Spin-orbit coupling induced spin dynamics in metals and semiconductors

Thesis booklet

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Introduction

Understanding the basic transport phenomena during the first half of the 20th century was vital in the success of conventional electronics, which in turn revolutionized all aspects of humankind. It was recognized back in 1965 that the computing capacity growth is exponential, which is now known as the Moore's law [1]. Although Moore's law has been followed quite well throughout the past 5 decades, this unparalleled growth of computing and storage power may come to an end soon, which is dictated by the fundamental limits of quantum transport phenomena.

Conventional electronics operates essentially with a control over the number of electrons (or flow of electrons) in the devices for both information storage and manipulation. The idea to use the intrinsic angular-momentum of electrons (also known as spin angular momentum or shortly spin), for the same purposes arose first in the 1990s with the first published appearance in 2001 by Wolf *et al.* [2], soon followed by an excellent review paper by Žutić, Fabian and Das Sarma [3]. The field was coined *spintronics* which reminds us that it uses *spin* and is related to elec*tronics*. The basic idea behind spintronics is that the electron spin is much less affected by the environment than the electron momentum. The earlier property is affected only through relativistic interactions (the spin-orbit coupling in this case), whereas the electron momentum is altered due to the much stronger Coulomb interaction. When devised and controlled wisely, the spin direction of an electron ensemble (or of a few electrons) could in principle be used for information storage and computing.

It turns out that the fundamental theory of spin relaxation needs to be developed prior to any successful implementation of spintronics. The reason is that a spin ensemble loses the coherence of its spin direction which is characterized by various spin-dephasing, spin-relaxation, or decoherence times (their origin and notations are clarified later). The longevity of the spin-relaxation time indicates how much time is allowed for the spin information manipulation and read-out. A fundamental property of spin relaxation is that it is a usually orders of magnitude slower process than the conventional momentum relaxation. As a result, spin transport is a diffusive process in most cases, i.e. the spin direction is retained over several momentum scattering events.

Two fundamental theories are known in the field which apply to the majority of cases: the so-called Elliott-Yafet theory [4, 5] is known to be valid in metals with inversion symmetry (which is the case for most elemental metals) and when momentum scattering is moderate, whereas the D'yakonov-Perel' theory [6, 7] applies when the inversion symmetry is broken (like in GaAs) and the momentum scattering is significant. Several questions might arise immediately from this description. To what extent can these theories be validated experimentally? What happens when the above conditions are not satisfied, i.e. for a metal with inversion symmetry when the momentum scattering is large or for GaAs when the momentum scattering is moderate? Can one provide a unified mathematical basis and a unified physical description for these two relaxation mechanisms?

Objectives

The present thesis was motivated by these open questions and herein I present my theoretical results which I made in this field along the above three questions. The results include an empirical verification of the Elliott-Yafet theory in metals with inversion symmetry [8], a Monte Carlo based approach which allows calculation of spin-relaxation time in materials without inversion symmetry for arbitrary value of the momentum scattering and spin-orbit interaction strength, it thus extends the D'yakonov-Perel' theory [9], and also an intuitive approach to unify the seemingly disparate theories which apply for materials with and without inversion symmetry [10].

This thesis is organized as follows: I introduce the basic theory of spin-orbit coupling and the theories of spin relaxation, which were known prior to this thesis. This includes the conventional Elliott-Yafet and D'yakonov-Perel' theories and also the advances made to the field in the group which has hosted me [11], as the present results are a continuation of those efforts. I present my results in three sections and conclude with presenting my thesis points. An Appendix is provided with algorithmic details and supplementary calculations.

Methods

I implemented a Monte Carlo method based simulation software for the calculation of spin-susceptibility and spin relaxation times in materials with broken spatial inversion symmetry. The time evolution of the electron states follow the Boltzmann equations, the individual electron spins are precessing around an intrinsic, $\boldsymbol{k}$-dependent magnetic field between scattering events due to the spin-orbit coupling. Momentum scatterings change the $\boldsymbol{k}$ wave number of an electron while it leaves its spin-state in place. The simulation keeps track of the random walk of the electron spins and the collective magnetization of the whole system. The spin susceptibility and the spin relaxation time can be deduced from the time-dependent magnetization of the electron ensemble.

New scientific results

1. I pointed out two shortcomings of the phenomenological Beuneu-Monod relation, which was developed to explain the spin-relaxation time in elemental metals by correlating the experimental electron spin resonance line-width with the so-called spin-orbit admixture coefficients and the momentum-relaxation theory. Namely that i) the momentum-relaxation involves the Debye temperature and the electron-phonon coupling whose variation among the elemental metals

was neglected, ii) the Elliott-Yafet theory involves matrix elements of the spin-orbit coupling (SOC), which are however not identical to the SOC induced energy splitting of the atomic levels, even though the two have similar magnitudes. I obtained refined values for the empirical spin-orbit admixture parameters for the alkali metals by considering the proper description of the momentum relaxation theory. [T1]

2. I developed a stochastic model for the calculation of the dynamic spin-susceptibility for materials without inversion symmetry for an arbitrary distribution of the spin-orbit coupling and for an arbitrary value of the quasiparticle scattering. The calculation yields numerically the spin-relaxation time. I validated the model by comparing its predictions to analytic calculations in the clean (no momentum scattering) and dirty limits (large momentum scattering) [T2].

3. Using the stochastic model, I studied the full phase space of spin relaxation as a function of SOC strength, its distribution, and the magnitude of the momentum relaxation rate. This allowed the identification of two novel spin-relaxation regimes; where spin relaxation is strongly non-exponential and when the spin relaxation equals the momentum relaxation. I also found a compelling analogy between the spin-relaxation theory and the NMR motional narrowing. Using the stochastic model, I calculated the dynamic

spin-susceptibility for a variety of SOC distributions [T2].

4. I developed an intuitive model which allowed the unification of the Elliott-Yafet and the D'yakonov-Perel' spin-relaxation mechanisms. I showed that the respective Hamiltonians of the two theories can be transformed to each other. I showed that the so-called generalized Elliott-Yafet theory, which was developed for the case of large momentum scattering, can be straightforwardly obtained using the D'yakonov-Perel' approach [T3].

5. I showed that the intuitive unification of the EY and DP theories not only provides an insight to the intimate relationship between the two theories but allows to numerically obtain spin-relaxation times using the stochastic approach, which was developed for the DP case. I presented that this can be successfully applied to calculate the experimentally determined spin-relaxation time in MgB_2, which shows a significant momentum scattering rate, it thus cannot be handled with the conventional Elliott-Yafet model [T3].

6. I developed an intuitive numerical tool which allows the separation of dephasing and spin-relaxation processes. The method essentially mimics the concept of the Loschmidt echo, i.e. it introduces a time reversal for the built-in magnetic fields and keeps track

of the resulting ensemble magnetization decay. I showed that the envelope of the Loschmidt echoes recovers the true spin-relaxation processes, which are otherwise unobservable due to strong dephasing [T4].

The publications related to the thesis points are as follows:

[T1] L. Szolnoki, A. Kiss, L. Forró, and F. Simon: *Empirical Monod-Beuneu relation of spin relaxation revisited for elemental metals*, Physical Review B **89**, 115113 (2014).

[T2] L. Szolnoki, A. Kiss, B. Dóra, and F. Simon: *Spin-relaxation time in materials with broken inversion symmetry and large spin-orbit coupling*, Scientific Reports **7**, 9949 (2017).

[T3] L. Szolnoki, B. Dóra, A. Kiss, J. Fabian, and F. Simon: *Intuitive approach to the unified theory of spin relaxation*, Physical Review B **96**, 245123 (2017).

[T4] L. Szolnoki, *et al.* manuscript in preparation

Additional publications

[T5] G. Fábián, B. Dóra, Á. Antal, L. Szolnoki, L. Korecz, A. Rockenbauer, N. M. Nemes, L. Forró, and F. Simon: *Testing the Elliott-Yafet spin-relaxation mechanism in KC_8: A model system of biased graphene*, Physical Review B **85**, 235405 (2012).

[T6] A. Kiss, L. Szolnoki, and F. Simon: *The Elliott-Yafet theory of spin relaxation generalized for large spin-orbit coupling*, Scientific Reports **6**, 22706 (2016).

[T7] B. G. Márkus, L. Szolnoki, D. Iván, B. Dóra, P. Szirmai, B. Náfrádi, L. Forró, and F. Simon: *Anisotropic Elliott-Yafet theory and application to* KC_8 *potassium intercalated graphite*, Physica Status Solidi B **253**, 2293 (2016)

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[8] L. Szolnoki, A. Kiss, L. Forró, and F. Simon, “Empirical monod-beuneu relation of spin relaxation revisited for elemental metals,” *Phys. Rev. B*, vol. 89, p. 115113, Mar 2014.

[9] L. Szolnoki, A. Kiss, B. Dóra, and F. Simon, “Spin-relaxation time in materials with broken inversion symmetry and large spin-orbit coupling,” *Sci. Rep.*, vol. 7, 2017.

[10] L. Szolnoki, B. Dóra, A. Kiss, J. Fabian, and F. Simon, “Intuitive approach to the unified theory of spin relaxation,” *Phys. Rev. B*, vol. 96, p. 245123, 2017.

[11] P. Boross, B. Dóra, A. Kiss, and F. Simon, “A unified theory of spin-relaxation due to spin-orbit coupling in metals and semiconductors,” *Scientific Reports*, vol. 3, p. 3233, 2013.