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Basic Principles of Nuclear Magnetic Resonance and Its Physical Applications

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Abstract. The general physical ideas of Nuclear Magnetic Resonance (NMR) and its some applications in physics are introduced in this paper. The NMR is crucial in probing molecular structure and interactions across chemistry, biology, and condensed-matter physics. Through method such as logical structuring, formula derivation, information integration, and systematic synthesis, the basic physics of NMR is illustrated, and its applications and advantages are comprehensively introduced, followed by a discussion of its significance and future prospects. Zeeman splitting and relaxation mechanisms are the physical foundations of NMR as a microscopic probe. Based on the above analysis, NMR can be used to measure relaxation rates and Knight shifts to identify non-trivial quantum effects, such as Majorana fermions and topological surface states. NMR has gradually been used to realize precise control of quantum coherence, and with the continuous development of technology, it is expected that future ultra-low-power quantum information storage devices and physical systems will be constructed based on this technology.

Keywords: Nuclear Magnetic Resonance; Zeeman Splitting; Relaxation Mechanisms; Quantum Sensing; Quantum Spin Liquids.

1. Introduction

Nuclear Magnetic Resonance (NMR) is a foundational branch of contemporary physics that can observe the small-scale quantum-mechanical features of matter in large-scale experiments. In recent years, NMR has achieved many notable results and can now be employed to study the basic characteristics of matter other than chemical structure. For example, in recent years, quantitative nuclear magnetic resonance technology has been applied broadly to determine the purity of compounds (such as the field of trace water content measurement), and it has good attributes such as non-destructive testing, rapid analysis, and minimal sample preparation [1]. The advantages of NMR include being non-destructive and highly sensitive to changes in the local magnetic environment. Using the spin of atomic nuclei as an internal quantum probe, many complex physical phenomena can be investigated, such as the dynamics of condensed matter and the coherence of quantum information systems; therefore, it is now an essential tool in contemporary research in physics.

Since the first work by Purcell and Bloch in recent years, many scholars have conducted studies on NMR and expanded its theoretical foundations and applications. Early studies focused on the basic physics of Zeeman splitting and the development of the Bloch equations for magnetic dynamics. Classical works by Mefed and Slichter provided the first rigorous quantum mechanical descriptions of resonance and relaxation processes and are still used today [2,3]. Recently, more attention has been paid to the application of NMR in frontier physics in the literature. Research has shown that it can describe strongly correlated systems well and has detected Majorana fermions in Kitaev-like materials [4]. In recent years, improvements in hyperpolarization and pulse-sequence design have extended the application scope of NMR to surface physics and topological insulators [5], and is used to study spin-momentum locking and low-dissipation electronic states.

This paper introduces the general ideas of NMR and some representative applications of NMR in current science. The organization of the text is as follows: Section 2 introduces the theoretical basis for NMR, begins with the micro-origin of nuclear spin and magnetic moments, and then systematically discusses Zeeman splitting, Larmor precession, and the quantum mechanics of

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radiofrequency coupling. Statistics of relaxation processes (T1 and T2) and the way a spin system reaches a steady state will also be presented here. Section 3 introduces some applications of the above ideas in physics and specifically studies NMR for investigating quantum spin liquids, its use as a memory unit in quantum information processing, and new research directions on catalysis and topological thin films. Finally, the last section will devote to the conclusion, summarizing the foregoing text and offering a perspective about ongoing development and the future of NMR.

2. Physical Principles of NMR

2.1. Nuclear Spin and Magnetic Moment: Microscopic Physical Origins

The physical root of the Nuclear Magnetic Resonance (NMR) phenomenon lies in the spin property of the atomic nucleus. According to quantum mechanical theory, the nucleus is composed of protons and neutrons. These fermions possess an intrinsic angular momentum, also known as spin. At the same time, they undergo relative motion within the nucleus, which gives rise to a corresponding orbital angular momentum. The vector sum of all nucleons' angular momenta (both intrinsic and orbital) constitutes the total angular momentum of the nucleus, denoted as P_I. Its magnitude is determined by the spin quantum number I:

$$P_I = \sqrt{I(I+1)}\hbar \tag{1}$$

Both protons and neutrons are fermions with a spin of $1/2$, and the total spin of a nucleus depends on the even-odd combination of the numbers of these two particles, while nuclear magnetic resonance only yields signals for nuclei with a non-zero total spin; therefore, atomic nuclei can be classified into four categories: if the mass number is even and the proton number is even, the nuclear spin quantum number $I = 0$, resulting in no signal; if the mass number is even and the proton number is odd, the nuclear spin quantum number I is an integer such as 1, 2, or 3, yielding a signal; if the mass number is odd and the proton number is even, I is a half-integer such as $1/2$, $3/2$, or $5/2$, yielding a signal; if the mass number is odd and the proton number is odd, I is also a half-integer such as $1/2$, $3/2$, or $5/2$, yielding a signal. When I is zero, the nucleus is regarded as a non-spinning sphere; when I is $1/2$, it is viewed as a spinning sphere with a uniform charge distribution; and when I is greater than $1/2$, it is seen as a spinning sphere with a non-uniform charge distribution. Since the nucleus is electrically charged, its spin inevitably generates an associated nuclear magnetic moment μ, and the proportional relationship between the magnetic moment and angular momentum is described by the gyromagnetic ratio γ

$$\vec{\mu} = \gamma \vec{P_I} \tag{2}$$

In physics, this can also be expressed through the nuclear magneton μ_N and the nuclear Landé g-factor g_N as:

$$\mu = g_N \mu_N \sqrt{I(I+1)} \tag{3}$$

The existence of such a microscopic magnetic moment enables the atomic nucleus to interact with an external magnetic field, much like a miniature magnetic needle. Although this interaction is extremely small, it provides an exceptionally precise microscopic probe for detecting the internal structure of matter, serving as the physical prerequisite for the occurrence of nuclear magnetic resonance [6].

2.2. Zeeman Level Splitting: Energy Quantization in a Static Magnetic Field

When an atomic nucleus is placed in a constant external magnetic field of strength B_0, the magnetic moment of the nucleus enables it to interact with the field, generating an additional energy:

$$W = -\vec{\mu} \cdot \vec{B}_0 \tag{4}$$

According to the theory of spatial quantization, the projection of the spin angular momentum onto the direction of the magnetic field (defined as the z-axis), P_{Iz}, can only take discrete values: $P_{Iz} = m_I\hbar,\ m_I = I, I-1, \ldots, -I$. This quantization of spatial orientation leads to the splitting of energy levels, known as Zeeman Splitting. For a nucleus with a spin quantum number $I = 1/2$ (such as the hydrogen nucleus), the originally degenerate energy level splits into two: a lower-energy parallel state ($\mathrm{m_I} = +1/2$) and a higher-energy anti-parallel state ($\mathrm{m_I} = -1/2$). The energy difference between adjacent levels is:

$$\Delta E = \gamma\hbar B_0 = \mu_H B_0/I \tag{5}$$

This level splitting not only establishes the image of energy quantization but also determines a slight excess of particles in the lower energy level under thermal equilibrium via the Boltzmann distribution; in other words, at a constant temperature, the distribution of particles between the high and low energy levels reaches a dynamically stable ratio, where the number of nuclei in the lower state slightly exceeds those in the higher state. This minute difference in particle numbers accumulates statistically to form the macroscopic magnetization vector M_0, which is the total magnetic field strength resulting from the vector sum of all microscopic magnetic moment (μ) in a sample—a net magnetic field aligned with the external field that establishes the potential energy foundation for subsequent signal excitation [7]. In detail, the receiving coil (detector) cannot directly detect the microscopic magnetic moment of a single nucleus; instead, the coil captures the electromagnetic induction current generated by the motion (precession) of M_0. The detected signal intensity is directly proportional to the magnitude of M_0: the larger M_0 is, the higher the signal-to-noise ratio (SNR), and the clearer the resulting image or spectrum.

2.3. Larmor Precession: The Perspective of Classical Dynamical Evolution

To understand the behavior of spin from a dynamical standpoint, a classical mechanical image can be introduced. When a magnetic moment μ is placed in an external magnetic field B_0, the field exerts a torque on the magnetic moment:

$$\vec{\tau} = \vec{\mu} \times \vec{B}_0 \tag{6}$$

According to the angular momentum theorem, the torque equals the time rate of change of the angular momentum ($dP_I/dt = \tau$), which causes the magnetic moment not to align directly with the magnetic field, but rather to rotate in a conical fashion around the magnetic field vector, a motion known as Larmor Precession. The angular frequency of this precession, ω_0, satisfies the relation $\omega_0 = \gamma B_0$, and the corresponding frequency,

$$\nu_0 = \omega_0/2\pi = \gamma B_0/2\pi \tag{7}$$

is called the Larmor frequency. This classical image intuitively demonstrates the steady-state motion of the nuclear magnetic moment in a static magnetic field. It predicts that to change this state of motion or to transfer energy within the system, one must introduce a time-varying field that matches this intrinsic precession frequency (in NMR experiments, the radiofrequency pulse (RF Pulse) applied is a magnetic field whose direction changes over time, i.e., a "time-varying field"), thereby achieving a stimulated response of the system [2], transitioning it from a low-energy equilibrium state to a high-energy non-equilibrium state.

2.4. RF Resonance and Energy Transitions: Quantum Mechanical Coupling

Building upon energy level splitting, if an alternating magnetic field B_1 (radio frequency field) is applied perpendicular to the static magnetic field B_0, and its frequency ν satisfies the resonance condition $h\nu = \Delta E$, the system absorbs photons and undergoes stimulated transitions. From a quantum mechanical perspective, this represents an energy exchange between RF photons and the nuclear spin system, forcing transitions to obey the selection rule $\Delta m = \pm 1$. Specifically, since the total angular momentum in the z-direction of the initial state must equal that of the final state (including the photon), one has z-angular momentum conservation $m_I + \sigma = m_I'$. Given that the photon's angular momentum projection along the z-axis is $\pm\hbar$, it follows that

$$m_I' - m_I = \pm 1, \tag{8}$$

meaning the nuclear spin flips between adjacent Zeeman levels. From a classical perspective, this is the effective manipulation of the magnetization vector by the RF field within a rotating reference frame. In this frame, B_1 appears as a static transverse magnetic field that exerts a continuous torque on the macroscopic magnetization M, causing it to precess around B_1 and gradually tip away from the equilibrium z-axis. These two descriptions are complementary—the quantum image explains "why a specific frequency" is required, while the classical image explains "how the magnetization vector moves." At this point, the magnetization M, originally in thermal equilibrium, deviates from its equilibrium position. When resonance occurs, nuclei in the lower energy level absorb energy and transition to the higher level. Because the initial population of the lower level is slightly larger than that of the higher level, the total number of photon absorptions exceeds that of stimulated emissions. The net absorption of photons at resonance—the difference remaining after subtracting stimulated emission from total absorption—results in a transverse component M_{xy} of the macroscopic magnetization. This transverse component induces a measurable electromotive force in the receiving coil, thereby converting microscopic energy level spacing into a macroscopic electromagnetic signal. This high frequency selectivity (Resonance) is the core logic enabling high-resolution detection in NMR, directly transforming microscopic energy gaps into measurable electromagnetic frequency signals and making the probing of atomic-scale environments possible [3].

2.5. Relaxation Processes: Statistical Physical Mechanisms for Returning to Equilibrium

After the RF pulse ceases, the excited spin system does not remain in a non-equilibrium state but returns to thermal equilibrium through interactions with the surrounding environment and between spins. This process, known as relaxation, is the non-radiative transition of nuclei from high-energy states back to low-energy states. Physically, relaxation consists of two independent yet simultaneous mechanisms. The first is spin-lattice relaxation (longitudinal relaxation), characterized by the time constant T_1. It involves the exchange of energy between the spin system and the surrounding thermal reservoir (the lattice or solvent), allowing the longitudinal magnetization M_z to recover to its equilibrium value M_0 as determined by the Boltzmann distribution. T_1 serves as a measure of the high-energy state's lifetime and relaxation efficiency; a smaller T_1 indicates higher efficiency. This process reflects the internal energy dissipation efficiency of the system and is closely related to the frequency of molecular thermal motion (Brownian motion). Molecules in the lattice undergo thermal motion, generating randomly fluctuating "stochastic magnetic fields." If these fluctuations contain frequency components near the Larmor frequency, they induce stimulated transitions between energy levels. Thus, T_1 reflects the dynamics of molecular motion. If molecular motion is too rapid (highly dispersed frequency components) or too sluggish (a rigid environment with low-frequency components), T_1 will increase; T_1 is minimized only when the "tempo" matches the Larmor frequency. Therefore, the duration of T_1 directly reflects the dynamical characteristics of molecular motion and is a vital parameter for studying molecular tumbling frequencies and environmental viscosity.

The second mechanism is spin-spin relaxation (transverse relaxation), characterized by T_2, which describes the decay of the transverse magnetization component M_{xy}. This process involves only the exchange of energy between similar magnetic nuclei without changing the total nuclear magnetic energy. Its essence lies in the microscopic inhomogeneity of local magnetic fields and dipolar interactions between spins, which cause the initially phase-coherent spins to gradually dephase during precession. Relaxation processes not only determine the signal duration (FID decay), but their parameters T_1 and T_2 also contain deep physical information regarding microscopic dynamical fluctuations, molecular motion rates, and spin correlations, making NMR a powerful tool for studying the condensed matter properties of materials [8]. In summary, the physical significance of T_1 and T_2 extends far beyond simple decay constants; they are sensitive measures of the microscopic environment. In biomedicine, differences in relaxation form the basis of contrast in Magnetic Resonance Imaging (with tissue relaxation times ranging from 10^{-5} to several seconds [9]), allowing for the differentiation of anatomical structures and pathological tissues. In materials science, the analysis of relaxation spectra enables the quantitative study of spatially confined molecular motion, adsorption states, and phase transition processes. Furthermore, relaxation dynamics not only determine the upper limit of the signal-to-noise ratio but also provide core timing parameters for pulse sequence design. In short, the relaxation process is the critical link that allows NMR to evolve from a pure physical phenomenon into a multi-disciplinary analytical tool.

3. Applications

3.1. The Logical Leap from Spin Dynamics to Quantum Sensing

The reason why NMR can be used to observe changes in a material's local environment and measure that change is due to the properties of the spin system. As shown in Section 2.5, relaxation rates (T1 and T2) are not merely decay constants but also dynamic fingerprints of the spectral density of physical fluctuations in the lattice that contain rich physical information. For example, Nuclear Magnetic Resonance (NMR) and Nuclear Quadrupole Resonance (NQR) have been used to study the charge-density wave (CDW) structure of CsV_3Sb_5 [10], as shown in Fig. 1.

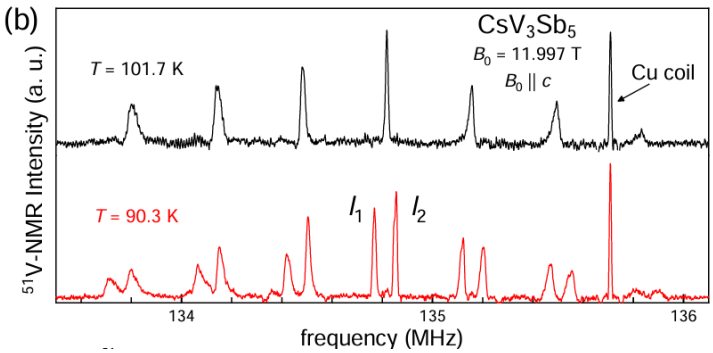

Fig. 1 Temperature dependence of the 51V-NMR spectra above TCDW (black color) and below TCDW (red color) with the external magnetic field applied along the c-axis [10].

NMR has gradually become a high-performance platform for quantum sensing in recent years and started as a tool for structural determination. Atoms are used as internal, non-destructive quantum probes to map the complex phase diagram of quantum materials and observe physical changes in a non-equilibrium state in real time [11]. Therefore, at present, NMR research is no longer focused on observing spin states passively but rather on manipulating quantum coherence in condensed matter systems actively. This change can be observed in many parts of physics; for instance, through high-precision measurements of the Knight shift in metals, which is a deviation in the magnetic field experienced by the nucleus due to free electrons, NMR has been applied to quantum sensing of the electronic density of states (i.e., the number of available states for electrons at a given energy level). Probe for free-electron information, study the mechanism of superconductivity, and observe changes in the structure of the atomic electron cloud.

3.2. Detection of Exotic Quantum Phases and Strongly Correlated Systems

One of the first and most important applications of NMR in the forefront of modern condensed matter physics is the study of strongly correlated electron systems and unconventional magnetism; these systems exhibit strong Coulomb interactions among electrons and therefore display complex collective behaviour rather than acting independently. In this context, physicists strive to find an exotic state of matter known as the Quantum Spin Liquid (QSL)(As one of the most promising Kitaev quantum-spin-liquid (QSL) candidates, α-RuCl3 has received a great amount of attention of physicists[12]). At a higher temperature, the atomic spins in a conventional magnetic material are randomly oriented. However, in a QSL, spins are still in a liquid-like, continuously fluctuating disordered state even at absolute zero. This state has a high degree of quantum entanglement and is a key route for topological quantum computing; that is, quantum information is stored in invariant "topological properties", and local external noise cannot destroy this data by altering the overall shape of the system. NMR can be used to study QSLs by measuring the spin-lattice relaxation rate (1/T1) precisely. The system is in a QSL state and, therefore, exhibits the phenomenon of fractionalized excitations. In short, a full electronic excitation is divided into several quasiparticles, and the characteristics of the electron, such as spin and charge, are separated into independent components. In the well-known Kitaev model, which describes spin interactions on a honeycomb lattice theoretically, these excitations are Majorana fermions.

These are special particles in physics that are identical to their antiparticles. NMR is employed to investigate the movement of Majorana fermions, and thus particular low-energy magnetic fluctuations are generated; these fluctuations are subsequently transmitted to the nucleus via hyperfine interaction. Measure how the temperature affects 1/T1 and determine what kind of excitation it is. Recently, using NMR, some scholars have successfully observed the signature of Majorana fermions in a honeycomb lattice [4]. The Size of the magnetic fluctuations can be obtained directly from the NMR relaxation rate. For example, the experimental 1/T1 curve shows a characteristic 'concave shape' with respect to temperature, and this is in good agreement with the theoretical predictions of the pure Kitaev model. It can be seen that the main relaxation path for $Na_2Co_2TeO_6$ is not through traditional phonons or magnons, but via Kitaev fractional excitations (cf. Fig. 2). That is, magnetic fluctuations resulting from Majorana fermions and visons [13].

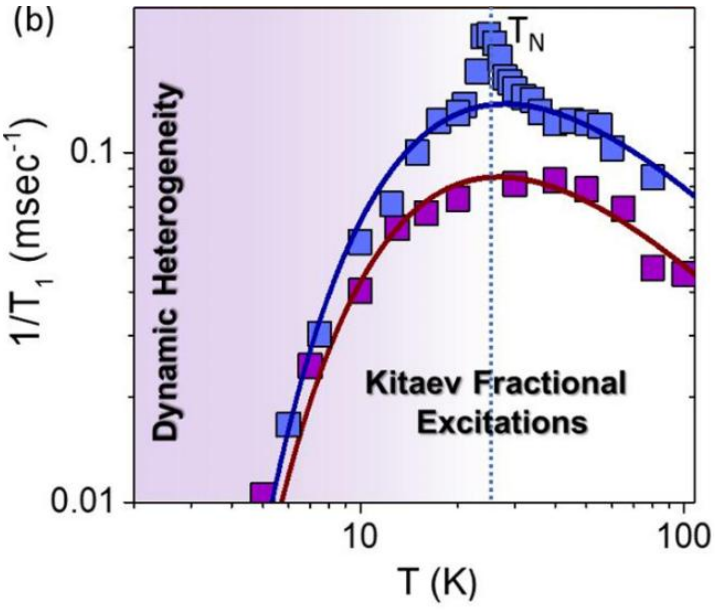

Fig. 2 The relaxation rate $1/T_1$ plotted against temperature in magnetic fields of 4.7 and 9.4 Tesla (blue and purple squares, respectively) [13].

Compared to another mainstream detection method, Inelastic Neutron Scattering (INS)—which calculates energy and momentum changes of neutrons to determine internal vibration frequencies—NMR possesses unique advantages. While neutron scattering provides information in momentum

space, NMR's local-field perspective can directly distinguish whether a system is "gapped" or "gapless." A "gap" refers to the minimum energy threshold required to excite a particle. Determining the existence of an energy gap is a decisive criterion for classifying different topological quantum models. Through this microscopic quantum detection, NMR provides the most direct experimental evidence for verifying complex quantum topological theories [4].

3.3. Quantum Information Processing and Coherent Manipulation

Nuclear spins have extremely weak coupling to their surroundings and are thus suitable for use as qubits. The first NMR quantum computers focused on liquid-state systems, but now most of the current physical research has moved to semiconductor-based spin qubits and hybrid quantum systems. Superconducting qubits and electron spins are employed to carry out high-speed logic operations, and nuclear spins, due to their very long coherence times, function as quantum memory elements. For example, there is a qubit register composed of a SiV electron spin those functions as a communication qubit and a strongly coupled silicon-29 nuclear spin that serves as a memory qubit with a quantum memory time exceeding two seconds [14]. NMR technology is now a high-precision device that can also be used to alter quantum states coherently through hyperfine interactions and is employed in the detection section.

3.4. Future Prospects: Sensitivity Enhancement and Surface Physics

An inherent challenge NMR has long faced is its relatively low sensitivity, which contemporary physics is addressing through cutting-edge methods such as spin hyperpolarization. These techniques increase the population difference between Zeeman levels by several orders of magnitude, making it possible to detect surface and interface physical processes that were previously elusive [5]. This leap in sensitivity opens new pathways for surface physics, enabling the clear characterization of catalytic reaction processes and the physical properties of topological insulator thin films at the molecular level. The former can observe chemical reactions at the reaction site in situ, and by observing changes in the signal of a particular atom (such as Carbon-13 or Hydrogen-1), researchers can see how reactant molecules adsorb onto the catalyst surface and how chemical bonds are broken and formed [15]. The latter are topological insulators; they are insulators in the bulk but conduct on the surface. Their surface currents are special: electrons do not scatter (no energy loss due to collisions) and are therefore very poor conductors of heat. It will help promote the development of new ultra-low-power chips.

4. Conclusion

In short, this paper has introduced the general physical basis of NMR and presented some applications in contemporary science. Through the investigation of the basic reasons for Zeeman splitting and relaxation processes, this paper has determined that NMR is not only a relatively simple spectroscopic technique but also a sophisticated microscopic probe based on the quantum-mechanical coupling of radiofrequency photons and nuclear spins. Relaxation rate and Knight shift analyses can be used to investigate how they serve as dynamic indicators of other quantum phenomena. As shown in the discussion of Strongly Correlated Electron Systems, NMR can provide necessary experimental support for identifying quantum spin liquids and their related fractionalized excitations, such as Majorana Fermions. It is an independent local-field view that can distinguish between gapped and gapless states, and thus reconcile the theoretical model of the Kitaev model with experimental results. In recent years, NMR has begun to explore the active manipulation of quantum coherence, thus emerging as a new field for quantum information technology.

In the future, hyperpolarization techniques will be used to enhance the inherent sensitivity of materials and catalysts for new applications in surface science. NMR can be used to observe topological surface states without scattering loss, and thus will be suitable for building low-dissipation physical devices. With continuous progress in technology, NMR will remain one of the indispensable instruments in condensed matter physics for some time, providing strong support for the development of next-generation quantum memory and ultra-low-power electronic devices.

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