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REZUMATUL TEZEI DE DOCTORAT

Engineering Spin Dynamics through Periodic Modulations: A Floquet-Theoretical Framework for Fast MAS NMR and Spintronics

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1 Introduction and motivation

Physics, when first encountered, often looks like a strange mixture of poetry and bookkeeping. Symbols parade across the page, equations stretch like railway tracks, and somewhere between a Greek letter and an integral sign, the reader begins to suspect that nature might be hiding behind mathematics simply for amusement.

Yet the true charm of physics lies elsewhere. It lies in the realization that complex physical behavior often arises from very simple underlying principles. Spins precess. Fields oscillate. Interactions compete. And from these deceptively modest ingredients arise everything: spectroscopy, magnetic resonance, quantum coherence, spintronics, and the entire technological playground of modern spin-based science.

This thesis lives precisely at that intersection. On one side stands solid-state Nuclear Magnetic Resonance (NMR), a technique born from the gentle wobbling of nuclear spins in magnetic fields, yet capable of revealing molecular structures, dynamics, and interactions with astonishing precision. On the other side stands spintronics, a field where electron spins, rather than charges alone, carry information, opening pathways toward new forms of computation, storage, and coherent control.

Before entering the technical landscape, a modest confession is necessary. The intention of this thesis was not merely to present results, equations, and simulations, but to tell a coherent physical story. Wherever possible, the discussion favors intuition over algebraic intimidation, explanation over formalism, and conceptual clarity over decorative complexity. In writing these pages, I attempted, perhaps recklessly, to construct a document that could be read with genuine curiosity by any ordinary reader possessing basic knowledge of physics. The equations remain essential, of course. Nature stubbornly insists on mathematics. But the mathematics is treated here as a language of explanation rather than an obstacle course. Physics, after all, should illuminate rather than obscure.

The first part of this thesis is devoted to the development of new heteronuclear decoupling pulse sequences for fast Magic-Angle Spinning NMR. Stated in more physical terms, the objective is to engineer methods for weakening the effect of the interactions between nuclear spins, thereby allowing high-resolution solid-state NMR spectra to emerge from what would otherwise be a forest of broadened lines. At its heart, this endeavor reflects one of the most charming paradoxes of magnetic resonance. Nuclear spins, by their very nature, insist on interacting. Dipolar couplings, chemical shift anisotropies, and a host of microscopic forces continuously entangle their motion. Spectral broadening is therefore not an experimental nuisance but a direct manifestation of underlying physics. And yet, a curious possibility arises, which is one of the two main central motivations of this thesis:

If interactions are fundamental, can they nevertheless be persuaded, gently, coherently, and without violence, to average themselves away?

Decoupling pulse sequences represent precisely such persuasion strategies. Rather than eliminating interactions, they orchestrate spin motion so that unwanted couplings cancel through symmetry, modulation, and interference. The spins are not silenced. They are choreographed. In this sense, heteronuclear decoupling becomes less an experimental technique and more an exercise in dynamical engineering. By designing suitable RF irradiation schemes synchronized with rotor motion, one reshapes the effective Hamiltonian experienced by the spins. The spectral lines sharpen not because interactions vanish, but because their observable consequences are carefully rearranged.

The second part of the thesis is a combination of NMR and spintronics, or an exotic application of NMR in spintronics. At first glance, these domains appear unrelated. One studies molecules in rotating rotors, and the other studies electrons in engineered materials. But physics rarely respects such boundaries. Spins remain spins. Hamiltonians remain Hamiltonians. And coherence, wherever it appears, obeys the same fundamental principles. Therefore, a second central motivation of this work is simple:

Can the theoretical language and physical intuition developed in nuclear magnetic resonance be used to understand and engineer coherent dynamics in interacting electron spin systems? Or, stated less formally: *If spins behave so elegantly in NMR, why shouldn't they perform similar dances in spintronics?*

Like any journey through spin dynamics, this thesis starts with an introduction, followed by six chapters, conclusions, and perspectives, proceeds step by step, beginning with foundations before venturing into increasingly rich dynamical regimes.

Every story requires a beginning, and physics insists that the beginning be honest. The first chapter establishes the conceptual and theoretical framework underlying the entire thesis. The fundamental principles of Nuclear Magnetic Resonance are introduced, followed by the essential mechanisms of Magic-Angle Spinning (MAS), spin interactions, density operator formalism, and Floquet theory. Rather than treating Floquet theory as an abstract mathematical construction, it is presented as a natural language for periodically driven quantum systems, which is a perspective that later becomes central for describing coherent spin manipulation beyond traditional NMR. The chapter concludes by extending these ideas toward electron spin dynamics in spintronics, laying the intellectual bridge between spectroscopic physics and driven spin systems.

After a brief introduction, the story enters the laboratory of the real spins and imperfect hardware. Chapter 2 introduces the ROSPAC heteronuclear decoupling pulse sequence, developed for fast MAS solid-state NMR. Both experimental investigations and theoretical analysis are combined to explore how symmetry, rotor synchronization, and phase alternation suppress unwanted effects of the spin interactions. The emphasis lies not only on performance but on mechanisms: understanding why the sequence works, when it works best, and how resonance conditions shape decoupling efficiency.

Exact symmetry is elegant. Slight asymmetry is often more useful. Chapter 3 introduces Slightly Desynchronized Phase-Alternated Cycles (SDPACs), a deliberate relaxation of strict rotor synchronization. Experiments reveal that optimal decoupling is not always achieved at perfect synchronization, while theoretical analysis explains how controlled detuning modifies the effective Hamiltonian. The result is a subtle but powerful lesson: deviations from idealized conditions can become design principles rather than imperfections.

With NMR intuition firmly established, the thesis turns to electron spins. Using a minimal two-spin Ising model, Chapter 4 investigates magnetic-field-driven coherent dynamics under exchange coupling and Dzyaloshinskii–Moriya interaction (DMI). Floquet theory becomes the central analytical tool, revealing how symmetric and antisymmetric interactions reshape spin trajectories. Even the simplest interacting system proves capable of remarkable dynamical richness.

Adding one spin changes everything. The introduction of a third spin, together with open boundary conditions, breaks equivalence and introduces intrinsic asymmetry. Edge-localized effects, nonlinear dynamics, and interaction-driven complexity emerge naturally. Chapter 5 highlights how topology, often treated as a technical detail, becomes an active dynamical parameter.

What if the edges disappear? This is the central question of the last chapter. By imposing periodic boundary conditions, the system transforms into a cyclic, symmetry-preserving network. The dynamics reorganize, collective modes emerge, and chiral interactions become globally distributed. Floquet control landscapes reveal that complexity does not obstruct control. It enriches it.

The reader will encounter equations, simulations, Bloch spheres, Fourier components, and Hamiltonians of various temperaments. Some will behave politely. Others will display stubborn eccentricity. But beneath every calculation lies a unifying theme: Coherent quantum dynamics is shaped by symmetry, interactions, and driving. Moreover, even minimal systems can reveal unexpectedly profound physical behavior. If, along the way, the mathematics occasionally appears intimidating, one may take comfort in a simple truth: the spins themselves do not worry about the equations. They simply obey them. Let us now follow their motion!

"I would rather have questions that can't be answered than answers that can't be questioned." - Richard P. Feynman

2 Scientific context and objectives

2.1 Heteronuclear decoupling under fast MAS

Magic-angle spinning (MAS) efficiently averages spatial anisotropies such as chemical shift anisotropies and dipolar couplings. However, even at spinning frequencies approaching 100-200 kHz, residual heteronuclear dipolar interactions persist. These residual terms arise from incomplete averaging and higher-order cross contributions, leading to line broadening and reduced spectral resolution in solid-state NMR.

Classical heteronuclear decoupling sequences, including TPPM, SPINAL, and related phase-modulated schemes, improve spectral quality but exhibit limitations at ultrafast MAS. Their performance becomes increasingly sensitive to RF inhomogeneity, chemical shift offsets, and resonance conditions that are not fully suppressed by intuitive pulse design. As spinning frequencies increase, the interplay between rotor modulation and RF irradiation becomes more subtle, and empirical optimization alone is insufficient.

These limitations motivate a symmetry-based engineering approach. Rather than relying solely on pulse modulation, decoupling can be treated as a problem of effective Hamiltonian design, where phase alternation, synchronization, and controlled detuning are used to suppress specific Floquet components responsible for residual dipolar couplings.

2.2 Periodic Hamiltonians and Floquet theory

Both MAS and RF irradiation introduce explicit time dependence into the spin Hamiltonian. The system can therefore be described as a periodically driven quantum system satisfying

$$\hat{H}(t) = \hat{H}(t + T)$$

Floquet theory provides a natural framework for analyzing such systems. Instead of following the full time-dependent evolution directly, the dynamics can be recast in terms of an effective time-independent Hamiltonian that governs the stroboscopic evolution over one modulation period. This effective Hamiltonian encodes the net influence of periodic driving, including resonance conditions, interference effects, and higher-order corrections [1, 2, 3, 4, 5, 6, 7].

Within this framework, decoupling efficiency and coherent control can be understood as consequences of constructive or destructive interference between Fourier components of the modulation. The same mathematical structure applies not only to MAS NMR, but also to magnetic-field-driven spintronic systems.

2.3 Spintronic Systems and Driven Spin Dynamics

Spintronics extends the concept of electronics by exploiting not only the charge of the electron but also its spin degree of freedom. Magnetic anisotropy, exchange coupling, and Dzyaloshinskii–Moriya interaction (DMI) govern the behavior of nanoscale magnetic systems, including magnetic tunnel junctions and chiral magnetic textures [8].

At the microscopic level, the dynamics of localized spins in such systems are often described by effective Hamiltonians structurally similar to those encountered in magnetic resonance. When external magnetic fields or microwave driving are applied, the resulting dynamics become explicitly time-periodic. Consequently, coherent manipulation of spin states in spintronic devices can be interpreted within the same Floquet framework traditionally used in NMR.

This structural analogy provides a powerful conceptual bridge. While solid-state NMR seeks to suppress unwanted interactions to obtain high-resolution spectra, spintronics often seeks to exploit interactions such as exchange and DMI to generate nontrivial magnetic states. In both cases, however, the central problem is identical: how to engineer and control the effective Hamiltonian governing spin motion.

2.4 Objectives of the thesis

The central objective of this thesis is to demonstrate that periodic modulation can be systematically engineered to control spin interactions in both spectroscopic and spintronic contexts. The specific goals are:

- To design and experimentally validate improved heteronuclear decoupling sequences for fast MAS solid-state NMR.
- To provide a rigorous operator-based Floquet analysis of these sequences, identifying the symmetry principles governing their performance.
- To transfer the theoretical machinery developed in NMR to interacting electron spin models, establishing a conceptual bridge between high-resolution spectroscopy and coherent spin manipulation in spintronic systems.

3 Theoretical framework

3.1 Spin Hamiltonian structure

The systems investigated in this thesis belong to the broader class of periodically driven spin Hamiltonians, although their microscopic origin differs between solid-state NMR and spintronic model systems.

In the context of MAS NMR, the Hamiltonian contains static Zeeman terms together with anisotropic interactions modulated by sample rotation and RF irradiation:

$$\hat{H}_{\mathrm{NMR}}(t) = \hat{H}_Z + \hat{H}_{CSA} + \hat{H}_{dip} + \hat{H}_{RF}$$

where $\hat{H}_Z$ denotes the Zeeman interaction, $\hat{H}_{CSA}$ and $\hat{H}_{dip}$ represent anisotropic interactions modulated by magic-angle spinning, and $\hat{H}_{RF}$ describes the interaction of the spin system with the oscillating magnetic field [9, 10].

In contrast, the spintronic models considered here are based on interacting spin chains driven by magnetic fields. Their Hamiltonian takes the form

$$\hat{H}_{\mathrm{spin}}(t) = \hat{H}_Z + \hat{H}_J + \hat{H}_{DMI} + \hat{H}_{RF}$$

where $\hat{H}_J$ represents isotropic exchange coupling, $\hat{H}_{DMI}$, the antisymmetric Dzyaloshinskii–Moriya interaction, and $\hat{H}_{RF}$ represent the interaction between the spin system and the externally applied oscillating magnetic field.

Despite their different physical origins, both classes of systems share a common structural feature: the Hamiltonian is explicitly time-periodic. Whether the modulation is generated mechanically (MAS), electronically (RF pulse sequences), or magnetically (driven spin chains), the resulting dynamics can be treated within a unified Floquet framework.

3.2 Operator-Based Floquet formalism

For periodically driven systems, the Floquet theory provides a rigorous framework for analyzing the resulting dynamics. The time-dependent Schrödinger equation can be recast in an extended Hilbert space, leading to the Floquet operator

$$\hat{H}_F = \hat{H}(t) - i\hbar\frac{\partial}{\partial t}.$$

Within this formalism, the Hamiltonian is expanded in Fourier components, and the dynamics are represented in a composite spin–Fourier space. Each Fourier index corresponds to a modulation, allowing systematic identification of resonance conditions and interaction pathways.

Rather than tracking the full-time evolution explicitly, the dynamics can be described through an effective time-independent Hamiltonian that governs the evolution over one modulation period. This effective Hamiltonian incorporates higher-order corrections arising from interference between Fourier components and provides direct access to the mechanisms responsible for averaging, enhancement, or reintroduction of spin interactions.

3.3 Effective Hamiltonians and control landscapes

The structure of the effective Hamiltonian is determined by resonance conditions of the form

$$n\omega_r + k\omega_m + l\omega_{\text{eff}} = 0,$$

where ω_r denotes the rotor frequency, ω_m the modulation frequency, and ω_{eff} the effective field.

Cross terms arising from combinations of spatial and RF modulations generate residual interactions that limit decoupling efficiency. Their magnitude can be quantified through logarithmic maps of the corresponding Fourier coefficients. These maps define control landscapes in parameter space (RF amplitude, offset, pulse spacing), identifying regions where destructive interference suppresses unwanted terms.

Symmetry plays a central role in this suppression. Rotor synchronization, phase alternation, and controlled detuning modify the selection rules governing allowed Fourier pathways. By engineering these symmetry properties, specific cross terms can be minimized or eliminated, thereby improving decoupling performance or enabling controlled coherent spin manipulation.

The same Floquet-based strategy applies beyond NMR spectroscopy. In interacting spin models, periodic driving reshapes the effective Hamiltonian in an analogous manner, demonstrating that MAS, pulse sequencing, and magnetic-field-driven spintronics are unified under a common theoretical framework of periodically driven quantum systems.

Part I: Heteronuclear decoupling pulse sequences design for fast MAS NMR

A significant part of my PhD years' work was devoted to experimental investigations of complex materials using solid-state Nuclear Magnetic Resonance (ss-NMR), understanding of NMR technique limitations, and fixing a part of these shortcomings. During the course of the PhD, I applied ss-NMR to characterize a variety of complex materials, ranging from archaeological ceramics and pharmaceutical compounds to polymer–biomolecule complexes and nanostructured inorganic materials. These studies demonstrated the unique capability of ss-NMR to probe local atomic environments in systems where conventional crystallographic techniques are often limited, particularly in the presence of structural disorder or amorphous phases.

For instance, ss-NMR methods were employed to investigate the structural features of archaeological ceramics from several Romanian sites, revealing variations in aluminum coordination and silicate network polymerization that reflect differences in ancient manufacturing technologies and firing conditions [11]. In parallel, ss-NMR spectroscopy contributed to the structural elucidation of biologically active aminonaphthoquinone derivatives with promising antitumor and antibacterial activity, providing insights into molecular packing and heterogeneity in the solid state [12]. Similar approaches were applied to the characterization of newly synthesized molecular complexes based on chitosan and thiamine hydrochloride, where ss-NMR confirmed the formation of new supramolecular structures following mechanochemical processing [13]. Further experimental work involved the investigation of functional materials such as silibinin fatty acid conjugates designed as potential prodrugs [14], as well as nanostructured silica–alumina core–shell systems containing paramagnetic gadolinium ions. In these systems, ss-NMR proved particularly sensitive to local structural modifications and magnetic interactions that arise from ion incorporation and interfacial diffusion processes [15]. Additional studies focused on the atomic-scale structure of polydopamine films and precipitates, where advanced ss-NMR techniques enabled the identification of structural differences between bulk material and ultra-thin coatings down to nanometer thicknesses [16].

While these experimental applications illustrate the versatility of solid-state NMR as a structural probe across diverse fields, they also highlight one of the fundamental challenges of the technique: the presence of strong anisotropic interactions that broaden spectral lines in solids. Among these interactions, heteronuclear dipolar couplings often represent a major limitation for achieving high spectral resolution. Magic-angle spinning (MAS) reduces a large part of this anisotropy, yet under fast MAS conditions additional radio-frequency pulse sequences are typically required to efficiently suppress the residual dipolar interactions.

Motivated by this challenge, a substantial part of the present work was dedicated to the theoretical design and analysis of improved heteronuclear decoupling sequences for fast MAS NMR. In particular, two novel pulse schemes were developed and investigated using a combination of Floquet theory and effective Hamiltonian analysis. The first sequence, termed *Rotor-Synchronized Phase-Alternated Cycles* (ROSPAC), exploits rotor synchronization and phase alternation to achieve enhanced cancellation of dipolar cross terms. The second sequence, *Slightly Desynchronized Phase-Alternated Cycles* (SDPACs), introduces controlled detuning from strict rotor synchronization, allowing additional suppression pathways for residual interactions (Figure 1).

The theoretical principles underlying these sequences, together with their performance and limitations under fast MAS conditions, constitute the central topic of the first part of this thesis. The physical design principles, Floquet-space analysis, and experimental validation of the ROSPAC and SDPACs heteronuclear decoupling schemes are presented in detail.

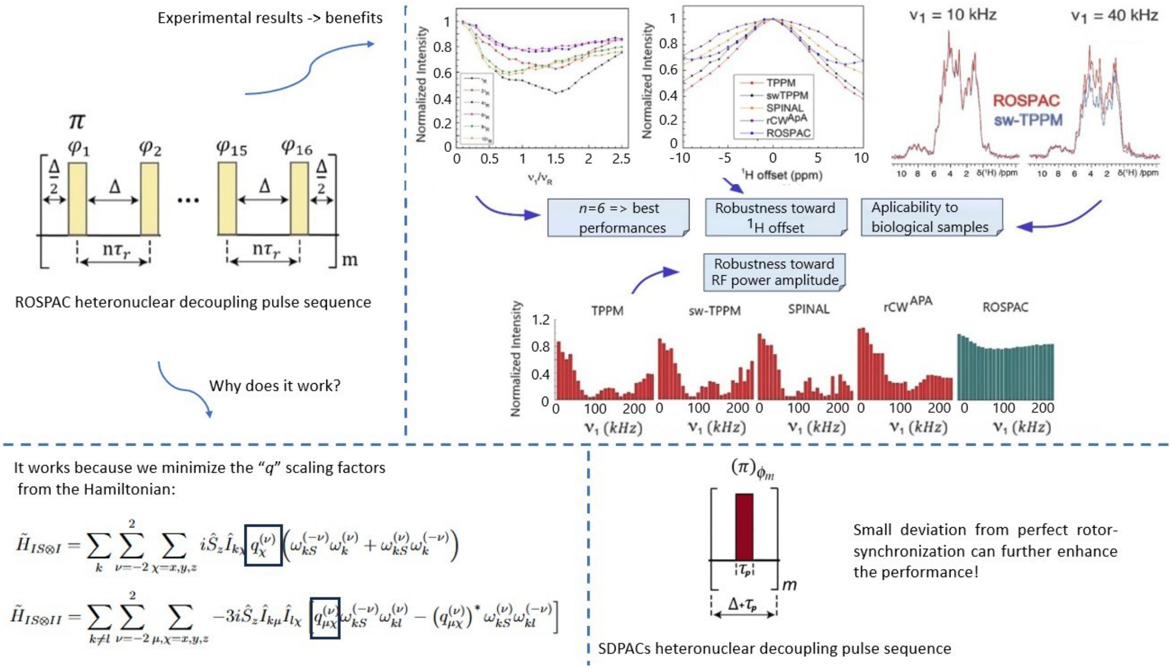


Figure 1. Schematic representation of the ROSPAC and SDPACs heteronuclear decoupling pulse sequences together with a part of the obtained results for the ROSPAC sequence

4 ROSPAC heteronuclear decoupling

4.1 Physical design principles

The Rotor-Synchronized Phase-Alternated Cycles (ROSPAC) sequence [17] was developed to address residual heteronuclear dipolar couplings under fast MAS conditions. The design is based on three core principles: rotor synchronization, controlled phase alternation, and symmetry-driven cancellation of unwanted effective Hamiltonian terms.

Rotor synchronization ensures that the interpulse spacing matches an integer multiple of the rotor period, enforcing a well-defined periodicity in the combined MAS–RF modulation. Phase alternation introduces controlled sign changes in successive π pulses, modifying the selection rules of the Fourier components in Floquet space. Together, these elements impose symmetry constraints that suppress specific cross terms responsible for incomplete dipolar averaging.

Rather than relying on empirical optimization alone, ROSPAC was constructed as an effective Hamiltonian engineering problem, where modulation symmetry is deliberately used to cancel residual interaction pathways.

4.2 Effective Hamiltonian analysis

Within the operator-based Floquet formalism, the decoupling efficiency can be quantified by analyzing second-order cross terms of the type $q^{(\nu)}_{IS\otimes I}$ and $q^{(\nu)}_{IS\otimes II}$ which arise from combined spatial and RF modulation pathways. These terms contribute directly to residual heteronuclear dipolar broadening. The Floquet expansion reveals that their magnitude is governed by resonance conditions of the form $n\omega_r + k\omega_m = 0$, where ω_r is the rotor frequency and ω_m the modulation frequency associated with the pulse sequence. By enforcing strict rotor synchronization and applying alternating phases, the Fourier coefficients corresponding to dominant cross terms are strongly attenuated. Logarithmic mapping of these terms as a function of RF nutation frequency and chemical shift offset identifies operating regions where destructive interference minimizes their contribution to the effective Hamiltonian. This analysis provides a quantitative explanation for the observed improvement in decoupling performance [18].

4.3 Experimental validation

The theoretical predictions were validated experimentally at MAS frequencies up to 100 kHz. Measurements of normalized signal intensity as a function of ^{1}H chemical shift offset demonstrated reduced offset sensitivity compared to conventional phase-modulated sequences such as TPPM and SPINAL.

The dependence of decoupling efficiency on MAS frequency and RF nutation amplitude confirmed the predicted resonance behavior. Across a broad parameter range, ROSPAC maintained higher signal intensity and improved robustness with respect to RF field inhomogeneity. These observations are consistent with the Floquet-based suppression of dominant cross terms.

4.4 Performance assessment

ROSPAC provides enhanced performance in fast MAS regimes where classical sequences become increasingly sensitive to offset and power miscalibration. The sequence demonstrates improved stability against RF inhomogeneity and retains efficiency over-extended offset ranges.

Its limitations arise in regimes where higher-order resonance conditions become dominant or when RF amplitudes deviate substantially from nominal values. Nevertheless, the results establish ROSPAC as a symmetry-engineered alternative to traditional phase-modulated decoupling schemes and provide a clear framework for further sequence optimization based on effective Hamiltonian analysis.

5 SDPACs: controlled desynchronization

5.1 Motivation

While rotor synchronization provides a powerful symmetry constraint, analysis of the Floquet spectra revealed that strict synchronization does not always minimize higher-order cross terms. In certain regimes, exact matching between the interpulse spacing and the rotor period places the system close to residual resonance conditions. This observation motivated the exploration of controlled desynchronization as a deliberate design parameter rather than an experimental imperfection.

5.2 Sequence structure

The Slightly Desynchronized Phase-Alternated Cycles (SDPACs) sequence [19] retains the phase-alternation pattern of ROSPAC but introduces a controlled detuning between the π-pulse spacing and the rotor period. The interpulse delay is written as

$$\Delta + \tau_p \neq n\tau_r,$$

where Δ is adjusted according to the MAS frequency and RF nutation amplitude. This slight detuning modifies the temporal symmetry of the combined MAS–RF modulation without breaking periodicity.

5.3 Floquet interpretation

Within the Floquet framework, desynchronization shifts the location of dominant Fourier components in frequency space. This alters the effective resonance conditions and reduces the magnitude of second-order cross terms contributing to residual dipolar couplings. In contrast to strict synchronization, where specific modulation pathways may constructively interfere, controlled detuning redistributes spectral weight and suppresses near-resonant contributions. Thus, SDPACs demonstrate that optimal decoupling can arise from carefully engineered asymmetry.

5.4 Experimental optimization rule

Experimental investigations at 100 kHz MAS identified a simple empirical relation linking the optimal interpulse delay to the RF nutation frequency:

$$\Delta = 8 \times \mathrm{round}\left(\frac{2\nu_r}{\nu_1}\right),$$

where ν_r is the MAS frequency and ν_1 the RF amplitude. This rule provides a practical guideline for sequence tuning under ultrafast MAS conditions.

5.5 Comparison with ROSPAC

Compared to ROSPAC, SDPACs exhibit improved performance in parameter regions where strict rotor synchronization approaches residual resonance conditions. Enhanced offset tolerance and increased robustness toward RF inhomogeneity were observed for selected RF amplitudes.

Together, ROSPAC and SDPACs establish a broader design principle: both symmetry and controlled symmetry breaking can be exploited to engineer the effective Hamiltonian in fast MAS decoupling.

Part II: NMR-based theory methods development for coherent electron spin manipulation in spintronic applications

The theoretical tools developed within nuclear magnetic resonance are not limited to spectroscopy alone. Over the decades, NMR has also provided a remarkably rich framework for understanding the dynamics of interacting spin systems under periodic driving. Many of the concepts routinely used in magnetic resonance—such as effective Hamiltonians, rotating frames, and Floquet representations—are, in fact, general tools for describing time-dependent quantum systems. This observation naturally raises an intriguing question: can the theoretical machinery developed in NMR be transferred to other fields where spin dynamics plays a central role?

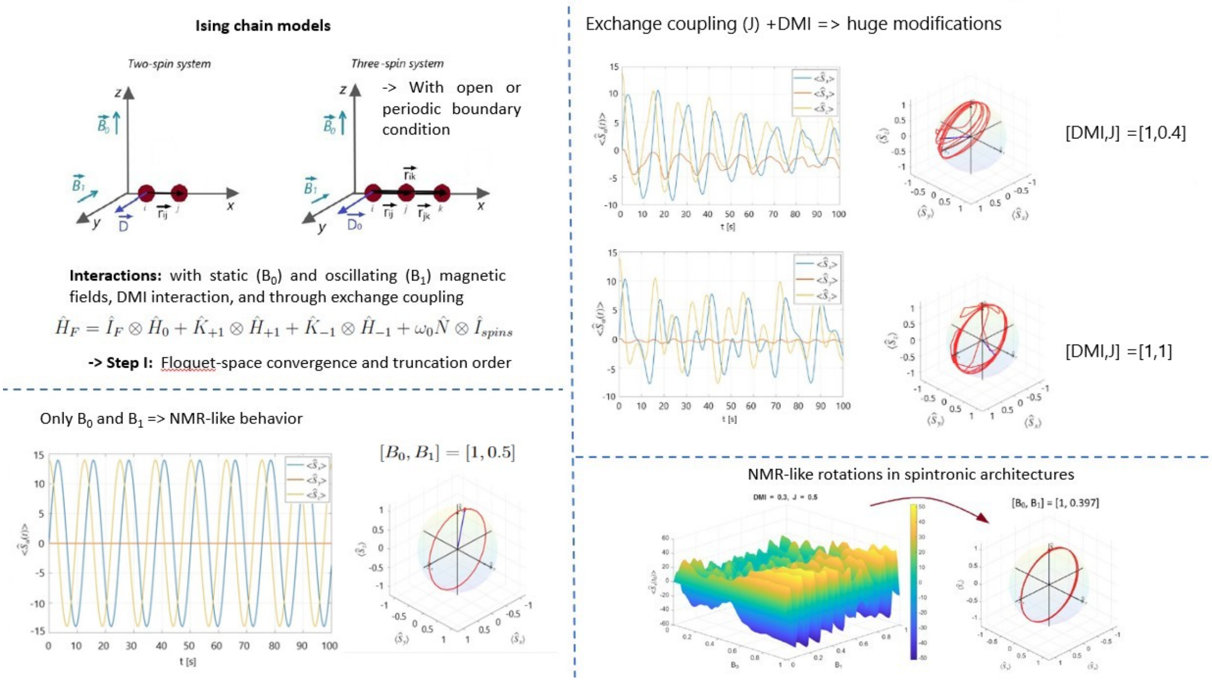
One such field is spintronics, where the control and manipulation of spin degrees of freedom forms the basis of emerging technologies. In contrast to conventional electronics, which relies on the charge of the electron, spintronics exploits the electron's spin and its associated magnetic moment to encode and process information. Understanding how spins interact, evolve under external fields, and respond to periodic driving is therefore essential for describing a wide class of spintronic systems.

From a theoretical perspective, many spintronic models share structural similarities with the spin Hamiltonians encountered in magnetic resonance. Exchange interactions, anisotropic couplings, and external magnetic fields all contribute to the collective dynamics of spins. When these systems are subjected to time-dependent driving fields, their behavior can often be described by periodically modulated Hamiltonians. In such cases, Floquet theory provides a natural framework for analyzing the resulting dynamics by transforming the explicitly time-dependent problem into an equivalent time-independent representation in an extended Hilbert–Floquet space.

Motivated by these parallels, the second part of this thesis explores how the theoretical formalism commonly used in NMR can be applied to driven spin systems relevant to spintronics. The central objective is to investigate how periodic driving and spin–spin interactions jointly shape the dynamics of small spin networks. Particular attention is given to minimal models that capture the essential physical mechanisms while remaining sufficiently simple to allow detailed theoretical analysis.

The study begins with the investigation of a two-spin Ising-type system subjected to periodic magnetic driving. Within this minimal model, the influence of isotropic exchange coupling and Dzyaloshinskii–Moriya interactions on the coherent evolution of the spins is analyzed using an operator-based Floquet formalism. The analysis is then extended to three-spin chains, where the role of system topology becomes particularly important. By comparing systems with open boundary conditions and periodic boundary conditions, it becomes possible to isolate the effects of boundary-induced asymmetry and symmetry restoration on the resulting spin dynamics.

Beyond the analysis of the intrinsic dynamics, the Floquet framework also allows the construction of control landscapes that reveal how external driving parameters can be tuned to engineer specific spin transformations. These results illustrate how periodic modulation can be used not only to understand the behavior of interacting spin systems, but also to manipulate their collective dynamics in a controlled manner (Figure 2).



Interactions: with static (B_0) and oscillating (B_1) magnetic fields, DMI interaction, and through exchange coupling

$$\hat{H}_F = \hat{I}_F \otimes \hat{H}_0 + \hat{K}_{+1} \otimes \hat{H}_{+1} + \hat{K}_{-1} \otimes \hat{H}_{-1} + \omega_0 \hat{N} \otimes \hat{I}_{spins}$$

-> Step I: Floquet-space convergence and truncation order

Figure 2. Schematic representation of the Ising chain models and the results obtained for the two-spin system when only the magnetic fields or the magnetic fields, exchange coupling, and DMI are considered, and demonstration of the NMR-like rotation for a particular case obtained for a three-spin system with OBC

The chapters that follow, therefore, aim to demonstrate that the theoretical language of magnetic resonance—originally developed to describe nuclear spins in spectroscopic experiments—can also provide valuable insight into the dynamics of driven spin systems encountered in spintronics. In this sense, the second part of the thesis represents a conceptual bridge between two domains of spin physics: the methodology of NMR and the emerging landscape of spin-based technologies.

6 Magnetic Field–Driven Spin Coherence under Dzyaloshinskii Moriya Interaction in a two-spin system Ising Chain model

6.1 Model Hamiltonian

To transfer the theoretical machinery of NMR to spintronic systems, a minimal two-spin Ising chain was considered under magnetic-field driving. The Hamiltonian is written as

$$\hat{H}(t) = \hat{H}_Z + \hat{H}_J + \hat{H}_{DMI} + \hat{H}_{RF},$$

where $\hat{H}_Z$ represents the static Zeeman term, $\hat{H}_J$ the isotropic exchange coupling, $\hat{H}_{DMI}$ the antisymmetric Dzyaloshinskii–Moriya interaction, and $\hat{H}_{RF}$ describes the interaction of the spin system with the oscillating magnetic field. The system, therefore, constitutes a periodically driven, interacting quantum model directly amenable to Floquet analysis.

6.2 Floquet convergence analysis

The Floquet Hamiltonian is formally infinite-dimensional, reflecting the fact that a time-periodic system contains, in principle, infinitely many Fourier harmonics. In practical calculations, this space must be truncated, and numerical convergence must be verified to ensure physical reliability.

Convergence was tested by increasing the Floquet truncation order m for a strongly interacting two-spin system ($B_0 = 1$, $B_1 = 0.5$, $J = 1$, and DMI $= 1$). At low truncation order ($m = 1$), the dynamics exhibit distortions, indicating incomplete representation of relevant frequency components. As m increases, the spin expectation values and Bloch-sphere trajectories stabilize, and for $m \geq 4$ the results become indistinguishable.

This confirms that a finite subset of Fourier modes governs the physically relevant dynamics. In the considered parameter regime, a truncation order of $m = 3$ is sufficient for subsequent simulations.

6.3 Role of Exchange and DMI

In the absence of interactions, the driven two-spin system exhibits regular, geometrically simple precessional dynamics. After introducing exchange coupling, the rotating-frame evolution for $J = 0$ and $J = 1$, with fixed driving parameters $[B_0, B_1] = [1, 0.5]$ and DMI $= 0$ was compared. Surprisingly, no qualitative differences are observed. The oscillation amplitudes, frequencies, and phase relations remain unchanged, and the Bloch-sphere trajectories coincide in both cases. This apparent insensitivity is explained by symmetry. The isotropic exchange Hamiltonian preserves rotational invariance and commutes with the collective spin operators under the chosen driving configuration. Consequently, although exchange modifies the microscopic energy structure, it does not generate new dynamical components in the measured collective expectation values.

In contrast, the Dzyaloshinskii–Moriya interaction introduces chirality into the system. Its antisymmetric structure produces asymmetric spin trajectories and multi-frequency components in the Floquet spectrum. The resulting motion becomes more structured, reflecting interference between symmetric (exchange) and antisymmetric (DMI) interaction pathways.

Despite this increased complexity, the dynamics remain bounded and deterministic across a broad parameter range. The two-spin model therefore provides a controlled theoretical foundation for understanding how competing interactions reshape periodically driven spin motion before extending the analysis to larger and topologically distinct systems [20].

7 Three-Spin Chain with Open Boundary Conditions

7.1 Edge-Induced Asymmetry

Extending the model to three spins with open boundary conditions introduces a fundamental change in symmetry. Unlike the two-spin system, the spins are no longer equivalent: the edge spins interact with only one neighbor, while the central spin couples to both. This loss of translational invariance generates intrinsic asymmetry in the energy landscape and modifies the collective response to external driving.

The topology of the chain, therefore, becomes a dynamical parameter. Even in the absence of additional interactions, the inequivalence between edge and central spins alters the redistribution of polarization and breaks the simple geometric structure observed in smaller systems.

7.2 Nonlinear Dynamics

When exchange coupling and Dzyaloshinskii–Moriya interaction are simultaneously present, their competition produces nonlinear collective behavior. Exchange favors symmetric polarization sharing, while DMI introduces chirality and antisymmetric coupling pathways.

The resulting dynamics exhibit multi-frequency motion, with interference between different interaction channels generating structured, time-dependent modulation of the spin expectation values. In contrast to the two-spin case, interactions now become dynamically visible. The collective magnetization no longer follows a simple circular trajectory but develops deformation and frequency mixing characteristic of nonlinear spin dynamics.

7.3 Floquet Control Landscapes

Despite the increased complexity, coherent control remains achievable. By mapping the transverse spin component as a function of driving parameters (B_0, B_1), Floquet control landscapes were constructed. These maps reveal structured regions where large transverse magnetization is generated after a fixed evolution time.

Selected points from these landscapes correspond to deterministic longitudinal-to-transverse rotations, analogous to $\pi/2$ rotations in NMR. Thus, even in the presence of edge-induced asymmetry and competing interactions, periodic driving enables controlled steering of collective spin polarization [20].

8 Three-Spin Chain with Periodic Boundary Conditions

8.1 Restored Symmetry

Imposing periodic boundary conditions reconnects the ends of the chain, transforming the linear three-spin system into a closed ring. In this cyclic topology, each spin interacts identically with two neighbors, restoring translational symmetry and eliminating edge-induced inequivalence.

Unlike the open chain, no spin occupies a privileged or reduced interaction environment. The Hamiltonian becomes invariant under cyclic permutation of spin indices, and topology ceases to generate intrinsic asymmetry. The system, therefore, transitions from a boundary-driven structure to a symmetry-governed network.

8.2 Collective Modes

Within this symmetric topology, the driven dynamics reorganize into collective modes. The spin expectation values evolve in a globally coherent manner, reflecting synchronized motion of the entire spin network.

Even in the presence of exchange coupling and Dzyaloshinskii–Moriya interaction, the cyclic symmetry constrains the redistribution of polarization. Chirality and multi-frequency effects persist, but they are distributed uniformly across the system rather than localized near boundaries. The Bloch-sphere trajectories remain structured and globally organized, illustrating symmetry-disciplined nonlinear dynamics.

8.3 Comparison: OBC vs PBC

The contrast between open and periodic boundary conditions reveals the decisive role of topology in interacting spin systems.

Under OBC, boundary-induced asymmetry amplifies nonlinear effects, produces inequivalent spin responses, and enhances trajectory distortion. Under PBC, restored symmetry redistributes complexity into collective modes and suppresses the localization of dynamical irregularities.

Thus, while the microscopic interactions remain formally similar, the macroscopic dynamics are fundamentally topology-dependent. Open chains generate asymmetry-driven dynamics. Cyclic chains produce symmetry-governed coherence. The comparison demonstrates that topology acts as an active control parameter in Floquet-driven many-body systems [20].

9 General Conclusions

9.1 Unified Perspective

Although the physical systems investigated in this thesis span solid-state NMR and driven spin models inspired by spintronics, a unifying conceptual framework emerges naturally: all problems addressed here are instances of periodic Hamiltonian engineering.

Magic-angle spinning (MAS) introduces mechanical modulation of anisotropic spin interactions through sample rotation. Radio-frequency (RF) irradiation generates controlled time-periodic transverse fields. Magnetic-field driving in spin chains produces coherent time-dependent evolution under externally imposed modulation. In all cases, the resulting dynamics are governed not only by static energy scales, but by the structured interference of the Fourier components in Floquet space.

From this perspective, MAS is not merely a technical tool for line narrowing, RF pulses are not merely experimental operations, and magnetic driving is not merely excitation. They are mechanisms for reshaping effective Hamiltonians. The apparent diversity of phenomena reduces to a single theoretical principle: coherent dynamics can be sculpted by engineering time periodicity.

This unified viewpoint enables direct conceptual transfer between high-resolution NMR methodology and interacting spin models. The same Floquet formalism that predicts suppression of heteronuclear dipolar couplings under fast MAS also describes chirality-induced nonlinear motion in three-spin Ising systems. The mathematical language remains unchanged. Only the physical interpretation evolves.

9.2 Original contributions

The main original contributions of this thesis can be summarized as follows:

1. **Development of the ROSPAC heteronuclear decoupling sequence.** A symmetry-based rotor-synchronized phase-alternated scheme was designed and analyzed using operator-based Floquet theory. Resonance conditions responsible for second-order cross terms were explicitly identified and suppressed. Experimental validation demonstrated improved robustness under fast MAS conditions.

2. **Introduction of SDPACs (Slightly Desynchronized Phase-Alternated Cycles).** A controlled detuning strategy was proposed, demonstrating that strict rotor synchronization is not universally optimal. A systematic relation between interpulse delay Δ and RF nutation frequency was established, enabling enhanced decoupling efficiency in high-frequency MAS regimes.

3. **Rigorous Floquet-space convergence analysis.** A structured truncation strategy was implemented and validated, demonstrating that physically relevant dynamics are governed by a finite subset of Fourier components. This analysis established methodological reliability for both NMR and spin-chain simulations.

4. **Floquet engineering of interacting two-spin and three-spin Ising models.** Exchange coupling and Dzyaloshinskii–Moriya interaction were analyzed within a periodically driven framework. It was shown that isotropic exchange alone remains dynamically silent under symmetry-protected conditions, whereas DMI introduces chirality-driven multi-frequency motion.

5. **Topology-dependent nonlinear dynamics.** A direct comparison between open and periodic boundary conditions demonstrated that topology acts as an active dynamical parameter. Open chains exhibit edge-induced asymmetry and enhanced nonlinear effects, while periodic chains redistribute complexity into symmetry-governed collective modes.

6. **Construction of Floquet control landscapes.** Global parameter-space maps were generated to identify driving conditions producing deterministic transverse spin rotations. The results establish a bridge between NMR pulse design and Floquet engineering of interacting spin systems.

7. **Conceptual transfer between NMR theory and spintronics.** The thesis demonstrates that theoretical tools developed for high-resolution solid-state NMR can be successfully extended to model and control coherent spin dynamics in interacting quantum systems relevant to spintronics.

Taken together, these contributions demonstrate that time-periodic control is not an auxiliary feature of spin physics, but a central organizing principle. From MAS rotors to RF phase alternation, from decoupling sequences to chiral spin chains, coherent dynamics can be understood, predicted, and engineered within a single unified Floquet framework.

10 Perspectives and Future Directions

The results presented in this thesis open up several promising and natural research directions, both at the experimental and theoretical levels.

- **MAS beyond 200 kHz.** Current state-of-the-art MAS technology allows spinning frequencies approaching 200 kHz using ultra-small rotors ($\sim$0.4 mm diameter). Further increases of the spinning frequency would enhance suppression of chemical shift anisotropy and dipolar interactions, pushing solid-state NMR toward liquid-like resolution. However, mechanical stability, sample volume, and fundamental constraints related to rotor size and acoustic limits pose significant challenges. Future developments in materials, rotor engineering, and pulse sequences design could redefine the practical limits of ultrafast MAS.

- **Extension to larger spin networks.** The three-spin models analyzed here represent minimal interacting systems. A natural extension involves larger spin chains and two-dimensional lattices, where topology, frustration, and collective modes become increasingly rich. Scaling Floquet-based approaches to larger Hilbert spaces will require advanced numerical strategies, but offers direct access to genuine many-body phenomena.

- **Application to skyrmionic and chiral systems.** The interplay between exchange coupling and Dzyaloshinskii–Moriya interaction explored in small spin chains provides a conceptual foundation for studying chiral magnetic textures such as skyrmions. Floquet engineering may offer routes to dynamically stabilize, manipulate, or reshape topologically non-trivial spin configurations in nanoscale systems.

- **Quantum control strategies in interacting systems.** The construction of Floquet control landscapes demonstrates that nonlinear interacting dynamics remain controllable. Future work may combine optimal control theory, machine-learning-assisted pulse design, and symmetry-based Hamiltonian engineering to achieve targeted transformations in strongly coupled spin networks.

Overall, the central message for future research is clear: time-periodic modulation is not merely a perturbation, but a powerful design principle. By combining mechanical rotation, RF engineering, and interaction control, it becomes possible to navigate complex spin dynamics in a structured and predictable manner.

The frontier, therefore, lies not only in pushing experimental limits, but in deepening the theoretical framework that allows coherent many-body motion to be engineered rather than merely observed.

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1. A. Simion, C. Filip, and C. Tiusan, "From Approximate Floquet Engineering to Full Floquet Theory: Coherent Control of Chiral Spin Systems in Spintronics", Phys. Rev. B, submitted manuscript, 2026. (IF=3.7, AIS=0.878)

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4. R. G. Stroia, M. Vasilescu, S. M. Cursaru Herlea, A. M. R. Gherman, L. Barbu-Tudoran, T. Tămaș, R. Hirian, C. Filip, and A. Simion, "Structural characterization of ceramic artifacts from three archaeological sites in Romania – an original approach by using various Nuclear Magnetic Resonance techniques", J. Cult. Herit., submitted manuscript, 2026. (IF=3.3, AIS=0.597)

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Conferences: oral contributions

1. Invited speaker, The Central European NMR Symposium & Bruker Users Meeting, Solid-State NMR Workshop (CEUM), 13-15 September 2023, Prague, Czech Republic. Presentation title: "Heteronuclear decoupling sequences for fast MAS NMR – from theory to applications"

Conferences: poster contributions

1. The 19th European Magnetic Resonance Congress 09 - 13 July 2023, Glasgow, Scotland, "Heteronuclear decoupling for fast MAS NMR: robustness toward ^{1}H offset, RF field irradiation and RF field inhomogeneity", A. Simion, M. Ernst, and C. Filip.

2. The 21th European Magnetic Resonance Congress 6-10 July 2025, Oulu, Finland, "Polarization transfer efficiency under spinning frequencies up to 150 kHz – an experimental approach", A. Simion, T. Franks, S. P. Brown, and C. Filip.

3. The 21th European Magnetic Resonance Congress 6-10 July 2025, Oulu, Finland, "New insights into Romanian archeological ceramics investigated by solid-state NMR spectroscopy", R. G. Stroia, M. Vasilescu, S. M. Cursaru Herlea, A. M. R. Gherman, L. Barbu, C. Filip, and A. Simion.

4. PIM 2025 International Conference, 16-19 September 2025, Cluj-Napoca, Romania, "Polarization transfer efficiency in solid state NMR at spinning frequencies up to 150 kHz", A. Simion, T. Franks, S. P. Brown, and C. Filip.

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7. PIM 2023 International Conference, 19-22 September 2023, Cluj-Napoca, Romania, "Cross-polarization under fast MAS NMR: from spin dynamics to experimental methods", A. Simion and C. Filip.

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Scientific papers

1. A.S. Farcasanu, M. Todea, M. Muresan-Pop, D.M. Petrisor, A. Simion, A. Vulpoi, and S. Simon, "Synthesis and structural characterization of silica particles doped with Dy and Gd paramagnetic ions as MRI contrast agents", Result Chem. 4, 100520, 2022, `https://doi.org/10.1016/j.rechem.2022.100520`. (IF=2.3, AIS=0.283)

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1. Zakopane Ampere NMR School, 19-25 June 2022, Zakopane, Poland, "Heteronuclear decoupling for ultra-fast MAS: Robustness toward ^{1}H offset and radio-frequency power", A. Simion, M. Ernst, and C. Filip.

2. PIM 2021 International Conference, 22-24 September 2021, Cluj-Napoca, Romania, "Structural changes in nanostructured silica core-alumina shell microspheres doped with iron and gadolinium investigated by Solid- State NMR Spectroscopy ", A. Simion, M. Vasilescu, M. Todea, M. Mureșan- Pop, A. Vulpoi, and S. Simon.