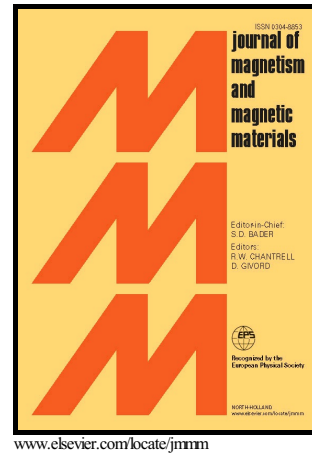


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Ekaterina D. Vtulkina, Ekaterina A. Elfimova



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# Thermodynamic and magnetic properties of ferrofluids in external uniform magnetic field.

Ekaterina D. Vtulkina, Ekaterina A. Elfimova

*Institute of Mathematics and Computer Sciences, Ural Federal University, 51 Lenin Avenue, Ekaterinburg 620000, Russia*

## Abstract

The work is devoted to the theoretical investigation of the thermodynamic and magnetic properties of ferrofluids in applied magnetic field. Analytical expressions for the second and the third virial coefficients of dipolar hard spheres model were obtained by using the least-squares approximation to the simulation data [Phys. Rev. E, 88, 2013, 04310]. The expressions for the virial coefficients are presented as functions of the dipolar coupling constant  $\lambda$  and the Langevin parameter  $\alpha$ . The analytical formulas for the virial coefficients were incorporated in to so-called logarithmic free energy theory [Phys. Rev. E, 86, 2012, 021126]. This theory yields the Helmholtz free energy and the magnetization. The comparison between theory and computer simulation shows good agreement for  $\lambda \leq 2$ . The analytical expression of the Helmholtz free energy was also used to obtain a sedimentation equilibrium concentration profile of ferrofluids subjected to uniform magnetic and gravitational fields.

## 1. Introduction

The simplest model of ferrofluids is the system of dipolar hard spheres (DHS). DHS is a hard sphere of diameter  $\sigma$  bearing a permanent dipole moment  $m$  at its center. The interaction between two DHSs  $i$  and  $j$  is given by a sum of hard sphere ( $U_{ij}^{HS}$ ) and dipolar ( $U_{ij}^D$ ) terms:

$$U_{ij}^{HS} = \begin{cases} \infty & , \quad r_{ij} < \sigma \\ 0 & , \quad r_{ij} \geq \sigma \end{cases}, \quad (1)$$

$$U_{ij}^D = - \left[ 3 \frac{(\mathbf{m}_i, \mathbf{r}_{ij})(\mathbf{m}_j, \mathbf{r}_{ij})}{r_{ij}^5} - \frac{(\mathbf{m}_i, \mathbf{m}_j)}{r_{ij}^3} \right], \quad (2)$$

where  $\mathbf{r}_{ij}$  is the interparticle separation vector and  $r_{ij} = |\mathbf{r}_{ij}|$ . In a uniform magnetic field  $\mathbf{H}$  the total interaction energy of the fluid is

$$U = \sum_{i < j} (U_{ij}^{HS} + U_{ij}^D) - \sum_{i=1}^N (\mathbf{m}_i, \mathbf{H}). \quad (3)$$

The strength of interparticle interactions is specified by the dipolar coupling constant  $\lambda = m^2/(\sigma^3 kT)$ , where  $kT$  is the thermal energy. The dipole-field interaction is measured by the Langevin parameter  $\alpha = mH/kT$ .

From the theoretical standpoint, there are many approaches to the general problem of how to describe the thermodynamic properties of DHSs in applied fields, including density functional theory [1, 2], integral equations [2, 3], and virial expansions [4, 5]. In the framework of virial expansion theory, the DHS free energy  $F$  of  $N$  particles in a volume  $V$ , and in an applied field  $H$  can be written as

$$\frac{F}{NkT} = \frac{F^{HS}}{NkT} - \ln \Psi + \sum_{n=1}^{\infty} n^{-1} \Delta B_{n+1} \rho^n, \quad (4)$$

where  $\Psi = \sinh(\alpha)/\alpha$ , and  $-NkT \ln \Psi$  and  $F^{HS}$  are the Helmholtz free energy of ideal paramagnetic gas and hard spheres respectively;  $\rho = N/V$  is the concentration, and  $\Delta B_n = B_n - B_n^{HS}$  is the difference between the virial coefficients of the DHS fluid ( $B_n$ ) and hard sphere system ( $B_n^{HS}$ ). The correct expressions for the second and third virial coefficients of a system in an applied field were derived in Ref. [4]. The second virial coefficient is given by

$$B_2 = -\frac{1}{2} \int d\mathbf{r}_{12} \langle f_{12} \rangle, \quad (5)$$

where  $f_{ij}$  is the Mayer function, and angular brackets denote an orientational average for each particle. The third virial coefficient is expressed conveniently as a sum of two terms:

$$B_3 = B_{3a} + B_{3b}, \quad (6)$$

$$B_{3a} = -\frac{1}{3} \int d\mathbf{r}_{12} \int d\mathbf{r}_{13} \langle f_{12} f_{13} f_{23} \rangle,$$

$$B_{3b} = \int d\mathbf{r}_{12} \int d\mathbf{r}_{13} [\langle f_{12} \rangle \langle f_{13} \rangle - \langle f_{12} f_{13} \rangle].$$

In the absence of an applied field  $B_{3b} = 0$ . For DHSs in the presence of finite fields,  $B_{3b}$  was found to give a negative contribution to  $B_3$  [4]. It is emphasized that these  $B_{3b}$  corrections to the third virial coefficients were first identified by Bruns and Caracciolo with co-authors. [6, 7] as arising from intramolecular degrees of freedom. The explicit analytical expressions of  $B_2$  and  $B_3$  for DHS fluid in applied magnetic field have been evaluated as expansion in dipolar coupling constant  $\lambda$  up to third order in Ref. [4]. For DHS fluid the rate of convergence of the virial series (4) is very slow and the sign of the virial coefficients  $B_n$  is alternate, frustrating attempts to improve the accuracy of the expansion simply by adding extra terms. One approach to this problem was suggested in recent works [4, 8] where so-called

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