

# High Temperature Dynamics of the Linear Chain Spin-One Model in a Transverse Field

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The dynamics of the spin-one model with single-ion anisotropy (the Blume-Capel model) in the presence of a transverse field is studied by means of the continued fraction of the longitudinal relaxation function. Within the approximations used the dynamics of the spin-one model is similar to the spin-1/2 model and the single-ion anisotropy enhances the central mode behavior.

## I. Introduction

The dynamics of quantum spin models has been an important subject in many-body physics for a long time. Among these models two have received considerable attention: the spin-1/2 Weisenberg model[1-13] and the spin-1/2 transverse Ising model[14-18]. The linear chain models[5,7,8,11-14,17,19-25] attracted considerable interest as simple non-trivial interacting many-body systems. Although some progress has been accomplished over the years, some dynamical properties of spin chains are still poorly understood. The objective of the present study is to look into some aspects that may influence the dynamics which have not been fully analyzed before. They are: the influence of the spin quantum number and of the anisotropies in the dynamics.

For this purpose we will study the spin-one model, with an exchange interaction ( $J$ ) and a single-ion anisotropy ( $D$ ), in the presence of a transverse field ( $O$ ), in the limit of high temperatures. As far as we know this model has not been studied before. A recent publication by Bohm and Leschke<sup>[26]</sup> has analyzed the high temperature dynamics of the isotropic spin-1 Heisenberg chain and the isotropic spin-1 XY chain. They conclude that "with increasing  $S$  (spin number) the dynamics should converge rapidly to the limit  $S = \infty$  be-

havior". Our calculation is based on Mori's continued fraction representation of the longitudinal relaxation-shape function<sup>[27,28]</sup>. We use the standard procedure to truncate the continued fraction, which is equivalent to a short memory approximation, and it is an  $N$ -pole approximation to a function with an infinite number of poles. The truncation will use the relaxation time form proposed by de Raedt and de Raedt<sup>[29]</sup> which has shown to be more consistent than other procedures for the isotropic spin-1/2 Heisenberg chain and spin-1/2 transverse Ising model chain.

The calculations were performed for the three- and four - pole approximations. The longitudinal relaxation function  $\Omega \text{Re} \psi^{zz}(\vec{q}, \omega)$  a function of  $\omega/\Omega$ , will be presented in two different schemes, both within the three-pole approximation: a) for three different values of the single ion anisotropy, we show the dependence with the exchange interaction  $J$ , both normalized to the transverse frequency. b) for three different values of the single ion anisotropy (normalized to  $J$ ) we show the dependence with the transverse frequency  $\alpha = \Omega/J$ . As a of comparison we present, within the three-pole approximation, in the same plot the results for the spin-1/2 transverse Ising model and the  $D = 0$  spin-1 model in the transverse field. In the following section the model and the methodology are described. Results and discussions are shown in the final section.

## II. The model and the method

The spin-1 model in one-dimension with an exchange interaction  $\mathbf{J}$ , a single-ion anisotropy  $D$  in the presence of a transverse field  $\Omega$ , is described by the Hamiltonian,

$$S_i^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_i^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & i \\ 0 & i & 0 \end{pmatrix} \quad \text{and} \quad S_i^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and  $\vec{S}_i^2 = s(s+1)1$ , where  $s = 1$ .

The dynamics of model (1) can be studied by means

$$R^{zz}(\vec{q}, t) = \int_0^\beta \langle e^{\lambda+H} S^z(\vec{q}, t) e^{-\lambda+H} S^z(-\vec{q}, t) \rangle d\lambda - \beta \langle S^z(\vec{q}, t) \rangle \langle S^z(-\vec{q}, t) \rangle \quad (3)$$

and  $\beta = 1/k_b T$ .

The longitudinal relaxation shape function will be calculated by means of Mori's method<sup>[27,28]</sup>. Mori has used the projection operator technique to express the Laplace transform of the autocorrelation function in the form of a continued fraction. Mori's method shows how time scales (fast and slow) arise from hamiltonian systems and how transport coefficients are related to the interaction energy of the spins. It is an exact method. But, it depends on the knowledge of all the moments of the spectral function. For example, when applied to the one-dimensional spin 1/2 isotropic XY-model or

$$\delta_1 = \langle \omega_q^2 \rangle, \quad \delta_1 \delta_2 = \langle \omega_q^4 \rangle - \langle \omega_q^2 \rangle^2, \quad \delta_1 \delta_2 \delta_3 = \langle \omega_q^6 \rangle - \langle \omega_q^4 \rangle^2 \langle \omega_q^2 \rangle, \text{ etc.} \quad (5)$$

and the moments are defined as

$$\langle \omega_q^n \rangle = \frac{1}{\pi} \int_{-\infty}^{\infty} \omega^n F^{zz}(\vec{q}, \omega) d\omega, \quad (6)$$

where

$$F^{zz}(\vec{q}, \omega) = \text{Re} \Psi^{zz}(\vec{q}, \omega) \quad (7)$$

$$H = -\frac{J}{2} \sum_{i=1}^N S_i^z S_{i+1}^z - \frac{D}{2} \sum_{i=1}^N (S_i^z)^2 - \Omega \sum_{i=1}^N S_i^x \quad (1)$$

where  $S_i^\alpha$  are components of a spin-1 operator at site  $i$  of an one-dimensional lattice. The spin operators are explicitly given by

of the longitudinal relaxation shape function,

$$\Psi^{zz}(\vec{q}, \omega) = \int_0^\infty \frac{R^{zz}(\vec{q}, t)}{R^{zz}(\vec{q}, 0)} e^{-i\omega t} dt \quad (2)$$

where

to the one-dimensional spin-1/2 transverse Ising model the method gives the exact result for the autocorrelation function. However, in most cases of physical interest the moments are not all known and one must rely on different approaches to terminate the continued fraction. The Mori continued fraction formalism expresses  $\Psi^{zz}(\vec{q}, \omega)$  as a continued fraction

$$\Psi^{zz}(I, \omega) = (i\omega + \delta_\ell f_\ell(i\omega))^{-1}, \quad (4.a)$$

$$f_\ell(i\omega) = (i\omega + \delta_{\ell+1} f_{\ell+1}(i\omega))^{-1}, \quad (4.b)$$

where

Among several methods used to cut-off the continued fraction we will use the n-pole approximation. It consists in approximating the function  $f_\ell(i\omega)$  by

$$f_\ell(i\omega) = (i\omega + \tau_\ell^{-1}(q))^{-1}, \quad (8)$$

where  $\tau_\ell(\vec{q})$  is the relaxation time expressed in terms of the moments. We will make use of the theoretical calculation proposed by de Raedt and de Raedt<sup>[29]</sup> for the relaxation time, which has proved to be more consistent than other type of calculations. They use up to  $\ell = 3$  the following form for the relaxation time,

$$\tau_2^{-1}(\vec{q}) = \delta_1 + \delta_2 \tag{9}$$

$$\tau_3^{-1}(\vec{q}) = \delta_2 + \delta_3 \tag{10}$$

which corresponds to the three- and four- pole approximations, respectively. It is assumed that all poles of  $\Psi^{zz}(\vec{q}, \omega)$  lie within the corresponding circle of radius  $\tau_\ell^{-1}(\vec{q})$ , in order to guarantee a good description of the short time processes. Yet, this condition does not ensure that the n-pole approximation will give good results.

The moments defined by (6) can be calculated using the relation

$$\langle \omega_q^n \rangle = (-1)^{m+1} \langle [L^{n-m-1} S^z(\vec{q}), L^m S^z(-\vec{q})] \rangle / R^{zz}(\vec{q}, 0) \tag{11}$$

where L is the Liouville operator,  $LS_i^z = [H, S_i^z]$ .

In the high temperature limit the  $\delta_i$  for the Hamiltonian (1), are given by

$$\begin{aligned} \delta_1 &= 2\Omega^2, \\ \delta_2 &= J^2 + D^2 - \Omega^2, \\ \delta_3 &= \frac{J^4\Omega^2 + 12J^2D^2\Omega^2 + 6D^4\Omega^2 - 2J^2\Omega^4 - 2D^2\Omega^4}{2(J^2\Omega^2 + D^2\Omega^2 - \Omega^4)} \end{aligned} \tag{12}$$

We can explicitly write down equation (4) in the three- and four- pole approximation. They are, respectively,

given by:

$$\begin{aligned} \Psi_3^z(\vec{q}, \omega) &= \frac{z^2 + \tau_2^{-1}z + \delta_2}{z^3 + \tau_2^{-1}z^2 + (\delta_1 + \delta_2)z + \delta_1\tau_2^{-1}} \\ \Psi_4^{zz}(\vec{q}, \omega) &= \frac{z^3 + \tau_3^{-1}z^2 + (\delta_2 + \delta_3)z + \delta_2\tau_3^{-1}}{z^4 + \tau_3^{-1}z^3 + (\delta_1 + \delta_2 + \delta_3)z^2 + (\delta_1 + \delta_2)\tau_3^{-1}z + \delta_1\delta_3} \end{aligned}$$

where  $z = i\omega$ ,  $\tau_2^{-1}$  and  $\tau_3^{-1}$  are given by (9) and (10).

### III. Results and discussions

In Fig. (1.a) we show the longitudinal relaxation function  $\Omega F^{zz}(\vec{q}, \omega)$  as a function  $\omega/\Omega$  for three different values of the exchange interaction  $J/\Omega$  and  $D/\Omega = 0$ . From the figure we see that for  $J/\Omega = 1.5$

the relaxation function shows a resonant structure. On the other hand for  $J/\Omega = 3.0$  the spectrum has a central peak structure. Therefore as  $J/\Omega$  increases the collective mode (resonant structure) type dynamics goes into a central mode (central peak) type dynamics. The physical interpretation of this crossover has to do with the root-mean-square internal field associated with the

spin-spin interaction and the value of the transverse frequency. The field due to the coupling in the infinite temperature limit is

$$\langle G_{iz}^2 \rangle = \sum_{jk} J_{ij} J_{ik} \langle S_i^z S_j^z \rangle \approx \sum_j J_{ij}^2 \langle (S_i^z)^2 \rangle$$

or

$$\langle G_{iz}^2 \rangle \approx 4 \times 2J^2 = 2J^2 (q=0)$$

The root-mean square goes as  $1.4 J(0)$ . Roughly speaking for large  $R$  (or  $J/\Omega$  small) the system behaves like independent spins precessing about  $R$ . The fluctuating internal field causes damping of the precessing spins and gives the relation function its breadth. The resonant (collective mode) structure disappears when the transverse field is less than the root-mean-square internal field (or  $J/\Omega$  large). The effect of the single-ion anisotropy shown in Fig. (1.b) and Fig. (1.c), for  $D/\Omega = -1$  and  $D/\Omega = -2$ , respectively, is to enhance the central mode dynamics. In Fig. (2), we show a comparison of the 3-pole and 4-pole approximations in the dynamics, for  $D/\Omega = -1$ ,  $J/\Omega = 1.5$  and  $J/\Omega = 3.0$ . This shows a good qualitative agreement between the two approximations, although quantitatively both the collective mode frequency and central mode width diminishes in the 4-pole approximation. In Fig. (3.a) we plot  $\Omega F^{zz}(\vec{q}, \omega)$  for two different values of the transverse frequency (field)  $a = \Omega/J$  and  $D/J = 0$ . Again, one can see from Figs. (3.b) and (3.c) that the effect of the single-ion anisotropy is to destroy the collective mode excitation, enhancing the central mode behavior. This effect is shown more explicitly in Fig. (4) where we present for a given value of  $a$ , namely  $a = 2/3$ , the relaxation function for  $D/J = 0, -1, -2$ . Fig. 5 is a comparison of the dynamics of the spin-1/2 transverse Ising model and the  $D = 0$  spin-1 model in a transverse field. This figure shows how the modulus of the spin affects the dynamics. As can be seen although quantitatively different both dynamics are qualitatively similar. In order to allow a comparison between these two models we used a renormalized exchange coupling defined by  $J_s = (3tr1/tr\vec{S}_0^2)^{1/2} J$ , where  $\vec{S}_0 = s(s+1)\mathbf{1}$  and  $s$  is the modulus of the spin. In conclusion, we have shown that the influence of a single-ion anisotropy on the high-temperature dynamics of spin chains is to enhance the central mode type behavior. Concerning the

influence of the spin quantum number  $S = 1$  is to exhibit a behavior similar to the  $S = 1/2$  model.

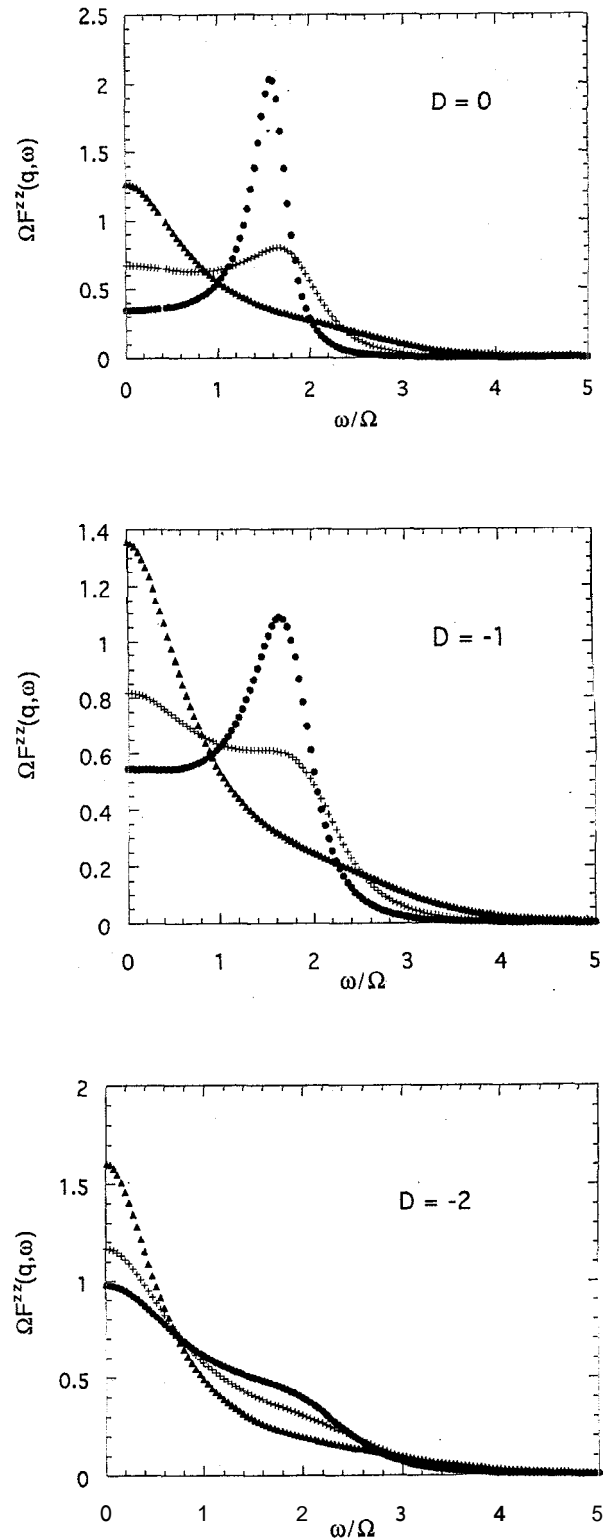


Figure 1: Longitudinal relaxation function  $\Omega F^{zz}(\vec{q}, \omega)$  as function of the frequency  $\omega/\Omega$  for  $J/\Omega = 1.5(0)$ ,  $J/\Omega = 2.0(+)$  and  $J/\Omega = 3.0(\Delta)$ , in the three-pole approximation. (a)  $D/\Omega = 0$ ; (b)  $D/\Omega = -1$ ; (c)  $D/\Omega = -2$ .

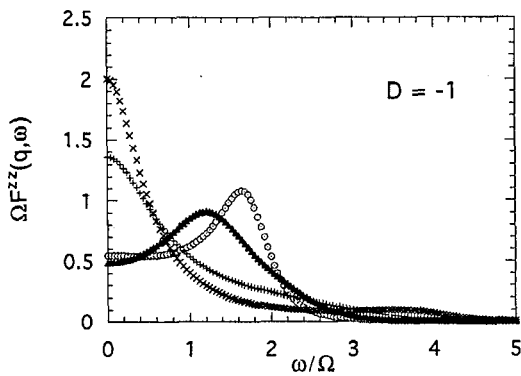


Figure 2: Longitudinal relaxation function  $\Omega F^{zz}(\vec{q}, \omega)$  as function of the frequency  $\omega/\Omega$  for  $D/\Omega = -1$ . In the three-pole approximation:  $J/\Omega = 1.5(0)$ ,  $J/\Omega = 3.0(+)$ . In the four-pole approximation:  $J/\Omega = 1.5(\Delta)$ ,  $J/\Omega = 3.0(x)$ .

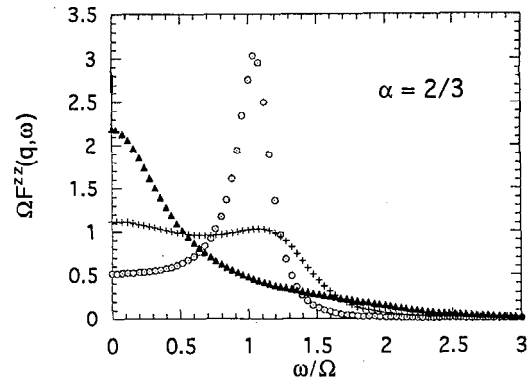


Figure 4: Longitudinal relaxation function  $\Omega F^{zz}(\vec{q}, \omega)$  as function of the frequency  $\omega/\Omega$  for  $\Omega/J = 2/3$  and  $D/J = 0(0)$ ,  $D/J = -1(+)$  and  $D/J = -2(\Delta)$ , in the three-pole approximation.

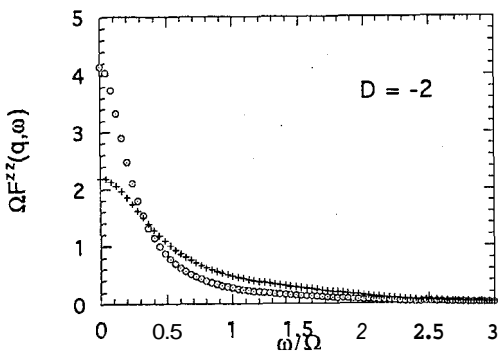
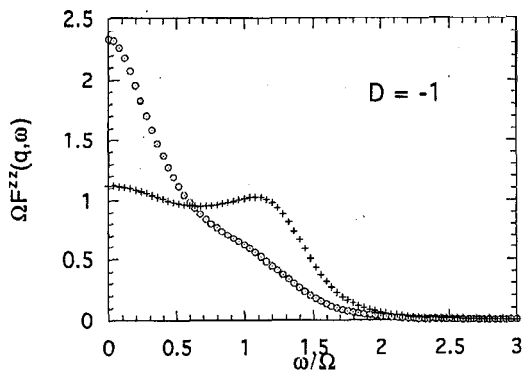
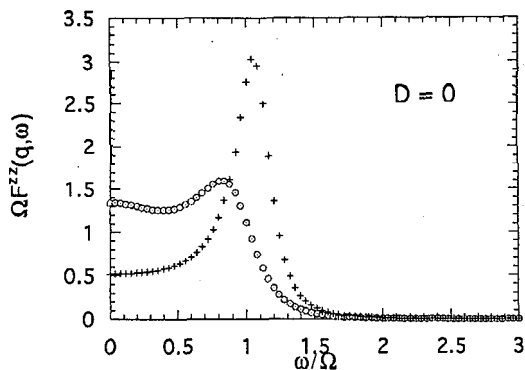


Figure 3: Longitudinal relaxation function  $\Omega F^{zz}(\vec{q}, \omega)$  as function of the frequency  $\omega/\Omega$  for  $\Omega/J = 0.5$  and  $\Omega/J = 2/3(+)$ , in the three-pole approximation. (a)  $D/J = 0$ ; (b)  $D/J = -1$ ; (c)  $D/J = -2$ .

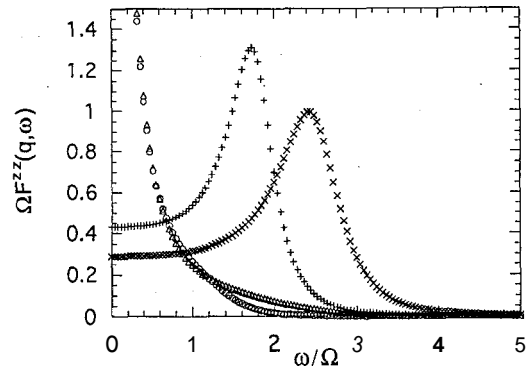


Figure 5: Longitudinal relaxation function  $\Omega F^{zz}(\vec{q}, \omega)$  as function of the frequency  $\omega/\Omega$ . For the spin-1/2 transverse Ising model for  $\Omega/J = 0.5(0)$  and  $\Omega/J = 1/5(+)$ . For the  $D = 0$  spin-1 model in a transverse field for  $R/J = 0.5(\Delta)$  and  $\Omega/J = 1.5(x)$ .

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