First principles approach to non-collinear magnetization dynamics

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The investigation of magnetization dynamics is a highly active field of research on both the experimental and the theoretical side. In our group, we focus on the computational description of condensed matter properties using the Korringa-Kohn-Rostoker (KKR) multiple scattering approach to Density Functional Theory (DFT)[1]. Central quantity of this technique is the KKR- Green's function, which is determined from a combination of single (atomic) site scattering quantities and expressions related to the finite or infinite structure. This clear separation, for instance, allows for the convenient investigation of disordered materials. Furthermore, the Green's function being this approach's central quantity, the framework can conveniently be extended to Linear Response Time Dependent DFT (LRTDDFT).

In the recent years, our group's main aim was the description of magnons, i.e. collective magnetic excitations, often referred to as spin waves, in collinear systems [2]. Our first-principles approach allows for the investigation of magnons and their lifetimes in collinear magnets, e.g. ferro or anti-ferromagnets on an equal footing. This capability is central for the interpretation of results from experimental techniques such as Spin Polarized Electron Energy Loss Spectroscopy (SPEELS) [3].

On my poster, I would like to present my current effort to extend our methods to non-collinear magnetic systems, i.e. those without a common spin quantization axis. The latter can either arise from competing exchange interactions or from relativistic effects. Investigating the dynamics of non-collinear magnets is of great interest as, in these systems, several magnetic degrees of freedom and charge density fluctuations can be coupled. This opens up new decay channels for the spin dynamics, which are absent in the collinear case. Additionally, the coupling of the spin and charge degrees of freedom is a step to paving the way to construct efficient interfaces between conventional electronics and spintronic devices.

So far, I generalized the our existing method to be able to self-consistently describe the ground state of non collinear systems. Furthermore, we are now able to treat Spin-Orbit Coupling in those systems. Currently, my focus lies on the last steps of implementing the LRTDDFT scheme described above. My poster will consequently include methodological details, preliminary results and an overview over future tasks yet to be tackled.

References

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