Anisotropic *XY* model on the inhomogeneous periodic chain

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The static and dynamic properties of the anisotropic *XY* model ($s=1/2$) on the inhomogeneous periodic chain, composed of N cells with n different exchange interactions and magnetic moments, in a transverse field h, are determined exactly at arbitrary temperatures. The properties are obtained by introducing the Jordan-Wigner fermionization and by reducing the problem to a diagonalization of a finite matrix of nth order. The quantum transitions are determined exactly by analyzing, as a function of the field, the induced magnetization $1/n\Sigma_{m=1}^{n}\mu_m\langle S_{j,m}^{z}\rangle$ (j denotes the cell, m the site within the cell, μ_m the magnetic moment at site m within the cell) and the spontaneous magnetization $1/n\Sigma_{m=1}^{n}\langle S_{j,m'}^{x}\rangle$ which is obtained from the correlations $\langle S_{j,m}^{x}S_{j+r,m}^{x}\rangle$ for large spin separations. These results, which are obtained for infinite chains, correspond to an extension of the ones obtained by Tong and Zhong [Physica B **304**, 91 (2001)]. The dynamic correlations, $\langle S_{j,m}^{z}(t)S_{j',m'}^{z}(0)\rangle$, and the dynamic susceptibility, $\chi_q^{zz}(\omega)$, are also obtained at arbitrary temperatures. Explicit results are presented in the limit $T=0$, where the critical behavior occurs, for the static susceptibility $\chi_q^{zz}(0)$ as a function of the transverse field h, and for the frequency dependency of dynamic susceptibility $\chi_q^{zz}(\omega)$.

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I. INTRODUCTION

The one-dimensional *XY* model introduced by Lieb, Schultz, and Mattis[1] is still one of the few quantum many-body problems that can be solved exactly. Although almost 45 years have passed since the original solution has been proposed, this old model continues to provide new information on the quantum behavior of magnetic systems.[2–6] In particular, it has shed some light on the quantum phase transitions,[7] since exact results can be obtained for most of its properties. The model has also been applied in the study of quantum entanglement, which plays an essential role in the quantum computation. Important results of this application can be found in the recent work by Amico *et al.*[8] and in the references therein.

In this paper we will consider the anisotropic *XY* model in a transverse field on the inhomogeneous periodic (closed) chain consisting of N cells composed of n sites, whose version on the open chain has been recently addressed by Feldman.[9] It has also been studied by Tong and Zhong[10] and Derzhko *et al.*,[11] who have restricted their analysis to the study of the thermodynamic properties. To the best of our knowledge, the work by Tong and Liu,[12] which concerns the study of the zeros of the partition function, at $T=0$, and its relation to the quantum phase transitions contains the latest results on the model.

The anisotropic model corresponds to an extension of the isotropic one recently studied by the authors.[13] Its study on the inhomogeneous periodic chain also corresponds to an extension of its version on the alternating superlattice,[14–19] and, in this work, we will solve exactly the model by considering n different exchange constants and magnetic moments. The aim of this work is to present a comprehensive study of its static and dynamic quantum critical behavior.

In Sec. II we introduce the model and diagonalize its Hamiltonian. An explicit expression is presented for $n=2$, and the results compared to the known ones obtained by various authors.[14–19] We also present the solution of the model for $n=8$, which has been obtained numerically.

The induced magnetization M^z and the isothermal susceptibility χ_T^{zz}, at arbitrary temperature, are obtained in Sec. III, and explicit expressions presented for $T=0$. By analyzing these quantities, the quantum critical behavior is studied and the critical exponents associated to the quantum transitions are obtained.

The spontaneous magnetization M^x is obtained in Sec. IV, from the two-spin correlation $\langle S_{l,m}^{x}S_{l+r,m}^{x}\rangle$, and the critical behavior is also obtained, with high accuracy, numerically, by means of a nonlinear regression of the data evaluated for finite values of r. This rather surprising result allows for the complete determination of M^x as a function of the field, and to determine the multiple quantum transitions undergone by the model.

The static and dynamic correlations $\langle \tau_l^z \tau_{l+r}^z\rangle$ are presented in Sec. V and, the dynamic susceptibility $\chi_q^{zz}(\omega)$, in Sec. VI. Finally, in Sec. VII, we summarize the main results of the paper.

II. THE MODEL

We consider the anisotropic *XY* model $\left(s=\frac{1}{2}\right)$ on the inhomogeneous periodic chain with N cells, n sites per cell, and

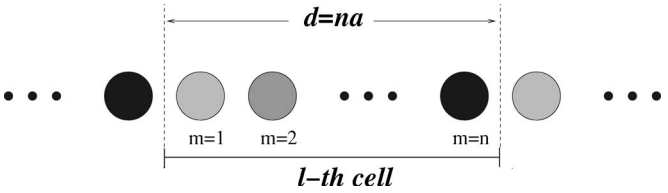

FIG. 1. Unit cell of the inhomogeneous periodic chain.

lattice parameter a, in a transverse field, whose unit cell is shown in Fig. 1, which corresponds to an extension of the isotropic model recently considered.[13] The Hamiltonian is given by

$$H = -\sum_{l=1}^{N}\left[\sum_{m=1}^{n}\mu_m h S_{l,m}^z + \left(\sum_{m=1}^{n-1} J_m(1+\gamma_m)S_{l,m}^x S_{l,m+1}^x + J_m(1-\gamma_m)S_{l,m}^y S_{l,m+1}^y\right) + J_n(1+\gamma_n)S_{l,n}^x S_{l+1,1}^x + J_n(1-\gamma_n)S_{l,n}^y S_{l+1,1}^y\right], \quad (1)$$

where the parameters $J_{l,m}$ are the exchange couplings between nearest neighbor, μ_m the magnetic moments, h the external field, and we have assumed periodic boundary conditions. If we introduce the ladder operators

$$S_{l,m}^{\pm} = S_{l,m}^x \pm iS_{l,m}^y, \quad (2)$$

and the generalized Jordan-Wigner transformation,[20]

$$S_{l,m}^{+} = \exp\left(i\pi\sum_{l'=1}^{l-1}\sum_{m'=1}^{n} c_{l',m'}^{\dagger}c_{l',m'} + i\pi\sum_{m'=1}^{m-1} c_{l,m'}^{\dagger}c_{l,m'}\right)c_{l,m}^{\dagger},$$

$$S_{l,m}^z = c_{l,m}^{\dagger}c_{l,m} - \tfrac{1}{2}, \quad (3)$$

where $c_{l,m}$ and $c_{l,m}^{\dagger}$ are fermion annihilation and creation operators, we can write the Hamiltonian as[21]

$$H = H^+P^+ + H^-P^-, \quad (4)$$

where

$$H^{\pm} = -\sum_{l=1}^{N}\left[\sum_{m=1}^{n}\mu_m h\left(c_{l,m}^{\dagger}c_{l,m} - \frac{1}{2}\right) + \sum_{m=1}^{n-1}\left(\frac{J_m}{2}(c_{l,m}^{\dagger}c_{l,m+1} + c_{l,m+1}^{\dagger}c_{l,m}) + \frac{J_m\gamma_m}{2}(c_{l,m}^{\dagger}c_{l,m+1}^{\dagger} + c_{l,m+1}c_{l,m})\right)\right] - \sum_{l=1}^{N-1}\left(\frac{J_n}{2}(c_{l,n}^{\dagger}c_{l+1,1} + c_{l+1,1}^{\dagger}c_{l,n}) + \frac{J_n\gamma_n}{2}(c_{l,n}^{\dagger}c_{l+1,1}^{\dagger} + c_{l+1,1}c_{l,n})\right) \pm \left(\frac{J_n}{2}(c_{N,n}^{\dagger}c_{1,1} + c_{1,1}^{\dagger}c_{N,n}) + \frac{J_n\gamma_n}{2}(c_{N,n}^{\dagger}c_{1,1}^{\dagger} + c_{1,1}c_{N,n})\right), \quad (5)$$

and

$$P^{\pm} = \frac{I \pm P}{2}, \quad (6)$$

with P given by

$$P = \exp\left(i\pi\sum_{l=1}^{N}\sum_{m=1}^{n} c_{l,m}^{\dagger}c_{l,m}\right). \quad (7)$$

As it is well known,[21–23] since the operator P commutes with the Hamiltonian, the eigenstates have definite parity, and $P^-(P^+)$ corresponds to a projector into a state of odd (even) parity.

Introducing periodic and antiperiodic boundary conditions on c's for H^- and H^+, respectively, the wave vectors in the Fourier transform,[14]

$$c_{l,m} = \frac{1}{\sqrt{N}}\sum_{q}\exp(-iqdl)a_{q,m},$$

$$a_{q,m} = \frac{1}{\sqrt{N}}\sum_{l=1}^{N}\exp(iqdl)c_{l,m}, \quad (8)$$

are given by $q^- = \frac{2l\pi}{Nd}$, for periodic condition and $q^+ = \frac{\pi(2l+1)}{Nd}$, for antiperiodic condition, with $l = 0, \pm 1, \ldots, \pm N/2$, and H^- and H^+ can be written in the form

$$H^{\pm} = \sum_{q^{\pm}} H_{q^{\pm}}, \quad (9)$$

where

$$H_{q^{\pm}} = -\sum_{m=1}^{n}\mu_m h\left(a_{q^{\pm},m}^{\dagger}a_{q^{\pm},m} - \frac{1}{2}\right) - \sum_{m=1}^{n-1}\frac{J_m}{2}[a_{q^{\pm},m}^{\dagger}a_{q^{\pm},m+1} + a_{q^{\pm},m+1}^{\dagger}a_{q^{\pm},m} + \gamma_m(a_{q^{\pm},m}^{\dagger}a_{q^{\pm},m+1}^{\dagger} + a_{q^{\pm},m+1}a_{q^{\pm},m})] - \frac{J_n}{2}\{a_{q^{\pm},n}^{\dagger}a_{q^{\pm},1}\exp(-idq^{\pm}) + a_{q^{\pm},1}^{\dagger}a_{q^{\pm},n}\exp(idq^{\pm}) + \gamma_m[a_{q^{\pm},n}^{\dagger}a_{q^{\pm},1}^{\dagger}\exp(-idq^{\pm}) + a_{q^{\pm},1}a_{q^{\pm},n}\exp(idq^{\pm})]\}. \quad (10)$$

Although H^- and H^+ do not commute, it can be shown that in the thermodynamic limit all the static properties of the system can be obtained in terms of H^- or H^+. However, even in this limit, some dynamic properties depend on H^- and H^+.[21–23] Since $[H_{q^{\pm}}, H_{-q^{\pm}}] \neq 0$, we consider the symmetrization

$$\widetilde{H}_{q^{\pm}} \equiv H_{q^{\pm}} + H_{-q^{\pm}}, \quad (11)$$

and the Hamiltonian $H^{\pm}$ can be written as

$$H^{\pm} = \frac{1}{2}\sum_{q^{\pm}} \widetilde{H}_{q^{\pm}}. \tag{12}$$

By making the identification $q^{\pm} \equiv q$, it follows immediately that $[\widetilde{H}_q, \widetilde{H}_{q'}]=0$. Therefore, following the procedure introduced by Lieb, Schultz, and Mattis,[1] we can diagonalize the Hamiltonian $H^{\pm}$ by introducing the canonical transformation

$$a_{q,m} = \sum_{k}^{n} \left(\frac{\psi^*_{q,k,m} + \phi^*_{q,k,m}}{2} \eta_{q,k} + \frac{\psi^*_{q,k,m} - \phi^*_{q,k,m}}{2} \eta^{\dagger}_{-q,k} \right),$$

$$a^{\dagger}_{q,m} = \sum_{k}^{n} \left(\frac{\psi_{q,k,m} + \phi_{q,k,m}}{2} \eta^{\dagger}_{q,k} + \frac{\psi_{q,k,m} - \phi_{q,k,m}}{2} \eta_{-q,k} \right), \tag{13}$$

where $\phi_{q,k,m}$ and $\psi_{q,k,m}$ are the components of the eigenvectors, $\mathbf{\Phi}_{q,k}$ and $\mathbf{\Psi}_{q,k}$, of the matrices $(\mathbb{A}_q - \mathbb{B}_q)(\mathbb{A}_q + \mathbb{B}_q)$ and $(\mathbb{A}_q + \mathbb{B}_q)(\mathbb{A}_q - \mathbb{B}_q)$, with $\mathbb{A}_q$ and $\mathbb{B}_q$ given by

$$\mathbb{A}_q = -\begin{pmatrix} \mu_1 h & \frac{J_1}{2} & 0 & \cdots & 0 & \frac{J_n}{2}\exp(iqd) \\ \frac{J_1}{2} & \mu_2 h & \frac{J_2}{2} & & & 0 \\ 0 & \frac{J_2}{2} & \mu_3 h & \frac{J_3}{2} & & \vdots \\ \vdots & & \frac{J_3}{2} & \ddots & \ddots & 0 \\ 0 & & & \ddots & \mu_{n-1} h & \frac{J_{n-1}}{2} \\ \frac{J_n}{2}\exp(-iqd) & 0 & \cdots & 0 & \frac{J_{n-1}}{2} & \mu_n h \end{pmatrix}, \tag{14}$$

$$\mathbb{B}_q = \begin{pmatrix} 0 & -\frac{J_1\gamma_1}{2} & 0 & \cdots & 0 & \frac{J_n\gamma_n}{2}\exp(iqd) \\ \frac{J_1\gamma_1}{2} & 0 & -\frac{J_2\gamma_2}{2} & & & 0 \\ 0 & \frac{J_2\gamma_2}{2} & 0 & -\frac{J_3\gamma_3}{2} & & \vdots \\ \vdots & & \frac{J_3\gamma_3}{2} & \ddots & \ddots & 0 \\ 0 & & & \ddots & 0 & -\frac{J_{n-1}\gamma_{n-1}}{2} \\ -\frac{J_n\gamma_n}{2}\exp(-iqd) & 0 & \cdots & 0 & \frac{J_{n-1}\gamma_{n-1}}{2} & 0 \end{pmatrix}. \tag{15}$$

The corresponding eigenvalues are $E^2_{q,k}$, the squares of the fermion energy levels, such that the Hamiltonian $H^{\pm}$, given in Eq. (10), can be written in the diagonal form

$$H^{\pm} = \sum_{q,k} E_{q,k}\left(\eta^{\dagger}_{q,k}\eta_{q,k} - \tfrac{1}{2}\right), \tag{16}$$

where for $H^{+}(H^{-})$ the wave vector q is identical to $q^{+}(q^{-})$, and the spectrum $E_{q,k}$ of $\widetilde{H}_q$ is determined from the determinantal equation

$$\det[(\mathbb{A}_q + \mathbb{B}_q)(\mathbb{A}_q - \mathbb{B}_q) - E^2_q \mathbb{I}] = 0. \tag{17}$$

Since we are interested in the thermodynamic limit, we will consider from here on H^{-} only, in all calculations.

Explicit expressions for the excitation spectrum can be determined for n equal to 2, 3, and 4, and for n greater than 4, it is determined numerically from Eq. (17). Since we are considering the particle-hole representation, this implies that $E_q \geqslant 0$.

Explicitly, for $n=2$, the excitation spectrum is given by

$$E_q^2 = \frac{\alpha_1 + \alpha_2 + (\lambda_1 + \lambda_2)\cos 2q}{2} \pm \frac{1}{2}\sqrt{[\alpha_1 - \alpha_2 + (\lambda_1 - \lambda_2)\cos 2q]^2 + 4[\delta_1^2 + \delta_2^2 + 2\delta_1\delta_2 \cos(2q)]}, \tag{18}$$

where

$$\alpha_1 = (\mu_1 h)^2 + \frac{J_1^2}{4}(1+\gamma_1)^2 + \frac{J_2^2}{4}(1-\gamma_2)^2,$$

$$\alpha_2 = (\mu_2 h)^2 + \frac{J_2^2}{4}(1+\gamma_2)^2 + \frac{J_1^2}{4}(1-\gamma_1)^2,$$

$$\lambda_1 = \frac{J_1 J_2}{2}(1+\gamma_1)(1-\gamma_2),$$

$$\lambda_2 = \frac{J_1 J_2}{2}(1-\gamma_1)(1+\gamma_2),$$

$$\delta_1 = \frac{J_1}{2}(1-\gamma_1)\mu_1 h + \frac{J_1}{2}(1+\gamma_1)\mu_2 h,$$

$$\delta_2 = \frac{J_2}{2}(1+\gamma_2)\mu_1 h + \frac{J_2}{2}(1-\gamma_2)\mu_2 h. \tag{19}$$

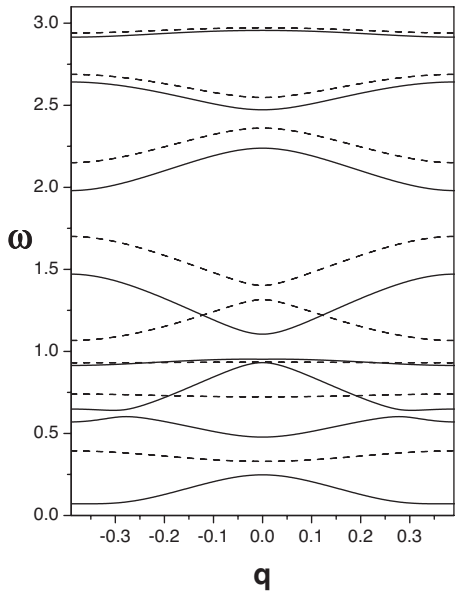

FIG. 2. Excitation spectrum for $n=8$, $J_1=J_6=J_8=1.5$, $J_2=3$, $J_3=1.5$, $J_4=J_5=J_7=2$, $h=1$, $\mu_1=\cdots=\mu_8=1$, and $\gamma_1=\cdots=\gamma_8=0.1$ (continuous line), and for $\gamma_1=0.1$, $\gamma_2=0.2$, $\gamma_3=0.3$, $\gamma_4=0.4$, $\gamma_5=0.5$, $\gamma_6=0.6$, $\gamma_7=0.7$, $\gamma_8=0.8$ (dashed line).

For $\gamma_1=\gamma_2=0$, the previous result reproduces the excitation spectrum obtained for the isotropic case,[13] provided we consider the particle representation which allows for negative energies. It also reproduces the result obtained by Siskens *et al.*[16]

As already pointed out, although explicit expressions can be determined for n equal to 3 and 4, they are not presented here since they are too cumbersome.

Even in the case where we have identical magnetic moments, differently from the isotropic case, the effect of the field does not correspond to a translation of the excitation spectrum for zero field, since the term of the field does not commute with the Hamiltonian.

The critical fields which characterize the quantum transitions are determined from the excitation spectrum by imposing the condition $E_q=0$ for $q=0$ and $q=\pi/d$.[13] The number of transitions is highly dependent on the anisotropy and varies from n to 1. In particular, the limit of a single transition always occurs for the transverse Ising model which corresponds to the γ's equal to 1.

The excitation spectrum for $n=8$ and identical magnetic moments is presented in Fig. 2 for identical and different γ's, where we have considered the lattice spacing $a=1$. As it can be seen, the energy of the modes is always positive and the effect of the spatial variation of the anisotropy is more pronounced in the low energy modes. Since there is no zero energy excitation, the model is not critical at the considered value of the transverse field.

III. THE INDUCED MAGNETIZATION AND ISOTHERMAL SUSCEPTIBILITY χ_T^{zz}

From Eqs. (3), the operator $S_{l,m}^z$ can be written as

$$S_{l,m}^z = -\tfrac{1}{2}A_{l,m}B_{l,m}, \tag{20}$$

with

$$A_{l,m} \equiv c_{l,m}^\dagger + c_{l,m},$$

$$B_{l,m} \equiv c_{l,m}^\dagger - c_{l,m}, \tag{21}$$

which can be expressed, from Eqs. (8) and (13), as

$$A_{l,m} = \frac{1}{\sqrt{N}}\sum_{q,k} e^{iqdl}\psi_{q,k,m}(\eta_{q,k}^\dagger + \eta_{-q,k}),$$

$$B_{l,m} = \frac{1}{\sqrt{N}} \sum_{q,k} e^{iqdl} \phi_{q,k,m} (\eta^{\dagger}_{q,k} - \eta_{-q,k}). \tag{22}$$

By using Eqs. (20) and (22), the local magnetization $M^z_{l,m}$ can be written as

$$M^z_{l,m} \equiv \mu_m \langle S^z_{l,m} \rangle = -\frac{1}{2N} \sum_{q,k} \mu_m \psi_{q,k,m} \phi^*_{q,k,m} (1 - 2n_{q,k}), \tag{23}$$

where the fermion occupation number $n_{q,k}$ is given by

$$n_{q,k} = \frac{1}{1 + e^{\bar{E}_{q,k}}}, \tag{24}$$

where $\bar{E}_{q,k} = \beta E_{q,k} \equiv E_{q,k}/k_B T$, and the calculation has been done by considering $H = H^-$,[21–23] since we are interested in the thermodynamic limit.

As in the isotropic model,[13] we define an average cell magnetization operator in the z direction, τ^z_l, as

$$\tau^z_l \equiv \frac{1}{n} \sum_{m=1}^{n} \mu_m S^z_{l,m}, \tag{25}$$

then the induced magnetization per site, M^z, is equal to $\langle \tau^z_l \rangle$ and, from Eq. (23), can be written in the form

$$M^z \equiv \langle \tau^z_l \rangle = -\frac{1}{2nN} \sum_{q,k,m} \mu_m \psi_{q,k,m} \phi^*_{q,k,m} \tanh\left(\frac{\bar{E}_{q,k}}{2}\right), \tag{26}$$

which at $T=0$ becomes

$$M^z = -\frac{1}{2nN} \sum_{q,k,m} \mu_m \psi_{q,k,m} \phi^*_{q,k,m}. \tag{27}$$

The isothermal susceptibility can be obtained from Eqs. (26) and (27) by means of the expression

$$\chi^{zz}_T \equiv \frac{1}{n} \frac{\partial M^z}{\partial h}, \tag{28}$$

which must be evaluated numerically.

At $T=0$, the isothermal susceptibility χ^{zz}_T diverges at the quantum critical points induced by the field. This result can be seen in Fig. 3 where M^z and χ^{zz}_T are presented as functions of the field h, at $T=0$, for a chain with $n=8$, identical μ's, $\gamma=0.1$ and 0.15. The magnetization, differently from the isotropic model, does not present plateaus but it does present inflexion points which induce the divergences of the susceptibility at the quantum phase transitions. As expected, the results also show that for n even there is the tendency of formation of a zero magnetization plateau in the limit $\gamma \to 0$, which is not present for n odd as shown in Fig. 4 for $n=5$.

At $T=0$, on the critical region, we have verified numerically that the isothermal susceptibility presents the behavior

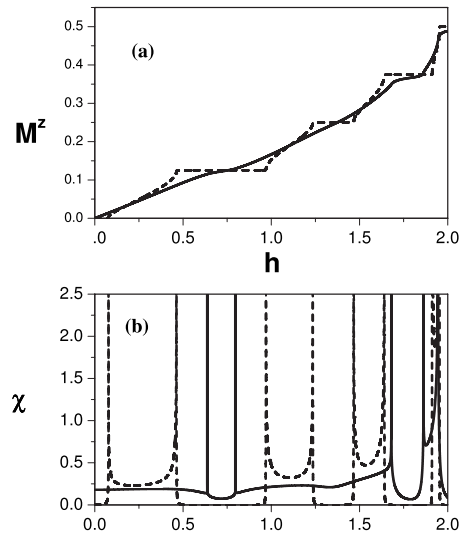

FIG. 3. (a) Magnetization M^z and (b) isothermal susceptibility χ^{zz}_T, at $T=0$, as functions of the field for $n=8$, $\mu_1=\cdots=\mu_8=1$, $J_1=J_6=J_8=1.5$, $J_2=3$, $J_3=1.5$, $J_4=J_5=J_7=2$, $\gamma=0.1$ (dashed line) and for $\gamma=0.15$ (continuous line).

$$\chi^{zz}_T \sim \ln|h - h_c| \quad (0 < \gamma_m \leq 1), \tag{29}$$

as it can be seen in the results presented in Fig. 5, for a chain with $n=4$, and identical μ's and γ's.

The transitions belong to the same universality class as the one in the homogeneous model.[24] For $T>0$ all these transitions are suppressed by the thermal fluctuations.

As already pointed out, the critical fields are associated with the zero-energy modes with $q=0$ and $q=\pi/d$, and the

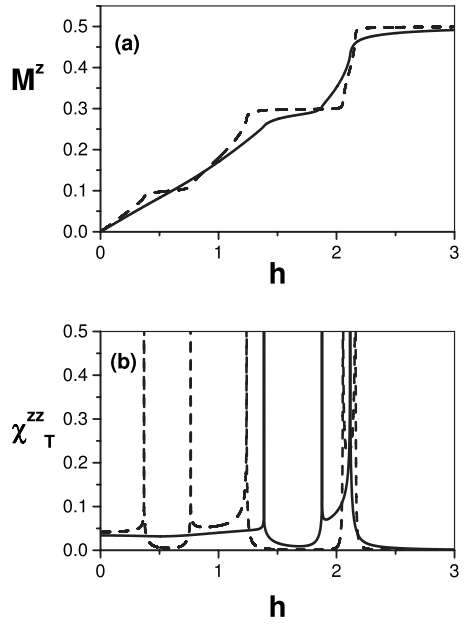

FIG. 4. (a) Magnetization M^z and (b) isothermal susceptibility χ^{zz}_T, at $T=0$, as functions of the field for $n=5$, $\mu_1=\cdots=\mu_5=1$, $J_1=1$, $J_2=1.5$, $J_3=2$, $J_4=2.5$, $J_5=3$, $\gamma=0.1$ (dashed line) and for $\gamma=0.3$ (continuous line).

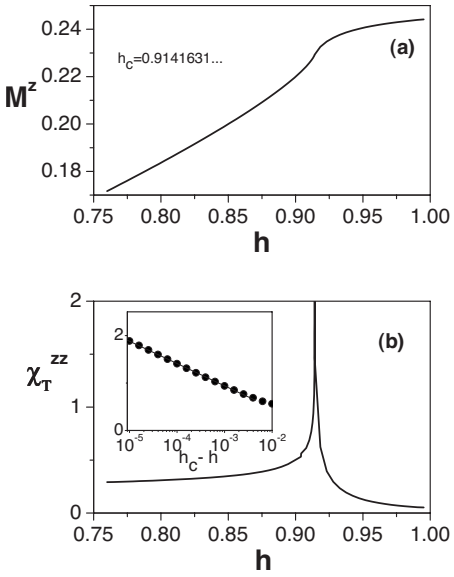

FIG. 5. (a) Magnetization M^z and (b) isothermal susceptibility χ_T^{zz}, at $T=0$ and $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$, $\gamma_1=\gamma_2=\gamma_3=\gamma_4=0.1$, as functions of the uniform field for $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2.0$. The logarithmic singular behavior of χ_T^{zz} is shown in the inset in (b) where the horizontal scale is decimal logarithmic.

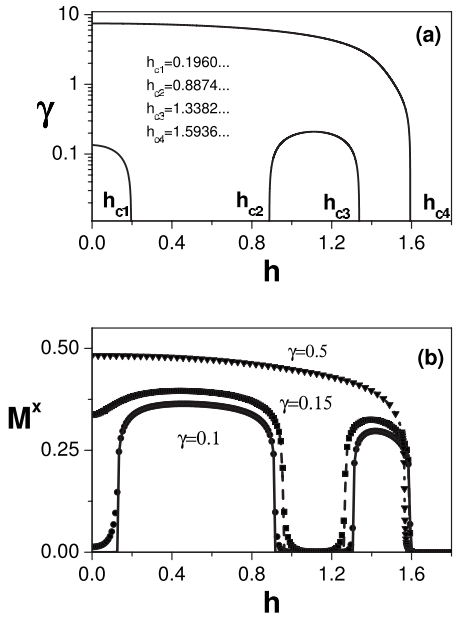

FIG. 6. (a) Critical lines, at $T=0$, for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$ and for $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$. (b) Spontaneous magnetization M^x as a function of the uniform field, for different γ, $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$ and $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$. The continuous line represents the extrapolation procedure.

number of critical points can vary from one in the transverse Ising model limit, for γ's equal to 1, to n, provided the μ's are positive. On the other hand, if we allow the μ's to assume negative values, we can have more than one phase transition even in the transverse Ising model limit, as has been shown by Derzhko *et al.*[11]

Then, the critical fields can be obtained numerically from the excitation spectrum and the results are shown in Fig. 6(a) for a chain with $n=4$, and identical μ's and γ's. As can be verified, the number of transitions depends on γ and its signature is present in the behavior of the spontaneous and induced magnetizations. From these results, we can also conclude that for n even we have two critical γ's, which can induce quantum transitions at zero field, whereas for n odd we have just a single critical γ, equal to zero, as in the uniform model.[25] This result is shown in Fig. 7 and, differently from the isotropic model, it constitutes the main effect of the cell size on the quantum critical behavior of the model.

IV. THE MAGNETIZATION M^x

Since the Hamiltonian is invariant under the transformation $S_{l,m}^x \to -S_{l,m}^x$, which means that the $\langle S_{l,m}^x \rangle$ is equal to zero, we cannot calculate the spontaneous magnetization directly by using the Hamiltonian shown in Eq. (1). On the other hand, the Hamiltonian after the introduction of an external field along the x direction, which would eliminate the mentioned symmetry property, is no more exactly soluble. Therefore, by using the original Hamiltonian, the spontaneous local magnetization, M_m^x, can be determined, from the static correlation function $\langle S_{l,m}^x S_{l+r,m}^x \rangle$, by means of the well-known decomposition[26]

$$\lim_{r\to\infty} \langle S_{l,m}^x S_{l+r,m}^x \rangle = \langle S_{l,m}^x \rangle \langle S_{l+r,m}^x \rangle. \tag{30}$$

Then we can write immediately the local spontaneous magnetization as

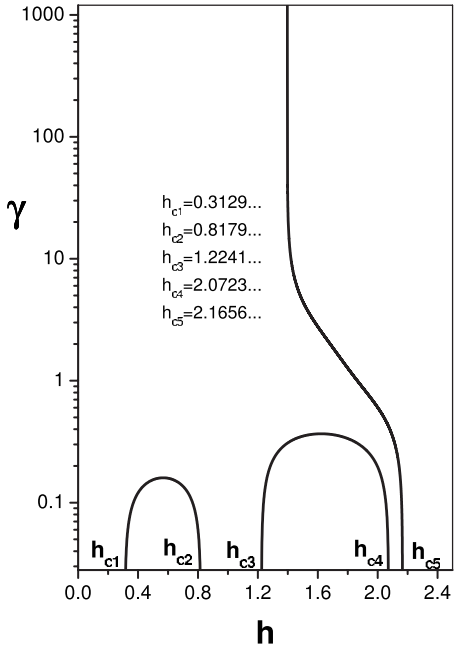

FIG. 7. Critical lines, at $T=0$, for $n=5$, $\mu_1=\mu_2=\mu_3=\mu_4=\mu_5=1$ and for $J_1=1$, $J_2=1.5$, $J_3=2$, $J_4=2.5$, $J_5=3$, where the vertical scale is decimal logarithmic.

$$M_m^x = \lim_{r\to\infty} \sqrt{\langle S_{l,m}^x S_{l+r,m}^x \rangle}, \tag{31}$$

and from this we obtain the average spontaneous magnetization per cell, M^x, given by

$$M^x = \frac{1}{n}\sum_{m=1}^{n} M_m^x. \tag{32}$$

Therefore, by using the Eqs. (2), (3), and (21), the correlation $\langle S_{l,m}^x S_{l+r,m}^x \rangle$ can be written as

$$\langle S_{l,m}^x S_{l+r,m}^x \rangle = \tfrac{1}{4}\langle B_{l,m}A_{l,m+1}B_{l,m+1}A_{l,m+2} \times B_{l,m+2}\cdots A_{l+r,m-1}B_{l+r,m-1}A_{l+r,m}\rangle. \tag{33}$$

Following Ref. 1 we can write $\langle S_{l,m}^x S_{l+r,m}^x \rangle$, by using the Wick's theorem, in terms of the determinant

$$\langle S_{l,m}^x S_{l+r,m}^x \rangle = \frac{1}{4}\det\begin{pmatrix} \langle B_{l,m}A_{l,m+1}\rangle & \langle B_{l,m}A_{l,m+2}\rangle & \cdots & \langle B_{l,m}A_{l,n}\rangle & \cdots & \langle B_{l,m}A_{l+r,m}\rangle \\ \langle B_{l,m+1}A_{l,m+1}\rangle & \langle B_{l,m+1}A_{l,m+2}\rangle & \cdots & \langle B_{l,m+1}A_{l,n}\rangle & \cdots & \langle B_{l,m+1}A_{l+r,m}\rangle \\ \langle B_{l,m+2}A_{l,m+1}\rangle & \langle B_{l,m+2}A_{l,m+2}\rangle & \cdots & \langle B_{l,m+2}A_{l,n}\rangle & \cdots & \langle B_{l,m+2}A_{l+r,m}\rangle \\ \vdots & \vdots & \ddots & & \ddots & \vdots \\ \langle B_{l,n}A_{l,m+1}\rangle & \langle B_{l,n}A_{l,m+2}\rangle & \cdots & \langle B_{l,n}A_{l,n}\rangle & \cdots & \langle B_{l,n}A_{l+r,m}\rangle \\ \vdots & \vdots & \cdots & \vdots & \cdots & \vdots \\ \langle B_{l+r,m-1}A_{l,m+1}\rangle & \langle B_{l+r,m-1}A_{l,m+2}\rangle & \cdots & \langle B_{l+r,m-1}A_{l+r,n}\rangle & \cdots & \langle B_{l+r,n}A_{l+r,n}\rangle \end{pmatrix}, \tag{34}$$

where the static contractions $\langle B_{l,m}A_{l',m'}\rangle$, at arbitrary T, are given by

$$\langle B_{l,m}A_{l',m'}\rangle = \frac{1}{N}\sum_{q,k} e^{-iqd(l'-l)}\phi_{q,k,m}\psi^*_{q,k,m'}(2n_{q,k}-1). \tag{35}$$

Therefore, in order to obtain the average spontaneous magnetization per cell, M^x, we must determine the asymptotic behavior of the determinant shown in Eq. (34). For finite temperature, it can be shown that the asymptotic behavior of the determinant is zero, which corresponds to the limit $r\to\infty$, and, as expected, there is no spontaneous magnetization at $T\neq 0$.

On the other hand, at $T=0$, the asymptotic behavior of the determinant is different from zero for values of the field where the ground state is ordered. This asymptotic behavior of the determinant can be estimated numerically by using the ε algorithm,[27] and, by using this method, we have obtained M^x for a lattice with $n=4$, identical μ's and γ's. In order to obtain the estimate of the asymptotic value of the determinant, we have considered a numerical series constructed by varying r from 56 to 80, and the results are shown in Fig. 6(b). The behavior of the magnetization close to the transition points has been obtained by adjusting the reliable numerical results in the critical region to the scaling function

$$M^x(h) = M_0|h-h_c|^{\bar{\beta}}. \tag{36}$$

By considering a nonlinear regression we have been able to obtain the adjustable parameters of the scaling function, namely, the critical field h_c, the critical exponent $\bar{\beta}$ and the amplitude M_0. These results are shown in Table I.

As it can be seen in Table I, the comparison of the numerical results, obtained from the nonlinear regression, with the exact known ones show that they are extremely precise. This rather surprising result means that the quantum critical region can be precisely described numerically by Eq. (36).

V. STATIC AND DYNAMIC CORRELATIONS $\langle \tau_l^z \tau_{l+r}^z \rangle$

The correlation function $\langle S_l^z(t)S_{l+r}^z(0)\rangle$, in the thermodynamic limit, can be obtained from the expression[21–23]

$$\langle S_{l,m}^z(t)S_{l+r,m'}^z(0)\rangle = \frac{\mathrm{Tr}[\exp(-\beta H^-)\exp(iH^-t)S_{l,m}^z\exp(-iH^-t)S_{l+r,m'}^z]}{\mathrm{Tr}[\exp(-\beta H^-)]}. \tag{37}$$

Therefore, the dynamic correlation between the effective spins in the field direction,

$$\langle \tau_l^z(t)\tau_{l+r}^z(0)\rangle = \frac{1}{n^2}\sum_{m,m'=1}^{n}\mu_m\mu_{m'}\langle S_{l,m}^z(t)S_{l+r,m'}^z(0)\rangle, \tag{38}$$

by using Eqs. (3) and (21), and Wick's theorem, can be expressed as

$$\langle \tau_l^z(t)\tau_{l+r}^z(0)\rangle = \frac{1}{4n^2}\sum_{m=1}^{n}\sum_{m'=1}^{n}\mu_m\mu_{m'}[\langle A_{l,m}(t)B_{l,m}(t)\rangle \times\langle A_{l+r,m'}(0)B_{l+r,m'}(0)\rangle - \langle A_{l,m}(t)A_{l+r,m'}(0)\rangle \times\langle B_{l,m}(t)B_{l+r,m'}(0)\rangle + \langle A_{l,m}(t)B_{l+r,m'}(0)\rangle \times\langle B_{l,m}(t)A_{l+r,m'}(0)\rangle], \tag{39}$$

where the dynamic contractions, obtained from Eq. (22), are given by

TABLE I. Numerical results for the fitting, in the scaling region, of the spontaneous magnetization M^x at $T=0$, as a function of the uniform field for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$, $\gamma_1=\gamma_2=\gamma_3=\gamma_4=\gamma$, $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$ and different γ. The parameters shown have been obtained from the nonlinear regression of the equation $M^x(h)=M_0|h_c-h|^{\bar{\beta}}$.

γ	h_c (exact)	M_0	h_c (calculated)	$\bar{\beta}$
$\gamma=0.1$	$h_{c1}=0.130554559\ldots$	0.479(8)	0.13050(1)	0.125(3)
	$h_{c2}=0.914163156\ldots$	0.465(4)	0.9142(1)	0.125(2)
	$h_{c3}=1.310209705\ldots$	0.436(8)	1.31017(6)	0.125(4)
	$h_{c4}=1.5922623078\ldots$	0.395(2)	1.59227(6)	0.126(1)
$\gamma=0.15$	$h_{c1}=0.9541874918\ldots$	0.488(12)	0.9542(3)	0.125(6)
	$h_{c2}=1.2687172332\ldots$	0.465(8)	1.26870(5)	0.125(4)
	$h_{c3}=1.5905738964\ldots$	0.423(5)	1.5906(1)	0.125(3)
$\gamma=0.5$	$h_c=1.5644253446\ldots$	0.501(9)	1.5644(2)	0.125(4)

$$\langle A_{l,m}(t)A_{l+r,m'}(0)\rangle = \frac{1}{N}\sum_{q,k} e^{-iqdr}\psi_{q,k,m}\psi^*_{q,k,m'}[e^{iE_{q,k}t}n_{q,k} + e^{-iE_{q,k}t}(1-n_{q,k})],$$

$$\langle A_{l,m}(t)B_{l+r,m'}(0)\rangle = \frac{1}{N}\sum_{q,k} e^{-iqdr}\psi_{q,k,m}\phi^*_{q,k,m'}[-e^{iE_{q,k}t}n_{q,k} + e^{-iE_{q,k}t}(1-n_{q,k})],$$

$$\langle B_{l,m}(t)B_{l+r,m'}(0)\rangle = \frac{1}{N}\sum_{q,k} e^{-iqdr}\phi_{q,k,m}\phi^*_{q,k,m'}[-e^{iE_{q,k}t}n_{q,k} - e^{-iE_{q,k}t}(1-n_{q,k})],$$

$$\langle B_{l,m}(t)A_{l+r,m'}(0)\rangle = \frac{1}{N}\sum_{q,k} e^{-iqdr}\phi_{q,k,m}\psi^*_{q,k,m'}[e^{iE_{q,k}t}n_{q,k} - e^{-iE_{q,k}t}(1-n_{q,k})]. \quad (40)$$

Then we can write the dynamic correlation $\langle \tau^z_l(t)\tau^z_{l+r}(0)\rangle$ in the form

$$\begin{aligned}\langle \tau^z_l(t)\tau^z_{l+r}(0)\rangle = \langle \tau^z_l\rangle^2 &+ \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\psi^*_{q,k,m'}\phi_{q',k',m'}\phi^*_{q',k',m}\\
&\times[e^{i(E_{q,k}+E_{q',k'})t}n_{q,k}n_{q',k'} + e^{-i(E_{q,k}+E_{q',k'})t}(1-n_{q,k})(1-n_{q',k'})\\
&+ e^{i(E_{q,k}-E_{q',k'})t}n_{q,k}(1-n_{q',k'}) + e^{-i(E_{q,k}-E_{q',k'})t}(1-n_{q,k})n_{q',k'}]\\
&- \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\phi^*_{q,k,m'}\psi_{q',k',m'}\phi^*_{q',k',m}\\
&\times[e^{i(E_{q,k}+E_{q',k'})t}n_{q,k}n_{q',k'} + e^{-i(E_{q,k}+E_{q',k'})t}(1-n_{q,k})(1-n_{q',k'})\\
&- e^{i(E_{q,k}-E_{q',k'})t}n_{q,k}(1-n_{q',k'}) - e^{-i(E_{q,k}-E_{q',k'})t}(1-n_{q,k})n_{q',k'}]. \quad (41)\end{aligned}$$

For $t=0$ we obtain the static correlation, which is given by

$$\begin{aligned}\langle \tau^z_l(0)\tau^z_{l+r}(0)\rangle = \langle \tau^z_l\rangle^2 &+ \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\psi^*_{q,k,m'}\phi_{q',k',m'}\phi^*_{q',k',m}\\
&- \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\phi^*_{q,k,m'}\psi_{q',k',m'}\phi^*_{q',k',m}(1-2n_{q,k})(1-2n_{q',k'}). \quad (42)\end{aligned}$$

At $T=0$, the dynamic and static correlation are given, respectively, by

$$\langle \tau_l^z(t)\tau_{l+r}^z(0)\rangle = \langle \tau_l^z\rangle^2 + \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\psi^*_{q,k,m'}\phi_{q',k',m'}\phi^*_{q',k',m}[e^{-i(E_{q,k}+E_{q',k'})t}]$$

$$-\frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\phi^*_{q,k,m'}\psi_{q',k',m'}\phi^*_{q',k',m}(e^{-i(E_{q,k}+E_{q',k'})t}) \quad (43)$$

and

$$\langle \tau_l^z(0)\tau_{l+r}^z(0)\rangle = \langle \tau_l^z\rangle^2 + \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\psi^*_{q,k,m'}\phi_{q',k',m'}\phi^*_{q',k',m}$$

$$-\frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\phi^*_{q,k,m'}\psi_{q',k',m'}\phi^*_{q',k',m}. \quad (44)$$

As in the homogeneous model,[25] the asymptotic behavior of the static correlation $\langle \tau_l^z(0)\tau_{l+r}^z(0)\rangle$, at $T=0$, as a function of r, can be oscillatory or monotonic depending on the values of the interaction parameters. For arbitrary n, these regions are separated by hypersurfaces in the parameter space and are called disordered surfaces, which collapse into disorder lines for identical γ's. For $n=4$, these disorder lines and the critical lines are shown in Fig. 8. Independently of the number of sites in the unit cell, in the plane $\gamma \times h$, the disorder lines are given by the equation

$$h^2 + \gamma^2 h_{jc}^2 = h_{jc}^2, \quad (45)$$

where h_{jc} is a critical field. Along these curves the anisotropic model is equivalent to an effective isotropic model.[25] For $n=2$, this equivalence is shown in the Appendix, and for $n>2$ it has been verified numerically. It is also shown that along this curve, the effective isotropic model is in a disordered state, which corresponds to the magnetization plateaus for the case where we have identical μ's.

The asymptotic behavior of the static correlation function, also for $n=4$ and at $T=0$, as a function of the distance r between cells, is presented in Fig. 9 for various values of h and γ in the different regions shown in Fig. 8. As can be seen, the behavior, as expected, alternates between oscillatory and monotonic.

At the critical point, as in the homogeneous case, the direct static correlation behaves asymptotically as r^{-2}.[25] This behavior is shown in Fig. 10(a), for $n=4$, and different critical fields. However, at the disorder line, differently from the homogeneous model where the direct static correlation is

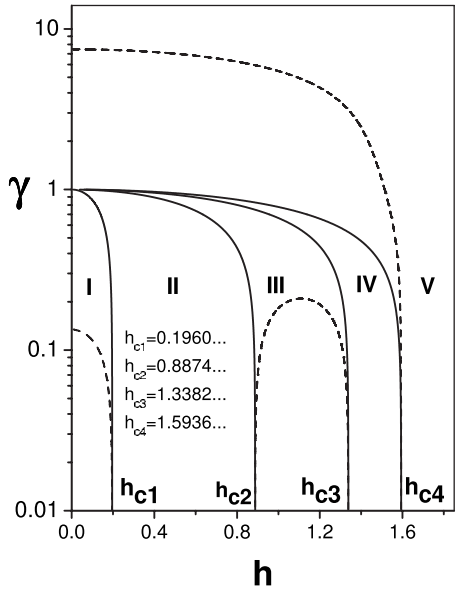

FIG. 8. Disorder lines (continuous line) and critical (dashed line), at $T=0$, for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$ and for $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$, where the vertical scale is decimal logarithmic. The asymptotic behavior alternates between monotonic and oscillatory as we go from region I to region V.

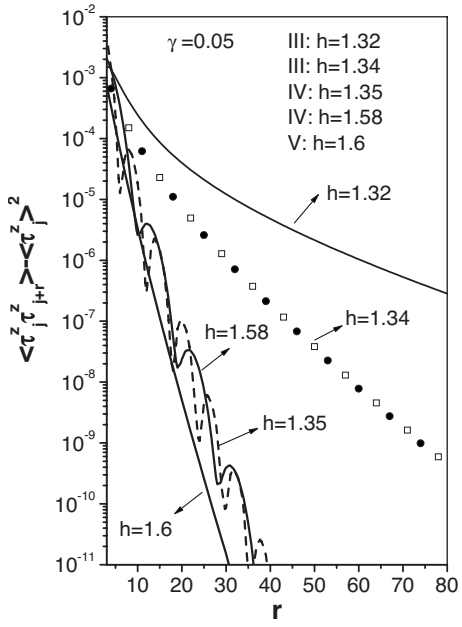

FIG. 9. Static correlation function in the field direction, at $T=0$, for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$ and for $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$, as function of r (distance between cells) for values of the field belonging to different regions shown in Fig. 8, where the vertical scale is decimal logarithmic.

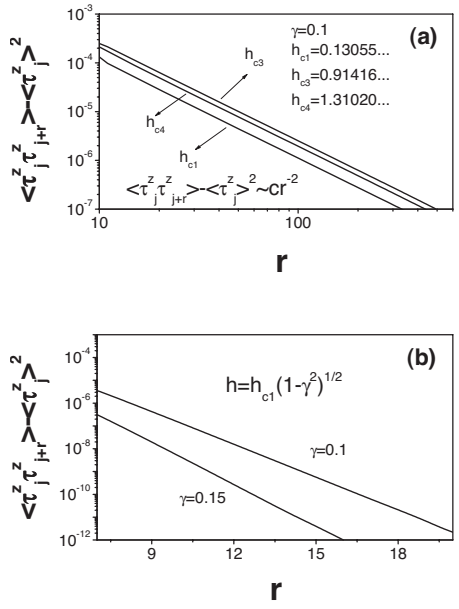

FIG. 10. Asymptotic behavior of the direct static correlation function in the field direction, at $T=0$, for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$ and for $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$, as a function of r (distance between cells) for values of the field belonging to the critical lines (a), where the scales are decimal logarithmic, and disorder lines (b), where the vertical scale is also decimal logarithmic.

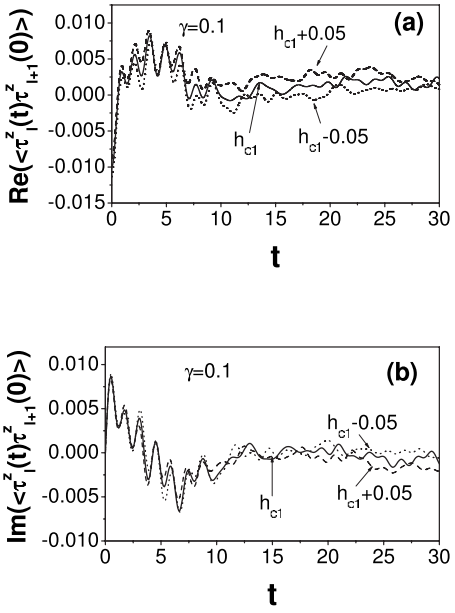

FIG. 11. (a) The real and (b) imaginary parts of the dynamic correlation function $\langle \tau_l^z(t)\tau_{l+1}^z(0)\rangle$, at $T=0$ for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$ and $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$, as function of time t.

zero, it behaves asymptotically as λ^{-r}, where λ is a function of the field and of the interaction parameters, as shown in Fig. 10(b), for identical γ's and different values of the field.

The real and imaginary parts of the dynamic correlation for a chain with $n=4$ and uniform μ's, at $T=0$, are presented in Fig. 11 for values of the field greater, smaller and equal to the critical field. As in the isotropic case, apart from the asymptotic behavior, no noticeable difference is observed in the dynamic correlation at different values of the field.

VI. DYNAMIC SUSCEPTIBILITY

From the dynamic correlation $\langle \tau_l^z(t)\tau_{l+r}^z(0)\rangle$, Eqs. (41), we can obtain the time Fourier transform of dynamic correlation $\langle \tau_l^z\tau_{l+r}^z\rangle_\omega$ from the equation

$$\langle \tau_l^z\tau_{l+r}^z\rangle_\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle \tau_l^z(t)\tau_{l+r}^z(0)\rangle e^{i\omega t}dt, \tag{46}$$

which is given by

$$\begin{aligned}\langle \tau_l^z\tau_{l+r}^z\rangle_\omega = {} & \delta(\omega)\langle \tau_l^z\rangle^2 + \frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\psi^*_{q,k,m'}\phi_{q',k',m'}\phi^*_{q',k',m}\\
& \times[\delta(\omega+E_{q,k}+E_{q',k'})n_{q,k}n_{q',k'}+\delta(\omega-E_{q,k}-E_{q',k'})(1-n_{q,k})(1-n_{q',k'})\\
& +\delta(\omega+E_{q,k}-E_{q',k'})n_{q,k}(1-n_{q',k'})+\delta(\omega-E_{q,k}+E_{q',k'})(1-n_{q,k})n_{q',k'}]\\
& -\frac{1}{4n^2N^2}\sum_{q,k,m}\sum_{q',k',m'}\mu_m\mu_{m'}e^{-i(q-q')dr}\psi_{q,k,m}\phi^*_{q,k,m'}\psi_{q',k',m'}\phi^*_{q',k',m}\\
& \times[\delta(\omega+E_{q,k}+E_{q',k'})n_{q,k}n_{q',k'}+\delta(\omega-E_{q,k}-E_{q',k'})(1-n_{q,k})(1-n_{q',k'})\\
& -\delta(\omega+E_{q,k}-E_{q',k'})n_{q,k}(1-n_{q',k'})-\delta(\omega-E_{q,k}+E_{q',k'})(1-n_{q,k})n_{q',k'}].\end{aligned} \tag{47}$$

By introducing the spatial Fourier transform

$$\langle \tau_q^z\tau_{-q}^z\rangle_\omega = \sum_r \langle \tau_l^z\tau_{l+r}^z\rangle_\omega e^{idrq}, \tag{48}$$

in the previous expression, we can write immediately

$$\langle \tau_q^z \tau_{-q}^z \rangle_\omega = N\delta_{q,0}\delta(\omega)\langle \tau_l^z \rangle^2 + \frac{1}{4n^2N}\sum_{q',k,m,k',m'} \mu_m \mu_{m'} \psi_{q',k,m} \psi^*_{q',k,m'} \phi_{q'-q,k',m'} \phi^*_{q'-q,k',m}$$
$$\times [\delta(\omega + E_{q',k} + E_{q'-q,k'}) n_{q',k} n_{q'-q,k'} + \delta(\omega - E_{q',k} - E_{q'-q,k'})(1-n_{q',k})(1-n_{q'-q,k'})$$
$$+ \delta(\omega + E_{q',k} - E_{q'-q,k'}) n_{q',k}(1-n_{q'-q,k'}) + \delta(\omega - E_{q',k} + E_{q'-q,k'})(1-n_{q',k}) n_{q'-q,k'}]$$
$$- \frac{1}{4n^2N}\sum_{q',k,m,k',m'} \mu_m \mu_{m'} \psi_{q',k,m} \phi^*_{q',k,m'} \psi_{q'-q,k',m'} \phi^*_{q'-q,k',m}$$
$$\times [\delta(\omega + E_{q',k} + E_{q'-q,k'}) n_{q',k} n_{q'-q,k'} + \delta(\omega - E_{q',k} - E_{q-q',k'})(1-n_{q',k})(1-n_{q-q',k'})$$
$$- \delta(\omega + E_{q',k} - E_{q'-q,k'}) n_{q',k}(1-n_{q'-q,k'}) - \delta(\omega - E_{q',k} + E_{q'-q,k'})(1-n_{q',k}) n_{q'-q,k'}]. \quad (49)$$

The dynamic susceptibility $\chi_q^{zz}(\omega)$ can be obtained by using the expression[28]

$$\chi_q^{zz}(\omega) = -\int_\infty^\infty \frac{(1-e^{-\omega'/k_BT})\langle \tau_q^z \tau_{-q}^z \rangle_{\omega'} d\omega'}{\omega - \omega'}, \quad (50)$$

and from this we obtain

$$\chi_q^{zz}(\omega) = -\frac{1}{4n^2N}\sum_{q',k,m,k',m'} \mu_m \mu_{m'} \left(P_{q',k,m,q'-q,k',m'} - Q_{q',k,m,q'-q,k',m'}\right)$$
$$\times \left(\frac{1}{\omega + E_{q',k} + E_{q'-q,k'}} - \frac{1}{\omega - E_{q',k} - E_{q'-q,k'}}\right)(n_{q',k} + n_{q'-q,k'} - 1)$$
$$- \frac{1}{4n^2N}\sum_{q',k,m,k',m'} \mu_m \mu_{m'} (P_{q',k,m,q'-q,k',m'} + Q_{q',k,m,q'-q,k',m'})$$
$$\times \left(\frac{1}{\omega + E_{q',k} - E_{q'-q,k'}} - \frac{1}{\omega - E_{q',k} + E_{q'-q,k'}}\right)(n_{q',k} - n_{q'-q,k'}), \quad (51)$$

where

$$P_{q',k,m,q'-q,k',m'} = \psi_{q',k,m} \psi^*_{q',k,m'} \phi_{q'-q,k',m'} \phi^*_{q'-q,k',m}, \quad (52)$$

$$Q_{q',k,m,q'-q,k',m'} = \psi_{q',k,m} \phi^*_{q',k,m'} \psi_{q'-q,k',m'} \phi^*_{q'-q,k',m}, \quad (53)$$

and we have used the identity

$$1 - n_{q,k} = e^{\beta E_{q,k}} n_{q,k}. \quad (54)$$

It should be noted that the previous result reduces to the known one for the isotropic model.[13]

The static susceptibility $\chi_q^{zz}(0)$ is obtained by making $\omega=0$ in Eq. (51), and is given by

$$\chi_q^{zz}(0) = -\frac{1}{2n^2N}\sum_{q',k,m,k',m'} \mu_m \mu_{m'} (P_{q',k,m,q'-q,k',m'} - Q_{q',k,m,q'-q,k',m'}) \left(\frac{1}{E_{q',k} + E_{q'-q,k'}}\right)(n_{q',k} + n_{q'-q,k'} - 1)$$
$$- \frac{1}{2n^2N^2}\sum_{q',k,m,k',m'} (P_{q',k,m,q'-q,k',m'} + Q_{q',k,m,q'-q,k',m'}) \left(\frac{1}{E_{q',k} - E_{q'-q,k'}}\right)(n_{q',k} - n_{q'-q,k'}). \quad (55)$$

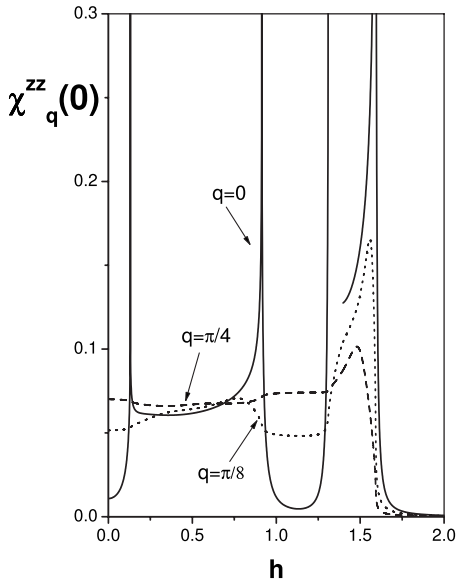

FIG. 12. Static susceptibility in the field direction, $\chi_q^{zz}(0)$, at $T=0$, as a function of the field for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$, $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$, $\gamma=0.1$ and different values of q.

The isothermal susceptibility can also be obtained by using the dynamic correlation given in Eq. (41), and can be written as[29]

$$\chi_T^{zz} = \sum_r \int_0^\beta (\langle \tau_l^z(-i\lambda)\tau_{l+r}^z(0)\rangle - \langle \tau_l^z\rangle^2) d\lambda, \tag{56}$$

where, as defined previously, $\beta=1/k_BT$. From this it can be shown that the isothermal susceptibility in the field direction is equal to the uniform static one $\chi_0^{zz}(0)$.

At $T=0$, the dynamic and static susceptibilities given in Eqs. (51) and (55) can be explicitly written as

$$\chi_q^{zz}(\omega) = \frac{1}{4n^2N} \sum_{q',k,m,k',m'} \mu_m\mu_{m'}(P_{q',k,m,q'-q,k',m'} - Q_{q',k,m,q'-q,k',m'}) \tag{57}$$

$$\times \left(\frac{1}{\omega + E_{q',k} + E_{q'-q,k'}} - \frac{1}{\omega - E_{q',k} - E_{q'-q,k'}} \right) \tag{58}$$

and

$$\chi_q^{zz}(0) = \frac{1}{2n^2N} \sum_{q',k,m,k',m'} \mu_m\mu_{m'}(P_{q',k,m,q'-q,k',m'} - Q_{q',k,m,q'-q,k',m'}) \left(\frac{1}{E_{q',k} + E_{q'-q,k'}} \right). \tag{59}$$

The static susceptibility $\chi_q^{zz}(0)$, at $T=0$ and for $n=4$, as a function of the field is presented in Fig. 12. For $q=0$, as expected, it diverges at the critical fields and it tends to zero as $h\to\infty$, which corresponds to the saturation of the model. However, for $q\neq 0$ differently from the isotropic model, no divergence is present, even for a wave vector at the zone boundary.

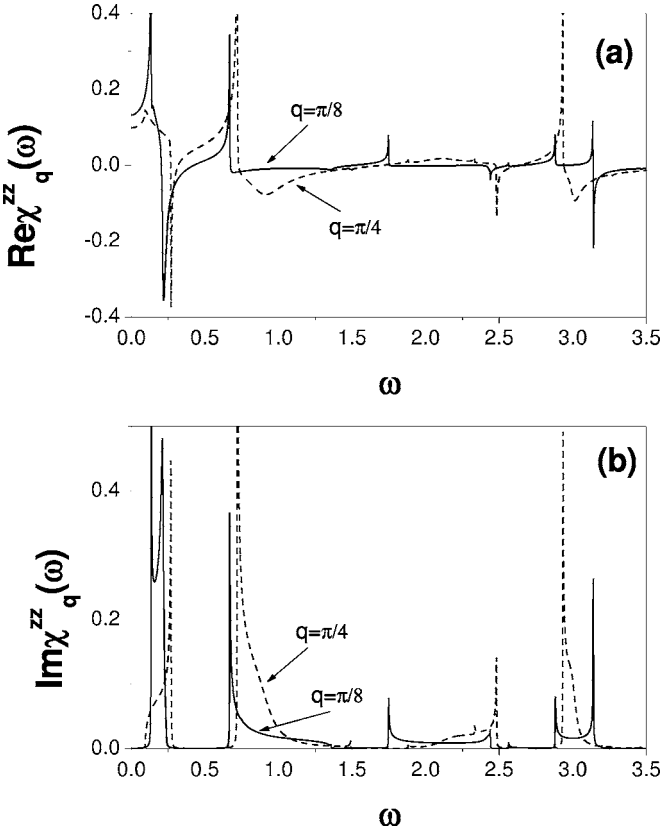

FIG. 13. (a) The real and (b) imaginary parts of the dynamic susceptibility $\chi_q^{zz}(\omega)$, at $T=0$, for $n=4$, $\mu_1=\mu_2=\mu_3=\mu_4=1$, $J_1=1$, $J_2=1.5$, $J_3=1.75$, $J_4=2$, $h=0.5$, and $\gamma=0.1$, as function of frequency ω and for different values of q.

The real and imaginary parts of $\chi_q^{zz}(\omega)$ are obtained by considering $\chi_q^{zz}(\omega-i\epsilon)$ in the limit $\epsilon\to 0$ in Eqs. (51) and (55). The results, at $T=0$ and for $n=4$, are shown in Fig. 13 for different wave vectors, as functions of ω. As expected, since the Hamiltonian of the model preserves the symmetry of the spin interactions of the homogeneous one, the divergences in the real part, for any wave vector, correspond to square-root singularities in the imaginary part.

VII. CONCLUSIONS

In this work we have considered the anisotropic XY model on the inhomogeneous periodic chain with N cells and n sites per cell. The model has been exactly solved, at arbitrary temperature, for the general case where we have n different exchange constants and n different magnetic moments. The number of branches of the excitation spectrum is equal to n, and analytical results can be found for $n\leqq 4$. For $n=2$, explicit expressions are presented for the excitation spectrum, and, for $n=8$, it is obtained numerically.

The induced magnetization M^z and the isothermal susceptibility χ_T^{zz} are also given by explicit expressions at arbitrary temperature. At $T=0$, where the quantum transitions induced by the transverse field occur, the spontaneous magnetization M^x is written in terms of the asymptotic behavior of the determinant of a Toeplitz matrix which corresponds to the

static two-spin correlation in the x direction, at large separation. The critical behavior is determined, in high numerical accuracy, by adjusting the numerical results obtained for finite Toeplitz matrices by using a nonlinear regression of the scaling relation and the ε algorithm. This is a rather remarkable result since it allows us to determine very precisely the critical behavior of the system within a numerical approach. As expected, we have shown from these results that the inhomogeneous model belongs to the same universality class of the homogeneous one.

For $n>1$, the system can present multiple phase transitions and it is shown that the divergence of the isothermal susceptibility χ_T^{zz}, which is associated to inflection points in the induced magnetization, is also a signature of the quantum transitions. These critical points, as usual, correspond to the points where the spontaneous magnetization, which is the order parameter characterizing the quantum transition, goes to zero.

Explicit results are presented for $n=4$ and $n=5$, where we show that, differently from the isotropic model where we always have n transitions, the number of quantum transitions is dependent on the values of the anisotropy parameters γ. We have also concluded that, for n even, there are two critical γ's, whereas, for n odd, there is just one critical γ equal to zero, and this constitutes the main effect of the cell size on the critical quantum behavior of the anisotropic model.

It has also been shown that the static two-spin correlation in the z direction, as in the homogeneous model, can present oscillatory or monotonic behavior depending on the values of γ's and the field. The limiting surfaces, in the parameter space, which separates the two regimes, are the so-called disorder surfaces. For the special case when we have different J's and identical γ's, the disorder surfaces collapse into disorder lines and, in this case, they have been determined analytically. In particular, for $n=2$, it has been proven exactly that these lines correspond to regions where the model can be mapped onto an equivalent isotropic model. It should be noted that along the disorder lines the direct static correlation $\langle\tau_l^z(0)\tau_{l+r}^z(0)\rangle-\langle\tau_l^z\rangle^2$ presents an exponential asymptotic behavior, differently from the homogeneous model where it is equal to zero.

We have also obtained the static and dynamic correlation on the field directions and, from these results, we have determined the dynamic wave-vector dependent susceptibility $\chi_q^{zz}(\omega)$. Finally, we have shown that, as in the homogeneous model, the static susceptibility $\chi_0^{zz}(0)$ is equal to the isothermal one χ_T^{zz}.

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APPENDIX

In this appendix we present analytically the mapping of the anisotropic model onto the isotropic one, for a given set of parameters, for a chain with $n=2$. This mapping will be obtained, as in the homogeneous model,[25] by imposing that the isotropic and the anisotropic models have the same spectrum. As it will be shown, this equivalence is only possible when $\gamma_1=\gamma_2$.

Therefore, let us consider the matrices $\mathbb{A}_q$ and $\mathbb{B}_q$, given by Eqs. (14) and (15), which in this case are explicitly given by

$$\mathbb{A}_q=-\begin{pmatrix} \mu_1 h & \frac{J_1}{2}+\frac{J_2}{2}\exp(-i2q) \\ \frac{J_1}{2}+\frac{J_2}{2}\exp(i2q) & \mu_2 h \end{pmatrix}, \tag{A1}$$

$$\mathbb{B}_q=-\begin{pmatrix} 0 & \frac{J_1\gamma_1}{2}-\frac{J_2\gamma_2}{2}\exp(-i2q) \\ -\frac{J_1\gamma_1}{2}+\frac{J_2\gamma_2}{2}\exp(i2q) & 0 \end{pmatrix}. \tag{A2}$$

From these results we obtain the matrix $(\mathbb{A}_q+\mathbb{B}_q)$ $(\mathbb{A}_q-\mathbb{B}_q)$, whose eigenvalues, determined from Eq. (17), which constitute the two branches of the spectrum of the chain, are given by

$$\begin{aligned} E_{q,k=1,2}^2 = {} & \tfrac{1}{2}[\alpha_1+\alpha_2+(c_1+c_2)\cos 2q] \pm \tfrac{1}{2}\{[\alpha_1+\alpha_2+(c_1 \\ & +c_2)\cos 2q]^2-4[(\alpha_1+c_1\cos 2q)(\alpha_2+c_2\cos 2q) \\ & -\beta^2-\delta^2-2\beta\delta\cos 2q]\}^{1/2}, \end{aligned} \tag{A3}$$

where

$$\begin{aligned} &\alpha_1\equiv\mu_1^2h^2+a_1^2+b_2^2, \quad \alpha_2\equiv\mu_2^2h^2+a_2^2+b_1^2, \\ &a_1\equiv\frac{J_1}{2}(1+\gamma_1), \quad a_2\equiv\frac{J_2}{2}(1+\gamma_2), \\ &b_1\equiv\frac{J_1}{2}(1-\gamma_1), \quad b_2\equiv\frac{J_2}{2}(1-\gamma_2), \\ &c_1\equiv\frac{J_1J_2}{2}(1+\gamma_1)(1-\gamma_2), \quad c_2\equiv\frac{J_1J_2}{2}(1-\gamma_1)(1+\gamma_2), \\ &\beta\equiv(\mu_1b_1+\mu_2a_1)h, \quad \delta\equiv(\mu_1a_2+\mu_2b_2)h. \end{aligned} \tag{A4}$$

From the previous result we can obtain the spectrum of the isotropic chain, with parameters $\mu_1'h'$, $\mu_2'h'$, J_1', J_2', by making $\gamma_1=\gamma_2=0$ and from this we can write

$$\begin{aligned} \varepsilon_{q,k=1,2}^2 = {} & \frac{1}{2}\left[(\mu_1'^2+\mu_2'^2)h'^2+\frac{J_1'^2}{2}+\frac{J_2'^2}{2}+J_1'J_2'\cos 2q\right] \\ & \pm\frac{1}{2}(\mu_1'+\mu_2')h' \\ & \times\sqrt{(\mu_1'-\mu_2')^2h'^2+J_1'^2+J_2'^2+2J_1'J_2'\cos 2q}. \end{aligned} \tag{A5}$$

By imposing the equivalence of the two spectra we conclude immediately that we should have $c_1=c_2\equiv c$, which implies that $\gamma_1=\gamma_2\equiv\gamma$. Introducing these conditions in Eq. (A3) we obtain

$$E^2_{q,k=1,2}=\tfrac{1}{2}[\alpha_1+\alpha_2+2c\cos 2q] \pm \tfrac{1}{2}\sqrt{(\alpha_1-\alpha_2)^2+4(\beta^2+\delta^2)+8\beta\delta\cos 2q}, \tag{A6}$$

and by comparing it with Eq. (A5) we can write immediately the mapping relations

$$(\mu_1'^2+\mu_2'^2)h'^2+\frac{J_1'^2}{2}+\frac{J_2'^2}{2}=(\mu_1^2+\mu_2^2)h^2+\frac{(J_1^2+J_2^2)}{2}(1+\gamma^2), \tag{A7}$$

$$J_1'J_2'=J_1J_2(1-\gamma^2), \tag{A8}$$

$$(\mu_1'^2-\mu_2'^2)^2h'^4+h'^2(\mu_1'+\mu_2')^2(J_1'^2+J_2'^2) =(\mu_1^2-\mu_2^2)^2h^4+\gamma^2(J_1^2-J_2^2)^2 +(J_1^2+J_2^2)[(\mu_1+\mu_2)^2h^2-\gamma^2(\mu_1-\mu_2)^2h^2], \tag{A9}$$

$$(\mu_1'+\mu_2')^2h'^2J_1'J_2'=J_1J_2[(\mu_1+\mu_2)^2h^2-\gamma^2(\mu_1-\mu_2)^2h^2]. \tag{A10}$$

This set of equations is not independent, and this means that the parameters of the equivalent isotropic model are not uniquely determined. Moreover, we can show that Eqs. (A7)–(A10) can only present a solution if the parameters of the anisotropic model satisfy the equation

$$(J_1^2-J_2^2)^2(1-\gamma^2)^2-8\mu_1\mu_2h^2(J_1^2+J_2^2)(1-\gamma^2)+16\mu_1^2\mu_2^2h^4=0. \tag{A11}$$

This expression is obtained after some lengthy but straightforward algebra, by using the result

$$(\mu_1'+\mu_2')^2h'^2=\frac{(\mu_1+\mu_2)^2h^2-\gamma^2(\mu_1-\mu_2)^2h^2}{1-\gamma^2}, \tag{A12}$$

which is obtained from Eqs. (A7) and (A10), and Eqs. (A7), (A8), and (A12). The solution of Eq. (A11) gives the result

$$h=\pm\frac{|J_1\pm J_2|\sqrt{1-\gamma^2}}{2\sqrt{\mu_1\mu_2}}\equiv\tilde{h}_c\sqrt{1-\gamma^2}, \tag{A13}$$

where $\tilde{h}_c$ are the critical fields of the anisotropic model in the limit $\gamma\to 0$. Although this result, for the disorder lines, is restricted to $n=2$, we have verified numerically that, for identical γ's, it is still valid for arbitrary n. In particular, for $n=4$, the numerical verification of Eq. (A13) is shown in Fig. 8.

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[1] H. E. Lieb, T. Schultz, and D. C. Mattis, Ann. Phys. **16**, 407 (1961).
[2] E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
[3] T. N. Nguyen, P. A. Lee, and H. C. Loye, Science **27**, 489 (1996).
[4] P. Gambardella, A. Dallmeyer, K. Maiti, M. C. Malagoli, W. Eberhardt, K. Kern, and C. Carbone, Nature (London) **416**, 301 (2002).
[5] C. J. Mukherjeea, R. Coldea, D. A. Tennant, M. Kozac, M. Enderlec, K. Habichtd, P. Smeibidld, and Z. Tylczynski, J. Magn. Magn. Mater. **272-276**, 920 (2004).
[6] M. Matsumoto, B. Normand, T. M. Rice, and M. Sigrist, Phys. Rev. B **69**, 054423 (2004).
[7] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 2000).
[8] L. Amico, F. Baroni, A. Fubini, D. Patanè, V. Tognetti, and P. Verrucchi, Phys. Rev. A **74**, 022322 (2006).
[9] K. E. Feldman, J. Phys. A **39**, 1039 (2006).
[10] P. Tong and M. Zhong, Physica B **304**, 91 (2001).
[11] O. Derzhko, J. Richter, T. Krokhmalskii, and O. Zaburannyi, Phys. Rev. E **69**, 066112 (2004).
[12] P. Tong and X. Liu, Phys. Rev. Lett. **97**, 017201 (2006).
[13] J. P. de Lima, T. F. A. Alves, and L. L. Gonçalves, J. Magn. Magn. Mater. **298**, 95 (2006).
[14] F. F. Barbosa Filho, J. P. de Lima, and L. L. Gonçalves, J. Magn. Magn. Mater. **226-230**, 638 (2001).
[15] J. P. de Lima and L. L. Gonçalves, Physica A **311**, 458 (2002).
[16] Th. J. Siskens, H. W. Capel, and J. H. H. Perk, Phys. Lett. **53A**, 21 (1975).
[17] J. H. H. Perk, H. W. Capel, M. J. Zuilhof, and Th. J. Siskens, Physica A **81**, 319 (1975).
[18] J. H. H. Perk and H. W. Capel, Physica A **100A**, 1 (1980).
[19] J. H. Taylor and G. Müller, Physica A **130**, 1 (1985).
[20] L. L. Gonçalves and J. P. de Lima, J. Magn. Magn. Mater. **140-144**, 1606 (1995).
[21] Th. J. Siskens and P. Mazur, Physica (Amsterdam) **71**, 560 (1974).
[22] H. W. Capel and J. H. H. Perk, Physica A **87**, 211 (1977).
[23] L. L. Gonçalves, thesis, University of Oxford, 1977.
[24] Th. Niemeijer, Physica (Amsterdam) **37**, 377 (1967).
[25] E. Barouch and B. M. McCoy, Phys. Rev. A **3**, 786 (1971).
[26] H. E. Stanley, *Phase Transitions and Critical Phenomena* (Oxford University Press, Oxford, 1971).
[27] M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by J. Lebowitz and C. Domb (Academic, London, 1983), Vol. 8, p. 146.
[28] D. N. Zubarev, Sov. Phys. Usp. **3**, 320 (1960).
[29] See, for instance, W. Marshall and S. W. Lovesey, *Theory of Ther mal Neutron Scattering* (Oxford University Press, Oxford, 1971), Appendix B.