

THE STOCHASTIC TREATMENT OF PARALLEL DIFFERENT SPINS

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Abstract

The considered system of parallel spins of different magnitudes with random distribution of spins requires statistical approach to the problem. So, we can find the most probable distribution. Using this distribution we substitute the system of random spins with simple system having the spins of equal magnitude, whose properties can be determined by usual methods.

Keywords: spin, statistical approach, probabilistic distribution.

1. Introduction

Real crystal structures contain between 5% and 15% of impurities. In standard analysis this fact is not taken into account, mainly. Even the problem of one impurity is relatively complicated in mathematical sense, while the problem with two impurities requires several pages of clear calculations. The problem with three impurities is three body problem and nobody tried to solve it. In the theory of magnetism Izjumov solved problems with one and two impurities [2, 3]. So, the problem of structures with large number of impurities which appear as random variables is very complicated. Having this in mind, we concluded that such structures must be treated by stochastically statistical method which cover all problems of random impurities and gives possibility to go over to an equivalent ideal structure with spins, as mathematical expectation of all ones, which are located in the lattice.

2. Stochastic model

We shall consider inter metallic compound consisting of several different ferromagnetic materials having different spins. Distribution of atoms of ferromagnetic materials is random and we assume that all different spins are parallel. In this situation the unique approach in

analysis is rather stochastically [4, 5]. It means that statistical probability of the system has to be determined as well as the laws of conservation.

We suppose that inter metallic compound contains n different spins and that N_λ atoms have spin S_λ , with $\lambda = 1, 2, \dots, n$. The corresponding statistical probability is given by:

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| | $P = \frac{N!}{\prod_{\lambda=1}^n N_\lambda!} \approx \frac{N^N}{\prod_{\lambda=1}^n N_\lambda^{N_\lambda}}.$ | (1) |
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In the considered system are conserved total number N of spins and total spin of the system. So we have the conservation laws: $\sum_{\lambda=1}^n N_\lambda = N = const$ and $\sum_{\lambda=1}^n N_\lambda S_\lambda = S = const$.

The thermodynamical potential is given by $\Phi = \ln P - \alpha N - \beta S$ and we can write:

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| | $\Phi = N \ln N - \sum_{\lambda=1}^n (N_\lambda \ln N_\lambda + \alpha N_\lambda + \beta S_\lambda N_\lambda),$ | (2) |
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where from it follows:

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| | $\delta\Phi = - \sum_{\lambda=1}^n (\ln N_\lambda + 1 + \alpha + \beta S_\lambda) \delta N_\lambda.$ | (3) |
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Equating the variation $\delta\Phi$ with zero, we obtain

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| | $N_\lambda = e^{-(\alpha+1)-\beta S_\lambda}.$ | (4) |
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After the determination of Lagrange multiplier α [6], by standard methods, we obtain the most probable distribution density of spins:

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| | $W_\lambda = \frac{N_\lambda}{N} = \frac{e^{-\beta S_\lambda}}{\sum_{\lambda=1}^n e^{-\beta S_\lambda}}.$ | (5) |
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It is obvious that every of spins S_λ can be represented as product of integer λ and spin $S=1/2$, i.e.: $S_\lambda = \lambda/2$, so that finally we obtain:

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| | $W_\lambda = \frac{N_\lambda}{N} = \frac{e^{-\frac{1}{2}\lambda\beta}}{\sum_{\lambda=1}^n e^{-\frac{1}{2}\lambda\beta}}.$ | (6) |
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Now we shall determine Lagrange multiplier β . By using the relations

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| $\frac{\sum_{\lambda=1}^n \frac{1}{2} \lambda e^{-\frac{1}{2} \lambda \beta}}{\sum_{\lambda=1}^n e^{-\frac{1}{2} \lambda \beta}} = -\frac{d}{d\beta} \ln \sum_{\lambda=1}^n e^{-\frac{1}{2} \lambda \beta} = \frac{S}{N};$ | $\sum_{\lambda=1}^n e^{-\frac{1}{2} \lambda \beta} = \frac{1 - e^{-\frac{1}{2} n \beta}}{e^{\frac{1}{2} \beta} - 1}$ | (7) |
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we obtain a transcendental equation defining β (which can be solved only numerically) :

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| | $\frac{1}{1 - e^{-\frac{1}{2} \beta}} - \frac{n}{e^{\frac{1}{2} \beta} - 1} = 2 \frac{S}{N}.$ | (8) |
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The average spin value is mathematical expectation of $S_\lambda = \lambda/2$ over probability densities W_λ , i.e.

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| | $\langle S_\lambda \rangle = \frac{\sum_{\lambda=1}^n \frac{1}{2} \lambda e^{-\frac{1}{2} \beta \lambda}}{\sum_{\lambda=1}^n e^{-\frac{1}{2} \beta \lambda}} = -\frac{d}{d\beta} \ln \sum_{\lambda=1}^n e^{-\frac{1}{2} \beta \lambda},$ | (9) |
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wherefrom it follows:

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| | $\langle S_\lambda \rangle = \frac{1}{2} \left(\frac{1}{1 - e^{-\frac{\beta}{2}}} - \frac{n}{e^{\frac{\beta}{2}} - 1} \right).$ | (10) |
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Our main goal is to find statistical average of spin with random distributed spins. This average enables us to treat the inter metallic compound with random distributed parallel, different spins as an ideal ferromagnetic spin lattice with average spin. This average value $\langle S_\lambda \rangle$ we shall considered as equivalent spin of ferromagnet with N identical spins: $\langle S_\lambda \rangle = S_{eq}$. Having an equivalent ideal infinite structure, we can cut off from it a rectangular and cylindrical nanostructure, which are equivalent to corresponding nanostructures cut off from metallic compound with random distributed parallel spins.

3. Illustrative examples

Now we shall quote two illustrative examples.

The first example is the following: inter metallic compound has 10% spins $S = 1/2$, 40% spins $S = 1$, 25% spins $S = 3/2$, 20% spins $S = 2$, and 5% spins $S = 5/2$. In this case we can write: $S = (1/2 \times 0.1 + 1 \times 0.4 + 3/2 \times 0.25 + 2 \times 0.2 + 5/2 \times 0.05)N$, and so, $2S/N = 2.70$. Putting this result into Eq. (10), and taking into account that $n = 5$, we obtain numerically that

$\beta = 0.303$. On the other hand, with this value we obtain: $S_{eq} = 1.350 \approx 3/2$. It follows that considered inter metallic compound behaves as ideal spin lattice with $S = 3/2$.

The second example is more realistic than above one. The inter metallic compound has 50% of atoms with spin $S = 1$, 40% of atoms with spin $S = 1/2$, and 10% of atoms with spin $S = 2$. These spins the most often appear in ferromagnetic materials. In this case we can write: $S = (1 \times 0.5 + 3/2 \times 0.4 + 2 \times 0.1)N = 1.13N$, wherefrom it follows $2S/N = 2.26$. Putting this result into Eq. (8), and taking into account that $n = 3$, we obtain, numerically, that $\beta = 4.256$. With this value for β we have: $S_{eq} = 0.565 \approx 1/2$. This means that considered inter metallic compound behaves as an ideal spin lattice with spin $S = 1/2$.

4. Conclusions

It is not quite clear whether the described spin systems appear in practice but it is sure that stochastically approach in analysis in such structures is unique possible.

Acknowledgements

This work was supported by the Serbian Ministry of Science and Technology: Grant No 141044, by Vojvodina Academy of Sciences and Arts and, partially, by National Council of Scientific Research in the Romanian Universities: Grant CNCSIS A 647 /2005-2007.

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