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Ferromagnetic model system with spin-orbit coupling: Dynamical gap and effective spin-flip scattering

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ABSTRACT

We investigate ultrafast magnetization dynamics due to electron-phonon interaction in a ferromagnetic Rashba model, which includes spin-orbit coupling and a Stoner mean-field splitting. By computing the reduced spin-density matrix including explicitly spin-independent electron-phonon scattering at the level of Boltzmann-type scattering integrals, we investigate the influence of a time-dependent Stoner mean field on the magnetization dynamics. We find that the dynamical gap increases the magnetization quenching on short timescales and slows down the remagnetization process. We further show how the noncollinear dynamics of electronic spins in the band structure with internal spin orbit fields can be approximated by effective spin-flip scattering matrix elements.

1. Introduction

The measurement of ultrafast (sub-ps) demagnetization in ferromagnetic materials after ultrashort laser pulses [1] has led to a new field of research with very promising prospects for applications in data storage. Different models are used to describe these ultrafast magnetization dynamics, one of the more prominent being the phenomenological three temperature model (3TM) that separates the three systems “spin”, “electrons” and “lattice” and couples them with different relaxation times to each other. Extensions to this model (e.g. the μ3TM [2]) or completely different approaches like the Langevin theory with stochastic fields [3], time-dependent density functional theory [4], or hot-electron transport [5] consider additional/different aspects, but there is yet no complete *microscopic* theory that can explain the observed ultrafast demagnetization and remagnetization behavior from first principles. This is mainly due to the large variety of effects that possibly play a role in these ultrafast dynamics (coherent interactions with the photons of the laser, redistribution of spin and orbital angular momentum, incoherent processes like scattering between electrons, phonons, magnons, etc.), and it is difficult to disentangle the different contributions.

Here, we analyze a simplified ferromagnetic model system with spin-orbit coupling. In this way, we can include the band structure of the model, the laser/heat-induced dynamics and the incoherent scattering with phonons in a unified framework, i.e., at the level of a quantum mechanical hamiltonian. We focus on incoherent electron-phonon scattering as the mechanism responsible for the incoherent electronic dynamics, as this is widely believed to be one of the most important contributions to demagnetization dynamics. A commonly used picture for magnetization dynamics resulting from electron–phonon scattering is the Elliot-Yafet mechanism, i.e., the change of the ensemble spin via microscopic spin-flip transitions, but as we have shown recently, this description is not always valid and depends on the internal effective fields and the momentum scattering time [6]. In Ref. [6] we also found that because of the large exchange splitting in ferromagnets, the precessional (noncollinear) electronic spin dynamics around internal fields can be approximated by a collinear spin-flip scattering process.

The purpose of this paper is twofold. First, we want to further investigate the approximation of the noncollinear electronic dynamics by spin-flip scattering. Second, we want to focus on the effect of a time-dependent Stoner mean-field splitting on the electronic spin dynamics. While the electron–phonon interaction is too weak to be responsible for ultrafast demagnetization in a fixed band structure [7,8], it has already been shown that the demagnetization can be accelerated and enhanced in a collinear dynamical calculation [9]. We go beyond this earlier work by including the internal effective magnetic fields and by investigating the effect of the dynamical Stoner gap in such a noncollinear calculation.

The paper is organized as follows. In Section 2 we introduce our model system and the dynamical equations for the reduced spin-density matrix. In Section 3 we present the excitation conditions for the

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magnetization dynamics and we investigate the effects of a time-dependent band structure on the electron spin dynamics in Section 4. Finally, in Section 5 we look at different simplifications/approximations to the dynamical equations that describe the spin dynamics in our model system and study their influence on the dynamics.

2. Model

We use a Rashba model with ferromagnetism at the level of a Stoner mean-field that has been discussed in Ref. [6]. It describes itinerant electrons in a thin ferromagnetic film with out-of-plane magnetization and Bychkov-Rashba spin-orbit coupling. It has a two-dimensional k-space and the electronic states are described by a model Hamiltonian that consists of three terms

$$\widehat{H}_{\mathrm{e}} = \widehat{H}_{\mathrm{kin}} + \widehat{H}_{\mathrm{Stoner}} + \widehat{H}_{\mathrm{Rashba}}. \tag{1}$$

In the spin $|\uparrow, \downarrow\rangle$-basis this Hamiltonian is given by

$$\widehat{H}_{\mathrm{e}} = \begin{pmatrix} E_{\mathrm{kin}} + \Delta_z & -i\alpha k e^{-i\varphi_{\mathbf{k}}} \\ i\alpha k e^{i\varphi_{\mathbf{k}}} & E_{\mathrm{kin}} - \Delta_z \end{pmatrix}, \tag{2}$$

where the $\varphi_{\mathbf{k}}$ and k correspond to the angle and the value of $\mathbf{k}$ in the x-y-plane respectively, α is the Bychkov-Rashba parameter and Δ_z the splitting due to the ferromagnetic Stoner contribution. Diagonalizing the hamiltonian (2) yields two bands (labeled "$\nu = +$" and "$\nu = -$"), which are separated by the Stoner (exchange) splitting. For more details regarding the different contributions to the Hamiltonian as well as its analytically known eigenstates and -energies refer to e.g. Refs. [6,10].

The important point for the following section is the spin-dependence of the Stoner splitting, i.e., $\Delta_z = -\frac{2}{3} U_{\mathrm{eff}} \langle \hat{\sigma}_z \rangle$ where U_{eff} is the Stoner parameter and the Pauli matrix in z-direction $\hat{\sigma}_z$ is directly connected to the dimensionless ensemble spin-expectation value $S = \frac{1}{2}\langle \hat{\sigma}_z \rangle$.

We derive the dynamics of the electronic system due to electron–phonon interaction for the reduced spin density matrix $\rho_{\mathbf{k}}^{\nu\nu'} = \langle c_{\mathbf{k}\nu}^{\dagger} c_{\mathbf{k}\nu} \rangle$ where $c_{\mathbf{k}\nu}^{\dagger}$ and $c_{\mathbf{k}\nu}$, respectively, create and annihilate an electron in the single-particle state $|\mathbf{k}, \nu\rangle$, which are the eigenstates of $\widehat{H}_{\mathrm{e}}$ and where $\nu \in \{+,-\}$ enumerates the bands. The equation of motion (EOM) for the reduced spin density matrix

$$\frac{\partial}{\partial t}\rho_{\mathbf{k}}^{\nu\nu'} = \frac{\partial}{\partial t}\rho_{\mathbf{k}}^{\nu\nu'}\bigg|_{\mathrm{coh}} + \frac{\partial}{\partial t}\rho_{\mathbf{k}}^{\nu\nu'}\bigg|_{\mathrm{scat}} \tag{3}$$

consists of two contributions, the first term describes a coherent precession around k-local effective fields, the second term describes spin-conserving electron–phonon scattering terms similar to Boltzmann-scattering integrals. For more details on the EOM as well as consequences arising from the spin-conserving nature of the scattering contribution see again Refs. [6,10].

As stated above, we focus here on the dynamic adjustment of the single-particle states throughout the dynamics due to the changing mean-field contribution from the ensemble spin expectation value S in the Stoner splitting Δ_z and compare them to earlier calculations done for fixed states.

3. Excitation conditions, effective temperatures, etc.

Here we describe the initial conditions for the dynamics and introduce quantities of interest that characterize the electronic dynamics. All calculations below use our standard parameters $U_{\mathrm{eff}} = 720$ meV and $\alpha = 30$ meV nm, an electron density $n_e = 1\ \mathrm{nm}^{-2}$ and an equilibrium temperature $T_{\mathrm{eq}} = 70$ K, which is also the temperature of the phonon bath and lies well below the Curie-temperature $T_{\mathrm{C}} = 514$ K.

We self-consistently calculate the equilibrium configuration of the system for our standard parameters by fitting the chemical potential μ_{C} so that the correct electron density is achieved. The laser excitation is modeled by an instantaneous heating of the electronic system to an elevated temperature $T_{\mathrm{e}} \gg T_{\mathrm{eq}}$ by adjusting the distribution functions to the higher temperature while maintaining the electron density *in each band*. This leads to a small change of the ensemble spin due to the different projections of the effective fields on the z-direction for different k, a difference of the chemical potentials between the + /−-bands and to a non-equilibrium between electronic system and phonon bath.

Starting from an instantaneous heating of the self-consistently determined equilibrium state, we solve the equations of motion (3). From the time-dependent reduced spin-density matrix, we compute three quantities to characterize the dynamics of the electronic system, the *ensemble spin* S, the effective *temperature* T and the chemical potentials $\mu_{\mathrm{C}}^{\pm}$ *for each band*. The ensemble spin is given by $S = \frac{1}{2}\langle \hat{\sigma}_z \rangle = \frac{1}{2}\sum_{\mathbf{k},\nu\nu'} \langle \mathbf{k}, \nu | \hat{\sigma}_z | \mathbf{k}, \nu' \rangle \rho_{\mathbf{k}}^{\nu\nu'}$. Note that our system is isotropic in the x-y-plane which is why the in-plane components cancel each other out. The effective temperature is defined by the following procedure. We calculate the total energy E of the system and then adjust the effective temperature T of a fictitious Fermi–Dirac equilibrium distribution so that its total energy matches the current energy of the system. The temperature determined in this way is a quantity suitable to describe energy relaxation for short times, where a strong non-equilibrium is present. The chemical potentials are calculated using the current temperature T of the system by fitting equilibrium distributions to the electron densities for each band separately. The chemical potentials are therefore a means to measure the extent of the non-equilibrium via the discrepancy between μ_{C}^{+} and μ_{C}^{-}.

4. Dynamical band structure

In Refs. [6,10], we determined the electronic band structure during the self consistent search for the ground state and kept it fixed throughout all calculations to this equilibrium configuration. In Fig. 1(a) we plot the dynamics, i.e., ensemble spin, chemical potentials and effective temperature for the dynamics computed including all terms of (3) and the excitation conditions described in the last section for this fixed band structure.

In Fig. 1(b) we plot the same quantities but now for a calculation with a time-dependent Stoner mean-field. This means that we use the ensemble spin S at each time step—modulo$\frac{1}{2}$—to determine the Stoner-splitting part Δ_z of the Hamiltonian (2). This changes the eigenenergies and states and thus the quasiparticle band structure. Because of this change of the quasiparticle energies and states we transform the spin density matrix at each time step to the instantaneous basis during the calculation. There are several similarities and differences regarding these two scenarios. The ensemble spin S reveals the most obvious difference: The demagnetization for the dynamic band structure is faster and more pronounced while the remagnetization takes about one order of magnitude longer. We can explain the stronger and faster demagnetization by an expanding scattering phase space during the beginning of the dynamics. The dominant contribution to the spin dynamics is the *inter*band scattering. Due to the shrinking exchange (Stoner) splitting, hot electrons in the high energy part of the lower (majority electron) band at larger k have more time to scatter to the low energy part of the upper (minority electron) band at smaller k and thus contribute to a reduction of spin polarization and thus demagnetization. In the case of the constant exchange splitting these states would already lie under the bottom of the upper band.

The longer remagnetization time can be explained with the same argument: The nearly equilibrated electrons in the upper (minority electron) band have less phase space to scatter into the lower (majority electron) band, since the possible final states are below the chemical potential resulting in a Pauli-blocking.

The dynamics of the temperature and thus the energy relaxation are very similar for the case without and with dynamic exchange splitting, so that the cooling effect of the electron–phonon scattering, which occurs dominantly by *intra*band scattering, is only weakly affected.