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THERMAL ACTIVATION, MAGNETIZATION DYNAMICS, DISSIPATION, NUMERICAL MODELLING

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In this lecture we will discuss different timescales in the magnetisation dynamics starting from femto-second ultra-fast demagnetisation and ending with long-time thermal stability (up to years). In the intermediate timescale the thermal magnetisation dynamics (nanoseconds) and the magnetic viscosity problem (seconds) will be described. We will outline relevant thermal and dissipation mechanisms and numerical models which could allow evaluation of the magnetisation dynamics at each timescale (see Fig.1). The necessity of multi-scale approaches [1] will be stressed.

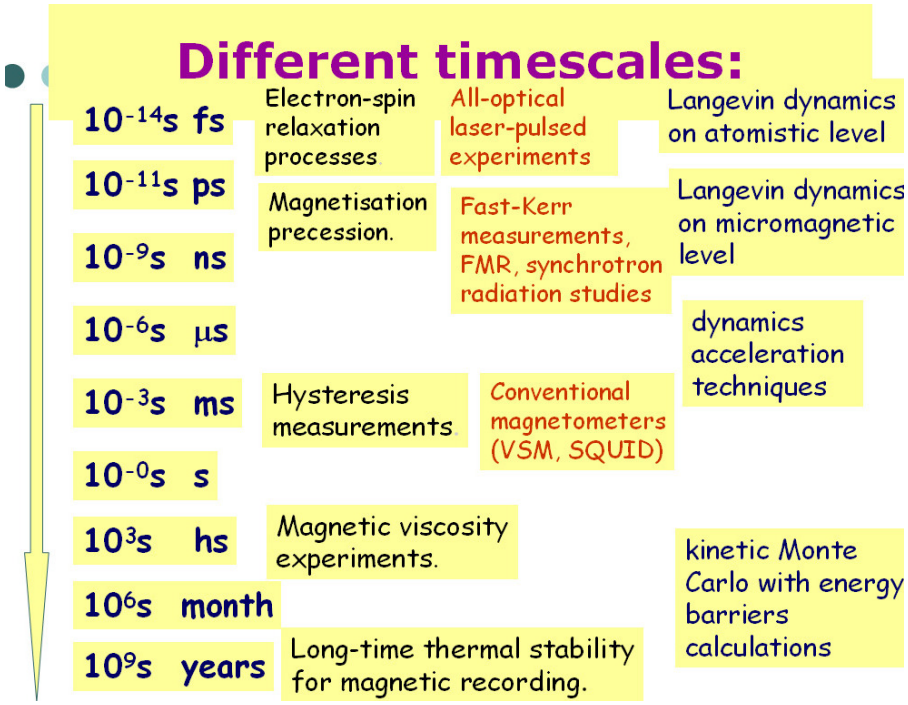

Fig.1 Different timescales for the magnetisation dynamics including typical measurements techniques and corresponding numerical methods.

We will start with **short-time magnetisation dynamics.** This first will be considered in relation to the classical problem of the ferromagnetic resonance (FMR) [2]. For the FMR problem we will discuss main energy relaxation processes such as spin-phonon, spin-impurity and spin-spin relaxation channels. The magnetisation dynamics is typically described in terms of the precessional equation of motion with Landau-Lifshitz (LL) phenomenological dissipation term :

$$\frac{d\vec{M}}{dt} = -\gamma'_0 \left[\vec{M} \times \vec{H}\right] - \alpha_{LL}\left[\vec{M} \times \left[\vec{M} \times \vec{H}\right]\right] \tag{1}$$

or the Gilbert damping term:

$$\frac{d\vec{M}}{dt} = -\gamma_0 \left[\vec{M} \times \vec{H}\right] - \alpha_G \gamma_0 \left[\vec{M} \times \frac{d\vec{M}}{dt}\right] \tag{2}$$

where $\vec{M}$ is the magnetisation vector satisfying $M^2 = M_s^2$ (saturation magnetisation value) and $\vec{H}$ is the effective magnetic field containing Zeeman, exchange, anisotropy and magnetostatic contributions. The two equations are mathematically equivalent provided that the parameters are renormalized:

$$\gamma'_0 = \frac{\gamma_0}{1 + \gamma_0^2 \alpha_G M_s^2}, \qquad \alpha_{LL} = \frac{\gamma_0^2 \alpha_G}{1 + \gamma_0^2 \alpha_G M_s^2} \quad . \tag{3}$$

The Gilbert form of the damping is known to give more physically reasonable results in terms of the dependence of the relaxation time on the damping parameter. The Gilbert equation transformed into the LL equation form is known as the Landau-Lifshitz-Gilbert (LLG) equation and is the most widely used model. An alternative macrospin approach historically used for nuclear and electron paramagnetic resonance is the Bloch-Bloembergen damping:

$$\left(\frac{d\vec{M}}{dt}\right)_{X,Y} = -\gamma_0 \left[\vec{M} \times \vec{H}\right]_{X,Y} - \frac{1}{T_2} M_{X,Y}$$

$$\left(\frac{d\vec{M}}{dt}\right)_{Z} = -\gamma_0 \left[\vec{M} \times \vec{H}\right]_{Z} + \frac{1}{T_1}(M_s - M_Z), \tag{4}$$

where T_1 and T_2 are the longitudinal and transverse characteristic relaxation times.

We will discuss the phenomenological character of the damping term and show several examples when its form can be justified.

Thermal fluctuations have been introduced to the magnetisation dynamics by W.F.Brown [3] for a collection of small non-interacting magnetic particles based on two approaches (i) the fluctuation-dissipation theorem and (ii) the Fokker-Plank (FP) equation. For a generalization to the system of interacting magnetic moments (and thermal micromagnetics) see Ref.[4]. The approach (known as the Langevin dynamics) consists of adding an additional random fluctuation term with the properties consistent with the thermodynamic equilibrium. Both the fluctuation-dissipation theorem and the requirement of the equilibrium Boltzman solution to the FP equation give the following properties of the random noise term (white noise) in Eq.(1) for field components and different atomic sites:

$$\left\langle h_{th}^{i} \right\rangle = 0, \quad \left\langle h_{th}^{i}(t) h_{th}^{j}(0) \right\rangle = \frac{2\alpha_{LL} k_B T}{\Delta t} \delta_{ij} \delta(t) \tag{5}$$

Here Δt is the integration time step. The white-noise properties of Eq.(5) effectively mean the separation of timescales, i.e. it assumes that spin dynamics is slower than the corresponding phonon and electron dynamics, whose role is to produce a thermal bath.

On the atomistic level (Heisenberg model) the thermal equation (1) with (5) correctly describes the Curie temperature. However, on the micromagnetic level this approach is not correct (see Fig.2). This happens due to the fact that the Curie temperature is defined by short wavelength spinwaves which are cut in the micromagnetic approach.

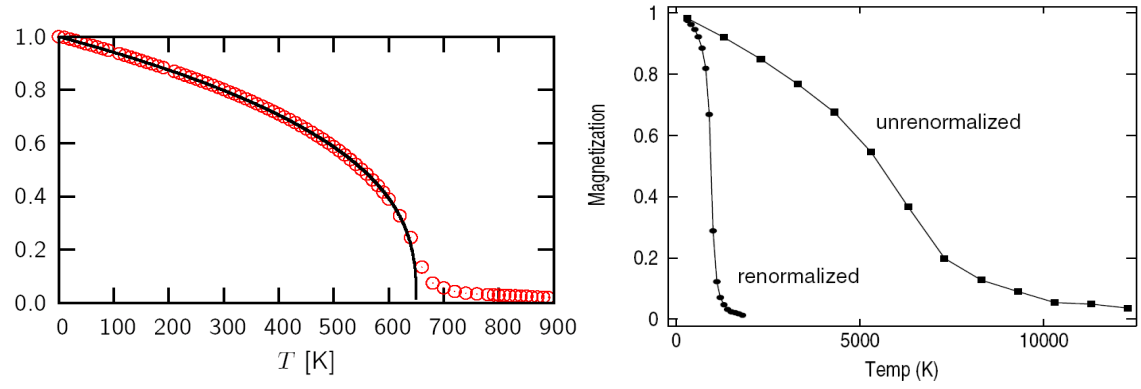

Fig.2 Numerical modelling results for magnetisation versus temperature using the Langevin dynamics: (left) from Ref.[1]: Atomistic model for FePt, showing the correct Curie temperature (right) from Ref.[5]: Micromagnetic model (unrenormalized). The renormalization group approach is suggested in this article to correct for the Curie temperature.

A more thermodynamically consistent approach is the Landau-Lifshitz-Bloch (LLB) micromagnetic equation, derived by D.Garanin [6] within mean field approximation (MFA) from the classical Fokker-Planck equation for atomistic spins interacting with a heat bath and from the corresponding density-matrix in the quantum case. The macrospin LLB equation has been shown to be a valid micromagnetic equation at all temperatures, even above T_c [7]. We write the LLB equation as follows:

$$\dot{\vec{m}} = \gamma_0 \left[\vec{m} \times \vec{H}_{eff}\right] + \frac{\gamma \alpha_{\parallel}}{m^2}\left[\vec{m} \cdot \left(\vec{H}_{eff} + \xi_{\parallel}\right)\right]\vec{m} - \frac{\gamma \alpha_{\perp}}{m^2}\left\{\vec{m} \times \left[\vec{m} \times \left(\vec{H}_{eff} + \xi_{\perp}\right)\right]\right\} \qquad (6)$$

Here $\vec{m} = \left\langle \vec{s} \right\rangle_{th}$ is the thermally averaged spin polarisation, the total effective field if given by the external, anisotropy, exchange fields and entropy correction, respectively:

$$\vec{H}_{eff} = \vec{H}_{ext} + \frac{1}{\chi_{\perp}}(m_x \vec{e}_x + m_y \vec{e}_y) + \vec{H}_{exch} + \begin{cases} \frac{1}{2\chi_{\parallel}}\left(1 - \frac{m^2}{m_s^2}\right)\vec{m} & T < T_c \\ \frac{J_0}{\mu_s}\left(1 - \frac{T}{T_c} - \frac{3}{5}m^2\right)\vec{m} & T > T_c \end{cases}$$

$\chi_{\perp}, \chi_{\parallel}$ are perpendicular and longitudinal susceptibilities; the longitudinal and transverse damping parameters are temperature dependent $\alpha_{\parallel} = 2\lambda T / 3T_c \quad \alpha_{\perp} = \lambda(1 - T/3T_c)$ for $T<T_c$ and $\alpha_{\perp} = \alpha_{\parallel}$ for $T>T_c$, λ is the atomistic coupling-to the bath constant, J_o is the zero-Fourier component of the exchange integral and μ_s is the atomic moment . The thermal fields have the following properties:

$$\left\langle \xi^i_{\parallel,\perp}(t)\xi^j_{\parallel,\perp}(t')\right\rangle = \frac{2k_B T}{\gamma \alpha_{\parallel,\perp} M_s(T=0)V_i}\delta_{ij}\ \delta(t-t')\delta_{\parallel,\perp} \qquad (7)$$

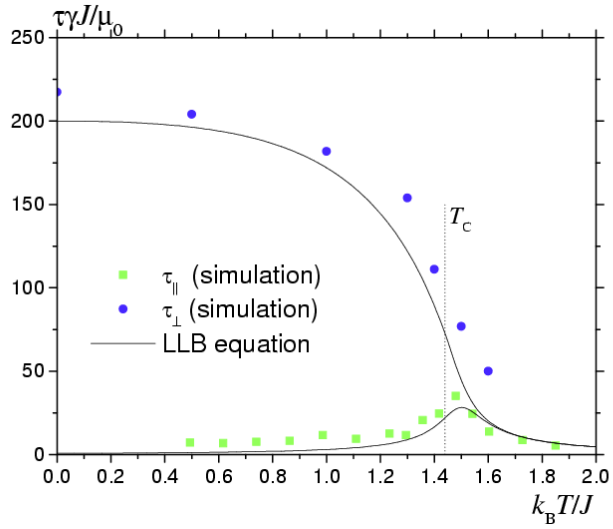

Fig.3 Longitudinal and transverse relaxation time as a function of temperature modelled within atomistic approach (symbols) and one macrospin LLB equation (line) from Ref.[7]

In the ultra-short timescale (femto-pico seconds) the dynamics is governed by the non-equilibrium electron, phonon and spin dynamics and the energy transfer (scattering processes) between different subsystems. The electron and phonon dynamics should be considered explicitly and is normally described in terms of the two-temperature (2T) model [9].

$$C_e \frac{dT_e}{dt} = -G_{el}(T_e - T_l) + P(t),$$

$$C_l \frac{dT_l}{dt} = G_{el}(T_e - T_l),$$

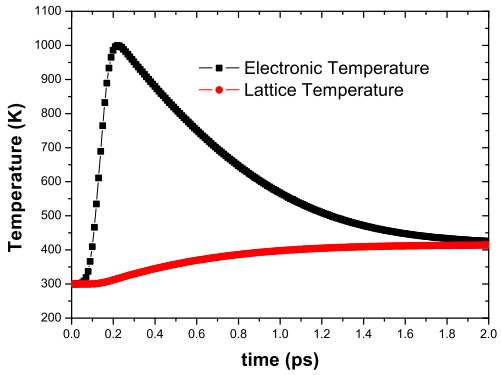

Fig.4 The two-temperature model (left) and the dynamics of the electron T_e and phonon T_l temperatures: The parameters are the following C_e and C_l are electron and phonon specific heats G_{el} – electron-phonon coupling constant, the function $P(t)$ describes the laser pulse.

During the laser-induced ultra-fast magnetisation dynamics the temperature is increased up to and even above Tc. The magnetisation dynamics could be coupled in the atomistic approach (or using the micromagnetic LLB equation (iii)) to the electron temperature T_e in the 2T model. This gives results in agreement with the experiment [9] (see Fig. 5)

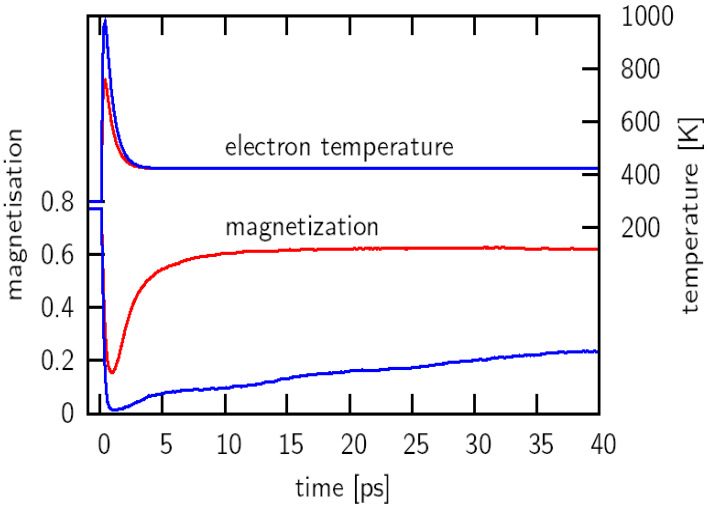

Fig. 5. Atomistic modelling of spin dynamics at the femto and pico-second timescale, for two laser pump fluencies, showing femto-second demagnetisation and pico-second magnetisation recovery (from Ref.[1]).

However at the femtosecond timescale the assumption of the separation of timescales for the white-noise approximation (5) may be violated. For this case we suggested the use of the Miazaki-Seki approach [10] which takes into account the correlated noise and avoids the application of the fluctuation-dissipation theorem directly to the spin system.

Finally, we will describe the problem of **long-time magnetisation dynamics,** related to magnetic viscosity measurements and long-time thermal stability. The long-time thermal decay occurs due to the possibility to overcome thermally energy barriers in magnetic systems. The probability is given by the Arrenius-Neél formula:

$$f = f_0 \exp\left(-\Delta E / k_B T\right) \tag{8}$$

Where f_0 is the temperature, field, etc.-dependent reversal frequency, ΔE is the energy barrier (normally also temperature dependent), k_B is the Boltzaman constant and T is the temperature. Thus, the most important part for the evaluation of the long-time thermal decay is the evaluation of energy barriers. At relatively low temperatures the temperature dependence of the energy barriers can be taken into account by temperature dependent parameters such as anisotropy and magnetisation with subsequent zero-temperature energy barrier evaluation. We will start with a well-known model of uniform energy barrier distribution and show that this leads to a widely measured logarithmic magnetisation decay . As a first model to evaluate energy barriers in slightly interacting system we will consider the Pfeiffer approximation for energy barriers evaluation [11] and to evaluate the magnetisation dynamics – the kinetic Monte Carlo approach [12].

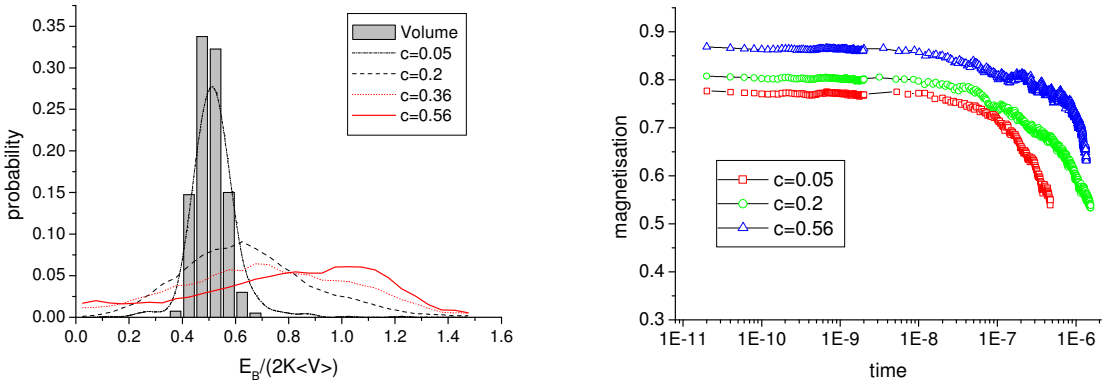

Fig. 6. (from Ref. [14]) Energy barrier distributions (normalized to average energy barrier in the non-interacting case) for magnetostatically interacting Co nanoparticles with different concentrations c (left) and the evaluated magnetisation decay (right).

However, generally speaking the magnetisation dynamics occurs in a complex magnetisation landscape and the evaluation of energy barriers should be done numerically in a multidimensional space. We will discuss the problem of energy barriers evaluation in magnetic systems and give several examples of energy barrier evaluation in magnetic nanoelements [13] and energy barrier distributions in systems of interacting nanoparticles [14], see Fig.6.

Finally, we will end with a full method to evaluate long-time magnetisation dynamics for completely interacting systems, based on a combined Metropolis-kinetic Monte Carlo approaches with multidimensional energy barrier evaluation [14].

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