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Quantum Stochastic Model for Spin Dynamics in Magnetic Systems

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Abstract. We develop a numerical model that reproduces the thermal equilibrium and the spin transfer mechanisms in magnetic materials. We analyze the coherent two-particle spin exchange interaction and the electron-electron collisions. Our study is based on a quantum atomistic approach and the particle dynamics is performed by using a Monte Carlo technique. The coherent quantum evolution of the atoms is interrupted by instantaneous collisions with itinerant electrons. The collision processes are associated to the quantum collapse of the local atomic wave function. We show that particle-particle interactions beyond the molecular field approximation can be included in this framework.

Our model is able to reproduce the thermal equilibrium and strongly out-of-equilibrium phenomena such as the ultrafast dynamics of the magnetization in nanomaterials.

AMS subject classifications: 81P20, 82D40

Key words: Quantum model, thermal equilibrium, spin dynamics.

1 Introduction

The study of the magnetism dynamics in a nanostructure is a rapidly developing area of research. The technological interest relies on the applications to magnetic data storage and sensing devices. The conventional way to record informations in a magnetic memory is to modify the local magnetization of a magnetic material [1]. Understanding the spin dynamics in magnetic materials is an issue of crucial importance for progress in information processing and recording technology. The use of a laser field has been proved to lead to a considerable speed up of the digital information recording. The elementary mechanisms that lead to the modification of the magnetic order triggered by laser pulses are at the center of an intense debate [2–4, 6–13].

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The physical properties of a magnetic system arise from the microscopic configuration of the angular momentum and the spin of the atoms. It is generally challenging to develop a framework capable of reproducing two important aspects of the solid state physics: the coherent quantum mechanical evolution of the system and the loss of quantum coherence due to collisions. Usually, the coherent quantum evolution of atoms and electrons is described at the single particle level by reversible Hamiltonian dynamics. Collisions are a complex many-particle effect and are usually approximated by classical mechanics or by a framework where quantum mechanics plays a minor role. As an example, in the Boltzmann kinetic theory the quantum mechanics is limited to the calculation of scattering parameters such as the effective cross sections. Concerning the study of systems at the nanometric scale, it seems natural to rely on a full ab initio many-body description, which is able in principle to describe at the same time the collisional and the purely coherent quantum mechanical evolution of electrons and atoms. However, due to the inherent extensive numerical effort, in many cases the application of ab initio approaches is limited to periodic structures or to small particle systems like molecules [14].

Such difficulties have encouraged the development of heuristic approaches. Coarse-grained methods and discrete mesoscopic models are adopted to assess the properties of materials at atomistic or continuum level. The so called atomistic models provide a simple and powerful framework capable to reproduce the microscopic spin dynamics of complex systems [15, 16]. Atomistic models are based on the classical description of the atomic spin provided by the phenomenological Landau-Lifshitz-Gilbert (LLG) equation. They have been used to reproduce the ultrafast evolution of the total magnetization in systems excited by laser pulses and the angular momentum transfer in alloys containing metals and rare earth elements [17]. Such models suffer of a serious theoretical limitation that reduces considerably their area of application. Atomistic models for magnetic materials are based on the classical spin theory. Electron spin is intrinsically a quantum mechanical phenomena, the classical description being valid only in the limit of large spin.

In the present contribution, we propose an atomistic-like approach based on the quantum mechanical framework. A cluster of atoms or, more generally, a nanomaterial is described by a network of quantum spin particles interacting via exchange interaction. We treat also the interaction of such particles with a gas of itinerant electrons. The main concern of our approach is to develop a Monte Carlo (MC) stochastic method able to reproduce the twofold aspect of the mesoscopic dynamics, the coherent and the collisional one. We observe that both the quantum and the classical collisional dynamics can be modeled by time-continuous stochastic processes. The central point of our approach is to assume that every collision among bounded atomic electrons and itinerant ones causes the Heisenberg collapse of the atomic particle wave function. In fact, the Heisenberg quantum measurement process is expected to take place every time a quantum system interacts with a classical apparatus or with an external system containing many degree of freedom. It this regards, we treat the delocalized electrons as a classical bath interacting with the open quantum system constituted by the net of interacting atoms.