Is Quantum Mechanics necessary for understanding Magnetic Resonance?

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Based on a Paper by Lars. G Hanson
Overview

- Introduction
- Misinterpretations
- Discussion
- Conclusion
Introduction

Transition from Classical Physics to Quantum Mechanics

Bohr–Einstein debates

Wolfgang Pauli and Niels Bohr look at a spinning top. Bohr and Pauli are pioneers of quantum mechanics, where the concept of spin is rooted.
Probabilistic Nature of Quantum Mechanics

Understanding and Interpreting Quantum Mechanics Phenomena

Role of QM in Explaining MR

MR and Correspondence Principle
Misinterpretations of Quantum Mechanics in MR and Myths

- First Myth: According to QM, Protons align Either Parallel or Antiparallel to the Magnetic field
  - A Classical Analogy
  - Spin States and Uncertainty

\[ |\psi\rangle = c_\uparrow |\uparrow\rangle + c_\downarrow |\downarrow\rangle \]
What is the Origin of Misconception?

- Magnetization of an Individual Proton
- Ensemble of Particles in a Magnetic Field
Comparing Two Illustrations of Spin Eigenstates
Analyzing the Problem for a two particle System

An MR measurement does not make the state of an Ensemble collapse into single particle eigenstates

Polarization = +1, 0, -1

\[ |\psi\rangle = c_{\uparrow\uparrow}|\uparrow\uparrow\rangle + c_{\downarrow\downarrow}|\downarrow\downarrow\rangle + c_{\uparrow\downarrow}|\uparrow\downarrow\rangle + c_{\downarrow\uparrow}|\downarrow\uparrow\rangle \]

Measurement of zero total Magnetization:

\[ |\psi\rangle = k(c_{\uparrow\downarrow}|\downarrow\uparrow\rangle + c_{\downarrow\uparrow}|\uparrow\downarrow\rangle) \]

\[ \rightarrow \text{Entanglement of the states of two particles} \]
Second Myth: **MR is a Quantum Effect**

- How is a Quantum Effect defined?
- Some examples of Quantum Phenomena
- [Bloch Vector and Two Quantum-Level Systems](#)

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**Journal of Applied Physics**

*January, 1957*

*Geometrical Representation of the Schrödinger Equation for Solving Maser Problems*

**Richard P. Feynman and Frank L. Vernon, Jr., California Institute of Technology, Pasadena, California**

**Robert W. Hellwarth, Microwave Laboratory, Hughes Aircraft Company, Culver City, California**

(Received September 18, 1956)

A simple, rigorous geometrical representation for the Schrödinger equation is developed to describe the behavior of an ensemble of two quantum-level, noninteracting systems which are under the influence of a perturbation. In this case the Schrödinger equation may be written, after a suitable transformation, in the form of the real three-dimensional vector equation \(dv/dt = \omega \times v\), where the components of the vector \(v\) uniquely determine \(\phi\) of a given system and the components of \(\omega\) represent the perturbation. When magnetic interaction with a spin \(s\) system is under consideration, \(\phi\) space reduces to physical space. By analogy, the techniques developed for analyzing the magnetic resonance precession model can be adapted for use in any two-level problems. The quantum-mechanical behavior of the state of a system under various different conditions is easily visualized by simply observing how \(v\) varies under the action of different types of \(\omega\). Such a picture can be used to advantage in analyzing various Maser-type devices such as amplifiers and oscillators. In the two illustrative examples given (the beam-type Maser and radiation damping) the application of the picture in determining the effect of the perturbing field on the molecules is shown and its interpretation for use in the complex Maxwell’s equations to determine the reaction of the molecules back on the field is given.
Quantum Mechanics and Classical Physics Give the Same Predictions

- Density operator formalism as an alternative to vector approach

\[ \rho = |\psi\rangle \langle \psi| \]

- Coherent evolution described by Liouville equation:

\[ \frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H, \rho] \]

- Density Operator and Coherency

\[ \rho = \begin{pmatrix} |c_\uparrow|^2 & c_\uparrow c_\downarrow^* \\ c_\downarrow^* c_\uparrow & |c_\downarrow|^2 \end{pmatrix} \]
X Component of Proton Magnetic Moment:

\[ \mathbf{\mu}_x = \frac{\hbar \gamma}{2} (S_+ + S_-) \]

\[ S_+ = S_x + iS_y \quad S_- = S_x - iS_y \]

Expectation value of Magnetic Moment:

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

Using Liouville Equation:

\[ \frac{\partial \langle \mu_x \rangle}{\partial t} = \frac{\hbar \gamma}{2i} \left( i \frac{\partial \rho_{\uparrow\uparrow}}{\partial t} + i \frac{\partial \rho_{\downarrow\downarrow}}{\partial t} \right) = \frac{\gamma}{2i} ([H, \rho]_{\uparrow\uparrow} + [H, \rho]_{\downarrow\downarrow}) \]

\[ = \frac{\gamma}{2i} ((H_{\uparrow\uparrow} - H_{\downarrow\downarrow})(\rho_{\downarrow\downarrow} - \rho_{\uparrow\uparrow}) + (\rho_{\downarrow\uparrow} - \rho_{\uparrow\downarrow})(H_{\downarrow\downarrow} - H_{\uparrow\uparrow})) \]
Having Dipole Hamiltonian as

\[ H = -\mu \cdot B \]

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

We can write the equation above as:

\[
\frac{\partial \langle \mu \rangle}{\partial t} = \gamma \langle \mu \rangle \times B
\]

Which is exactly equivalent to the Classical Evolution.

\[ \frac{dr}{dt} = \omega \times r \]
- Counter_Feynman approach in MR
- Zeeman Splitting and RF Field
- Coherent Evolution as the Crucial point of Understanding Magnetic Resonance
Third Myth: RF Pulses Bring the Precessing Spin into Phase

- RF field never changes the relative orientation between noninteracting proton spins
- RF field never changes Coherence (nonrandom phase relations)
- T1 as Real source of Coherence
Visualization of Spin Precession in Magnetic Fields

$B_0$ and $B_1$
Equilibrium Magnetization for Small Degrees of Polarization

Classical and QM Predictions

Relative population expressed in diagonal elements of equilibrium density operator:

\[
P_{\uparrow} = \frac{\exp(-E_{\uparrow}/kT)}{\exp(-E_{\uparrow}/kT) + \exp(-E_{\downarrow}/kT)}
\]

\[
= \frac{\exp(h\gamma B_0/2kT)}{\exp(h\gamma B_0/2kT) + \exp(-h\gamma B_0/2kT)}
\]

\[P_{\downarrow} \text{: Same expression with different sign of numerator exponent}\]

The net magnetization per nucleus

\[
\langle \mu_z \rangle = \frac{h\gamma}{2} (P_{\uparrow} - P_{\downarrow}) \approx \frac{h^2\gamma^2 B_0}{4kT}
\]
The approximation for small Degree of Polarization $\Rightarrow \hbar \gamma B_0 < kT$

$$E(\theta) = -\mu B_0 \cos \theta$$

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

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

$$= \mu \frac{\int_{-1}^1 \exp(\mu B_0 u/kT) u \, du}{\int_{-1}^1 \exp(\mu B_0 u/kT) \, du} \approx \frac{\hbar^2 \gamma^2 B_0}{4kT}$$

For small degrees of polarization we get the same result from Classical Mechanics and QM.
Nature, Reality, our Perception
Different approaches

- Mental Representation, Simplification of Reality
- Intuitiveness, simplicity and Prediction as Criteria
- Classical and Quantum Mechanics Approach of MR
Conclusion

- MR is not extremely complicated and QM is not responsible because MR is a classical phenomena.

- Basic NMR can be explained by QM but the interpretation is often problematic.

- A classical introduction to MR can provide intuition and predictive power.
Thank you for your Attention
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