1. SIMULATIONS OF ELECTROMAGNETIC FIELDS, AND FIELD MATTER INTERACTIONS – TOWARD ENGINEERING QUANTUMELECTRODYNAMICS

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In this report we present (i) two applications of short wavelength spin-waves, (ii) a case study on excitation energy transfer between two-state atoms, and (iii) a study on stimulated emission microscopy.

To simulate micromagnetic spin-waves we use OOMMF – Object Oriented Micromagnetic Framework and electromagnetic simulations to estimate the generated wave amplitudes for different geometries and at different frequencies.

To simulate room temperature molecular systems subject to optical frequency electromagnetic excitations we introduce equivalent quantum circuit models composed of (i) two-state 'atoms', (ii) ideal lossless harmonic oscillators and (iii) transmission lines coupled to (iv) heat baths representing the environment, and illuminated by (v) electromagnetic excitation. The temporal dynamics of the system is obtained by the numerical solution of the Liouville–von Neumann master equation describing the dynamics of the reduced density operator.

(I) SHORT-WAVELENGTH SPIN-WAVE GENERATION [1], [2].

We investigate the use of microstrip lines for short-wavelength spin-wave generation in magnetic thin films. We use micromagnetic (OOMMF – Object Oriented Micromagnetic Framework) and electromagnetic simulations to estimate the generated wave amplitudes for different geometries and at different frequencies. Our results suggest that in applications where coherent wavefronts need to be generated a microstrip line might also be used instead of more complicated devices (e.g. spin-torque oscillators) with comparable efficiency.

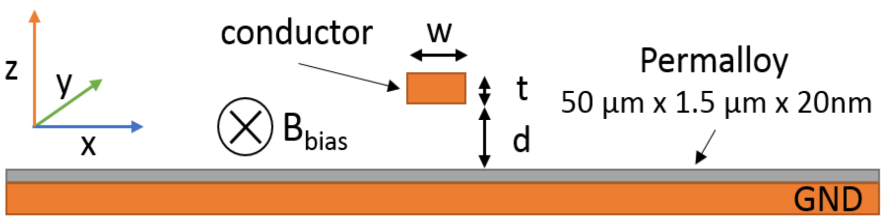

Fig. 1 *Geometry of the simulated microstrip line (cross section).*

As a first approach, we calculated the magnetic field generated by the microstrip line using Ampere's law, assuming a uniform current distribution through the wire, and ignoring the effect of the ground plane and the dielectric. For the simulations, we assumed 1 mA current. We applied the calculated spatial field distribution as an external magnetic field in OOMMF multiplied by a time-dependent sinusoidal function at microwave frequencies.

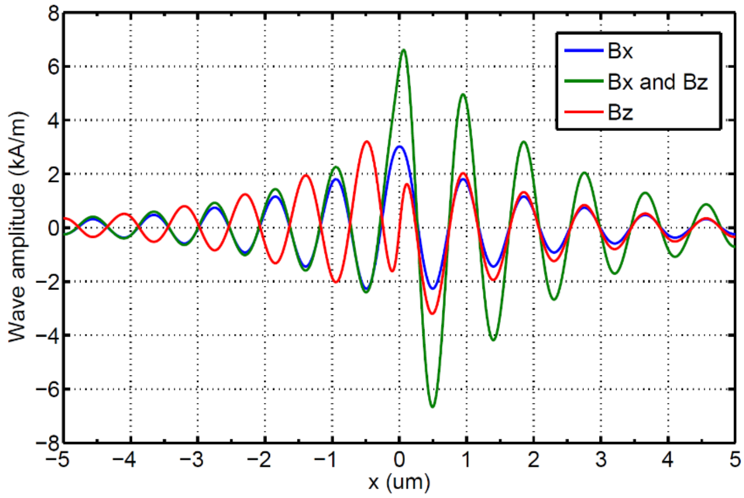

Fig. 2 *Anisotropic spin-wave generation by the microstrip line centered at x = 0 µm (green), and spin waves generated by applying only the x (blue) or z (red) field component of the line.*

We found that the wavelength of the generated spin waves is independent of the physical dimensions of the microstrip line in the investigated range of the physical dimensions, but it depends on the applied biasing magnetic field B_{bias} and the frequency f. However, there is strong correlation between the spin-wave amplitude and the physical dimensions of the microstrip line, the generation efficiency decays as the physical dimensions of the microstrip increase (for the same spin-wave wavelength).

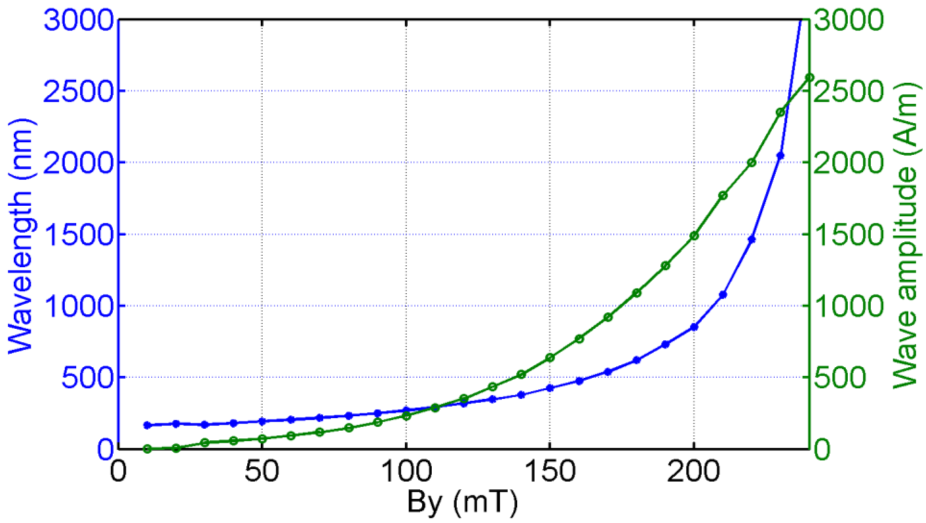

Fig. 3 *Wavelength and amplitude of the generated spin waves in function of B_{bias} (f = 15 GHz, w = 100 nm, d = 100 nm, t = 50 nm)*

We have studied the use of spin waves for computing and signal processing purposes. Spin waves are propagating excitations of the spins in magnetic materials that can represent and carry information. The idea of utilizing spin waves for computing is not new, however, it got special interest in the last decade in nanoscale devices. Spin-wave devices promise high speed, low power devices with relatively simple fabrication.

While most devices presented so far aim to create novel switches to replace transistors in logic applications, we focus on wave-based approaches where the spin waves are used to perform linear transformations on analog signals. We borrow ideas from the well-established optical computing theory, but instead of light we use spin waves in magnetic films which can be integrated on-chip straightforwardly. We propose spin-wave elements analogous to optical elements like lenses, mirrors and gratings [2]. Using micromagnetic simulations (OOMMF) we demonstrate that although there are many differences between light and spin waves, it is possible to redesign the optical computing concepts to be realized on magnetic medium. One of the most important concept in optical computing is the Fourier transform property of a lens which is the basis of many optical algorithms, like signal filtering and pattern matching. We show that a spin-wave lens can also realize these functions. We design a GRIN lens for spin waves and demonstrate the Fourier transformation with the GRIN lens using micromagnetic OOMMF simulations.

Our calculations suggest that in both speed and power consumption multiple orders of magnitude improvement is achievable (not including the supporting circuitry). Although there are many proposed devices for spin-wave generation and readout, these are still the bottleneck of the energy consumption of the envisioned system, but even considering these losses our proposed device has a significant gain compared to state-of-the-art CMOS realizations.

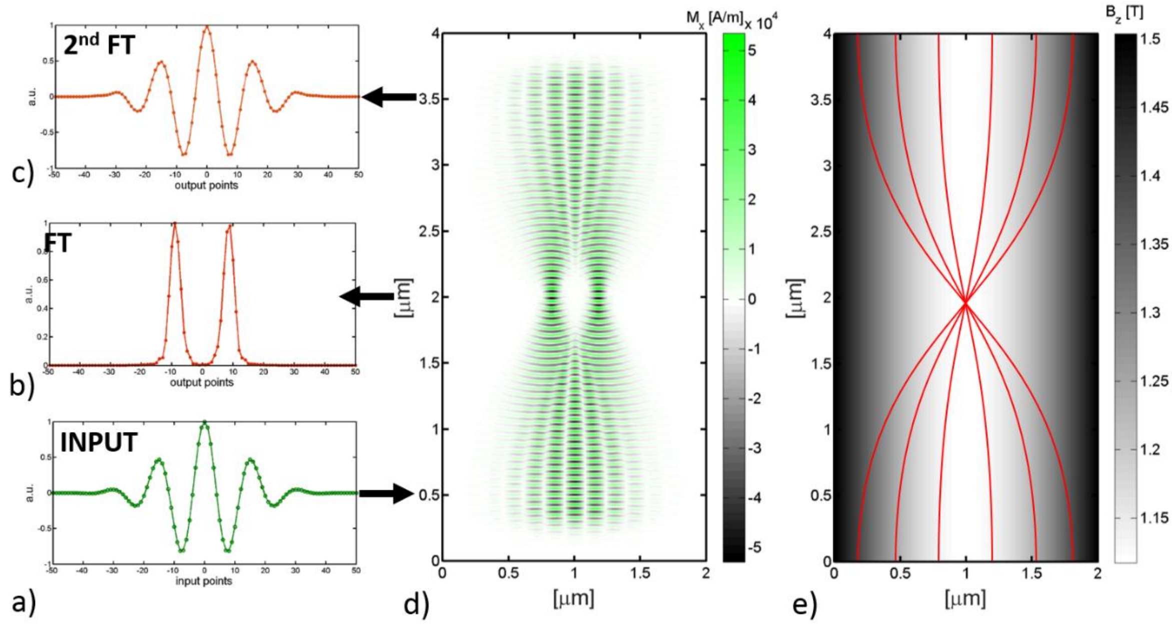

Fig. 4 *Micromagnetic simulation of a GRIN lens performing Fourier transform. a) Morlet wavelet as input. b) Fourier transform performed by the GRIN lens @ ½ pitch length. c) 2^{nd} Fourier transform performed by the GRIN lens @ 1 pitch length. d) Snapshot of the waves propagating in the magnetic film. e) Applied magnetic field distribution to realize GRIN lens.*

(II) SIMULATION OF EXCITATION ENERGY TRANSFER BETWEEN COUPLED TWO-STATE ATOMS [3], [4]

We developed a quantum mechanical model and implemented a simulator program using Quantum Toolbox in Python (QuTiP) to investigate the energy transfer between coupled atoms. The simulator solves the Lindblad master equation of a system consisting of N coupled two-state atoms, defined by energy, coupling and dissipation parameters.

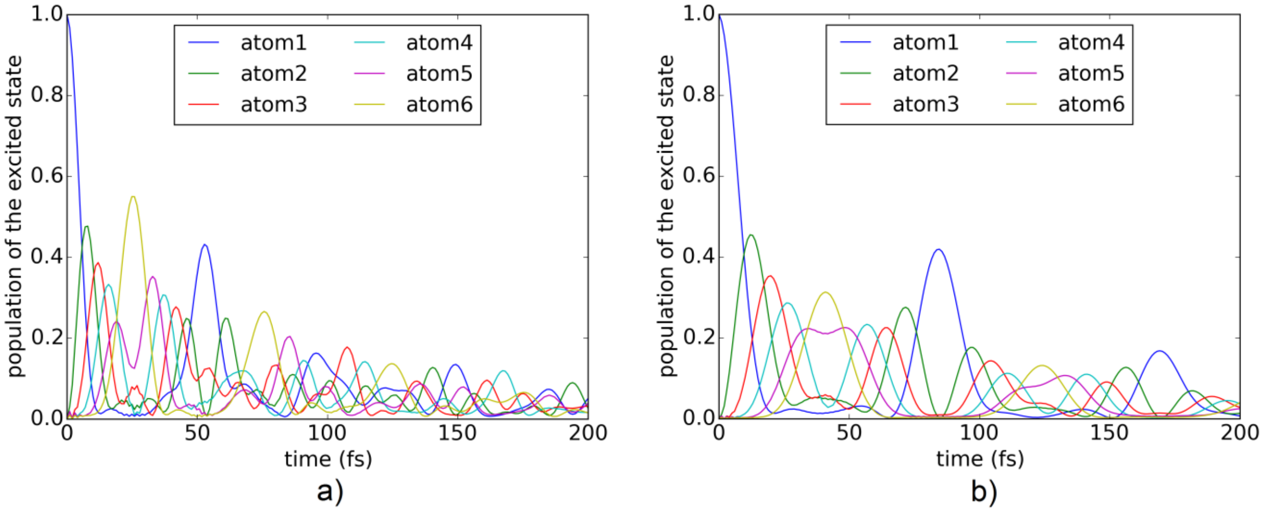

Fig. 5 *Energy transfer in a chain built up of six linearly coupled two-state atoms. The curves depict the population of the excited state of each atom over time. At the beginning of the simulations, the first atom was in the excited state, while all the other atoms were in the ground state. The site energies of the atoms were 1.08, 1.06, 1.04, 1.02, 1.00, and 0.98 eV, respectively; that is, they formed a decreasing sequence. The decay rate characterizing the irreversible energy transfer from the excited state of the atoms towards the environment was 0.01 fs^{-1}. The coupling strengths between the adjacent atoms were set to a) 0.1 or b) 0.06, which resulted in a faster (a) or a slower (b) energy transfer.*

(III) MODELING AND SIMULATION RELATED TO STIMULATED EMISSION MICROSCOPY [5]

We illustrate the modeling and simulation of a published measurement by developing a new QED model and comparing the measured data with simulations. The experiment demonstrated the principle of a new stimulated emission microscope which can perform label-free detection of non-fluorescent molecules forcing them to emit stimulated photons (“seeing in the dark”).

In the experiment a non-fluorescent bio-chromophore (crystal violet) molecule was subject (i) to a strong short laser pulse generating excitation by absorption. (ii) Then photon emission was stimulated by a second weak laser pulse, and the spectrum of relative excitation as a function of stimulating wavelength was measured.

We created a quantum-electrodynamic QED model and computationally feasible simulation program to understand the dynamics of stimulated emission microscopy.

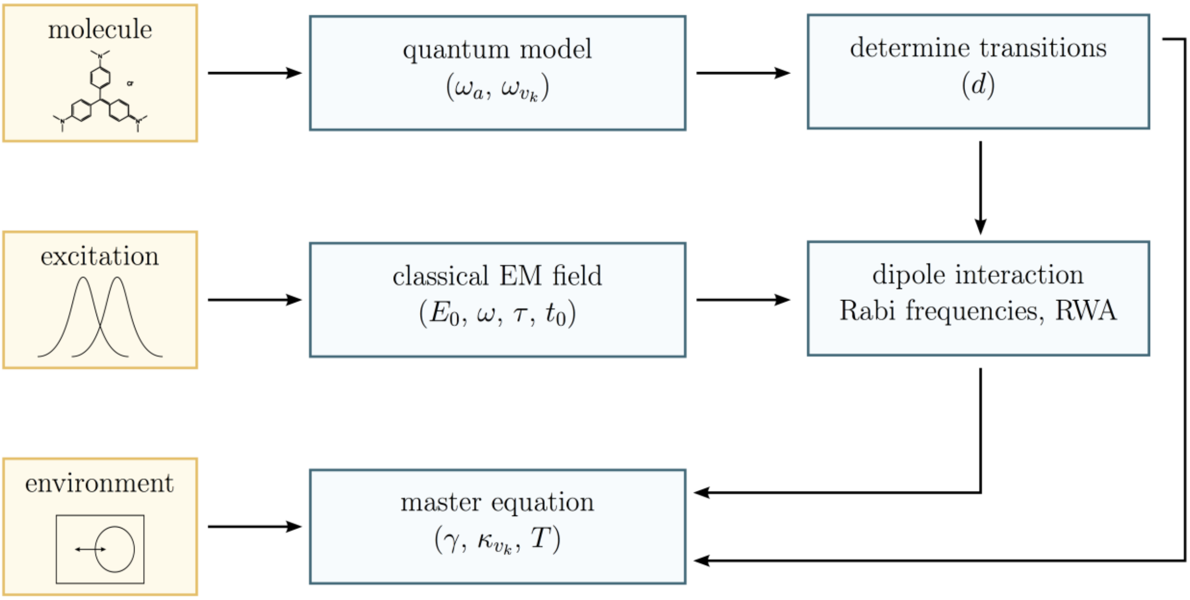

Fig. 6 *Block diagram of the main parts of model and the corresponding variables.*

Based on the new model we have performed simulations verifying the published experimental results. Entanglement between vibrational states turned to be significant. We could reproduce the experimental results of spectroscopic measurements by taking into account entanglement between two vibrational states. High correlation between calculated and measured data confirmed the validity of the proposed model.

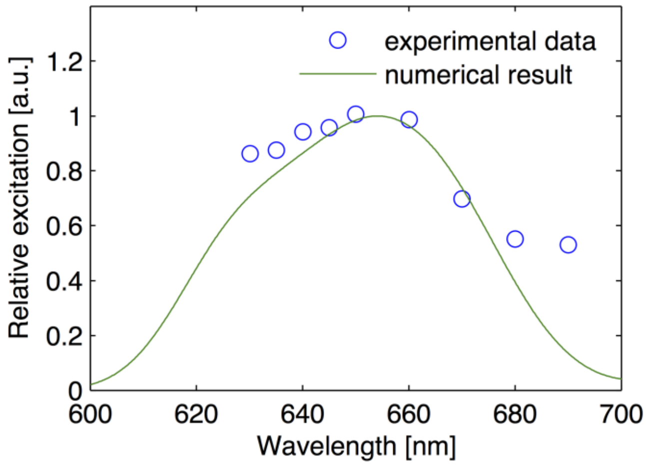

Fig. 7 *Numerical results of spectrum calculation shows the relative excitation as a function of wavelength in the simulation model compared to the experimental data presented by Min at al.*

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