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Magnon-electron scattering and non-Landau magnon decay, *ab initio* theories

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The highest activity a human being can attain is learning for understanding, because to understand is to be free.

Baruch Spinoza (1632 – 1677)

Wir müssen wissen, wir werden wissen.

David Hilbert (1862 – 1943)

Men wanted for hazardous journey. Low wages, bitter cold, long hours of complete darkness. Safe return doubtful. Honour and recognition in event of success.

Ernest Shackleton (1874 – 1922), apocryphal

Contents

Abstract

This habilitation treatise is concerned with the description of the spin dynamics in solids using linear response time-dependent density functional theory going beyond the ferromagnetic spin waves. First, the application of the method to ferri- and antiferromagnets is presented. Following this, the studies of paramagnons and longitudinal spin excitations are outlined. Following this, the non-Landau magnon decay channels, in particular disorder and multi-magnon processes, are assessed in order to establish the hierarchy of the spin dynamics attenuation in itinerant magnets. In the second part, the theory of magnon-electron interaction based on the time-dependent density functional theory is exposed and applied to several relevant magnetic systems. This interaction leads to a range of measurable and important phenomena, including band structure renormalization, the emergence of non-quasiparticle states, the unconventional superconducting pairing, and the impact on the spin dynamics itself, which are addressed from an *ab initio* perspective.

1. Context and motivation

This cumulative habilitation treatise summarizes author's scientific output following his doctorate with a particular focus on the *ab initio* description of the spin dynamics and magnon-electron interaction in solids. This introductory chapter provides the motivation for his work, its context, and, in Sec. 1.2, outlines his contribution to the theoretical description of Landau damping of magnons in ordered collinear magnets along with the literature review of the state of the art in this field. The latter research, conducted during his doctorate, constitutes one of the prerequisites for the subsequent scientific activities described in this treatise. The following chapters, briefly summarized in Sec. 1.3, detail on the corresponding developed methodology and the results obtained. The cumulative list of authors pertinent published scientific contributions can be found in the Appendix "Own works". These are marked with prefix "C", e.g. [C1].

1.1 Introduction

The magnetism was known in antiquity and used as early as 200 BC during the Han dynasty in China to construct compasses made of naturally occurring lodestone, i.e., magnetite [1]. In modern times, the compass, together with sextant and chronometer, allowed the European sailors to navigate the entire globe. Towards the end of industrial revolution, the description of electromagnetism and the discovery of dynamo gave this niche science a central position in modern science and technology. The triumphal march of magnetism continues throughout the quantum era with the experiments of Gerlach and Stern [2] and theoretical foundations by Pauli [3] heralding the discovery of the spin degree of freedom.

Apart from the energy generation, storage, transmission, and transformation, the honored applications of classical electrodynamics, the magnetism is pivotal in medical imaging [4] and high-density information storage [5, 6]. Furthermore, the fields of *spintronics* [7–10] and *magnonics* [11–14] use the spin degrees of freedom and their dynamics to process information, promising a new generation of low-power computers. Last but not least, spins can become a basis for the physical realization of quantum computers [15–19].

The *ab initio* quantum theory of magnetism in solids, in particular in the metallic, or itinerant, magnets, faces two major challenges [20, 21]. These are the faithful description of the magnetic ground state, including quasiparticle dynamics [22], and the reliable prediction of spin excitation properties.[1] Unquestionably, both are of paramount importance in the design of functional magnetic materials.

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[1] Several specific aspects of the theory for insulating magnets will be discussed in Sec. 4 but these challenges appear there as well.

In metallic magnets, the magnetism emerges from the coexisting localized (typically, of d-type) and band electrons which has proven to elude simple theoretical treatment [23]. A considerable success has been achieved by the density functional theory (DFT) [24], even in the local spin density approximation (LSDA), but the theory fails to grasp the remnants of atomic-like properties, e.g., the multiplet structure. Here, the combination of the DFT and the dynamical mean field theory (DMFT) [25–30] considerably improved the description of quasiparticle states.

Nevertheless, a systematic joint experiment-theoretical analysis of the angle resolved photoemission spectroscopy (ARPES) spectra of transition metals [31–34] revealed that the DFT+DMFT framework, resorting to the local approximation for the electron self-energy, despite overall improvement, fails to account fully for the wave-vector quasiparticle renormalization in many systems, most notable example being body centered cubic (bcc) Fe.

Inevitably, this already rich physics is augmented with further correlations effects. An ingredient partially missed by the DFT+DMFT theory is the impact of magnetic fluctuations on the electronic structure, castable in the language of electron-boson interaction (in this case electron-magnon). Other examples of such many-body effects are already known for some time. The screening of the Coulomb potential can be understood as electron-plasmon interaction [35] while the electron-phonon coupling leads to both the renormalization of the electronic bands as well as the conventional superconductivity [36]. The *electron-magnon coupling*, a subtle and weakly understood but equally important many-body effect, turns out to be the missing, even if not the only, piece of this puzzle.

The *magnons* (or *spin waves*), the collective excitations or a magnetic system, [C23, 37–42] manifest themselves in collinear magnets as coherent precession of magnetic moments. In metals, they hybridize with the single electron-hole pairs of opposite spins (*Stoner excitations*) which leads to the pronounced decay of the magnons, called *Landau damping*, a mechanism analogous to the plasmon attenuation put forth by Landau [43].

The spin waves exert a tremendous impact on the properties of functional magnets. Their interaction with the electrons leads not only to the band-structure renormalization but also to the shortening of the electronic mean-free path [44–47]. In addition to phonons, magnons can support the Cooper pair formation in unconventional superconductors [48–51]. The spin excitations drive the magnetic phase transitions determining the Curie, or Néel, temperatures [20, 52] and contribute to the materials specific heat [53]. Unquestionably, their faithful theory is of much scientific interest.

Historically, the spin-wave in ordered magnetic systems were described first resorting to the mapping onto the Heisenberg model (*adiabatic* approximation) [54–62] This approach yields numerically cheap schemes. However, the mapping involves a certain ambiguity and neglects Landau damping as well as the corresponding magnon energy renormalization associated with the latter.

The Landau damping is natively captured when resorting to the *linear response time-dependent density functional theory* (LRTDDFT) [63, 64] which allows to find, in principle exactly, the transverse magnetic susceptibility $\chi(\mathbf{q}, \omega)$. The poles of this function on the complex plane allow to determine the dispersion and damping of the magnons. Alternatively, the magnetic susceptibility can be also computed in the framework of first principles many-body perturbation theory [65–69]. A more detailed exposition of these formalism is presented in Sec. 2.

The observations provided above became the motivation for the author to develop the scientific program following his PhD devoted, among others, to the deeper understanding of the spin dynamics and magnon-electron interaction in solids taking advantage of the time-dependent density functional theory.

The program builds upon the theoretical advances made in his PhD thesis. In order to facilitate a clear division between the results obtained during his doctorate and the content of this treaty, the former are briefly described in the following subsection alongside the literature review of the state of the art in this field.

1.2 First principles non-adiabatic spin dynamics

The properties of collective modes, including magnons and plasmons, can be extracted from the density-density response function which in its general form can be written as [22]

$$\chi^{ij}(\mathbf{x}, \mathbf{x}', t - t') = -i\theta(t - t')\left\langle \left[\hat{\sigma}^i(\mathbf{x}t), \hat{\sigma}^j(\mathbf{x}'t')\right] \right\rangle. \tag{1}$$

This so called *susceptibility* describes the linear charge or magnetization density change $\delta n^i(x)$ of a system to the applied external field $\delta V^j(\mathbf{x}')$. $\hat{\sigma}^i$ are charge ($i = 0$) and magnetization density operators ($i = x, y, z$), $[A, B] \equiv AB - BA$, and the $\langle \hat{o} \rangle$ is the expectation value of the operator $\hat{o}$ for the system without external perturbation.

Even in the linear regime, the computation of the response for the interacting electron gas is as complex as the solution of the many-body problem itself, i.e., currently not feasible in the exact manner. There are two lines of the approximation attack. The first one relies on the linear response time-dependent density theory (LRTDDFT) and the other resorts to the many-body perturbation schemes.

1.2.1 Linear response time-dependent density theory

The LRTDDFT allows to find χ from an integral equation formally resembling the Dyson one [63, 70]:

$$\chi = \chi_{KS} + \chi_{KS}(\nu_C + K_{xc})\chi \tag{2}$$

Here, χ_{KS} is the susceptibility of the formally non-interaction Kohn-Sham system of the ground state, v_C is the Coulomb interaction ("Hartree response"), and K_{xc} is the so called *exchange correlation kernel*. In the above equation, for simplicity, the spatial, time, and spin arguments were dropped for clarity. Despite the simple random phase approximation (RPA) appearance, the equation is exact but, sadly, not easy to solve. It is so because, in most cases, neither the Kohn-Sham system is known exactly (due to the necessary approximations to the ground state exchange-correlation potential) nor the K_{xc} is available. One might resort to the established adiabatic local spin density approximation (ALSDA) [71] which, however, fails to yield important physical excitonic effects.

However, the ALSDA is less critical in the case of spin-wave description where the kernel does not diverge in the $q \to 0$ regime. In the case of collinear magnets and negligible spin-orbit coupling (SOC), the spin-wave signature is given by the transverse susceptibility (*spin-flip propagator*)

$$\chi^{\pm} = \chi^{xx} \mp i\chi^{xy} \tag{3}$$

and the susceptibility Dyson equation (2) does not involve the Coulomb interaction.

1.2.2 Many-body perturbation schemes

Another line of attack is facilitated by the time-dependent quantum perturbation theory applied to a many-body electronic Hamiltonian. In an early study, Callaway and Wang [72–74] took a simplified Hubbard-like model as a starting point. A series of studies concerned with the spin dynamics of ultra-thin magnetic films [75–81] appeared along this line as well. In parallel, more faithful approaches taking advantage of a realistic LSDA-based ground state band structure and screened Coulomb interaction were developed [66–68].

One anticipates that this formalism will allow in the future for a systematic and possibly easier incorporation of many-body effects into the description of spin dynamics. However, the currently available implementations use approximations making them practically equivalent to the LRTDDFT in the ALSDA. These are the use of the LSDA for the electronic ground state, local and static approximation to the screened Coulomb interaction W, as well as approximations to the perturbation terms included, i.e., the choice of Feynman diagrams yielding the RPA-like equation for the dynamics susceptibility resembling formally the equation (2) of the LRTDDFT. Additionally, unless W is not used to self-consistently generate the ground state itself, the method suffers from a violation of the rotational symmetry [69, 82].

1.2.3 Landau damping of magnons in ordered collinear complex bulk magnets and ultra-thin magnetic films

Staunton *et al.* [83–85] deployed the LRTDDFT to investigate the spin-fluctuations of (disordered) paramagnets (*paramagnons*) while Savrasov addressed [86] the magnons and their Landau damping in elementary magnets. However, the method turned out to be algorithmically complex and computationally expensive, especially for complex bulk systems and ultrathin magnetic films. In a series of publications following the PhD thesis of the author, a methodology for treating the spin dynamics of such complex solids films was developed and applied to a series of ordered collinear ferromagnets. (An overview of these results relevant to this treaty is given below.) Later, Lounis *et al.* [81, 87–89] successfully applied the LRTDDFT to adatoms and other zero-dimensional nanomagnets. In the meantime, the approach has been successfully implemented in several further numerical frameworks [90, 91]. Also, a non-perturbative treatment of spin precession (a full time-dependent density functional theory (TDDFT) treatment) was reported [92]. Still, studies of complex systems featuring many non-equivalent atoms are scarce.

At the same time, such calculations are of great interest since they can be related to experimental results. The measurements of spin waves provide an extremely valuable insight into the nature of the exchange interaction governing the formation of the magnetic ground state. The inelastic neutron scattering (INS) [93–102] and the resonant inelastic X-ray scattering (RIXS) [103–105] play the pivotal role for the bulk magnets here. However, the corresponding cross section is often too small to allow for a reliable study of magnons in ultra-thin films. In the latter case, the long wave-length spin waves can be studied using Brillouin light scattering [106]. Additionally, inelastic scanning tunneling microscopy can recover the signature of magnetic excitations [C23, 41, 42]. The magnon dispersion and damping in the entire two-dimensional Brillouin zone can be probed reliably using the spin-polarized electron energy loss spectroscopy (SPEELS) [C15, C22, C25, C26, 40, 107–123].

The early theories of Landau damping in ultra-thin magnetic films based on model Hamiltonians postulated an extremely strong impact of non-magnetic substrates on the attenuation [75–81]. At the same time, a very strong sensitivity of the results to the details of orbital parameterization showed that only an *ab initio* theory can provide reliable predictions concerning the spin dynamics of ultra-thin films.

In order to achieve it, a first principles computational scheme for the evaluation of the dynamical transverse susceptibility within LRTDDFT was developed during the PhD program of the author [124] using the Korringa-Kohn-Rostoker (KKR) Green's function (GF) method [88, 125–133]. This approach showed two decisive advantages. First, the Kohn-Sham susceptibility is evaluated as convolution of the two Kohn-Sham Green's functions. This can be achieved using a suitable complex energy integration contour allowing for the evaluation of this quantity away from its singularities on the real axis. This improves the convergence of the numerical scheme by orders of magnitude[2]. Second, the Green's function method operates natively in the real space, making it perfectly suitable for the description of systems with broken translational symmetry, e.g., featuring surfaces or interfaces. The detailed exposition of the formalism was provided in Ref. [134]. With the efficient numerical scheme at hand, complex bulk magnets and ultra-thin films were addressed.

In the case of bulk Heusler phases, the intricate interplay of magnon shapes, energies, and the Landau damping was unveiled [135, 136]. Many of the phases are half-metallic [137] meaning that the spectrum of Stoner excitations features a gap. In the limit of the negligible spin-orbit interaction, the low energy spin waves are not Landau damped.

A careful critical analysis of spin dynamics and its damping in magnetic films supported on non-magnetic substrates was carried out as well. Among the key results, the applicability of standing spin waves for spintronic applications was appraised [138] alongside with the detailed analysis of the impact of the electronic structure at the film-substrate interface on the Landau damping [115, 139]. In the latter case, one of the central observations was that the electronic states of the substrate localized at the surface ("surface states") [140] can hybridize strongly with the magnetic states of the film leading to the formation of so called *interface complexes* inducing the enhanced Landau damping. However, interestingly, the transition between the parent bulk and and a two-dimensional magnet supported on a non-magnetic surface does not automatically involve the enhancement of the Landau damping. As shown on the example of Fe, Ni, and Co, the relationship is strongly system and geometry dependent [134], paving the way for the engineering of magnon life-time in nanostructures.

1.3 Overview

The treatise is organized as follows. Sec. 2 presents further developments in the description of spin dynamics in solids using LRTDDFT going beyond the ferromagnetic spin-wave description. First, the application of the method to ferri- and antiferromagnets is presented. Following this, the studies of paramagnons and longitudinal spin excitations are outlined. It is shown how the paramagnons can lead to unconventional Cooper-paring being an example of the magnon-electron interaction. The non-Landau magnon decay channels constitute the topic of section 3. Here, the hierarchy of the spin dynamics attenuation is established taking into account the disorder and multi-magnon processes. Section 4 outlines the studies performed on several families of complex functional magnetic materials. The investigations of the corresponding ground states are included as well as they are the indispensable basis for the spin dynamics investigations which, in some cases, are not yet completed at the time of writing.

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[2] However, at the price of necessary careful analytic continuation.

The theory of magnon-electron interaction based on the TDDFT is presented in section 5 and applied to a range of magnetic systems. This interaction leads to a range of measurable and important phenomena, including band structure renormalization, the emergence of non-quasiparticle states, and the impact on the spin dynamics itself, which are addressed from an *ab initio* perspective. The final section 6 provides a summary and a overview of ongoing scientific activities.

❧

Scientific and human motivation remain two different reasons to embark on a scholar career and let us carry out a brief investigation into the latter. In “The Collected Poems of Dylan Thomas”, the poet’s own foreword contains the following passage:

> I read somewhere of a shepherd who, when asked why he made, from within fairy rings, ritual observances to the moon to protect his flocks, replied: “I’d be a damn’ fool if I didn’t!” These poems, with all their crudities, doubts, and confusions, are written for the love of Man and in praise of God, and I’d be a damn’ fool if they weren’t.

Scientists might mention social good, grants, fame, drive for understanding out of curiosity, or cold buffets at conferences but, at the end, they are blessed with having no choice.

2. Developments in the *ab initio* description of spin excitations

2.1 Ferri- and antiferromagnetic magnons

In two publications [C24, C29], the LRTDDFT methodology described in the preceding section was applied to ferri- and antiferromagnetic magnons for the first time. Here, the major findings are reported on.

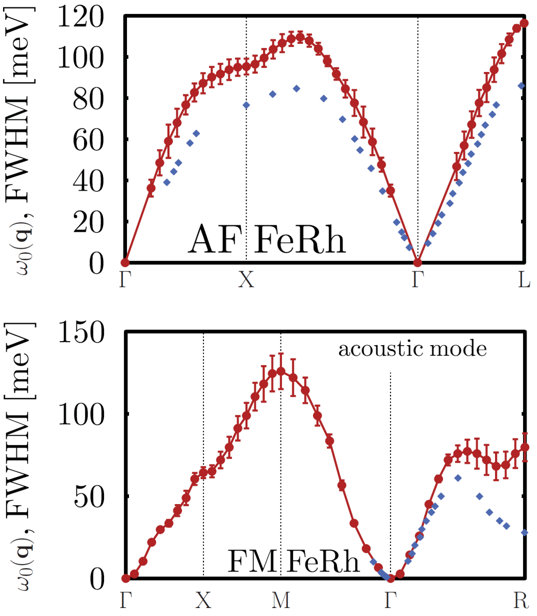

Figure 1: The energies and FWHMs of magnon peaks in AF (upper panel) and FM (lower panel) phases obtained from LRTDDFT (dots • and error bars) compared to the experimental data (♦) from [141]. The figure is reproduced from [C29].

A particularly interesting system in this context is the FeRh which can feature, at varying external conditions, both the FM and AF phases [142–145], allowing to contrast easily the spin dynamics of these orderings. Fig. 1 presents the dispersions and FWHMs of spin waves in these two cases. One observes that the magnons are well defined in the entire Brillouin zone, their Landau damping remaining moderate for all momenta. (No other decay channels are considered.) As expected, the damping vanishes in the center of the Brillouin zone for acoustic magnons in both phases, but, in the case of the FM ordering, in contrast to the AF one, there is a critical momentum below which the damping is practically inoperative. On the other hand, the weakly dispersive optical magnons at energy of around 750 meV (not shown) are substantially stronger Landau damped. They are separated from the acoustic magnons by a gap and arise due to the two magnetic Fe atoms in the primitive cell of the compound[3].

These results illuminate the complexity of the interactions between the Stoner and spin-wave spectrum. We refer to Fig. 2 now. In the FM case, the intensity of low energy Stoner excitations is small, since they arise mostly from the transitions between bands of the same spatial character but separated by the Stoner splitting ("intraband transitions"). In general, the "interband transitions", between energetically close, or overlapping, bands yield Stoner excitations of vanishing activation energy. These transitions, however, have typically a low inten-

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[3] This makes FeRh, strictly speaking, an example of *magnonic crystal*, an interesting concept which we will, however, not follow any further here.

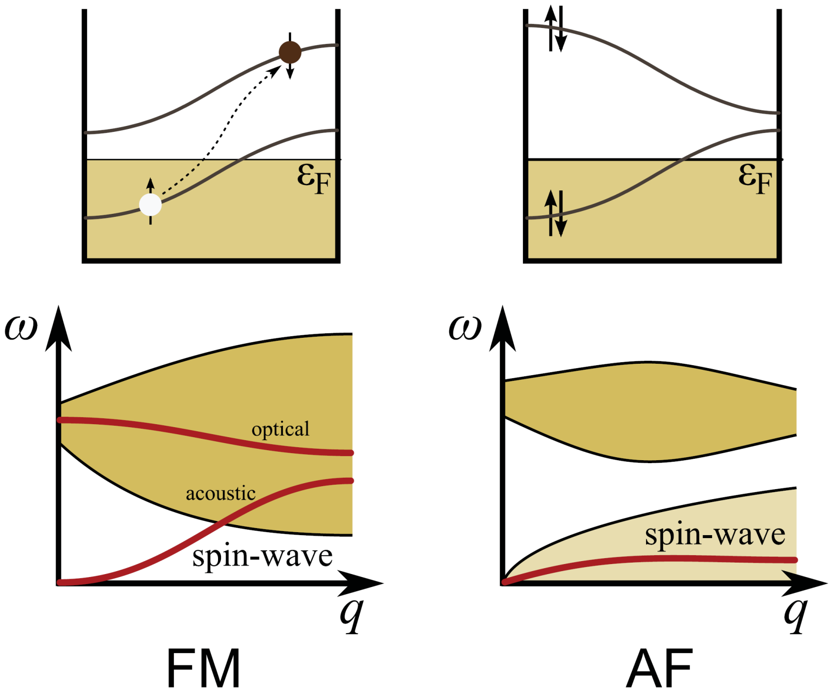


Figure 2: Spin polarized electronic band structures and corresponding Stoner spectra shown schematically for FM (left panel) and AF phases (right panel). The figure is reproduced from [C29].

sity due to the small spatial overlap of wave functions in these bands of different character. This explains why the acoustic spin waves can be practically Landau undamped below certain energy and why higher energy magnons, in particular the optical ones, engage in this hybridization. The up and down spin bands of an AF system are degenerate and of the same spatial character, except that the up and down orbitals are more strongly localized on two different atomic sites. This leads to relatively weak overlap between the two bands and results in small intensity of Stoner excitations, even though the AF magnons involve in the hybridization with them at any energy. In short, these are the details of the band structures and the hybridization matrix elements which finally govern the magnon attenuation. Therefore, realistic *ab initio* calculations are indispensable here.

Magnons feature an additional degree of freedom, the *chirality*. It determines the polarization, or angular momentum, associated with a magnon. In FM phases, there is only one type of magnons corresponding to an effective "up-to-down" spin spin-flip. However, in systems composed of magnetic moments pointing in different directions, even in the collinear case, there appear also magnons of "down-to-up" spin spin-flip signature precessing in the opposite sense [146, 147].

Remarkably, the chirality can be used to control the Landau damping [C24]. In the compensated ferrimagnet CrMnSb, the Cr and Mn atoms are opposite spin-polarized but the half-metallicity of the systems forces the equal magnitudes of

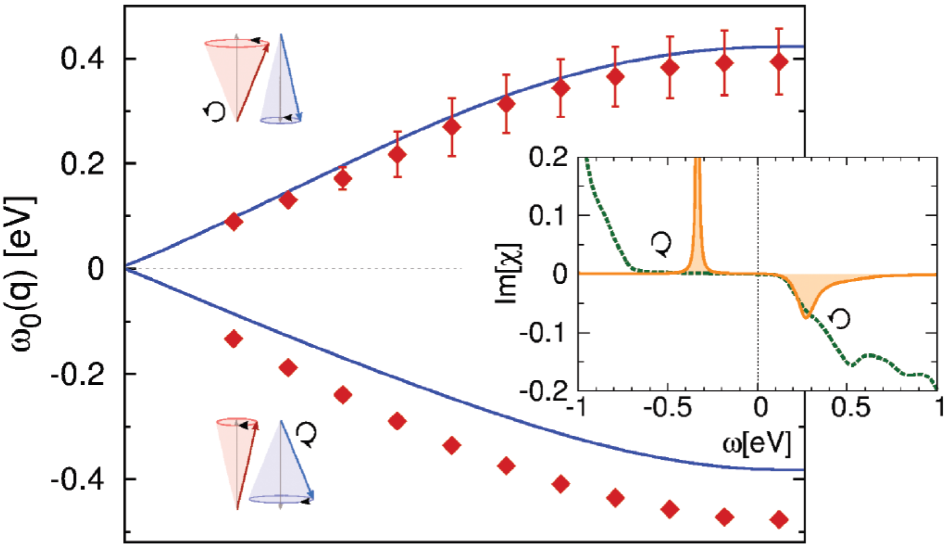


Figure 3: Spin waves of CrMnSb. The diamonds and error bars are positions and FWHMs of the magnon peaks while the solid lines depict the adiabatic calculations. The inset shows an example of magnons forming outside or within the Stoner continuum based on the magnon polarization. The figure is reproduced from [C24].

their magnetic moments. Still, the atoms are not identical and the two AF-like magnon branches are not of the same frequencies, cf. Fig. 3. More remarkably, however, the damping signature of these two magnon modes is qualitatively different. The counterclockwise precessing magnon is not damped, as it emerges in the Stoner spectrum gap caused by the system's half-metallicity. On the other hand, the clockwise magnon can hybridize with the Stoner excitations and undergo the attenuation.

2.2 Paramagnons in unconventional superconductors

Up to now, the LRTDDFT studies were devoted to the faithful description of the Landau damping. The qualitative picture of magnons in FM and AF phases can, however, be obtained in the adiabatic mapping of the magnetic system onto Heisenberg Hamiltonian. Nevertheless, there are magnetic excitations of the electron gas which cannot be grasped in the latter model: the *paramagnons* and *longitudinal spin excitations* which are addressed in the following two sections.

The paramagnons are the spin-flip excitations of non-magnetic solids. They involve the dynamic emergence of local fluctuating magnetization and are particularly pronounced when a system is in the proximity of its magnetic phase. A prototypical example of such phase is Pd [148, 149].

Interestingly, strong paramagnon-like excitations were reported in the large class of unconventional superconductors including FeSe [150–153] and we investigated those fluctuations using LRTDDFT [C27]. Experimentally, at ambient pressure, FeSe is non-magnetic but the proximity of the magnetic phase manifests itself in the sensitivity of the ground state ordering to the positions of the Se atoms with respect to the Fe-plane. Below the critical value of $z^{\mathrm{c}}_{\mathrm{Se}} \approx 1.18$, which can be regarded as the onset of a quantum phase transitions, the system does not spin-polarize but still shows strong paramagnon excitations which intensify upon approaching $z^{\mathrm{c}}_{\mathrm{Se}}$, cf. Fig. 5. (Above $z^{\mathrm{c}}_{\mathrm{Se}}$, FeSe features the so called stripe AF phase.) One observes that the magnetic response of the system is strongly enhanced by the exchange interactions leading, close to the critical point, to the paramagnon excitations of clear dispersion becoming almost linear for the low energy excitations which resembles strongly the spin-flip picture of the proximal AF ordering. As discussed in Sec. 5.5, these intense paramagnon excitations can provide strong enough electron-electron pairing for the superconducting state to form.

2.3 Magnetic second sound

Within the ALSDA, in collinear magnets, and upon neglecting the SOC, the response to the scalar and magnetic fields along different directions is given by the matrix of the following structure

$$\chi_{\mathrm{KS}} = \begin{pmatrix} \chi^{xx}_{\mathrm{KS}} & \chi^{xy}_{\mathrm{KS}} & 0 & 0 \\ -\chi^{xy}_{\mathrm{KS}} & \chi^{xx}_{\mathrm{KS}} & 0 & 0 \\ 0 & 0 & \chi^{00}_{\mathrm{KS}} & \chi^{0z}_{\mathrm{KS}} \\ 0 & 0 & \chi^{0z}_{\mathrm{KS}} & \chi^{00}_{\mathrm{KS}} \end{pmatrix}. \tag{4}$$

(The magnetization is assumed to point along the z direction.) The x and y channels describe the transverse response including the magnons (spin waves and Stoner states). We have already encountered them in the preceding sections. Decoupled from them are the longitudinal and charge excitations in the charge (0) and z channels [154]. The charge fluctuations are typically dominated by plasmons [155–164] but in magnetically ordered systems they couple, at least formally, to the fluctuations of the longitudinal magnetization.

Little is known about the nature of the excitations in this longitudinal spin channel, and we investigated them in Ref. [C16] for elementary and 3d transition metals and magnetically ordered FeSe. The results for the latter are presented in Fig. 4. In the work cited we showed that the excitations correspond to the fluctuations of the order parameter and are thus akin to *second sound* in liquid He [165–167]. Furthermore, they bear a resemblance to the paramagnons, corresponding to the exchange-correlation (xc)-enhancement of single electron-hole pair excitations. Interestingly, the magnetization fluctuations in the z channel are effectively decoupled from the charge excitations (plasmons). The reason for that is the large difference between the energy scales on which these two types of excitations form. This situation might change in two dimensional structures where

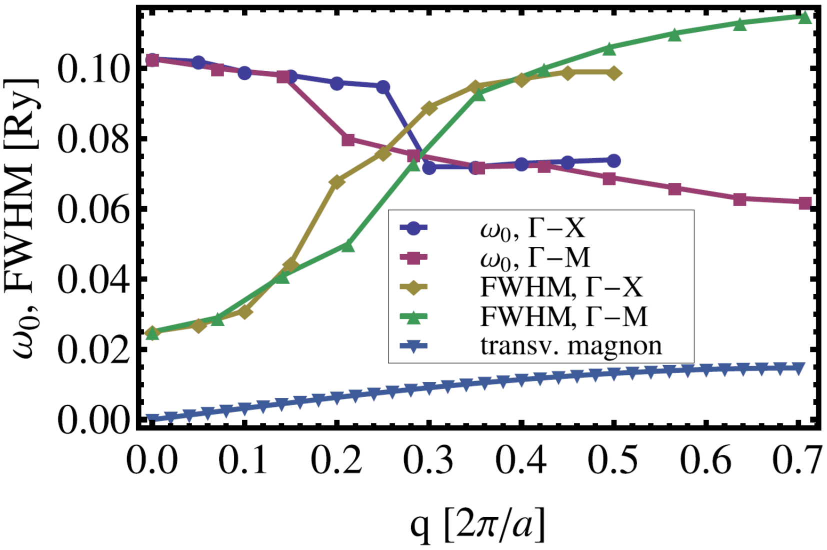
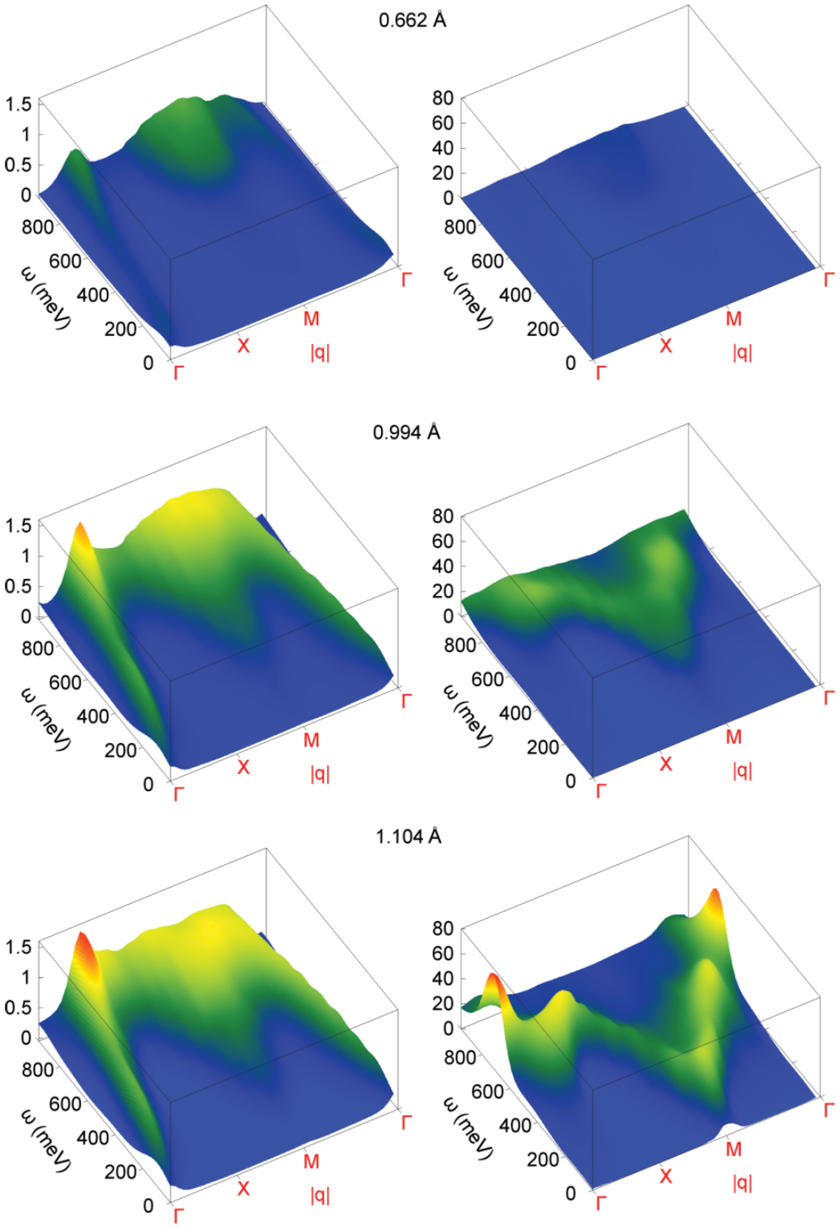


Figure 4: The energies and FWHMs of longitudinal spin excitations (*magnetic second sound*) in FeSe along different crystallographic directions compared to the energies of the transverse AF magnons. The figure is reproduced from [C16].

plasmons do not feature the activation energy and could hybridize with these longitudinal fluctuations.


0.662 Å

0.994 Å

1.104 Å

Figure 5: The paramagnons of FeSe approaching its quantum critical point. Shown are the intensities of spin-flip excitations of the formally non-interacting KS system (left figures) and those associated with the full susceptibility (right figures). The numbers in Å correspond to the positions of the Se atoms, z_{Se}, with respect to the Fe-plane, gradually approaching the onset of the magnetic ordering, from top to bottom. The figure is reproduced from [C27].

3. Non-Landau magnon decay channels

As argued in the introduction, the damping of the magnetization dynamics is of paramount importance in the applied field of spintronics. Moreover, the phenomenon allows an insight into the microscopic nature of interactions between spin and other degrees of freedom in solids.

What are the conceivable decay channels? We have already encountered the interaction of collective spin wave modes with the single electron spin-flips in Sec. 1.2, the Landau damping. Further effects include magnon-magnon scattering [168] appearing, among others, in the non-linear regime of large magnetic precession, spin-orbit coupling [169, 170] and scattering off lattice imperfections [171]. They are depicted schematically in Fig. 6. Other degrees of freedom, e.g., phonons [172], couple to magnons as well and open further decay channels. The list is hardly an exclusive one.

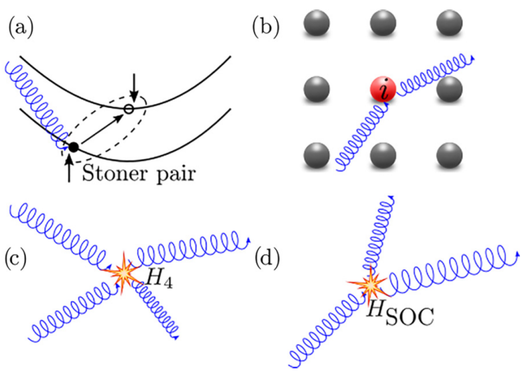


Figure 6: Several spin wave decay channels: (a) Landau mechanism, (b) scattering off lattice imperfections (disorder induced damping), (c) non-linear four-magnon process, (d) SOC mediated magnon-to-two-magnon decay. The figure is reproduced from [C3].

A general heuristic theory of “damping”, or, equivalently, “friction”, is constructible following Boltzmann treatment allowing for the microscopic irreversibility [173]. As a result, a set of few empirical damping parameters enters the Landau–Lifshitz–Gilbert equation [174, 175] allowing to investigate the effect of the attenuation [C11]. However, another ambitious goal is to compute these parameters *ab initio*.

Often, such direct calculations are unfeasible, especially when the microscopic mechanism of the friction is not fully known. The numerical aspects turn out to be challenging, too, since the figures to be determined are small and thus prone to numerical errors.

Luckily, in many cases, there are available models allowing us to tackle the damping from first principles. The Landau damping arises naturally in the LRTDDFT. The magnon-magnon scattering, absent in the linear response regime, is accessible from the Heisenberg Hamiltonian analysis using higher term of the Holstein-Primakoff transformation. The disorder can be treated on the level of the linearized Heisenberg Hamiltonian or using the disordered ground state in the LRTDDFT directly. In the following sections, the contribution of the author to the quantification of these effects are outlined.

3.1 The inclusion of disorder effects

The magnets feature often structural imperfections being result of the deviation from perfect stoichiometry caused by alloying, doping, diffusion (intermixing) processes, the presence of contaminants during the preparation, and many more. All these effects break the translational invariance. A magnon with a well-defined crystal momentum (Bloch wave) ceases to be an eigenstate of the disordered Hamiltonian. Pictorially, it collides with the impurities and gets scattered in other eigenstates while the quasi-momentum conservation is provided by the crystal, cf. Fig. 6b. In the limit of small scattering, the Bloch states can still be seen as approximate solutions but of a finite lifetime due to the scattering now.

There is no conceptual difficulty in incorporating the structural disorder into the LRTDDFT. Starting from the disordered ground state, e.g., described within a large supercell, one might attempt to compute the KS ground state and, subsequently, the magnetic susceptibility. However, the approach is computationally unfeasible as one would have to use prohibitively extensive supercells in order to describe the impact of disorder on larger length scales. Luckily, the description of the electronic disorder can be achieved using computationally realistic coherent potential approximation (CPA). Alas, it comes at a cost of algorithmic complexity and up to now, in the context of LRTDDFT, it has been applied to study paramagnons only [84, 85, 176] but not the spin excitations of ordered magnets yet.

In a series of publications, we provided the description of the disorder-induced magnon-damping within the Heisenberg model built upon the disordered ground state described within the CPA [C13, C14, C20] capable of treating complex lattice geometries and arbitrary mixtures of magnetic and non-magnetic atoms. We will expose the formalism now.

The simplest model of a disordered magnetism arises from the consideration of dilution, cf. Fig. 7 for a two-dimensional example of simple lattice with vacancy concentration evolving across the percolation threshold [177–179]. Certain magnetic atoms are removed together with the magnetic couplings (exchange integrals) originating from them. We note that this gives rise not only to the substitutional disorder (an atom replaced, possibly by a vacancy) but also to the off-diagonal one (disordered couplings between the magnetic atoms). The latter constitutes a serious challenge in the CPA-treatment of the problem. The generalization of the description to arbitrary mixtures of magnetic and non-magnetic atoms and lattices with complex bases is tedious but we gave it in the works cited.

The original CPA description of the Heisenberg model with the proper treatment of the off-diagonal disorder was given by Yonezawa and Matsubara [180, 181] and used in subsequent studies of simple systems [171, 182, 183]. In short,

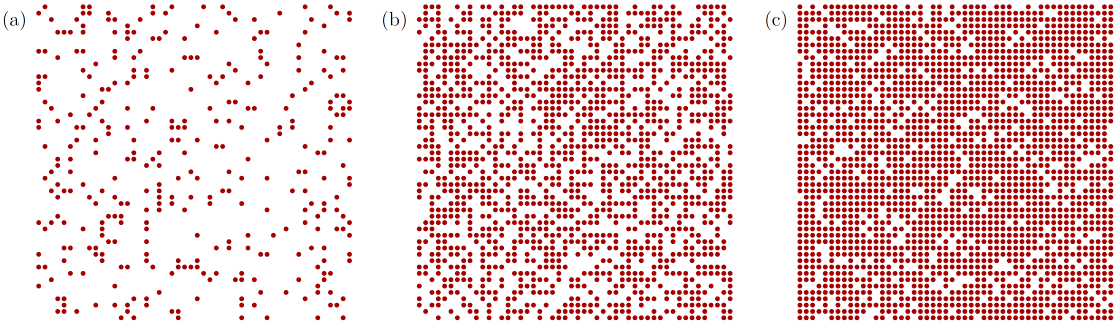


Figure 7: Examples of disordered two-dimensional magnetic structures at different concentrations of defects: (a) $\zeta = 0.15$, (b) $\zeta = 0.85$ (the vicinity of the percolation threshold), (c) $\zeta = 0.59$. There are no correlations between occupation of sites. The figure is reproduced from [C20].

it relies on, at this state exact, the development of the disordered Heisenberg model's GF in cumulant series. Now, CPA chooses the set of *non-crossing* cumulants and sums them up self-consistently, cf. Fig. 8, yielding the best single-site approximation to the magnon self-energy arising from the scattering off impurities. Even simplest approximation emerges in the virtual crystal approximation (VCA), which includes only disconnected cumulants, but we will see that it is, in general, a qualitatively poor model.

A numerically exact treatment of the disordered Heisenberg model arises from direct averaging of the magnetic susceptibility over different configurations of the disorder (Monte Carlo treatment) [C20]. At this level, with modern supercomputers, this direct line of attack is possible but still costly. (It continues to be impractical on the level of the electronic structure.) Thus, it is of interest to inquire how doe the CPA performs compared to this exact solution. The agreement is mostly satisfactory, especially in higher dimensions, cf. Fig. 9. The CPA gives a faithful account of the magnon dynamics away from the percolation threshold for the diluted magnets, with the agreement being better in three than in two dimensions, as expected considering the mean-field nature of the approximation. In one dimension, not shown, CPA tends to fail qualitatively. Still, the approximation "senses" the vicinity of percolation threshold and correctly reproduces the dimensionality trends for both the energy and the FWHM of the magnon peak, the latter being proportional to the inverse lifetime of the collective mode. For non-diluted magnets the agreement tends to be even better. On the other hand, the VCA fails qualitatively. It is unable to differentiate between dimensions and predicts exclusively magnons of infinite lifetimes.

For non-diluted magnets and moderate regime of disorder, the almost free Bloch wave picture works well, cf. Fig. 10. The disorder induced damping is pronounced only at elevated energy where the density of states a magnon can decay into is substantial.

Is is relatively easy to include the impact of the temperature on the magnon

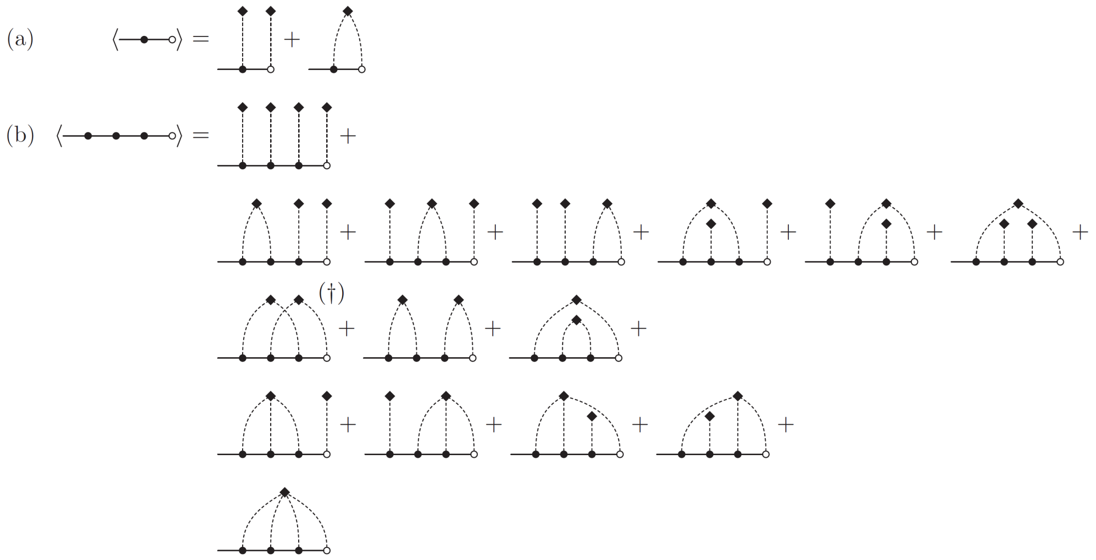


Figure 8: The diagrammatic expansion of the Dyson series corresponding to the magnetic susceptibility of the disordered Heisenberg model on the example of: (a) second and (b) fourth order average. An infinite series of such averages much be summed up self-consistently to obtain the full spin-flip propagator. The CPA corresponds to neglecting "crossed" cumulants, marked with dagger (†). The VCA keeps only the *disconnected* cumulants in the expansion. The figure is reproduced from [C20].

spectra on the level of the RPA [C14, 52]. The latter predicts the magnon softening as the temperature rises (with their energy vanishing at the critical temperature) but fails to yield the magnon peak broadening due to the temperature effects.

3.2 Magnon-magnon collisions

The SPEELS experiments we are concerned in are performed at very low temperatures compared with the Curie one. This means that there are practically no thermally excited magnons the one we consider can interact with. However, the SPEELS process itself continuously excites the magnons (although at presumably low rate) by the constant bombardment of the sample with spin polarized electrons. A magnon can interact with the bath which facilitates its decay.

When the SOC is neglected, the conservation of the angular momentum requires that two colliding (incoming) magnons must produce a pair of outgoing magnons, cf. Fig. 6c. With SOC operative, the excessive angular momentum can be absorbed by the lattice. In the latter case, a magnon can decay into two, as depicted in Fig. 6d. (A magnon could also collide with a partner from the SPEELS-bath but such process is much less probable.) Of course, there are also higher

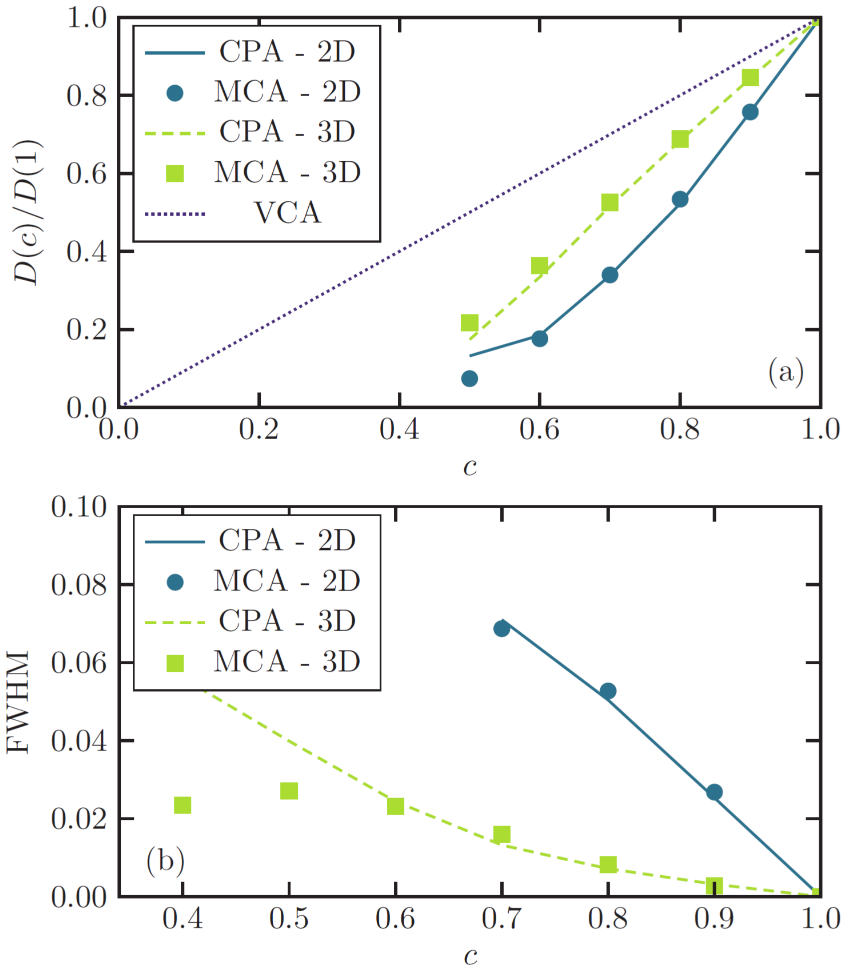


Figure 9: The dependence of the spin dynamics on the concentration of magnetic atoms c ($c = 1$ being perfect magnet) in two (three) dimensions for simple quadratic (cubic) lattice with nearest neighbor interactions. The performance of the VCA, CPA, and Monte Carlo approach (MCA) is compared concerning (a) the normalized spin wave stiffness and (b) the FWHM of the spin wave peak. The figure is reproduced from [C20].

order processes but they become less probable with the increasing number of magnons involved.

The observations can be mathematically formulated in an effective Hamiltonian

$$H = \sum_{\mathbf{k}ij} a_i^\dagger(\mathbf{k}) T_{ij}(\mathbf{k}) a_j(\mathbf{k}) + H_4 + H_{SOC} \tag{5}$$

The first sum represents free magnons. The term H_4 arises from the consideration of higher terms in the Holstein-Primakoff transformation. It corresponds to the non-linearity of the underlying dynamical equations or, equivalently, to the increased precession amplitude associated with the increased number of magnon states. Finally, H_{SOC} describes the SOC mediated 3-magnon decay process. Again, it appears naturally in the Heisenberg Hamiltonian when anisotropy terms or the Dzyaloshinskii–Moriya interaction (DMI) are considered.

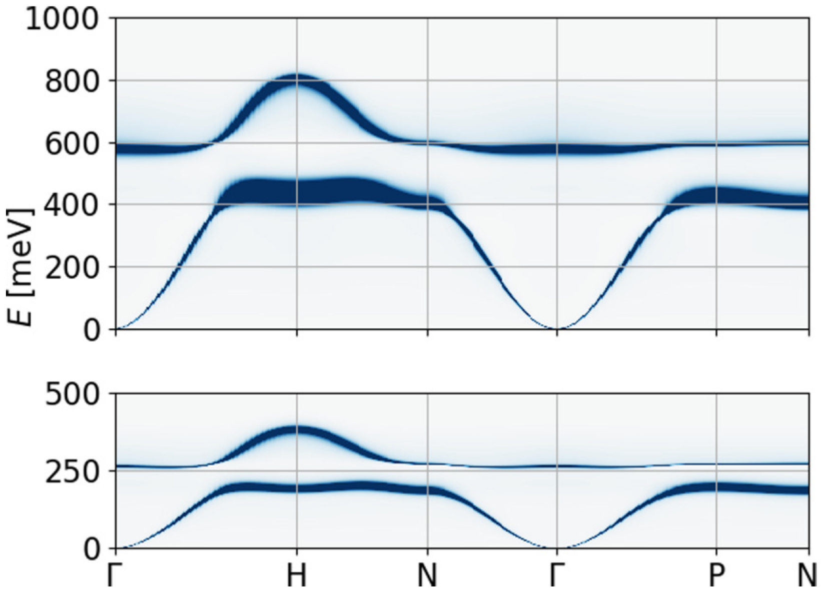


Figure 10: The spectral power of magnon excitations in $Fe_{0.8}Co_{0.2}$ at $T = 0$ (upper panel) and $T \approx 1200K$ (lower panel). The figure is reproduced from [C14].

H_4 and H_{SOC} appear to be small and can be treated as perturbations. The lifetime of a magnon state can be obtained from the Fermi golden rule upon the evaluation of the matrix element of the perturbing term on initial and final magnon states. (Note that these are many-magnon states involving the investigated state and the magnons from the SPEELS-bath.)

For the specific example of 3 monolayer (ML) of Co/Ir(001) considered in Ref. [C3], the magnon-magnon-induced attenuation rate is orders of magnitude smaller than the Landau damping: $\Gamma_4 < 5$meV and $\Gamma_{SOC} < 1$meV. No other systematic *ab initio* studies of these effects in magnetic nanostructures are known to the author.

3.3 The hierarchy of spin dynamics attenuation mechanisms

The results reported in the preceding sections allow us to establish the hierarchy of magnon decay channels in the metallic nanostructures. Unless the systems are half-metallic [135, 136], which happens rarely for ultrathin magnetic films, the Landau damping is expected to be the dominating attenuation mechanism. However, the impact of disorder must not be neglected. In general, its role will strongly vary depending on the concentration and the type of impurities. On the other hand, the multi-magnon processes in the low temperature regime appear to be of practically no importance compared with the two others mechanisms. Further effects, like magnon-phonon interaction [172, 184], may be of importance as well and require further studies.

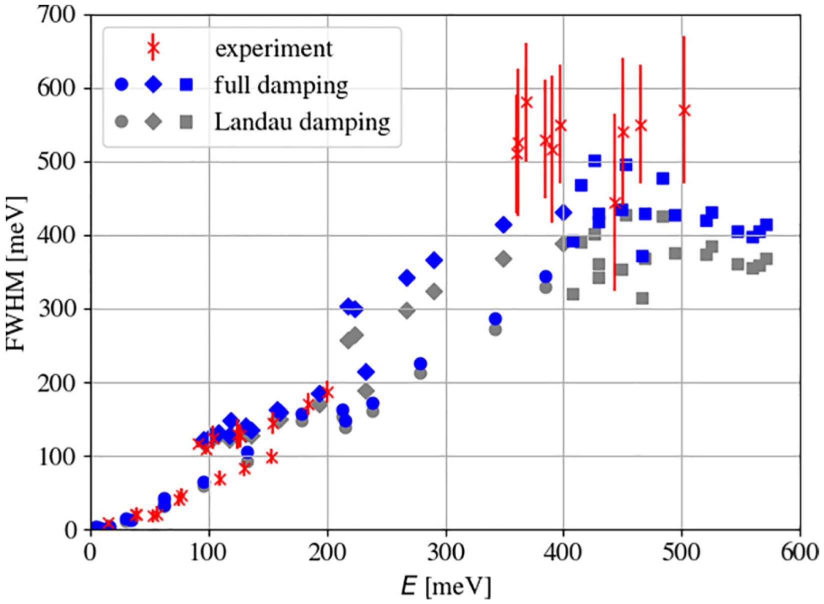


Figure 11: The comparison of the experimental data and the theoretical prediction of damping for 3 ML of Co/Ir(001). The inclusion of disorder improves the description of the spin wave decay rates at elevated energies. The multi-magnon processes are found to be irrelevant. The figure is reproduced from [C3].

In any case, the actual magnitude of the attenuation and the ratio of different processes will necessarily be strongly material specific. Therefore, let us consider the example of 3 ML of Co/Ir(001). It is an ultrathin metallic magnetic film and its magnon damping was characterized by means of SPEELS [C3]. The results are presented in Fig. 11. While the damping of low energy magnon branches can be fully explained through the Landau damping, the neglecting of other decay channels clearly underestimates the attenuation of the optical magnons above 350meV. The gap can be partially closed by considering the disorder induced damping. However, a certain disagreement persists, and it cannot be explained by minuscule magnon-magnon interaction. The role of magnon-phonon interaction, or other, in this system has not been investigated so far.

4. Complex oxides and other functional magnets

4.1 The structure and magnetic properties of complex oxides

The fascinating interplay between the structural, electronic, magnetic properties of insulating perovskites has gained a substantial attention in recent years [185–190]. In a series of publications [C6, C8–C10, C12], we have contributed to the understanding of the electronic structure and magnetism in these systems. In this section, a short discussion concerning the tunable two-dimensional electron gas (2DEG) is given.

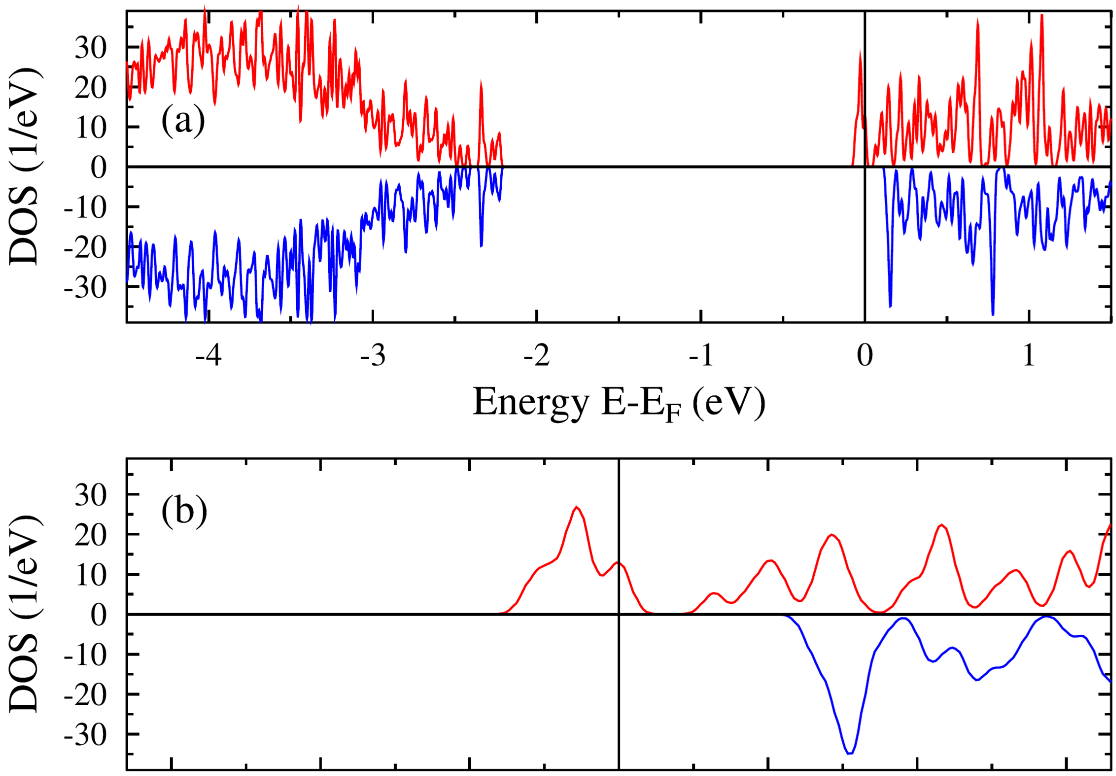


Figure 12: The density of states calculated for LaAlO3/Li1.17NbO3. (a) large energy scale showing the band gap. (b) zoom around the Fermi level showing the clear appearance of the spin polarized 2DEG. The figure is reproduced from [C12].

The possibility of the formation of the latter is a particularly striking feature of the interfaces in the perovskite heterostructures. Initially observed beneath polar $LaAlO_3$ (LAO) grown on TiO_2-terminated $SrTiO_3$(001), it was suggested by us to take advantage of a solid electrolyte $LiNbO_3$ (LiNO) instead of $SrTiO_3$ to induce a robust and switchable magnetic 2DEG in LAO/LiNO. Our strategy is based on the controlled introduction of defects (simulated *ab initio* using the CPA) providing the necessary charge accumulation at the interface. Furthermore, it can be demonstrated that the application of an electric field can dynamically charge and discharge the LiNO layers influencing the magnetoelectric properties via the Rashba-Edelstein effect.

4.2 The magnetism of digital alloys in two and three dimensions

In several papers [C28, C30, C31] we analyzed systematically a family of so called *digital alloys*, an example of 12-ML-thick Si/Mn superlattice is shown in Fig. 13. We resorted to the *ab initio* calculations of the electronic structure and the exchange interactions and focused particularly on the the dependence of magnetic properties on the morphology of the Mn monolayer. Subsequently, the Heisenberg model was deployed to determine the magnetic stability of the collinear FM phase and determine the energies and shapes of the magnonic modes. The critical temperatures of the magnetic phase transitions were calculated using the Monte Carlo simulations taking into account the SOC-induced anisotropy, strongly influencing it in two dimensions following the Mermin-Wagner-theorem [191].

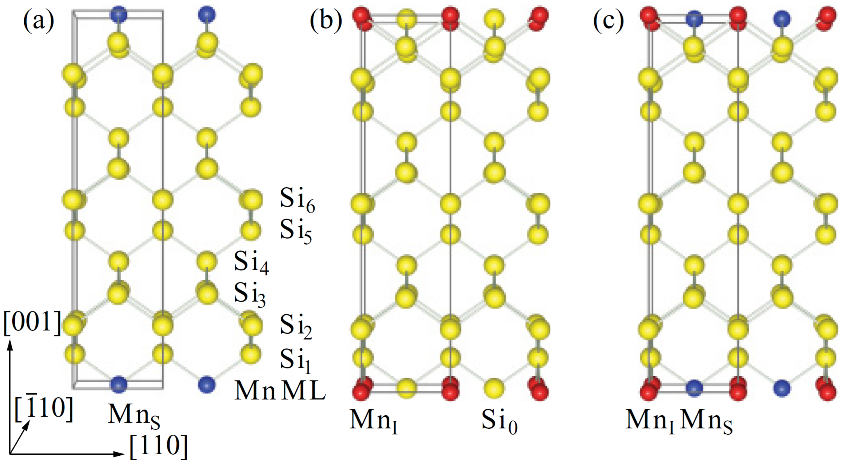


Figure 13: 12-ML-thick Si/Mn superlattices, with the substitutional Mn_S (a) and interstitial Mn_S (b) or both (c). The figure is reproduced from [C31].

In general, the magnetic properties of the digital magnetic alloy are decisively governed by the structural properties of the underlying crystal. Furthermore, stable ferromagnets and non-collinear structures coexist in the same parent material phases. The critical temperatures vary sensitively following the variations of the exchange parameters and anisotropy constants between 150K and the room temperature.

4.3 Altermagnetic phases

Let us conclude this section with a brief account of our studies [C1] concerning the novel magnetic phases termed *altermagnets* [192, 193]. Altermagnets are akin to AFMs but the Kramers degeneracy of their band structure is lifted, and the staggering of the magnetization takes place both in momentum and real space. The discovery of new functional materials in this class, microscopic electronic details of AFM ordering, its coupled charge and spin dynamics, as well as means of engineering and controllable switching the phases of these exotic materials are far from full explanation and pose an exciting emerging research field.

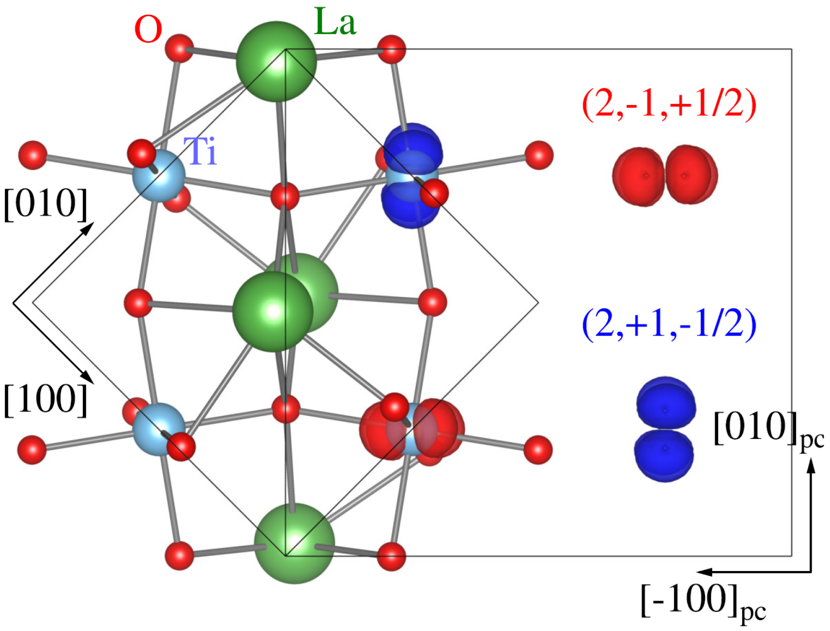


Figure 14: Top view of the magnetic unit cell of orthorhombic $LaTiO_3$. The figure is reproduced from [C1].

Resorting to *ab initio* calculations, we predicted that the Mott insulator $LaTiO_3$ (LTO), not known previously as an altermagnetic material, shows the characteristic features of these phases, in particular, the fully compensated antiferromagnetism and **k**-dependent spin-split electron bands in the absence of SOC. The altermagnetism occurs when Ti become occupied by single electrons with rotated orbitals, cf. Fig. 14. In this case, the system develops the band structure with the characteristic altermagnetic symmetry, i.e., involving the joint spin-inversion and crystal rotation, cf. Fig. 15.

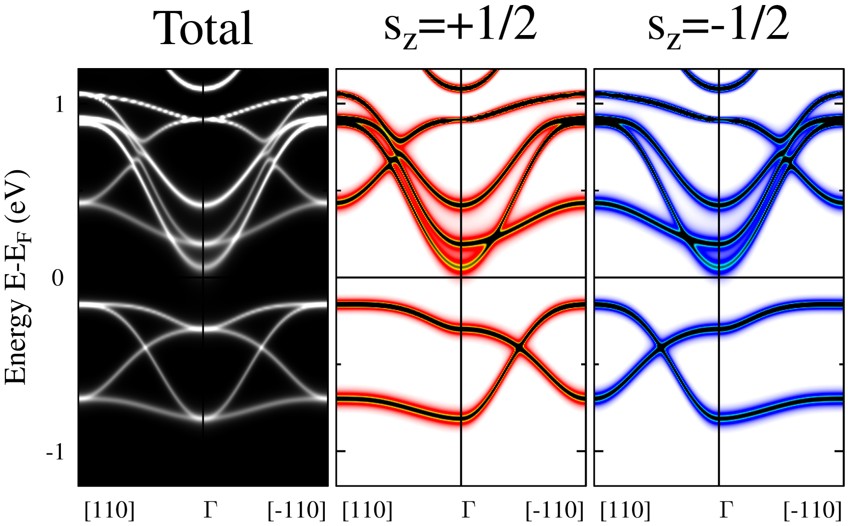


Figure 15: Total and spin-resolved Bloch spectral functions of altermagnetic $LaTiO_3$. The figure is reproduced from [C1].

5. Magnon-electron scattering

5.1 The physical picture and the many-body mathematical description of the interaction

The long-range magnetic order emerges as a genuine many-body quantum effect but, remarkably, our primary understanding of it is facilitated by the mean field treatment, the Slater-Stoner theory formulated first for ferromagnetic metals [20, 194–196]. In short, in itinerant magnets, the electronic bands magnetically split, or spin-polarize, despite the associated gain of their kinetic energy because the symmetry break lowers their mutual interaction arising from the Coulomb repulsion. In the Hartree-Fock approximation, the magnetization gives rise to the effective magnetic field which self-consistently stabilizes the spin-polarization. This picture echoes in the LSDA of the DFT where the spin density induces the xc magnetic field [24, 197]. Necessarily, the description must be complemented with a careful treatment of higher-order many-body effects [27, 29, 31, 32]. Nevertheless, for the sake of initial understanding, it pays off to bear with the mean-field concept for a second.

Can it give us a hint on how to construct the electron-magnon coupling theory? The answer turns out to be yes. The mean field fluctuates following the oscillations of the magnetization. The elementary excitations of the latter are magnons. Thus, the electrons can be imagined interacting with magnons by following the dynamic field induced by them. An equivalent interpretation of electron-photon scattering in the quantum electrodynamics provided by Feynman involves the interaction of the electron with the electromagnetic field corresponding to the photon [198]. The magnons are bosons and carry the angular momentum of $2\mu_B$ which must be conserved in the electron-magnon collision. Thus, the initial and final electron state must be of opposite spins when the magnon is absorbed or emitted. Furthermore, this implies that the xc-field associated with magnons is orthogonal to the ground state magnetization direction in the collinear magnets, as only such a field is capable of flipping ground state electron spins. This is consistent with the fact that magnons are transverse fluctuations of the ground state magnetization. In ALSDA, they induce the transverse xc-field given by the xc-kernel K_{xc}, cf. Sec. 1.2.1:

$$\delta B^{\perp}_{xc} = K_{xc} \delta B^{\perp}_{\text{magnon}}. \tag{6}$$

So emerges an intuitive physical picture of the interaction and, actually, the only formal treatment the solid-state physics can currently propose essentially mirrors it. Nevertheless, it cannot be the final one, at least because magnons and electrons are not separate entities like electrons and photons: magnons emerge as collective excitations of the electron gas.

A mathematical description of the phenomenon may be formulated on the ground of the many-body perturbation theory [199–201]. The influence of magnon scattering on the electronic quasiparticles is quantified by the self-energy. Since it cannot be computed in its full complexity, a set or relevant Feynman diagrams is chosen in order to approximate it. In metals, following Hedin [35, 202], the expansion is developed in the screened Coulomb interaction W. Since the latter, following the manner of the bare Coulomb interaction itself, cannot mediate spin-flip, the simplest term in the expansion, GW, cannot account for the electron-magnon collisions, cf. Fig. 16a.

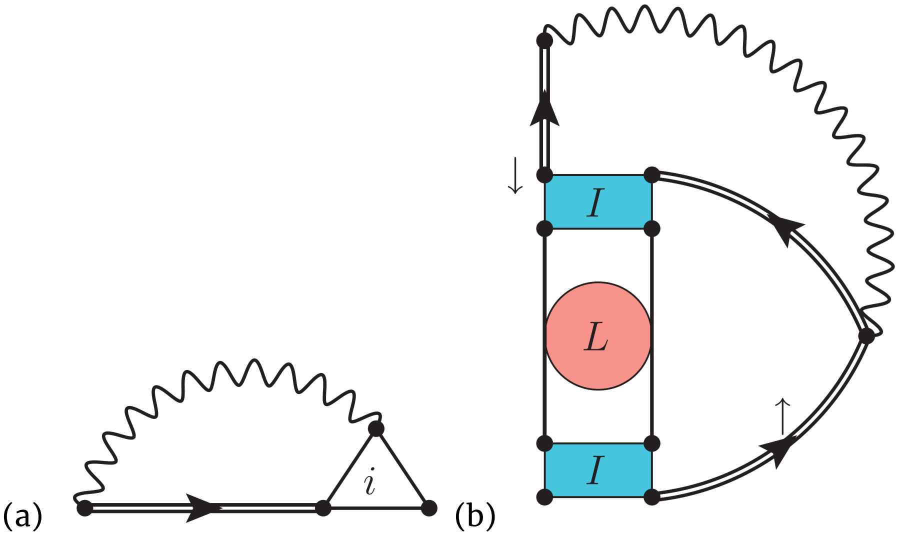


Figure 16: (a) The general form of the electronic self-energy Σ following Hedin's theory, following [C7]. The wavy line denotes the screened Coulomb interaction W while i is the vertex. (b) A selected set of Feynman diagrams in the expansion of the latter gives rise to the simplest possible electron-magnon interaction theory. The figure is reproduced from [C7].

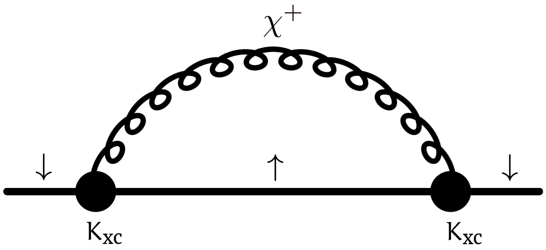


Figure 17: The contribution to the electronic self-energy arising from the magnon-electron scattering approximated using numerically cheap *ab initio* quantities obtainable from the LRTDDFT. The solid line pertains to the electron (electronic Green's function) while the wiggly one denotes magnon (spin-flip propagator). They couple by means of the exchange-correlation kernel $\mathrm{K_{xc}}$.

The magnon electron-interaction is recovered upon choosing a suitable set of Feynman diagrams in the expansion of the vertex in the self-energy [82, 203, 204], cf. Fig. 16. It turns out that this set of diagrams can be related to the transverse magnetic susceptibility expansion which is readily obtainable from the LRTDDFT [65, 66, 201].

We leveraged this observation to evaluate the strength of the electron-magnon coupling in solids [C7, 205]. The corresponding self-energy attains the structure depicted in Fig. 17. A down electron couples to the up electron in a process mediated by magnon (the dominating process in strong ferromagnets) described using the spin-flip propagator.

Since the LRTDDFT susceptibility is numerically cheaper than the corresponding quantities of many-body perturbation theory (MBPT) and, with our scheme, obtainable even for complex magnetic structures, the resulting novel formalism opened the possibility for evaluating the magnon-electron coupling even in these intricate cases. The remaining part of this section describes the results obtained.

5.2 Correlations effects in elementary and complex ferromagnetic phases

In [C7], we applied the formalism outlined in the preceding to study the electron-magnon interaction in several bulk systems. The results for bcc Fe and face centered cubic (fcc) Ni are summarized in Fig. 19. The coupling leads to a sizable renormalization of the electronic band structure: the broadening of the electron peaks, their shift, and the appearance of additional (satellite) states. For Fe, our result compares favorably to existing MBPT [82, 203, 204] and the DMFT [27, 31–34] results. In Ni, contrary to the DMFT approach, we are able to account for the nonlocality of the self-energy which appears to be important for achieving a better agreement with experiments concerning the value of **k**-dependent exchange splitting [29].

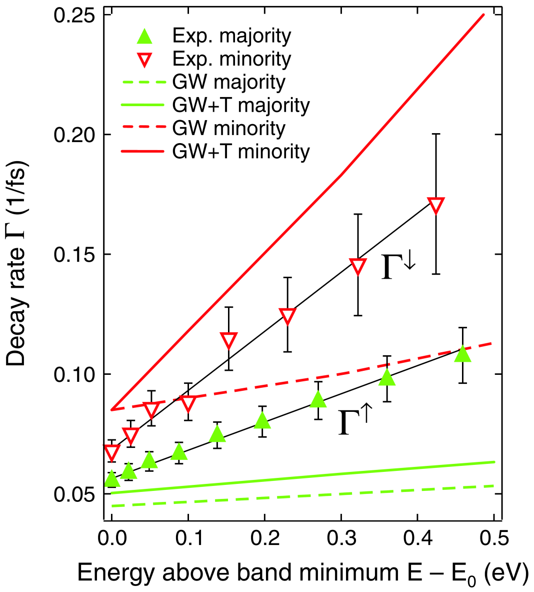


Figure 18: The decay rate of majority and minority electrons in the the first image-potential-state band of 3ML Fe/Cu(100) film. The figure is reproduced from [C32].

The relatively moderate numerical costs of our scheme allow to address also complex bulk materials as shown on the example of the weak itinerant ferromagnet $LaCo_2P_2$ [C5] where we were able to address both the impact on

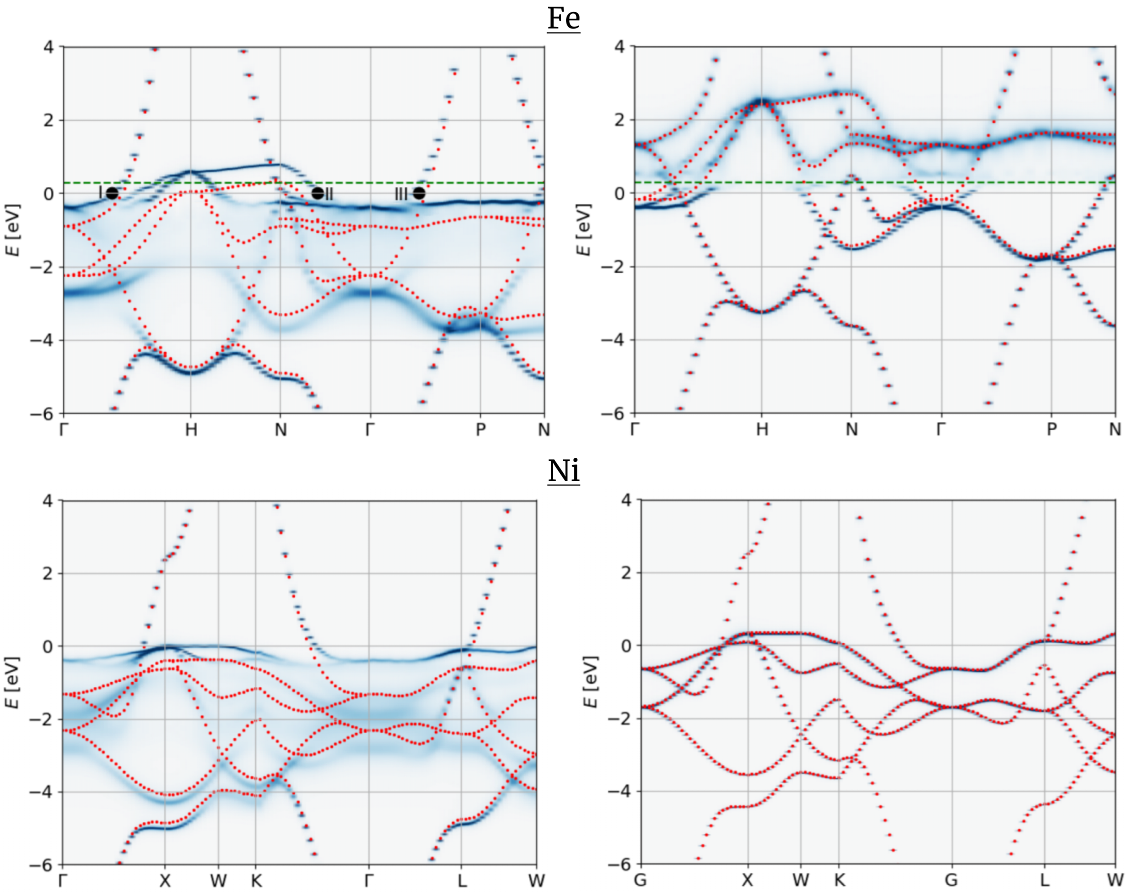


Figure 19: Effect of the magnon-electron interaction on the band structure of bcc Fe and fcc Ni for the majority (left) and minority (right) spin electrons. The red dots represent the electronic dispersion within ALSDA while the blue density plot is the spectral density renormalized due to the interaction of electrons with the virtual gas of magnons. The figure is reproduced from [C7].

phonons and *magnons* on the electronic structure of this compound, cf. Fig. 20. One of the central results obtained is the observation that phonons and electrons tend to affect the band structure in two largely distinct ways. The phonons lead to the emergence of "kinks" in the energy window around the Fermi level E_F corresponding to the approximate 50meV phonon bandwidth. This strong interaction leads, in a multitude of other systems, to the emergence of superconductivity. On the other hand, the magnons do not seem to induce such striking energy-localized features. Their influence causes a strong renormalization of the entire band. Interestingly, in $LaCo_2P_2$, these are predominantly majority spin holes engaging in the interactions with the virtual magnon gas which is a consequence of the enhanced number of final minority states below E_F. As evident from Fig. 20b, this leads to the sizable life-times shortening below the Fermi level. We see that the majority spin electrons (above E_F) do not decay but their energy is re-normalized. (By the virtue of the Kramers-Kronig relations, the imaginary part of the self-energy below below $\mathrm{E_F}$ leads to the real part observable above it.) On the other hand, the minority spin particles practically do not couple to magnons, cf. Fig. 20c.

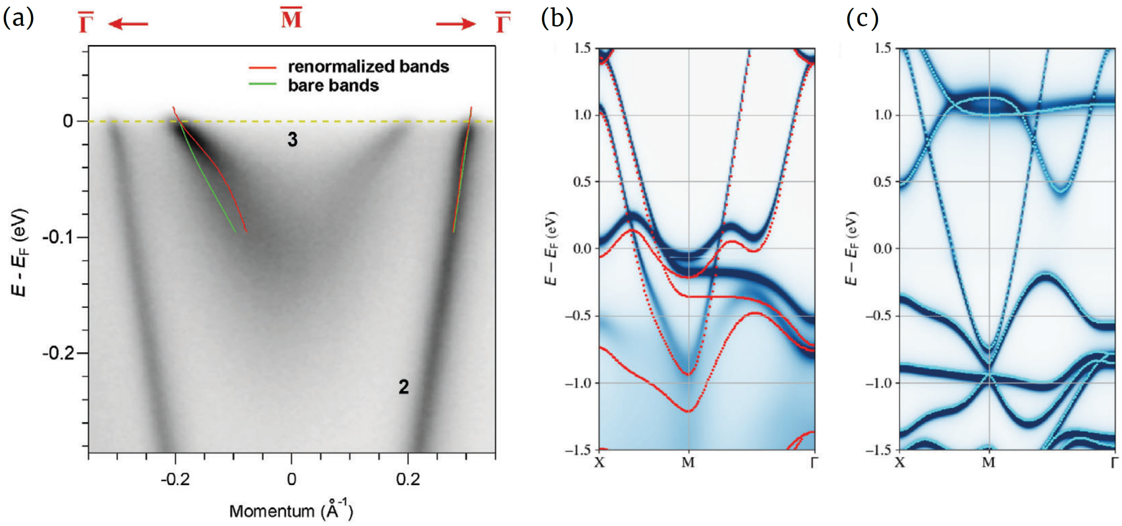


Figure 20: The electron-boson interaction in weak itinerant ferromagnet $LaCo_2P_2$. (a) The band renormalization ("kinks") due to the electron-phonon scattering. (b) and (c) The band structure renormalization due to the magnon induced self-energy, respectively majority and minority bands. The figure is reproduced from [C5].

Let us conclude this section by noting that the magnon-assisted decay of excited electrons can be directly experimentally observed as we showed in our earlier study of 3ML Fe/Cu(100) film [C32], cf. also Fig. 18. In the two-photon photoemission experiments, an electron is excited into an image-potential-state band and subsequently its lifetime can be measured. It turns out that the decay rate of the minority electrons exceeds strongly the one of minority ones. A careful theoretical analysis reveals that in this system the only process capable of selectively affecting spin channels is the magnon assisted electron decay, operative primarily for the minority electrons above the Fermi level.

5.3 Non-quasiparticle states of half-metals

The *half-metals* constitute an intriguing family of magnets [136, 206–210]. One of its spin channels (the minority one in the case of NiMnSb which we will focus on) shows the semi-conducting behavior while the second one remains metallic. This makes half-metals exciting candidates for spintronic applications and renders the Landau damping, of at least low energy magnons, strictly inoperative in the absence of SOC [135, 211].

Another intriguing effect observable in half-metals is the emergence of the *non-quasiparticles states* [212, 213]. It pertains to the superposition of electron and

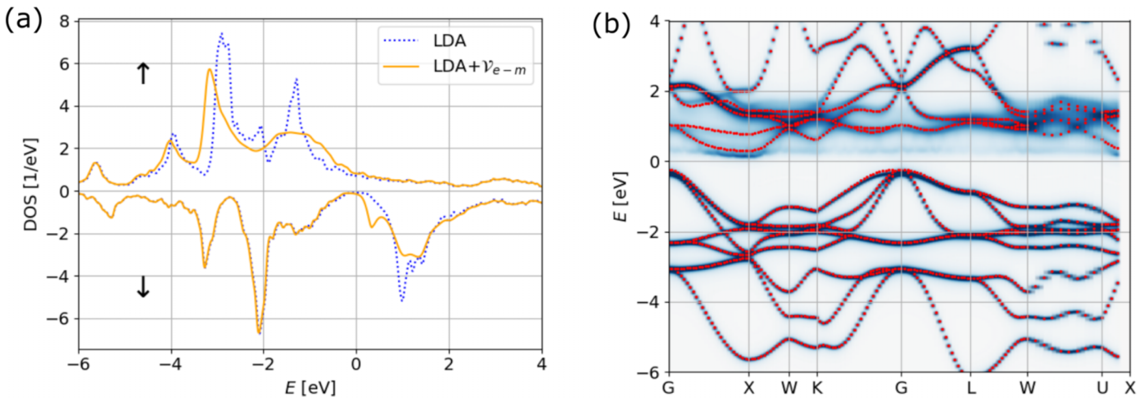


Figure 21: The electron-magnon interaction in NiMnSb. (a) Density of states in LSDA and under the influence of the electron-magnon scattering. (b) Bloch spectral function of the minority spin channel. The figure is reproduced from [C7].

virtual magnon particles, the "spin polaron". As a consequence, electron states (minority in the case of NiMnSb) emerge in the half-metallic gap in which they otherwise are absent. They can be described theoretically using the DMFT [214] or our approach to study electron-magnon interaction, cf. Fig. 21. One clearly notices the appearance of electronic states in the half-metallic gap. These states do not emerge as a perturbative evolution of the KS bands but form as a bound state of a majority electron and magnons, a genuine many-body phenomenon. Note the conservation of the angular momentum given by the sum of the up electron spin and $-2\mu_B$ one of the magnon yielding effectively a down electron spin.

5.4 Magnon-electron scattering in antiferromagnets

Our studies could not be complete without considering another important family of magnets, the antiferromagnets [C4]. In collinear magnets, there are four conceivable scattering processes of this type, depicted in Fig. 22, when one considers the low temperature regime in which there are no thermally excited magnons such that only their generation, but not absorption, is possible. Up hole (below the Fermi level) and down electron (above the Fermi level) generate magnons lowering the system's magnetization in the $\mathcal{C}^+$-type process dominating in ferromagnets. Down holes and up electrons could generate a magnon which would effectively increase the system's magnetization. This *anti-Stoner scattering* ($\mathcal{C}^-$) is strictly absent in strong ferromagnets but emerges in the weak ones (like Ni) and in the antiferromagnets.

It turns out that in AF systems the magnon-electron interaction is governed not only by the density of available final particle states but also by the shapes of the magnon modes influenced by their chirality, cf. Fig. 23, where we consider specifically the example of CrSb. We observe that electrons as well as holes in all spin channels engage in the magnon scattering since both $\mathcal{C}^+$ and $\mathcal{C}^-$ Stoner

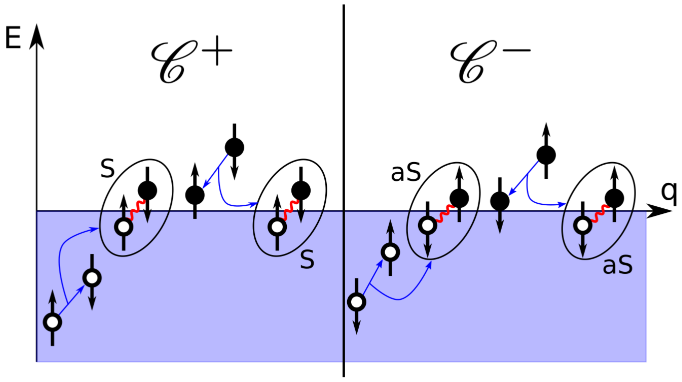


Figure 22: Stoner ($\mathscr{C}^+$) and anti-Stoner ($\mathscr{C}^-$) electron-magnon scattering processes. The figure is reproduced from [C4].

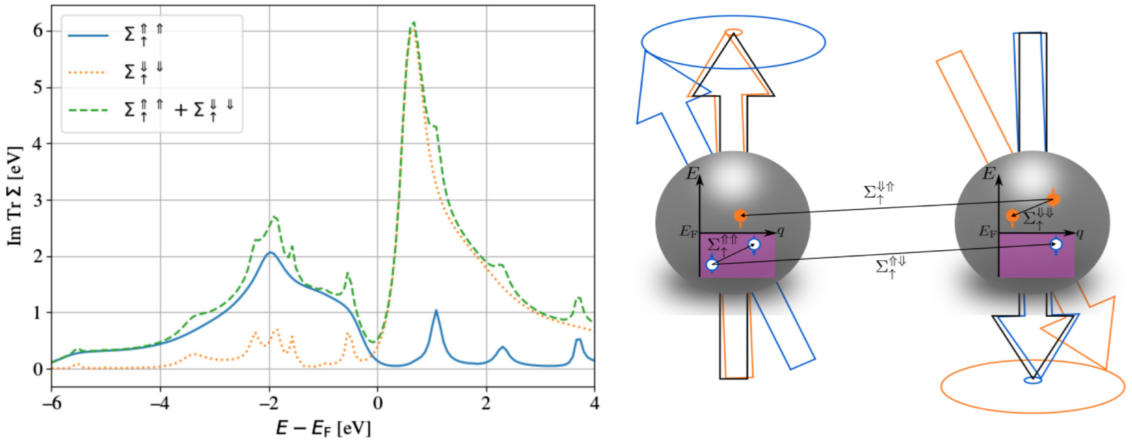


Figure 23: (left) The imaginary part of the up particle self-energy on up (⇑⇑) and down (⇓⇓) Cr sites. (right) Corresponding electron-magnon processes. The figure is reproduced from [C4].

processes are equally available. An up hole decays by emitting a Stoner-type magnon which occurs primarily on the Cr⇑ sites owing to the large amplitude for these magnons there. An up electron couples to an anti-Stoner magnons, featured primarily on the Cr⇑ atoms.

5.5 Paramagnon-driven superconductivity

In [C21] we investigated whether the electron-paramagnon coupling emerging from our theory is capable to drive superconducting phase transitions in the pnictide family [51, 151, 215–218], taking FeSe as a representative example. The coupling can hardly originate from the very weak electron-phonon coupling [219]. A challenge in the description of FeSe is the sensitivity of its electronic structure and magnetism to the position of Se, z_{Se}. Standard functionals of the DFT are unable to predict the position correctly from the total energy calculations. The missing ingredient is believed to be the spin fluctuations themselves [216] but no detailed calculations seem to be available for FeSe. In order to overcome this difficulty, we investigated different $z_{\mathrm{Se}} < z^{c}_{\mathrm{Se}}$, cf. Sec. 2.2. It turns out that the transition temperature $T_c(z_{\mathrm{Se}})$ saturates before z^{c}_{Se} is reached. In this regime, the large paramagnon fluctuations described in Sec. 2.2 yield $T_c = 32\mathrm{K}$ which is reduced to $T_c = 24\mathrm{K}$ by including detrimental effects as Coulomb repulsion. Thus, it turns out that the spin-fluctuation mediated paring is capable of inducing the superconducting order. However, the predicted value is higher than the experimental one of 8K which shows that the full understanding of this material family is yet to be achieved, in particular concerning the faithful description of its ground state.

5.6 The impact of magnon-electron scattering on spin dynamics

In the preceding sections we have seen that the coupling of magnons to electrons clearly renormalizes the properties of the latter. On the other hand, we can legitimately ask whether the coupling memorializes the magnon properties as well. We already considered the first obvious consequence at length, the Landau damping. Here, the single particle Stoner excitations couple to magnons augmenting them with a self-energy which leads to the damping and the energy renormalization. However, there is one further, more subtle influence of the electron-magnon coupling on the spin dynamics. Indirectly, the magnon-induced renormalization of the electronic bands self-consistently impacts the spin-wave spectrum as well and focused on this issue in our recent paper [C3].

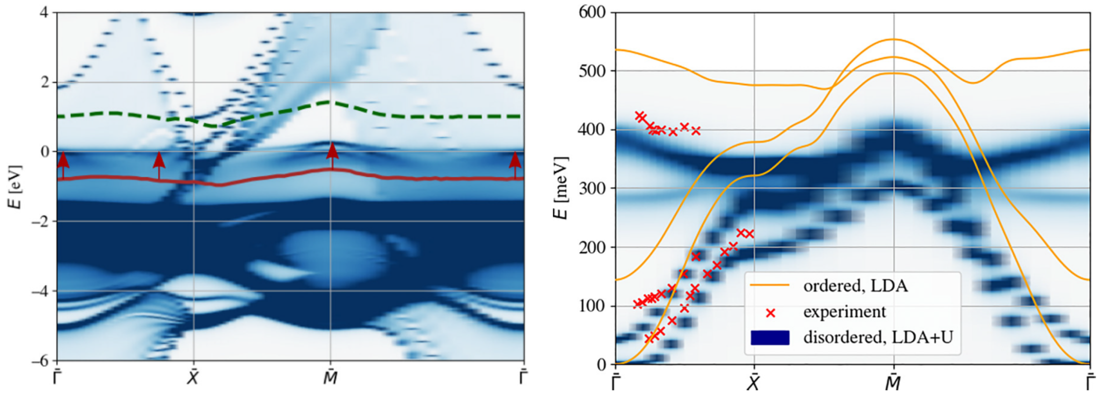


Figure 24: 3 ML Co/Cu(100). (left) The majority spin carrier band structure renormalization due to the magnon-electron interaction. The red line denotes the LSDA d-band and the red arrows its shift following the inclusion of the magnon-electron interaction. (right) The resulting softening of the magnon modes. The figures are reproduced from [C3].

The magnons affect primarily the majority spin holes and lead to the sizable reduction of the Stoner splitting, as evident from Fig. 24a. In turn, this leads to the softening of the magnons modes, bringing them into much better agreement with the existing SPEELS data, Fig. 24b. In short, this is a result of self-consistency. The magnons affect the electrons which in turn modify the magnon spectrum, etc.

5.7 Towards the *ab initio* theory of SPEELS

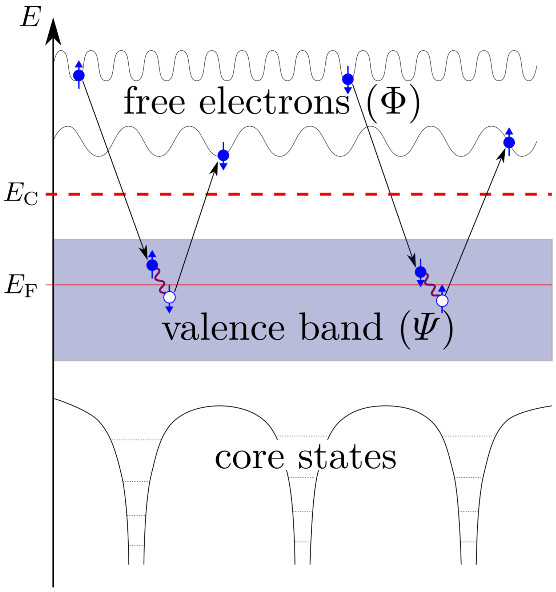


Figure 25: The SPEELS process and its characteristic energy scales, from [205]. Of interest here are processes in which the outgoing SPEELS electron is of spin opposite to the incoming one, as only those lead to the magnon excitations in the sample.

As discussed in the introduction section 1.2.3, the magnons of ultra-thin films cannot be efficiently investigated using INS. However, the magnetic scattering of electrons (SPEELS) allows to probe them in the entire two-dimensional Brillouin zone [C22]. As carefully discussed by Hong and Mills [220] this arises due to the different nature of the interaction of neutrons and SPEELS electrons with the sample. The long-ranged dipolar interaction of neutrons makes them mostly sensitive to spin-wave excitations. On the other hand, the electrons can uncover the signature of the Stoner excitations as well [221]. In short, this arises due to the strong Coulomb nature of the scattering between impinging electrons and the ones residing in the sample. As a consequence, the energy and momentum dependence of the cross-section in the INS is given (up to several factors) by the imaginary part of the transverse susceptibility $\chi^{\pm}(\mathbf{q},\omega)$ while in the case of SPEELS it involves substantially altered response function $\chi^{\mathrm{SPEELS}}(\mathbf{q},\omega)$.

Since the Coulomb interaction conserves the spin, the SPEELS process is necessarily of exchange character [108, 222, 223], cf. Fig. 25. A high-energy incoming SPEELS electron occupies a free state sample state above the Fermi level expelling an electron from below. The sample is left in an excited state with energy and momentum given by the corresponding losses of the SPEELS beam. The electron-hole undergoes repeated scattering leading to the formation of magnons. The ground state of the system must be understood as a true man-body wave function involving single electron states in a possibly broad energy window around the Fermi level E_F. However, it is assumed that both the incoming and outgoing SPEELS electrons dwell above the cut-off energy E_C being in essentially free single particle states (plane-waves) and not contributing the ground state of the sample. The last assumption allows to an easier perturbative treatment of the scattering processes.

The evaluation of χ^{SPEELS} involves thus not only the repeated scattering of electron and hole of opposite spins, the physical content of $\chi^{\pm}$, but also the Coulomb interaction of electrons in the sample and those in the beam. The evaluation of χ^{SPEELS} has been performed on the model level by Hong and Mills and the corresponding *ab initio* formulation within the KKR GF formalism has been given in [205]. The actual implementation is formidable due to the complicated form of the KKR GF and the convergence issues has not been fully solved so far. Thus, the first principles description of SPEELS process remains a work in progress.

6. Summary and outlook

This habilitation treatise exposed the author's works in several areas of contemporary theoretical solid-state physics. Advances in the *ab initio* description of spin excitations were presented concerning the ferri- and antiferromagnetic magnons [C24, C29], paramagnons [C27], the magnetic second sound (longitudinal spin excitations) [C16], and skyrmionic structures [C11, C18]. The description of non-Landau spin-wave damping was given [C3, C19, C20], in particular involving disorder and multi-magnon processes, establishing the hierarchy of the spin dynamics attenuation in conducting magnets. Next, the magnetic ground state and spin excitations of diverse functional materials were discussed [C6, C8–C10, C12, C15, C17, C21–C23, C25, C28, C30, C31], including altermagnets [C1]. Finally, an extended *ab initio* theory of the magnon-electron scattering was exposed [C3–C5, C7, C32]. Here, it is shown how the spin excitations can lead to the unconventional Cooper-paring, the spin-dependent band structure renormalization, the emergence of non-quasiparticle states, and the renormalization of the spin dynamics.

The field of *ab initio* description of spin dynamics has not reached its boundaries. The current goals of the theory are two-fold. On one hand, one strives to provide a faithful description of excitations in materials where the local spin density approximation fails. A prominent example here is provided by exotic superconductors, e.g., cuprates [153]. To achieve it, one must take into account a wide range of correlations effects both in the picture of the ground state as well as in the exchange correlation kernel. Especially the second task is far from its completion for magnets in contrast to the more mature approaches available for charge excitations [71]. One believes that the inclusion of correlations arising from electron-magnon coupling constitutes an important puzzle piece here [C3, 91].

On the other hand, there is an important physics waiting to be uncovered even upon staying with the local spin density approximation. Here, the spin dynamics of non-collinear magnets remains far from being fully charted. The ground state of such systems is relatively well understood [55, 58, 197] but much less is known about their spin excitations. At the same these excitations are believed to be of pronounced topological character [224–227] and likely to set new trends in the spintronics [10]. Closely related is the impact of relativistic corrections [89, 176, 228]. In particular, the SOC allows for a coupling of transverse magnons to the low-energy charge fluctuations, giving rise to the SOC-induced Landau damping. The magnitude of this effect is in general unknown and likely to bear strong material dependence. Last but not least, the magnons can interact with further quasiparticles and collective modes in solids which opens new decay channels for them. Currently, an actively investigated example is their coupling to phonons [184, 229, 230]. Last but not least, the description of the spin dynamics in the magnetic but atomically disordered systems has not been achieved within the LRTDDFT yet. (This is in in contrary to the paramagnetic case [84, 85].) Thus, the interplay between the disorder-induced and Landau damping is still not well understood. The methodology outlined in this treatise is currently being extended to account for all the aforementioned effects.

Ultimately, the quest for faithful description of yet a broader class of materials brings one to the realm of quantum chemistry. The electronic structure of molecules can hardly be realized using the methods developed for close packed solids. For this purpose, an implementation of the linear combination of atomic orbitals (LCAO) approach is currently being pursued [231–233]. To provide specific examples, this method paves the way to describe molecules absorbed on surfaces [234] and understand complex chemical processes, e.g., the photocatalytic water splitting [235].

Let us finally mention the extraordinary chance for the *ab initio* magnetism associated with the advent of quantum computing. The new paradigm promises to decisively alleviate the exponential algorithmic complexity associated with the exact solution of the electronic many-body problem [236–240]. With the true correlated many-body wave-functions at hand, the spectrum and further properties of spin excitations of a system can be extracted exactly. Alas, the dawning noisy intermediate-scale quantum (NISQ) era [241, 242] will hardly be able to treat the electronic system of solids in its full complexity. Nevertheless, the field of magnetism has already embraced the quantum computers and actively investigates complex correlated magnetic textures using them [243–245].

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List of Acronyms

2DEG two-dimensional electron gas

AF antiferromagnetic

ALSDA adiabatic local spin density approximation

ARPES angle resolved photoemission spectroscopy

bcc body centered cubic

CPA coherent potential approximation

DFT density functional theory

DMFT dynamical mean field theory

DMI Dzyaloshinskii–Moriya interaction

fcc face centered cubic

FM ferromagnetic

FWHM full-width at half-maximum

GF Green’s function

INS inelastic neutron scattering

KS Kohn-Sham

KKR Korringa-Kohn-Rostoker

LRTDDFT linear response time-dependent density functional theory

LSDA local spin density approximation

MBPT many-body perturbation theory

ML monolayer

RIXS resonant inelastic X-ray scattering

RPA random phase approximation

SOC spin-orbit coupling

SPEELS spin-polarized electron energy loss spectroscopy

TDDFT time-dependent density functional theory

VCA virtual crystal approximation

xc exchange-correlation

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Eidesstattliche Erklärung

Hiermit erkläre ich, dass ich die Habilitationsschrift selbstständig und ohne fremde Hilfe verfasst und andere als die angegebenen Quellen und Hilfsmittel nicht benutzt und die den benutzten Werken wörtlich oder inhaltlich entnommenen Stellen als solche kenntlich gemacht habe.

Linz, 17. Juni 2025

Dr. Paweł Adam Buczek

Appendix: Own works

This appendix contains the cumulative list of author's works accrued after the completion of his doctorate and constituting this habilitation treatise.

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