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# Distribution of Exchange Interaction Fields for 2D and 3D Systems of Spherical Dipoles

A.G. Makarov[1,2,*], K.V. Nefedev[2,†]

[1] *Far Eastern Federal University, The School of Natural Sciences, Department of theoretical and experimental physics, 8-43, Sukhanova Str., 690950 Vladivostok, Russian Federation*
[2] *Far Eastern Branch Russian Academy of Science, Institute of Applied Mathematics, 7, Radio Str., 690041 Vladivostok, Russian Federation*

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By the method of numerical simulation have been shown that the dipole-dipole interaction in the high-anisotropic spherical magnetic dipole moments can result in the case of the particle distribution on the plane to poorly defined ferromagnetism, and for the distribution in the volume to the equality of ferromagnetic and antiferromagnetic interactions. Results are consistent with the results of the random exchange interaction field calculation method, i.e. in 3D systems with random distribution of the particles is no ferromagnetism.

**Keywords:** Ferromagnetism, Antiferromagnetism, Superspin, Spin glass, Numerical experiments.

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## 1. INTRODUCTION

Interaction effects can lead to interesting collective phenomena, such as superferromagnetism. This phenomenon is the magnetism of an ensemble of magnetically interacting super-moment-bearing material particles that would be superparamagnetic if they were not interacting [1]. It should be noted that until today the influence of the magnitostatical interaction and its combination with another types interactions is not well defined and demand additional research [2]. The ground state of such systems was studied in [3-6]. Therefore, it is of interest to find a solution for the problem of magnetic state of the system of magnetostatically interacting dipoles, randomly distributed in the space of the sample. Random particle method in various forms has been used successfully to simulation of magnetic phenomena and solving the other problems of mathematical physics [7-11].

Thus, the theoretical research and computer modeling of the magnetic states of a disordered system of dipoles in 2D and 3D sample space are of interest.

## 2. DIPOLE-DIPOLE INTERACTION

### 2.1 Formalization

Let us to consider a system of spherical highly anisotropic uniaxial magnetic single-domain particles randomly distributed on a plane. The interaction energy of a pair of magnetic dipole moments $\mathbf{m_1}$ and $\mathbf{m_2}$, which coordinates are $(x_1, y_1, z_1)$ and $(x_2, y_2, z_2)$, respectively, is defined as follows:

$$E = \frac{\left(\vec{m_1}\vec{m_2}\right)}{r_{12}^3} - 3\frac{\left(r_{12}\vec{m_1}\right)\left(r_{12}\vec{m_1}\right)}{r_{12}^5} \qquad (2.1)$$

Since the unit vectors of the vector of the summary field of interaction are orthogonal, then the following equations can be derived:

$$E_{tot} = E_x + E_y + E_z \qquad (2.2)$$

The ground state of the system is determined according to the principle of minimum energy $\min\{E_{tot}\}$. Such state will have the highest probability at $T = 0$. The type of ordering at zero temperature depends on the competition between the ferromagnetic and antiferromagnetic type of exchange interaction.

The total value of the exchange integrals $\gamma$, i.e. multipliers before multiplication $m_1 m_2$ is calculated as follows:

$$J_{12xx} = \frac{1}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}\left[\frac{3x_{12}^2}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)} - 1\right], \qquad (2.3)$$

$$J_{12xy} = \frac{3x_{12}y_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \qquad (2.4)$$

$$J_{12xz} = \frac{3x_{12}z_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \qquad (2.5)$$

$$J_{12yx} = \frac{3y_{12}x_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \qquad (2.6)$$

$$J_{12yy} = \frac{1}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}\left[\frac{3y_{12}^2}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)} - 1\right], \qquad (2.7)$$

$$J_{12yz} = \frac{3y_{12}z_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \qquad (2.8)$$

$$J_{12zx} = \frac{3z_{12}x_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \qquad (2.9)$$

* makarov_age@students.dvfu.ru
† nefedev.kv@dvfu.ru

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$$J_{12zy} = \frac{3z_{12}y_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \quad (2.10)$$

$$J_{12zz} = \frac{1}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{3/2}}\left[\frac{3z_{12}^2}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)} - 1\right]. \quad (2.11)$$

For this pair of magnetic moments $\boldsymbol{m}_1$ and $\boldsymbol{m}_2$ defines a parallel (ferromagnetism) with $\gamma > 0$, antiparallel (antiferromagnetic) for $\gamma < 0$, or frustrated (spin glass) the orientation of the magnetic moments at $\gamma = 0$.

Generally for a system of $N$ magnetic dipoles, the value

$$\gamma_{3D} = \frac{1}{N}\sum_{i=1}^{N-1}\sum_{i+1}^{N}\begin{pmatrix} J_{ijxx} + J_{ijxy} + J_{ijxz} + J_{ijyx} + \\ + J_{ijyy} + J_{ijyz} + J_{ijzx} + J_{ijzy} + J_{ijzz} \end{pmatrix} \quad (2.12)$$

could be the order parameter calculated per spin.

For the two-dimensional case we have

$$\gamma_{2D} = \frac{1}{N}\sum_{i=1}^{N-1}\sum_{i+1}^{N}\left(J_{ijxx} + J_{ijxy} + J_{ijyx} + J_{ijyy}\right), \quad (2.13)$$

where

$$J_{12xx} = \frac{1}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{3/2}}\left[\frac{3x_{12}^2}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)} - 1\right], \quad (2.14)$$

$$J_{12xy} = \frac{3x_{12}y_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \quad (2.15)$$

$$J_{12yx} = \frac{3y_{12}x_{12}}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{5/2}}, \quad (2.16)$$

and

$$J_{12yy} = \frac{1}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{3/2}}\left[\frac{3y_{12}^2}{\left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)} - 1\right]. \quad (2.17)$$

Let us average the absolute values of the exchange integrals and to proceed with the reduced values:

$$\gamma_{3D}^* = \frac{\gamma_{3D}}{|\gamma_{3D}|} = \frac{\sum J}{\sum |J|}\frac{\sum_{i=1}^{N-1}\sum_{i+1}^{N}\left(J_{ijxx} + J_{ijxy} + J_{ijxz} + J_{ijyx} + J_{ijyy} + J_{ijyz} + J_{ijzx} + J_{ijzy} + J_{ijzz}\right)}{\sum_{i=1}^{N-1}\sum_{i+1}^{N}\left(|J_{ijxx}| + |J_{ijxy}| + |J_{ijxz}| + |J_{ijyx}| + |J_{ijyy}| + |J_{ijyz}| + |J_{ijzx}| + |J_{ijzy}| + |J_{ijzz}|\right)}. \quad (2.18)$$

where $|J_{ij}|$ is an absolute values of the exchange integral and $\gamma_{3D}^* \in [-1,1]$ by definition.

For the two-dimensional case we now have:

$$\gamma_{2D}^* = \frac{\gamma_{2D}}{|\gamma_{2D}|} = \frac{\sum J}{\sum |J|}, \quad (2.19)$$

$$\gamma_{2D}^* = \frac{\sum_{i=1}^{N-1}\sum_{i+1}^{N}\left(J_{ijxx} + J_{ijxy} + J_{ijyx} + J_{ijyy}\right)}{\sum_{i=1}^{N-1}\sum_{i+1}^{N}\left(|J_{ijxx}| + |J_{ijxy}| + |J_{ijyx}| + |J_{ijyy}|\right)}, \quad (2.20)$$

where $\gamma_{2D}^* \in [-1,1]$.

### 2.2 The Algorithm for Distributing Magnetic Particles

A sequential algorithm was developed by authors. It was designed for simulation of disordered array of spherical dipoles and then it was implemented in C++ language. The algorithm as defined as follows

1. The type of the sample is selected to perform calculations for 2D or 3D.

2. The length of the particles array is determined (it is $N = 10000$ by default).

3. The radius of a particle is set up (it is 0.5 nm by default).

4. It is determined the concentration limit C. For 2D sample it must not be higher than 0.5 and for 3D – than 0.3. If one sets it to a higher value, there is a possibility, that with given uniform distribution all particles won't fit the sample's size, as the distance between them may vary and the significant part of the sample might be taken by empty space.

5. The lengths of the sides of the samples are calculated. As long as square (for 2D) and cubic (for 3D) samples are used, the lengths of the sides are similar.

The following concentration formulas for 2D and 3D length calculation are used:

$$C_{2D} = \frac{\sum S_p}{S_{tot}} = \frac{S_p n}{a^2} = \frac{\pi r^2 n}{a^2}, \quad (2.21)$$

and

$$C_{3D} = \frac{\sum V_p}{V_{tot}} = \frac{V_p n}{a^3} = \frac{\pi r^3 n}{a^3}, \quad (2.22)$$

where $C$ – concentration, $S_p$ – particle area, $S_{tot}$ – sample area, $a$ – sample side length, $r$ – particle radius, $n$ – the number of particles, $V_p$ – particle volume, $V_{tot}$ – sample volume.

6. The coordinates $(x, y, z)$ are picked randomly. Random numbers are generated with the standard library function rand(). It generates the pseudorandom integer number. To generate the non repeated sequence of numbers command srand (time(NULL)) is used. It initializes the random numbers generator depending on starting count time.

7. For each new particle intersections with other particles and with the boundaries of the sample are checked. If there are intersections, the coordinates of a particle are generated randomly and checked again.

8. The magnetic moments are randomly distributed along the directions (the kind of magnetic configuration does not affect the total value of the exchange integrals).

To construct a visual model, the particle parameters are written to the file. For 2D modelling the freeware utility "gnuplot" is used and 3D modelling is performed with the help of computer algebra system - Wolfram Research "Mathematica".

9. The sum value of exchange integrals between the particle pairs of different configurations is calculated. Then we average the absolute value of the exchange integral. Then, results are written to a file for later use with "gnuplot".

### 2.3 Results for 2D Sample

Numerical modeling allows us to create a sample with a random uniform distribution of particles in the plane. For example, let's take the sample with $0.01 \times 0.01$ μm size, particle's diameter of $d = 1$ nm, concentration of $C = 0.5$ and the number of particles $N = 60$. In Figure 1, arrows indicate directions of magnetic moment vectors.

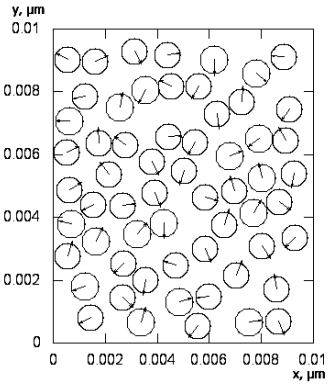


**Fig. 1** – The sample with randomly uniformly distributed particles on a plane

For calculating sum values of exchange integrals in systems with varying density of dipoles, arrays of size $N = 10000$ were used. Density then was increased up to 0.5 by decreasing the area of the surface with the constant particle area. It is obvious, that increasing the density will cause increasing the sum of the exchange integrals, which is shown on Figure 2.

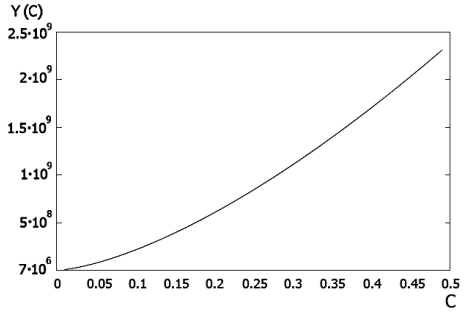


**Fig. 2** – A plot of the sum of the exchange integrals of the concentration of particles for 2D sample

Let us reduce the value of the sum of the exchange integral to a relative value see Figure 3.

Relatively small values of exchange integrals are very close to each other and have small deviation, therefore in the small scale they can merge on the plot.

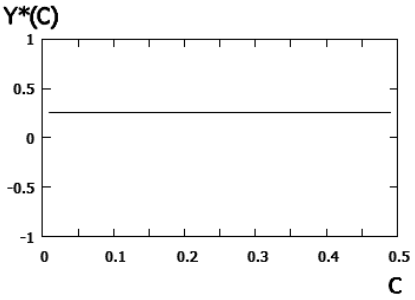


**Fig. 3** – The reduced value of the exchange integral for 2D sample

Thus, in this system of randomly uniformly distributed spherical dipole particles on a surface, there is a weak ferromagnetic interaction. However, theoretically, dipolar interactions cannot yield a ferromagnetic ground state in a disordered system [12]. So further research is required.

### 2.4 Results for 3D Sample

Let us to consider what magnetic state could a 3D system of randomly distributed spherical dipoles have. Using a numerical modeling, the sample with random uniform particles distribution in 3D was successfully visualised. This sample is a cube of the size $0.004 \times 0.004 \times 0.004$ μm, see Figure 4 for details. The diameter of each particle is $d = 1$ nm, the concentration is 0.3 and the number of particles is $N = 60$.

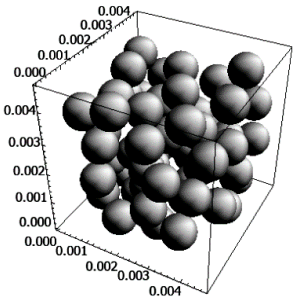


**Fig. 4** – The 3D sample with randomly uniformly distributed particles

Numerical experiments for 3D were conducted and values of sums of exchange integrals were reduced to relative values see Figure 5.

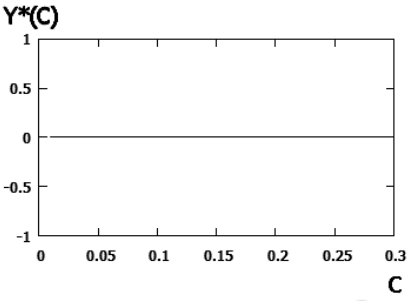


**Fig. 5** – Average of the absolute value of an exchange integral for 3D sample

The particles array with size $N = 10000$ was used for calculations. The sum value of exchange integrals

between all pairs of dipoles in the array was calculated for different density values. The density was increased up to 0.3 by decreasing the volume of the sample with the constant particle volume.

It can be seen from the plot that in 3D sample with random distribution of magnetic particles there is a competition of antiferromagnetic and ferromagnetic interactions, which could cause the spin-glass magnetic configuration of the system at zero temperature.

## 3. CONCLUSIONS

This paper describes, that dipole-dipole interactions in a system of two-level magnetic moments on a surface could cause the weak ferromagnetism. For 3D case it could cause the equality of ferromagnetic and antiferromagnetic interactions, i.e. the spin-glass state, which is consistent with the results obtained by the method of calculation of the random fields of the exchange interaction. For reliability of this conclusion it is necessary to carry out the research of samples with greater number of particles. Check for convergence of the results for large amount of experiments with the similar parameters is also required along with calculation of the average relative exchange integral and standard deviation from the mean value.

Further research will include the problem of search of the lowest energy state for the systems with $J \sim r^{-3}$ and arbitrary value of the superspin, and study of the degree of degeneracy of this state for such systems.

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