# Effects of a magnetic field on the dynamics of the one-dimensional Heisenberg model with Dzyaloshinskii-Moriya interactions

Maria Eugênia Silva Nunes*
*Universidade Federal de Ouro Preto, Departamento de Física, ICEB, Campus Universitário Morro do Cruzeiro, 35400-000 Ouro Preto, MG, Brazil*

Érica de Mello Silva† and Paulo H. L. Martins‡
*Universidade Federal de Mato Grosso, Instituto de Física, Av. Fernando Corrêa da Costa, 2367, Bloco F, Sala 209, 78060-900 Cuiabá, MT, Brazil*

J. A. Plascak§
*Universidade Federal da Paraíba, Departamento de Física, CCEN, Campus I, s/n, Cidade Universitária, 58051-090 João Pessoa, PB, Brazil;*
*Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, C.P. 702, 30123-970 Belo Horizonte, MG, Brazil;*
*and Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602, USA*

João Florencio‖
*Universidade Federal Fluminense, Departamento de Física, Av. Litorânea s/n, 24210-340 Niterói, RJ, Brazil*

(Received 11 May 2018; published 15 October 2018)

We use the method of recurrence relations to investigate the dynamics of the one-dimensional spin-1/2 Heisenberg model with Dzyaloshinskii-Moriya (DM) interaction in a magnetic field perpendicular to the DM axis. Our results are valid in the high-temperature limit. We determine exactly the first four recurrants, which produce the time-dependent correlation functions. In order to extend our results to longer times, we introduce a new extrapolation procedure for obtaining higher-order recurrants. Our extrapolation mechanism produces good results when compared to the well-known behavior of the relaxation function in the limit of the $XY$ and isotropic Heisenberg models. The relaxation function and the spectral density function are then analyzed for several values of the external field $B$ for the Heisenberg model with DM interactions in one dimension, in the $T \to \infty$ limit. We find that the external field produces stronger and faster oscillations in relaxation functions and a suppression of the central peak in the spectral density. That is accompanied by the appearance of a peak centered at a finite frequency, due to enhancement of the collective mode of spins precessing about the external field.

DOI: 10.1103/PhysRevE.98.042124

## I. INTRODUCTION

Quantum spin models are very important tools in the study of magnetic properties of matter [1]. The exchange interactions play an important role in the microscopic arrangements of the spin states, which can result, for example, in ferromagnetic, antiferromagnetic, ferrimagnetic, and several other types of more complex phases. However, some antiferromagnetic crystals and carbonates do exhibit, in addition, a weak ferromagnetic behavior. This mechanism was first explained by Dzyaloshinskii [2] on a phenomenological ground. Later, Moriya [3] put it in a more elegant theoretical basis by extending Anderson's superexchange interaction theory [4] to include the spin-orbit coupling.

The Dzyaloshinskii-Moriya (DM) interaction, which arises from the impurities in the system, is very important in low-symmetry crystals, while it vanishes in higher symmetric materials. Since asymmetry is quite ubiquitous in nature, this interaction exists in many real systems and can lead to some special phenomena, not only in three-dimensional compounds. As a two-dimensional example, in the superconductor $LaCu_2O_4$, this interaction induces a slight spin canting out of the $CuO_2$ plane [5].

From a theoretical point of view, quantum spin models in lower spatial dimensions are also important to consider. In fact, Heisenberg spin chains with DM interaction have been of great interest to describe magnetically ordered systems. Recent experimental realizations of this model have been found in a family of spin chains materials with the general formula $K_2CuSO_4Ha_2$, where Ha represents the halogen atom Cl or Br [6]. These compounds are interesting cases of Heisenberg spin chains with uniform DM interactions $D$. Although

*mariaeugenia@ufop.edu.br
†erica@fisica.ufmt.br
‡pmartins@fisica.ufmt.br
§pla@physast.uga.edu
‖jfj@if.uff.br

 

the magnitude of the DM interaction is expected to be small compared to intrachain coupling $J$, it may become considerable in compounds such as cooper benzoate [7,8] and hexagonal perovskite $CsCuCl_3$ [9,10]. The dynamical structure factor for a quantum spin Heisenberg chain with Dzyaloshinskii interactions was investigated with spin wave theory [11], mean-field [12], and projection operator techniques [13].

In the present work we study the effects of an external magnetic field on the dynamics of the spin-1/2 one-dimensional Heisenberg model with DM interaction, where the magnetic field is perpendicular to the DM axis. Our goal is to obtain the time-dependent autocorrelation function and its Fourier transform, the spectral density. We use the method of recurrence relations (RR), proposed by Lee [14] several years ago. The method exploits the geometric properties of a realized Hilbert space, in which the time evolution of a given Hermitian operator takes place. The basis vectors are static, whereas the time evolution is placed on the coefficients representing the projections of the time-dependent operator onto the basis vectors. The dimensionality $d$ and the shape $\sigma$ of the realized Hilbert space are the static properties that characterize time correlation functions of a dynamical variable in its relaxation process towards equilibrium. The time-dependent coefficients are identified as relaxation functions and obey a second recurrence relation. Knowledge of the basis vectors together with their associated coefficients amounts to the solution of a Heisenberg equation of motion for a given operator. The Hilbert space is realized by a suitable inner product, defined in terms of the Kubo formula [14–17]. The method has been used to investigate the dynamics of quantum and classical systems [18–23], such as electron gas [24–29], spin systems [30–40], classical harmonic oscillator chains [41–47], and a two-dimensional plasmonic Dirac system [48,49].

The paper is organized as follows. The model and the method are introduced in Sec. II. Section III is devoted to the exact results we have obtained by directly computing the first four vectors that span the realized Hilbert space in which the dynamical variable of interest evolves. In Sec. IV we present an extrapolation procedure for obtaining the remaining recurrants and a comparison one gets when applying this scheme to the well-known $XY$ and Heisenberg models. Section V presents the behavior of the autocorrelation function for several values of the external field and the corresponding spectral densities for the Heisenberg model with DM interaction in the presence of an external magnetic field. Finally, we present concluding remarks in the last section.

## II. MODEL AND METHOD

The Hamiltonian of the Heisenberg chain with DM interactions in an external magnetic field is given by

$$\mathcal{H} = -J\sum_{i=1}^{N}\vec{\sigma}_i\cdot\vec{\sigma}_{i+1} - \vec{D}\cdot\sum_{i=1}^{N}(\vec{\sigma}_i\times\vec{\sigma}_{i+1}) - \vec{B}\cdot\sum_{i=1}^{N}\vec{\sigma}_i, \tag{1}$$

where $J$ is the nearest-neighbor exchange interaction, $\vec{D}$ is the DM interaction, and $\vec{B}$ is an external magnetic field. The model is defined on a chain of $N$ sites, where $\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ are spin operators defined by Pauli matrices. By considering DM interactions of the form $\vec{D} = D\hat{z}$ and an external perpendicular field $\vec{B} = B\hat{x}$, the above Hamiltonian can be written as

$$\mathcal{H} = -J\sum_{i=1}^{N}\left(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z\right) - D\sum_{i=1}^{N}\left(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x\right) - B\sum_{i=1}^{N}\sigma_i^x. \tag{2}$$

We shall be interested in the study of the time evolution of the $z$ component of the spin operator $\sigma_j^z(t)$, which obeys the usual Heisenberg equation $d\sigma_j^z(t)/dt = i\,[\mathcal{H}, \sigma_j^z(t)]$, with formal solution $\sigma_j^z(t) = \exp(i\mathcal{H}t)\sigma_j^z\exp(-i\mathcal{H}t)$, where $\hbar = 1$.

In the method of recurrence relations, one builds a Hilbert space $\mathcal{S}$ for $\sigma_j^z(t)$ in order to study its time evolution in a geometric frame. The positive-definite scalar product in $\mathcal{S}$ is defined by the Kubo product (see, for instance, Refs. [14–17])

$$(A, B) = \beta^{-1}\int_0^\beta d\lambda\langle A(\lambda)B^\dagger\rangle - \langle A\rangle\langle B^\dagger\rangle, \tag{3}$$

where $A$ and $B \in \mathcal{S}$ are Hermitian operators, $\beta = 1/kT$ is the inverse temperature, $A(\lambda) = \exp(\lambda\mathcal{H})A\exp(-\lambda\mathcal{H})$, and $\langle AB^\dagger\rangle$ is the canonical ensemble average, $\langle AB^\dagger\rangle = \mathrm{Tr}AB^\dagger\exp(-\beta\mathcal{H})/\mathrm{Tr}\exp(-\beta\mathcal{H})$.

In the present work, we are concerned with the time evolution of a tagged spin operator $\sigma_j^z(t)$ in a chain governed by Hamiltonian (2). For times $t \geqslant 0$, we can express $\sigma_j^z(t)$ as an orthogonal expansion

$$\sigma_j^z(t) = \sum_{\nu=0}^{d-1} f_\nu a_\nu(t), \tag{4}$$

where $\{f_\nu\}$ constitutes a set of time-independent orthogonal basis vectors, and the time dependence is placed in the coefficients $a_\nu(t)$. Accordingly, the dimensionality $d$ of $\mathcal{S}$ is yet to be determined.

In the infinite temperature limit, where all the eigenstates of $\mathcal{H}$ enter with the same statistical weight in the canonical averages, the inner product, Eq. (3), reduces to [14,15,17]

$$(A, B) = \frac{1}{Z}\mathrm{Tr}AB^\dagger. \tag{5}$$

The realization of $\mathcal{S}$ by this inner product leads to a recurrence relation for the basis vectors

$$f_{\nu+1} = i\mathcal{L}f_\nu + \Delta_\nu f_{\nu-1}, \quad 0 \leqslant \nu \leqslant d-2, \tag{6}$$

where $\mathcal{L}$ is the Liouville operator,

$$\mathcal{L}A = [\mathcal{H}, A] \equiv \mathcal{H}A - A\mathcal{H}. \tag{7}$$

The quantity $\Delta_\nu$ is the ratio between the norms of consecutive basis vectors,

$$\Delta_\nu = \frac{(f_\nu, f_\nu)}{(f_{\nu-1}, f_{\nu-1})}. \tag{8}$$

We choose $f_0 = \sigma_j^z(0)$ as the dynamic variable of interest, and by definition $f_{-1} \equiv 0$ and $\Delta_0 \equiv 1$. From now on, the recurrence relation Eq. (6) shall be referred to as RR I. The corresponding $\Delta_\nu$ shall be termed the $\nu$th recurrant. Once $f_0$

is defined, the remaining basis vectors are determined by RR I and Eq. (8).

The coefficients $a_\nu(t)$, which are the relaxation functions, satisfy a second recurrence relation (RR II),

$$\Delta_{\nu+1}a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t), \quad 0 \leqslant \nu \leqslant d-2, \tag{9}$$

where $\dot{a}_\nu(t) = da_\nu(t)/dt$ and $a_{-1} \equiv 0$.

Since the zeroth basis vector has been chosen as the dynamic variable of interest $f_0 = \sigma_j^z(0) \equiv \sigma_j^z$, it follows that the coefficient $a_0(t)$ can be identified as the time-dependent autocorrelation function $C_z(t)$,

$$a_0(t) = \left(\sigma_j^z, \sigma_j^z(t)\right) = \frac{1}{Z}\mathrm{Tr}\sigma_j^z\sigma_j^z(t) \equiv C_z(t), \tag{10}$$

where $Z = 2^N$ is the partition function at infinite temperature. Here $C_z(t)$ can be interpreted as the amplitude probability that the stochastic variable $\sigma_j^z$, initially in equilibrium in a canonical ensemble at infinite temperature, will remain the same at some later time $t$. The recurrence relation RR II leads also directly to a generalized Langevin equation (GLE) [50]. It reflects the geometric shape $\rho = (\Delta_1\Delta_2\ldots\Delta_{d-1})$ of the realized space $\mathcal{S}$ for the Hamiltonian dynamics of $\sigma_j^z(t)$. Note that the initial state of the tagged spin $\sigma_j^z$ of the chain is a linear combination of all the eigenstates of the Hamiltonian, where each state enters with the same probability (Boltzmann factor unity at infinite temperature). In the initial state, there are energy eigenstates from the ground state up to the highest energy state of the chain. Nevertheless, since we are dealing with the correlation function, at $t = 0$ one has $\langle\sigma_i^z(0)^2\rangle = 1$, and $C_z(t)$ is thus independent of any particular initial condition of the tagged spin.

The correlation function $C_z(t)$, which is both real and even in $t$ and its time derivative is zero at $t = 0$, can be Taylor expanded about $t = 0$ as

$$C(t) = \sum_{\nu=0}^{\infty}\frac{(-1)^\nu}{(2\nu)!}\mu_{2\nu}t^{2\nu}, \tag{11}$$

where the moments $\mu_{2\nu}$ are defined in terms of a trace over iterated commutators

$$\mu_{2\nu} = \frac{1}{2}\mathrm{Tr}\left(\sigma_i^z\mathcal{L}^{2\nu}\sigma_i^z\right). \tag{12}$$

Since the correlation function is even in $t$, only even powers of $t$ appear in the Taylor expansion.

It is often convenient to take the Laplace transform of RR II. Note that with the choice $f_0 = \sigma_i^z$, it follows from Eq. (4) that $a_0(t=0) = 1$, and $a_\nu(t=0) = 0$ for $\nu \geqslant 1$. The result is

$$1 = z\tilde{a}_0(z) + \Delta_1\tilde{a}_1(z), \tag{13a}$$

$$\tilde{a}_{\nu-1}(z) = z\tilde{a}_\nu(z) + \Delta_{\nu+1}\tilde{a}_{\nu+1}(z), \tag{13b}$$

where $\tilde{a}_\nu(z)$ is the Laplace transform of $a_\nu(t)$.

After some manipulations of Eqs. (13a) and (13b), we obtain

$$\tilde{a}_0(z) = \frac{1}{z+\phi(z)}, \tag{14}$$

where $\phi(z)$ is the memory function, given as the continued fraction

$$\phi(z) = \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots}}}. \tag{15}$$

In those cases where the recurrants are known, inspection of RR II can effectively be used to uncover the relaxation functions $\tilde{a}_\nu(z)$. On the other hand, if one knows the basal relaxation function $\tilde{a}_0(z)$, the remaining relaxation functions can be readily obtained using RR II.

There are also conversion formulas connecting the recurrants to the moments defined in Eq. (12) [51]. Without loss of generality we can set $\mu_0 = 1$, which is consistent with the normalized time-dependent correlation function defined in Eq. (10). Having the first $\nu$ recurrants $\Delta_1, \ldots, \Delta_\nu$, the conversion formulas yield the first moments up to order $2\nu$ from

$$\Delta_1 = \mu_2, \quad \Delta_2 = \mu_2 + \mu_4/\mu_2,$$
$$\Delta_3 = \left(\mu_4^2/\mu_2 - \mu_6\right)/\left(\mu_2^2 - \mu_4\right), \ldots, \tag{16}$$

where lengthier expressions are obtained for higher-order recurrants. The previous equations enable us to get the $\mu_{2\nu}$ in terms of $\Delta_\nu$.

As can be seen from the above equations, the crucial quantities that enter the analysis are the recurrants $\Delta_\nu$. In practice, only a very small number of nontrivial models allow for a complete knowledge of them. For most cases, however, one must resort to extrapolation. There are several extrapolation schemes found in the literature, such as the Gaussian terminator [51] and different numerical methods [34,35]. In the present work we shall use a numerical extrapolation scheme which interpolates between known limit cases, from which we obtain reliable results.

## III. EXACT RESULTS FOR THE BASIS VECTORS

We have exactly calculated the first four basis vectors of the Hilbert space of $\sigma_j^z(t)$, $\mathcal{S}$, using the recurrence relations RR I and RR II for the Heisenberg model defined in Eq. (2). The first basis vector $f_0$ is the dynamic variable of interest,

$$f_0 = \sigma_j^z.$$

Its norm is simply $(f_0, f_0) = 1$. Next we use RR I, with $\nu = 0$, to determine the next vector $f_1$:

$$f_1 = i\mathcal{L}f_0 = i[\mathcal{H}, f_0] = i[\mathcal{H}, \sigma_j^z]. \tag{17}$$

The result is given by

$$\begin{aligned} f_1 = {} & -2B\sigma_j^y - 2J\sigma_j^y\sigma_{j+1}^x - 2J\sigma_{j-1}^x\sigma_j^y \\ & + 2J\sigma_j^x\sigma_{j+1}^y + 2J\sigma_{j-1}^y\sigma_j^x - 2D\sigma_j^y\sigma_{j+1}^y \\ & + 2D\sigma_{j-1}^x\sigma_j^x - 2D\sigma_j^x\sigma_{j+1}^x + 2D\sigma_{j-1}^y\sigma_j^y. \end{aligned} \tag{18}$$

The first recurrant is then obtained,

$$\Delta_1 = \frac{(f_1, f_1)}{(f_0, f_0)} = 4B^2 + 16J^2 + 16D^2. \tag{19}$$

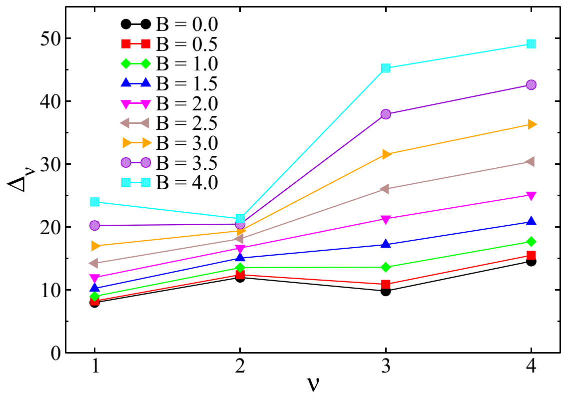


FIG. 1. Recurrants for the Heisenberg chain with DM coupling with $D = 1$ and several values of the magnetic external field $B$. Here and in the next figures, the energy unit is set by $J = 1$. (The lines connecting the points are just an aid to the eye.)

In an analogous way, the next three vectors $f_2$, $f_3$, $f_4$, and the corresponding recurrants $\Delta_2$, $\Delta_3$, and $\Delta_4$ were calculated exactly. However, their expressions are too lengthy to be reproduced here.

In order to have a picture of the these recurrants, we show in Fig. 1 the first four $\Delta_\nu$ ($\nu = 1, 2, 3, 4$) for $D = 1$ and several values of the external magnetic field. In this case, and in what follows, we have set the exchange interaction $J = 1$ and measured the parameters $D$ and $B$ in units of $J$.

Figure 2 shows the autocorrelation functions $C_z(t)$, given by Eq. (11) for different values of the magnetic field, where the moments have been obtained from relations as given in (16) by employing those four recurrants only. One can see that the magnetic field promotes a faster decay. However, in this case with only four recurrants, we were able to get reliable results up to time $t \approx 0.4$ (the time is measured in units of the inverse of the exchange interaction $J^{-1}$). Due to the fact that only a short time dynamics can be achieved from the present exact data, we expect the results depicted in Fig. 2 will not change noticeably if one includes higher-order recurrants in the calculations.

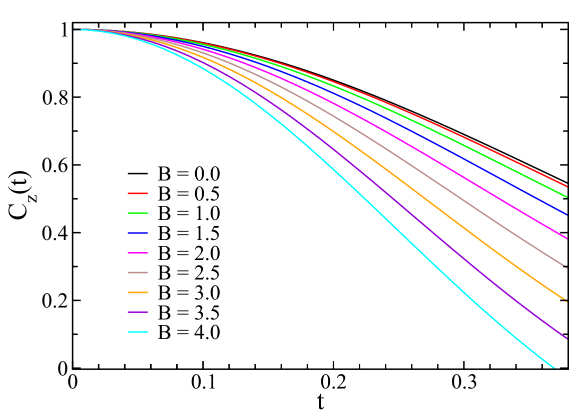


FIG. 2. Time-dependent spin autocorrelation function $C_z(t)$ obtained from the first four recurrants, for DM coupling $D = 1$ and several values of the magnetic field $B$.

As discussed above, since we know analytically only the first four recurrants, the ensuing relaxation function is valid for relatively short times only. On the other hand, the obtention of more recurrants is quite prohibitive for the Hamiltonian given in (2). Therefore, in order to extend the time range, we must use some sort of approximation in order to use higher-ordered recurrants. Below we present an extrapolation scheme to carry out that task.

## IV. EXTRAPOLATION SCHEME FOR THE HIGHER-ORDER RECURRANTS

In order to extrapolate the recurrants $\Delta_\nu$ for $\nu > 4$, we must consider what is already known regarding the dynamics of other systems which are somewhat related to our problem. Take, for example, the dynamics of $\sigma_j^z$ in the $XY$ model, for which the time-dependent correlation function is exactly known [52], $C_z(t) = J_0^2(t) \sim t^{-1}$ for large times ($J_0$ is a Bessel function of first kind). In that case, the recurrants level off as $\nu$ increases, approaching a finite value. If, on the other hand, one has a system where the recurrants grow indefinitely as $\nu$ increases, the ensuing $C_z(t)$ decays faster than any power law. For example, linear growth $\Delta_\nu = \nu\Delta$ produces a Gaussian relaxation function [30]. On the other hand, there are strong numerical indications that $C_z(t)$ for the isotropic Heisenberg chain decays slower than the squared Bessel function of the $XY$ model [53]. This indicates that the recurrants of the Heisenberg chain must be bounded, hence it is not appropriate to extrapolate linearly or, equivalently, to use a Gaussian terminator. Therefore, we construct an extrapolation scheme in which the recurrants of the Heisenberg model (with or without DM interactions or external magnetic fields) is bounded by a finite asymptotic value $\Delta_\infty$ as $\nu \to \infty$.

Our procedure is as follows. We first define $\Delta_\nu^<$ for $\nu \leqslant n_c$ and $\Delta_\nu^>$ for $\nu > n_c$, where $n_c$ is the number of exactly known recurrants. Figure 1 shows the first four exact recurrants for $D = 1$ and several values of $B$. We estimate $\Delta_\infty$ by extrapolating the straight line of the behavior of $\Delta_3^<$ and $\Delta_4^<$ as a function of $1/\nu$. The value thus obtained for vanishing external field and $D = 1$ is $\Delta_\infty \approx 28.8$.

To obtain the extrapolated recurrants, we assume that both $\Delta_\nu^<$ and $\Delta_\nu^>$ have power-like behavior of the form

$$\Delta_\nu^< = a\nu^\alpha, \qquad \Delta_\nu^> = \Delta_\infty - \frac{b}{\nu^\beta}, \tag{20}$$

where $a$, $b$, and the exponents $\alpha$ and $\beta$ are determined as follows. The constants $a$ and $\alpha$ are determined by using a numerical fit for the first known exact recurrants. To find $b$ and $\beta$, we impose continuity in $\Delta_\nu^<$ and $\Delta_\nu^>$ and their derivatives at $\nu = n_c$.

It is then possible with the above procedure to get as many recurrants as needed for obtaining the relaxation functions. It would be worthwhile to test the scheme by applying it to known problems, like the $XY$ model, which allows exact solutions [52], and the isotropic Heisenberg chain, where several recurrants have already been computed exactly [54]. For the $XY$ model one can extract all the recurrants from the exact solution by Niemeijer [52]. Figure 3 shows the time dependence of the relaxation function as obtained from the first four exact recurrants and the results for the relaxation

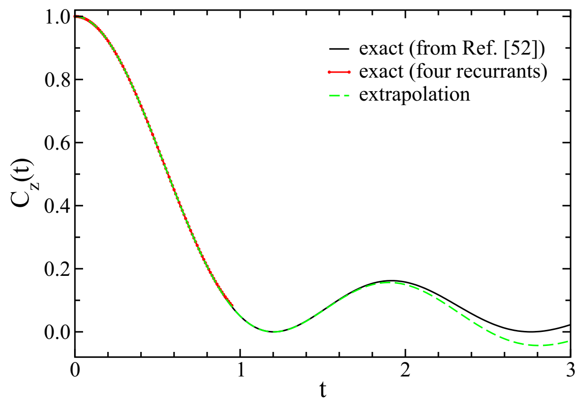


FIG. 3. Time-dependent autocorrelation function of the $z$ component of the spin for the one-dimensional $XY$ model. Full line (black): exact result of Ref. [52]; circle-dashed line (red): result using the first four exact recurrants; long-dashed line (green): result using extrapolation.

function stemming from 100 recurrants (four exact plus 96 extrapolated values). Those curves can be compared with the exact result, the squared Bessel function $J_0^2(t)$, also shown in Fig. 3. One can clearly see that the present extrapolation procedure not only is able to extend the time interval from $t \sim 0.9$ to $t \sim 3.0$, but also it is quite close to the exact result up to $t \sim 2.5$.

In Fig. 4 we have a similar comparison, but now for the Heisenberg chain. The results for the time dependence of the $z$ component of the relaxation function obtained from different ways are presented. The proposed extrapolation scheme gives quite nice results in the time interval considered when compared to the values coming from the 15 recurrants computed in Ref. [54].

In obtaining the correlation functions above, as well those in the next section, we consider only extrapolated recurrants and moments that give significant contribution to $C_z(t)$. It happens that the higher the moment the smaller its value, making the cutoff for large $\nu$ quite irrelevant in the present case.

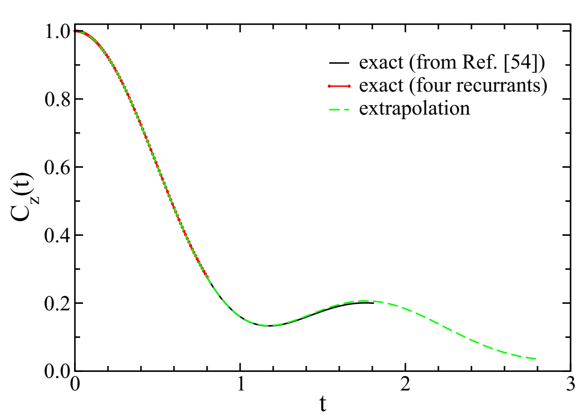


FIG. 4. Time-dependent spin autocorrelation function of the one-dimensional Heisenberg model. Full line (black): result from 15 exact recurrants obtained from Ref. [54]; circle-dashed line (red): result from four exact recurrants from our calculations with $D = B = 0$; long-dashed line (green): result from extrapolation.

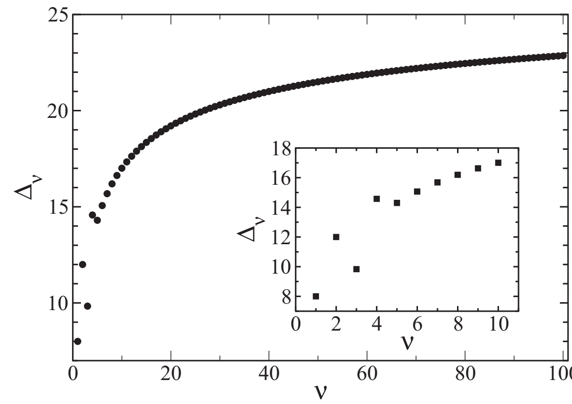


FIG. 5. Extrapolated recurrants for $5 \leqslant \nu \leqslant 100$ for the Heisenberg model with DM interaction $D = 1$ and zero external magnetic field $B = 0$. The inset shows the behavior for $\nu \leqslant 10$.

## V. RESULTS FOR HEISENBERG MODEL WITH DM INTERACTION IN AN EXTERNAL FIELD

Figure 5 shows the extrapolation results for the recurrants up to $\nu = 100$ for the case $D = 1$ and $B = 0$. Similar results are also obtained for several values of the external field $B$. Our results for the relaxation function for $D = 1$ and several values of $B$ are depicted in Fig. 6. We find that for $B = 0$ the relaxation function is always positive and oscillates with decreasing amplitude as time increases. This is a typical behavior of the dynamics of the $XXZ$ model [53]. In fact, for $B = 0$ one has the Heisenberg model with DM interactions only. In that case, a suitable rotation of the spin variables can show that this model is equivalent to the $XXZ$ model [55]. This explains the anisotropic Heisenberg behavior obtained for $B = 0$. The procedure can then be repeated for other values of $B$, each case having its own extrapolated recurrants. We notice in Fig. 6 that for $B < 1.5$ the autocorrelation function is always positive but oscillates with decreasing amplitude, similar to the $XXZ$ model. However, for $B \gtrsim 1.5$ the relaxation function can become negative in some time intervals. As $B$ increases, both oscillations amplitudes and frequencies become larger, indicating a strong response to the applied field.

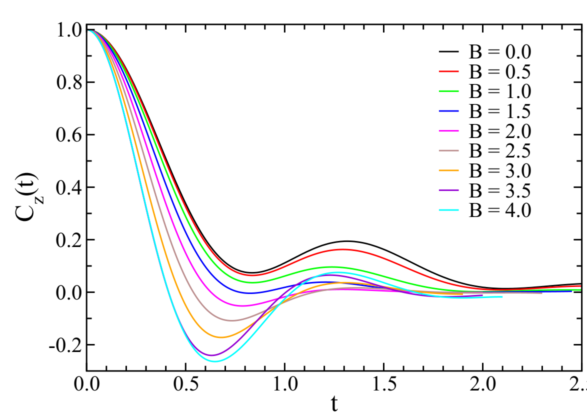


FIG. 6. Time-dependent relaxation function for $D = 1$ and several values of the field $B$. We used the first four exact recurrants and extrapolated ones up to $\nu = 100$.

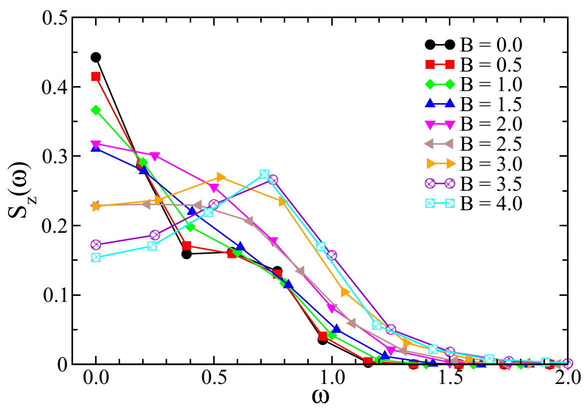


FIG. 7. Frequency-dependent spectral density for $D = 1$ and several values of the external magnetic field $B$.

Classically, such a case corresponds to the scenario where the precession of each spin around the external magnetic field starts to dominate the dynamics. Indeed, the spins are still tied to each other via the exchange coupling $J$ and the DM interactions, which try to drive the spins away from the field direction. For large enough $B$ we expect the dynamics to be completely dominated by the collective precession of the spins around the field.

The spectral density $S_z(\omega)$ is defined as the time Fourier transform of the relaxation function $C_z(t)$,

$$S_z(\omega) = \int_{-\infty}^{+\infty} C_z(t) e^{-i\omega t} dt, \tag{21}$$

and is shown in Fig. 7 for different values of the magnetic field. This spectral density was calculated numerically from the discrete Fourier transform of the correlation function $C_z(t)$. The distance between two consecutive frequencies is determined by the total time interval $T$ of $C_z(t)$, in such a way that $\Delta\omega = 1/T$. As one can see in Fig. 6, $T$ is of order of 4, if we consider the symmetric interval $-2 \lesssim t \lesssim 2$. Although the curves are not smooth by using this simple numerical procedure, the general trend of the frequency behavior of $S_z(\omega)$ is apparent from the figure.

For $B < 1.5$ one can see that a shoulder is present in $S_z(\omega)$. For external fields in the range 1.5–2.5 only a central peak is present and the shoulder is suppressed. On the other hand, for larger values of $B > 2.5$, the central peak decreases and an additional peak appears, centered at a finite value of the frequency. This extra peak should be attributed to the precession of the spins around the large magnetic field, when it is large enough to counterbalance the exchange and DM interactions.

## VI. CONCLUDING REMARKS

In this work we have studied the dynamics of the spin-1/2 one-dimensional Heisenberg model with Dzyaloshinskii-Moriya (DM) interaction in the presence of an external magnetic field perpendicular to the DM axis. We obtained the autocorrelation function in the high-temperature limit by means of the method of recurrence relations. We exactly computed the first four recurrants and used an extrapolation procedure to obtain higher-order recurrants. Our extrapolation scheme produces good results when compared to the well-known behavior of the relaxation functions of the *XY* and isotropic Heisenberg chains. The relaxation function and its associated spectral density were analyzed for several values of the external field $B$ keeping the DM interaction $D = 1$. For small values of the field the behavior is similar to the *XXZ* chain. For intermediate values only a central peak and a shoulder appear in the spectral density function, while for large values of the field a nonzero frequency peak results from the precession of the spins around the magnetic field, with suppression of the central peak and its shoulder. Although the central mode behavior versus collective dynamics is an old feature of the dynamics of spin systems, they are in some sense not universal. Some systems do not show those behaviors, and one could not expect, *a priori*, the results we have just obtained for the present system.

It should be stressed that our procedure is in fact exact for short times, as is shown in Figs. 3 and 4. Our extrapolation covers then the remaining time domain. There our results are approximate, and we have implemented a procedure guided by known numerical results from the literature. Although a Gaussian termination, i.e., a linear growth of the expansion coefficients, will produce a similar result, at least for zero external field [56], we used herein only the finite asymptotic value approach, which is physically more suitable for the present more general model.

We have discussed here results only for $D = 1$. However, as the DM interaction effect is just to rescale the *XY* components of the exchange interaction, similar results are obtained for different values of $D$.

Regarding the extrapolation procedure, it has been used in the present model where only four recurrants were able to be exactly computed. Nonetheless, the method can be perfectly extended to the study of other systems and with a general number of exact recurrants, even to the case where the recurrants oscillate for even and odd indices $\nu$. In order to implement our extrapolation scheme for finite temperatures one must first obtain a few exact recurrants using the full Kubo formula (with $\beta = 1/kT \neq 0$). Finally, the goal is to obtain the long-time dynamics of the system. Some of the problems that can be addressed are the characterization of diffusive or nondiffusive behavior, which is intimately related to the approach to equilibrium at long times.

As a final remark, it is known that there has been recently much activity concerning the dynamics of spin chains extended to the context of ergodicity, ergodicity breaking, and the evolution at long times towards thermal equilibrium. In fact, besides the usefulness of the present approach in the study of dynamical properties of Hermitian systems, a relevant result has also been derived from the recurrence relations method in the direction of the formulation of an ergodicity condition in terms of an infinite product [57]. It is worth mentioning that connections between this ergodic condition and the Birkhoff ergodic theorem and Khinchin theorem were additionally established to a new formulation for irreversibility in many-body Hermitian systems [58]. Since then, the ergodic hypothesis has been revisited in different perspectives. Concerning the model we consider here, the ergodicity of the dynamical variable $\sigma_i^z$ and its consequences will be investigated in a future work in the light of the recurrence relations method. Nevertheless, even though we do not discuss ergodicity in the present study, or the approach to equilibrium at long times, our results may be of interest to those working in this exciting field.

## ACKNOWLEDGMENTS

The authors would like to thank the Brazilian agencies CNPq (BR), CAPES (BR), and FAPEMAT (BR) for financial support. The Universidade Federal de Minas Gerais is also acknowledged for hosting a meeting of the Dynamical Group (GRUDI). We would like to thank M. Howard Lee for making us interested in the recurrence relations method.

[1] See, for example, J. B. Parkinson and D. J. J. Farnell, *An Introduction to Quantum Spin Systems*, Lecture Notes in Physics Vol. 816 (Springer, Berlin, 2010).
[2] I. Dzyaloshinskii, Phys. Chem. Solids **4**, 241 (1958).
[3] T. Moriya, Phys. Rev. **120**, 91 (1960).
[4] P. W. Anderson, Phys. Rev. **115**, 2 (1959).
[5] D. Coffey, K. S. Bedell, and S. A. Trugman, Phys. Rev. B **42**, 6509 (1990).
[6] M. Hälg, W. E. A. Lorenz, K. Y. Povarov, M. Mansson, Y. Skourski, and A. Zheludev, Phys. Rev. B **90**, 174413 (2014).
[7] M. Oshikawa and I. Affleck, Phys. Rev. Lett. **79**, 2883 (1997).
[8] I. Affleck and M. Oshikawa, Phys. Rev. B **60**, 1038 (1999).
[9] U. Schotte, A. Kelnberger, and N. Stüsser, J. Phys.: Condens. Matter **10**, 6391 (1998).
[10] A. E. Jacobs and T. Nikuni, J. Phys.: Condens. Matter **10**, 6405 (1998).
[11] Q. Xia and P. S. Riseborough, J. Appl. Phys. **63**, 4141 (1988).
[12] L. S. Lima and A. S. T. Pires, J. Magn. Magn. Mater. **320**, 2316 (2008).
[13] A. S. T. Pires and M. E. Gouvêa, J. Magn. Magn. Mater. **212**, 251 (2000).
[14] M. H. Lee, Phys. Rev. Lett. **49**, 1072 (1982).
[15] M. H. Lee, J. Hong, and J. Florencio, Phys. Scr. **T19**, 498 (1987).
[16] M. H. Lee, Phys. Rev. E **61**, 3571 (2000).
[17] U. Balucani, M. H. Lee, and V. Tognetti, Phys. Rep. **373**, 409 (2003).
[18] S. Sen, Physica A (Amsterdam) **315**, 150 (2002).
[19] A. V. Mokshin, Theor. Math. Phys. **183**, 449 (2015).
[20] I. Sawada, Physica A (Amsterdam) **315**, 14 (2002).
[21] S. Sen, Physica A (Amsterdam) **360**, 304 (2006).
[22] A. S. T. Pires, Helv. Phys. Acta **61**, 988 (1988).
[23] A. V. Mokshin, Discontinuity Nonlinearity Complexity **2**, 43 (2013).
[24] M. H. Lee, J. Hong, and N. L. Sharma, Phys. Rev. A **29**, 1561 (1984).
[25] N. L. Sharma and M. H. Lee, J. Math. Phys. **27**, 1618 (1986).
[26] N. L. Sharma, Phys. Rev. B **45**, 3552 (1992).
[27] M. H. Lee and J. Hong, Phys. Rev. B **32**, 7734 (1985).
[28] M. H. Lee and J. Hong, Phys. Rev. B **30**, 6756 (1984).
[29] M. H. Lee and J. Hong, Phys. Rev. Lett. **48**, 634 (1982).
[30] J. Florencio and M. H. Lee, Phys. Rev. B **35**, 1835 (1987).
[31] J. Florencio and M. H. Lee, Nucl. Phys. B **5A**, 250 (1988).
[32] J. Florencio, S. Sen, and M. H. Lee, Braz. J. Phys. **30**, 725 (2000).
[33] M. E. S. Nunes, J. A. Plascak, and J. Florencio, Physica A (Amsterdam) **332**, 1 (2004).
[34] M. E. S. Nunes and J. Florencio, Phys. Rev. B **68**, 014406 (2003).
[35] S. Sen, Z.-X. Cai, and S. D. Mahanti, Phys. Rev. E **47**, 273 (1993).
[36] Z.-Q. Liu, X.-M. Kong, and X.-S. Chen, Phys. Rev. B **73**, 224412 (2006).
[37] S.-X. Chen, Y.-Y. Shen, and X.-M. Kong, Phys. Rev. B **82**, 174404 (2010).
[38] X.-J. Yuan, X.-M. Kong, Z.-B. Xu, and Z.-Q. Liu, Physica A (Amsterdam) **389**, 242 (2010).
[39] Y.-F. Li and X.-M. Kong, Chin. Phys. B **22**, 037502 (2013).
[40] J. Florencio, S. Sen, and Z.-X. Cai, J. Low. Temp. Phys. **89**, 561 (1992).
[41] J. Florencio and M. H. Lee, Phys. Rev. A **31**, 3231 (1985).
[42] M. H. Lee, Symmetry **8**, 22 (2016).
[43] M. B. Yu, Phys. Lett. A **380**, 3583 (2016).
[44] M. B. Yu, Eur. Phys. J. B **90**, 87 (2017).
[45] M. B. Yu, Eur. Phys. J. B **91**, 25 (2018).
[46] A. Wierling, Eur. Phys. J. B **85**, 20 (2012).
[47] A. Wierling and I. Sawada, Phys. Rev. E **82**, 051107 (2010).
[48] E. M. Silva, Phys. Rev. E **92**, 042146 (2015).
[49] E. M. Silva, Acta Phys. Pol. B **46**, 1135 (2015).
[50] M. H. Lee, J. Math. Phys. **24**, 2512 (1983).
[51] V. S. Viswanath and G. Müller, *The Recursion Method—Application to Many-Body Dynamics*, Lecture Notes in Physics Vol. 23 (Springer-Verlag, Berlin, 1994).
[52] T. Niemeijer, Physica **36**, 377 (1967).
[53] K. Fabricius, U. Löw, and J. Stolze, Phys. Rev. B **55**, 5833 (1997).
[54] M. Böhm and H. Leschke, J. Phys. A **25**, 1043 (1992).
[55] F. C. Alcaraz and W. F. Wreszinski, J. Stat. Phys. **58**, 45 (1990).
[56] M. Böhm, V. S. Viswanath, J. Stolze, and G. Müller, Phys. Rev. B **49**, 15669 (1994).
[57] M. H. Lee, Phys. Rev. Lett. **87**, 250601 (2001).
[58] M. H. Lee, Phys. Rev. Lett. **98**, 190601 (2007).