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Mini Review

Revisiting the holstein-primakov transformations

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Abstract

It is shown that in addition to the Holstein-Primakov transformations in the theory of magnetism, a number of other transformations can be proposed which also lead to very interesting and consistent results. In particular, with the help of the transformation proposed in the paper for spin operators, it turns out to be possible to strictly analytically calculate the temperature dependence of the ferromagnet magnetization in a wide temperature range from zero and up to the Curie temperature. It is shown that for these transformations in the Curie temperature area, the magnetization tends to zero exponentially.

Thus, the aim of this study is to describe magnetization over a wide range of temperatures using a new transformation for electron spin operators.

Introduction

The issue that we would like to focus on in this paper relates to the classical theory of magnetism. The essence of the problem which will be discussed below, is to clarify some types of transformations for operators of atomic spins in magnetic materials. The fact is that the well-known Holstein-Primakov transformations give a correct answer to the issue of the temperature dependence of magnetization in the low-temperature area which however does not mean their uniqueness at all. In fact, if we calculate the commutator of spin operators S^+, S^- for spin S = (S_x, S_y, S_z) $S^{\pm} = S_x \pm iS_y$ it is defined as $[S^-, S^+] = 2S_z$ [1,2].

Therefore, any set of transformations makes it possible to find operators S_z by the type of operators S^+, S^-. In this case, dependence S_z can be any, but in the limiting case of large spins, it should lead to equality $S_z = S - a^+ a$ where a^+ (a) – is the operator of the birth (destruction) of the spin deviation (magnon). As a result of the averaged spin component, (S_z) we arrive at Bloch's law in the low-temperature area (the so-called «three-second law» for a ferromagnet [3,4].

In general, the form of Hermitian-conjugate operators S^+, S^- can be represented as $S^+ = \sqrt{2S}a^+ f(n)$, $S^- = \sqrt{2S} f(n) a$ where $n = a^+ a$ and $f(n)$ – is an arbitrary operator function.

According to the switching rule, the longitudinal spin operator therefore is defined as

$$S_z = \frac{1}{2}\left[(1+n) f^2(n) - a^+ f^2(n) a\right].$$

In the special case of the Holstein-Primakov transformations the function is $f(n) = \sqrt{1 - \frac{n}{2S}}$, and after calculating the corresponding commutators we come to an exact expression for the longitudinal spin operator $S_z = S - a^+ a$.

It is quite clear that such dependence $f(n)$ is hardly the only and we can also consider some other quite possible cases one of which, in our opinion, should be discussed in more detail.

Non-root dependency of the operator $f(n)$

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Indeed, let

$$\begin{cases} S^{+} = \sqrt{2S}a^{+}e^{-\frac{a^{+}a}{4S}}, \\ S^{-} = \sqrt{2S}e^{-\frac{a^{+}a}{4S}}a. \end{cases} \quad (1)$$

Then due to the switching equality [1]

$$K = \left[S^{-}, S^{+}\right] = 2S_{z} \quad (2)$$

Taking into account the definitions (1) after a simple calculation we have the following from here

$$K = 2S\left(aa^{+} - a^{+}ae^{\frac{1}{2S}}\right)e^{-\frac{n}{2S}}.$$

Note that the result obtained is easily obtained using the rule of «dragging» the operator a behind the exponent according to equality

$$e^{-\frac{a^{+}a}{2S}}a = ae^{-\frac{aa^{+}}{2S}}.$$

This relation is easy to prove due to the expansion of function e^{-x} into a series by the indicator exponents and at the same time take into account the rules of switching operators for bosons

$$aa^{+} - a^{+}a = 1. \quad (3)$$

As a result for z - spin operator components we arrive at the following relation:

$$S_{z} = S\left[1 + n\left(1 - e^{\frac{1}{2S}}\right)\right]e^{-\frac{n}{2S}}. \quad (4)$$

From this, it can be seen that in the limiting case when the condition $2S >> 1$ is met expression (4) is converted to the form

$$S_{z} \approx S\left(1 - \frac{n}{2S}\right)\left(1 - \frac{n}{2S} + \frac{n^{2}}{8S^{2}}\right) = S\left(1 - \frac{n}{S} + \frac{3n^{2}}{8S^{2}}\right) = S - n + \frac{3n^{2}}{8S} \quad (5)$$

According to the ratio (5) we also come to Bloch's «three-halves» law which does not contradict the Holstein-Primakov theory as well as a lot of experimental facts confirming it. However, as can be seen from (5) we can also calculate additional temperature corrections to the «three-halves» law. They are determined by the last summand standing on the right side of expression (5) but which is not the last in the literal sense since it is a consequence of the exponential expansion if we proceed from formula (4).

This fact can be considered one of the advantages of transformations (1). Another advantage in our opinion is that these transformations allow us to calculate the temperature behavior of magnetization not only in the low-temperature area but also in the high-temperature area in particular in the Curie temperature area. In order to prove this statement, we will focus on this issue in more detail.

Temperature behavior of magnetization

As is well known (see for example [3] as well as the monograph [5]) the average value of magnetization is obtained by averaging the observed magnitude according to the equilibrium density matrix which was first introduced by Bloch and Landau. It is on the basis of this definition that the average value of magnetization can be easily calculated.

Indeed, we follow the general thermodynamic definition of the average magnetic moment of an atom then in accordance with formula (4) it should be represented as

$$\left\langle S_{z}\right\rangle = S\left[\left\langle e^{-\frac{n}{2S}}\right\rangle + \left(1 - e^{\frac{1}{2S}}\right)\left\langle ne^{-\frac{n}{2S}}\right\rangle\right], \quad (6)$$

Where angle brackets mean averaging by the basic state of a ferromagnet with an equilibrium density matrix.

To introduce the magnon energy ε (k) where k - is its wave vector we should write down a general expression for the energy of a ferromagnet placed in a constant and uniform magnetic field H = (0,0, H) with an axis z selected along the ferromagnet anisotropy axis direction.

As an illustrative example consider a easy axial ferromagnet with cubic symmetry. The general expression for its magnetic energy can be represented then as the following Hamiltonian (see for example [6] as well as review [7]):

$$\mathrm{H} = -\frac{1}{N^{2}}\sum_{i,j}^{N} J_{ij}\mathbf{S}_{i}\mathbf{S}_{j} - \frac{H}{N}\sum_{i=1}^{N} S_{iz} - \frac{\beta}{2N}\sum_{i=1}^{N} S_{iz}^{2}, \quad (7)$$

Where β - the characteristic energy of magnetic anisotropy J_{ij} - is the Heisenberg exchange integral.

In $a^{+}a$ operator-quadratic approximation from (7) we have

$$\mathrm{H}_{0} = -\frac{S^{2}}{N^{2}}\sum_{i,j}^{N} J_{ij} - \frac{S}{N^{2}}\sum_{i,j}^{N} J_{ij}a_{i}^{+}a_{j} + \frac{S}{2N^{2}}\sum_{i,j}^{N} J_{ij}\left(a_{i}^{+}a_{i} + a_{j}^{+}a_{j}\right) - \frac{H}{N}\sum_{i=1}^{N}\left(S - a_{i}^{+}a_{i}\right) - \frac{\beta}{2N}\sum_{i=1}^{N}\left(S - a_{i}^{+}a_{i}\right)^{2}$$

Or in a compact form

$$\mathrm{H}_{0} = U_{0} + H_{0}, \quad (8)$$

Where

$$U_{0} = -\frac{S^{2}}{N^{2}}\sum_{i,j}^{N} J_{ij} - HS - \frac{\beta S^{2}}{2}, \quad (9)$$

and the energy operator

$$H_{0} = \frac{S}{2N^{2}}\sum_{i,j}^{N} J_{ij}\left(a_{i}^{+}a_{i} + a_{j}^{+}a_{j}\right) - \frac{S}{N^{2}}\sum_{i,j}^{N} J_{ij}a_{i}^{+}a_{j} + \frac{\mu_{e}H + \beta}{N}\sum_{i=1}^{N} a_{i}^{+}a_{i}. \quad (10)$$

The transition in (10) to k - representation using the expansion of the exchange integral and the birth and destruction operators into a Fourier series allows us to rewrite operator (10) in a compact form as

$$H_{0} = \frac{1}{N}\sum_{\mathbf{k}}\varepsilon(k)a_{k}^{+}a_{k}, \quad (11)$$

Where the magnon energy is

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$$\varepsilon(k)=2S\left(J(0)-J(k)\right)+\beta+\mu_e H\cdot \tag{12}$$

Therefore taking into account (12) returning to formula (6) in which the averaging can now be concretized using a transition to k - space for averaged thermodynamic values we have the right to write that

$$\left\langle e^{-\frac{n}{2S}}\right\rangle=\sum_{\mathbf{k}}\frac{\sum_{n=0}^{\infty}e^{-\left(\frac{1}{2S}+\frac{\varepsilon_k}{T}\right)n}}{\sum_{n=0}^{\infty}e^{-\left(\frac{\varepsilon_k}{T}\right)n}}=\sum_{\mathbf{k}}\frac{1-e^{-\lambda}}{1-e^{-\gamma}}, \tag{13}$$

$$\left\langle ne^{-\frac{n}{2S}}\right\rangle=\sum_{\mathbf{k}}\frac{\sum_{n=0}^{\infty}ne^{-\left(\frac{1}{2S}+\frac{\varepsilon_k}{T}\right)n}}{\sum_{n=0}^{\infty}e^{-\left(\frac{\varepsilon_k}{T}\right)n}}=\sum_{\mathbf{k}}\frac{e^{-\gamma}\left(1-e^{-\lambda}\right)}{\left(1-e^{-\gamma}\right)^2}, \tag{14}$$

Where parameters are

$$\begin{cases}\gamma=\dfrac{\varepsilon_k}{T},\\ \lambda=\dfrac{\varepsilon_k}{T}+\dfrac{1}{2S}.\end{cases} \tag{15}$$

Here and everywhere below the Boltzmann constant k_B is considered equal to one.

As a result, taking into account the (13) – (15) formula (6) can be rewritten as follows

$$\langle S_z\rangle=\frac{Se^{\frac{1}{2S}}}{N}\sum_{\mathbf{k}}\frac{e^{\lambda}-1}{e^{\gamma}-1}+\frac{Se^{\frac{1}{2S}}\left(1-e^{\frac{1}{2S}}\right)}{N}\sum_{\mathbf{k}}\frac{e^{\lambda}-1}{\left(e^{\gamma}-1\right)^2}.$$

Or after simplification we have

$$\langle S_z\rangle=\frac{Se^{\frac{1}{S}}}{N}\sum_{\mathbf{k}}\left(\frac{e^{\lambda}-1}{e^{\gamma}-1}\right)^2. \tag{16}$$

If $S >> 1$ then it follows from formula (16) in linear approximation by S that

$$\langle S_z\rangle\approx\frac{Se^{\frac{1}{S}}}{N}\sum_{\mathbf{k}}\left(1-\frac{1}{S}-\frac{1}{S\left(e^{\lambda}-1\right)}\right)\approx S-\frac{1}{N}\sum_{\mathbf{k}}\overline{n}_k, \tag{17}$$

Where

$$\overline{n}_k=\frac{1}{e^{\frac{\varepsilon_k}{T}}-1}.$$

To analyze the general formula (16) it is convenient to rewrite it in non-dimensional form taking into account explicit expressions for parameters λ and γ according to (15) as well as the magnon dispersion law (12). Since in the simplest case dependence $J(k)$ can be approximated by a periodic function

$J(k) = J(0)(1 - \cos ak)$,

Where a - is the interatomic distance it follows from (12) that in the long-wave approximation, the magnon dispersion has a well-known quadratic form

$$\varepsilon(k)=SJ(0)(ak)^2+\beta+\mu_e H. \tag{18}$$

Therefore for the temperature area from the range $T\gg\beta+\mu_e H$ we get

$$y(x)=\frac{\langle S_z\rangle}{S}=3x^3e^{2p}\int_0^{\frac{1}{x}}\frac{\left(e^{t^2}-1\right)^2t^2dt}{\left(e^{t^2+p}-1\right)^2}. \tag{19}$$

Where the dimensionless argument is $x=\frac{2}{\pi}\sqrt{\frac{T}{J_{ex}}}$ and a parameter is $p=\frac{1}{2S}$.

Numerical analysis of integral dependence (18) makes it possible to illustrate the behavior of function $y(x)$ graphically using visual Figure 1 in the case of three selected values of the parameter $p=\frac{1}{3},\ \frac{1}{5},\ \frac{1}{101}$ and over the entire range of $x\in[0,\infty)$ argument variation.

It can be seen from the presented figures, in particular, that the proposed transformation for spin operators makes it possible to describe the dependence of the average spontaneous magnetization of a ferromagnet in a fairly large range of temperature changes almost to the Curie temperature. It can also be seen from these figures that for each spin value, a ferromagnetic material must have its own Curie temperature, which is quite natural.

To relate Curie's temperature T_C to exchange energy J_{ex}, which according to (18) is defined as

$$J_{ex}=SJ(0), \tag{20}$$

Let us proceed as follows.

We will find the asymptotic behavior of function $y(x)$ according to the obtained dependence (19), and we will «link» them.

Indeed if $x << 1$ then

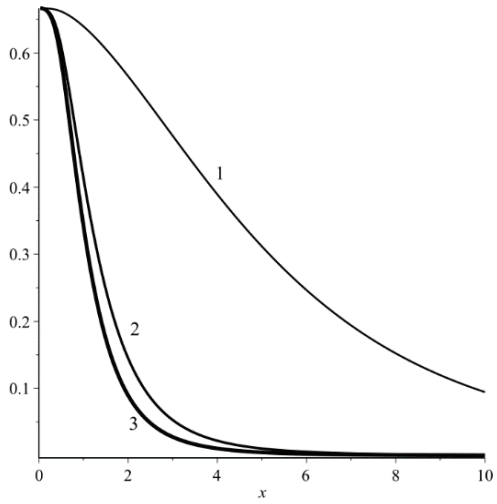

Figure 1: Line 1 corresponds to the value of an infinitely large spin, i.e. S ⇒ 1. Curve 2 corresponds to the value of the spin $S=\frac{5}{2}$, and curve 1 corresponds to the value of the spin $S=\frac{3}{2}$.

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$$y(x) \approx 1 - x^3 . \quad (21)$$

In the opposite extreme case if $x \gg 1$

$$y(x) \approx \frac{6S}{7x^4} . \quad (22)$$

From condition, $x^3 \sim \frac{6S}{7x^4}$ we get that $x \approx \left(\frac{6S}{7}\right)^{\frac{1}{7}}$. In dimensional units, the «linking» point is determined by the temperature

$$T_0 = J_{ex}\left(\frac{\pi}{2}\right)^2 \left(\frac{6S}{7}\right)^{\frac{2}{7}} . \quad (23)$$

The Curie temperature is in the area $T \ T_o$ and its value can be estimated from Figure 1 which is shown by a dot with a designation T_c along the abscissa axis.

If we use for example the classical monograph [1] then following it the Curie temperature is associated with the exchange integral by ratio

$$T_C \approx ZSJ(0) , \quad (24)$$

Where Z - is the number of nearest neighbors? If for example a cubic crystal lattice is volume-centered then $Z = 8$, and if it is simply cubic then $Z = 6$.

From the comparison of formulas (23) and (24) it can be seen that ratio $Z > \left(\frac{\pi}{2}\right)^2 \left(\frac{6S}{7}\right)^{\frac{2}{7}}$ must be observed which is well performed for almost any value of spin S.

The temperature dependence for the average magnetization in the region of high temperatures as is well known (see [1]) is described by Curie's law, i.e.

$$\langle S_z \rangle \approx \frac{A}{T} \quad (25)$$

According to the Brillouin function [5].

As can be seen from the above figure, at high temperatures, according to dependence (22) the behavior of the average magnetization is fully correlated with the classical law (25).

The disadvantage of the proposed transformation is apparently the qualitative difference between the hyperbolic dependence (22) and the root dependence which is characteristic in close proximity to the Curie point. According to (19) in temperature area $T > T_c$ due to the asymptotics of (22), it is quite possible to assume that $<S_z> \approx 0$.

Conclusion

Concluding this message, the following is worth noting.

If we use the transformation of electron spin operators which differs from the Holstein-Primakov transformations, we are finding Bloch's «three halves» law in the low-temperature area. And in the field of high temperatures, we come to a slightly refined Curie's law. Figure 1 shows the dependence of the average magnetization over the entire temperature region.

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