Mean-Field Theories of Immobilised Superparamagnetic Nanoparticles: Problems and Possible Solutions

<u>Кэмп Ф. Дж.</u>^{1, 2}, Елфимова Е. А.², Иванов А. О.²

¹Школа химии, Университет Эдинбурга, Эдинбург, Шотландия ²Институт естественных наук и математики, Уральский федеральный университет, Россия Электронная почта ответственного автора: <u>philip.camp@ed.ac.uk</u>

Modified mean-field (MMF) theories provide a systematic, statistical-mechanical approach to the properties of magnetic nanoparticles dispersed in liquids (ferrofluids, magnetorheological fluids) or soft solids (ferrogels, magnetic elastomers) [1]. The main idea is that interactions between particles are described by an effective field H_{eff} experienced by each single particle. Once H_{eff} is known, the magnetisation curve M(H) and initial susceptibility χ can be computed using simple, one-particle formulas. The accuracy of MMF theories depends on the calculation of H_{eff} arising from the dipole-dipole interactions, and the pair correlations (spatial and orientational), between particles. In a first approximation, the pair correlations can be ignored. This is justified for systems in which the particle dipole moments are free to rotate, and orientational averaging gives rise to weak, short-range $(1/r^6)$ correlations. Such an approach is adequate for systems such as typical ferrofluids with Langevin susceptibilities $\chi_L \leq 3$ [2].

The magnetic properties of superparamagnetic nanoparticles (SNPs) immobilised in a solid matrix are studied with MMF theory [3]. It is shown that with small anisotropy (magnetically soft particles) and/or random orientations of the particle easy axes, the magnetic properties are described accurately with MMF theory. But with large anisotropy (magnetically hard particles), and alignment of the particle easy axes, the MMF theory is not very accurate. This is because there is restricted orientational averaging, giving strong, long-range $(1/r^3)$ correlations between the particles. Hence, to describe such cases, strong correlations must be described more accurately.

To illustrate the problems and possible solutions, a 1D chain of SNPs is considered, in which the particle easy axes are aligned with the chain [4]. By changing the anisotropy parameter σ , it is possible to connect a 1D Heisenberg model with long-range dipolar interactions ($\sigma = 0$, weak anisotropy), to a 1D Ising model with long-range dipolar interactions ($\sigma = \infty$, strong anisotropy). MMF theories for both cases are considered using the normal, no-correlation approximation. For the $\sigma = \infty$ case, a MMF theory is also formulated with the known pair correlations in the 1D nearest-neighbour Ising model. It is shown that, with $\sigma = 0$, the normal MMF theory is quite reliable. With $\sigma = \infty$, the MMF theory based on the Ising model gives superior results to the normal MMF theory. This simple 1D model illustrates how MMF theories can be improved, and the remaining challenges in describing 3D systems of SNPs.

[1] A. O. Ivanov and O. B. Kuznetsova, Physical Review E, 64 (2001) 041405.

- [3] E. A. Elfimova, A. O. Ivanov, and P. J. Camp, Nanoscale, 11 (2019) 21834.
- [4] P. J. Camp and A. O. Ivanov, Ukrainian Journal of Physics, 65 (2020) 691.

^[2] A. O. Ivanov, S. S. Kantorovich, E. N. Reznikov, C. Holm, A. F. Pshenichnikov, A. V. Lebedev, A. Chremos, and P. J. Camp, Physical Review E, 75 (2007) 061405.