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## ACCEPTED MANUSCRIPT

### Spin-lattice relaxation beyond Gilbert damping

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#### Abstract

A combined dynamics for the spin and lattice degrees of freedom is proposed. For that we couple a Heisenberg spin Hamiltonian via a distance dependent exchange integral and an anisotropic correction to the lattice, where the latter is formed by a harmonic potential. With these extensions the transfer of energy as well as angular momentum between lattice and spins is possible. We test this model successfully by reproducing the Einstein-De Haas effect for a free cluster. On the other hand we find severe differences of the temperature dependent demagnetization dynamics of the new approach as compared to the well-established magnetization dynamics covered by Gilbert damping.

Keywords: Magnetic damping, Spin-lattice coupling, Classical spin models

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#### 1. Introduction

Since the discovery of ultrafast magnetization processes [1] the flow of energy and angular momentum between spin, electron, and phonon degrees of freedom, their underlying microscopic mechanisms and associated time scales move in the focus of current research. Experiments lead to the conclusion [2] that efficient channels exist for the spin angular moment to dissipate into the lattice. However, this phenomenon and its underlying mechanisms are still controversially discussed [3, 4, 5, 6, 7].

Improved imaging techniques allow to track even atomic movement on ultrashort time scales during magnetization processes[8, 9, 10]. These experiments are available now to examine the mechanisms of spin-lattice coupling fundamentally, fostering an interest in theory and modeling of these interactions. Furthermore, spin-lattice coupling is very important in the field of spin-caloritronic transport in insulators, where the lattice and spin subsystem are on different temperatures, leading to a flow of energy and angular momentum between both systems [11].

The most common way for modeling dissipative magnetization dynamics is to assume one single phenomenological damping parameter which represents the coupling of the magnetic systems to a heat-bath. This parameter is used in the equation of motion, normally the Landau-Lifshitz-Gilbert equation (LLG) [12, 13]. This approach completely neglects any subtleties coming from the interactions of the spins with the electrons and the lattice, respectively. The challenge in this context is to explain the damping processes on a microscopic basis. While the coupling to the electronic reservoir [14, 15, 16, 17] and the intrinsic magnon scattering processes [18] have been discussed before, atomistic models which determine the coupling to the lattice directly are still rare [19, 20, 21, 22, 23]. The reason for that is the enormous effort in *ab-initio* calculations to treat the spin-orbit interaction, which allows for the necessary transfer of spin angular momentum into the lattice. As one needs the full electronic structure of the material, the numerical complexity restricts the size of the samples to a few atoms. Otherwise one has to assume perfect lattice symmetries and cannot take distortions through, e.g.,

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