cdot\omega t}$ alakú, végtelen idejű BÁZIS ELEMEK végtelen frekvenciatartományú sorává

$$f(t)=\frac{1}{2\pi}\cdot\int_{-\infty}^{\infty}F(\omega)\cdot e^{i\cdot\omega t}\cdot d\omega$$



$\underline{A}\cdot e^{i\omega t}$

$\underline{A}\cdot e^{i\omega t}$

$\underline{A}\cdot e^{i\omega t}$

$\underline{A}\cdot e^{i\omega t}$

$\underline{A}\cdot e^{i\omega t}$

$\underline{A}\cdot e^{i\omega t}$

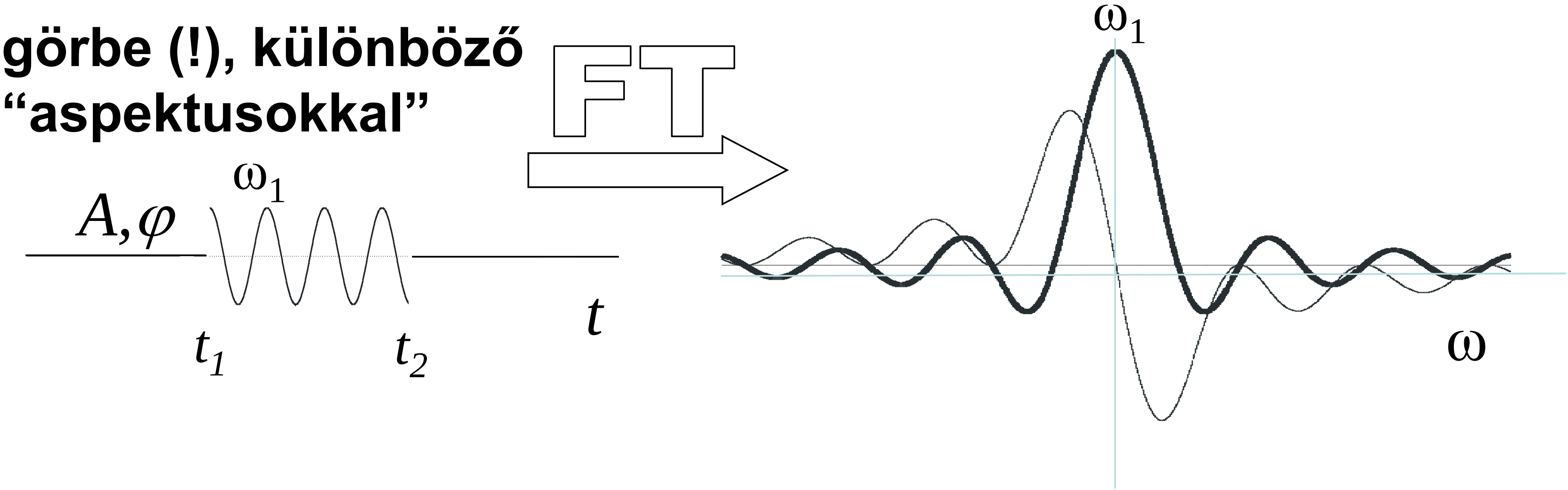
$\underline{A}\cdot e^{i\omega t}$

$\underline{A}\cdot e^{i\omega t}$

$\underline{F}(\omega)$

Bázis elem = matematikai absztrakció, aminek NINCS inherens fizikai jelentése! A fizikai jelentést MI (emberek) rendeljük hozzá, nem pedig belőle fakad!

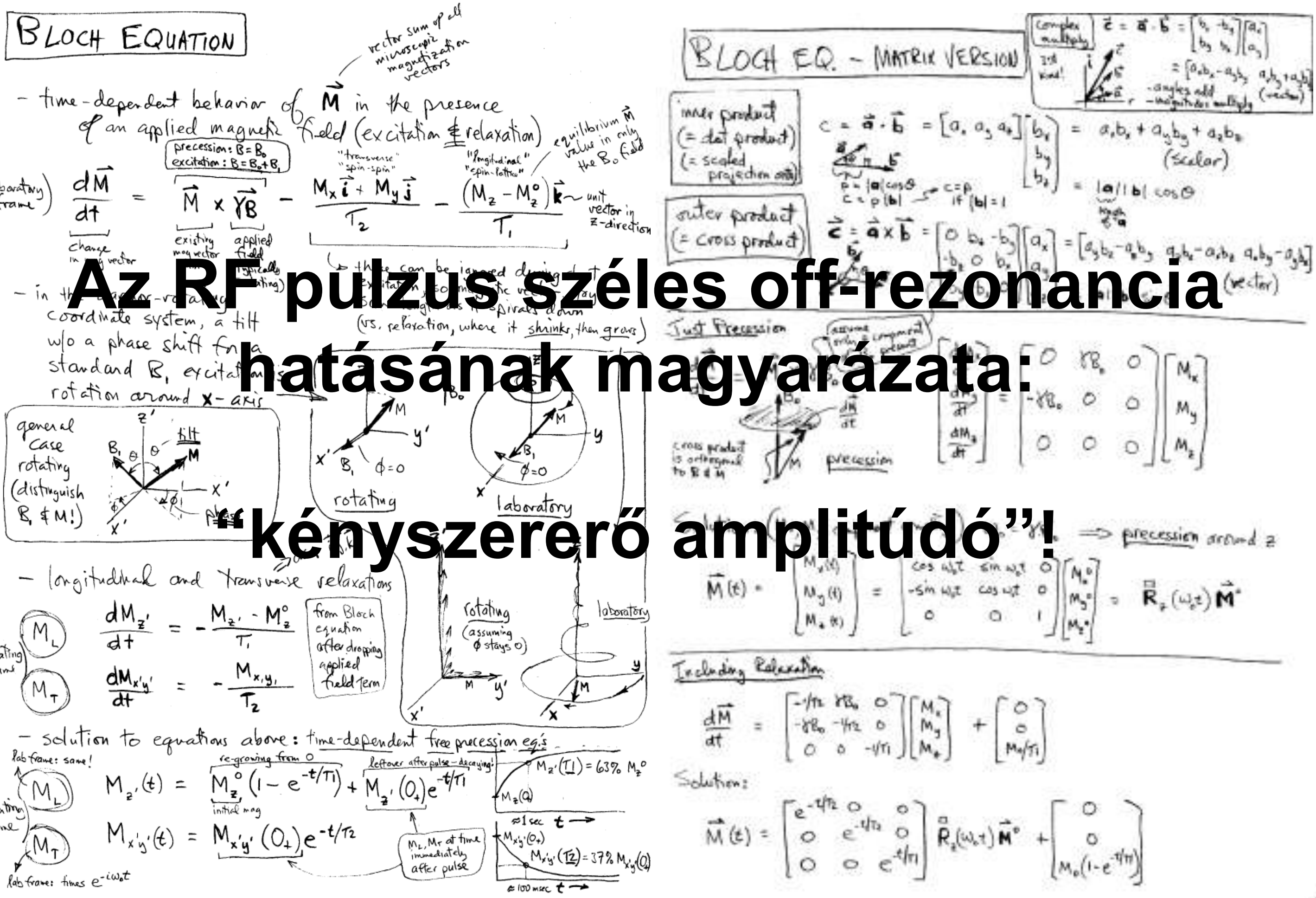
görbe (!), különböző “aspektusokkal”



Az információ csomag van átkódolva!

A “spektrum” a kódok összessége!

(a fizikai értelmezést MI adjuk, az NEM a “kódok” sajátja!)

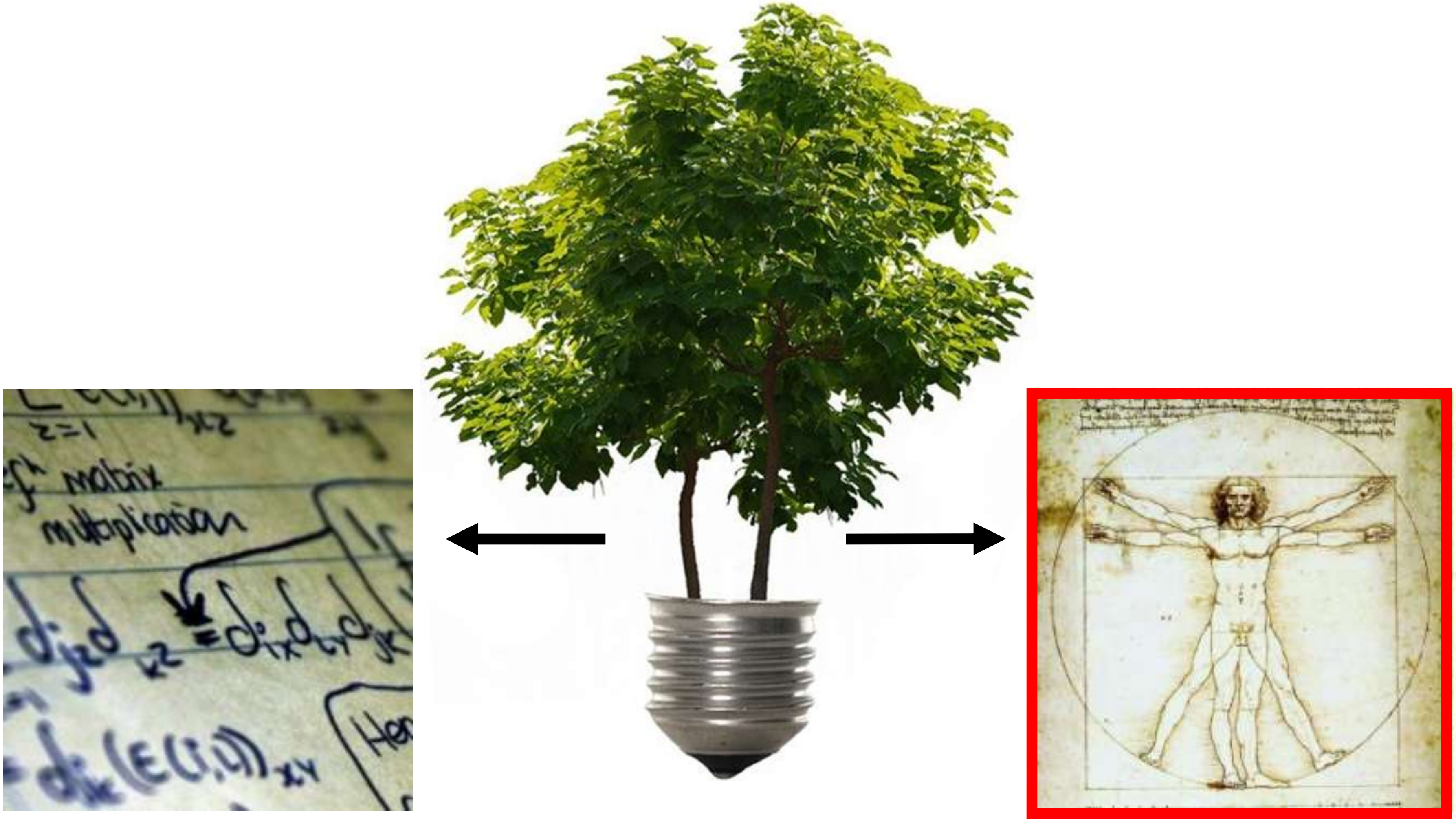


Az RF pulzus széles off-rezonancia hatásának magyarázata:

“kényszererő amplitúdó”!

lineáris határeset: pulzus FT spektruma ~
~ NMR gerjesztési profil (Szuperpozíció Elv)

A MEGOLDÁS



#3

antrópikusan árnyalt tudományos gondolkodás

#1

#2

#1

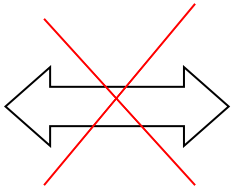
~~A *tudomány* alapja az *abszolút igazság*.~~
~~A tudomány célja a világ tőlünk függetlenül létező objektív igazságainak a feltárása.~~

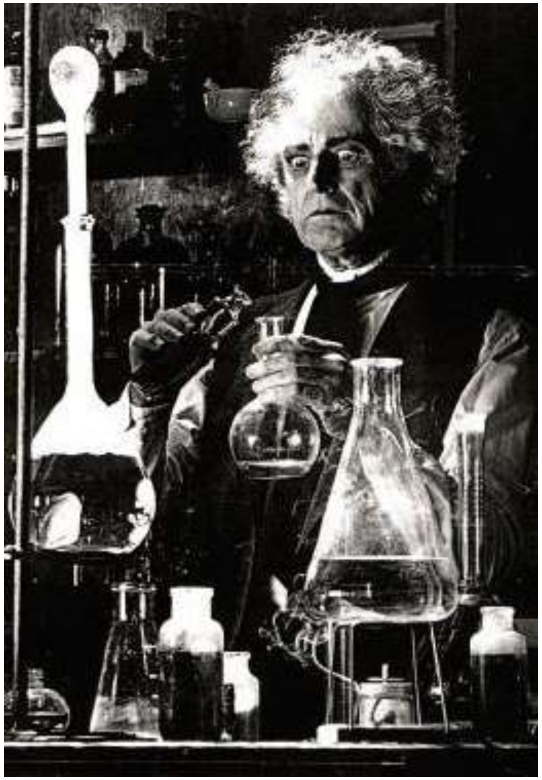
Az “igazság” nem létezhet az *emberi* értelemtől függetlenül: a világról nem, csak a világ *általunk* alkotott *LEÍRÁSÁRÓL* állíthatjuk, hogy igaz, vagy hamis. *Tudományos igazság* alatt valójában nem “abszolút igazságot” kell értenünk, hanem a világnak egy olyan *leírását*, amely a megerősítésére és cáfolatára tett kísérletek egész sorát kiállta, ezért helyesnek tekinthető.

(Richard Rorty, John Webb)

#2

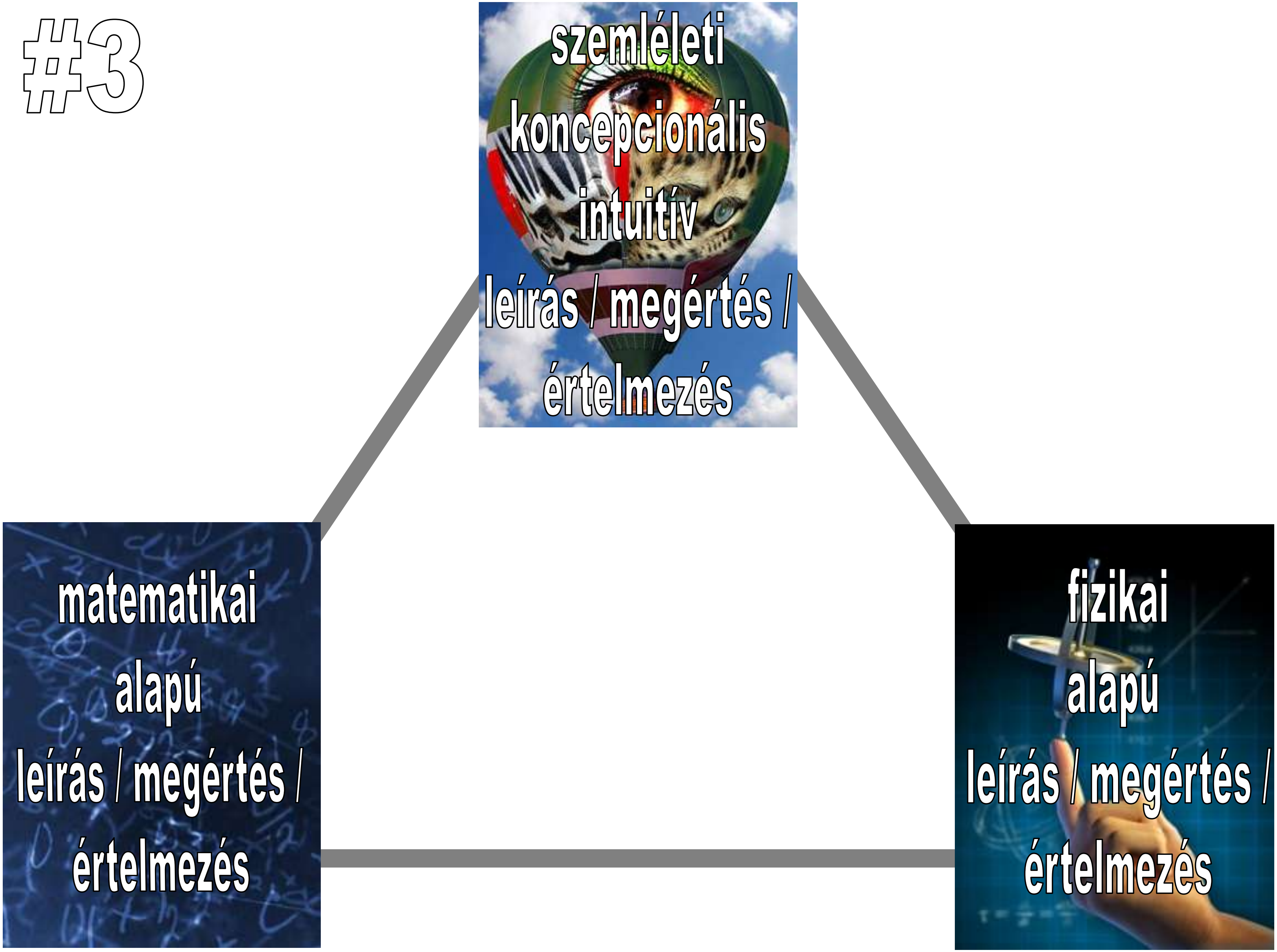
“átlagember”





“képzett tudós”

#3



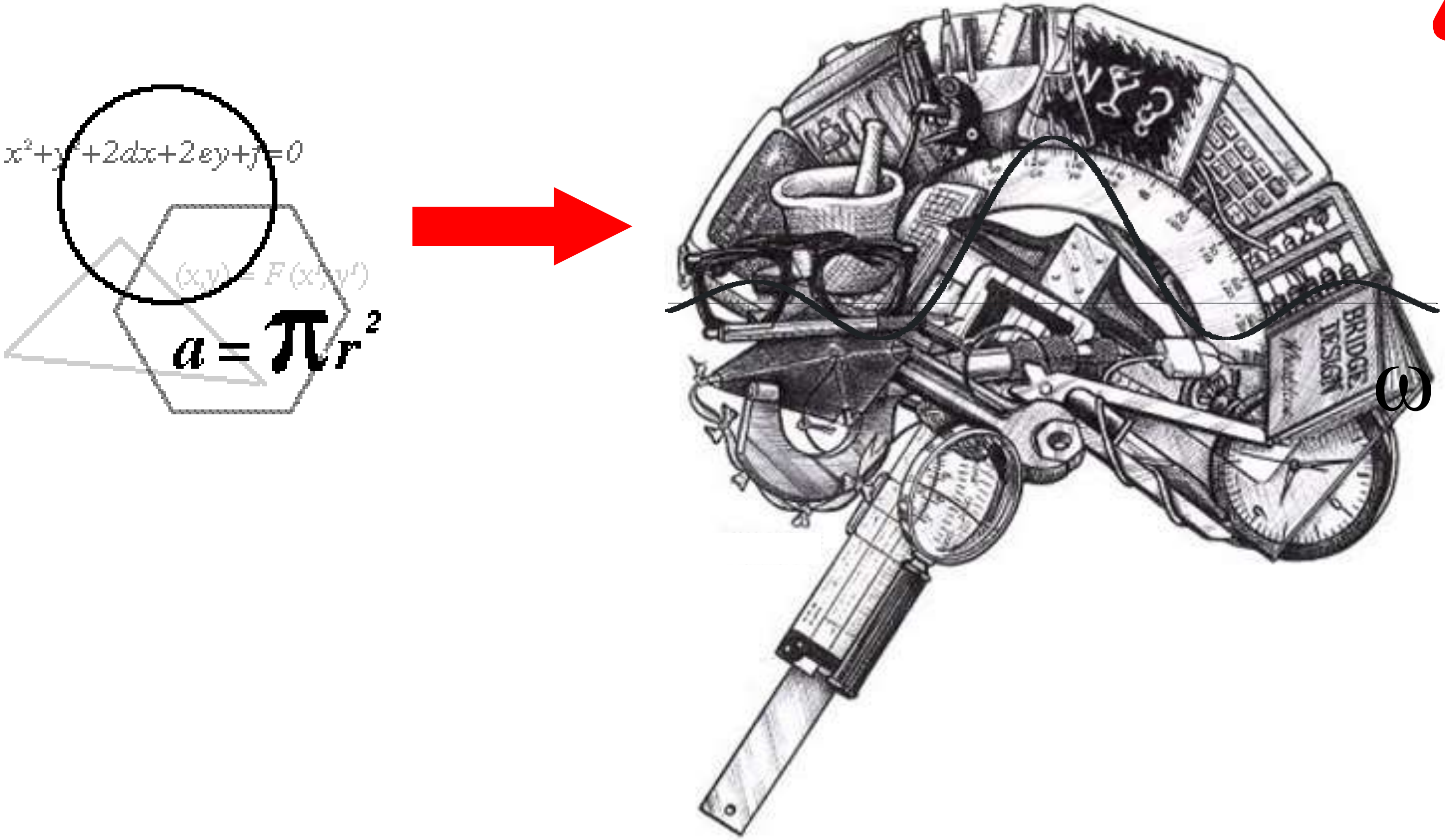
szemléleti
koncepcionális
intuitív
leírás / megértés /
értelmezés

matematikai
alapú
leírás / megértés /
értelmezés

fizikai
alapú
leírás / megértés /
értelmezés

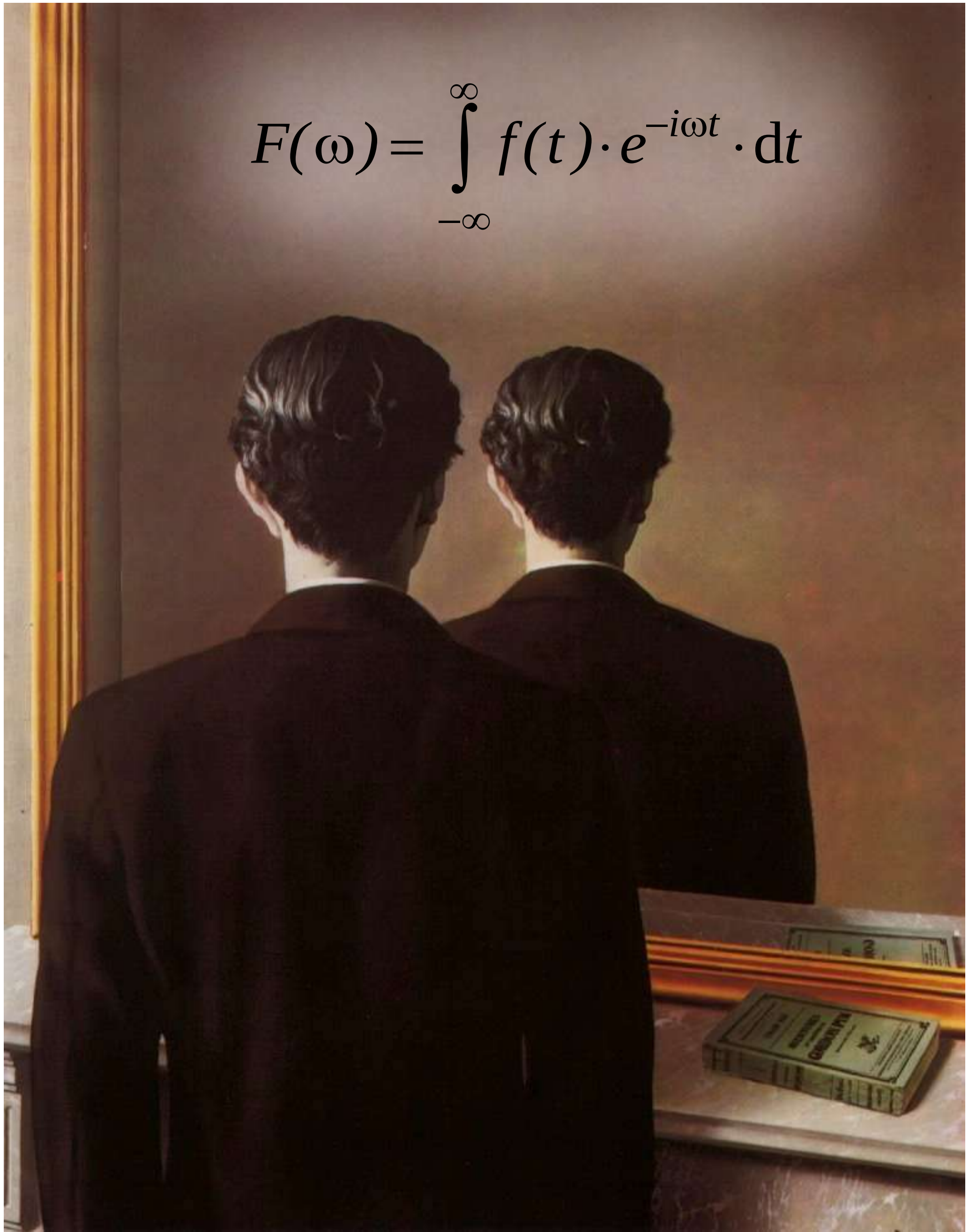
“reflexszerű de-absztrahálás”

kognitív veszély



“ismeretlen ismerős”

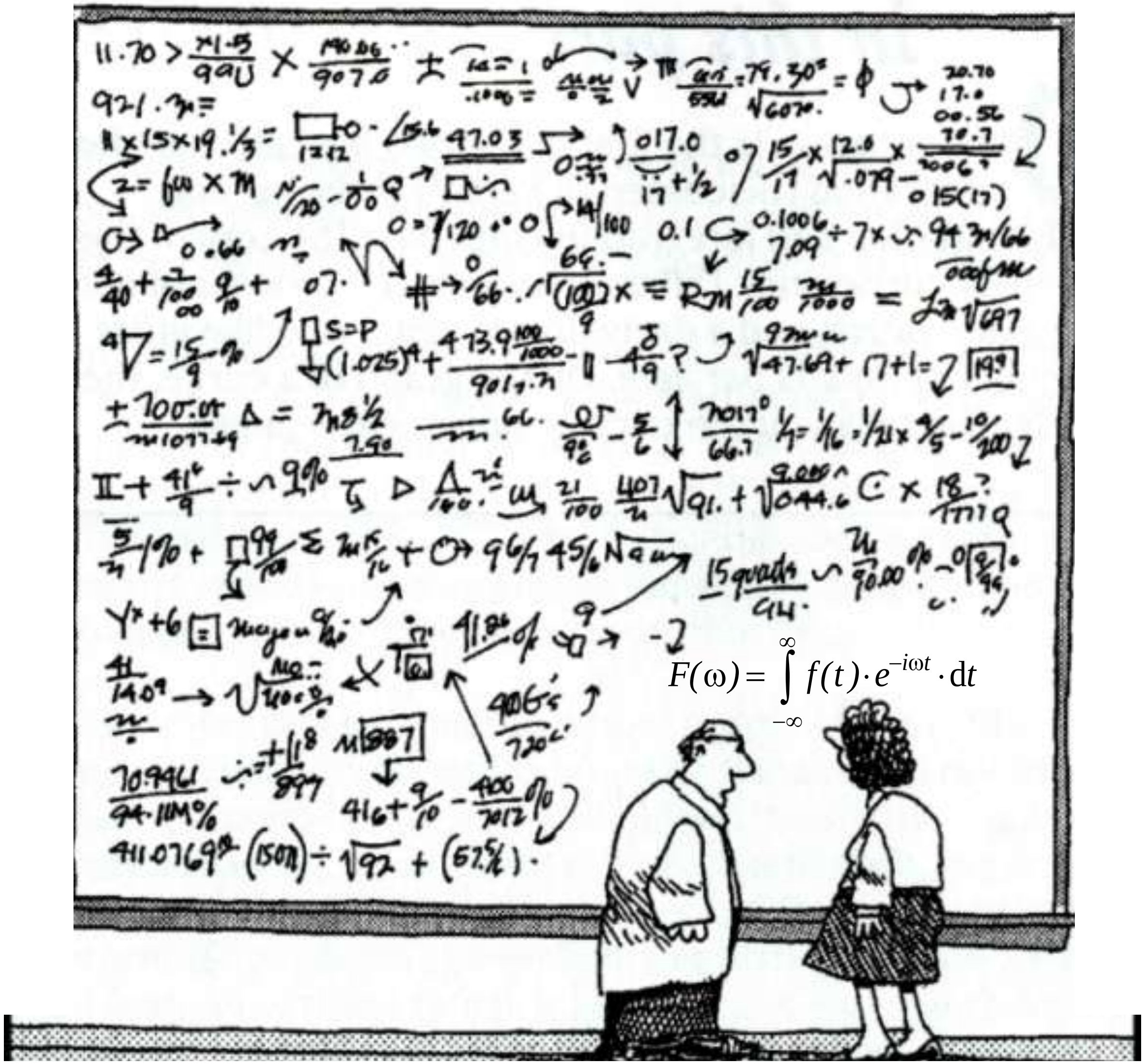
kognitív veszély



$$F(\omega)=\int_{-\infty}^{\infty} f(t)\cdot e^{-i\omega t}\cdot \mathrm{dt}$$

“(matematikai) fa vs. (fizikai) erdő”

kognitív veszély



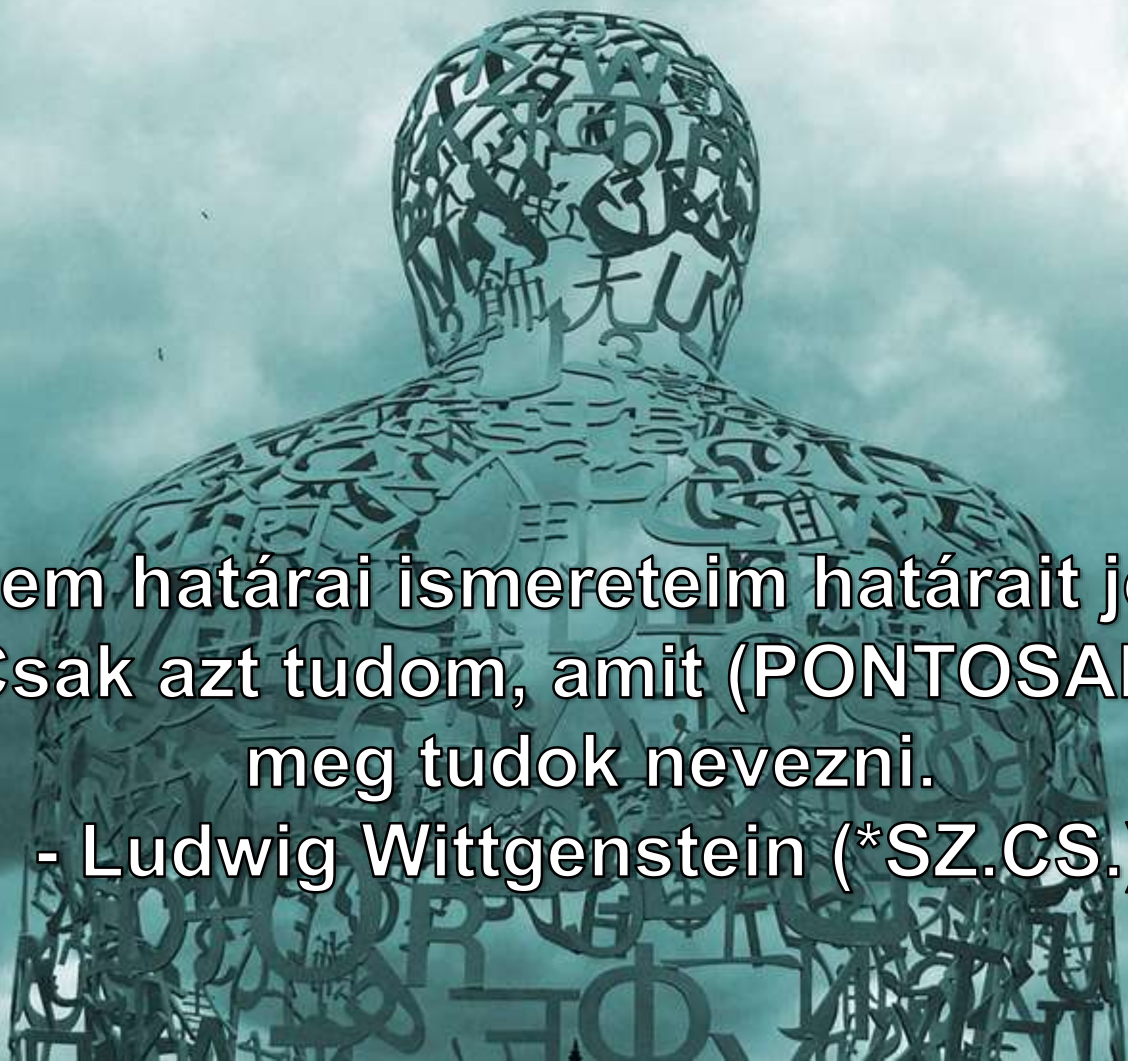
$$F(\omega) = \int_{-\infty}^{\infty} f(t) \cdot e^{-i\omega t} \cdot \mathrm{d}t$$

“Pontosan mit is akartunk itt mondani?”

“enjoy your flight”

“elveszett jelentés”

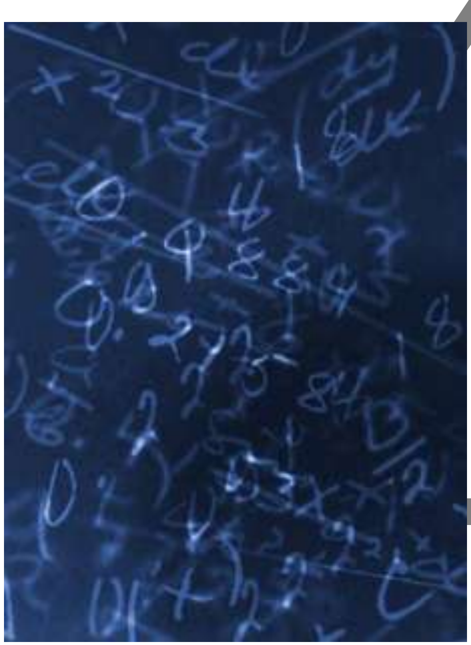
kognitív veszély



Nyelvem határai ismereteim határait jelentik.
Csak azt tudom, amit (PONTOSAN*)
meg tudok nevezni.
- Ludwig Wittgenstein (*SZ.CS.)

JELENTŐSÉG + MERRE VEZET MINDEZ?

FOURIER
TRANSFORMS
APPROACH TO SCIENTIFIC PRINCIPLES




Ó! PARADIGMAVÁLTÁS!

KÖSZÖNÖM A FIGYELMET

Honnan tudná az ember, hogy melyik a saját útja, ha csak járt utakon jár?

– Reinhold Messner