Classical magnetism and an integral formula involving modified Bessel functions

Orion Ciftja
E-mail ogciftja@pvamu.edu[1]
[1]*Department of Physics, Prairie View A&M University, Prairie View, Texas 77446, USA*
(Dated: February 19, 2018)

We study an integral expression that is encountered in some classical spin models of magnetism. The idea is to calculate the key integral that represents the building block for the expression of the partition function of these models. The general calculation allows one to have a better look at the internal structure of the quantity of interest which, in turn, may lead to potentially new useful insights. We find out that application of two different approaches to solve the problem in a general case scenario leads to an interesting integral formula involving modified Bessel functions of the first kind which appears to be new. We performed Monte Carlo simulations to verify the correctness of the integral formula obtained. Additional numerical integration tests lead to the same result as well. The approach under consideration, when generalized, leads to a linear integral equation that might be of interest to numerical studies of classical spin models of magnetism that rely on the well-established transfer-matrix formalism.

PACS numbers: 01.55.+b, 73.43.Cd, 02.30.-f

I. INTRODUCTION

Magnetic spin systems, in particular, one-dimensional (1D) lattice models of classical spins have been widely studied in recent decades[1] since: (i) In some cases they can be solved exactly; and (ii) In some cases they approximate well real magnetic materials. An example of such real materials is the case of molecular magnets which typically are artificial magnetic structures containing a small number of magnetic ions[2,3]. Molecular magnetism has attracted considerable recent interest since molecular magnetic clusters have desirable properties for technological applications as nanoscale magnetic devices and/or sensors. Many molecular magnets consist of a finite number of magnetic ions, each possesing a large value of spin[4,5]. Because of the large value of spin, many magnetic properties for such structures can be reproduced to high accuracy by using the classical Heisenberg spin model where a spin, $\vec{S}_i$ is treated as a three-dimensional (3D) vector of unit length ($|\vec{S}_i|^2 = 1$). A typical classical molecular magnet consists of a certain small finite number of classical spins interacting with each other via various coupling parameters. The simplest case would be that of a cluster with a finite number, N of spins all coupled equally (via a coupling constant, J) to each other:

$$H_{Cluster} = -J \sum_{i<j}^{N} \vec{S}_i \, \vec{S}_j \ . \tag{1}$$

It is easy to see that the spin Hamiltonian in Eq.(1) (for $N \geq 3$) is different from another standard classical model of magnetism known as the open linear chain model:

$$H_N = -J \sum_{i=1}^{N-1} \vec{S}_i \, \vec{S}_{i+1} \ , \tag{2}$$

where J is the isotropic exchange interaction energy between neighbouring spins. Note that the partition function for the case of Eq.(2) is written as:

$$Z_N = \int d\Omega_1 \cdots \int d\Omega_N \, \exp\left(\beta \, J \sum_{i=1}^{N-1} \vec{S}_i \, \vec{S}_{i+1}\right) \ , \tag{3}$$

where $\int d\Omega_i = \int_0^{\pi} d\theta_i \, \sin\theta_i \int_0^{2\pi} d\varphi_i$ is the integral over the solid angle for the i-th vector, θ_i is the polar angle and φ_i is the azimuthal angle. The parameter β in Eq.(3) is written as $\beta = 1/(k_B \, T)$ where k_B is Boltzmann's constant and T is the absolute temperature of the system. It is a well-known fact that the partition function can be calculated exactly for the open linear chain model case[6]:

$$Z_N = (4\pi) \, [4\pi \, i_0(\beta \, J)]^{N-1} \ , \tag{4}$$

where

$$i_l(x) = \sqrt{\frac{\pi}{2\,x}} \, I_{l+\frac{1}{2}}(x) \ , \tag{5}$$

are modified spherical Bessel functions of the first kind (see for example pg.733 of Ref. 7) and $l = 0, \pm 1, \ldots$. The function $I_\nu(x)$ denotes the modified Bessel function of the first kind. Note that $i_0(x) = \sinh(x)/x$ where $\sinh(x)$ is the hyperbolic sine function. This striking result hinges solely on the observation that the integrals in Eq.(3) will separate if the polar coordinates, $(\theta_{i+1}, \varphi_{i+1})$ for $\vec{S}_{i+1}$ are referred to $\vec{S}_i$ as polar axis of a 3D coordinative system. For instance, by choosing $\vec{S}_1$ as lying in the z-direction, one immediately has:

$$\int d\Omega_2 \, \exp\left(\beta \, J \, \vec{S}_1 \, \vec{S}_2\right) = 4\pi \, i_0(\beta \, J) \ . \tag{6}$$

As pointed out earlier, a typical molecular magnet system cannot be described as an open linear chain of spins since the positions of the magnetic ions generally define a 3D structure. Tetrahedron-shaped magnetic molecules[8,9] represent one of the simplest examples of this type of structure[10] consisting of only $N = 4$ spins where each spin is coupled to the three other spins. Since the simple approach that works fine for the calculation of the partition function of an open linear chain spin model is not possible for a system like that in Eq.(1) (as long as $N \geq 3$) one asks if anything new can be learned by: (i) Firstly, solving the resulting integral expression in Eq.(6) quite generally for a totally arbitrary choice of the 3D coordinative system where neither $\vec{S}_1$, nor $\vec{S}_2$ lie in the z-direction; and (ii) Secondly, see to relate the solution to other treatments of the problem that might lead to new insights.

In this work, we show that the problem can be solved in general terms using two methods as layed out, respectively, in Section II and Section III. The results obtained by the application of these two different methods lead to an interesting formula involving modified Bessel functions of the first kind. This formula was verified via various simulations and numerical tools. In addition, the results derived lead to a kernel that might be of interest within the framework of the transfer-matrix approach, a tool widely used in studies of classical spin systems. Some discussions and conclusions are presented in Section IV.

II. GENERAL CASE SCENARIO

Let's assume that the two classical spin vectors have an arbitrary orientation in a 3D spherical system of coordinates (namely, none of the spins lies along the z-direction). In such a case, one has:

$$\vec{S}_1\,\vec{S}_2 = \cos\gamma = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2)\ . \tag{7}$$

At this juncture, one uses the following expansion formula (see for example pg.445 of Ref. 11 or pg.308 of Ref. 12) for:

$$\exp\left(x\,\cos\gamma\right) = \sum_{l=0}^{\infty}(2\,l+1)\ i_l(x)\,P_l(\cos\gamma)\ , \tag{8}$$

where $P_l(\cos\gamma)$ are Legendre polynomials. With help from Eq.(8) one writes:

$$\int d\Omega_2\,\exp\left(\beta\,J\,\vec{S}_1\,\vec{S}_2\right) = \int d\Omega_2\sum_{l=0}^{\infty}(2\,l+1)\ i_l(\beta\,J)\,P_l(\cos\gamma)\ . \tag{9}$$

At this point, we apply the addition theorem for spherical harmonics (see pg.796 of Ref. 7) which allows us to write:

$$P_l(\cos\gamma) = \frac{4\,\pi}{2\,l+1}\sum_{m=-l}^{+l}Y^{*}_{l\,m}(\theta_1,\varphi_1)\,Y_{l\,m}(\theta_2,\varphi_2)\ , \tag{10}$$

where $Y_{l\,m}(\theta,\varphi)$ are spherical harmonics. In the above expression, the asterisk may go on either spherical harmonic. By substituting the result from Eq.(10) into Eq.(9), one has:

$$\int d\Omega_2\,\exp\left(\beta\,J\,\vec{S}_1\,\vec{S}_2\right) = = 4\,\pi\sum_{l=0}^{\infty}i_l(\beta\,J)\sum_{m=-l}^{+l}Y^{*}_{l\,m}(\theta_1,\varphi_1)\int d\Omega_2 Y_{l\,m}(\theta_2,\varphi_2) \tag{11}$$

We recall that:

$$\int d\Omega_2\,Y_{l\,m}(\theta_2,\varphi_2) = \sqrt{4\,\pi}\,\delta_{l0}\,\delta_{m0}\ , \tag{12}$$

where $\delta_{i\,j}$ is a Kronecker's delta function. Based on the result from Eq.(12) and using the fact that $Y_{00}(\theta,\varphi) = 1/\sqrt{4\,\pi}$ we calculate that:

$$\int d\Omega_2\,\exp\left(\beta\,J\,\vec{S}_1\,\vec{S}_2\right) = 4\,\pi\,i_0(\beta\,J)\ . \tag{13}$$

This conclusion represents the proof of validity of the formula in Eq.(6) for the general case of an arbitrarily chosen 3D coordinative system.

The advantages of the prescribed method become clearer when one recognizes that the expansion in Eq.(8) in conjunction with the expansion in Eq.(10) may be readily used to calculate a more general integral of the type listed below:

$$\int d\Omega_2\,\exp\left(\beta\,J\,\vec{S}_1\,\vec{S}_2\right)Y_{l\,m}(\theta_2,\varphi_2) = \lambda_l\,Y_{l\,m}(\theta_1,\varphi_1)\ , \tag{14}$$

where

$$\lambda_l = 4\,\pi\,i_l(\beta\,J)\ \ ;\ \ l=0,1,\ldots\ \ ;\ \ m=0,\pm1,\ldots,\pm l\ . \tag{15}$$

Note that Eq.(14) represents what is known as a Fredholm homogeneous linear integral equation of the second kind. As such, this linear integral equation defines the exact eigenfunctions, in this case $Y_{l\,m}(\theta,\varphi)$ and exact eigenvalues, in this case λ_l of the kernel, $K(\vec{S}_1,\vec{S}_2) = \exp\left(\beta\,J\,\vec{S}_1\,\vec{S}_2\right)$. We remark that different notations are used in the literature to describe linear integral equations of this type. For example, a common choice in literature is to write the equation in such a way that parameter, λ multiplies the integral. Note that the kernel, $K(\vec{S}_1,\vec{S}_2)$ appearing in Eq.(14) is symmetric (and real). As a result, the Hilbert-Schmidt theory[13] for linear integral equations with symmetric (and real) kernels can be immediately applied in this case. This observation leads to an exact calculation of the partition function not only for the open linear chain of Eq.(2), but also for a closed ring model of N classical spins with nearest-neighbour isotropic interactions[14]. If we assume that the number of spins in the system is $N \geq 3$, a closed ring spin model differs from an open linear chain spin model in that, in the ring, there is interaction between spins $\vec{S}_N$ and $\vec{S}_1$ (while, such an interaction term is absent in the open linear chain). As a result, the Hamiltonian for a closed ring of classical Heisenberg spins interacting with nearest-neighbour isotropic exhange interaction is written as:

$$H_N^{Ring} = -J \sum_{i=1}^{N-1} \vec{S}_i \, \vec{S}_{i+1} - J \, \vec{S}_N \, \vec{S}_1 \quad ; \quad N \geq 3 \; . \qquad (16)$$

Obviously, use of $\vec{S}_i$ as polar axis for $\vec{S}_{i+1}$ will not help in the calculation of the partition function for a closed ring as in Eq.(16). However, the result in Eq.(14) is extremely important since it allows one to expand the kernels, $K(\vec{S}_i, \vec{S}_{i+1})$ appearing in the expression of the partition function in terms of the corresponding eigenfunctions given from Eq.(14) with the eventual final result for the partition function reading:

$$Z_N^{Ring} = \sum_{l=0}^{\infty} (2\,l+1) \, \lambda_l^N \; , \qquad (17)$$

where the factor, $(2\,l+1)$ comes from the fact that each eigenvalue, λ_l is $(2\,l+1)$-fold degenerate. In essence, these are the general features of the transfer-matrix formalism[15]. Obviously, the problem is much more difficult when the systems (either the linear chain, or the closed ring) are in an external magnetic field. In such a case, the partition function can be calculated analytically only for systems consisting of a very small number of spins[16,17].

III. DIFFERENT APPROACH

Let's now consider the problem in Section II with a different approach that is more direct in the sense that it does not make use of the addition theorem for spherical harmonics. This is important since application of different methods to solve a given mathematical problem may potentially result in interesting transformations and identities that otherwise are not so obvious[18–20]. We explicitly write the expression under consideration as:

$$\int d\Omega_2 \, \exp\Big(\beta \, J \, \vec{S}_1 \, \vec{S}_2\Big) = \int_0^{\pi} d\theta_2 \, \sin\theta_2 \int_0^{2\,\pi} d\varphi_2 \, \exp\Big\{\beta \, J \, \Big[\cos\theta_1 \, \cos\theta_2 + \sin\theta_1 \, \sin\theta_2 \, \cos(\varphi_1 - \varphi_2)\Big]\Big\} \qquad (18)$$

We simplify the notation by denoting $a = \beta \, J$ and, hence, rewrite Eq.(18) as:

$$\int d\Omega_2 \, \exp\Big(a \, \vec{S}_1 \, \vec{S}_2\Big) = \int_0^{\pi} d\theta_2 \, \sin\theta_2 \, \exp\Big(a \, \cos\theta_1 \, \cos\theta_2\Big) \times \int_0^{2\,\pi} d\varphi_2 \, \exp\Big[a \, \sin\theta_1 \, \sin\theta_2 \, \cos(\varphi_1 - \varphi_2)\Big] \; . \qquad (19)$$

At this point, we apply the formula:

$$\int_0^{2\,\pi} d\varphi_2 \, \exp\left[x \, \cos(\varphi_1 - \varphi_2)\right] = 2\,\pi \, I_0(x) \; , \qquad (20)$$

where $I_0(x)$ is a modified Bessel function of the first kind of order zero. We are left with the following integral:

$$\int d\Omega_2 \, \exp\Big(a \, \vec{S}_1 \, \vec{S}_2\Big) = 2\pi \int_0^{\pi} d\theta_2 \sin\theta_2 \exp\Big(a \cos\theta_1 \cos\theta_2\Big) \, I_0\Big(a \sin\theta_1 \sin\theta_2\Big) \qquad (21)$$

We simplify Eq.(21) by introducing a new variable, $y = \cos\theta_2$ so that:

$$\int d\Omega_2 \, \exp\Big(a \, \vec{S}_1 \, \vec{S}_2\Big) = 2\,\pi \, F(a, \theta_1) \; , \qquad (22)$$

where

$$F(a, \theta_1) = \int_{-1}^{+1} dy \, \exp\Big(a \, \cos\theta_1 \, y\Big) \, I_0\Big(a \, \sin\theta_1 \, \sqrt{1-y^2}\Big) \; . \qquad (23)$$

At first sight, the integral above does not look extremely challenging. However, despite the efforts, we could not find a simple way to calculate it analytically. Because of this reason we chose to calculate the integral in Eq.(23) numerically by adopting the standard Monte Carlo simulation method. Numerical integration via the Monte Carlo simulation method is a well-established robust technique that generally leads to very accurate results when the number of sampling points is reasonably large. To this effect, we selected different values of the parameter, a (for the sake of simplicity, we show the results for only four values, $a = 1, 2, 3$ and 4). For each of the values of a we calculated numerically the integral for several different values of the variable, θ_1. We performed several Monte Carlo simulation runs with a large number of sampling points to the extent that we believe that all the numerical simulation results are accurate to the fourth digit after the decimal point (the fourth digit after the decimal point is rounded). The Monte Carlo integration results were later verified (to the same degree of accuracy) by numerical integration of the expression in question using other schemes (not Monte Carlo). The numerical results obtained are listed in Table. I. The numerical results indicate without any ambiguity that the value of the integral function in Eq.(23) does not depend on variable, θ_1. This means that we can suitably choose $\theta_1 = 0$ and calculate the integral $F(a, \theta_1) = F(a, \theta_1 = 0)$. This observation leads to:

$$F(a, \theta_1) = \int_{-1}^{+1} dy \, \exp(a\,y) \; = \; \frac{\exp(a) - \exp(-a)}{a} \; . \qquad (24)$$

We searched some of the most authorative books that contain tables of integrals[21,22] but could not find an integral of the form of Eq.(23). Even standard computational packages based on symbolic

TABLE I: Numerical estimate of the integral, $F(a, \theta_1)$ for selected values of the parameters, a and θ_1. The numerical results are rounded at the fourth digit after the decimal point.

a	$\theta_1 = \frac{\pi}{6}$	$\theta_1 = \frac{\pi}{5}$	$\theta_1 = \frac{\pi}{4}$	$\theta_1 = \frac{\pi}{3}$	$\theta_1 = \frac{\pi}{2}$	$\theta_1 = \pi$
1	2.3504	2.3504	2.3504	2.3504	2.3504	2.3504
2	3.6269	3.6269	3.6269	3.6269	3.6269	3.6269
3	6.6786	6.6786	6.6786	6.6786	6.6786	6.6786
4	13.6450	13.6450	13.6450	13.6450	13.6450	13.6450

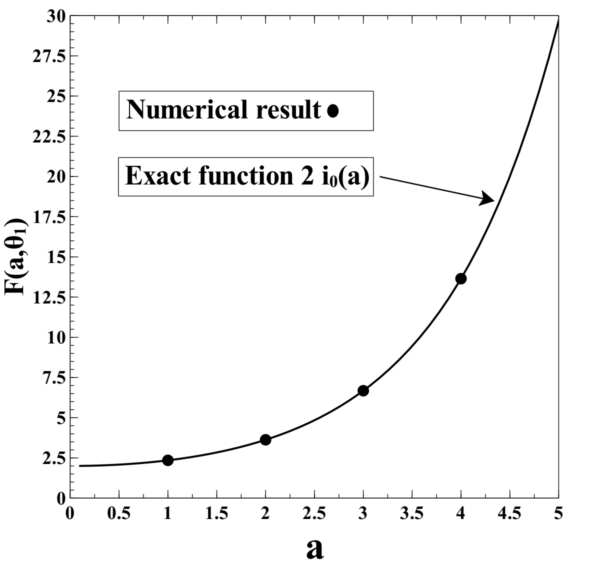

FIG. 1: Comparison of the numerically obtained results from Table. I (filled dots) to the exact function, $2\,i_0(a) = \frac{[\exp(a) - \exp(-a)]}{a}$ (solid line). The uncertainty of the numerical results (of the order of 10^{-4}) is much less than the size of symbols (drawn as large filled dots for better visual clarity).

mathematical manipulations like Mathematica[23] were unable to do it analytically. On the other hand, our numerical simulations clearly suggest that the integral expression in question has the value as given from Eq.(24). It appears that this new approach (which avoids the use of the addition theorem for spherical harmonics) has led us to an interesting integral involving the modified Bessel function. This fact is quite interesting since we can obtain the correct answer in Eq.(24) in another way by looking at the result in Eq.(13).

A comparison of Eq.(22) to Eq.(13) leads to the conclusion that:

$$F(a, \theta) = \int_{-1}^{+1} dy \, \exp\left(a \, \cos\theta \, y\right) I_0 \left(a \, \sin\theta \, \sqrt{1 - y^2}\right) = 2\, i_0(a). \quad (25)$$

Note that we now dropped the subscript "1" from the notation for angle θ_1 in Eq.(23). It can be checked that the result in Eq.(25) is in agreement with Eq.(24) since by definition, $i_0(a) = \sinh(a)/a$ where $\sinh(a) = \left[\exp(a) - \exp(-a)\right]/2$. It can be seen in Fig. 1 that the numerically obtained results in Table. I are in perfect agreement with what we believe to be the exact analytical value of the integral as written in Eq.(25). The expression in Eq.(25) appears to be a novel integral formula involving modified Bessel functions of the first kind.

IV. DISCUSSIONS AND CONCLUSIONS

We applied different mathematical methods to solve a problem encountered in studies of classical magnetism. The approach of using different mathematical transformations of a given quantity is known to be extremely useful with the potential benefits of helping to uncover novel formulas or identities[24]. This approach allows one to derive interesting alternative analytic expressions for a given quantity of interest. In our case, a comparison of the results obtained by by using different approaches leads to an interesting integral expression involving modified Bessel functions. The result obtained appears to constitute a novel integral formula involving modified Bessel functions of the first kind, therefore, it might be of interest to researchers working in the field of mathematical physics and/or applied mathematics. We checked the correctness of the result obtained numerically via an accurate Monte Carlo calculation of the integral expression under consideration. We also caculated the integral expression in Eq.(25) numerically via other tools (not Monte Carlo) ending with identical results for the accuracy adopted. The numerical approach is unambigous, we chose arbitrary values of the variables a and θ in the expression for $F(a, \theta)$ in Eq.(25) and then verified numerically that the formula in question is always true and the final result does not depend on the variable θ. In a nutshell, the numerical results leave no doubt to the correctness of the formula in Eq.(25). For an analytical proof see the Appendix.

Note that Eq.(13) and Eq.(25) are related and

both represent special cases of more general linear integral equations. For example, Eq.(13) is a special case of Eq.(14) for $l = 0$ and $m = 0$. However, it is important to note that their respective kernels are quite different. Differently from the kernel $K(\vec{S}_1, \vec{S}_2) = \exp\left(\beta\, J\, \vec{S}_1\, \vec{S}_2\right)$ in Eq.(13) which is a function of four variables, the kernel, $K(\theta, y) = \exp\left(a\, \cos\theta\, y\right)\, I_0\left(a\, \sin\theta\, \sqrt{1-y^2}\right)$ in Eq.(25) is a function of only two variables. Thus, extension of Eq.(25) to a more general linear integral equation of the form:

$$\int_{-1}^{+1} dy\, K(\theta, y)\, f(y) = \lambda\, f(\theta)\ , \tag{26}$$

may be deemed of interest within the framework of standard linear integral equation methods[13]. Note that Eq.(26) represents a typical homogeneous Fredholm linear integral equation of the second kind. Linear integral equations of the type in Eq.(26) are the key ingredients of the transfer-matrix method that can be used to solve (numerically) more complex situations involving interacting spins. Hence, a kernel like the one in Eq.(26) may be appealing to the broad audience of researchers that work in numerical studies of such problems.

Acknowledgement

This research was supported in part by National Science Foundation (NSF) Grants No. DMR-1410350 and DMR-1705084. The author thanks the anonymous referee for suggesting an analytical proof of the result as outlined in the Appendix.

APPENDIX: CALCULATION OF $F(a, \theta)$

The relation in Eq.(25) can be written as:

$$F(a, \theta) = \int_{-1}^{+1} dy\, e^{a\, \cos\theta\, y}\, I_0\left(a\, \sin\theta\, \sqrt{1-y^2}\right) = \sqrt{\frac{2\,\pi}{a}}\, I_{\frac{1}{2}}(a) \tag{A.1}$$

based on the general definition of $i_l(x)$ from Eq.(5). We expand the modified Bessel function of the first kind that appears inside the integral sign by using Eq.(10.25.2) of Ref. 25 that reads:

$$I_\nu(z) = \left(\frac{z}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{\left(\frac{z^2}{4}\right)^k}{k!\,\Gamma(\nu+k+1)}\ , \tag{A.2}$$

where Γ represents the gamma function. For $\nu = 0$ one has:

$$I_0(z) = \sum_{k=0}^{\infty} \frac{z^{2k}}{2^{2k}\,(k!)^2}\ . \tag{A.3}$$

We substituting the result from Eq.(A.3) into Eq.(A.1) and interchange summation and integration:

$$F(a, \theta) = \sum_{k=0}^{\infty} \frac{a^{2k}\, \sin^{2k}\theta}{2^{2k}\,(k!)^2} \int_{-1}^{+1} dy\, e^{a\, \cos\theta\, y}\, (1-y^2)^k\, dy\ . \tag{A.4}$$

We now rely on Eq.(10.32.2) of Ref. 25 which reads:

$$I_\nu(z) = \frac{\left(\frac{z}{2}\right)^\nu}{\sqrt{\pi}\,\Gamma(\nu+\frac{1}{2})} \int_{-1}^{+1} (1-t^2)^{\nu-1/2}\, e^{\pm z\, t}\, dt\ . \tag{A.5}$$

For $\nu = k + 1/2$ such a formula leads to:

$$\int_{-1}^{+1} (1-t^2)^k\, e^{\pm z\, t}\, dt = \frac{\sqrt{\pi}\, k!}{\left(\frac{z}{2}\right)^{k+\frac{1}{2}}}\, I_{k+\frac{1}{2}}(z)\ . \tag{A.6}$$

With help from Eq.(A.6), one transforms Eq.(A.4) into:

$$F(a, \theta) = \sqrt{\frac{2\,\pi}{a\, \cos\theta}} \sum_{k=0}^{\infty} \frac{1}{k!} \left[\frac{a\, \sin^2\theta}{2\, \cos\theta}\right]^k I_{k+\frac{1}{2}}\left(a\, \cos\theta\right)\ . \tag{A.7}$$

We now use Eq.5.7.6.(1) of Ref. 22 (pg.660) that gives:

$$\sum_{k=0}^{\infty} \frac{t^k}{k!}\, J_{k+\nu}(z) = z^{\nu/2}\, (z - 2\,t)^{-\nu/2}\, J_\nu\left(\sqrt{z^2 - 2\,t\, z}\right)\ , \tag{A.8}$$

where $J_{k+\nu}(z)$ is a Bessel function of the first kind. This formula suggests that for $\nu = 1/2$ we should have:

$$\sum_{k=0}^{\infty} \frac{t^k}{k!}\, J_{k+\frac{1}{2}}(z) = \left(\frac{z}{z-2\,t}\right)^{1/4} J_{\frac{1}{2}}\left(\sqrt{z(z-2\,t)}\right)\ . \tag{A.9}$$

The formula in Eq.(10.27.6) of Ref. 25 explains how a Bessel function of the first kind with imaginary argument is related to a modified Bessel function of the first kind:

$$I_\nu(z) = e^{-\nu\frac{\pi}{2}i}\, J_\nu\left(z\, e^{\frac{\pi}{2}i}\right)\ . \tag{A.10}$$

This implies that, for our specific case, we have:

$$J_\nu(i\, z) = e^{\nu\frac{\pi}{2}i}\, I_\nu(z)\ . \tag{A.11}$$

The next step is to write $z = i\,\xi$, $t = -i\,\tau$ and use Eq.(A.11) to transform Eq.(A.9) in terms of modified Bessel functions of the first kind. After some careful algebraic manipulations of Eq.(A.9) (note that a factor $e^{\frac{\pi}{4}i}$ appears in both sides of the equation and, thus, cancels out), one obtains:

$$\sum_{k=0}^{\infty} \frac{\tau^k}{k!}\, I_{k+\frac{1}{2}}(\xi) = \left(\frac{\xi}{\xi+2\,\tau}\right)^{1/4} I_{\frac{1}{2}}\left(\sqrt{\xi(\xi+2\,\tau)}\right)\ . \tag{A.12}$$

The formula in Eq.(A.12) can be immediately applied to Eq.(A.7) with the understanding that:

$$\tau = \frac{a\,\sin^2\theta}{2\,\cos\theta} \quad ; \quad \xi = a\,\cos\theta\ . \qquad \text{(A.13)}$$

As a result, one obtains $F(a,\theta) = \sqrt{\frac{2\pi}{a}}\, I_{\frac{1}{2}}(a)$ as in Eq.(A.1).

---

[1] H. E. Stanley, Phys. Rev. **158**, 537 (1967).
[2] *Nanomagnetism*, (NATO Asi Series E: Applied Sciences, Vol. 247) edited by A. Hernando (Kluwer Academic, Dordrecht, 1993).
[3] O. Kahn, *Molecular Magnetism*, (Wiley-VCH, New York, 1993).
[4] K. L. Taft, C. D. Delfs, G. C. Papaefthymiou, S. Foner, D. Gatteschi, and S. J. Lippard, J. Am. Chem. Soc. **116**, 823 (1994).
[5] D. Gatteschi, A. Caneschi, L. Pardi, and R. Sessoli, Science **265**, 1054 (1994).
[6] M. E. Fisher, Am. J. Phys. **32**, 343 (1964).
[7] Mathematical Methods For Physicists, Fifth Edition, G. B. Arfken and H. J. Weber, Harcourt/Academic Press, San Diego (2001).
[8] A. L. Barra, A. Caneschi, A. Cornia, F. Fabrizi de Biani, D. Gatteschi, C. Sangregorio, R. Sessoli, and R. Sorace, J. Am. Chem. Soc. **121**, 5302 (1999).
[9] A. Bino, D. C. Johnston, D. P. Goshorn, T. R. Halbert, and E. I. Stiefel, Science **241**, 1479 (1988).
[10] O. Ciftja, Physica A **286**, 541 (2000).
[11] Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, 9th Edition, Edited by M. A. Abramowitz and I. A. Stegun, Dover Publications Inc, New York (1972).
[12] Special Functions of Mathematics for Engineers, Second Edition, L. C. Andrews, Oxford University Press, Oxford (1998).
[13] Methods of Mathematical Physics, Volume 1, Chapter 3, R. Courant and D. Hilbert, Wiley-Interscience, New York (1953).
[14] G. S. Joyce, Phys. Rev. **155**, 478 (1967).
[15] M. Blume, P. Heller, and N. A. Lurie, Phys. Rev. B **11**, 4483 (1975).
[16] O. Ciftja, M. Luban, M. Auslender, and J. H. Luscombe, Phys. Rev. B **60**, 10122 (1999).
[17] P . J. Cregg, J. L. Garcia-Palacios, and P. Svedlindh, J. Phys. A: Math. Theor. **41**, 435202 (2008).
[18] P. A. Martin, J. Phys. A: Math. Theor. **41**, 015207 (2008).
[19] O. Ciftja, Physica B **407**, 2803 (2012).
[20] A. Al-Sharif, M. Hajja, and P. T. Krasopoulos, Results Math. **55**, 231 (2009).
[21] Table of Integrals, Series and Products, I. S. Gradshteyn and I. M. Ryzhik, Fourth Edition, Academic Press, New York (1965).
[22] Integrals and Series, Volume 2, Special Functions, A. P. Prudnikov, Yu. A. Brychkov and O. I. Marichev, Third Printing, Gordon & Breach Science Publishers, New York (1992).
[23] See http://www.wolfram.com/mathematica/
[24] M. L. Glasser and E. Montaldi, J. Math. Anal. and Appl. **183**, 577 (1994).
[25] F. W. J. Olver and L. C. Maximon, Chapter 10: Bessel Functions in NIST Handbook of Mathematical Functions, pages 215-286, Cambridge University Press, New York (2010). http://dlmf.nist.gov/10.