Quantum Mechanical Description of NMR: From Wave Function to Bloch Equation

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Summary

This report outlines steps in deriving the Bloch Equation, beginning by applying the principles of relativistic and non-relativistic quantum mechanics to simple physical models of the proton, and deriving the two-component Schrödinger Equation, which describes the interaction of a single proton with externally applied magnetic fields. The off-diagonal entries of the Bloch equation matrix are derived by taking the time derivative of the expectation values of the solutions (spinors) of the Schrödinger Equation that describe the dynamics of the collection (ensemble) of protons in each voxel. Derivations of the Boltzmann distribution, which determines the thermal equilibrium magnetization, and of the mechanisms of magnetization relaxation, are also described to complete the entries of the Bloch Equation. The mathematical foundations of proton intrinsic spin and magnetic moment from relativistic and non-relativistic quantum mechanics will be described, and an intuitive understanding of the proton gyromagnetic ratio, and of the physical origin of the Nuclear Magneton fundamental constant, is obtained from non-relativistic quantum mechanics. The paragraphs below briefly describe these topics, which will be elaborated in the talk.

Relativistic Dirac equation predicts intrinsic spin and intrinsic magnetic moment

The intrinsic spin of the electron (or any charged point particle) was elegantly predicted by P.A.M. Dirac. By requiring that the quantum mechanical wave function of the electron obey a first order differential equation, and by requiring that the differential equation be invariant under Lorentz Transformations, a magnetic coupling term between the electron and externally applied magnetic field emerged in the differential equation. The coupling term generated behavior of the electron consistent with the electron having an intrinsic magnetic moment and an intrinsic spin. Prior to this derivation by Dirac, Pauli had imposed the same magnetic field interaction term into a scalar non-relativistic Schrödinger differential equation. Wave functions solving this equation represented particles that demonstrated intrinsic magnetic moment and intrinsic spin in experiments. Dirac's equation was more elegant and profound in that it produced the interaction term, along with the concepts of intrinsic spin and intrinsic magnetic moment, only from the requirements of differential equation linearity and Lorentz invariance.

Although work by Dirac, Pauli and others, e.g. Zeeman, was motivated by the challenge of understanding the electrons' influences on the atomic spectrum of the hydrogen atom, experiments with the proton demonstrated that it also had an intrinsic spin and intrinsic magnetic moment. The intrinsic spin of the proton was the same value (½) as that for the electron, but the strength of the magnetic moment that resulted from the intrinsic spin was not predicted by the prior theoretical work of Dirac and Pauli. The numerical value of the proton's magnetic moment predicted by this prior theoretical work became known as the Nuclear Magneton (which appears in most tables of Fundamental Physical Constants), and the adjective "anomalous" became accepted to indicate that the magnetic moment's strength was not as predicted for true point particles, but instead had to be determined experimentally. Like the proton, the neutron also behaved as a spin ½ particle and possessed an anomalous magnetic moment, and in ensuing research, other hadrons were found to have half-integer spin and anomalous magnetic moments. While there currently exists no satisfactory nuclear theory to accurately predict (e.g. to 2-3 decimal places) these anomalous values across the family of hadrons,

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the quark model of these particles (in which the proton is composed of two up and one down quark, and the neutron is composed of two down and one up quark) provides the most accurate predictions. It is interesting that the strength of the proton magnetic moment, the most fundamental parameter upon which MRI depends, cannot be theoretically explained.

Spinors represent the quantum mechanical properties of single protons
The non-relativistic approximation of the Dirac equation, with the inclusion of an anomalous magnetic moment replacing the Nuclear Magneton in the equation, accurately predicts the action of a single proton under the influence of external magnetic fields such as those applied in an MRI system. This equation is also well-known as the two-component Schrodinger equation (in some references, it is known as the two-component Pauli equation). The two-component solutions of this equation representing single protons are called spinors, not vectors, in recognition of the fact that these solutions do not transform as vectors under coordinate rotations. The spinors have two distinct complex-valued components, and different specific values for these components are identifiable with the spin-up proton or spin-down proton, possessing positive or negative magnetic moment, respectively, and possessing low or high energy, respectively, if in a static magnetic field. In general, specific values for the spinor components are identifiable with specific probabilities that the proton represented by the spinor will be detected with a positive or negative magnetic moment. The non-relativistic approximation of the Dirac equation and its spinor solutions can also be derived from first quantization of a simple classical model of a charged particle in a magnetic field revolving around a virtual point. This classical model provides greater intuitive physical insight into the relationship between spin, angular momentum, magnetic moment and the gyromagnetic ratio possessed by the proton.

The collection of protons in each voxel develops a thermal equilibrium magnetization
In the presence of a static magnetic field, a greater number of spin-up (low energy) protons than spin-down (high energy) protons will develop, provided there is a mechanism for energy exchange between the spin system and the system consisting of quantum states of the surrounding molecules (the lattice). This slight excess of spin-up protons produces a net magnetic moment in each voxel, which at equilibrium is called the thermal equilibrium magnetization. Deriving the specific numerical value for the thermal equilibrium magnetization requires a model in which the quantum mechanical states in the spin system and in the surrounding molecules can be separately enumerated (counted), for any partition of energy between the two systems. The partition of energy that yields the greatest number of assessable quantum states will be the partition of energy that is observed in MRI experiments. Using binomial terms for counting the number of spin-up and spin-down proton combinations for any specific energy in the spin system, and a free-particle kinetic energy model for counting states for any specific energy in the lattice, the well-known Boltzmann equation can be derived. The Boltzmann equation reveals that at thermal equilibrium the number of protons in the low energy state exceeds the number in the high energy state by small fraction. For a 1.5T system, this fraction is approximately 5 protons excess per million protons in the spin system.

The protons in each voxel can be represented using a common probabilitistic spinor
At thermal equilibrium, the protons in each voxel are accurately represented by spinors with a common mathematical form, and the spinors representing different protons differ only with respect to complex phase factors multiplying each spinor component. Summing the magnetic moments of all protons, the correct thermal equilibrium magnetization is obtained, provided that across all protons the phase angles of these

factors are randomly and uniformly distributed over their full range of possible values. In MRI, it is often assumed that a small number of excess spin-up protons, generated by energy exchange with the lattice in the static magnetic field, are unchanging in time and solely constitute the observed magnetization. However, in reality at any given time during the pulse sequence, any of the protons in the voxel might contribute to the observed magnetization. So, it is more realistic to consider that all of the protons are contributing to the magnetization but that the majority of the contributions are canceling each other out. Mathematically, this cancellation is shown to result from the statistical distribution of the phase angles assigned to the spinors.

The RF coil detects the net magnetic moment (magnetization) of the protons in each voxel

Immediately after nutation of the magnetization by an RF pulse, and throughout the pulse sequence, the values of the spinors representing the individual protons in each voxel are rapidly changing due to the interaction of the proton magnetic moments with the external magnetic fields. The RF coil detects the magnetic moment of each precessing proton as a quantized unit of induced electromotive force (emf), in accordance with Faraday's classical law of electromagnetic induction, and each magnetic moment is detected as either positive or negative, as either a positive or negative unit of induced emf, respectively. At any given time, the net magnetic moment (the magnetization) from the entire collection of protons is detected by the total induced electromotive force (emf) in the coil. In a large collection of protons, the total induced emf is proportional to the number of positive magnetic moments detected, minus the number of negative magnetic moments detected. The number of positive magnetic moments detected is equal to the probability that a single proton is detected with positive magnetic moment, multiplied by the total number of protons. A similar statement applies to calculating the number of negative magnetic moments detected. For example, if each proton in a collection of 10^{12} protons has a 50.00025% probability of being detected with positive magnetic moment along the direction of sensitivity of the RF coil, and a 49.99975% probability of being detected with negative magnetic moment along that direction, then a positive net magnetic moment, corresponding to the combined moments of $5x10^6$ protons, will be detected as a net positive induced emf in the coil. Although the magnetic moment of each proton is quantized, and detected through a positive or negative unit of induced emf, the total induced emf in the RF coil appears to have a continuum of possible values, because an extremely large number of protons contribute to the emf. The total induced emf is not observed as being quantized.

Magnetization decay caused by random time-varying magnetic fields acting on each proton

It is well established from theory and experiment that a negative exponential characteristic time, defined T2, is identifiable as the time constant for decay of transverse proton magnetization during signal detection, and a negative exponential characteristic time, defined T1, is identifiable as the time constant for decay of longitudinal magnetization, as well as the time constant for recovery of longitudinal magnetization towards thermal equilibrium. These characteristic times can be derived using a Gaussian random process model of time-varying microscopic magnetic fields, acting locally and independently at each proton. These random time-varying magnetic fields result in a gradual loss of similarity of spinors representing the protons, and the characteristic times can be directly calculated from the correlation time and temporal variance of the fields. In addition, tissues are composed of a multitude of water compartments, each with unique T1s and T2s, and water molecules typically exchange very rapidly between the different compartments relative to the typical intervals for data collection in an MRI experiment. Consequently, the characteristic times observed in the MRI experiment are the weighted average of the times in each of the compartments.

Putting the effects together to construct the Bloch equation

By linearly combining the independent contributions to the time derivatives of proton magnetization arising from (1) the two-component Schrödinger equation describing the dynamics of single protons interacting with external magnetic fields, (2) the recovery of longitudinal magnetization based on energy exchange between the spin system and the lattice and (3) the decay of magnetization due to the action of microscopic random magnetic fields, the well-known Bloch Equation is obtained. See [Buonocore 2010] for the mathematical details of this construction.

QED used to describe the interaction between proton and RF coil

A limitation of the model presented above of induced emf in the RF coil is that it treats the effect of the precessing proton magnetic moment on the RF coil in accordance with classical electromagnetism, rather than in accordance with quantum mechanics. At the point in the model when the induced emf in the RF coil is calculated, we ignore the inherent quantum mechanical interaction that exists. Specifically, we do not consider quantized energy and or magnetic moment exchange between the quantum states of the proton and those of the current or emf in the coil. Instead, the protons in the voxel are seen as creating a classical net magnetic moment, which creates a classical dipole magnetic field with field lines that cut through the circular loop of the RF coil, inducing (mainly during precession) a current and voltage in accordance with Faraday's law of electromagnetic induction. The quantum mechanical interaction between the spin and coil is neither explained nor modeled. Quantum Electrodynamics (QED) has been used to describe the interaction of one or a collection of protons with an RF coil. This formulation of signal detection includes a description of the quantum states of the current or emf in the RF coil, and of the quantum states of the protons in the voxel that interact with the coil, and represents the interactions of these quantum states as virtual photons. Another approach has been developed in which the RF coil and proton magnetic moment are modeled through a common energy equation (Hamiltonian equation), and in which the quantum states are coupled not through a virtual photon field but empirically through specific interaction terms in the Hamiltonian. See [Sykora 2010] and [Engelke 2010] for details regarding these and other formulations.

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