



Dynamic properties of a classical anisotropic Heisenberg chain under external magnetic field

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Abstract

We investigate the dynamic properties of a classical anisotropic Heisenberg chain interacting with an external magnetic field at different temperatures. Properties such as time-dependent energy autocorrelation and space–time spin–spin correlation are obtained by solving the dynamic equation $\dot{\mathbf{S}}_i = \mathbf{S}_i \times \nabla_{\mathbf{S}_i} \mathcal{H}$. While the static spin–spin correlation length decreases as the system is heated up, it increases when an external magnetic field is present. The time-dependent spin–spin correlation decreases when the system is heated up, resulting in a decrease of the spin-diffusion speed. The presence of the magnetic field contributes to the order, and therefore produces an increase of the spin-diffusion speed. In contrast, the single-ion type anisotropy behaves dynamically as a local field, inducing disorder in the chain.

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1. Introduction

Since the discovery and fabrication of molecular magnets composed by a small number of particles, there has been a renewed and growing interest in

low-dimensional magnetism [1]. In fact, nowadays a wide number of molecular clusters containing relatively a small number of magnetic ions can be synthesized. In these structures, for example, the magnetic moments can be symmetrically positioned in a simple ring, forming a unidimensional ring-shaped magnetic structure [2–4]. It appears that in most cases the magnetic properties of these molecules are rather well described by the Heisenberg model with possibly small anisotropy corrections [5,6]. From a theoretical point of view, these

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models are not only able to explain the measured properties, but also provide some general understanding of higher-dimensional magnetic systems.

In addition to those new molecular magnets, there are several systems which are well represented by the one-dimensional Heisenberg model within some range of temperature [7]. For instance, the system CsNiF_3 can be modeled by a ferromagnetic Heisenberg chain with easy-plane anisotropy for a temperature $T > 4.4$ K and spin $S = 1$. Also, the compound tetramethyl ammonium manganese trichloride (TMMC) is well represented by an antiferromagnetic Heisenberg chain for temperatures above 1.3 K. Notice that although one-dimensional magnetic systems have in general a low-spin number S , and therefore should be treated as quantum systems, the classical approximation (i.e. $S \rightarrow \infty$) is a good approximation in some cases [8].

Thermodynamical properties of one-dimensional magnetic systems have been widely studied from a theoretical point of view. In the classical limit, analytical results exist when the number of spins tend to infinity, such as the one by Fisher [9] and Parsons [10] for the isotropic Heisenberg model. Other results include the case of the Heisenberg chain under external magnetic field by Blume et al. [11], and with anisotropy by Loveluck et al. [12]. When the analytical procedure is not possible (for example, in a system with a finite number of spins) the preferred technique has been the Monte Carlo (MC) method [13].

Dynamical properties of classical Heisenberg chains have been studied both analytically and numerically [7,14]. The main interest in these studies is the understanding of diverse dynamical phenomena, such as spin waves and spin diffusion processes, as well as inelastic neutron scattering and spin-lattice dynamics. An important quantity which allows to study such properties is the time-dependent correlation function at different temperatures. From a theoretical point of view, the spin dynamics method, based on the numerical solution of a Landau–Lifshitz-like equation, has been proved to be very useful in the study of these problems [15–18].

In this paper we are interested in the dynamic spin–spin correlations and their dependence on the

anisotropy and magnetic field intensity, for several different temperatures. We use a numerical procedure which combines MC and spin dynamics simulation. A description of the model and details of the computational procedures are given in Section 2. The results of the simulation are presented in Section 3 and the conclusions are drawn in Section 4.

2. Model and method

Our starting point is the classical one-dimensional Heisenberg model with nearest-neighbor interaction, planar anisotropy and external magnetic field, as described by the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^N \mathbf{S}_i \mathbf{S}_{i+1} + D \sum_{i=1}^N (S_i^z)^2 - h \sum_{i=1}^N S_i^x, \quad (1)$$

where the \mathbf{S}_i are three-dimensional classical vectors of unit length and N is the number of spins. The (ferromagnetic) exchange-coupling constant is $J > 0$, the (easy-plane) single ion anisotropy is represented by $D > 0$, and $h = g\mu_B H$ is an external magnetic field in the x direction. All calculations were done on systems with up to $N = 1000$ spins, with periodic boundary conditions. The value of J is taken to be 1 and the relevant parameters of the model are D and h . A sketch of the system is displayed in Fig. 1.

Spin dynamics is studied by solving a Landau–Lifshitz-like equation [7], $\dot{\mathbf{S}}_i = \mathbf{S}_i \times \nabla_{\mathbf{S}_i} \mathcal{H}$, obtained from the classical limit of the quantum dynamic equation $i\hbar \dot{\mathbf{S}}_i = [\mathbf{S}_i, \mathcal{H}]$. For our model this equation takes the form

$$\dot{\mathbf{S}}_i = \mathbf{S}_i \times [J(\mathbf{S}_{i+1} + \mathbf{S}_{i-1}) + 2DS_i^z \hat{z} - h\hat{x}], \quad (2)$$

which is a set of coupled first-order-differential equations. Here \hat{z} and \hat{x} are the unit vectors in the z and x directions, respectively. These equations are solved using the fourth-order Runge–Kutta method, and the total integration time was $1000\Delta t$ (time unit and integration step are explicated below). As initial condition we choose a single array of spins generated by standard Metropolis Monte Carlo method [13] corresponding to a particular set of parameters and temperature.

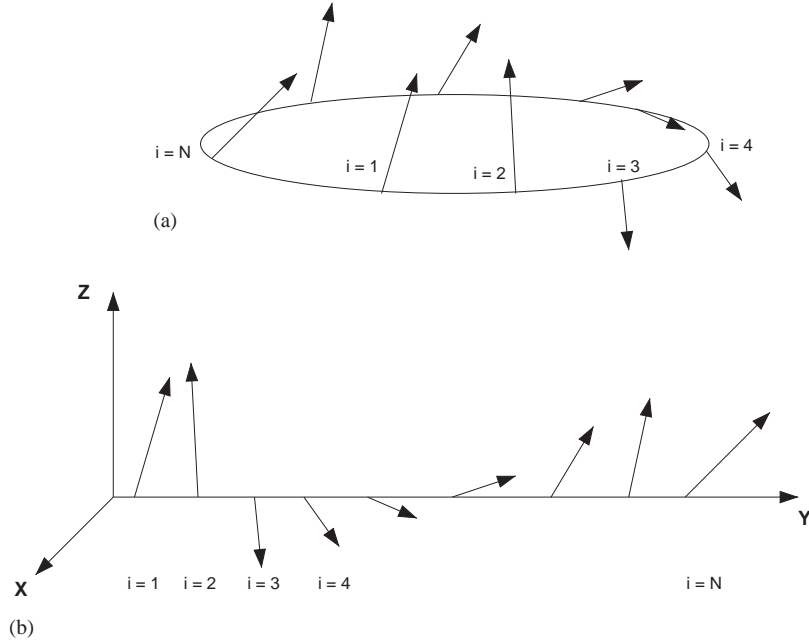


Fig. 1. (a) The actual system, represented as a closed chain due to its periodic boundary conditions. (b) The equivalent system in its reference frame, with the chain laying along the y -axis.

From the time evolution of these arrays of spins, time-correlation functions are calculated, and therefore the dynamical properties can be obtained.

3. Results

The results we present are given in dimensionless units corresponding to the values of the system CsNiF_3 , which is taken for reference purposes. Hence, the temperature is measured in terms of $J/k_B = 18 \text{ K}$, the energy in units of $J = 1.551 \text{ meV}$, and the time unit is $\tau = \hbar/J = 0.424 \text{ ps}$. The typical value for the anisotropy is $D = 0.33J$ and for the magnetic field is $h = 0.1J$, and the time step used to integrate Eq. (2) is $\Delta t = 0.01\tau$.

The most useful quantity concerning dynamic properties is the spin–spin time-dependent correlation function. This kind of correlation functions give information about the behavior of the system in time. For example, Fig. 2 shows the space–time

energy autocorrelation function, computed

$$C_e(r, t) = \left\langle \frac{1}{N} \sum_i \frac{E_i(0)E_{i+r}(t)}{E_i(0)^2} \right\rangle \quad (3)$$

for three different temperatures. It can be seen that the energy of a given site fluctuates in time for all three cases. This can be explained by analyzing the dynamic Equation (2). In the isotropic case ($D = h = 0$), these fluctuations are associated to the spin rotation of the site due to misalignments with its nearest neighbors. The size of these fluctuations increases with temperature.

We can gain further insight into the nature of dynamic properties by means of the space–time spin–spin correlation function $C_s(r, t)$ defined as

$$C_s(r, t) = \left\langle \frac{1}{N} \sum_i \mathbf{S}_i(0)\mathbf{S}_{i+r}(t) \right\rangle, \quad (4)$$

where r denotes the spin sites. This is equivalent to the van Hove correlation function used in the case of a particle system.

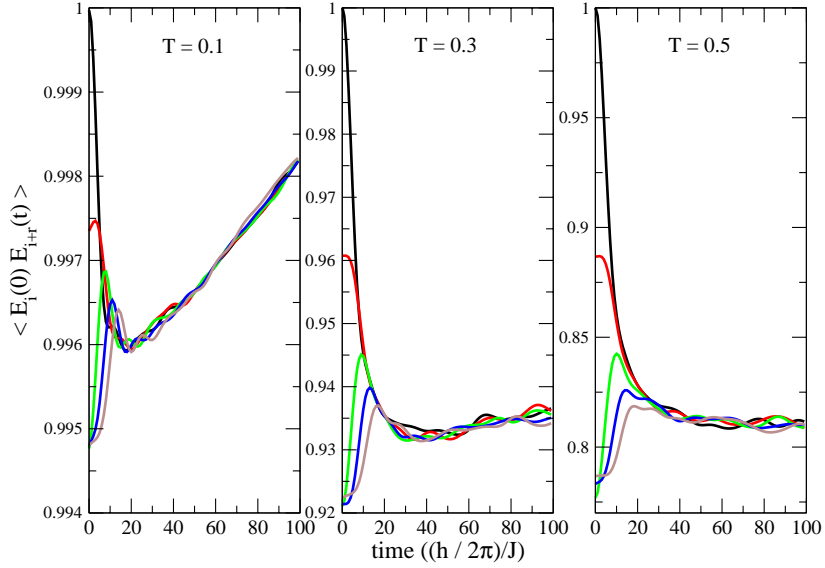


Fig. 2. Space–time energy autocorrelation function for three different temperatures and $D = h = 0$. The curves represent, from top to bottom, the correlation between sites $r = 0, 1, 2, 3$ and 4 , respectively.

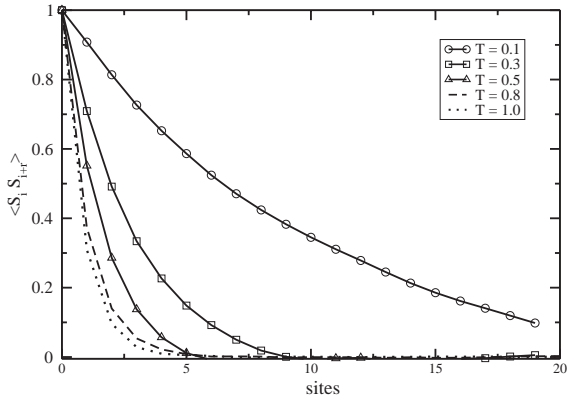


Fig. 3. Spatial dependence of the spin–spin correlation function for the isotropic case ($D = h = 0$), at five different temperatures.

Interestingly, the evaluation of Eq. (4) at $t = 0$ leads to the spatial spin–spin correlation, $C_s(r)$, computed as $C_s(r) = \langle (\sum_i S_i(0) S_{i+r}(0)) / N \rangle$. It is well known [19] that this correlation function decays exponentially with distance,

$$C(r) \propto e^{-r/\xi}, \quad (5)$$

where ξ is the so called *correlation length*, which measures the range of the magnetic order. Fig. 3 shows the results for the isotropic case. It can be seen that each spin–spin correlation curve in Fig. 3 follows approximately an exponential decay, like Eq. (5), with a particular value of ξ . Thus, in general, the correlation length ξ depends on the temperature, decreasing when the temperature increases. For the isotropic case with $N \rightarrow \infty$ the result can be obtained analytically [9], given by $\xi = -(\ln(\coth(1/T) - T))^{-1}$.

3.1. Static spin–spin correlations

Fig. 4 shows the spatial dependence of the spin–spin correlation with applied magnetic field for the x (parallel to the magnetic field) and yz (perpendicular to the magnetic field) components of \mathbf{S} . In the former case, the applied magnetic field increases the ordering range due to its global behavior, correlating spins between distant sites. However, the decay of the spin–spin correlation function is slower than an exponential and therefore expression (5) with the definition of ξ is no longer valid. In contrast, the correlations in the yz

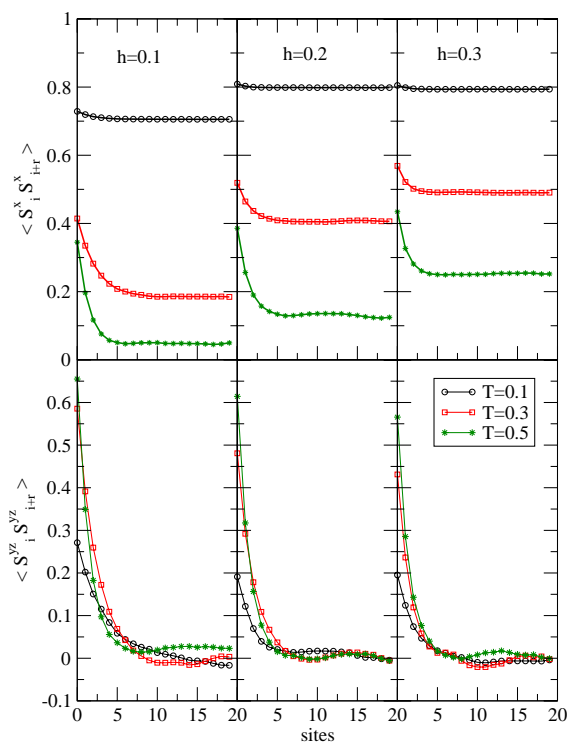


Fig. 4. Spatial dependence of the spin–spin correlation function for zero planar anisotropy, three different temperatures and three values of the applied magnetic field h .

plane are not affected by the presence of the magnetic field, presenting a behavior which looks similar to the one seen in the isotropic case.

Fig. 5 shows the results obtained for the anisotropic case with $D = 0.1, 0.2$ and 0.3 , at three different temperatures. Although anisotropy drives the spins to be aligned in the xy plane, we can see that the higher the anisotropy, the lower the spin–spin correlation length for the xy components. In the case of the z component, the decay is faster than the former case, presenting a change of sign, which means that the S_z component after ~ 5 sites points in the opposite direction. Spin–spin correlation decreases in both xy and z components that indicates a loss of the magnetic order in the chain, due to the local behavior of the single-ion type anisotropy. Thus, the emerging picture is that the anisotropy induces

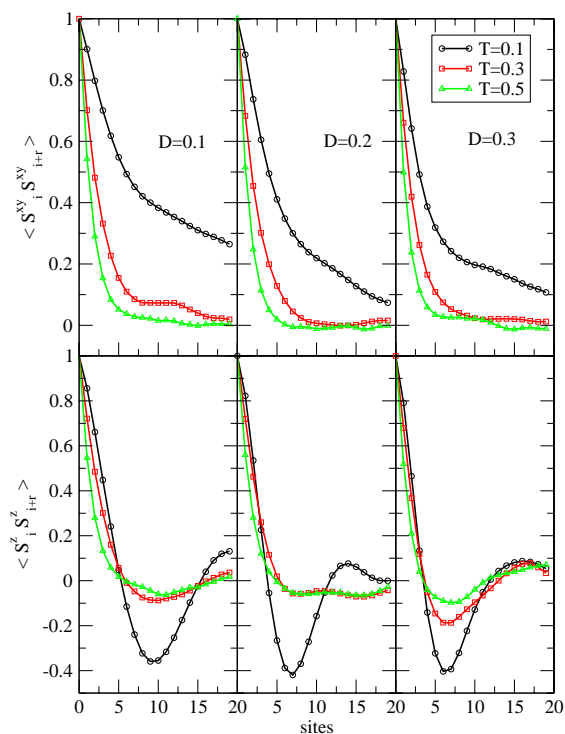


Fig. 5. Spatial dependence of the spin–spin correlation function for zero applied magnetic field, three different temperatures and three values of the planar anisotropy D .

disorder in the chain. The temperature enhances this behavior.

3.2. Dynamic spin–spin correlations

The space–time spin–spin correlation function for the isotropic case is shown in Fig. 6. The correlation function decays with distance just like the static one, and also decays in time in an oscillating way. From the position of the first maximum for each site ($r=0, r=1$ and so on) we can conclude that the spin value of any given site propagates to its neighbors with constant speed, decreasing when the temperature increases. This is a dynamic expression of the fact that temperature induces disorder in the chain.

The results for space–time spin–spin correlation function for anisotropy $D \neq 0$ and applied

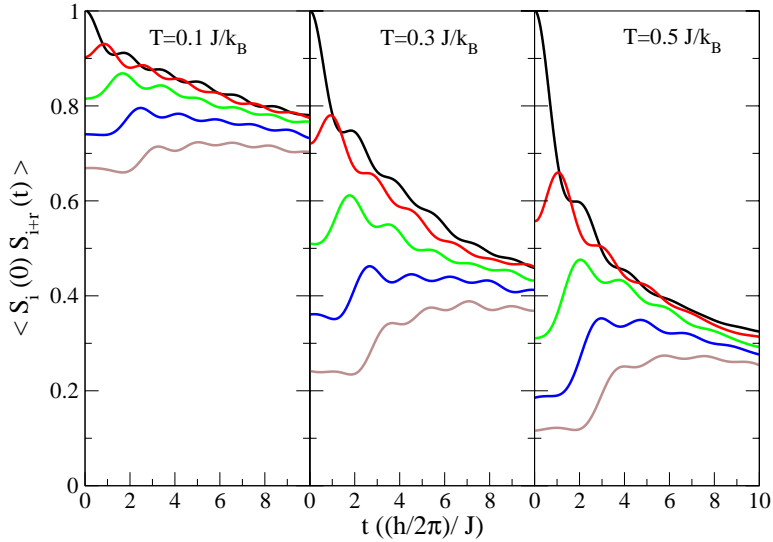


Fig. 6. Spin–spin correlation function for the system at three different temperatures and $D = h = 0$. The curves represent, from top to bottom, the correlation between sites $r = 0, 1, 2, 3$ and 4 , respectively.

magnetic field $h \neq 0$ are displayed in Fig. 7(a) for temperature $T = 0.1$, in Fig. 7(b) for $T = 0.3$ and in Fig. 7(c) for $T = 0.5$.

At low temperatures (Fig. 7(a)) the effects of the external magnetic field and anisotropy can be seen clearly. We can observe that the external magnetic field has almost no influence on the spin diffusion speed, but as a global effect it contributes to correlate the system, increasing the correlation in space and in time. Increasing the magnetic field causes the system to reach a site-independent state of correlation faster, in which the curves for different values of r converge, and only decay in time. In contrast, the anisotropy D makes the spins become spatially decorrelated, decreasing the time-dependent spin–spin correlation function. If we increase the anisotropy, the differences between the spins at different sites at long times increase, reaching a highly site-dependent, but time-independent state of correlation. Thus the anisotropy, unlike the magnetic field, behaves dynamically as a local field, inducing disorder in the chain.

At intermediate and high temperatures (Fig. 7(b) and (c)) the effects of both the external

magnetic field and the anisotropy are qualitatively the same. However, they weakly affect the time-dependent spin–spin correlation, which is dominated by the effects of the temperature, already seen in Fig. 6. This picture is consistent with the fact that, when temperature increases, the interaction among neighboring spins or with an external field becomes less important.

4. Concluding remarks

Static and dynamic properties for the classical Heisenberg chain have been obtained by means of the Monte Carlo method combined with spin dynamic techniques, in good agreement with the available analytical results for specific cases. In particular, for the isotropic case we found that higher the temperature lower the order in the chain. This becomes manifested in the static properties as a decrease of the correlation length, and in the dynamic properties as a decrease of the spin diffusion speed.

According to our findings, the external magnetic field and the easy-plane anisotropy

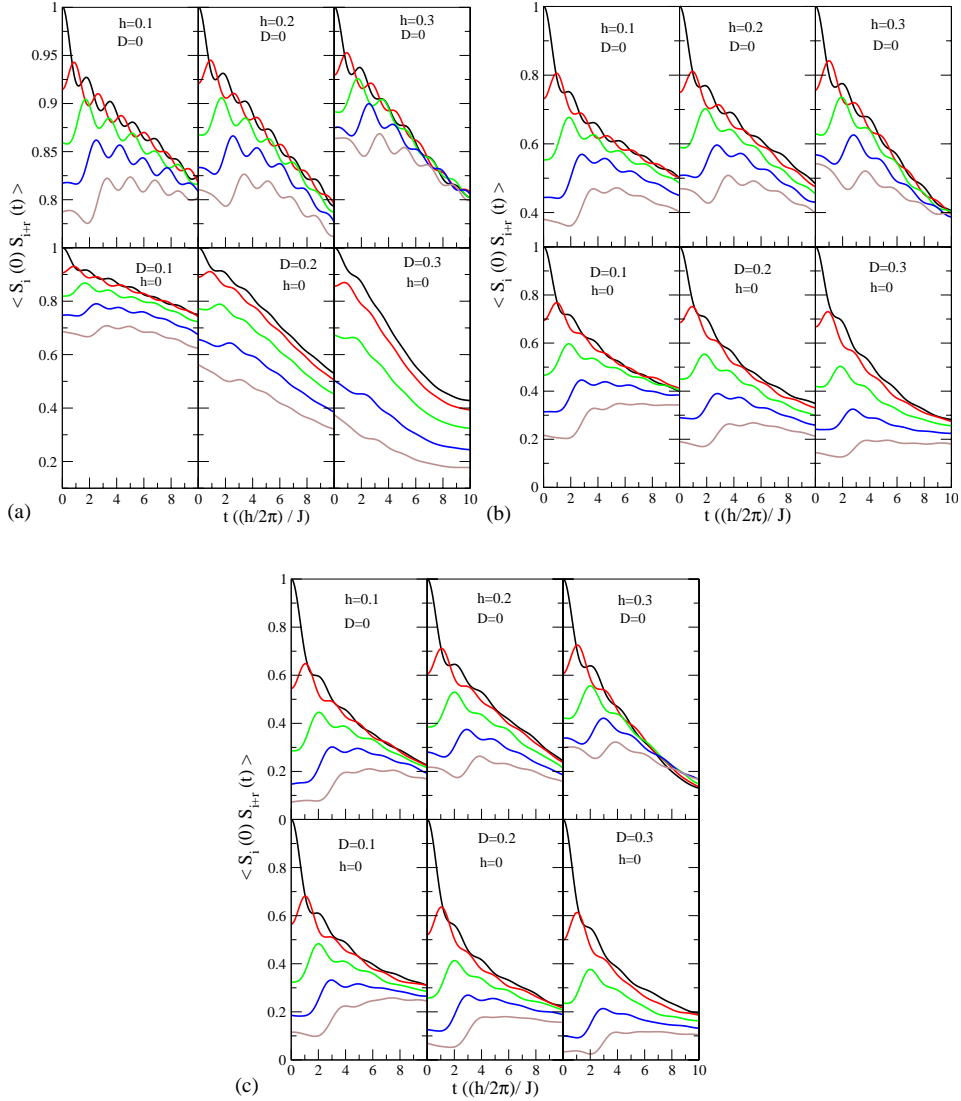


Fig. 7. Spin–spin correlation function for three different values of h and D , at temperatures: (a) $T = 0.1$, (b) $T = 0.3$, and (c) $T = 0.5$. In each plot, the five curves represent, from top to bottom, the correlation between sites $r = 0, 1, 2, 3$ and 4 , respectively.

affect in opposite ways the spin–spin correlation of the chain. While the magnetic field contributes to the order of the chain, increasing the correlation length and the spin diffusion speed, the anisotropy behaves dynamically as a local field, inducing spatial disorder which can be observed in the decrease of the time-dependent spin–spin correlation. In summary, we found that the increase of temperature and/or anisotropy induces

disorder, whereas the presence of an external magnetic field induces order in the chain.

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References

- [1] E. Coronado, P. Delhaes, D. Gatteschi, J. Miller (Eds.), *Localized and Itinerant Molecular Magnetism: From Molecular Assemblies to the Devices*, vol. 321, Series E: Applied Sciences, NATO, Kluwer Academic, Dordrecht, 1996.
- [2] D. Gatteschi, A. Caneschi, L. Pardi, R. Sessoli, *Science* 265 (1994) 1054.
- [3] L. Thomas, F. Lonti, R. Ballou, D. Gatteschi, B. Barbara, *Nature* 383 (1996) 145.
- [4] J. Friedman, M.P. Sarachik, J. Tejada, R. Ziolo, *Phys. Rev. Lett.* 76 (1996) 3830.
- [5] A. Bencini, D. Gatteschi, *Electron Paramagnetic Resonance of Exchange Coupled Systems*, Springer, Berlin, 1990.
- [6] M. Axenovich, M. Luban, *Phys. Rev. B* 63 (2001) 100407.
- [7] M. Steiner, J. Villain, C.G. Windsor, *Adv. Phys.* 25 (1976) 87.
- [8] V. Díaz, G. Gutiérrez, R. Ferrer, *Phys. Stat. Sol. B* 183 (2) (1994) 557.
- [9] M.E. Fisher, *Am. J. Phys.* 32 (1964) 343.
- [10] J.D. Parsons, *Phys. Rev. B* 16 (1977) 2311.
- [11] M. Blume, P. Heller, N.A. Lurie, *Phys. Rev. B* 11 (1975) 4483.
- [12] J.M. Loveluck, S.W. Lovesey, S. Aubry, *J. Phys. C* 8 (1975) 3841.
- [13] D.P. Landau, K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, Cambridge University Press, Cambridge, 2000.
- [14] H.-J. Mikeska, M. Steiner, *Adv. Phys.* 40 (1991) 191.
- [15] This method, devised by Watson et al. [16], has been employed extensively since then, notably by Landau and his coworkers [17].
- [16] R.E. Watson, M. Blume, G.H. Vineyard, *Phys. Rev.* 181 (1969) 811.
- [17] S.-H. Tsai, D.P. Landau, *Phys. Rev. B* 67 (2003) 104411.
- [18] S.K. Oh, C.N. Yoon, J.S. Chung, H.J. Kang, *J. Korean Phys. Soc.* 44 (2004) 491.
- [19] J. Yeomans, *Statistical Mechanics of Phase Transitions*, Oxford University Press, Oxford, 1994.