On the analytical evaluation of the magnetization of ferromagnetic lattices

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Abstract

We investigate analytically the magnetization of Heisenberg ferromagnetic lattices in one and two dimensions, and we derive approximate expressions that are valid at high and low temperatures. In the case of the spin-$\frac{1}{2}$ Heisenberg XX chain in a transverse field, we show that, when the applied magnetic field $h$ exceeds its critical value $h_c = J$, where $J$ is the exchange coupling constant, the magnetization per site deviates at low temperatures from its saturation value, $\frac{1}{2}$, following a power series with terms involving the power laws $T^{1/2}$, $T^{3/2}$, $T^{5/2}$..etc. When $h < h_c$, the zero temperature magnetization per spin turns out to be equal to $\frac{1}{\pi} \arcsin\left(\frac{h}{h_c}\right)$. In this case, the temperature dependence of the magnetization is given by a series expansion with power laws of the form $T$, $T^3$, $T^5$,..etc. In both cases, the coefficients of the expansions are temperature-dependent and are explicitly derived. Using the properties of the Eulerian polynomials, we show that, because of the fast convergence of the derived series for the Fermi-Dirac and the Bose-Einstein distributions, it is possible (in particular in strong magnetic fields) to express the magnetization of the Heisenberg model in a simple analytical form. Furthermore, the analytical results are compared with the exact numerical ones.

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I. INTRODUCTION

The Heisenberg model plays an important role in the study of the magnetic properties of many materials [1]. Its success in providing ample explanations for various phenomena occurring in many-body spin systems made it a fundamental tool that has been extensively used by many physicists. Historically, these investigations were motivated by the need to explore the properties of matter that arise from its periodic structure on the one hand, and the effect of the accompanying quantum degrees of freedom of the individual atoms or molecules on the other hand. For instance, the Heisenberg model has been employed to investigate the low temperature properties of ferro and anti-ferromagnetic materials, where the notions of the quasi-particles called magnons and spinons naturally emerge. This is the reason for which a great deal of attention has been given to the investigation of the transition form an ordered ferromagnetic phase to a paramagnetic one, which is characterized by the so-called Curie temperature, and, also, to the transition from an ordered antiferromagnetic phase to a paramagnetic phase, to which is associated the so-called Néel temperature [2]. Needless to mention also the study of the quantum phase transitions that occur at zero temperature, when a parameter of the system’s Hamiltonian crosses its critical value [3]. These processes are relevant to a large number of applications, as is the case in the emerging field of quantum information technology. Indeed, in recent years, research in quantum theory has been widely oriented towards this new field. The interest in spin systems stems from the fact that they are considered the most suitable candidates for the implementation of quantum computers, and quantum devices in a scalable manner [4].

The large number of the degrees of freedom characterizing, in general, many-body systems, makes it quite difficult to study their properties in a full analytical manner. Spin lattices, in particular, are no exception to this fact. As a general rule, the starting point in the study of the dynamical and statistical behavior of a quantum system is the Hamiltonian operator; once the latter is determined, one seeks a suitable diagonalization technique of the Hamiltonian, from which the relevant information about the system may be deduced. Unfortunately, this is not the case in the majority of the problems involving many particles. This is the reason for which numerical diagonalization techniques are invoked in order to gain more insight into the problem studied. The methods used vary, depending on the nature of the degrees of freedom one is dealing with. There exist, however, some techniques
like the powerful Beth ansatz, and the Jordan-Wigner transformations that lead to exact results. It is obvious that such exact results are of great usefulness in obtaining a clear and plausible description of many-spin systems. Another important fundamental result is the Mermin-Wagner theorem which excludes any long-range order in low dimensional isotropic spin ferromagnets, due to the thermal and quantum fluctuations. In other cases, it turns out that some simplifications and approximations may give rise to analytical results. A typical example is the long-wavelength approximation applied to the three-dimensional Heisenberg ferromagnet which yields the famous Bloch’s law, valid only at low temperatures. Corrections to the latter law are obtained by taking into account magnon-magnon interactions, which Dyson called dynamical interactions between magnons. He also introduced what he named the kinematical interactions, which arise from the finite dimensionality of the spin spaces of the atoms. The result is a power series with respect to the temperature, which includes obviously the Bloch law as a special case.

The one-dimensional Heisenberg chain has been the subject of a large number of investigations. In particular, the XY chain has been thoroughly studied by Katsura in [15], and later generalized by Perk et al [17]. In most instances, the magnetization cannot be expressed in a simple mathematical form. The aim of this paper is to fill this gap by deriving simple approximate expressions for the magnetization of some lattices in one and two dimensions, which are described by the Heisenberg model. The paper is organized as follows: In section II, we treat the XY spin-1/2 chain, and we explore mathematically the low and the high temperature behavior of the magnetization. The emphasis is on the isotropic XX model. Section III deals with the general spin-S Heisenberg lattice in two dimensions. We end the paper with a brief conclusion.

II. HEISENBERG XY SPIN-1/2 CHAIN

Let us begin our investigation with the one dimensional spin-1/2 Heisenberg XY chain described by the Hamiltonian operator:

$$\mathcal{H} = -J \sum_{i=1}^{N} \left( (1 + \gamma)S_i^x S_{i+1}^x + (1 - \gamma)S_i^y S_{i+1}^y \right) - \hbar \sum_{i}^{N} S_i^z,$$

where $\vec{S}_i$ is the spin vector operator of the particle that is located at site $i$ of the chain, while $J$ and $\gamma$ refer to the exchange integral and the anisotropy constant, respectively. The
parameter \( h \) denotes the strength of the applied magnetic field which is pointing along the \( z \) direction. In the case where \( J \) is positive, the interaction between the spins is of ferromagnetic nature. On the contrary, when \( J < 0 \), one is dealing with an antiferromagnetic model. By setting \( \gamma = 0 \), we obtain the Heisenberg XX model, whereas \( \gamma = 1 \) yields a transverse Ising-like model. In what follows, we shall mainly be interested in the transverse magnetization per site:

\[
M_z = \frac{1}{N} \langle S_z \rangle,
\]

(2)
in the limit of an infinite chain, with \( S_z = \sum_i S_z^i \), and \( \langle \cdot \rangle \) is the thermal average with respect to the Gibbs thermal equilibrium state of the chain at temperature \( T \). For convenience, we shall use, unless stated otherwise, the inverse temperature \( \beta = 1/k_B T \) where \( k_B \) is Boltzmann’s constant.

### A. XX model with \( \gamma = 0 \)

The XX model obtained by setting \( \gamma = 0 \) in equation (1) can be exactly diagonalized by using the Jordan-Wigner transformation [6]

\[
S_j^+ = c_j^\dagger \exp\left\{ -i\pi \sum_{k=1}^{j-1} c_k^\dagger c_k \right\},
\]

(3)

\[
S_j^- = \exp\left\{ -i\pi \sum_{k=1}^{j-1} c_k^\dagger c_k \right\} c_j,
\]

(4)

\[
S_j^z = c_j^\dagger c_j - \frac{1}{2},
\]

(5)

where \( S_\pm = S_x \pm iS_y \), and the \( c_j \)'s are fermionic operators satisfying \( \{c_j, c_k^\dagger\} = \delta_{jk}, \{c_j, c_k\} = \{c_j^\dagger, c_k^\dagger\} = 0 \). In terms of the latter operators the Hamiltonian can be written as:

\[
\mathcal{H} = -J \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) - h \sum_i (c_i^\dagger c_i - \frac{1}{2}).
\]

(6)

Then by imposing the periodic boundary condition \( c_{N+1} = c_1 \), and after the following Fourier transform:

\[
\eta_k = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{ijk} c_j,
\]

(7)

\[
\eta_k^\dagger = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-ijk} c_j^\dagger,
\]

(8)
the resulting Hamiltonian reads (we set $\hbar = 1$)

$$H = \sum_k \omega_k \eta_k^\dagger \eta_k + \frac{hN}{2},$$

with the dispersion relation:

$$\omega_k = -J \cos(k) - h,$$

where $k = \frac{2\pi m}{N}$ such that $m = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1, \frac{N}{2}$ when $N$ is odd. For the case of $N$ even, the possible values of $k$ are slightly different, since in this instance $m = -\frac{N-1}{2}, -\frac{N-2}{2}, \ldots, \frac{N-2}{2}, \frac{N-1}{2}$. Nevertheless, in the limit of $N$ very large ($N \to \infty$), the two cases become indistinguishable, in the sense that $k$ becomes a continuous variable whose domain determines the first Brillouin zone of the chain $-\pi \leq k \leq \pi$. Therefore, the procedure described above, enables one to map the $XX$ spin chain into a system of spinless free (non-interacting) fermions; this can be seen by checking that the operators $\eta_k$ satisfy the same anti-commutation relations as those of the operators $c_j$.

The magnetization per spin at temperature $T$ can be expressed in terms of the new operators as:

$$M_z = -\frac{1}{2} + \frac{1}{N} \sum_k \langle n_k \rangle, \quad n_k := \eta_k^\dagger \eta_k,$$

where the mean number of the fermions in mode $k$ is given by the Fermi-Dirac distribution:

$$\langle n_k \rangle = \frac{1}{e^{\beta \omega_k} + 1}.$$  

Hence, for an infinite chain, we may write:

$$M_z = -\frac{1}{2} + \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{e^{-\beta(h + J\cos(k))} + 1}. $$

The difficulty with the above expression resides in the fact that the integral cannot be carried out analytically, and one has to make recourse to numerical integration. As one may notice, the dispersion relation of the model is valid for all values of the temperature, which means that the integral should be carried out with respect to the full first Brillouin zone. Our aim is to derive analytical expressions that approximate, as good as possible, the magnetization $M_z$, at high, as well as, at low temperatures, taking into account the whole range of the wave vector $k$.

For this purpose, let us first make the change of variable $\cos(k) = z$; then, we have

$$M_z = -\frac{1}{2} + \frac{1}{\pi} \int_{-1}^{1} \frac{dz}{\sqrt{1 - z^2}} \frac{1}{e^{-\beta(h + Jz)} + 1}. $$
The latter expression suggests that the function $1/\pi \sqrt{1 - z^2}$ plays the role of a density of states for the spin chain. The points $z = \pm 1$ where the above function diverges represent the Van Hove singularities of the chain. For convenience and ease of notation, we shall denote the density of states by $D(z)$, i.e. (see the appendix for more details):

$$D(z) = \frac{1}{\pi \sqrt{1 - z^2}}. \quad (15)$$

1. Case of $h > J$

Let us assume for now that $h > h_c = J$. Then, we can formulate the following result:

**Proposition 1.** When $h > J$, the magnetization per spin of the $XX$ infinite chain satisfies:

$$M_z \sim -\frac{1}{2} + \frac{1}{4} \left[ \frac{1}{e^{-\beta(J+h)}} + \frac{1}{e^{-\beta(h-J)}} + 2 \right], \quad (16)$$

as $\beta \to 0$ or $\beta \to \infty$.

**Proof.** To prove the above proposition, we first establish the following lemma:

**Lemma 1.** Let $a$ and $b$ be arbitrary positive real numbers satisfying $a > b$, and let $z \in [-1, 1]$; then:

$$\frac{1}{\pi} \int_{-1}^{1} \frac{dz}{\sqrt{1 - z^2}} \frac{1}{e^{-(a+b)z} + 1} = \frac{1}{e^{-a} + 1} - \sum_{n=1}^{\infty} \frac{A_{2n}(e^a)}{(2n)!(1 + e^a)^{2n+1}} b^{2n} G(n), \quad (17)$$

where $A_n(x)$ is the Eulerian polynomial of degree $n$ and

$$G(n) := \frac{\Gamma(n + \frac{1}{2})}{\sqrt{\pi} \Gamma(n + 1)}. \quad (18)$$

Here, $\Gamma(x)$ denotes the complete gamma function.

**Proof.** To proceed with the proof, we begin by noting that, since $a > b > 0$ and $|z| < 1$, we can write

$$\frac{1}{e^{-(a+b)z} + 1} = \sum_{k=0}^{\infty} (-1)^k e^{-k(a+b)z} = \sum_{k=0}^{\infty} (-e^{-a})^k \sum_{\ell=0}^{\infty} (-b z)^\ell \frac{k^\ell}{\ell!}$$

$$= 1 + \sum_{\ell=0}^{\infty} \frac{(-b z)^\ell}{\ell!} \sum_{k=1}^{\infty} (-e^{-a})^k k^\ell. \quad (19)$$

On the other hand, by taking into account the generating function of the sequence of n’th powers, it follows that:

$$\sum_{k=1}^{\infty} (-e^{-a})^k k^\ell = (-1)^{\ell+1} \frac{A_\ell(e^{-a})}{(1 + e^a)^{\ell+1}}, \quad (20)$$
where $A_\ell(x)$ is the Eulerian polynomial of degree $\ell$. By direct substitution into equation (19), we find that

$$\frac{1}{e^{-(a+ bz)} + 1} = \frac{1}{e^{-a} + 1} + \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell+1} A_\ell(-e^a)}{\ell!(1 + e^a)^{\ell+1}} (-bz)^\ell.$$  (21)

Multiplying the two sides of the latter equation by the density of states, and integrating term by term yield:

$$\int_{-1}^{1} \frac{D(z)dz}{e^{-(a+ bz)} + 1} = \int_{-1}^{1} \frac{D(z)dz}{1 + e^{-a}} + \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell+1} A_\ell(-e^a)}{\ell!(1 + e^a)^{\ell+1}} (-b)^\ell \int_{-1}^{1} z^\ell D(z)dz.$$  (22)

The density of states is clearly an even function of its argument; this means that the contribution of the terms with odd powers of $b$ in the previous series identically vanishes, and one needs only to calculate:

$$\int_{-1}^{1} z^{2\ell} D(z)dz = \frac{1}{\pi} \int_{-1}^{1} \frac{z^{2\ell}dz}{\sqrt{1 - z^2}}.$$  (23)

By the change of variable $z^2 = t$, the latter integral becomes

$$\int_{-1}^{1} z^{2\ell} D(z)dz = \frac{1}{\pi} \int_{0}^{1} t^{\ell - \frac{1}{2}} (1 - t)^{-\frac{1}{2}} dt = \frac{1}{\pi} B(\ell + \frac{1}{2}, \frac{1}{2}),$$  (24)

where $B(z, w)$ is the beta function, which is defined by

$$B(z, w) = \int_{0}^{1} t^{z-1}(1 - t)^{w-1}dt.$$  (25)

Now it suffices to use the fact that the beta function can be expressed in terms of the gamma function as

$$B(z, w) = \frac{\Gamma(w)\Gamma(z)}{\Gamma(w + z)},$$  (26)

and the property:

$$\int_{-1}^{1} D(z)dz = 1$$  (27)

to arrive at expression (18), which concludes the proof of the lemma. $\square$
Lemma (1) implies that the magnetization per spin of the $XX$ chain described by the Hamiltonian $H$ can be expressed as

$$M_z = -\frac{1}{2} + \frac{1}{e^{-\beta h} + 1} + \sum_{\ell=1}^{\infty} B_{2\ell} (\beta J)^{2\ell} G(\ell)$$

$$= -\frac{1}{2} + \frac{1}{e^{-\beta h} + 1} + G(1) \sum_{\ell=1}^{\infty} B_{2\ell} (\beta J)^{2\ell} + \sum_{\ell=2}^{\infty} B_{2\ell} (\beta J)^{2\ell} (G(\ell) - G(1)), \quad (28)$$

where we have introduced the quantity

$$B_{\ell} := \frac{(-1)^{\ell+1} A_{\ell} (-e^{\beta h})}{\ell!(1 + e^{\beta h})}\ell+1. \quad (29)$$

The sums in the right-hand side of equation (28) involve only even powers of $J\beta$. Therefore, we can write

$$M_z = -\frac{1}{2} + \frac{1}{e^{-\beta h} + 1} + \frac{1}{2} G(1) \sum_{\ell=1}^{\infty} B_{\ell} [((\beta J)^{\ell} + (-\beta J)^{\ell}]$$

$$+ \sum_{\ell=2}^{\infty} B_{2\ell} (\beta J)^{2\ell} (G(\ell) - G(1)). \quad (30)$$

By virtue of the expansion (21), it follows that

$$M_z = -\frac{1}{2} + \frac{1}{e^{-\beta h} + 1} + \frac{1}{2} G(1) \left[\frac{1}{e^{-\beta (h+J)} + 1} + \frac{1}{e^{-\beta (h-J)} + 1} - \frac{2}{e^{-\beta h} + 1}\right]$$

$$+ \sum_{\ell=2}^{\infty} B_{2\ell} (\beta J)^{2\ell} (G(\ell) - G(1)). \quad (31)$$

Afterwards, by taking into account the fact that $G(1) = \frac{1}{2}$, we obtain

$$M_z = -\frac{1}{2} + \frac{1}{4} \left[\frac{1}{e^{-\beta (h+J)} + 1} + \frac{1}{e^{-\beta (h-J)} + 1} + \frac{2}{e^{-\beta h} + 1}\right] + \Lambda(h, J, \beta), \quad (32)$$

where

$$\Lambda(h, J, \beta) = \sum_{\ell=2}^{\infty} B_{2\ell} (\beta J)^{2\ell} (G(\ell) - \frac{1}{2}). \quad (33)$$

Clearly, at high temperatures, we have

$$\Lambda(h, J, \beta) = O(\beta^5), \quad (34)$$

which is assured since, on the one hand:

$$\forall \ell \geq 2, \quad G(\ell) < G(1) \equiv \frac{1}{2}, \quad (35)$$

and, on the other hand, as $\beta \to 0$

$$B_{2\ell} \sim \frac{2^{2\ell+1}}{(2\ell)!} A_{2\ell} (-1 + O(\beta)) = O(\beta). \quad (36)$$
This follows from the fact that the Eulerian polynomial of degree \( \ell \) can be expressed in terms of the Eulerian numbers \( A(\ell, m) \) as \( A_\ell(x) = \sum_{m=0}^{\ell} A(\ell, m)x^{\ell-m} \), along with the property \( A(\ell, m) = A(\ell, \ell - m - 1) \), which imply that for all integers \( \ell \geq 1 \), \( A_{2\ell}(-1) = 0 \).

In the limit of low temperatures, \( \beta \to \infty \), the Eulerian polynomial is dominated by the term with the greatest exponent, meaning that \( A_{2\ell}(e^{\beta h}) \sim e^{2\ell \beta h} \); therefore, since \( A(\ell, 0) = 1 \), we have

\[
B_{2\ell} \sim \frac{e^{-\beta h}}{(2\ell)!},
\]

which means that \( \Lambda(h, J, \beta) \) assumes negligible values as \( \beta \to \infty \).

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FIG. 1. The magnetization per spin \( M_z \) as a function of the inverse temperature \( \beta \): numerical values (solid curve) and the approximation (16) (dashed curve) for \( J = 1 \), and \( h = 1.5 \).

In figures (1) and (2) we represent the variation of the magnetization per site as a function of \( \beta \) obtained numerically, and compare it with the approximate expression (16) derived in proposition (1) for different values of \( h \) and \( J \). We see that the agreement is excellent for high as well as for low temperatures. In fact the more the magnetic field is strong, the better the analytical expression reproduces the exact values of \( M_z \). Another point worth mentioning is that when \( h > J \) there exists no Fermi level for the system of fermions, because the spectrum does not change sign. This fact is crucial because otherwise the sums in equation (19) do not converge. We shall see bellow that when \( h < J \) the situation is slightly different. But before that, let us investigate in more detail the low temperature limit; more precisely we shall prove that:
FIG. 2. The magnetization per spin $M_z$ as a function of the inverse temperature $\beta$: numerical values (solid curve) and the approximation (16) (dashed curve) for $J = 1$, and $h = 1.2$.

**Proposition 2.** At low temperatures, when $h > J$:

$$M_z \sim \frac{1}{2} + \frac{1}{\sqrt{2\pi \beta J}} \text{Li}_2\left(-e^{-\beta(h-J)}\right) + \frac{1}{8\sqrt{2\pi \beta J}^3} \text{Li}_3\left(-e^{-\beta(h-J)}\right) + \frac{9}{2! \times 8^2 \sqrt{2\pi \beta J}^5} \text{Li}_5\left(-e^{-\beta(h-J)}\right) + \ldots$$

(38)

where $\text{Li}_n(x)$ denotes the polylogarithm function.

**Proof.** For our purpose, we express the magnetization $M_z$ in the form

$$M_z = -\frac{1}{2} + \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{k=0}^{\infty} (-1)^k e^{-\beta k(h+J \cos(z))} dz$$

$$= \frac{1}{2} + \frac{1}{2\pi} \sum_{k=1}^{\infty} (-1)^k e^{-k\beta h} \int_{-\pi}^{\pi} e^{-k\beta J \cos(z)} dz$$

$$= \frac{1}{2} + \sum_{k=1}^{\infty} (-e^{-\beta h})^k I_0(kJ\beta),$$

(39)

where $I_n$ designates the modified Bessel function of the first kind of order $n$, namely, for positive integers $n$:

$$I_n(z) = \frac{1}{\pi} \int_0^{\pi} e^{z \cos \theta} \cos(n\theta) d\theta.$$  

(40)

Using the asymptotic expansion of the modified Bessel functions [21]:

$$I_\nu(z) \sim \frac{e^z}{\sqrt{2\pi z}} \left(1 - \frac{4\nu^2 - 1}{8z} + \frac{(4\nu^2 - 1)(4\nu^2 - 9)}{2!(8z)^2} - \frac{(4\nu^2 - 1)(4\nu^2 - 9)(4\nu^2 - 25)}{3!(8z)^3} + \ldots \right),$$

(41)
for large $|z|$, provided that $|\arg z| < \frac{\pi}{2}$, we obtain
\[
M_z \sim \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \sum_{k=1}^{\infty} \frac{(-e^{-\beta(h-J)})^k}{\sqrt{\beta J k}} \left(1 + \frac{1}{8J\beta} + \frac{9}{2!(8J\beta k)^2} + \cdots\right). \tag{42}
\]

Now observing that the polylogarithm function is defined by
\[
\text{Li}_n(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^n}, \tag{43}
\]
we arrive at expression (38).

By inspection we see that the term of order $n$ in $1/\sqrt{k}$ of the series \((42)\) is proportional to:
\[
\frac{[(2n-1)!!]^2}{n! \times 8^n \sqrt{2\pi(\beta J)^{2n+1}}} \quad n = 0, 1, 2, \ldots, \tag{44}
\]
where $x!! = x(x-2)(x-4)\cdots1$. The above result enables us to express the magnetization per spin in terms of the temperature as:
\[
M_z = \frac{1}{2} - Q_{\frac{1}{2}}(T)T^{\frac{1}{2}} - Q_{\frac{3}{2}}(T)T^{\frac{3}{2}} - \cdots \text{ as } T \to 0, \tag{45}
\]
where:
\[
Q_{\frac{2n+1}{2}}(T) = -\frac{k_B^{2n+1}[(2n-1)!!]^2}{n! \times 8^n \sqrt{2\pi J^{2n+1}}} \text{Li}_{2n+1} \left(-\frac{e^{-(h-J)/k_BT}}{2}\right). \tag{46}
\]

\[\text{FIG. 3. The low-temperature variation of the magnetization per spin } M_z: \text{ numerical values (solid curve) and the approximation \((45)\) up to order 3 in } J^{1/2} \text{ (dashed curve) for } J = 1.5, \text{ and } h=1.\]
2. Case of $h < J$.

Now let us investigate the case of $h < J$. Under this condition, the spectrum of the chain becomes gapless, the Fermi level of which is characterized by

$$k_F = \pm \arccos \left( -\frac{h}{J} \right), \quad E_F = 0. \quad (47)$$

Hence:

$$M_z = -\frac{1}{2} + \frac{1}{\pi} \int_{-h/J}^{1} \frac{dz}{\sqrt{1 - z^2}} \sum_{k=0}^{\infty} (-1)^k e^{-k \beta (h+Jz)} - \frac{1}{\pi} \int_{-1}^{-h/J} \frac{dz}{\sqrt{1 - z^2}} \sum_{k=1}^{\infty} (-1)^k e^{k \beta (h+Jz)}, \quad (48)$$

from which we can deduce:

**Proposition 3.** When $h < J$, the following holds:

$$M_z \sim -\frac{1}{2} + \frac{1}{4} \left[ \frac{1}{e^{-\beta(J+h)}} + \frac{1}{e^{-\beta(h-J)}} + \frac{2}{e^{-\beta h} + 1} \right], \quad (49)$$

as $\beta \to 0$.

**Proof.** The proof proceeds in a manner similar to that of proposition (1).

![FIG. 4. The magnetization per spin $M_z$ as a function of the inverse temperature $\beta$: numerical values (solid curve) and the approximation (49) (dashed curve) for $J = 1.5$, and $h=1$.](image)

We illustrate this result in figures (4) and (5), where we display the magnetization per spin calculated numerically and via the approximation (49) for some values of $h$ and $J$. It is clearly noticed that for low values of $\beta$ the agreement is good; but as $\beta$ increases
FIG. 5. The magnetization per spin $M_z$ as a function of the inverse temperature $\beta$: numerical values (solid curve) and the approximation (solid curve) for $J = 2$, and $h=1$.

the difference between the two curves representing the exact and the approximate values of the magnetization becomes important and the approximation gets quite poor at low temperatures.

The limit of $T \to 0$ when $h < J$ bears a quite different character as compared with that corresponding to $h > J$; more precisely we show that in this case:

**Proposition 4.** If $J > h$, then at $T = 0$,

$$M_z = \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right).$$

(50)

The same result has been obtained in Ref. [15]; we shall prove it using a different method, namely:

**Proof.** From equation (48) it follows, after some simplifications, that

$$M_z = \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) = \frac{1}{\pi} \sum_{k=1}^{\infty} (-1)^k 2 \sinh(k\beta h) \int_{-1}^{\frac{h}{J}} \frac{e^{\beta J z} dz}{\sqrt{1 - z^2}}$$

$$+ \frac{1}{\pi} \sum_{k=1}^{\infty} (-1)^k \int_{-\frac{h}{J}}^{\frac{h}{J}} \frac{e^{-k\beta(h-Jz)} dz}{\sqrt{1 - z^2}}.$$  

(51)

In obtaining the last equation we have used the fact that

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dz}{\sqrt{1 - z^2}} = \frac{\pi}{2} + \arcsin \left( \frac{h}{J} \right).$$

(52)
As $\beta \to \infty$, we can set $\sinh(k\beta h) \sim \exp(k\beta h)/2$; but by the mean value theorem, we now that:

$$\exists \xi \in (J,1[, \quad \int_{-1}^{\frac{J}{2}} \frac{e^{k\beta Jz}}{\sqrt{1-z^2}} \, dz = e^{-k\beta J\xi} \int_{-1}^{\frac{J}{2}} \frac{dz}{\sqrt{1-z^2}},$$

whence:

$$\lim_{\beta \to \infty} e^{k\beta h} \int_{-1}^{\frac{J}{2}} \frac{e^{k\beta Jz}}{\sqrt{1-z^2}} \, dz = 0$$

for $k > 0$, since by assumption $J > h$. With the same method, it can be shown that the second integral in equation (51) vanishes as $\beta$ approaches infinity.

In figure (6) we display an example of the dependence of the magnetization on the temperature, along with the asymptotic value as given by equation (50). For temperatures close to the absolute zero, it turns out that:

**Proposition 5.** When $J > h$, then

$$M_z \sim -\frac{1}{\pi \beta J} \text{Li}_1(-e^{\beta h}) - \frac{1}{\pi (\beta J)^3} \text{Li}_3(-e^{\beta h}) - \frac{9}{\pi (\beta J)^5} \text{Li}_5(-e^{\beta h}) - \cdots$$

as $\beta \to \infty$.

**Proof.** From equation (51), we deduce that:

$$M_z = \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) - \frac{1}{\pi} \sum_{k=1}^{\infty} (-1)^k 2 \sinh(k\beta h) \int_{-1}^{0} \frac{e^{k\beta Jz}}{\sqrt{1-z^2}} \, dz + \mathcal{F}(h, J, \beta),$$

FIG. 6. The magnetization per spin $M_z$ as a function of the inverse temperature $\beta$: numerical values (solid curve) and the saturation value (50) (dashed curve) for $J = 2$, and $h=1$.
where we have introduced the function

$$\mathcal{F}(h, J, \beta) = -\frac{1}{\pi} \sum_{k=1}^{\infty} (-1)^k 2 \sinh(k \beta h) \int_0^h \frac{e^{-k \beta J z}}{\sqrt{1-z^2}} dz + \frac{1}{\pi} \sum_{k=1}^{\infty} (-1)^k \int_{-h}^h \frac{e^{-k \beta (h-J) z}}{\sqrt{1-z^2}} dz. \quad (57)$$

Consequently, for large values of $\beta$:

$$M_z = \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) - \frac{1}{\pi} \sum_{k=1}^{\infty} (-1)^k e^{k \beta h} \int_0^0 \frac{e^{k \beta J z}}{\sqrt{1-z^2}} dz + \mathcal{F}(h, J, \beta)$$

$$= \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) - \frac{1}{2} \sum_{k=1}^{\infty} (-1)^k e^{k \beta h} \left( I_0(\beta J k) - L_0(\beta J k) \right) + \mathcal{F}(h, J, \beta), \quad (58)$$

where $L_0(x)$ is the modified Struve function of order zero [21]; notice that in general:

$$L_n(z) = \frac{2(z/2)^n}{\sqrt{\pi} \Gamma(n + \frac{1}{2})} \int_0^{\frac{\pi}{2}} \sinh(z \cos \theta) \sin^{2n} \theta d\theta. \quad (59)$$

Now, we may use the asymptotic expression:

$$L_n(z) - I_{-n}(z) \sim \frac{1}{\pi} \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu+1} \Gamma(\nu + \frac{1}{2})}{\Gamma(-\nu + n + \frac{1}{2}) (\frac{z}{2})^{2\nu-n+1}}, \quad (60)$$

when $|z|$ is large, from which it follows that:

$$M_z \sim \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) + \frac{1}{2\pi} \sum_{k=1}^{\infty} (-1)^k e^{k \beta h} \left( -\frac{2}{\Gamma(\frac{1}{2}) \beta J k} + \frac{2^3}{\Gamma(\frac{3}{2}) \Gamma(-\frac{1}{2}) (J \beta k)^3} - \frac{2^5}{\Gamma(\frac{5}{2}) \Gamma(-\frac{3}{2}) (J \beta k)^5} + \cdots \right) + \mathcal{F}(h, J, \beta). \quad (61)$$

Therefore:

$$M_z \sim \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) + \mathcal{F}(h, J, \beta) - \frac{1}{\pi \beta J} \text{Li}_1(-e^{\beta h}) - \frac{1}{\pi (\beta J)^3} \text{Li}_3(-e^{3h})$$

$$- \frac{9}{\pi (\beta J)^5} \text{Li}_5(-e^{5h}) - \cdots. \quad (62)$$

Next, we show that

$$\mathcal{F}(h, J, \beta) \sim -\frac{1}{\pi} \arcsin \left( \frac{h}{J} \right), \quad \beta \to \infty. \quad (63)$$

To do so, we use the property [22]:

$$\text{Li}_s(-e^\mu) \sim -\frac{\mu^s}{\Gamma(s+1)}, \quad \mu \to \infty, \quad (64)$$
which implies that close to the absolute zero:

\[ M_z \sim \frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) + \mathcal{F}(h, J, \beta) + \sum_{n=0}^{\infty} \frac{(h/J)^{2n+1}[(2n-1)!!]^2}{\pi(2n+1)!} \]

\[ = \frac{2}{\pi} \arcsin \left( \frac{h}{J} \right) + \mathcal{F}(h, J, \beta), \tag{65} \]

where we can recognize the power series expansion of the arcsin function. It immediately follows from proposition (4) that \( \mathcal{F}(h, J, \beta) \sim -\frac{1}{\pi} \arcsin \left( \frac{h}{J} \right) \), which concludes the proof. \( \square \)

Hence, by analogy with equation (45), we express the low-temperature behavior of the magnetization as

\[ M_z \sim -\mathcal{Q}_1(T)T - \mathcal{Q}_3(T)T^3 - \cdots \text{ as } T \to 0, \tag{66} \]

where in this case

\[ \mathcal{Q}_{2n+1}(T) = \frac{k^{2n+1}[(2n-1)!!]^2}{\pi J^{2n+1}} \text{Li}_{2n+1}(-e^{h/k_BT}). \tag{67} \]

Figure (7) displays the low temperature variation of \( M_z \) obtained exactly and compares it with the expansion (66). We see that the latter reproduces qualitatively and quantitatively the exact values at sufficiently low temperatures.

\[ \text{FIG. 7. The low-temperature magnetization per spin } M_z: \text{ numerical values (solid curve) and the asymptotic (55) up to fifth order in } J^{-1} \text{ (dashed curve) for } J = 3, \text{ and } h=1. \]

\[ \text{with the expansion (66). We see that the latter reproduces qualitatively and quantitatively the exact values at sufficiently low temperatures.} \]

**B. High-temperature expansion in the case of } \gamma = 1**

As we have already mentioned, the value \( \gamma = 1 \) of the anisotropy parameter corresponds to a transverse Ising model. The Hamiltonian can still be diagonalized by using the Jordan-
Wigner transformation combined with a Bogoliubov transformation to eliminate the non-diagonal quadratic terms in fermion operators. For more details on the derivation, the reader may consult Refs. 11 and 15. The spectrum resulting from the diagonalization of the Hamiltonian is described by the relation

$$\omega_k = \sqrt{J^2 + h^2 + 2Jh \cos(k)}. \quad (68)$$

The transverse magnetization per site in this case is given by [15]

$$M_z = \frac{1}{2\pi} \int_0^\pi \frac{(h + J \cos(k)) \tanh \left(\frac{1}{2}\beta\omega_k\right)}{\omega_k} dk. \quad (69)$$

For this model we shall treat only the high temperature behavior of the chain. To this end, we invoke the generating function of the Euler polynomials $E_n(x)$ (not to be confused with the Eulerian polynomials $A_n(x)$ used above) which enables us to write:

$$\frac{1}{e^z + 1} = \frac{1}{2} \sum_{n=0}^{\infty} E_n(0) z^n / n!, \quad (70)$$

which is valid for $|z| < \pi$. Thus, when

$$\beta < \frac{\pi}{J + h}, \quad (71)$$

corresponding obviously to high temperatures, the following expansion holds:

$$\frac{1}{e^{\beta\omega_k} + 1} = \frac{1}{2} \sum_{n=0}^{\infty} E_n(0)(\beta\omega_k)^n / n!. \quad (72)$$

Using the density of states $D(z)$, we can express the magnetization as

$$M_z = -\frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{E_{2n+1}(0)(h + Jz)(h^2 + J^2 + 2hJz)^n}{(2n + 1)!} \int_{-1}^{1} \frac{\beta^{2n+1}(h + Jz)(h^2 + J^2 + 2hJz)^n}{\sqrt{1 - z^2}} dz, \quad (73)$$

where we have used the fact that the Euler polynomial $E_n(x)$ vanishes at $x = 0$ for $n$ even. The latter integral can be expressed in terms of the hypergeometric function, and we find that

$$M_z = -\frac{h}{2} \sum_{n=0}^{\infty} \frac{E_{2n+1}(0)(J^2 + h^2)^{n-1}\beta^{2n+1}}{(2n + 1)!} \times \left(J^2 n \, _2F_1\left(\frac{1-n}{2}, \frac{2-n}{2}; 2; \frac{4J^2h^2}{(J^2 + h^2)^2}\right) + (J^2 + h^2) \, _2F_1\left(\frac{1-n}{2}, -\frac{n}{2}; 1; \frac{4J^2h^2}{(J^2 + h^2)^2}\right)\right). \quad (74)$$
We have thus obtained a series in powers of $\beta$, that could be truncated at a chosen order for high values of the temperature, which is permissible because of condition (71). Hence, at temperatures high enough, we may write:

$$M_z = \frac{h}{4} \beta - \frac{h}{48} (h^2 + 2J^2) \beta^3 + \frac{h}{480} (h^4 + 6J^2 h^2 + 3J^4) \beta^5$$

$$- \frac{17h}{80640} (h^6 + 12h^4 J^2 + 18h^2 J^4 + 4J^6) \beta^7 + \cdots .$$  \hspace{1cm} (75)

Let us have a look at the general form of the terms of the latter expansion. We see that it can be written as

$$M_z = h\beta \sum_{n=0} C_{2n} Q_{2n}(h, J) \beta^{2n},$$  \hspace{1cm} (76)

where the polynomials $Q_{2n}(h, J)$ are given by:

$$Q_0(h, J) = 1,$$
$$Q_2(h, J) = h^2 + 2J^2,$$
$$Q_4(h, J) = h^4 + 6J^2 h^2 + 3J^4,$$
$$Q_6(h, J) = h^6 + 12h^4 J^2 + 18h^2 J^4 + 4J^6,$$
$$Q_8(h, J) = h^8 + 20h^6 J^2 + 60h^4 J^4 + 40h^2 J^6 + 5J^8,$$

$$\vdots$$  \hspace{1cm} (77)

These polynomials can be expressed with the help of the binomial coefficients in the form:

$$Q_{2n}(h, J) = \sum_{\ell=0}^{n} \left( \begin{array}{c} n + 1 \\ \ell \end{array} \right) \left( \begin{array}{c} n \\ \ell \end{array} \right) h^{2(n-\ell)} J^{2\ell}.$$  \hspace{1cm} (78)

The coefficients $C_{2n}$ are equal to:

$$C_0 = \frac{1}{4},$$
$$C_2 = -\frac{1}{48},$$
$$C_4 = \frac{1}{480},$$
$$C_6 = -\frac{17}{80640},$$
$$C_8 = \frac{31}{1451520},$$

$$\vdots$$  \hspace{1cm} (79)
It can easily be verified by virtue of equation (74) that:

\[ C_{2n} = -\frac{E_{2n+1}(0)}{2(2n+1)!}. \]  

(80)

Figure (8) shows the magnetization \( M_z \) for small values of \( \beta \) as obtained by the numerical integration, and compares it with the values obtained from the expansion (74) truncated to fifth order in \( \beta \). It can be seen that the latter reproduces well the exact values at sufficiently high temperatures. Let us finally note that the zero-temperature magnetization in this case is equal to (15)

\[ M_z = \frac{1}{2\pi} \left( \frac{h - J}{h} K \left( \frac{2\sqrt{Jh}}{J+h} \right) + \frac{h + J}{h} E \left( \frac{2\sqrt{Jh}}{J+h} \right) \right), \]

(81)

with \( K(k) \) and \( E(k) \) being the complete elliptic integrals of the first and the second kind.

III. HEISENBERG ANISOTROPIC FERROMAGNETIC LATTICE IN \( d \geq 1 \)

The Hamiltonian describing a \( d \)-dimensional ferromagnetic lattice of \( N \) sites can be written as

\[ \mathcal{H} = -\sum_{ij} J_{ij} \left( S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z \right) + g\mu_B H \sum_{i} S_i \]

(82)

where \( \vec{S}_i \) is the spin vector operator of the particle that is located at site \( i \) of the lattice, while the parameter \( \Delta \) refers to the anisotropy constant (without loss of generality, we
shall assume that $\Delta > 1$). In the above equation, the quantities $\mu_B$, $g$ and $H$ denote the Bohr magneton, the Landé factor, and the strength of the magnetic field applied along the $z$-direction, respectively. Moreover, the coupling constants $J_{ij}$ are such that

$$J_{ij} > 0, \quad J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|).$$

(83)

(84)

Here, $\mathbf{R}_i$ designates the $d$-dimensional vector specifying the position in real space of the spin at site $i$ of the lattice. Notice that the ground state of Hamiltonian $\mathcal{H}$ when the magnetic field is pointing in the positive direction, is the Weiss state $|G\rangle = |-S, -S, \ldots, -S\rangle$, whose energy is $E_G = -NS\mu_B gH - N\Delta S^2 \sum_{ij} J_{ij}$. In order to study the magnetic properties of the lattice, it is instructive to introduce the states:

$$|m\rangle = |-S, -S, \ldots, -S + 1, -S, \ldots, -S\rangle.$$  

(85)

Actually, the above states are the one-excitation states, for which the eigenvalue $-NS$ of the operator $S_z$ corresponding to the ground state of the lattice as a whole, has increased by unity. One can easily verify that for a translation-invariant lattice (which is a reasonable assumption for $N$ sufficiently large), the Bloch states:

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_m e^{i\mathbf{k}\cdot\mathbf{R}_m} |m\rangle,$$

(86)

are eigenvectors of the Hamiltonian $\mathcal{H}$, with eigenenergies $E_\mathbf{k} + E_G$, where the excitation energy is given by:

$$E_\mathbf{k} = 2S \left( \Delta J(0) - J(\mathbf{k}) \right) + g\mu_B B,$$

(87)

with

$$J(\mathbf{k}) = \sum_{\delta} J(\delta)e^{i\delta\cdot\mathbf{k}}.$$  

(88)

The states (86) describe the propagation of nonlocal excitation modes throughout the lattice, which appear in the form of quantized spin waves or magnons, similar to phonons propagating in crystal lattices. By analogy, magnons are bosons satisfying to Bose-Einstein statistics. Every boson is characterized by a wave vector $\mathbf{k}$, and is created or annihilated through the action of the bosonic operators $a_\mathbf{k}$ and $a_\mathbf{k}^\dagger$, which fulfill $[a_\mathbf{k}, a_\mathbf{k'}^\dagger] = \delta(\mathbf{k} - \mathbf{k'})$. In the low-energy excitation approximation, the Hamiltonian $H$ can be put in the form:

$$H = \sum_\mathbf{k} E_\mathbf{k} a_\mathbf{k}^\dagger a_\mathbf{k} + E_G$$

(89)
where $E_k$ is given by formula (87). In the particular case where the coupling between the spins in the lattice involves only the nearest-neighbors, the number of which is denoted by $\eta$, the expression of $E_k$ simplifies drastically to take the form:

$$E_k = 2\eta JS(\Delta - \tau_k) + g\mu_B B$$ \hspace{1cm} (90)$$

where the form factor $\tau_k$ is given by

$$\tau_k = \frac{1}{\eta} \sum_{\delta} e^{i\delta\vec{k}}.$$ \hspace{1cm} (91)$$

In the above equation, the summation is carried out with respect to the vectors $\vec{\delta}$ linking every spin to its nearest neighbors only. For the one-dimensional linear chain, for which $\eta = 2$, one obtains $\tau_k = \cos(ak)$, where $a = ||\vec{\delta}||$ is the lattice constant. The square lattice in two dimensions is characterized by $\eta = 4$, which implies that $\tau_k = (1/2)\left(\cos(ak_x) + \cos(ka)\right)$. For a simple cubic lattice ($\eta = 6$), one simply gets $\tau_k = (1/3)\left(\cos(k_xa) + \cos(ka) + \cos(k_z a)\right)$.

At finite temperature, the magnetization of the lattice reads:

$$M = -g\mu_B NS + g\mu_B \sum_{n_k} \langle n_k \rangle$$ \hspace{1cm} (92)$$

where $\langle n_k \rangle$ is the thermal average number of magnons in mode $k$, which is given by the Bose-Einstein distribution:

$$\langle n_k \rangle = \frac{1}{\exp(\beta E_k) - 1}.$$ \hspace{1cm} (93)$$

It follows that the average magnetization deviation per spin with respect to the saturation state of the lattice reads:

$$\mathcal{M} := \frac{M + g\mu_B SN}{gN\mu_B} = \frac{1}{N} \sum_k \frac{1}{\exp(\beta E_k) - 1}.$$ \hspace{1cm} (94)$$

Notice that, by virtue of equation (A3), we conclude that the magnetization deviation per spin [Eq.(94)], in the thermodynamic limit can be expressed as:

$$\mathcal{M} = \int_{-1}^{1} \frac{\mathcal{D}(x)dx}{\exp[\beta E(x)] - 1}.$$ \hspace{1cm} (95)$$

where

$$E(x) := 2\eta JS(\Delta - x) + g\mu_B H.$$ \hspace{1cm} (96)$$
Therefore, the knowledge of the density of states $D$, allows one to evaluate the magnetization in the full first Brillouin zone, going thus beyond the long-wave approximation usually carried out \[23\]. In order to lighten the notation, we set:

$$B := 2\eta JS\Delta + g\mu_B H. \quad (97)$$

Then, we show that:

**Proposition 6.** The magnetization deviation per spin of the two-dimensional lattice is given at low temperatures by the series:

$$M = \sum_{n=0}^{\infty} \frac{A_{2n}(e^{\beta B})}{(2n)! (e^{\beta B} - 1)^{2n+1}} (8\beta JS)^{2n} F(n), \quad (98)$$

where the function $F(n)$ is defined by

$$F(n) = \frac{2}{(2n+1)\pi^2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; n + \frac{3}{2}; 1\right). \quad (99)$$

The proof of the latter proposition is almost identical to that of lemma \[11\]; the only difference resides in the use of the geometric series:

$$\frac{1}{1-x} = \sum_{k=0}^{\infty} x^k, \quad |x| < 1. \quad (100)$$

For the two-dimensional lattice, we show in the appendix that the density of states is given by

$$D(z) = \frac{2}{\pi^2} K(\sqrt{1-z^2}), \quad (101)$$

where $K(x)$ is the complete elliptic integral of the first kind. The remaining of the proof is based on the following lemma:

**Lemma 2.** For any non-negative integer $n$:

$$\int_{-1}^{1} x^{2n} K(\sqrt{1-x^2}) dx = \frac{\pi}{(2n+1)^2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; n + \frac{3}{2}; 1\right). \quad (102)$$

**Proof.** The complete elliptic integral of the first kind is related to the hypergeometric function through the relation:

$$K(z) = \frac{\pi}{2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; z^2\right). \quad (103)$$
Hence by noting that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$, we have for $n$ positive:

$$\int_{-1}^{1} x^{2n} K(\sqrt{1-x^2}) dx = \frac{1}{2} \sum_{k=0}^{\infty} \frac{\Gamma(k + \frac{1}{2})^2}{\Gamma(k + 1)^2} \int_{-1}^{1} (1 - x^2)^k x^{2n} dx$$

$$= \frac{1}{2} \sum_{k=0}^{\infty} \frac{\Gamma(k + \frac{1}{2})^2}{\Gamma(k + 1)^2} \int_{0}^{1} (1-t)^k t^{n-\frac{k}{2}} dt,$$

where, in the last equality, we have made the change of variable $t = x^2$. The integral in the last equation can be expressed in terms of the beta function [see equation (25)]. This means that

$$\int_{-1}^{1} x^{2n} K(\sqrt{1-x^2}) dx = \frac{1}{2} \sum_{k=0}^{\infty} \frac{\Gamma(k + \frac{1}{2})^2}{\Gamma(k + 1)^2} B(k + 1, n + \frac{1}{2})$$

$$= \frac{\Gamma(n + \frac{1}{2})}{2} \sum_{k=0}^{\infty} \frac{\Gamma(k + \frac{1}{2})^2 \Gamma(k + 1)}{\Gamma(k + 1)^2 \Gamma(k + n + \frac{3}{2})}$$

$$= \frac{\pi}{2n + 1} \sum_{k=0}^{\infty} \frac{(\frac{1}{2})_k (\frac{1}{2})_k}{k! (n + \frac{3}{2})_k},$$

where $(x)_k = \Gamma(x + k)/\Gamma(x)$ is the rising Pochhammer symbol, and where we have used the fact that $x\Gamma(x) = \Gamma(x + 1)$.

**Proposition 7.** In any dimension, at low temperatures, the magnetization deviation $\mathcal{M}$ satisfies:

$$\mathcal{M} \leq C \left[ \frac{1}{e^{\beta(2JS\eta + B)}} - 1 \right] + \frac{1}{e^{\beta(B - 2JS)}} - 1 - \frac{(2 - \frac{1}{C})}{e^{\beta B} - 1},$$

where:

$$C = \frac{1}{2} \int_{-1}^{1} z^2 D(z) dz.$$

The proof is quite similar to that of proposition (1). For $d = 2$, the constant $C$ is given by

$$C = \frac{\mathcal{F}(1)}{2} = \frac{1}{8}.$$

The inequality in equation (106) arises because we obtain an expansion with exclusively positive terms which was not the case for the Fermi-Dirac distribution. Let us also point out that the usual method to calculate $\mathcal{M}$ consists in replacing the sum in equation (94) by an integral over $\vec{k}$, and assuming that, at low temperatures, the resulting integral is
dominated by the low values of $k = ||\vec{k}||$ [11, 23]. Mathematically speaking, this is equivalent to setting:

$$E_k = J S a^2 k^2 + 2 J S \eta (\Delta - 1) + g \mu_B B,$$

yielding for the linear chain ($d = 1$):

$$M = \frac{1}{2 \pi} \int_0^\infty \frac{dk}{\exp[\beta (J S a^2 k^2 + g \mu_B \tilde{H})] - 1} = \frac{1}{4 (\pi \beta a^2 S)^{1/2}} \text{Li}_{1/2} (e^{\beta g \mu_B \tilde{H}}),$$

where for ease of notation we have set $g \mu_B \tilde{H} =: 2 J S \eta (\Delta - 1) + g \mu_B B$. In the same way, one finds that for the square lattice ($d = 2$):

$$M = \frac{1}{(2 \pi)^2} \int_0^\infty \frac{2 \pi k dk}{\exp[\beta (J S a^2 k^2 + g \mu_B \tilde{H})] - 1} = \frac{1}{4 \pi \beta a^2 S} \log \frac{1}{1 - e^{-\beta g \mu_B \tilde{H}}},$$

Finally, for the simple cubic lattice in three dimensions ($d = 3$),

$$M = \frac{1}{(2 \pi)^3} \int_0^\infty \frac{4 \pi k^2 dk}{\exp[\beta (J S a^2 k^2 + g \mu_B \tilde{H})] - 1} = \frac{1}{8 (\pi \beta a^2 S)^{3/2}} \text{Li}_{3/2} (e^{\beta g \mu_B \tilde{H}}).$$

All the above formulas were obtained under the assumption that $ka \ll 1$, which may not be suitable for strong magnetic fields.

In figures (9) and (10) we compare the analytical results with the numerical ones in the case of the two-dimensional lattice for particular values of the parameters at sufficiently low temperatures. We see that the agreement is good with the series expansion (98) truncated to order 4, as compared with the long-wavelength approximation (110). We see also that the accordance with the bound given by equation (110) becomes better as the strength of the magnetic field increases.

IV. CONCLUSION

In conclusion, we presented a analytical treatment of the magnetization of some Heisenberg spin lattices in one and two dimensions. By expanding the Ferm-Dirac and the Bose-Einstein distributions in power series, that are valid in the whole range of the first Brillouin
FIG. 9. The magnetization deviation $\mathcal{M}$ as a function of temperature obtained by numerical integration (solid curve), truncation of the series [98] (dotted curve), the approximation [106] (dot-dashed curve), and the approximation [110] (dashed curve). The parameters are $J = 20$, $H = 10$, $S = 7$, and $\Delta = 1.5$.

FIG. 10. The magnetization deviation $\mathcal{M}$ as a function of temperature obtained by numerical integration (solid curve), truncation of the series [98] (dotted curve), the approximations [106] (dot-dashed curve), and the approximation [110] (dashed curve). The parameters are $J = 20$, $H = 100$, $S = 7$, and $\Delta = 1.5$.

zone, we were able to gain many interesting mathematical results that facilitate the investigation of the magnetic properties of these systems. Such analytical results reduce the computational effort, and allow for a deeper understanding of the behavior of the magne-
tization at low and hight temperatures. For the special case of the XX spin-1/2 chain, the study presented here, reveals that the way the magnetization approaches its saturation value close to the absolute zero, varies as the applied magnetic field crosses its critical value. We have found the exact power law with respect to the temperature in each region, along with the temperature dependence of the corresponding coefficients in the expansion. The explicit analytical form of the expansion at hight temperatures has been identified in the case of the transverse ising model. In order to investigate the two-dimensional Heisenberg lattice, we used a truncated series expansion to calculate the magnetization deviation at low temperature. We found that the analytical expressions reproduce well the exact values calculated numerically especially for strong magnetic fields. This investigation may open further perspectives towards gaining more insight into the behavior of spin systems.

### Appendix A

In an explicit way, we may define the density of states \( D(x) \) through the Dirac delta function as:

\[
D(x) = \lim_{N \to \infty} \frac{1}{N} \sum_k \delta(x - \tau_k).
\]  

This function is usually calculated using the Green’s function \([24]\). We use a simpler method to derive it. Observing that in the first Brillouin zone \(-1 \leq \tau_k \leq 1\), we infer that for any function \( f(\tau_k) \), we have

\[
\lim_{N \to \infty} \frac{1}{N} \sum_k f(\tau_k) = \lim_{N \to \infty} \int_{-1}^{1} dx \frac{1}{N} \sum_k f(x) \delta(x - \tau_k),
\]

meaning that

\[
\lim_{N \to \infty} \frac{1}{N} \sum_k f(\tau_k) = \int_{-1}^{1} f(x)D(x)dx.
\]

In one dimension \((d = 1)\), we can easily derive the expression of \( D(x) \) as follows:

\[
D(x) = \lim_{N \to \infty} \frac{1}{N} \delta(x - \tau_k) = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \delta(x - \cos(ka))dk
\]

\[
= \frac{1}{\pi} \int_{-1}^{1} \delta(x - z)dz \sqrt{1 - z^2}.
\]

It immediately follows that

\[
D(x) = \frac{1}{\pi \sqrt{1 - x^2}}.
\]
Similarly, the expression of $\mathcal{D}(x)$ for the two dimensional lattice can be derived as

$$
\mathcal{D}(x) = \lim_{N \to \infty} \frac{1}{N} \delta(x - \tau_k) = \frac{a^2}{(2\pi)^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \delta\left(x - \frac{\cos(k_1a)}{2} - \frac{\cos(k_2a)}{2}\right) dk_1 dk_2
$$

$$
= \frac{2}{\pi^2} \int_1^1 \int_{-1}^1 \frac{dy dz}{\sqrt{1 - y^2} \sqrt{1 - z^2}} \delta(2x - y - z) = \frac{2}{\pi^2} \int_{-1}^1 \frac{dy}{\sqrt{1 - y^2} \sqrt{1 - (2x + y)^2}}.
$$

(A6)

Let us stress that the density of states is an even function of its argument if $\tau_k = \tau_{-k}$, which is true for the linear, the square, and the simple cubic lattices considered here. Hence, when $x > 0$, the condition $-1 \leq y \leq 1 - 2x$ should be satisfied in the above equation, which leads to

$$
\mathcal{D}(x) = \frac{2}{\pi^2} \int_{-1}^{1-2x} \frac{dy}{\sqrt{1 - y^2} \sqrt{1 - (2x + y)^2}}.
$$

(A7)

The transformation

$$
y = -1 + (1 + 2x)(1 - x) \frac{\sin^2 t}{1 - \sin^2 t}, \quad 0 \leq t \leq \frac{\pi}{2},
$$

(A8)

leads to

$$
\mathcal{D}(x) = \frac{2}{\pi^2} K(\sqrt{1 - x^2}),
$$

(A9)

where $K(k)$ is the elliptic integral of the first kind, which is defined by

$$
K(k) = \int_0^{\frac{\pi}{2}} \frac{dt}{\sqrt{1 - k^2 \sin^2 t}}.
$$

(A10)

For the three dimensional case, we may write

$$
\mathcal{D}(x) = \frac{a^3}{(2\pi)^3} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \delta(x - \cos(k_1a)/3 - \cos(k_2a)/3 - \cos(k_3a)/3) dk_1 dk_2 dk_3
$$

$$
= \frac{3}{2\pi^3} \int_{-\pi}^\pi \int_{-1}^1 \int_{-1}^1 \frac{d\rho dy dz}{\sqrt{(1 - y^2)(1 - z^2)}} \delta(3x - y - z - \cos(\rho))
$$

$$
= \frac{3}{2\pi^3} \int_{-\pi}^\pi \int_{-1}^1 \frac{dy}{\sqrt{1 - y^2}} \frac{1}{\sqrt{1 - (3x - \cos(\rho) + y)^2}}.
$$

(A11)

Note that in this case, the density of states cannot be written in a simple closed form.

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