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Prof. Jan Trlifaj
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Re: Opponent review of the habilitation thesis of RNDr. Karel Carva, Ph.D.

The presented thesis deals with comprehensive theoretical investigations of the magnetization dynamics of conventional ferromagnets. This is an important topic of current interest, with many unresolved fundamental issues. Since the experimental discovery of the ultrafast demagnetization, there have been many attempts at its theoretical understanding. Several mechanisms for this phenomenon, which has a potential for applications in magnetic memory, have since been proposed. The difficulty in finding the relevant mechanism lies in the fact that there are many processes, either competing or working together, which occur in the dynamics of nonequilibrium magnetization. The thesis of Dr. Carva presents significant efforts by the author and collaborators towards the resolution of the problem, providing the physics community with quantitative arguments for assessing some of the relevant processes.

The thesis begins with a brief presentation of the physics foundations behind the research of Dr. Carva, on the magnetization dynamics and equilibrium magnetic properties of ferromagnets (and antiferromagnets). Dr. Carva gives an honest account of the approximations used in various state-of-the art methods. I find this chapter informative and I like the authoritative statements on the techniques, which are expected from an experienced researcher.

In chapter 3 the results of the extensive research on equilibrium properties of magnetic impurities in topological insulators, and of ferromagnets are given. Based on DFT calculations, Dr. Carva has mapped the spectra of these magnetic systems to a Heisenberg model, and obtained critical temperatures using Monte-Carlo simulations. These are standard approaches in this field, the results obtained are reasonable considering the approximations made. The analysis is rather insightful. Chapter 4 deals with DFT calculations of the spin torque of magnetic systems. In particular, the spin-mixing conductance, which is the key quantity for evaluating the torque according to a leading interfacial spin-polarized transport model, is computed. These calculations are highly nontrivial, and very useful for estimating spin dynamics due to spin-polarized current.

The author has made most important contributions in the field of ultrafast demagnetization, presented in chapter 5, which is most extensive. This topic has attracted great interest on the part of theory, although the ultimate mechanism remains, in my view, still elusive, despite great strides towards a unified picture. Nonequilibrium magnons, phonons, and electron spins are all involved. Their interplay is a rather complex process whose realistic quantitative evaluation is likely beyond the current computational abilities. One approach, executed by the author, invokes spin-flip processes due to spin-orbit coupling. In a crystal lattice, spin-orbit coupling itself does not relax spin. One needs momentum scattering as well. This usually comes from phonons (impurities tend to play a role at low temperatures). To faithfully evaluate phonon-induced spin relaxation in realistic systems requires knowledge of the electronic and phonon spectra, as well as the electron-phonon coupling, modulated by spin-orbit interactions. Modern DFT codes are capable of rendering this interaction, thus allowing to obtain quantitative estimates for spin relaxation. Previously, such calculations were performed for nonmagnetic systems. Dr. Carva has pioneered this field for magnetic metals, by conducting first investigations of this particular demagnetization mechanism. Although the results show that this is not the mechanism behind the ultrafast demagnetization, the evaluated spin lifetimes are very important for understanding the diffusion and relaxation of the nonequilibrium spin in the linear response regime in ferromagnets. I am impressed with the corresponding publication, in which Dr. Carva is the first author [Physical Review Letters, 107, 207201 (2011)] in which a specific calculation of the spin-flip Eliashberg function for Ni is given. Such a calculation is difficult both conceptually and numerically, and was done previously using semiempirical approaches. The methodology of Dr. Carva is based on relativistic density functional techniques, whose implementation for the particular problem of the Elliott-Yafet scattering is particularly challenging. Dr. Carva has succeeded this pioneering task.

In addition, Dr. Carva also performed important simulations of the magnetization dynamics in realistic settings, including optical excitations, using kinetic equations approaches.

I find the research contributions of Dr. Carva to the field of magnetization dynamics as pioneering, important for interpreting ongoing experiments and for motivating further theoretical research. The papers of Dr. Carva on these topics are very well cited and recognized internationally. Dr. Carva has been using and developing state-of-the-arts methods within the first-principles codes, extending the application of DFT techniques to study a variety nonequilibrium processes.

To conclude, considering the high scientific quality of the research summarized in the thesis, and of the scholarship demonstrated in the many publications on which the thesis is based, I recommend granting the habilitation (DrSc) title to Dr. Carva.

Sincerely,

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Prof. Dr. Jaroslav Fabian