Magnetic properties of a classical XY spin dimer in a "planar" magnetic field

Orion Ciftja^{1,*} and Dode Prenga²

¹*Department of Physics, Prairie View A&M University, Prairie View, Texas 77446, USA*

²*Department of Physics, University of Tirana, Bul. Zog I, Tirana, Albania*

(Dated: April 23, 2016)

Single-molecule magnetism originates from the strong intra-molecular magnetic coupling of a small number of interacting spins. Such spins generally interact very weakly with the neighbouring spins in the other molecules of the compound, therefore, inter-molecular spin couplings are negligible. In certain cases the number of magnetically coupled spins is as small as a dimer, a system that can be considered the smallest nanomagnet capable of storing non-trivial magnetic information on the molecular level. Additional interesting patterns arise if the spin motion is confined to a two-dimensional space. In such a scenario, clusters consisting of spins with large-spin values are particularly attractive since their magnetic interactions can be described well in terms of classical Heisenberg XY spins. In this work we calculate exactly the magnetic properties of a nanomagnetic dimer of classical XY spins in a "planar" external magnetic field. The problem is solved by employing a mathematical approach whose idea is the introduction of auxiliary spin variables into the starting expression of the partition function. Results for the total internal energy, total magnetic moment, spin-spin correlation function and zero-field magnetic susceptibility can serve as a basis to understand the magnetic properties of large-spin dimer building blocks.

PACS numbers: 01.55.+b, 73.43.Cd

Keywords: Molecular magnetism; Heisenberg spins; XY model.

I. INTRODUCTION

Molecular magnets exhibit negligible inter-molecular magnetic interactions when compared to the values of the intra-molecular magnetic couplings present within the individual molecule¹⁻⁶. As a result, the magnetic behavior of the bulk system basically reflects the magnetic properties of a single magnetic molecule^{7,8}. The rather small number of the interacting spins makes these systems amenable to exact theoretical calculations⁹. Depending on the value of the spin, a molecular magnet manifests outstanding properties that tend to become classical for clusters containing spins with large values. Because of the large value of spins it turns out that many magnetic properties of such systems can be reproduced to very high accuracy¹⁰ by using the classical Heisenberg model which treats the spins as unit vectors. The simplest classical Heisenberg model to consider is the one-dimensional (1D) open linear chain model of $N \geq 2$ classical spins in zero magnetic field:

$$H_N = -J \sum_{i=1}^{N-1} \vec{S}_i \vec{S}_{i+1}, \quad (1)$$

where J is an isotropic exchange interaction energy between nearest-neighbouring spins and $\vec{S}_i$ are typically three-dimensional (3D) unit spin vectors. Note that one should not confuse the dimensionality of the lattice (that in this case is 1D) with that of spin vectors. The exact solution of the model in Eq.(1) for zero magnetic field is known for classical spins of an arbitrary dimensionality¹¹. The Hamiltonian in Eq.(1) reduces to an Ising model, classical planar model, and classical Heisenberg model, respectively for dimensionality of spin, $D = 1, 2$ and 3 ¹¹.

If one subjects the system to a nonzero external magnetic field ($\vec{B} \neq 0$), one must amend the Hamiltonian in Eq.(1) by adding a term of the form: $-\vec{B} \sum_{i=1}^N \vec{S}_i$ which results in:

$$H_N(B) = -J \sum_{i=1}^{N-1} \vec{S}_i \vec{S}_{i+1} - \vec{B} \sum_{i=1}^N \vec{S}_i. \quad (2)$$

Application of an external magnetic field to the system leads to formidable challenges for exact calculations. To our knowledge, no classical spin models of the form of Eq.(2) have been solved exactly in analytic form for a nonzero magnetic field. Addition of the field-dependent term in the Hamiltonian leads to nontrivial mathematical analysis and one must resort to numerical methods in order to obtain results for a system with an arbitrary number N of spins¹². Despite the fact that there are no general analytic results possible in a nonzero magnetic field for systems with arbitrary number N (and/or $N \rightarrow \infty$) of spins, one may hope to obtain closed-formed exact expression in a nonzero magnetic field ($\vec{B} \neq 0$) if N is relatively small. The simplest such system would be a dimer system of $N = 2$ classical spins in a nonzero magnetic field. Starting with a dimer system also makes sense since such a system represents an important building block for more complicated spin dimerized structures. Dimer systems under a variety of conditions ranging from classical to quantum regimes have always drawn great interest with the majority of studies treating the spin variables as 3D vectors¹³⁻¹⁷.

However, recent progress in nano-fabrication techniques has made possible the fabrication of ultra-small spin systems where the spin motion is further confined to a two-dimensional (2D) space. In such a case, the

essential physics of spin systems is captured by the classical XY spin model^{18,19}. Within the general framework of the classical XY spin model, the spins occupy the sites of a regular lattice in an arbitrary dimension. Each XY spin, $\vec{S}_i$ is represented as a 2D unit-length vector, $\vec{S}_i = (S_{ix}, S_{iy})$ and is free to point along any direction on the 2D plane. As it turns out, even when dealing with a 1D open linear chain system with an arbitrary number of N classical XY spins, the partition function can be readily evaluated only in zero magnetic field¹². Since the study area of molecular nano-magnetism is relatively new there have been comparatively fewer studies done on low-dimensional 2D classical XY spin systems in a nonzero magnetic field. In this work, we investigate the properties of a dimer system of classical XY spins in presence of a "planar" external magnetic field. It is shown that the exact calculation of various quantities in presence of a "planar" magnetic field is extremely challenging but achievable in closed-form. The exact analytic results obtained are useful not only because there is a scarcity of them, but also because spin dimer systems represent an important building block for various layered magnetic structures and/or spin dimer compounds²⁰⁻²².

II. MODEL AND THEORY

We consider a dimer system of classical XY spins whose interactions are described by a classical Heisenberg Hamiltonian with isotropic exchange interaction energy. The spins are also subject to a uniform "planar" external magnetic field, $\vec{B} = (B, 0)$ where the direction of $\vec{B}$ serves to define the x axis and $B = |\vec{B}| \geq 0$ is the magnitude of the magnetic field. We write the Hamiltonian of the system as:

$$H(B) = -J \vec{S}_1 \vec{S}_2 - \vec{B} \cdot (\vec{S}_1 + \vec{S}_2) . \quad (3)$$

The spins, $\vec{S}_i = (S_{ix}, S_{iy})$ are unit vectors whose orientations are specified by the angle, φ_i measured relative to the x axis (thus, magnetic field). The coupling constant, J can be either ferromagnetic (F), $J = |J| > 0$ or antiferromagnetic (AF), $J = -|J| < 0$. For the model under consideration, the partition function for an arbitrary value of the magnetic field is written as:

$$Z(\beta, B) = \int_0^{2\pi} d\varphi_1 \int_0^{2\pi} d\varphi_2 \exp[-\beta H(B)] , \quad (4)$$

where $\beta = 1/(k_B T)$ is the inverse temperature parameter, k_B is Boltzmann's constant and T is the absolute temperature of the system.

All relevant quantities such as total internal energy, heat capacity, free energy, entropy, total magnetic moment (magnetization), spin-spin correlation function and zero- or nonzero-magnetic field susceptibility can be calculated from the partition function. For example, the

total internal energy of the system is written as:

$$U(\beta, B) = \langle H(B) \rangle = -\frac{\partial}{\partial \beta} \ln Z(\beta, B) , \quad (5)$$

where $\langle \dots \rangle$ represents the canonical ensemble average. Heat capacity can be written as

$$C(\beta, B) = \frac{\partial U(\beta, B)}{\partial T} = -k_B \beta^2 \frac{\partial U(\beta, B)}{\partial \beta} , \quad (6)$$

while free energy and entropy are, respectively written as $F(\beta, B) = -\ln Z(\beta, B)/\beta$ and $S(\beta, B) = -\frac{\partial F(\beta, B)}{\partial T} = -k_B \beta^2 \frac{\partial F(\beta, B)}{\partial \beta}$.

With a similar logic, if one defines, $\vec{M} = \vec{S}_1 + \vec{S}_2$, then the total magnetic moment induced by the magnetic field at an arbitrary temperature will be given by:

$$\langle M_x \rangle(\beta, B) = \frac{1}{\beta} \frac{\partial}{\partial B} \ln Z(\beta, B) . \quad (7)$$

The spin-spin correlation function for arbitrary values of the magnetic field and arbitrary temperature is calculated from:

$$\langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B) = \frac{1}{\beta} \frac{\partial}{\partial J} \ln Z(\beta, B) . \quad (8)$$

If quite generally one defines the total magnetization vector as $\vec{M} = \sum_{i=1}^N \vec{S}_i$, then the N -spin zero-field magnetic susceptibility of the system is calculated from:

$$\chi_N(\beta, B=0) = \lim_{B \rightarrow 0} \frac{\partial}{\partial B} \langle M_x \rangle(\beta, B) . \quad (9)$$

An equivalent definition of $\chi_N(\beta, B)$ is also provided by the fluctuation-dissipation relation:

$$\chi_N(\beta, B) = \beta \sum_{i=1}^N \sum_{j=1}^N \left[\langle S_{ix} S_{jx} \rangle(\beta, B) - \langle S_{ix} \rangle(\beta, B) \langle S_{jx} \rangle(\beta, B) \right] . \quad (10)$$

In the zero-field limit, we have $\langle S_{ix} S_{jx} \rangle(\beta, B=0) = (1/2) \langle \vec{S}_i \vec{S}_j \rangle(\beta, B=0)$ (in 2D) and $\langle S_{ix} \rangle(\beta, B=0) = 0$. So the zero-field susceptibility per spin may be written as:

$$\frac{\chi_N(\beta, B=0)}{N} = \frac{\beta}{2} \tilde{\chi}_N(\beta) , \quad (11)$$

where

$$\tilde{\chi}_N(\beta) = 1 + \frac{2}{N} \sum_{i < j} \langle \vec{S}_i \vec{S}_j \rangle(\beta, B=0) , \quad (12)$$

represents a reduced zero-field susceptibility. In the absence of a magnetic field, all spin-spin correlation functions, $\langle \vec{S}_i \vec{S}_j \rangle(\beta, B=0)$ vanish in the high-temperature limit ($\beta \rightarrow 0$) for $i < j$. As a result, one can verify that the expression in Eq.(11) correctly reduces to Curie's law in such a limit. For the present case ($N = 2$), we have:

$$\tilde{\chi}_2(\beta) = 1 + \langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B=0) , \quad (13)$$

a quantity that can be calculated with help from Eq.(8).

III. PARTITION FUNCTION

The exact calculation of the partition function is facilitated if one notes that the Hamiltonian of the system may be rewritten solely in terms of the total spin vector, $\vec{S} = \sum_{i=1}^{N=2} \vec{S}_i$ as:

$$H(B) = -\frac{J}{2} (S^2 - 2) - \vec{B} \cdot \vec{S}. \quad (14)$$

The next step is to multiply the integral in Eq.(4) by:

$$1 = \int d^2 S \int \frac{d^2 k}{(2\pi)^2} \exp \left[i \vec{k} \cdot \left(\vec{S} - \sum_{i=1}^{N=2} \vec{S}_i \right) \right], \quad (15)$$

$$Z(\beta, B) = (2\pi)^2 \int d^2 S \exp \left[\frac{\beta J}{2} (S^2 - 2) + \beta \vec{B} \cdot \vec{S} \right] \int \frac{d^2 k}{(2\pi)^2} \exp \left(i \vec{k} \cdot \vec{S} \right) [J_0(k)]^2, \quad (16)$$

where $J_0(x)$ is a zero-th order Bessel function of the first kind. Integration over the angular variables appearing in

where we used a standard expression for the D -dimensional Dirac delta function^{23,24}. Although we are now faced with a seemingly more complicated multi-dimensional integral, the subsequent calculations are straightforward:

Eq.(16) is simple and one immediately obtains:

$$Z(\beta, B) = (2\pi)^2 \int dS S \exp \left[\frac{\beta J}{2} (S^2 - 2) \right] I_0(\beta B S) \int_0^\infty dk k J_0(k S) [J_0(k)]^2, \quad (17)$$

where $I_0(x)$ is a zero-th order modified Bessel function of the first kind. Integration over the variable, k gives:

$$\int_0^\infty dk k J_0(k S) [J_0(k)]^2 = \frac{2}{\pi} \frac{1}{S \sqrt{4 - S^2}}; \quad 0 \leq S \leq 2. \quad (18)$$

One can clearly see from the expression obtained in Eq.(18) that nonzero contributions to the integral come only for values, $0 \leq S \leq 2$. The final expression of the partition function may be conveniently written in 1D integral form as:

$$Z(\beta, B) = (8\pi) \exp(-\beta J) \int_0^2 dS \exp \left(\frac{\beta J}{2} S^2 \right) \frac{I_0(\beta B S)}{\sqrt{4 - S^2}} \quad (19)$$

For zero magnetic field ($B=0$), one has:

$$Z(\beta, B=0) = (2\pi)^2 I_0(\beta J). \quad (20)$$

Calculation of total internal energy, total magnetization, spin-spin correlation function, magnetic susceptibility, etc, follows from the partition function.

IV. ENERGY, MAGNETIZATION AND SPIN-SPIN CORRELATION FUNCTION AT ZERO TEMPERATURE

Before listing the general results, let's consider the special case when the system is subject to an arbitrary value of the magnetic field, $\vec{B}$ at absolute zero temperature, $T = 0$ K (for such a case, $\beta = \infty$). Total energy is minimized when the total spin vector $\vec{S}$ is parallel to the external magnetic field $\vec{B}$. In this case, the Hamiltonian in Eq.(14) is written as a function of the total spin as: $H(B) = -\frac{J}{2} (S^2 - 2) - B S$. For a given arbitrary value, $B \geq 0$, the ground state configuration of the spins depends on the sign of J (namely, whether the coupling is F or AF) as well as magnitude of B relative to $|J|$. Below we list separately some results that apply to F and AF coupling cases.

A. Ferromagnetic coupling

For F coupling ($J = |J| > 0$), the ground state energy of the system is:

$$E_F(B) = -|J| - 2B. \quad (21)$$

FIG. 1: Total internal energy, $U(\beta, B)$ in units of $|J|$ as a function of the magnetic field parameter, $\frac{B}{|J|}$ for a dimer system of classical XY spins with F (solid line) and AF (dashed line) exchange interaction. The value of the temperature parameter is $\beta|J| = 1$. Note that B is the magnitude of the "planar" magnetic field in the x direction, $\beta = \frac{1}{k_B T}$ is the inverse temperature parameter and T is the absolute temperature.

The total magnetization is:

$$\langle M_x \rangle(\beta = \infty, B) = 2. \quad (22)$$

The spin-spin correlation function is:

$$\langle \vec{S}_1 \vec{S}_2 \rangle(\beta = \infty, B) = +1. \quad (23)$$

B. Antiferromagnetic coupling

On the other hand, the corresponding quantities for AF coupling ($J = -|J| < 0$) are:

$$E_{AF}(B) = \begin{cases} -|J| - \frac{1}{2} \frac{B^2}{|J|}; & 0 \leq \frac{B}{|J|} \leq 2 \\ +|J| - 2B; & 2 \leq \frac{B}{|J|} < \infty \end{cases} \quad (24)$$

$$\langle M_x \rangle(\beta = \infty, B) = \begin{cases} \frac{B}{|J|}; & 0 \leq \frac{B}{|J|} \leq 2 \\ 2; & 2 \leq \frac{B}{|J|} < \infty, \end{cases} \quad (25)$$

and

$$\langle \vec{S}_1 \vec{S}_2 \rangle(\beta = \infty, B) = \begin{cases} -1 + \frac{1}{2} \left(\frac{B}{|J|} \right)^2; & 0 \leq \frac{B}{|J|} \leq 2 \\ +1; & 2 \leq \frac{B}{|J|} < \infty. \end{cases} \quad (26)$$

V. GENERAL RESULTS

The total internal energy of the dimer system of classical XY spins at an arbitrary temperature and magnetic field is calculated from Eq.(5) and can be written as:

$$U(\beta, B) = J - \frac{J}{2} \frac{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_0(\beta B S)}{\sqrt{4-S^2}} S^2}{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_0(\beta B S)}{\sqrt{4-S^2}}} - B \frac{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_1(\beta B S)}{\sqrt{4-S^2}} S}{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_0(\beta B S)}{\sqrt{4-S^2}}}. \quad (27)$$

Other quantities such as heat capacity, entropy or free energy can be calculated similarly. In Figure 1 we show the total internal energy of the dimer system in units of $|J|$ as function of $B/|J|$ at a temperature corresponding to $\beta|J| = 1$. Temperatures are measured by the dimensionless parameter, $\beta|J|$, where $\beta = 1/(k_B T)$. The behavior of $U(\beta, B)$ for both F and AF exchange interaction at this temperature seems to follow the general pattern seen at $T = 0$. For example, the behavior of $U(\beta, B)$ for $B/|J| \geq 2$ closely reflects that seen at $T = 0$ where $E_{AF}(B) - E_F(B) = 2|J|$ for $B/|J| \geq 2$.

The total magnetic moment induced by the magnetic field is calculated from Eq.(7) and one finds:

$$\langle M_x \rangle(\beta, B) = \frac{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_1(\beta B S)}{\sqrt{4-S^2}} S}{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_0(\beta B S)}{\sqrt{4-S^2}}}. \quad (28)$$

Figure 2 shows the total magnetic moment induced by the magnetic field for the dimer system of classical XY spins as function of $B/|J|$ for the case of F exchange interaction between spins at various temperatures. The same quantities are plotted in Figure 3 for the case of an AF coupling between spins. As expected, the total magnetization of the system is zero at any given finite

FIG. 2: Total magnetic moment, $\langle M_x \rangle(\beta, B)$ as a function of the magnetic field parameter, $\frac{B}{|J|}$ for a dimer system of classical XY spins with F exchange interaction. The values of $\beta|J|$ range from 10 (low temperature ; solid line) to 0.2 (high temperature ; dotted line). Note that B is the magnitude of the "planar" magnetic field in the x direction, $\beta = \frac{1}{k_B T}$ is the inverse temperature parameter and T is the absolute temperature.

FIG. 3: Total magnetic moment, $\langle M_x \rangle(\beta, B)$ as a function of the magnetic field parameter, $\frac{B}{|J|}$ for a dimer system of classical XY spins with AF exchange interaction. The values of $\beta|J|$ range from 10 (low temperature ; solid line) to 0.2 (high temperature ; dotted line). Note that B is the magnitude of the "planar" magnetic field in the x direction, $\beta = \frac{1}{k_B T}$ is the inverse temperature parameter and T is the absolute temperature.

temperature ($\beta|J| \neq \infty$) in absence of a magnetic field (when $B = 0$). The spin-spin correlation function is calculated from Eq.(8) resulting in the following expres-

FIG. 4: Spin-spin correlation function, $\langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B)$ for a dimer system of classical XY spins with F exchange interaction as a function of the magnetic field parameter, $\frac{B}{|J|}$ for values of $\beta|J| = 10$ (solid line), 1 (dashed line) and 0.2 (dotted line). The dimensionless parameter $\beta|J| = |J|/(k_B T)$ measures the absolute temperature of the system.

FIG. 5: Spin-spin correlation function, $\langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B)$ for a dimer system of classical XY spins with AF exchange interaction as a function of the magnetic field parameter, $\frac{B}{|J|}$ for values of $\beta|J| = 10$ (solid line), 1 (dashed line) and 0.2 (dotted line). The dimensionless parameter $\beta|J| = |J|/(k_B T)$ measures the absolute temperature of the system.

sion:

$$\langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B) = -1 + \frac{1}{2} \frac{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_0(\beta B S)}{\sqrt{4-S^2}} S^2}{\int_0^2 dS \exp\left(\frac{\beta J}{2} S^2\right) \frac{I_0(\beta B S)}{\sqrt{4-S^2}}} . \quad (29)$$

In Figure 4 we show the spin-spin correlation function, $\langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B)$ for a dimer system of classical XY spins

FIG. 6: Reduced zero-field susceptibility per spin, $\tilde{\chi}_2(\beta)$ for a dimer system of classical XY spins as a function of the dimensionless temperature parameter, $\beta|J|$ for the case of F exchange interaction (solid line) and AF exchange interaction (dashed line).

with F exchange interaction as a function of the magnetic field, $B/|J|$ for several values of $\beta|J|$ ranging from a low temperature ($\beta|J| = 10$) to a high temperature value ($\beta|J| = 0.2$). The same quantity, but for AF coupling between spins, is shown in Figure 5.

Note that at $B = 0$, the pair of AF-coupled spins can be pictured as tending to orient anti-parallel to each other, $\langle \vec{S}_1 \vec{S}_2 \rangle(\beta, B = 0) \approx -1$ at low temperature (the case of $\beta|J| = 10$). This order is modified as the magnetic field is applied. For instance, in the case of $\beta|J| = 10$, one clearly sees how the spin-spin correlation function gradually increases from approximately -1 to approximately $+1$ as the magnetic field increases. For large magnetic field values (theoretically, for values of $B/|J| \geq 2$ at $T = 0$) the spins tend to orient parallel to each other. In Figure 6 we show the reduced zero-field susceptibility per spin, $\tilde{\chi}_2(\beta)$ for a dimer system of classical XY spins as a function of the dimensionless temperature parameter, $\beta|J|$ for F and AF coupling between spins.

VI. CONCLUSION

To conclude, we calculated exactly the magnetic properties of a dimer system of classical XY spins in a "planar" external magnetic field. The partition function, total internal energy, total magnetic moment, spin-spin correlation function and other related quantities were obtained as closed-form 1D integral expressions that depend only on the total spin variable. Despite its simple appearance, this model hints to the difficulties faced when dealing with exact calculations of interacting spin sys-

tems in an external magnetic field. The exact calculation of the partition function even for a 1D open linear chain of classical XY spins in an external magnetic field is yet to be achieved analytically and the current work serves as a good illustration of the challenges faced in this direction. Not totally surprisingly, we found out that the calculation of the partition function even for the case of a dimer system of classical XY spins in a nonzero magnetic field seems to defy a more explicit analytical expression than the one provided by Eq.(19). As easily deduced, the case of AF coupling between spins is more interesting than that of F coupling in presence of a "planar" external magnetic field. Differently from the F case, alignment of the AF-coupled individual spins with the external magnetic field at $T = 0$ occurs only for values of the magnetic field that are larger or equal than a critical one. Other small clusters of N classical XY spins described by an Hamiltonian of the form: $-J \sum_{i<j}^N \vec{S}_i \vec{S}_j - \vec{B} \sum_{i=1}^N \vec{S}_i$ can be solved by applying the same solution method (using $\vec{S} = \sum_i^N \vec{S}_i$ as an auxiliary variable) and we expect them to manifest qualitatively similar patterns. Overall, the behaviour characterized in this study can be helpful on understanding the magnetic properties of various layered compounds that have built-in spin dimers as building blocks²⁵. The results obtained also provide useful benchmarks to gauge the accuracy of various numerical methods used in studies of classical XY spin systems of this nature and can be related to phenomena dealing with small molecular dimerized clusters featuring high-spin magnetic ions.

For instance, an important numerical method widely used in numerical studies is the Monte Carlo method²⁶. Within the framework of this method, one has a way to sample the configuration integral (that represents the canonical ensemble average of a desired quantity):

$$\langle O \rangle = \frac{\int d\Gamma O \exp \left[-\beta H(\{\vec{S}_i\}) \right]}{\int d\Gamma \exp \left[-\beta H(\{\vec{S}_i\}) \right]}, \quad (30)$$

where $d\Gamma = \prod_{i=1}^N d\vec{S}_i$ is the integral element for N spin variables, $H(\{\vec{S}_i\})$ is a N -spin classical Hamiltonian and O is a given dynamical variable (such as total magnetization, energy, etc.) that depends on the N -spin variables. If one can generate states of the system with a probability given by the canonical probability density, $p(\{\vec{S}_i\}) = \frac{\exp[-\beta H(\{\vec{S}_i\})]}{\int d\Gamma \exp[-\beta H(\{\vec{S}_i\})]}$, one estimates the canonical ensemble average as:

$$\langle O \rangle \approx \frac{1}{N_c} \sum_{n=1}^{N_c} O(n), \quad (31)$$

where $O(n)$ is the value of the dynamical variable O in the n -th state and N_c ($\rightarrow \infty$) represents the number of spin configurations considered in the averaging process. In practice, one starts with a system of spins in a given spin configuration. Each spin is then in turn rotated by

FIG. 7: Total magnetic moment, $\langle M_x \rangle(\beta, B)$ as a function of the magnetic field parameter, $\frac{B}{|J|}$ for a dimer system of classical XY spins with F exchange interaction at a temperature corresponding to $\beta |J| = 0.5$. Numerical data obtained from a Monte Carlo simulation (solid circles) with a small number of spin configurations are compared to the exact analytic result (solid line). The statistical uncertainty of the Monte Carlo simulations is of the order of the size of solid circles.

a random angle and the change in total energy, ΔE , is calculated. If one adopts one commonly used algorithm such as the Metropolis algorithm, the new configuration is accepted with probability 1 if $\Delta E < 0$ and accepted

with probability $\exp(-\beta \Delta E)$ if $\Delta E > 0$. This process is repeated for a chosen number of configurations, N_c depending on the available computer time. The convergence of $\langle O \rangle$ to its limiting value as $N_c \rightarrow \infty$ is typically of the order $\propto 1/\sqrt{N_c}$, thus, larger the N_c , better it is. Despite its technical difficulties, one of the advantages of the Monte Carlo method is that it can be used to treat arbitrarily large systems (that cannot be solved analytically). Availability of exact analytic results is very useful at this juncture. Exact results can help one gauge the accuracy of numerical methods such as the Monte Carlo technique. This idea is illustrated in Figure 7 where we display the Monte Carlo values of the total magnetization of a dimer system of classical XY spins with F exchange interaction obtained numerically using a small number of few thousand spin configurations. The numerically obtained Monte Carlo values are then compared the exact analytic result. One notes that, despite the small number of spin configurations used in the simulation, the Monte Carlo results have a satisfactory accuracy for small magnetic fields. However, the results suggest that one must a better numerical work (increase the number of spin configurations used in the sampling of the average) to obtain the corresponding values of the total magnetization at higher magnetic fields where variation of magnetization as function of the magnetic field is not pronounced.

Acknowledgments

This research was supported in part by US Army Research Office (ARO) grant no. W911NF-13-1-0139 and National Science Foundation (NSF) grant DMR-1410350.

-
- * Electronic address: ogciftja@pvamu.edu
- ¹ *Nanomagnetism*, (NATO Asi Series E: Applied Sciences, Vol. 247) edited by A. Hernando (Kluwer Academic, Dordrecht, 1993).
 - ² O. Kahn, *Molecular Magnetism*, (Wiley-VCH, New York, 1993).
 - ³ K. L. Taft, C. D. Delfs, G. C. Papaefthymiou, S. Foner, D. Gatteschi, and S. J. Lippard, *J. Am. Chem. Soc.* **116**, 823 (1994).
 - ⁴ 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).
 - ⁵ O. Ciftja, *J. Phys. A: Math. Gen.* **34**, 1611 (2001).
 - ⁶ R. R. Chrichton, *Inorganic Biochemistry of Iron Metabolism* (Horwood, New York, 1991).
 - ⁷ A. Bino, D. C. Johnston, D. P. Goshorn, T. R. Halbert, and E. I. Stiefel, *Science* **241**, 1479 (1988).
 - ⁸ A. Lascialfari, D. Gatteschi, F. Borsa, and A. Cornia, *Phys. Rev. B* **55**, 14341 (1997).
 - ⁹ O. Ciftja, *Physica A* **286**, 541 (2000).
 - ¹⁰ J. Luscombe, M. Luban, and F. Borsa, *J. Chem. Phys.* **108**, 7266 (1998).
 - ¹¹ H. E. Stanley, *Phys. Rev.* **179**, 570 (1969).
 - ¹² M. Blume, P. Heller, and N. A. Lurie, *Phys. Rev. B* **11**, 4483 (1975).
 - ¹³ D. Mentrup, J. Schnack, and M. Luban, *Physica A* **272**, 153 (1999).
 - ¹⁴ M.-H. Whangbo, D. Dai, and H.-J. A. Koo, *Solid State Sci. B* **7**, 827 (2005).
 - ¹⁵ D. O. Soares-Pinto, A. M. Souza, R. S. Sarthour, I. S. Oliveira, M. S. Reis, P. Brandão, J. Rocha, and A. M. Dos Santos, *Europhys. Lett.* **87**, 40008 (2009).
 - ¹⁶ A. Furrer, *J. Phys.: Conf. Ser.* **325**, 012001 (2011).
 - ¹⁷ L. M. Perez, O. J. Suarez, D. Laroze, and H. L. Mancini, *Cent. Eur. J. Phys.* **11**(12), 1629 (2013).
 - ¹⁸ H. E. Stanley, *Introduction to phase transitions and critical phenomena*, Oxford University Press, NY (1971).
 - ¹⁹ D. C. Mattis, *Phys. Lett.* **104A**, 357 (1984).
 - ²⁰ E. C. Samulon, K. A. Al-Hassanieh, Y. -J. Jo, M. C. Shapiro, L. Balicas, C. D. Batista, and I. R. Fisher, *Phys. Rev. B* **81**, 104421 (2010).
 - ²¹ E. C. Samulon PhD thesis (Stanford University), 2011 "Magnetic phases of the frustrated spin dimer compounds $Ba_3Mn_2O_8$ " available on line at <http://purl.stanford.edu/qh243cb9446>
 - ²² D. V. Dmitriev and V. Ya. Krivnov, *Phys. Rev. B* **86**, 134407 (2012).
 - ²³ O. Ciftja, M. Luban, M. Auslender, and J. H. Luscombe, *Phys. Rev. B* **60**, 10122 (1999).
 - ²⁴ O. Ciftja, *Nanoscale Res. Lett.* **2**, 168 (2007).

- ²⁵ S. Haravifard, A. Banerjee, J. van Wezel, D. M. Silevitch, A. M. dos Santos, J. C. Lang, E. Kermarrec, G. Srajer, B. D. Gaulin, J. J. Molaison, H. A. Dabkowska, and T. F. Rosenbaum, Proc. Nat. Acad. Sciences **111**, 14372 (2014).
- ²⁶ K. Binder, *Monte Carlo Methods in Statistical Mechanics*, 2nd Ed. Springer-Verlag, Berlin (1986).