Skyrmion dynamics and topology of spin fields for logic gates in semi-quantum processing

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Magnetic skyrmions are promising spin textures for fundamental physics, the next-generation devices and dense data storage. The objective of this project is to develop a code to simulate the skyrmions dynamics in low thickness materials and in narrow nanowires, in order to use of skyrmions in logic gates. The project is distributed over 3 years plus a flexibility period of 6 months to allow the exploration of adjacent topics.

I. PROJECT DESCRIPTION

Magnetic skyrmions[1] are promising spin textures[2] for fundamental physics, the next-generation devices[3–5], and dense data storage[6]. Recent measurements shows that they can be generated at room temperature[7] with finite life-time[8], so that they can be used as individual computation bits[9–12]. Furthermore, skyrmions are less energy consuming than current memories, then can improve the efficiency of devices and avoid the heat up of future computers[13].

Skyrmions have been observed in chiral helimagnets presenting a lack of inversion symmetry. This includes crystals with the cubic B20 structure and MnSi[14] and FeGe crystals[15]. Magnetic skyrmion can also arise at interfaces[16] or in heterostructures such as LaAlO3/SrTiO3[17], where they are stabilized by the so called chiral Dzyaloshinskii-Moryia interaction (DMI)[18–21].

There is a unique coupling between the electronic and the magnetic structure of those materials that allows to efficiently manipulate skyrmions by external electromagnetic fields such as laser light[22,23]. Furthermore, it has been shown that they can be driven and displaced[24–26] but also tuned with laser pulses[27] .

II. OBJECTIVES AND EXPECTED AWARDS

The micromagnetic description of skyrmions currently uses continuous spin fields which do not match the discrete inter-sites Hamiltonian representing the interaction of magnetic moments with each other. This second principle-based description of the skyrmions requires heavy analytics which often do not have solutions, but can be explored throughout numerical simulations.

The main objective of this project is to develop computational methods to simulate the skyrmions dynamics in low thickness materials and in narrow nanowires[28–30]. The outline of this work is to exhibit the necessary conditions required in the use of skyrmions as semi-quantum bits, instead of magnetic domains, for quantum computing and nano-devices.

A secondary objective is to train the student (Antoine Herrmann) develop a theoretical understanding of the physics underlying the skyrmions dynamics such that connections with other fields of physics and experimental protocols to verify the numerical predictions can be proposed.

Three intermediate goals drive the project :

1. Determine the stability diagram for temperatures of 0.001°K, 4°K, 72°K and 300°K. These temperatures correspond to almost absolute zero, liquid Helium, liquid nitrogen and room temperature respectively.

2. Determine the electronic structure of skyrmions under the optical excitations introduced by the use of a Rashba-like perturbation modeling the action of an electric field.

3. Determine the energy barrier to merge two skyrmions in an infinite plane, and the energy needed to transmit a skyrmion through a narrow nanowire.

The achievement of these goals takes the form of five publications over the entire project :

- Stability of skyrmions in thin films via three phase diagrams for each temperature : first comparing the DMI with respect to the magnetic field oriented along the directions perpendicular to the interface and parallel to the interface in 2D films; second showing the penetration of the topological charge field in the nearest layers with respect to the thickness of the film, third estimating the radius of the skyrmion with respect to the DMI compared to the exchange and also the DMI compared to the magnetic field.

- Stability of skyrmions under the action of an external magnetic field and provide two phase diagrams for each temperatures : first a comparison between the magnetic field amplitude and the electric field amplitude when they are both parallel perpendicular to the plane of the film, parallel in the plane of the film and perpendicular to each other; second the penetration of the topological charge field in the thickness of the material with respect to the amplitude of the electric field.

- Phenomenological analysis of the motion of the center of the skyrmion under the action of the external electric field, and the dependence of the radius of the skyrmion on the electric field. This publication could be completed by a calculation of the electronic structure and the splitting between the bands corresponding to spin up and spin downs, and an estimate of the electric field effects on the effective mass of the skyrmion.

- Critical parameters (magnetic field, electric field and DMI) acting as threshold parameter in the diffusion of skyrmions through a nanowire connecting two finite planes, and calculate the energy barrier in the merge of two skyrmions. An other point is to propose a phenomenological model to estimate the loss of energy in magnon modes during this process.

- Electronic structure response in laser pulse experiments and the typical time required to relax the thermal energy such that the skyrmion fluctuations become negligible at zero temperature and propose an experimental protocol to confirm the use of skyrmions in logic gates.

III. IMPACT AND BENEFITS

Nanoscale skyrmions can be addressed with electric currents[31], however this technique creates a large Slonczewski torque[32] leading to a energy dissipation by adding a damping term in the LLG equation[33] and creating incoherent Joule effect. The use of laser pulses reduces the heat up of the free electrons and reduce this power loss, improving the efficiency of devices.

This work will also provide a better understanding of the deformation of the skyrmion under the laser pulse and compare it to recent literature[34–37]. Furthermore, the project can explore different designs for logic gates like for example simple wires, double wires or constriction regions and act in collaboration with experimental group to determine what design can be used for each kind of gate[38–41].

IV. METHODS

The system will be modeled with a Hamiltonian including two sites interactions :

$$H = -\sum_{i,j} J_{i,j}\, \mathbf{S_i}\cdot\mathbf{S_j} - \sum_{i,j} \mathbf{D_{i,j}}\cdot(\mathbf{S_i}\times\mathbf{S_j}) - \sum_i \mathbf{H}\cdot\mathbf{S_i} - \sum_i (\mathbf{S_i}\cdot\mathbf{K})^2 - \mu_0 M_S^2 \sum_{i,j} \frac{3(\mathbf{S_i}\cdot\mathbf{r_{ij}})(\mathbf{S_j}\cdot\mathbf{r_{ij}}) - \mathbf{S_i}\cdot\mathbf{S_j}}{|\mathbf{r_{ij}}|^3}\Bigg]$$

From left to right, the terms in this Hamiltonian describes the direct Heisenberg exchange, the DMI[42], the Zeeman interaction, the effect of the anisotropy[43,44] at the interface and the dipole-dipole interaction respectively. The Heisenberg, Zeeman and anisotropy terms favors an alignment of the spins along a single direction. The DMI and the dipole-dipole interaction competes with them and do not favor an alignment of the spins. This competition can lead to the appearance of non-colinear spin structures of non trivial topology when none of these interactions clearly dominates[45].

The detection of Skyrmions will be performed with the Chern-Simons number also called topological charge[46,47] :

$$Q^\gamma = \frac{1}{4\pi}\oint_S \mathbf{S}\cdot\left(\frac{\partial\mathbf{S}}{\partial\alpha}\times\frac{\partial\mathbf{S}}{\partial\beta}\right)ds$$

where α and β are two orthogonal direction in the plane perpendicular to the direction γ. Skyrmions are associated to a charge $+1$ and anti-skyrmions are associated to a charge -1. Other magnetic textures can occur and be associated with fractional charges like for instance merons[48].

The temperature effects will be modeled by introducing corrections in the coupling constants[49] and by using an effective stochastic uncorrelated Langevin field[50] verifying the properties :

$$\langle\xi(t,\mathbf{r})\rangle = 0\ , \quad \langle\xi(t,\mathbf{r})\xi(t',\mathbf{r}')\rangle = 2k_BT\delta(t-t')\delta(\mathbf{r}-\mathbf{r}')$$

It will be coded using a Metropolis Monte-Carlo algorithm to make sure that all excited states remains accessible[51,52].

The Dynamics of the spins will first obey the Landau-Lifschitz-Gilbert (LLG) equation[53] and will be extended to the Inertial LLG equation[54] :

$$\frac{d}{dt}\langle\vec{\mathbf{S}}\rangle = \gamma\langle\vec{\mathbf{S}}\rangle\times\vec{\mathbf{H}} - \lambda\langle\vec{\mathbf{S}}\rangle\times\frac{d}{dt}\langle\vec{\mathbf{S}}\rangle + \lambda\tau\langle\vec{\mathbf{S}}\rangle\times\frac{d^2}{dt^2}\langle\vec{\mathbf{S}}\rangle$$

where nutation effects presented in the objectives emerges from the last term of the ILLG equation.

V. TIMELINE

The project is distributed over 3 years plus a flexibility period of 6 months to allow the exploration of adjacent topics that could re-orient the work, prepare conferences and invite external researchers for collaborations, write the final dissertation and prepare the graduation interview.

The first year is devoted to the implementation of solvers of the ILLG equation, the Metropolis Monte-Carlo algorithm and the calculation of observables and leads to the production of the phase diagrams expected in the first publication. The second year focus on integrating the laser pulse effects via a Rashba spin-orbit coupling, the calculation of the electronic structure and to the recognition of skyrmion structures in the spin field. The initial model will be extended to indirect interactions like RKKY interactions and fine temperature effects will be introduced via the two (or three) temperatures model. The second publication is expected once the electronic structure can be calculated and the third publication, once the tracking of skyrmions is effective. Finally, the third year will explore the propagation of skyrmions in logic gates and the decay of skyrmions in lower energy modes. The fourth publication is expected once different designs have been determined for experimental tests. Finally, the last publication will not require new implementations and is to be seen as an exploitation of the up-to-here built code.

The timeline 1 describes the different objectives, the time scales allowed for each of them in units of months and the submission of expected papers. Solvers and Hamiltonian-related elements are in blue, temperature-related elements are in orange as well as transport and electronic-structure elements. Observables are in green and publications and final dissertation and presentation are in red. Acronyms are explicated in the table I.

Code	Implementation
LLG	LLG equation using an Euler solver of order 1
ILLG	Inertial LLG equation using a Runge-Kutta solver of order 2 or 4
M-MC	Metropolis-Monte Carlo algorithm and defining the thermalization period
O-MTE	Observables : Magnetization, Temperature, Energy
O-Skr/Pl	Observables : Skyrmion radius and Penetration length
TCF	Topological Charge Field for a surface and a volume
ES	Electronic structure
R-SOC	Rashba Spin-Orbit Coupling as a perturbation
TTM	Three Temperatures Model
CT	Charge Transport and charge channels openings
NW	Nanowires architecture and design for logic gates
OE/MM	Optical Excitations and Magnon Modes
O-F/RT	Observables : Fluctuations / Relaxation time
P1/P2/P3/P4/P5	Publications 1/2/3/4/5
D/FP	Dissertation / Final Presentation
GI	Graduation Interview

TABLE I: Table of codes and expected implementations

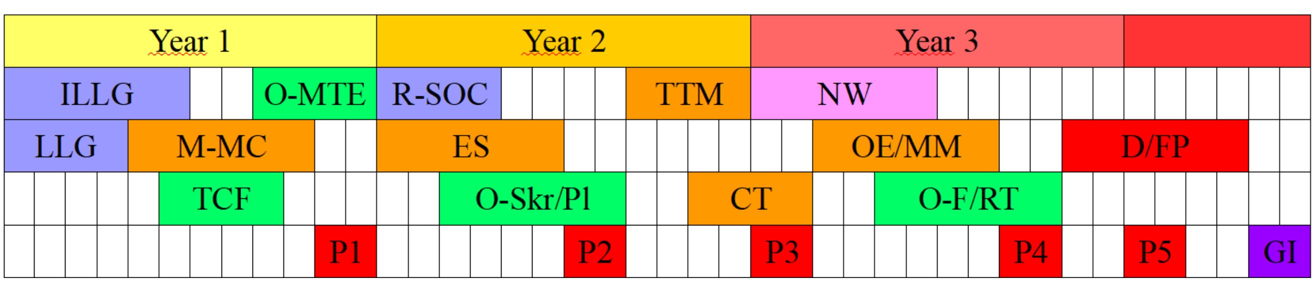

FIG. 1: Timeline of implementation of key concepts and estimate publication dates

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