HEISENBERG ANALYTICAL-NUMERICAL MODEL OF NANOPARTICLE WITH PARA- AND FERROMAGNETISM

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(received: 10 April 2019; revised: 6 May 2019;
accepted: 31 May 2019; published online: 28 June 2019)

Abstract: Two models of two- and three-layers of a magnetic nanoparticle are presented applying the Heisenberg theory with the parameter (exchange integral and closest neighbors) values for surface layers, which differ from the bulk layer values. The difference in the numbers of closest neighbors is taken into account. The corresponding distribution and partition functions are constructed. The magnetization of the particles is calculated by the conventional transition to thermodynamics. The results are illustrated by plots, representing magnetization curves and hysteresis loops for the layer contributions. The magnetization curves for both models are compared.

Keywords: magnetic nanoparticle, Heisenberg partition function, magnetization curves, hysteresis loop

DOI: https://doi.org/10.17466/tq2019/23.3/c

1. Introduction

A nanoparticle or a nanobody usually means a body composed of tens or thousands of atoms on a scale from a nanometer size up to 100 nanometers. Well-known single-walled and multi-walled nanotubes (where the distance between the neighboring walls is about 0.34 nm) are fullerenes, fullerites, even nanoonions, nanoloops, nanotoruses and nanofilms [1]. For nano-scaled objects it is hardly possible to determine the exact conditions, where the exertion of a micro-world turns into a macro-world and vice versa, which poses a problem for the theoretical modeling of such objects.

For instance, they are investigated primarily with an aim of studying therapeutic (in some sources called 'ferromagnetic', 'superparamagnetic') nanoparticles, to be used for diagnostics and treatment of diseases. These are magnetites,

maghemites, ultrafine suspensions made from ferro-, ferri-, superparamagnetic nanoparticles reagents – nanofluids, adding some stabilization, *etc.* [2]. Such metals as Fe, Co, Ni, Gd, Tb, Dy, Ho, Er, *etc.*, as well as compounds containing these elements, are considered as ferromagnetic.

The fundamental significance of the Heisenberg theory lies in its quantum interpretation of the electron interaction and application of the Pauli principle based on the permutation symmetry group. Its irreducible representations are used as a solid tool for the energy spectrum parameters evaluation. Nevertheless, it should be noted that free electrons appropriate for metals with high conductivity are not taken into account.

After the first publication of Heisenberg's theory in 1928 [3] it was noted by subsequent sources as a non-comporting with the experimental data. Videlicet for iron at the border of switching from the paramagnetic into ferromagnetic magnetization pattern was marked by Inglis in 1932 [4]. For most other cases (where the number of closest neighbors from the material lattice structure (marked by z) is more than 8) the so called Curie point slightly deviates or distinctly matches. In 1928 and 1932 the theory was developed by Heisenberg himself, including few valence electrons [5] and the study of the impact of domains [6]. In 1953 Huzio Nakano represented the results with the lowest ferromagnetism border $z = 6$, which gave a possibility of further using this model for iron [7]. The whole story of the ferromagnetism theory is outlined in [8].

It is known that the continuous version of the Heisenberg chain equation with the Gilbert term account [9] may explain the existence of the domain walls (DW) [10]. The energy of a DW and the conditions of its creation may be estimated in terms of the exchange integral and the anisotropy coefficient. The former is proportional to the so-called exchange stiffness and the latter relates to the distribution of atoms in space [2].

In this paper we present two models of a nanoparticle that exhibit ferromagnetic properties, studying its behavior in a magnetic field as a multi-electron system, the pairs of which may have a unit spin due to exchange interaction.

Nevertheless, the border conditions between scales and relevant parameters are to be established for further improvement of a recently mentioned science branch. For the studies described in this article we propose a simplified model of a nano-scaled body of a spherical shape, containing the surface atomic layer (marked by index S), the energy of the spin state which becomes significant comparatively to the distinct bulk atom (marked by B) model.

A thermodynamic description of such a multi-electron system is based on the conventional statistical physics formalism. Such procedure is followed using the Gibbs distribution [3], the partition function Z which is split up into two components $Z = Z_S Z_B$ – accounted for by the central atoms of a nano-body and by its edge atoms.

The quantum equilibrium distribution operator (density matrix) rendered by the Gibbs formula [11] reads

$$\hat{f} = \frac{1}{Z} e^{-\frac{\hat{H}}{k_B T}} \tag{1}$$

where $\hat{f}$ is the Gibbs operator, $\hat{H}$ is the Hamiltonian, k is the Boltzmann constant, T is temperature, Z is a normalization constant. The normalization constant is expressed further as

$$Z = Tr\left[e^{-\frac{\hat{H}}{kT}}\right] \tag{2}$$

and plays the role of a partition function [11]. Hence, if $\hat{H}$ is a function of the magnetic field $\mathcal{H}$ (say, along z), the magnetization along the same coordinate M is calculated by

$$-kT\frac{\partial \ln Z}{\partial \mathcal{H}} = M \tag{3}$$

In the energy representation the distribution function reads

$$f_n = \frac{1}{Z} e^{-\frac{E_n}{k_B T}} \tag{4}$$

so that the trace in (2) is evaluated as

$$Z = \sum_n e^{-\frac{E_n}{k_B T}} \tag{5}$$

In the model we take into account one "magnetic" electron per atom only.

The algorithm of magnetization curves and hysteresis loops (HL) construction is developed during the studies of the subject inasmuch as the Heisenberg model implies a transcendental system of equations. The intersection points of graphs (IP) are fixed automatically, clearly determining the pattern of magnetization in most cases. They are simple curves, loops of a classical shape, double loops with a central symmetry. The Maplesoft programming platform was used (Figures 2, 8, 9).

2. Partition function for a nanoparticle

2.1. Surface and bulk atoms division

To start with, we simplify the model of a nanoparticle as in Figure 1.

For nanobodies made from carbon, gold and silver (commonly used in a wide range of bio-medical nanotechnology applications), we list the approximate properties of atoms of elements as an example of atom dimensions to be compared with our calculations of ferromagnetic elements [12].

Table 1. Common elements used in bio-medical applications

Designation	Atom radius size	Element name
C	$67\,[\text{pm}] = 67 \cdot 10^{-12}\,[\text{m}]$	Carbon
Ag	$165\,[\text{pm}] = 165 \cdot 10^{-12}\,[\text{m}]$	Silver
Au	$174\,[\text{pm}] = 174 \cdot 10^{-12}\,[\text{m}]$	Gold

Table 2. Common ferromagnetic elements

Designation	Atom radius size	Element name
Fe	$156\,[\text{pm}] = 156 \cdot 10^{-12}\,[\text{m}]$	Iron
Co	$152\,[\text{pm}] = 152 \cdot 10^{-12}\,[\text{m}]$	Cobalt
Ni	$149\,[\text{pm}] = 149 \cdot 10^{-12}\,[\text{m}]$	Nickel
Gd	$233\,[\text{pm}] = 233 \cdot 10^{-12}\,[\text{m}]$	Gadolinium
Tb	$255\,[\text{pm}] = 255 \cdot 10^{-12}\,[\text{m}]$	Terbium
Dy	$228\,[\text{pm}] = 228 \cdot 10^{-12}\,[\text{m}]$	Dysprosium
Ho	$226\,[\text{pm}] = 226 \cdot 10^{-12}\,[\text{m}]$	Holmium

The information is taken from general sources, so the radius values can differ depending on the source used. Despite this, the approximate data was enough to get orientated in the theoretical base.

To find out the number of atoms at the surface, we use such an estimation, based on the spherical shell volume formula [13] taking into account a mono-atomic layer of the thickness:

$$n_S = \frac{4}{3}\pi \frac{R^3 - (R-d)^3}{d^3} = 4\pi \frac{R^2 - Rd + \frac{1}{3}d^2}{d^2} \tag{6}$$

where R is the size (radius) of a whole nanoparticle, d is the diameter of an atom, which represents a single layer.

For the bulk part we proceed similarly

$$n_B = \frac{\frac{4}{3}\pi(R-d)^3}{d^3} = \frac{\frac{4}{3}\pi R^3 - 4\pi R^2 d + 4\pi R d^2 - \frac{4}{3}\pi d^3}{d^3} \tag{7}$$

The example of nickel atom which is approximately $d = 2 \cdot 149 \cdot 10^{-12}\,[\text{m}]$ is given for more complex calculations with substitution of α, proportional to the magnetic field H, and developing a three-layer model (Figure 5) The next values are obtained changing the nanoparticle size (R – the nanoparticle radius).

Table 3. Nanoparticle radius and electrons number relation estimation for iron

R in [nm]	1	3	5	10	15	50	100
R in [m]	$1 \cdot 10^{-9}$	$3 \cdot 10^{-9}$	$5 \cdot 10^{-9}$	$1 \cdot 10^{-8}$	$1.5 \cdot 10^{-8}$	$5 \cdot 10^{-8}$	$1 \cdot 10^{-7}$
n^S	93	1045	3030	$1.25 \cdot 10^4$	$2.84 \cdot 10^4$	$3.2 \cdot 10^5$	$1.28 \cdot 10^6$
n^B	44	2678	14209	$1.25 \cdot 10^5$	$4.37 \cdot 10^5$	$1.69 \cdot 10^7$	$1.36 \cdot 10^8$

As it is shown, the described model is applicable from the size with radius 3 [nm].

2.2. The bulk and surface partition function

We neglect the interaction between layers, hence, the Hamiltonian of the body is the sum of the Hamiltonians of the layers. The property of the exponent

$$e^{-\frac{\hat{H}_B}{kT} - \frac{\hat{H}_S}{kT}} = e^{-\frac{\hat{H}_B}{kT}} \cdot e^{-\frac{\hat{H}_S}{kT}} \tag{8}$$

allows writing

$$Z = Z_B Z_S \tag{9}$$

It leads to the expression of the distribution function:

$$\hat{f}_n = \hat{f}_n^B \cdot \hat{f}_n^S = \frac{1}{Z_B Z_S} e^{-\frac{\hat{H}_B + \hat{H}_S}{kT}} \tag{10}$$

where

$$Z_B = \sum_n e^{-\frac{E_n^B}{kT}} \tag{11}$$

and

$$Z_S = \sum_n e^{-\frac{E_n^S}{kT}} \tag{12}$$

where E_n^S, E_n^B – energy spectra for bulk and surface parts.

2.3. Heisenberg partition function

We reproduce the partition function from Heisenberg's paper [3], built by means of the group representation theory that yields

$$\begin{aligned} Z = \sum_{s=0}^{n} \sum_{m=-s}^{+s} \int_{-\infty}^{+\infty} d\Delta E \frac{f_\sigma}{\sqrt{2\pi \overline{\Delta E_\sigma^2}}} e^{\alpha m + \beta \frac{s^2}{2\pi} - \frac{\Delta E}{kT} - \frac{\Delta E^2}{2\Delta E_\sigma^2}} = \\ \sum_{s=0}^{n} \sum_{m=-s}^{+s} f_\sigma e^{\alpha m + \beta \frac{s^2}{2\pi} - \frac{\overline{\Delta E_\sigma^2}}{2k^2T^2}} \end{aligned} \tag{13}$$

where m – is a magnetic quantum number which denotes spin projections, while

$$\alpha = \frac{\hbar e}{\mu k T} H \tag{14}$$

$$\beta = \frac{z J_0}{kT} \tag{15}$$

After the procedure of summation we arrive at

$$Z = F \left[2 \cosh \frac{\alpha + \beta \frac{m_0}{n} - \beta^2 \frac{m_0}{nz} + \beta^2 \frac{m_0^3}{2n^3 z}}{2} \right]^{2n} \tag{16}$$

here z – the number of closest neighbors, $\hbar$ – Plank constant, e – electron charge, J_0 – exchange integral, μ – electron mass, H – magnetic field force, k – Boltzmann constant, T – temperature, m_0 – the mean value of m, n – the number of electrons.

For comparison with the experimental data we reevaluate the dimensionless variable α into H in such a way:

$$H = \frac{\mu k T \alpha}{|e| \hbar} \tag{17}$$

According to this reevaluation, the next analysis is made:

Table 4. Relation estimation of α and H through the T contribution.

T	1400	1400	1400	1400	400	400	400	400
α	13	1.3	0.13	0.013	13	1.3	0.13	0.013
H	13549	1354	135	13	3871	387	38	3

The range of the magnetization saturation point is taken from Table 4 which is equal to $\alpha = 1.5$ in most of the cases for the represented elements.

2.4. Surface and bulk atomic layer parameters

The partition functions for the layers are written similar to (16)

$$Z_B = F_A \left[2\cosh\Omega_B\right]^{2n_B} \tag{18}$$

for bulk, and

$$Z_S = F_D \left[2\cosh\Omega_S\right]^{2n_S} \tag{19}$$

for the surface. We denote the arguments as

$$\Omega_B = \frac{\alpha + \beta_B \frac{m_0^B}{n_B} - (\beta_B)^2 \frac{m_0^B}{n_B z_B} + (\beta_B)^2 \frac{(m_0^B)^3}{2(n_B)^3 z_B}}{2} \tag{20}$$

for the bulk, while for the surface it is:

$$\Omega_S = \frac{\alpha + \beta_S \frac{m_0^S}{n_S} - (\beta_S)^2 \frac{m_0^S}{n_S z_S} + (\beta_S)^2 \frac{(m_0^S)^3}{2(n_S)^3 z_S}}{2} \tag{21}$$

It is denoted:

$$\beta_B = \frac{z_B J_B}{kT} \tag{22}$$

$$\beta_S = \frac{z_S J_S}{kT} \tag{23}$$

In the expressions, z_B, z_S – the number of closest neighbors (bulk, surface), J_B, J_S – exchange integrals (bulk, surface), m_0^B, m_0^S – mean values of the m magnetic quantum number (bulk, surface), n_B, n_S – the number of electrons (bulk, surface), F_A, F_D – some other functions which can be omitted.

3. To thermodynamics: nanoparticle magnetization

3.1. Two-layer model

From the general expression ((16)) we derive

$$m_0 = \frac{\partial \ln(F[2\cosh\Omega]^{2n})}{\partial\alpha} = n\tanh\Omega \tag{24}$$

where

$$\Omega = \frac{\alpha + \beta\frac{m_0}{n} - \beta^2\frac{m_0}{nz} + \beta^2\frac{m_0^3}{2n^3 z}}{2} \tag{25}$$

the modification of which could be similarly done for the Z^B and Z^S partition functions:

$$\begin{aligned} m_0^{[BS]} = &\frac{\partial \ln(Z_B Z_S)}{\partial\alpha} = \frac{\partial \ln(Z_B)}{\partial\alpha} + \frac{\partial \ln(Z_S)}{\partial\alpha} = \\ &\frac{\partial \ln(\left[2\cosh\Omega_B\right]^{2n_B})}{\partial\alpha} + \frac{\partial \ln(\left[2\cosh\Omega_S\right]^{2n_S})}{\partial\alpha} = \\ &\frac{2n_B(2\cosh\Omega_B)^{(2n_B-1)}\cdot 2\sinh\Omega^B}{2(2\cosh\Omega_B)^{2n_B}} + \frac{2n_S(2\cosh\Omega_S)^{(2n_S-1)}\cdot 2\sinh\Omega_S}{2(2\cosh\Omega_S)^{2n_S}} = \\ &n_B\tanh\Omega_B + n_S\tanh\Omega_S \end{aligned} \tag{26}$$

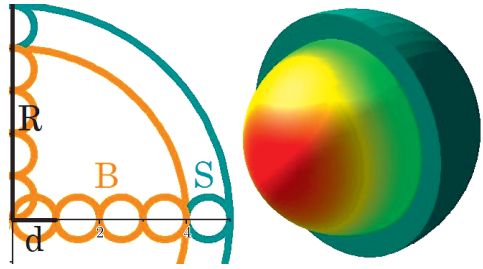

Figure 1. Spherical simplification of a nanobody (nanoparticle). The central part stands for the bulk part (Index B), while the outside layer is the surface area (Index S). R is the radius of the whole nanoparticle, d is the diameter of a single atom.

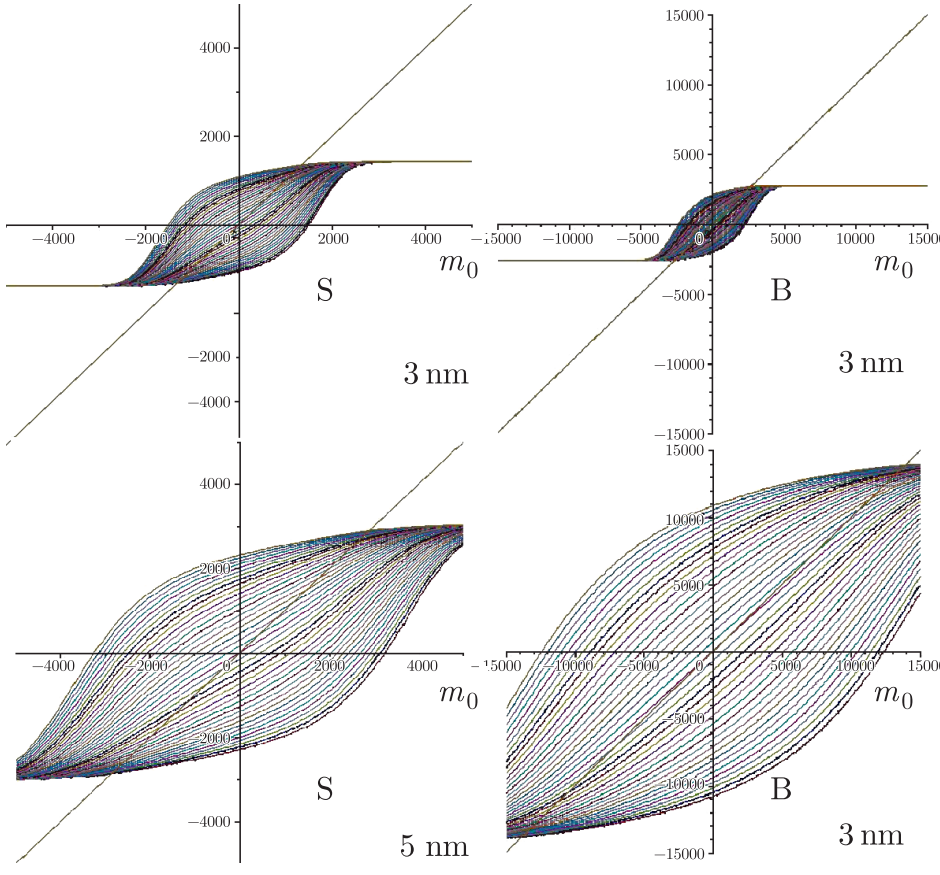

Figure 2. Element – Iron. Comparing $R = 3$ [nm] and $R = 5$ [nm]. $T = 1400$ [K]. The same scale is made for both bulk parts and for both surface parts to make a more clear comparison of the layer impact relations. The first peculiarity is when the nanoparticle size is smaller than presented – the bulk layer becomes insignificant

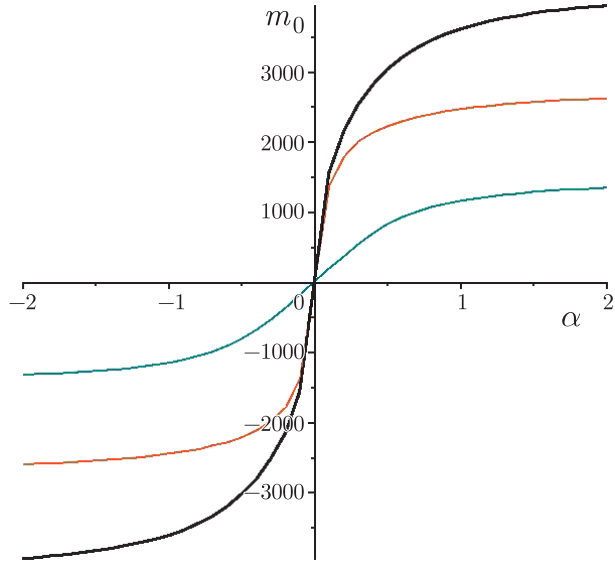

Figure 3. $m_0(\alpha)$. Element – Iron. $R = 3$ [nm]. $T = 1400$ [K]. Comparing with a bigger size (Figure 4), here the impact of the surface is significant

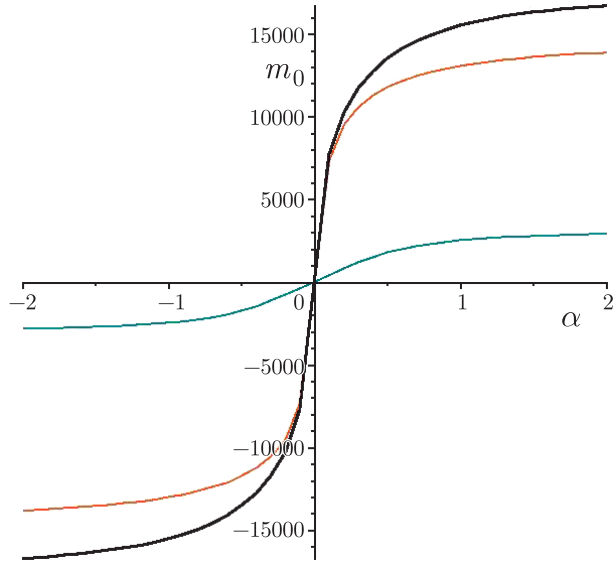

Figure 4. $m_0(\alpha)$. Element – Iron. $R = 5$ [nm]. $T = 1400$ [K]. The bigger the size – the smaller the impact of the surface, that is why surface phenomena are usually omitted and our model becomes less relevant

where $m_0^{[BS]}$ is a mean value of the magnetic quantum number for joint bulk and surface parts.

By converting the Curie-Weiss formula with the substitution of β and accounting for the θ temperature point, which is a critical point for switching between para- and ferromagnetic magnetization, we obtain:

$$J_B = \frac{\theta k(1-\sqrt{1-\frac{8}{z}})}{2} \tag{27}$$

which is used to find the value of the exchange integral for the bulk part, based on the estimations of Heisenberg [3]. Unfortunately, there is no exact analog for the surface part, hence, the simplified calculation is done for J_S. Thus, we enhanced J_B in a quarter of its value.

According to the geometry of the corresponding atomic positions the exchange integral for the surface part has to be bigger than for the bulk part. The reason for this is that the atom, surrounded by a smaller number of neighbors, comparing with the atoms inside the nanoparticle, is free from one side of space diminishing the distance between atoms and, hence, enhancing the exchange interactions.

For iron $\theta = 1043K, z = 8$, the bulk case gives

$$J_B = \frac{1043 \cdot 1.38 \cdot 10^{-23}(1-\sqrt{1-\frac{8}{8}})}{2} = 7.19 \cdot 10^{-21} \tag{28}$$

Then, the enlarged exchange integral for the surface is

$$J_S = 1.25 \cdot 7.19 \cdot 10^{-21} = 8.98 \cdot 10^{-21} \tag{29}$$

For nickel $\theta = 627K, z = 12$, in the direct analogue for the bulk

$$J_B = \frac{627 \cdot 1.38 \cdot 10^{-23}(1-\sqrt{1-\frac{8}{12}})}{2} = 1.82 \cdot 10^{-21} \tag{30}$$

and for the surface:

$$J_S = 1.25 \cdot 1.82 \cdot 10^{-21} = 2.28 \cdot 10^{-21} \tag{31}$$

The results of the magnetization curves for iron construction are shown in Figures 2, 3, 4.

3.2. Three-layer model

The further development of the nanoparticle model is the introduction of an intermediate layer in which the exchange integrals may differ from the surface and bulk exchange integrals, while the number of closest neighbors differs from those within the surface layer.

The intermediate layer is located between the surface layer and the bulk part – all the three layers are used in a three-layer model (Figure 5). The summing graphs are presented in Figure 6, 7, 9.

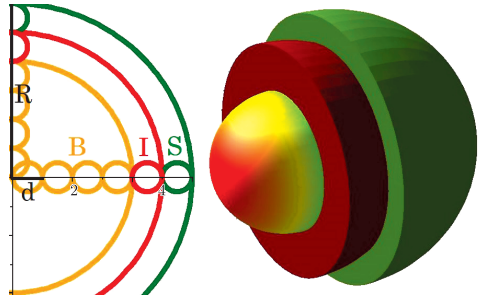

Figure 5. Three-layer model. R is a radius of the whole nanoparticle, d is a diameter of a single atom. B – bulk, I – intermediate, S – surface layers. Intermediate and surface layers do not have hysteresis, due to an insufficient number of neighbors

Repeating the previous succession of actions for a two-layer model, we distinguish a new – intermediate – layer (relevant values marked by index 'I'), which is to be significant in precisely 1-10 nanometer-sized nanoparticles. Its advantage is in the ambiguity of exchange interactions between atoms, where surface and bulk featuring characteristics are combined. The intermediate exchange integral (J_I) is responsible for this combination.

For iron we put

$$J_I = 1.15 \cdot 7.19 \cdot 10^{-21} = 8.27 \cdot 10^{-21} \tag{32}$$

while for nickel,

$$J_I = 1.15 \cdot 1.82 \cdot 10^{-21} = 2.1 \cdot 10^{-21} \tag{33}$$

Then, the total partition function Z for a three-layer model is found similar to the two-layer one:

$$Z = Z_B Z_I Z_S \tag{34}$$

where the partition function for the intermediate layer is built as

$$Z_I = F_G \left[2\cosh \Omega_I\right]^{2n_I} \tag{35}$$

where

$$\Omega_I = \frac{\alpha + \beta_I \frac{m_0^I}{n_I} - (\beta_I)^2 \frac{m_0^I}{n_I z_I} + (\beta_I)^2 \frac{(m_0^I)^3}{2(n_I)^3 z_I}}{2} \tag{36}$$

$$\beta_I = \frac{z_I J_I}{kT} \tag{37}$$

Here z_I – the number of closest neighbors (intermediate), J_I – exchange integral (intermediate), m_0^I – the mean value of m, the magnetic quantum number (intermediate), n_I – the number of electrons (intermediate), F_G – some other function, which is omitted.

For the partition functions Z_B, Z_I and Z_S we write:

$$m_0^{[BIS]} = \frac{\partial \ln(Z_B Z_I Z_S)}{\partial \alpha} = \frac{\partial \ln(Z_B)}{\partial \alpha} + \frac{\partial \ln(Z_I)}{\partial \alpha} + \frac{\partial \ln(Z_S)}{\partial \alpha} = n_B \tanh \Omega_B + n_I \tanh \Omega_I + n_S \tanh \Omega_S \tag{38}$$

where $m_0^{[BIS]}$ is a mean value of the magnetic quantum number for joint bulk, intermediate and surface parts.

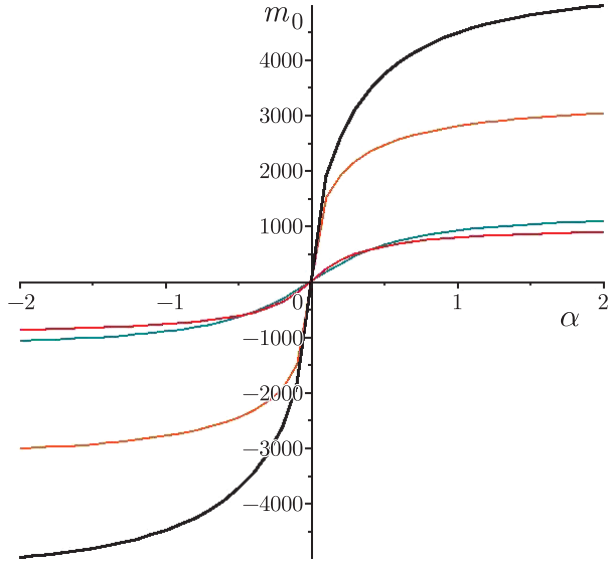

Figure 6. $m_0(\alpha)$. Element – Nickel. $R = 3$ [nm]. $T = 660$ [K]. Blue line – the surface layer. Red line – the intermediate layer. Orange line – the bulk layer. Surface and intermediate layers show similar magnetization that illustrates the importance of each layer thickness

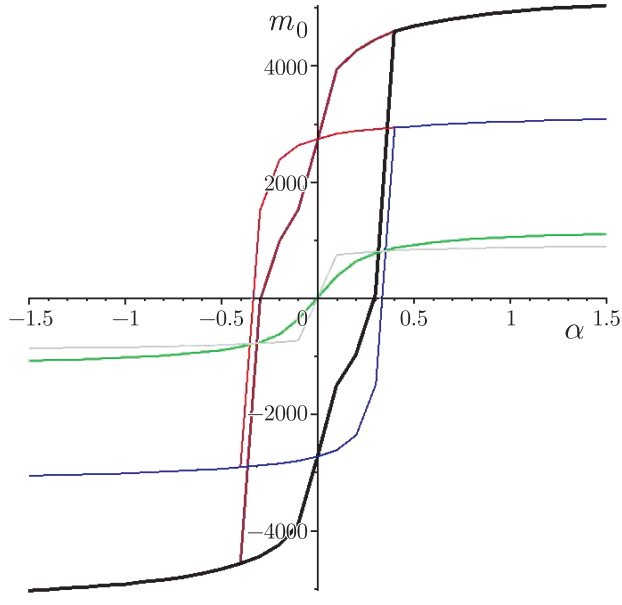

Figure 7. $m_0(\alpha)$. Element – Nickel. $R = 3$ [nm]. $T = 400$ [K]. $\alpha = -1.5..1.5$, where $\alpha = 1$ corresponds to the magnetic field value $297 \frac{A}{m}$. $m_0 \cdot \mu_B = M$, where μ_B is a Bohr magneton, M is magnetization. As the magnetization pattern of the bulk part is a loop (red and blue), then the total magnetization of all the three layers is a loop – black and brown. The green curve is the magnetization of the surface part, grey – an intermediate layer. As the intermediate layer is considered the smallest, thus, the saturation point for its magnetization is the smallest. Therefore, it looks fractured. Both impacts of our additional layers make the total loop fractured and deformed

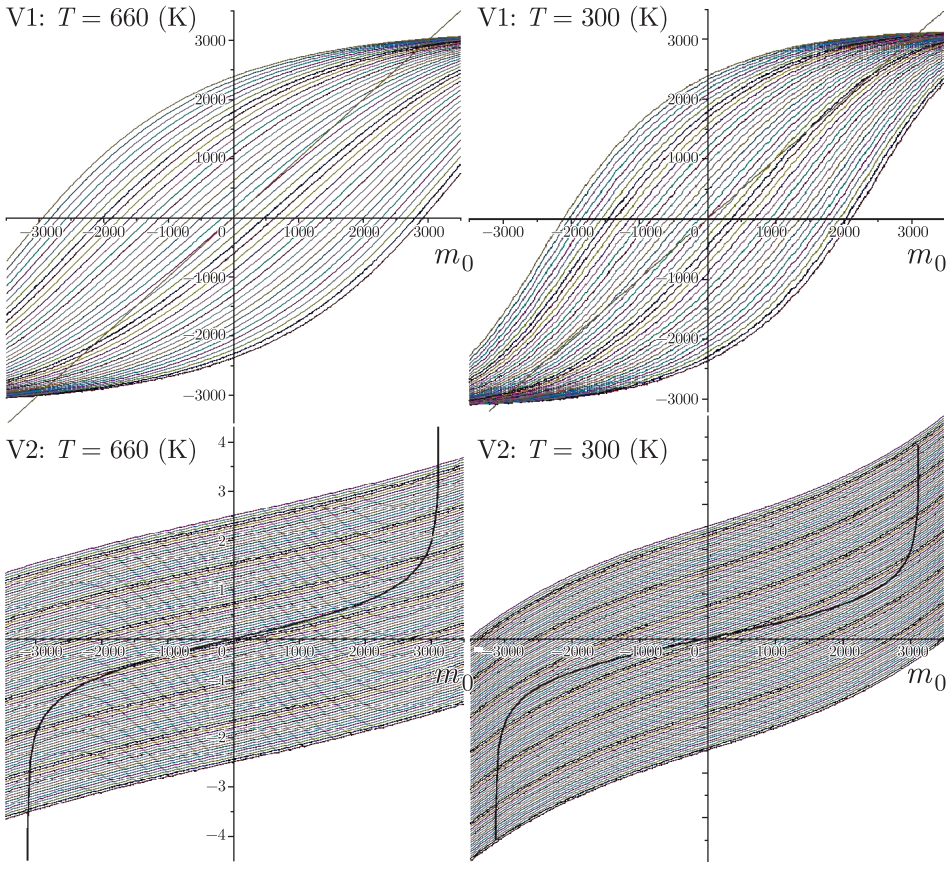

Figure 8. Element – Nickel. $R = 3$ [nm]. $T = 660$ [K] and $T = 300$ [K]. The given comparison illustrates an alternative method of building a magnetization curve in case of hysteresis (or even – hysteresis with double loops). According to variant 1 (V1) the intersection points (IP) are taken from the next graphs: the curves and the line. While variant 2 (V2) is based on taking the IP from curves instead of a line. This gives a possibility to catch the hysteresis theoretically not only for nickel or cobalt, but for iron as well. Iron is marked as the element with which it is sometimes hard to operate. For switching between the presented variants, hyperbolic tangent is algebraically replaced by hyperbolic arc-tangent

Finally, the last needed formula based on finding the spherical shell:

$$n_I = \frac{4}{3}\pi \frac{(R-d)^3 - (R-2d)^3}{d^3} \tag{39}$$

where n_I is the number of electrons for the intermediate layer.

3.3. Comparison of two- and three-layer models

The three-layer model would take into account the exchange integral variation in transition from layer to layer more exactly. The two-layer model is applicable in a wider range of nanoparticles, thus, it considered to be general. While a three-layer model is a particular case, applicable in cases of 1-10 nanometer sizes, where the intermediate layer contribution is essential.

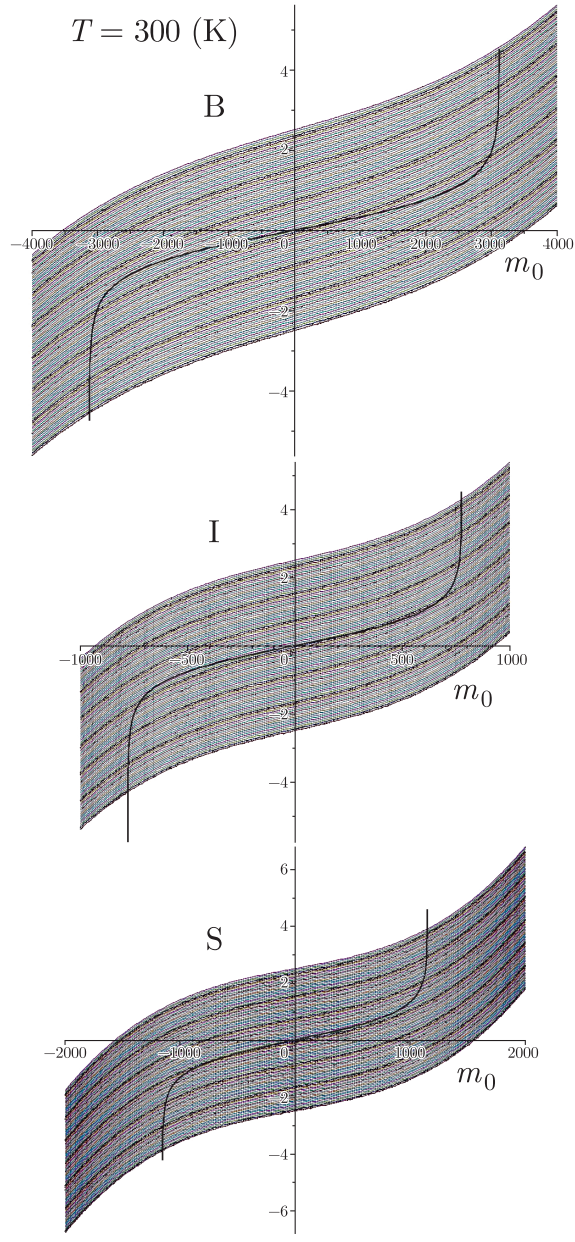

Figure 9. Algorithm of further construction of total $m_0(\alpha)$. Element – Nickel. $R = 3$ [nm]. $T = 300$ [K]. $n_B = 3122$, $n_I = 927$, $n_S = 1151$, $z_B = 12$, $z_I = 9$, $z_S = 7$. Loops from Figure 7 appear only in the bulk part, as the additional layers do not have the required number of neighbors (z). In the bulk part there is more than one intersection point (IP) of two curves, which are taken from the following graph and then fixed in two arrays of maximum and minimum IPs. Hence, multiple intersections (usually 5) are the key element for building hysteresis loops in any cases by using the described Heisenberg model

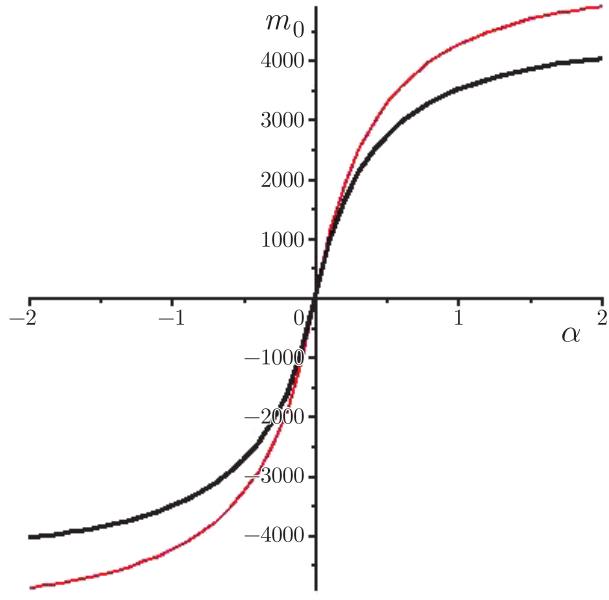

Figure 10. Comparison of two- and three- layer models without hysteresis. $m_0(\alpha)$. Element – Nickel. $T = 700$. $\alpha = -2..2$, where $\alpha = 1$ corresponds to the magnetic field value $521\frac{A}{m}$. $m_0 \cdot \mu_B = M$, where μ_B is the Bohr magneton, M is magnetization. Black curve – the two-layer model sum, red curve – the three-layer model sum

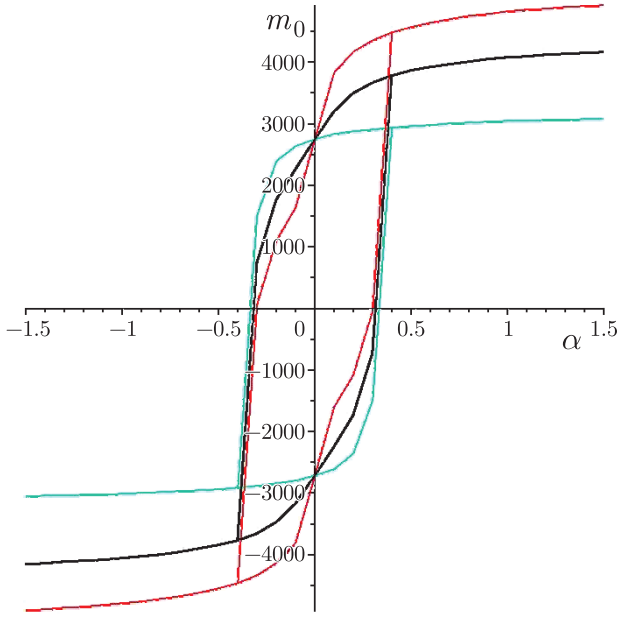

Figure 11. Comparison of two- and three- layer models with hysteresis. $m_0(\alpha)$. Element – Nickel. $T = 400$. $\alpha = -1.5..1.5$, where $\alpha = 1$ corresponds to the magnetic field value $297\frac{A}{m}$. Black loop – the two-layer model sum, red loop – the three-layer model sum. Mint loop – the magnetization pattern without taking into account any additional layers and applying our model

The comparison of the magnetization curves of models is presented in Figure 10 and the hysteresis curves are shown in Figure 11.

4. Conclusions

The main result of this paper is a generalization of the Heisenberg theory for the case of a nanoparticle. We built two models of partition functions applying the results of the Heisenberg theory to its construction.

The models use a division of a particle into two- and three layers which differ by basic parameters, the exchange integrals and numbers of closest atoms. We built and compared the magnetization and hysteresis curves.

References

[1] Series Editor: Palmer R E 2016 *Frontiers of Nanoscience: The Nanoscale Physics Research Laboratory, The School of Physics and Astronomy, The University of Birmingham*, UK Elsevier

[2] Schollẅock U, Richter J, Farnell D J J and Bishop R F 2004 *Quantum Magnetism, Lecture Notes in Physics 645*, Springer-Verlag, Berlin

[3] Heisenberg W 1928 *Zur Theorie des Ferromagnetismus*, *Zs. Phys.* **49** 619

[4] Inglis D R 1932 *The Heisenberg Theory of Ferromagnetism*, Landheim Pulvermuhle, Dusslingen bei Tubingen

[5] Heisenberg W 1928 *Zur Quantentheorie des Ferromagnetismus*, *Probleme der Modernen Physik. Arnold Sommerfeld zum 60. Geburtstage gewidmet von seinen Schülern* Debye P, Ed., Leipzig, Hirzel S 114

[6] Heisenberg W 1931 *Zur Theorie des Magnetpstriktin und der Magnetisierungkurve*, *Zs. Phys.* **69** 287

[7] Nakano H 1953 *The Heisenberg Theory of Ferromagnetism of the Crystal constituted by the Atoms with Spin One*, *Progress of Theoretical Physics* **9** (4) 403

[8] Navinder Singh *The story of magnetism: from Heisenberg, Slater, and Stoner to Van Vleck, and the issues of exchange and correlation*, arXiv:1807.11291 [cond-mat.str-el]

[9] Lakshmanan M 2011 *The fascinating world of the Landau–Lifshitz–Gilbert equation: an overview*, *Phil. Trans. R. Soc. A* **369** 1280

[10] Hayashi N, Inoue T, Nakatani Y and Fukushima H 1988 *Direct solution of Landau-Lifshitz-Gilbert equation for domain walls in thin Permalloy films*, *IEEE Transactions on Magnetics* **24** (6) 3111
[online] `https://ieeexplore.ieee.org/xpl/tocresult.jsp?isnumber=3040`

[11] Reichl L E *A Modern Course in Statistical Physics, 2nd Edition*, A Wiley-interscience publication, John Wiley and Sons, inc.

[12] *Element atom radius, [online]* `www.fxyz.ru`

[13] *Spherical shell, [online]* `wikipedia.org`