THEORY OF PROTON RELAXATION INDUCED BY SUPERPARAMAGNETIC NANOPARTICLE: A CLASSICAL APPROACH TO NMRD

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Superparamagnetic nanoparticles are particles that are smaller than a magnetic Weiss domain. They have no remnant magnetization and become highly magnetized under a magnetic field. Their properties render them ideal for a broad spectrum of applications, such as hyperthermia, where they act as nanoheaters to kill tumor cells, or magnetic particle imaging, an imaging technique where they are used as tracers. They have been widely used in magnetic resonance imaging (MRI) as negative contrast agents: they produce a strong dipolar magnetic field which interacts with proton spins and accelerates their relaxation [1].

The magnetic moment of these particles is aligned along a preferential axis called the "anisotropy axis" to which an anisotropy energy is associated. Another important parameter is the Néel time, which characterizes the alternation of the magnetic moment between the two directions of the anisotropy axis. These properties influence the dipolar magnetic field produced by these particles and consequently affect proton relaxation. Thus, the proton NMRD of an aqueous solution containing superparamagnetic nanoparticles is significantly impacted by the anisotropy energy, the Néel time, as well as the nanoparticle size and magnetization.

The usual approach to developing theoretical NMRD models is to use the Redfield formalism, which is a full quantum framework. The current models of NMRD induced by superparamagnetic nanoparticles are developed within this quantum formalism [2,3]. In this work, we propose to develop a full classical theory, which has the advantage of being more intuitive to understand. In this theory, the superparamagnetic spin is modeled by a classical magnetic moment that obeys the Landau-Lifshitz-Gilbert equation [4]. This equation describes the time evolution of the magnetic moment and includes thermal fluctuations. We demonstrate that this approach can reproduce the quantum NMRD, paving the way for a more general model that would include phenomena such as nanoparticle aggregation or Brownian rotational motion.

References

[1] Q. L. Vuong, P. Gillis, A. Roch, et Y. Gossuin, *WIREs Nanomedicine Nanobiotechnology*, vol. 9, nº 6, Art. nº 6, nov. 2017, doi: 10.1002/wnan.1468.
[2] A. Roch, R. N. Muller, et P. Gillis, *J. Chem. Phys.*, vol. 110, nº 11, Art. nº 11, mars 1999, doi: 10.1063/1.478435.
[3] M. Lévy, F. Gazeau, C. Wilhelm, S. Neveu, M. Devaud, et P. Levitz, *J. Phys. Chem. C*, vol. 117, nº 29, Art. nº 29, juill. 2013, doi: 10.1021/jp404199f.
[4] W. F. Brown, *Phys. Rev.*, vol. 130, nº 5, Art. nº 5, juin 1963, doi: 10.1103/PhysRev.130.1677.