Monte Carlo Simulations of the T_2 relaxation induced by cubic-shaped superparamagnetic nanoparticles

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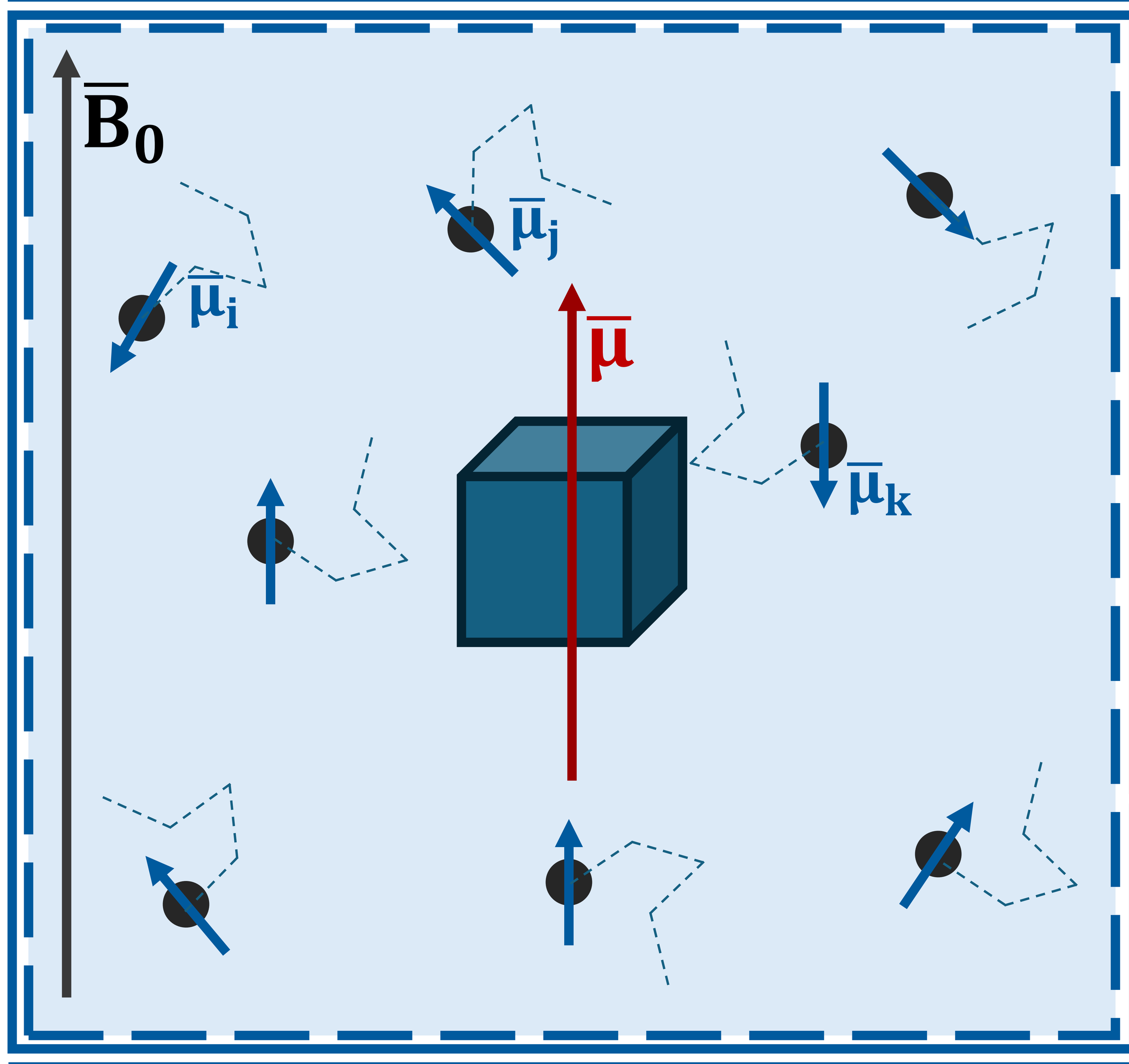
I. Introduction and research context

The transverse relaxation (T_2) of water protons induced by cubic-shaped superparamagnetic nanoparticles (NP), used as negative contrast agents in MRI, has been studied with Monte Carlo simulations considering a high static magnetic field (B_0). The comparison between spherical and cubic-shaped nanoparticles, at equal volumes, revealed minor deviations in the transverse relaxation (T_2) within the Motional Average Regime [d < 30nm] whereas no deviation was observed for larger particles. Magnetic Field Analysis of both cubic and spherical shaped Np's correlates with simulations results.

II. Monte Carlo Simulation Methodology

II. a. Simulation Setup [1]

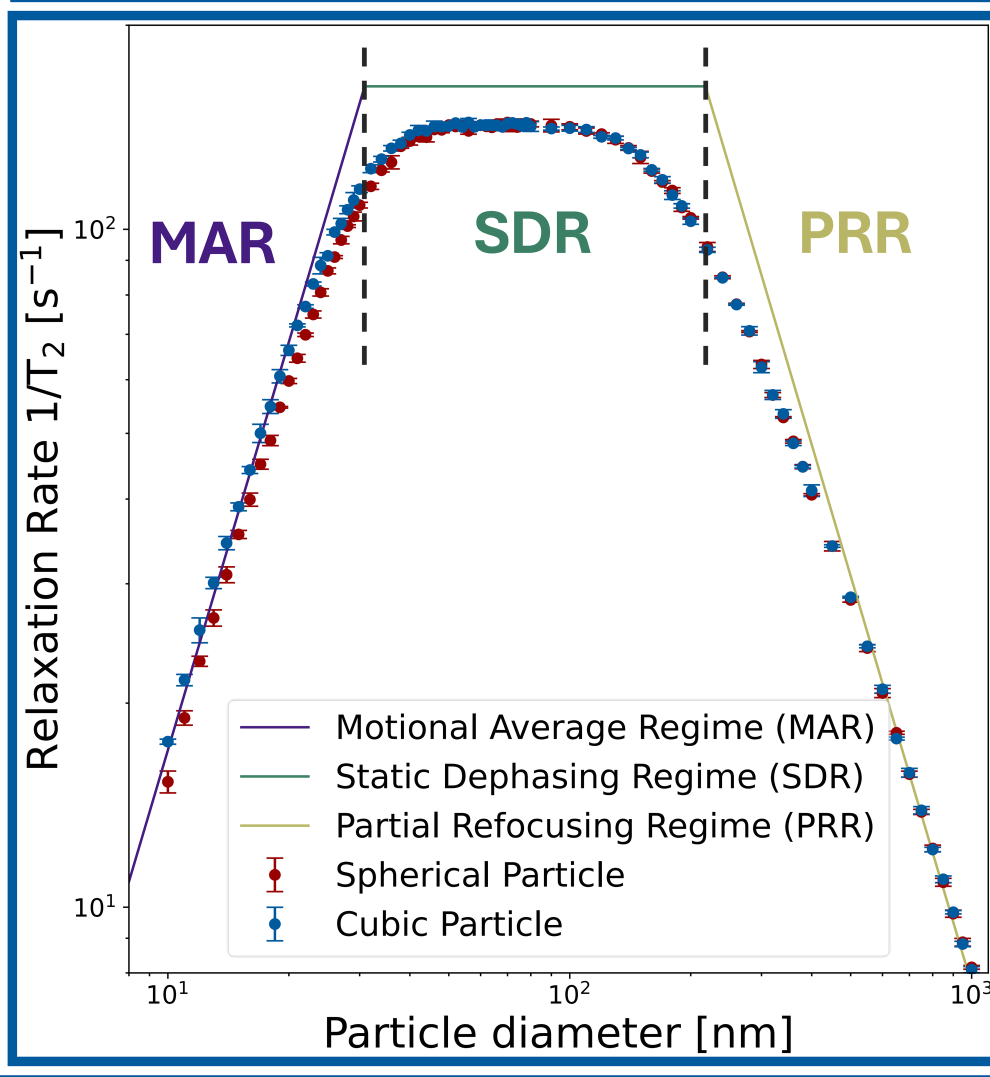


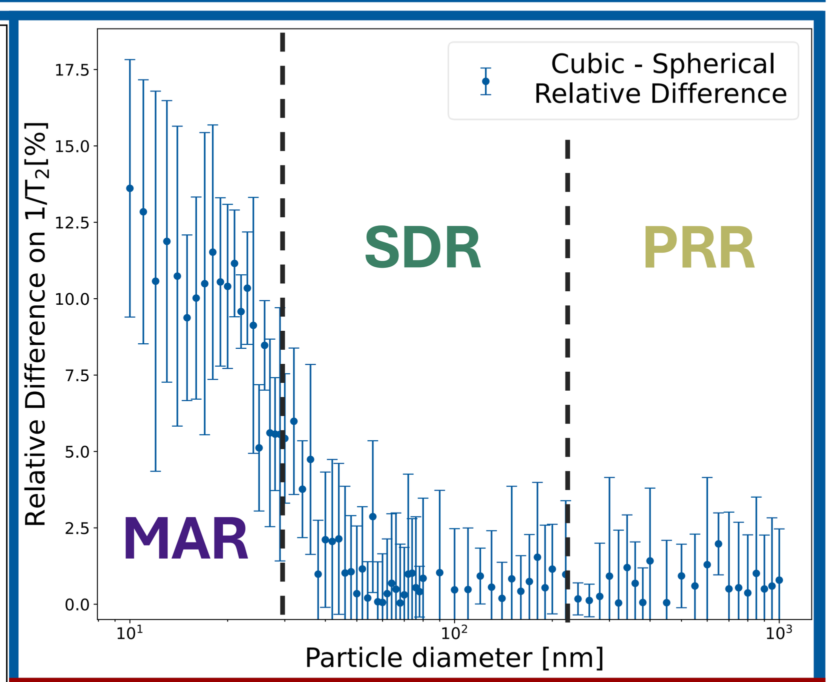
- 1 Cubic Magnetite NP
- 10 000 Water Protons

- Static magnetic field $\bar{B}_0$
- Random walk diffusion ($D = 3.10^{-9}\ m^2s^{-1}$)
- Periodic boundaries
- CPMG Sequence ($T_E = 1$ ms)
- Constant volume fraction ($f = 3.14\ 10^{-6}$)

- Larmor Precession of proton spins around cubic B_z magnetic field

II. b. Bell Curve





- Increase in $1/T_2$ in the MAR for cubes
  - Up to 15% for 10 nm cubes
- Magnetic field analysis

SDR. $[1/T_2 \propto p(B_z)]$[2]
PRR. $[1/T_2 \propto \sigma^2 = 1/V \int |\vec{\nabla} B_z|^2 dV]$[3]
MAR. $[1/T_2 \propto \langle B_z^2 \rangle]$[Redfield]

III. Magnetic Field Analysis

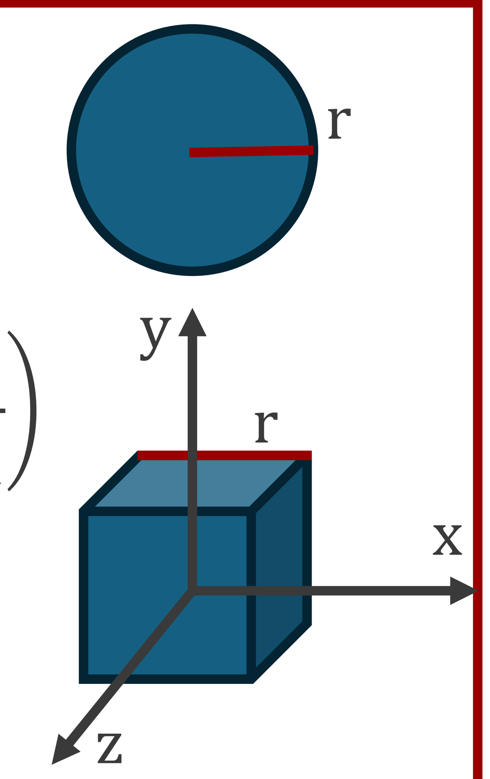
- Spherical / Dipolar Magnetic Field

$$B_z^{Sphere} = \left(\frac{\mu_0}{4\pi}\right)\frac{\mu}{r^3}(\cos^2\theta - 1)$$

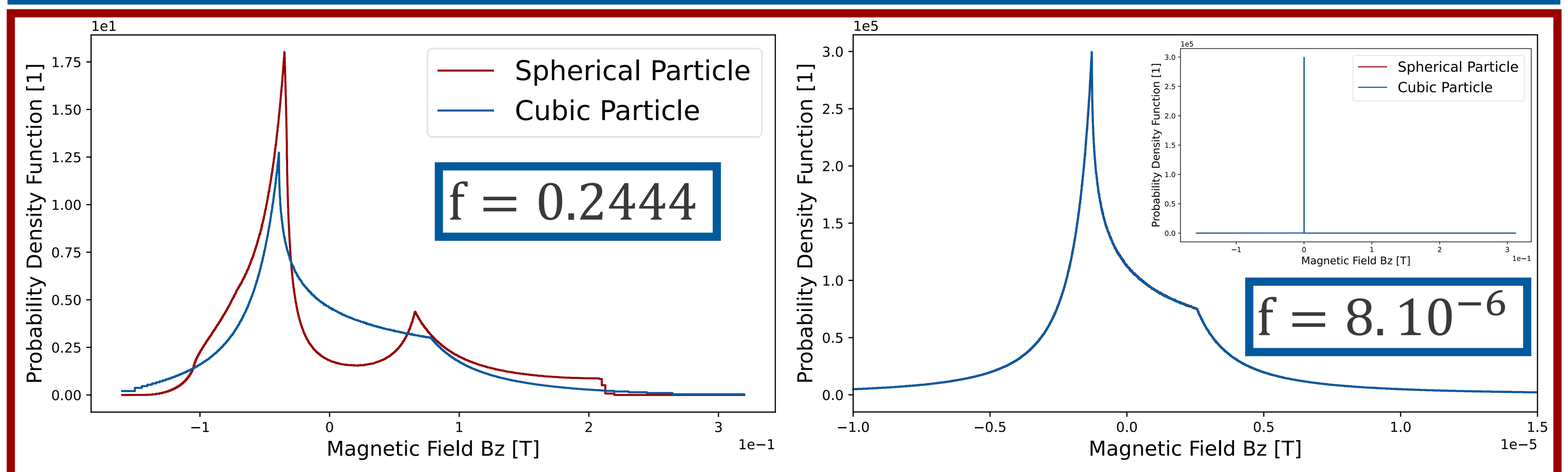
- Cubic Magnetic Field [4]

$$B_z^{Cube} = \left(\frac{\mu_0}{4\pi}\right)\frac{\mu}{V}\sum_{k,l,m=0}^{1}(-1)^{k+l+m}\,\mathrm{arctg}\left(\frac{x_k y_l}{z_m r_{klm}}\right)$$

$$\begin{cases} x_k = x + (-1)^k r \\ y_l = y + (-1)^l r \\ z_m = z + (-1)^m r \end{cases} \qquad r_{klm} = \sqrt{x_k^2 + y_l^2 + z_m^2}$$

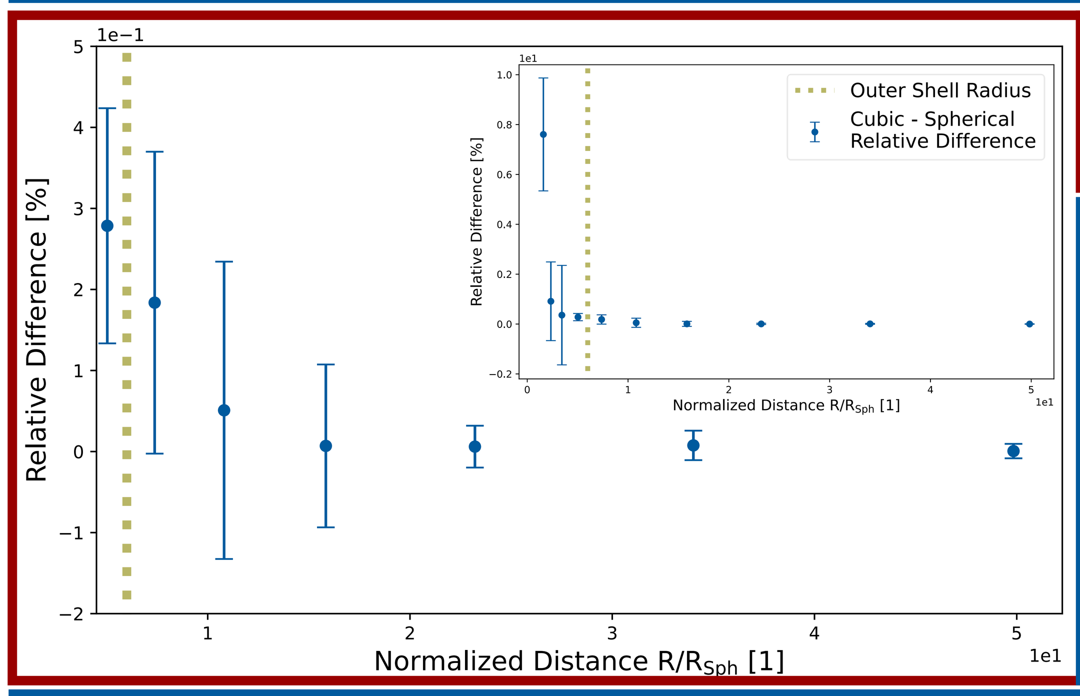


III. a. SDR



- Similar magnetic field statistical distribution for volume fraction of 10^{-3} and below. (MRI experiments : $f \sim 10^{-6}$)

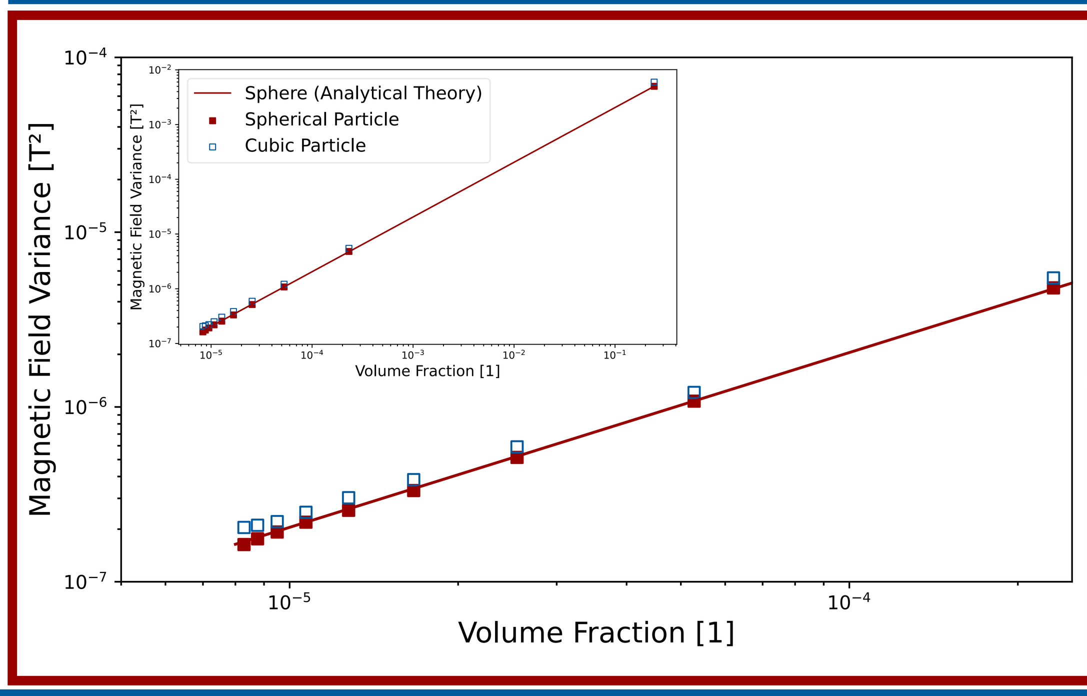
III. b. PRR



- Outer shell integration ($r_{outer} \approx 6R$)

- Protons diffusing below r_{outer} are directly lost from the signal [3].
- Dipolar approximation is valid in almost all the outer shell region leading to close to no differences

III. c. MAR



- Small Particles (< 30 nm)

→ Low magnetic field intensity
- Proton diffusion detects the nanoparticle shape without signal decorrelation

- Relative Differences of 15%
- Simulation yield same order of magnitude in differences

IV. Summary and Future Directions

- Monte Carlo Simulations demonstrate that the NP shape has little to no impact on T_2 for particles larger than 30 nm. However, an increase of up to 15% is observed for small particles below 30 nm within the Motional Average regime.
- The magnetic field analysis correlates with simulation results and provides insight into why differences are observed only in the MAR.
- Future studies will focus on other shapes, starting by cylinder-shaped particles which are believed to strongly impact $1/T_2$.
- Introduction of multiple nanoparticles into the simulation will provide a more accurate representation of the non-uniformity in solutions.

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