

# Is Quantum Mechanics necessary for understanding Magnetic Resonance?

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## Abstract

Educational material introducing magnetic resonance typically contains sections on the underlying principles. Unfortunately the explanations given are often unnecessarily complicated or even wrong. Magnetic resonance 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 magnetic resonance are often obscured by explanations that make the subject difficult to understand. Typical problems are addressed and alternative intuitive explanations are provided.

**Key words:** magnetic resonance imaging, education, quantum mechanics, classical mechanics, tutorial, spin, myths

## Introduction

Since the beginning of the 20th 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 since orbiting electrons radiate energy and hence lose 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 conditions must generally be reflected in uncertainty of the future). What *is* bizarre and non-intuitive, however, is that QM is not generally reducible to a non-probabilistic theory, even when initial conditions can be controlled perfectly, unless other equally bizarre additions to the theory are made (*1*). Hence, according to QM, measurements are associated with some intrinsic uncertainty, even when the state of the system is not. This indeterminism of nature has been tested extensively and experimentally verified.

That a complete description of the world has aspects that are considered bizarre by humans is not surprising, as phenomena encountered during species evolution all fall within a very narrow range: Until recently no creature made detailed observations of phenomena on other length and time scales than their own macroscopic scale, humans being the first known exception. The laws of classical mechanics that are based on macroscopic observations describe most phenomena on this scale well, but typically fail when applied to atomic and cosmological length and time scales. Hence, it is not surprising that QM occurs as a rather difficult theory to learn and understand. In fact, even physicists perfectly capable of

applying the laws of QM to make right predictions about results of experiments, may make misleading interpretations of the same experiments. QM is, in other words, easier to apply than to understand and explain, probably because little emphasis is put on interpretation in most contexts including education that is typically rooted in pragmatism.

This problem is unfortunately evident in the field of magnetic resonance (MR), and it is amplified by the diversity of people who teach and write books about this subject. Physicists, medical doctors, radiographers, electrical engineers and chemists are among the most common authors of books that include sections on the basic physics of MR. Many of these people are not trained in QM. Hence, even excellent books and lectures on MR may contain statements that are misleading, overly complicated, or downright wrong. Examples can be found in early MR literature, and some are repeated so often that alternative formulations are not given sufficient consideration. Precise formulations of MR basics exist, e.g. as presented by Levitt (2) or advocated on the *ReviseMRI* web site (3), but they are unfortunately a minority. Many texts aimed at physicists and other people trained in quantum mechanics do not make the mistakes pointed out here, but they often fail to mention that most aspects of MR are perfectly understandable from a classical perspective. It is a purpose of this article to challenge some of the myths and misleading explanations appearing in MR tutorials.

It was argued above that QM has bizarre aspects that must be acknowledged to apply and interpret the theory. It is important to note, however, that most aspects of QM are *not* surprising. In particular, the so-called *correspondence principle* must hold true: In the macroscopic limit QM typically reduces to classical mechanics, i.e., give similar predictions to those of Newton's and Maxwell's equations (macroscopic quantum phenomena exist, but they are few or non-obvious). Luckily the consequence in the context of MR is that a classical description is adequate, and overwhelmingly so in tutorials for non-physicists. Typically neither students, nor teachers of MR, have the background for meaningful discussions of QM. It is fortunate that they can refrain from engaging in such, since quantum phenomena are difficult to observe with MR hardware, and since QM play

no role for the vast majority of MR measurements. In addition to challenging myths, it is therefore a purpose of this article to suggest alternative, yet correct explanations and graphs based on classical mechanics only.

Quantum mechanics is here used to show that classical mechanics is fully adequate for almost all purposes related to MR. Using one formalism to demonstrate that the same formalism should be avoided in favor of something simpler, may seem counter-intuitive. QM *is* the more complete theory, however, and only by demonstrating that QM reduces to classical mechanics in the relevant situations, can the case be made rigorously. Consequently this text contains outlines of calculations that require QM knowledge to be understood, even though the target audience is people in need of explaining or understanding MR of which many are non-physicists. The rigor is needed, especially since the subject covered is potentially controversial, considering the large number of authors and educators that may feel targeted. The aim of this article is not to warn against typical presentations, however. The tutorials referenced for problematic propositions are, for example, all excellent in other respects. Rather it is the aim to avoid the continuous repetition of misleading arguments in MR literature and to avoid the confusion it causes among students that are already sufficiently challenged without such. An article on this matter is consequently considered long due. The references were chosen among many similar to exemplify that the problem is neither new, nor seems to be diminishing.

The theory section provides examples of common misconceptions, prove them wrong or misleading, and gives alternative explanations. The possible origins and consequences of the myths are also discussed. Sections requiring a detailed knowledge of QM are relegated to appendices that may be skipped by readers who accept the given arguments without reading the proofs.

The discussed phenomena are common to most magnetic resonance effects, e.g., electron spin resonance. All examples will be drawn from nuclear magnetic resonance, however, as this phenomenon is commonly explained for non-physicists in introductions to magnetic resonance imaging (MRI).

## Theory

### **Myth 1: According to quantum mechanics, protons align either parallel or anti-parallel to the magnetic field**

This myth reflects a misinterpretation of QM and it is found in numerous texts on MR, e.g. (4–9). The problem is realized by making a classical analogy. If a collection of non-interacting compasses were subject to the earth magnetic field, and they behaved as described, we would be surprised: Some would swing to the north as expected and some would swing south, which is not seen experimentally. QM is not classical mechanics, and as argued in the introduction, we do expect surprises, but this is not one of them, neither for compasses, nor for nuclei.

From a technical point of view, it is easy to track the origin of the misconception: According to QM, a proton in a magnetic field has only two spin-states with a well-defined energy (energy eigenstates). These are typically called spin-up and spin-down where up and down refers to parallel and anti-parallel to the magnetic field. These eigenstates are written as  $|\uparrow\rangle$  and  $|\downarrow\rangle$  by physicists. Despite their name, these states have elements of magnetization perpendicular to the magnetic field in addition to longitudinal components. Hence the spin-up and spin-down states are often illustrated by two cones as shown in Figure 1 e.g. in references (5–7, 10).

The energy eigenstates form a so-called basis for all possible states. Spin orthogonal to the field can, for example, be written as a weighted sum of spin-up and spin-down. To explain the concept of a basis, a highschool-level example will be given: Consider a particle moving in the two-dimensional  $xy$ -plane. The orthogonal unit vectors  $\hat{x}$  and  $\hat{y}$  form a basis for the two-dimensional vector space, so any velocity vector  $\mathbf{v}$ , for example, can be decomposed into velocity along the  $x$ -direction and velocity along the  $y$ -direction. Just as any two-dimensional vector in the  $xy$ -plane (for example velocity) can be written as a weighted sum of  $\hat{x}$  and  $\hat{y}$ , any spin-state  $|\psi\rangle$  can be written as a weighted sum of spin-up

and spin-down (the Greek letter  $\psi$  pronounced *psi* is typically used in this context):

$$\mathbf{v} = v_x \hat{\mathbf{x}} + v_y \hat{\mathbf{y}} \quad [1]$$

$$|\psi\rangle = c_\uparrow |\uparrow\rangle + c_\downarrow |\downarrow\rangle \quad [2]$$

The possible states are weighted sums of the eigenstates which indicate that there are many more states available to the protons, than spin-up and spin-down. The weights  $c_\uparrow$  and  $c_\downarrow$  are complex numbers that express the direction of spins as precisely as nature allows in accordance with QM. Considering the properties of the weights, it can be shown that there are two degrees of freedom for the spin of a proton (azimuthal and polar angle) just as there are in classical mechanics, i.e. a spin can point in any direction in three-dimensional space, although, as described in the introduction, the directions are associated with some intrinsic uncertainty. When the magnetizations of isochromats (groups of protons experiencing the same magnetic field) are considered rather than of individual nuclei, the relative uncertainty vanishes. This is the case for samples with more than a few atoms.

It is important for the understanding of QM that addition of states differs from addition of spin vectors. Adding equal amounts of spin-up and spin-down in the sense expressed by equation [2], for example, does not lead to cancellation, but amounts to a state of transversal magnetization.

Probably any physicist would agree to the above so this does not explain how **myth 1** occurred. The origin is the following: If the spin of an *individual* proton is measured along the direction of the magnetic field, it will be found to be either in the spin-up or spin-down state, no matter which mixed state  $|\psi\rangle$  it was in before. Furthermore, it will stay in that new state until the proton is subject to more interactions with environment (e.g. another measurement). This so-called collapse into an eigenstate is a consequence of QM. It apparently implies that a measurement of the net magnetization (e.g. by MRI), will force each proton into either the spin-up or the spin-down state in agreement with **myth 1**. This is wrong, however. The emphasized word *individual* above is important in the present context, as we can only infer from QM that the protons are forced into single-spin eigenstates, if we measure their magnetization one-by-one as can be done with a Stern-Gerlach apparatus,

for example (11). In contrast, that is never done in MR spectrometers or scanners: In order to get a measurable MR-signal the total magnetization of many nuclei is always measured, and **myth 1** does not follow. It could be true nevertheless, but in fact it is not, which is shown in appendix (proposition 1) by employing the QM formalism: A measurement of the net magnetization causes a perturbation of the system that is insufficient to affect the individual protons significantly. In particular, they are *not* brought into their eigenstates by the measurement process.

It is worth noting that even though the arguments above may occur complicated for the non-technical reader, they are what many students of MR more or less implicitly lay ears to, and for no good reason, as QM is not needed for understanding basic MR. Moreover, the students often hear the wrong version of the argument.

The lifetime of **myth 1** may have been prolonged by an observation that many working with MR have made: When subject to a magnetic field, an oblong piece of magnetizable material have a strong tendency to align itself in one of two opposite directions parallel to the field (in contrast to permanently magnetized material that orient itself in one direction only). Despite a superficial resemblance, this well-known phenomenon has nothing to do with the effect expressed in **myth 1**. Rather it is a consequence of reorientation of magnetic constituents inside the metal. This gives rise to the existence of two low-energy states for the orientation of the metallic piece, parallel and anti-parallel to the field. The magnetic constituents are in either case parallel to the field, since they have only one low-energy state. Similarly, the proton spin has only one low-energy state. Nothing but MR-irrelevant single-proton measurements give spins a tendency to align anti-parallel to the field.

Consequently, spins can point in any direction and the energy eigenstates are not more relevant to MR than any other state (the eigenstates form a convenient basis for computations, but they are irrelevant for the understanding). Hence Figure 1 that illustrates the nature of spin eigenstates, do not contribute much but confusion in an MR context. QM is later shown to imply that the spin-evolution of individual protons happens as expected classically unless perturbed, e.g., by a single-spin measurement.



Finally, replacements for Figure 1 are discussed. According to both classical and quantum mechanics, spins are expected to point in all directions in the absence of field as shown in Figure 2. Except for precession, the situation does not change much when the polarizing  $B_0$ -field used for MR is applied as shown in Figure 3. The energies associated with the orientation of the individual spins are much smaller than the thermal energies so the spins only have a slight tendency to point along the direction of the field (and no increased tendency to point opposite the field, neither classically, nor quantum mechanically). The situation can be compared to the one described earlier involving a hypothetical collection of compasses placed in the earth magnetic field. All compasses will swing to the north, if they are non-interacting and not disturbed. The situation changes if the compasses are placed in a running tumble-dryer or similar device increasing the collisional energies above those associated with changing the direction of the compass needles. The bouncing and interacting compasses will no longer all point toward north but there will still be a slight tendency for them to do so. If the net magnetization is measured, it will point toward north. The situation is like that of the moving protons in a liquid sample where the magnetic interactions between neighboring nuclei cause reorientation of the magnetic moments (relaxation). In the absence of a magnetic field, the angular distribution of spins is spherical in either case. When a field is added, the distribution is skewed slightly toward the field direction by relaxation.

It is important to understand that precession of the individual nuclei starts as soon as the sample is placed in the field (not only after excitation by RF fields, as frequently stated). The nuclei therefore emit radio waves at the Larmor frequency as soon as they are placed in the field. Similarly, however, they absorb radio waves emitted by their neighbors and surroundings. Since the distribution of spin directions is even in the transversal plane, the net transversal magnetization is zero, and there is no net exchange of energy between the sample and its surroundings. The exchange of radio waves within the sample is nothing but magnetic interactions between neighboring nuclei. These are responsible for relaxation.

## **Myth 2: Magnetic resonance is a quantum effect**

A quantum effect is a phenomenon that cannot be adequately described by classical mechanics, i.e., one where only QM give predictions in accordance with observations. In the introduction it was stated that atom formation is a quantum effect since atoms are not expected to be stable according to classical mechanics, whereas experiments have proven that they are. This does not imply that all phenomena involving atoms are defined as quantum effects, since such a broad definition would be quite useless. Instead, phenomena are hierarchically divided into classical and quantum phenomena, so a classical phenomenon can involve atoms that are themselves inexplicable by classical mechanics. Similarly, proton spin is a quantum effect but magnetic resonance is not since the latter is accurately described by classical mechanics. This is the subject of the present section.

It is often and correctly said that spin is a quantum effect. From a classical perspective it cannot be explained why protons apparently all rotate with the same constant angular frequency, which result in an observable angular momentum (spin) and associated magnetic moment. Despite the fact that this is really mind-boggling, it is usually not perceived so by students of MR. Just as atoms are taken for granted, it is typically accepted without argument that protons appear to be rotating and that they as a result behave as small magnets with a north and a south pole, i.e. they have angular and magnetic moments. Most books state this correctly and there is no apparent reason to elaborate, as a deeper understanding of spin is typically of little use in the context of MR.

Even though spin is a quantum effect, magnetic resonance is not, according to the definition given above, as it does not necessitate a quantum explanation. Classically, a magnetic dipole  $\mathbf{M}$  with an associated angular momentum  $\mathbf{M}/\gamma$  (spin) will precess in a magnetic field  $\mathbf{B}_0$  at the Larmor frequency  $f = \gamma B_0$ . The gyro-magnetic ratio  $\gamma$  is specific for the type of nucleus. If subject to an additional, orthogonal, magnetic field rotating at the Larmor frequency, the magnetization will also precess around the rotating field vector  $\mathbf{B}_1(t)$ . This is most easily appreciated in a rotating frame of reference (12), where  $\mathbf{B}_1$  appears stationary and the effect of  $\mathbf{B}_0$  is not apparent except for its influence

on relaxation. This is classical magnetic resonance, as visualized for example in published animations (9, 13, 14).

It was shown by the famous physicist and Nobel laureate Richard Feynman and co-workers (15) that the class of phenomena called two-level quantum dynamics can be understood in the light of classical MR. Specifically, the paper showed that these phenomena are described by the same math that applies to classical MR, and that an abstract vector quantity (the Bloch vector) descriptive of the quantum state moves like a magnetic dipole in a magnetic field. For the special case of the spin-up/spin-down two-level system, the Bloch vector is indeed proportional to the expected magnetization, which was shown to move as predicted by classical mechanics. Hence Feynman and co-workers pointed out that the dynamics of a proton in a time-varying magnetic field is easy to understand since it behaves classically.

In that light, it is difficult to understand the rationale of many introductory MR books that explain MR to students with non-technical backgrounds by use of quantum mechanical concepts, i.e., do the opposite of what Feynman suggested. The remaining part of this paragraph summarizes a typical QM-inspired, unsatisfying explanation of MR: The spin-up and spin-down states have an energy difference proportional to the magnetic field (Zeeman splitting). In equilibrium, they are almost equally populated with a small surplus of nuclei in the low-energy spin-up state. If the two-level system is subject to RF fields and if the photon energy matches the energy difference, transitions between the spin-up and spin-down state will be induced according to QM. Hence the population of the low-energy state can be excited to the high-energy state.

Even if this superficially sounds like a simple explanation, it is not. First of all, it requires familiarity with concepts such as energy eigenstates, Zeeman splitting and photons, concepts that are notoriously difficult to understand. Furthermore, the explanation does not give any hint of the importance of coherent evolution, which is crucial for the QM understanding of MR. So the above has character of a pseudo-explanation, unless the reader is familiar with the QM equations of motion. These describe smooth transitions between

spin-up and spin-down states (16) in contrast to the flips or jumps that are often highlighted in MR-tutorials (4–6) but are not occurring since the protons are not forced into eigenstates by MR measurements.

### **Myth 3: RF pulses brings the precessing spins into phase**

It is sometimes said that the effect of a resonant RF field is to bring the precessing spins into phase (4, 6, 17) as indicated in Figure 4 that has no basis in reality. It is a result of the wrong belief that the spins can only be in the energy eigenstates shown in Figure 1, combined with an attempt to explain how a magnetization can nevertheless be transverse.

In contrast, it is easy to demonstrate using either classical or quantum mechanics (see appendix, proposition 3) that a homogeneous RF field can never change the relative orientation between non-interacting proton spins. Hence RF fields can only rotate the spin-distribution as a whole. This immediately explains why it is sufficient to keep track of the local net magnetization in MR experiments and why RF fields cannot be used to change the size of this, even though Figure 4 wrongly seems to indicate that this might be possible. Another immediate consequence is that RF fields can never change coherence if this is defined as non-random phase relations generally (order). The concept of coherence, however, is typically used for non-random phase relations in the transverse plane only, a somewhat unfortunate definition that will nevertheless be adopted here (see appendix, proposition 3, for explanation). Only the combination of a polarizing field and additional inhomogeneous fields associated with nuclear interactions create the skewness of the spherical spin-distribution needed for having population differences and coherences. For the QM literate, it is worth noting that coherence and population differences are two aspects of order: What appears as population differences in one basis are coherences in another and vice versa. Hence there is no conceptual problem in field-assisted T1-relaxation to be the real source of coherence, though relaxation is normally considered a source of coherence loss.

Figure 4 is plain wrong, while Figure 1 is not when interpreted as a visualization of the somewhat irrelevant eigenstates. Since RF fields can only rotate the spin-distribution as a

whole, a better alternative to Figure 4 is one showing a rotation of the distribution shown in Figure 1 so the cones end up in the horizontal plane. This too would seem highly non-intuitive, but would nevertheless not be wrong in the sense that experimental observations match predictions. Yet another – and much better – alternative to Figure 1 is a nearly spherical, precessing spin-distribution somewhat skewed toward magnetic north, as predicted by both quantum and classical mechanics, and shown in Figure 3. The corresponding Figure 5 replacing the misleading Figure 4 is similar except rotated so the slight overweight of spins, and therefore the net magnetization, is pointing in a new direction.

## Discussion

QM and other laws of nature cannot necessarily tell us what really happens – they only describe our perception of nature. Some interpretations of QM imply that one should, in principle, not speak about what is *really* happening but only speak about past and future outcomes of measurements (experience and predictions, (1)). This can be used to argue that the two views expressed in Figures 1 and 3 are equally good as the predictions they give rise to, are the same. It could even be argued that no such mental representation should be made. The latter extreme view, however, does not help the MR student in establishing an intuitive feel of how MR works or what results are expected. Even though such pictures (and all other mental representation of the world) represent simplifications of reality and should be interpreted as such, they can still be immensely useful. The quality criteria are intuitiveness, simplicity and prediction accuracy of which the latter is most important. In the present case, the prediction accuracy of the mental representations shown in Figures 1 and 3 are the same, *if* the user has sufficient insight to understand both. In particular, coherent evolution as expressed in the Schrödinger equation must be understood rather than just the semi-random spin-flipping that is wrongly associated with the resonance phenomenon in some tutorials. In contrast, classical mechanics as expressed in Figures 2, 3 and 5 give intuitive and correct predictions understandable by most people.

It is often said that the classical explanation is adequate for most purposes but insufficient to really understand MR. This disregards the fact that QM translates directly into classical mechanics in the present context. Such statements are often followed by misinterpretations of QM based on Figures 1 and 4 that raise more questions than they answer: Why are spins only oriented parallel or anti-parallel to the field? In particular, why would nearly half the spins align opposite to the field? Why do RF fields reduce the phase spread on the two cones? How does the phase of the RF field translate into an azimuthal phase? How does the figure look for flip-angles different from 90 degrees? These questions cannot be answered satisfactorily from the figures that are not consistent with QM, nor with classical mechanics. The problems mentioned typically only occur on the very first pages of MR introductions. The explanations get back on track after a (semi-)classical picture is introduced and it is stated (typically without argument) that RF fields in a classical picture rotate the net magnetization, which is inconsistent with Figure 4.

In this article, it was argued that the spins are not forced into eigenstates by their interactions with environment. It is interesting to note, however, that if, by some means, the individual spins were brought into eigenstates before an MR-experiment as indicated by Figure 1, subsequent observations would not be changed. The expectation is, in other words, independent of whether they are based on the non-intuitive Figure 1 or the preferred counterpart Figure 2. This is not surprising, but it raises a question: In which sense is the latter picture more correct? First of all, there is nothing in QM telling us that the overall state collapses into a single-spin eigenstate as argued in appendix (proposition 1). Secondly, the appendix shows that the relative orientation is not changed by RF fields (proposition 3), so even if Figure 1 does not seem all that non-intuitive, it certainly does after rotation of the shown distribution around a horizontal axis. Such a rotation is induced by a  $90^\circ$  excitation pulse. Another blow against Figure 1 and excessive use of QM is delivered by Occam's Razor that can be described as follows: If there are two explanations for the same set of observations, choose the simpler. Using a scanner, it is extremely difficult to do experiments that reveal the quantum aspects of magnetic resonance. Hence, the natural consequence is

to acknowledge that MR is accurately described as a classical phenomenon and leave QM to the few, who can appreciate both the subtle differences and the overwhelming agreement with classical mechanics.

QM is considered somewhat exotic and intriguing by many, and should this motivating factor not be exploited? Should students not get a glimpse of the underlying physics, even if not needed? Even though QM is underlying classical mechanics, the physics underlying MR are classical. If MR is not sufficiently challenging for the students, or if they are sufficiently capable, they may indeed benefit from learning the quantum physics of MR and how the classical limit is approached as expressed in the correspondence principle (MR provides an excellent example of that). But it is not justified to take any odd explanation and call it quantum mechanics. Physics students, for example, may definitely benefit from a QM derivation, especially if it is preceded by a classical explanation, that in addition to being intuitive express the same physics in the case of MR. A good example of this approach is provided by Levitt (2), who also advocate some of the views expressed in the present paper.

It is also important to note that QM plays a role in magnetic resonance, especially when described quantitatively. QM governs the nuclear interactions that are responsible for relaxation, for example. While relaxation is consistent with classical mechanics, the observed sizes of relaxation rates are not. Only if these are calculated based on quantum mechanics do they match experiment. Normally, however, relaxation rates are measured rather than calculated from first principles. Hence, examples like this do not warrant the use of QM for non-physicists. The differences are subtle and detailed knowledge is required to acknowledge them.

## **Conclusion**

Quantum mechanics often get the blame for basic magnetic resonance appearing complicated or even incomprehensible. This is doubly unjust: Magnetic resonance is not as

complicated as it is often claimed to be, and quantum mechanics is not responsible since MR is a classical phenomenon.

It is not only a matter of the classical description being preferable to the quantum counterpart for educational purposes. It is also an issue that QM-inspired descriptions often include non-intuitive interpretations that are not supported by QM. In particular, there is little basis in QM for the non-intuitive proposition that spins are forced into the spin-up and spin-down states during MR experiments. As MR is a classical phenomenon, MR educators fortunately do not have to engage in QM-inspired descriptions that raise more questions than they answer when presented in simplified forms.

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## Appendix

This appendix contains sections that involve too much QM formalism to be understandable by most. QM is here used to show that MR is adequately described by classical mechanics. Each section heading below is a true proposition appearing in the main text, and it is followed by a QM-based justification. The basis for the calculations can be found in several textbooks including (2, 18, 19).

**Proposition 1** *An MR measurement does not make the state of an ensemble collapse into single-particle eigenstates.*

It is shown that a measurement of the total spin (or magnetization) of an ensemble of protons does not force the individual particles into their energy eigenstates unless a polarization of  $\pm 1$  is measured (full alignment), which never happens in MR where the polarization is close to 0. For the sake of clarity the argument is made for just two protons, but it is straightforward to extend to more.

The combined state vector for a system of two non-interacting protons is introduced.

$$|\psi\rangle = c_{\uparrow\uparrow} |\uparrow\uparrow\rangle + c_{\downarrow\uparrow} |\downarrow\uparrow\rangle + c_{\uparrow\downarrow} |\uparrow\downarrow\rangle + c_{\downarrow\downarrow} |\downarrow\downarrow\rangle$$

The four-dimensional state space is spanned by the product-states spin-up and spin-down for each of the two particles. The total spin operator is the sum of the individual spin operators for the two particles,  $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ . Any measurement will project the state vector onto the eigenspace associated with the measured eigenvalue of the measurement operator. A measurement of the spin of particle 1 along a direction will therefore force the state vector into a corresponding eigenstate of the associated operator. However, a measurement of the total spin along the same direction will not necessarily force the system into an eigenstate of the individual corresponding spin operators. Looking at the equation above, it is seen only to be the case if a polarization of  $\pm 1$  is measured, corresponding to parallel spins. Depending on the measured value, the state vector will collapse into  $|\uparrow\uparrow\rangle$  or  $|\downarrow\downarrow\rangle$  after such a measurement. These are indeed eigenstates of both spin operators. A measurement of

zero total magnetization, however, will not force the system into an eigenstate of any single spin-operator. Introducing a renormalization constant  $k$ , the new state is

$$|\psi'\rangle = k (c_{\downarrow\uparrow} |\downarrow\uparrow\rangle + c_{\uparrow\downarrow} |\uparrow\downarrow\rangle)$$

The terms correspond to the two ways that a total spin of zero can result from protons being in eigenstates, but  $|\psi'\rangle$  is not itself a single-particle eigenstate: It cannot be factorized and the states of particle 1 and 2 are said to be entangled. Also it is seen that the coherence is partially preserved. If more particles are present, there are more possible states with a polarization near zero, and hence the measurement-induced loss of coherence becomes insignificant when the total spin of many particles is measured (the dimensionalities of the associated subspaces increase). Consequently the individual protons are never forced into their eigenstates by MR, and **myth 1** is not supported.

**Proposition 2** *QM and classical mechanics give the same predictions.*

The state vector formalism used so far becomes impractical when more protons are considered as the dimensionality of the problem increases as  $2^N$  where  $N$  is the number of particles. A highly appropriate alternative to the vector approach is the density operator formalism that has significant advantages when ensembles of identical systems are described and when classical uncertainty and quantum indeterminism occur simultaneously (18). It is beyond the scope of this article to describe this commonly used formalism in detail, but a few important points must be made in this context.

The density operator defined for a pure state  $|\psi\rangle$  as  $\rho = |\psi\rangle\langle\psi|$ , is descriptive of the QM state just as the the state vector itself. Coherent evolution under the influence of a Hamiltonian  $H$  is described by the Liouville equation, which is the density operator analogue of the Schrödinger equation (18):

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H, \rho] \quad [3]$$

The expectation value of an operator  $A$  is given by the trace of the product  $\rho A$ :

$$\langle A \rangle = \text{Tr}(\rho A) \quad [4]$$

In the basis of spin-up and spin-down states, the density operator has the matrix representation

$$\rho = \begin{pmatrix} |c_{\uparrow}|^2 & c_{\uparrow}c_{\downarrow}^* \\ c_{\uparrow}^*c_{\downarrow} & |c_{\downarrow}|^2 \end{pmatrix}$$

It is an important advantage of density matrices over state vectors that they can be averaged over statistical ensembles in a meaningful way, i.e. so that equations [3] and [4] are still valid. The density operator for an ensemble of  $N$  particles labeled  $i$  is defined as  $\rho = 1/N \sum_{i=1}^N \rho_i$ . For individual nuclei, the probabilities of measuring energies corresponding to the energy eigenstates are present in the diagonal elements of the operator, whereas the complex phase of the off-diagonal holds the information about the direction of the transverse magnetization. The averaged density operator is independent of whether it is calculated for an ensemble of nuclei prepared with random phase as indicated in Figure 2 or of nuclei each being in spin-up or spin-down as indicated in Figure 1. In the first case, the off-diagonal elements average to zero, whereas each nuclear density matrix is itself diagonal in the latter. As predictions only depend on the density matrix, the two situations cannot be distinguished by experimental observations alone.

If the density operator is diagonal, the state is said to be incoherent. The distinction between coherent and incoherent states is somewhat arbitrary, however, as population differences (differing diagonal elements of the density operator) can be exchanged for off-diagonal coherence terms if a simple change of basis is performed by applying a unitary transformation.

The components of the proton magnetic moment  $\mu$  are conveniently expressed in terms of raising and lowering operators  $S_+ = S_x + iS_y$  and  $S_- = S_x - iS_y$ . Since the operator associated with magnetic moment along the  $x$  direction is  $\mu_x = \frac{\hbar\gamma}{2} (S_+ + S_-)$ , the expectation value of  $\mu_x$  is

$$\langle \mu_x \rangle = \text{Trace}(\mu_x \rho) = \frac{\hbar\gamma}{2} (\rho_{\downarrow\uparrow} + \rho_{\uparrow\downarrow}) \quad [5]$$

The Liouville equation provides the associated time evolution:

$$\begin{aligned}\frac{\partial\langle\mu_x\rangle}{\partial t} &= \frac{\hbar\gamma}{2i} \left( i\frac{\partial\rho_{\downarrow\uparrow}}{\partial t} + i\frac{\partial\rho_{\uparrow\downarrow}}{\partial t} \right) = \frac{\gamma}{2i} ([H, \rho]_{\downarrow\uparrow} + [H, \rho]_{\uparrow\downarrow}) \\ &= \frac{\gamma}{2i} ((H_{\downarrow\uparrow} - H_{\uparrow\downarrow})(\rho_{\downarrow\downarrow} - \rho_{\uparrow\uparrow}) + (\rho_{\downarrow\uparrow} - \rho_{\uparrow\downarrow})(H_{\downarrow\downarrow} - H_{\uparrow\uparrow}))\end{aligned}\quad [6]$$

Consequently, for the dipolar Hamiltonian,  $H = -\boldsymbol{\mu} \cdot \mathbf{B}$ ,

$$\frac{\partial\langle\mu_x\rangle}{\partial t} = \hbar\gamma^2 \left( \frac{-B_y(\rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow})}{2} + \frac{B_z(\rho_{\downarrow\uparrow} - \rho_{\uparrow\downarrow})}{2i} \right) = -\gamma B_y\langle\mu_z\rangle + \gamma B_z\langle\mu_y\rangle \quad [7]$$

Cyclic permutation finally provides the general formula.

$$\frac{\partial\langle\boldsymbol{\mu}\rangle}{\partial t} = \gamma\langle\boldsymbol{\mu}\rangle \times \mathbf{B} \quad [8]$$

This equation is remarkable: The individual magnetic moments and the macroscopic magnetization of a sample evolve according to the classical equations of motion. In particular,  $\langle\boldsymbol{\mu}\rangle$  will precess around  $\mathbf{B}$  at the Larmor frequency. The equation is equally valid for a single proton, but in that case it must be acknowledged that it describes the mean of expected outcomes of magnetization measurements rather than a definite nuclear magnetization, as the existence of the latter is not consistent with QM.

**Proposition 3** *A homogeneous RF field preserves the relative orientation of spins.*

It is shown that a homogeneous magnetic field never changes the relative spin-orientation of non-interacting protons. This is true for both static and RF fields. It implies that RF fields can only rotate the spin distribution as a whole. This proposition follows from commutator relations: If a Hermitian operator commutes with the Hamiltonian, the corresponding observable is constant in time. For two nuclei with spins  $\mathbf{S}_1$  and  $\mathbf{S}_2$ , the Hamiltonian in a magnetic field  $\mathbf{B}(t)$  is  $H = -\gamma(\mathbf{S}_1 + \mathbf{S}_2) \cdot \mathbf{B}(t)$ . This expresses that the energy is low when the nuclei are parallel to the field. The scalar product  $\mathbf{S}_1 \cdot \mathbf{S}_2$  is proportional to the cosine of the angle between the two spins. Hence it suffices to show that the commutator  $[H, \mathbf{S}_1 \cdot \mathbf{S}_2]$  is zero. This follows from relations for products of the components of spin components (19):

$$S_x^2 = S_y^2 = S_z^2 = \frac{\hbar^2}{4} \text{ and } S_i S_j = \frac{i\hbar}{2} S_k \quad [9]$$

where indices  $i, j, k = x, y$  or  $z$ , in cyclic order. Since the relation is true for any two nuclei, it is true generally, as expected on classical grounds also: The axis of precession may fluctuate, but the shape of the spin distribution remains unchanged as it is merely rotated at any instant in time. In contrast, the inhomogeneous fields created by the nuclei themselves change the relative orientation of nuclei and hence also the magnitude of the net magnetization. These fields are responsible for relaxation.

Starting from the incoherent equilibrium state, application of a  $90^\circ$  pulse makes the state coherent in the above mentioned sense. So the  $90^\circ$  pulse can be perceived as the source of the coherence. This is true in a trivial sense, but is misleading. What appears as a population difference in one basis, is coherence in another. The  $90^\circ$  pulse rotates the state vector so as to transform the population difference in the spin-up/spin-down basis into coherence. With another choice of basis, the same situation will be interpreted quite differently, e.g. opposite. The real source of the coherence is therefore not the  $90^\circ$  pulse but the field-associated longitudinal relaxation that created the population difference – the  $90^\circ$  pulse only made the population difference detectable as expressed in the coherence terms of the density operator. The typical use of the word coherence as referring to azimuthal, non-random phase relations thus unfortunately implies an apparent ability for RF pulses to change coherence whereas homogeneous RF fields in reality only can rotate the ensemble as a whole and therefore never can change the coherence generally defined as non-random phase relations (azimuthal or polar angles).

**Proposition 4** *Classical and quantum mechanics predict the same equilibrium magnetization for small degrees of polarization.*

The equilibrium magnetization is first calculated using QM and equation [4]: When expressed in the basis of energy eigenstates, the expectation value of the energy is the sum of eigenenergies each weighted by the probability of measuring that energy. From an energy accounting point of view, it therefore appears as if all nuclei are in their eigenstates, even when they are not. Hence the relative populations expressed in the diagonal elements

of the equilibrium density operator are given by the Boltzmann distribution:

$$P_{\uparrow} = \frac{\exp(-E_{\uparrow}/kT)}{\exp(-E_{\uparrow}/kT) + \exp(-E_{\downarrow}/kT)} = \frac{\exp(\hbar\gamma B_0/2kT)}{\exp(\hbar\gamma B_0/2kT) + \exp(-\hbar\gamma B_0/2kT)} \quad [10]$$

The similar expression for  $P_{\downarrow}$  differs only by the sign of the numerator exponent. The net longitudinal magnetization per nucleus  $\mu_z$  is calculated from equation [4]:

$$\langle \mu_z \rangle = \frac{\hbar\gamma}{2} (P_{\uparrow} - P_{\downarrow}) \simeq \frac{\hbar^2\gamma^2 B_0}{4kT} \quad [11]$$

The last approximation is valid when the thermal energies far exceed the energies associated with spin orientation, i.e. when the degree of polarization is small.

All spin orientations are possible according to QM but as argued above, the partition function nevertheless reduces to the sum of just two terms. In contrast, the classical partition function remains an infinite sum (integral). The energy  $E(\theta) = -\mu B_0 \cos \theta$  depends on the angle  $\theta$  between the field  $\mathbf{B}_0$  and the magnetic moment  $\boldsymbol{\mu}$ . The angular distribution again obeys Boltzmann statistics:

$$P(\theta) = \frac{\exp(-E(\theta)/kT)}{\int_0^\pi \exp(-E(\theta)/kT) \sin \theta d\theta} \quad [12]$$

The magnetic moment of a proton is  $\mu = \sqrt{3/4}\hbar\gamma$  which follows from equation [9]. These properties are used to calculate the equilibrium magnetization:

$$\langle \mu_z \rangle = \int_0^\pi P(\theta) (\mu \cos \theta) \sin \theta d\theta \quad [13]$$

$$= \mu \frac{\int_{-1}^1 \exp(\mu B_0 u/kT) u du}{\int_{-1}^1 \exp(\mu B_0 u/kT) du} \simeq \frac{\hbar^2\gamma^2 B_0}{4kT} \quad [14]$$

The last approximation is valid for small degrees of polarization. For high polarizations, e.g. for  $\hbar\gamma B_0 > kT$ , the classical and quantum predictions differ, which is easily appreciated: Classically, the maximum net magnetization is reached at zero temperature when the nuclei are perfectly aligned and each contributes a magnetization of  $\mu$ . But even at zero temperature, the spins are not perfectly aligned in agreement with quantum mechanics. Hence, each nucleus only contributes a longitudinal magnetization of  $\hbar\gamma/2$ . At temperatures and fields relevant for liquid state nuclear MR, polarizations are small (e.g.,  $10^{-6}$ ), and quantum and classical predictions are equal as shown.

Interestingly, the quantum derivation appears simpler than the classical counterpart, which can be used as an argument for choosing a QM approach to MR-teaching. Whereas the quantum derivation is easier with respect to the use of calculus, it requires more insight *a priori*. It is unfortunate that the math may seem to indicate that all spins are in eigenstates, which is not the case as explained in the appendix (proposition 1). Another unfortunate aspect of the quantum derivation is that it implicitly relies on the validity of classical mechanics since classical Boltzmann-statistics are employed rather than Fermi-statistics that describes the properties of ensembles of half-integer spin particles (20). Hence, there is no guarantee that the quantum derivation is valid in the domain where classical mechanics fail.

For MR-tutorials aimed at non-physicists, it is consequently suggested that the expression for the resulting net magnetization,  $\frac{\hbar^2 \gamma^2 B_0}{4kT}$  that is common to quantum and classical mechanics, is presented as a result of the slight skewness of the field-generated orientational spin-distribution. This is logical and true in both cases. Neither derivation contributes much clarity for non-physicists anyway.

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## Figure Captions

Figure 1: These figures illustrating the same situation are frequently seen in MR-tutorials but they do not contribute much but confusion. They illustrate the spin eigenstates which are of little relevance to MR, as the state reduction induced by measurement is only partial and does not bring single nuclei into eigenstates.

Figure 2: In the absence of magnetic field, the spins are pointing randomly hence giving a spherical distribution of spin orientations. This is illustrated to the right by a large number of example spins in an implicit magnetization coordinate space similar to that of Figure 1.

Figure 3: Better alternative to Figure 1 showing the spin distribution in a magnetic field. The spins will precess as indicated by the circular arrow and a longitudinal equilibrium magnetization (large vertical arrow) will gradually form as the distribution is skewed slightly toward magnetic north by T1-relaxation (uneven density of arrows). The equilibrium magnetization is stationary, so even though the individual spins are precessing, there is no net emission of radio waves in equilibrium.

Figure 4: This figure sometimes seen in MR literature is misleading. It shows how spins in the eigenstates (left) can be reoriented as to form a transversal magnetization (right). However, a homogeneous RF field never changes the relative orientations of spins which contradicts the validity of the figure.

Figure 5: This figure shows how an RF field on resonance can rotate the spin distribution of Figure 3. As all spins precess, the distribution and the net magnetization rotates around the  $B_0$  field direction. So does the orthogonal magnetic field vector associated with a resonant, circularly polarized RF field. Seen from a frame of reference rotating at the common frequency, all appear stationary except for a slow rotation of the spin distribution around the RF field vector. If this is pointing toward the reader, the magnetization will be rotated in the direction indicated.

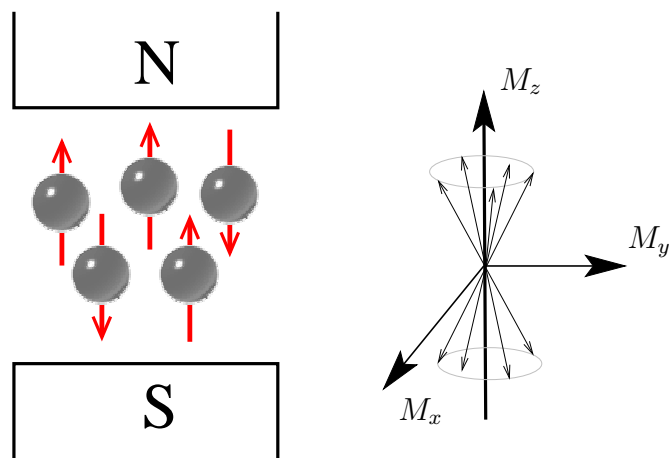


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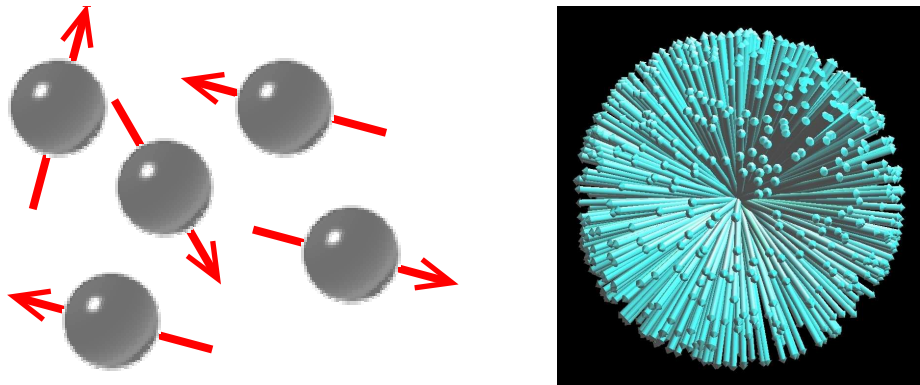


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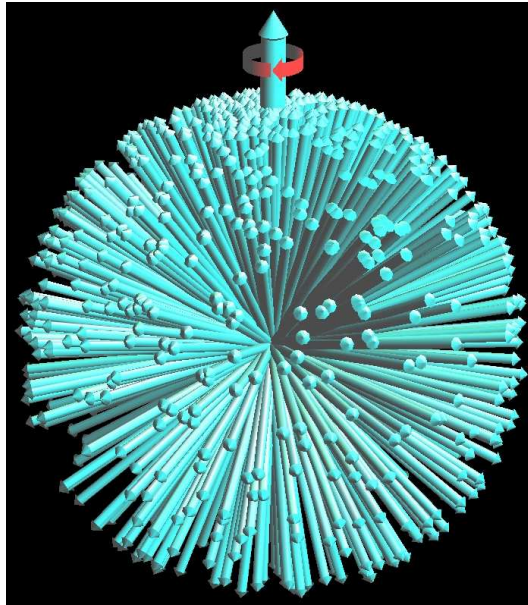


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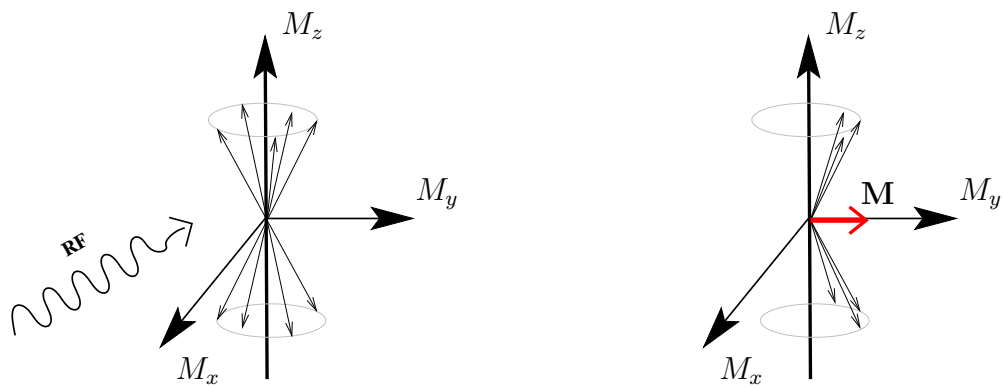


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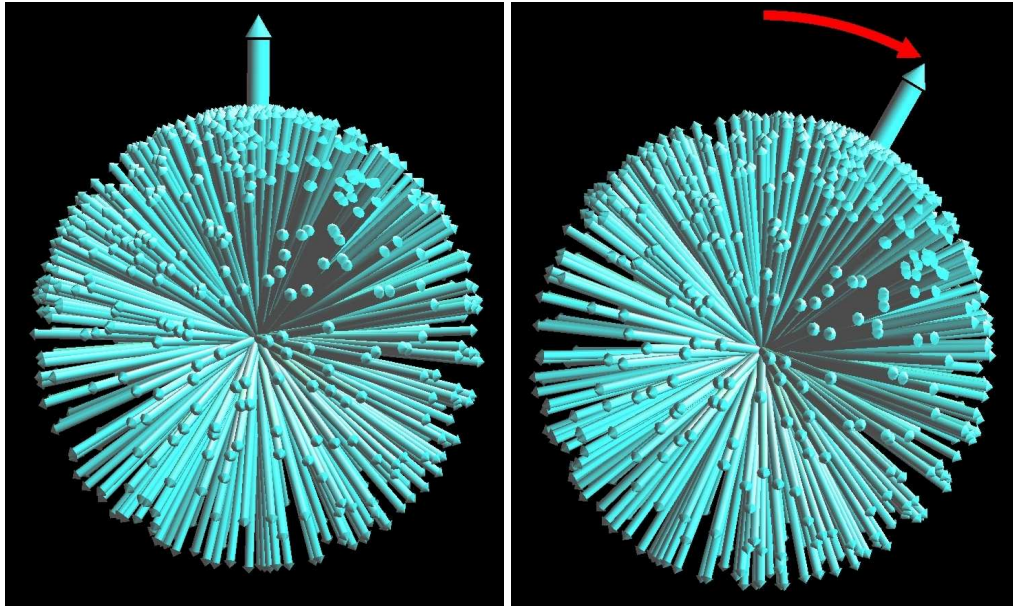


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