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HYSTERESIS LOOPS FOR A BULK FERROMAGNETIC BY HEISENBERG MODEL

In a framework of Heisenberg theory, that link quantum-statistical description taking Gauss distribution into account, explicit form is obtained by permutations group theory, the division paramagnetic/ferromagnetic is studied. The magnetization curves are built for a given set of parameters, such as exchange integral, number of closest neighbours and temperature. In a special range of the parameters a transition from unique solution of the resulting Heisenberg equation to multi-valued is observed. For this case exemplary hysteresis loops are built. The expression for Curie temperature allows to evaluate the exchange integral and proceed into temperature range above the critical temperature.

В рамках теории Гейзенберга, связывающей квантово-статистическое описание с учетом распределения Гаусса, явная форма получается с помощью теории групп перестановок, изучается парамагнитное / ферромагнитное разделение. Кривые намагниченности построены для заданного набора параметров, таких как обменный интеграл, число ближайших соседей и температура. В специальной области параметров наблюдается переход от единственного решения полученного уравнения Гейзенберга к многозначному. Для этого случая построены примерные петли гистерезиса. Выражение для температуры Кюри позволяет учесть обменный интеграл и перейти в температурный диапазон выше критической температуры.

Keywords: hysteresis loop, ferromagnetism, paramagnetism, Curie temperature, Curie point, magnetisation curve, Curie — Weiss law, transcedental equation.

Ключевые слова: петля гистерезиса, ферромагнетизм, парамагнетизм, температура Кюри, точка Кюри, кривая намагничивания, закон Кюри — Вейсса, трансцедентное уравнение.

Introduction

The problem of theoretical description of magnetization takes the significant place in modern studies, beginning from seminal results of Weiss [2]. In the famous paper of Heisenberg [3] on ferromagnetism it was established that the Weiss electric forces are originated from exchange effect of quantum mechanics primarily introduced in textbooks' Heitler — London results. This paper [3] contains also very deep results of general significance. Multielectron terms theory was built using the very common symmetry: in respect to group of electrons permutations. It has its extension based on joint symmetry group of permutations and space symmetry group [9], where the exchange integral notion is «lifted» up the Hartree — Fock equations level. The permutation group theory allows to express energy via its irreducible representations characters [6] and, in same context, statistical distribution function is constructed. Its derivative gives the internal parameter (magnetisation M value conjugate to magnetic field H, that results in equation of state $M(H)$).

The microscopic Heisenberg model goes to macroscopic Landau — Lifshits — Gilbert (LLG) equations as in [7]. For example, in the article of Rivas [1] the ferromagnetic alloy $Co_{66}Fe_4Mo_2Si_{16}B_{12}$ is studied. They explore such LLG-based model for hysteresis loop building with the help of LLG differential equations of the second order. Experimentally, the alloy was isothermally annealed: the following material was heated, then slowly cooled, in order to change the structural organisation of molecules in it. When the lattice (or other amorphous analog of it) changes, that changes the distance between units (atom or molecule), the properties of a material change too. The result is obtained at 530 degrees Celsium heating — there were some agglomerates of only 1—6 particles surrounded by the amorphous material. The group proceeded to the tests of its magnetic properties, changing the angle of applied magnetic field and other characteristics. Moreover, the bias of HL was detected.

In our paper we experienced two alike ways of graphical solutions of the resulting transcendent Heisenberg equations for the paramagnetism and ferromagnetism cases. It admits unique solution in the paramagnetism range, that gives the magnetisation curve. In the ferromagnetism domain few branches of solutions take place, that yields the loops.

Practically, notching the intersection points (IP) of functions into the so called matrix of values, which depends on the changes of external magnetic field strength and characteristics of the material. Connecting the extreme values of the matrix in case of multiple intersection between the same graphs, we managed either to build a hysteresis loop for a bulk ferromagnetic, or to identify some special cases, such as double loops with the central symmetry [10; 11].

In the last section we study a transition between para- and ferro-magnetics, parametrized by Curie temperature, that generalizes the Curie — Weiss relation.

Para-magnetic materials. On theoretical base

The Heisenberg equations, derived in [3—5] result in a couple of explicit functions, depending on M [9]:

$$y_1 = M, \tag{1}$$

$$y_2 = \tanh\left(\frac{\alpha + \beta M - \beta^2 \frac{M}{z} + \beta^2 \frac{M^3}{2z}}{2}\right), \tag{2}$$

where

$$\alpha = \frac{e\hbar}{mk_B T} H, \tag{3}$$

$$\beta = \frac{zJ}{k_B T}, \tag{4}$$

z — a number of closest neighbours; e — an electron charge; $\hbar$ — Plank constant; m — an electron mass; k_B — Boltzmann constant; T — temperature; J — an exchange integral.

The values of the parameters $e, m, \hbar$ are quite definite, while the z, J, T ones choice need some discussion. So, Heisenberg [3—5] estimates the parameter J by the note, that the exchange energy should be about $k_B T$, giving the value $J \approx 10^{-13}\, erg$. For such the value the parameter β is of order of 1 for the room temperature.

The paramagnetic case domain in $z\beta$ plane is fixed by the condition:

$$\beta(1 - \frac{\beta}{z}) < 2. \tag{5}$$

The magnetisation curve construction

To build the magnetisation curve the values of M for each α are required. We take them by the means of solving the system of equations (1) and (2) graphically (Fig. 1). There is one intersection point between the line and the curve for para-magnetic materials, for the choice of z, β, such that (5) holds.

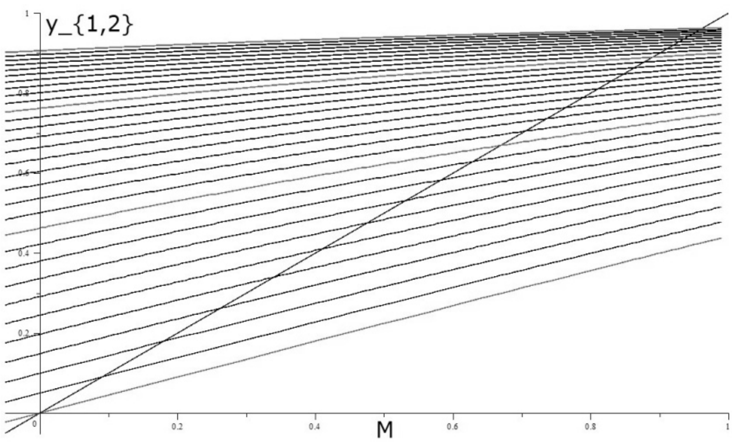

Fig. 1. The choice of parameters: $\beta = 1; z = 10$

The intersection points (IP) of a diagonal line with curves are the solution of the system of equations (1) and (2). The curves correspond to α, that is proportional to the magnetic field H, substitution from 0 value (the lowest curve) to 3 (the highest curve). The value of α between the closest curves differs in 0.1.

Next, the magnetization curve by the mentioned algorithm is built in Figure 2.

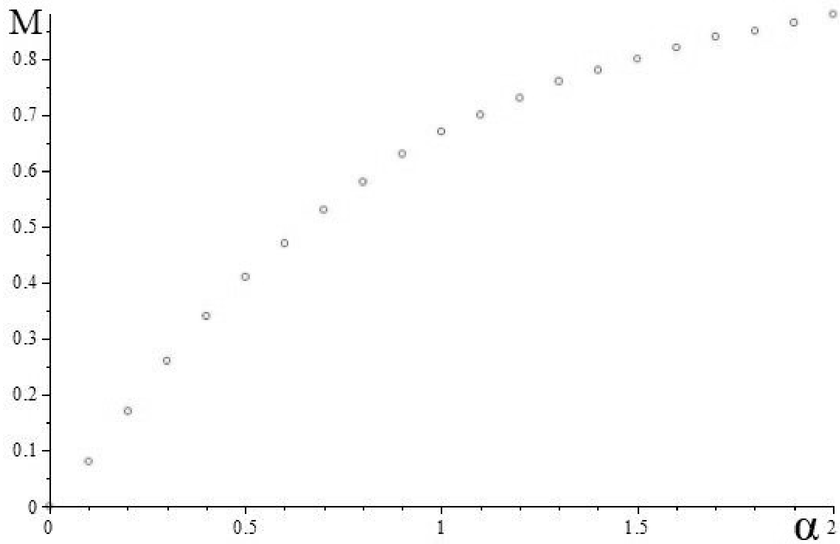

Fig. 2. Magnetisation curve for para-magnets looks typical [8]

The dependence of M on α in a range of $\alpha = 0..2$, shown for the same parameter values $\beta = 1; z = 10$ as in Figure 1. With the increase of α value the curve changes like a linear. The thickening of intersection points is observed.

Ferromagnetic materials

In the case of ferromagnetic state the domain by (5) is above the curve $z(\frac{J}{k_B T})$, whence the solution of the Eq. 2 is not unique. In order to find out the values of joint points of (1) and (2) graphs, we should follow the bends of hysteresis loop curves more accurately, using the alternative variant of graphical solution of the following equivalent equations:

$$\widetilde{y_1} = \arctan h(M), \tag{6}$$

$$\widetilde{y_2} = \frac{\alpha + \beta M - \beta^2 \frac{M}{z} + \beta^2 \frac{M^3}{2z}}{2}. \tag{7}$$

As it is observed in Figure 3 — the resultant loops, built by the means of (6) and (7) system, are rather convex and curved, comparing with (1) and (2) variant. The results of two different cases are presented in Figures 3—5.

Grey curves show the change of α value in 0.25 one by one. The black curve (6), unlike its possible alternative (1), gives the resultant thickening of intersection points in fracture areas of the function. There are cases of 5 intersections of a single grey curve with the black — this is a critically needed condition to obtain the loop, illustrated at Figure 4.

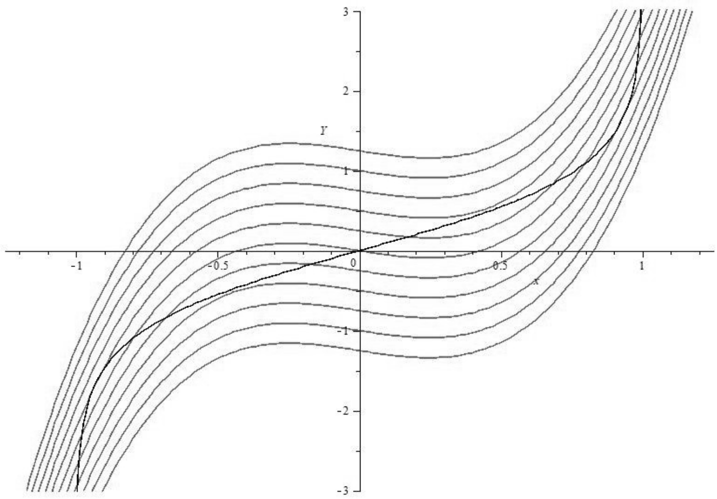

Fig. 3. The intersection points of (6) and (7) are carried out for $\alpha = -0.75..0.75; \beta = 10; z = 8$

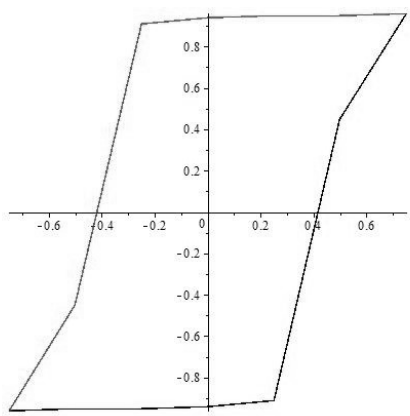

Fig. 4. The hysteresis loop for common ferromagnetic materials. The values for its compilation are obtained from Figure 3. The presence of 5 intersection points (IP) described at Figure 3, gives the expansion of a loop at the approaching area to abscissa axis

The further away from each other are the extreme points from the set of 5 IP (for a single grey tangensoid curve), the wider is the entire loop. The medium IP are not pictured and are not taken into account here. Though, medium IP are all inside the loop area.

The Heisenberg theory do not take into account domain walls presence in explicit form. It uses the Gauss distribution of states per energy level with parameters expressed in terms of characters of the universal symmetry group, the group of permutations. Few interesting properties however are exhibited in some range of the parameters z and T, see again [10; 11].

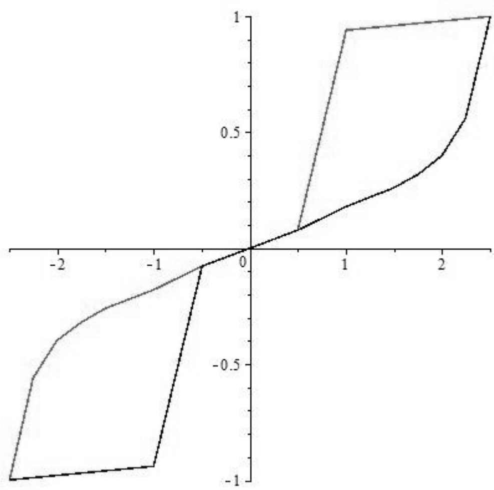

Fig. 5. The double loop with the center symmetry of sub-loops

The represented graph is the Hysteresis loop in case of maximum 3 intersections of (1) with the single curve (2) $(\alpha = -2.50..2.50; \beta = 11; z = 8)$. There is no tangible difference if we take either ((6) and (7)) or ((1) and (2)) system for compilation. The vivid peculiarity is in 3 IP at once for a single curve ((2) and (7)) with the auxiliary functions from appropriate for each system of equations. The critical condition of double loop compilation: all three IP must be found in the same quarter area. The curves have a central symmetry for positive and negative α values, so the sub-loop at the third quarter $(-\alpha)$ always repeats the sub-loop at the first $(+\alpha)$ if α value is the same, having the difference only in its sign.

Towards the Curie law

To add, the Ferromagnetism existence is demonstrated via the set of features, including the Curie law [8]. Its analog is derived at Heisenberg's paper [3] as well. According to it, there exists the critical temperature for switching from paramagnetic into ferromagnetic properties appearance and vice versa, by the boundary of the domain (5). It is marked as θ at original text:

$$\theta = \frac{2J}{k_B(1-\sqrt{1-\frac{8}{z}})}. \qquad (8)$$

As well, the author emphasizes the similarity of the Curie Law with modification to the Weiss theory. Thus, the critical point is taken from the following conclusion, where M, T, z are mathematically connected.

As a result of following the Heisenberg's algorithm of transformations, we have obtained the resembling formula (9). We use it for graphical analysis and further substitutions of contingent constants, proceeding the imitations of practical situations with real materials.

$$M = \frac{4\alpha T^2}{z(1-\sqrt{1-\frac{8}{z}})(T-\theta)(T(1+\sqrt{1-\frac{8}{z}})-\theta(1-\sqrt{1-\frac{8}{z}}))}. \quad (9)$$

Iron (Fe) was chosen as the primary sample of the corresponding section of this article out of its lattice structure. The approximation formula got vastly simplified (10) throughout the graphing procedure, because of the number of closest neighbours, which is 8 in our graphical imitation.

$$M = \frac{\alpha T^2}{2(T-\theta)^2}. \quad (10)$$

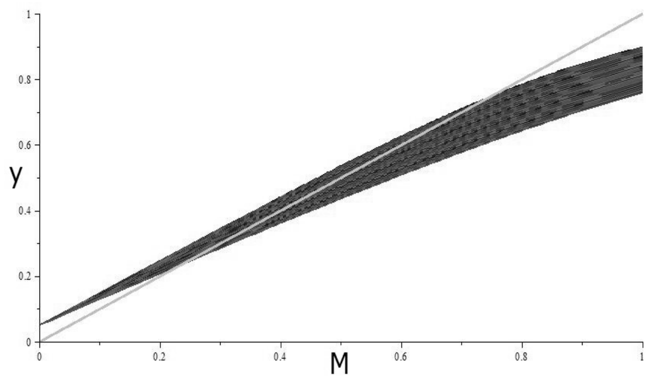

Fig. 6. The IP-printing for building (A) from Figure 7 with the usage of (1) and (2) system of equations. The horizontal axis shows the designation of magnetisation recession $(z = 8; \alpha = 0.1; \theta = 1043[K]; T = 1143..1903[K])$

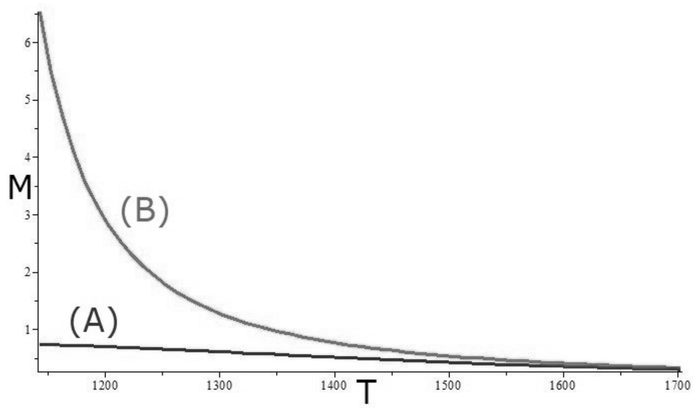

Fig. 7. The dependence of magnetisation on temperature (for Iron), where $T > \theta$. The comparison of two methods is graphed $(z = 8; \alpha = 0.1; \theta = 1043[K]; T = 1143..1703[K])$

(A) — the solutions of the equation system (1) and (2); (B) — the result plotted by (10)

Conclusions

We have built the magnetisation curves for paramagnetic and ferromagnetic ranges for temperatures below and above Curie temperature, appropriate for chosen material. We would note that microscopic Heisenberg model has its continuous analog, named Landau — Lifshits — Gilbert equations. It could be used in making description of domain walls dynamics [12] and hysteresis phenomenon as well [1].

References

1. *Martinez-Garzia J.C., Rivas M, Garcia J.A.* Induced ferro-ferromagnetic exchange bias in nanocrystalline systems // Journal of magnetism and magnetic materials. 2015. Vol. 377. P. 424—229.

2. *Weiss P.* Molecular field and ferromagnetic property // Journ. de phys. 1907. Vol. (4) 6. P. 661.

3. *Heisenberg W.* Zur Theorie des Ferromagnetismus // Zs. Phys. 1928. Vol. 49. P. 619—636.

4. *Heisenberg W.* Zur Quantentheorie des Ferromagnetismus // Probleme der Modernen Physik, A. Sommerfeld Festschrift. Leipzig, 1928. P. 114—122.

5. *Heisenberg W.* Zur Theorie des Magnetpstriktin und der Magnetisierungkurve // Zs. Phys. 1931. Vol. 69. P. 287—297.

6. *Heitler W.* Stäorungsenergie und Austausch beim Mehrkäorperproblem // Zs. Phys. 1927. Vol. 46. P. 47.

7. *Lakshmanan M.* The fascinating world of the Landau — Lifshitz — Gilbert equation: an overview // Phil. Trans. R. Soc. A. 2011. Vol. 369. P. 1280—1300.

8. *Kittel C.* Introduction to Solid State Physics. Wiley, 2004.

9. *Leble S.* Heisenberg chain equations in terms of Fockian covariance with electric field account and multiferroics in nanoscale // Nanosystems: physics, chemistry, mathematics. 2019. Vol. 10 (1). P. 18—30.

10. *Hirsch A.* Double hysteresis loops in ferromagnetic crystals // J. Phys. Radium. 1959. Vol. 20 (2—3). P. 262—263.

11. *Brandão J., Dugato D.A., Seeger R.L. et al.* Observation of magnetic skyrmions in unpatterned symmetric multilayers at room temperature and zero magnetic field // Sci Rep. 2009. Vol. 9. 4144. doi:10.1038/s41598-019-40705-4.

12. *Leble S.* Waveguide Propagation of Nonlinear Waves. Impact of Inhomogeneity and Accompanying Effects. Springer, 2019.

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