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A mean-field and propagation-of-chaos approach to magnetic nanoparticles

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There exist various methods for the analytical description of the collective behavior of a system of dipoles in magnetic fluids, including the use of mean fields, for example MMFM [1]. The applicability of mean-field approximations is limited to the case of low concentrations, and even in this case, the methods are justified primarily by physical assumptions and heuristic approximations. However, on the other hand, a mathematical approach is known for obtaining McKean-Vlasov type equations [5] for the distribution of "agents" from a system of stochastic differential equations. Additionally, problems regarding interacting Brownian particles have been investigated in general formulations [4].

In this work, starting from the classical overdamped Langevin stochastic equations for the coordinates x_i and orientations e_i of N particles:

$$dx_i = b_i^x(x_j, e_j, t)dt + \sqrt{2D_t}dW_i^x$$
$$de_i = b_i^e(x_j, e_j, t)dt + \sqrt{2D_r} \circ dW_i^e$$

the drift terms b^i are determined by the gradients of the total potential energy, including the Zeeman energy U_H and the dipole potential U_{dip}.

Under certain assumptions about the properties of the system (e.g., low concentration), Fokker-Planck type equations for the orientations of the dipole system are mathematically derived, assuming a uniform spatial distribution. The derivation is based on adapting classical theorems on the propagation of chaos [2] to the corresponding configuration space. Furthermore, a Fokker-Planck equation accounting for translational degrees of freedom is derived and rigorously proven for the case of a regularized dipole potential with the addition of a Lennard-Jones type potential to the drift. The theory is generalized to the case where the space is bounded by a container: using the penalty method, the problem is reduced to the Skorokhod problem, for which results on the propagation of chaos exist [3]. From this problem, a Fokker–Planck type equation with the corresponding boundary condition is derived.

An expression for the collective response and relaxation time is also obtained for the problem where the external magnetic field propagates as a traveling wave with an initial condition of an isotropic non-magnetized state.

Analytical investigation of such problems is possible only in the proposed translational variant of the equation. The obtained response values are consistent with known experimental data. Further paths for the development of the theory are discussed.

The research was supported by the Ural Mathematical Center, project No. 075-02-2026-1315.

References

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Type:

Poster