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Explicit thermostatics of Stanley's *n*-vector model on the harmonic chain by Fourier analysis

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Abstract

Thermostatic properties of Stanley's classical n-vector model on the harmonic chain are studied. It is shown that this model belongs to a rather general class of classical spin models in one dimension. The members of this class are characterized by spins which are elements of a homogenous space with transformation group G and a G-invariant and exchange-invariant spin-pair interaction. For the derivation of basic thermostatic quantities and correlation functions we use the method of abstract Fourier analysis. This allows to derive rather explicit results for any member of the aforementioned class of spin models. We present an exact closed-form expression as well as a high- and a low-temperature expansion for the free energy of Stanley's n-vector model on the harmonic chain. From this basic thermostatic quantities like internal energy, entropy and heat capacity are obtained. Furthermore, we present results for expectation values of one-spin and two-spin functions. From the latter it is possible to derive the zero-field susceptibility and it also allows for a discussion of magnetostrictive effects.

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1. Introduction

Exactly solvable one-dimensional models have always been and still are of considerable interest in statistical mechanics [1]. These models often may serve to caricature the behaviour of certain quasi-one-dimensional substances. Moreover, they "give us some insight into what is going on and also provide a valuable testing ground for approximation methods which are often applied to higher dimensional problems" [2]. Both arguments even apply in the classical limit. In contrast to one-dimensional quantum models, classical ones often allow for a complete analytical treatment.

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The aim of this paper is to provide in detail exact and explicit thermostatic results for a one-dimensional classical "spin" model, namely, Stanley's classical n-vector model on the harmonic chain [3]. In particular, the influence of the coupling between rotational and vibrational degrees of freedom is obtained for all values of $n \geqslant 1$. For the Ising case ($n = 1$) this has been done earlier by Mattis and Schultz (see Appendix of [4] and also p. 108 of [5] and references therein) with emphasis on the phenomenon of magnetostriction. Clearly, for zero coupling our results reduce to those of Stanley [6] for all n.

The method we are going to use is that of abstract Fourier (or harmonic) analysis known from the theory of group representation. The application of group-theoretical methods for the evaluation of spin models has, according to our knowledge, for the first time been used by Joyce [7] in an exact solution for the one-dimensional and in a high-temperature expansion of the higher-dimensional classical Heisenberg ($n = 3$) and planar rotator model ($n = 2$). For a more general class of classical models in one dimension a group-theoretical approach is due to Romerio and Vuillermot [8]. These authors have calculated the eigenvalues of the transfer matrix using the method of abstract Fourier analysis. Unfortunately, these group-theoretical methods have not found much attention for the evaluation of classical spin models. Only in connection with lattice-gauge theories the Fourier analysis has been used in strong-coupling expansions [9]. For this reason, we will present the method of abstract Fourier analysis as applied to a rather general class of classical spin models in full detail.

We proceed as follows. In the next section, we introduce Stanley's n-vector model on the harmonic chain and derive an effective spin Hamiltonian which takes into account the effect of the vibrational degrees of freedom. In Section 3 we construct a rather general class of classical spin models of which the n-vector model is a particular member. One characteristic property of this class of models is that their spins take values in a homogeneous space. This property together with a transformation-invariant and exchange-invariant spin-pair interaction allows for an explicit evaluation of basic thermostatic properties. Section 4 presents explicit results for the partition function and static expectation values of one-spin and two-spin functions. A general formula for the correlation length is also presented. In Section 5 we discuss these results for the particular n-vector model we are interested in. Finally, in Section 6 we compare our approach with that of Romerio and Vuillermot [8] and also point out further possible applications of the method presented. In two appendices we discuss the effect of boundary conditions on thermostatic properties of the finite chain (Appendix A) and consider (Appendix B) a particular subclass of models whose spins take values in a group.

2. The n-vector model on the harmonic chain

The many-body system the thermal equilibrium properties of which we want to derive can be described as follows. Consider the one-dimensional Bravais lattice $\ell\mathbb{Z}$

with lattice constant $\ell > 0$ and a set of $N+1$ point particles all of mass $m > 0$ spaced along the Euclidean line $\mathbb{R}$ at positions $j\ell + q_j$ $(j = 1,\dots,N+1)$. Denoting the momentum of the jth particle by $p_j \in \mathbb{R}$, the Hamiltonian H_0 defined by

$$H_0 := \frac{1}{2m}\sum_{j=1}^{N+1} p_j^2 + \frac{m}{2}\,\omega_0^2 \sum_{j=1}^{N}(q_j - q_{j+1})^2 \tag{2.1}$$

characterises the nearest-neighbour coupled *harmonic chain* with "spring constant" $m\omega_0^2$. It models the energy of the vibrational degrees of freedom of a (quasi-)one-dimensional monoatomic crystal in the harmonic approximation, that is, under the assumption that for any two atoms the difference $q_j - q_{j'}$ of their deviations from their respective lattice sites $j\ell$ and $j'\ell$ is sufficiently small [10].

We assume now that each particle carries a set of internal rotational degrees of freedom which we collectively represent by a classical *spin*, that is, by a unit vector $\boldsymbol{S}_j$ in the n-dimensional Euclidean space $\mathbb{R}^n$ for some fixed $n \in \{1,2,\dots\}$. The simplest rotational invariant interaction between the spins of two nearest neighboured particles corresponds to an energy of the form $-W_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}$, where the interaction strength W_j should vary with the actual interparticle distance according to $W_j = W(\ell + q_{j+1} - q_j)$ with some real-valued even function $x \mapsto W(x)$ independent of j. In accordance with the harmonic approximation we retain only the first two terms in a Taylor expansion of W:

$$W(\ell + q_{j+1} - q_j) \approx J + (q_{j+1} - q_j)\eta\ . \tag{2.2}$$

Here we have set $J := W(\ell)$ and $\eta := W'(\ell)$. Under these assumptions the total spin-interaction energy is given by the Hamiltonian

$$H_1 := -\sum_{j=1}^{N}\Big(J + (q_{j+1} - q_j)\eta\Big)\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \tag{2.3}$$

and the total Hamiltonian for the vibrational and rotational degrees of freedom is the sum

$$H := H_0 + H_1\ . \tag{2.4}$$

It characterises the many-body system we are actually going to study in a purely classical treatment.

By introducing the new particle coordinates (cf. [4,5] for $n = 1$)

$$x_1 := q_1\ , \qquad x_j := q_j - \frac{\eta}{m\omega_0^2}\sum_{k=1}^{j-1}\boldsymbol{S}_k \cdot \boldsymbol{S}_{k+1}\ , \quad j = 2,3,\dots,N+1\ , \tag{2.5}$$

the Hamiltonian (2.4) can be rewritten as

$$H = H_{vib} + H_{spin} \tag{2.6}$$

with a vibrational part

$$H_{vib} := \frac{1}{2m}\sum_{j=1}^{N+1} p_j^2 + \frac{m}{2}\,\omega_0^2\sum_{j=1}^{N}(x_j - x_{j+1})^2 \tag{2.7}$$

and a spin part

$$H_{spin} := -\sum_{j=1}^{N}\left(J\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1} + K(\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1})^2\right)\,, \qquad K := \frac{\eta^2}{2m\omega_0^2}\geqslant 0\,. \tag{2.8}$$

Obviously, the vibrational and rotational degrees of freedom are decoupled in the new coordinates. Since the thermal properties of the harmonic chain are well known (see, for example, [10]), we will concentrate on the derivation of those related to the spin-chain Hamiltonian (2.8). To this end, we will employ abstract Fourier analysis in the spirit of Joyce [7] and Romerio and Vuillermot [8].

Special cases of the spin-chain Hamiltonian (2.8) have already been discussed in the literature. In the absence of spin-vibrational coupling, $K = 0$, it corresponds to the well-known n-vector model introduced [6] and extensively discussed [6, 11] by Stanley. For vanishing spin-spin coupling, $J = 0$, and $n \in \{2, 3\}$ the thermostatic properties of the spin chain (2.8) have been derived by Vuillermot and Romerio [12]. As for the Ising case ($n = 1$), we remark that the biquadratic term in (2.8) lowers the specific free energy of the Ising chain simply by the constant K. However, even for $n = 1$ this term is responsible for magnetostrictive effects of the full system (2.6), as discussed by Mattis and Schultz [4, 5]. As an aside we mention that a quantum version of (2.8) is of interest in connection with Haldane's conjecture [13].

3. Generalization of the model

In this section we will embed the model (2.8) into a class of one-dimensional classical spin systems previously suggested by Romerio and Vuillermot [8]. We are going to describe this class in three steps.

Let us begin with the definition of the "spin space" M. We will assume that this space is a homogeneous space with transformation group G. That is, for each pair $(S, S_0) \in M \times M$ there exists a group element $g \in G$ such that

$$S = gS_0\,. \tag{3.1}$$

An element or point S of the space M will be called "spin" throughout this paper. Furthermore, we will assume that the group G is compact. This assumption assures the existence of a unique normalized invariant measure $\mathrm{d}g$ on G [14, p. 131; 15, p. 67], i.e., the normalized Haar measure. Normalization means that

$$\int_G \mathrm{d}g = 1 \tag{3.2}$$

and invariance means invariance under left and right shifts as well as under inversion:

$$\int_G \mathrm{d}g\, f(g) = \int_G \mathrm{d}g\, f(g_0 g) = \int_G \mathrm{d}g\, f(g g_0) = \int_G \mathrm{d}g\, f(g^{-1}) \tag{3.3}$$

for all integrable complex–valued functions $f : G \to \mathbb{C}$ and all $g_0 \in G$.

The normalized Haar measure $\mathrm{d}g$ induces a G-invariant probability measure $\mathrm{d}S$ on the spin space M [14, p. 143; 15, p. 128], which may be defined by

$$\int_M \mathrm{d}S\, F(S) := \int_G \mathrm{d}g\, F(gS_0)\,, \tag{3.4}$$

where $S_0 \in M$ is fixed and $F : M \to \mathbb{C}$ is such that the mapping $g \mapsto F(gS_0)$ is integrable with respect to $\mathrm{d}g$. The measure $\mathrm{d}S$ is independent of the particular choice of S_0. Its normalization

$$\int_M \mathrm{d}S = 1 \tag{3.5}$$

and G-invariance

$$\int_M \mathrm{d}S\, F(g_0 S) = \int_M \mathrm{d}S\, F(S) \tag{3.6}$$

are direct consequences of the properties (3.2) and (3.3) of $\mathrm{d}g$ and guarantees a uniform *a priori* probability distribution on M.

As any homogeneous space, M can be identified with the group quotient G/G_0 where

$$G_0 := \{g \in G \,|\, gS_0 = S_0\} \tag{3.7}$$

is the isotropy group of some fixed $S_0 \in M$. Different choices for the particular point S_0 correspond to different but equivalent realizations of M in terms of G/G_0. In the following we will consider only the case where G_0 is non-trivial in the sense that G_0 does not only consist of the unit element e, $G_0 \neq \{e\}$. For the special case $G_0 = \{e\}$ see Appendix B.

Having set up the spin space $M = G/G_0$ we can, in a second step, introduce a G-invariant and exchange-invariant spin-pair interaction $V : M \times M \to \mathbb{R}$:

$$V(gS, gS') = V(S, S') = V(S', S) \quad \text{for all } g \in G\,. \tag{3.8}$$

It is also convenient to define for a given S_0 the following function

$$v(g) := \int_G \mathrm{d}\tilde{g}\, V(\tilde{g} g S_0, \tilde{g} S_0) = V(S_0, gS_0)\,. \tag{3.9}$$

It can easily be verified using (3.8) that

$$V(S, S') = v(g^{-1} g') = v({g'}^{-1} g)\,, \tag{3.10}$$

where $S =: gS_0$ and $S' =: g'S_0$. It is obvious that v is invariant under arbitrary left and right shifts of G_0:

$$v(g) = v(hgh') \quad \text{for all} \quad h, h' \in G_0 \,. \tag{3.11}$$

Such functions on G are called *zonal spherical functions* [16, 17, p.31; 14, p. 227]. Therefore, for a non-trivial isotropy group G_0 we will assume that the pair interaction is characterized by a zonal spherical function.

In a third step for the definition of the class of spin chains we set up the Hamiltonian. To a given set of $N+1$ spins $\{S_1, \ldots, S_{N+1}\} \subset M$ and an invariant pair interaction (3.8) we associate an interaction energy by the sum

$$\mathscr{H} := \sum_{j=1}^{N} V(S_j, S_{j+1}) = \sum_{j=1}^{N} v(g_j^{-1} g_{j+1}) = \sum_{j=1}^{N} v(g_{j+1}^{-1} g_j) \,. \tag{3.12}$$

When one views S_j as the spin attached to the jth lattice site of the one-dimensional Bravais lattice $\mathbb{Z}$, the energy (3.12) can be interpreted as the Hamiltonian of a classical spin chain with nearest-neighbor interaction.

The basic thermostatic properties of such a spin chain can be derived from the canonical partition function Z for the finite chain, as a function of β, in the macroscopic limit $N \to \infty$. Here $k_B\beta$ denotes the inverse absolute temperature and k_B Boltzmann's constant. Clearly, for the finite chain one has to impose boundary conditions the dependence of which will disappear for $N \to \infty$ (see also Appendix A). Here we will work with open boundary conditions for which the partition function is defined as

$$\begin{aligned} Z &:= \int_M \mathrm{d}S_1 \cdots \int_M \mathrm{d}S_{N+1} \, \exp\{-\beta \mathscr{H}\} \\ &= \int_G \mathrm{d}g_1 \cdots \int_G \mathrm{d}g_{N+1} \prod_{j=1}^{N} \exp\{-\beta v(g_j^{-1} g_{j+1})\} \,. \end{aligned} \tag{3.13}$$

In the above we have utilized (3.4) and (3.12) to express the integrals over the spin space M by integrals over the group G.

Correspondingly, the equilibrium expectation value of a general complex–valued $(N+1)$-spin function $A : (S_1, \ldots, S_{N+1}) \mapsto A(S_1, \ldots, S_{N+1})$ is defined by

$$\langle A \rangle := \frac{1}{Z} \int_G \mathrm{d}g_1 \ldots \int_G \mathrm{d}g_{N+1} \, A(g_1 S_0, \ldots, g_{N+1} S_0) \prod_{j=1}^{N} \exp\{-\beta v(g_j^{-1} g_{j+1})\} \,. \tag{3.14}$$

Up to now we have used a notation which implicitly assumes that the transformation group G is continuous. Even so, the formulations are easily changed to the case of finite groups. For a finite group the group integrals have to be understood as normalized sums over the group elements, that is, $\int_G \mathrm{d}g\,(\cdot) = (1/|G|) \sum_{g \in G} (\cdot)$ where $|G|$ stands for the order of the group G. For example, in the Ising model where $M \simeq Z_2 := \{-1, +1\}$, we have $\int_G \mathrm{d}g\,(\cdot) \equiv \frac{1}{2}\sum_{g\in Z_2}(\cdot)$ (see also Appendix B). More general classical discrete spin models with finite symmetry groups are extensively discussed by Moraal [18].

It is obvious that the model we are mainly interested in, the n-vector model defined by (2.8), belongs to the class of models characterized in this section. For M one has to choose the $(n-1)$-dimensional unit sphere embedded in $\mathbb{R}^n$, which may be identified with the quotient $SO(n)/SO(n-1)$. For the spin-pair interaction characterized by (3.10) one has to choose

$$v(g) = -J\,(\boldsymbol{S}_0 \cdot g\boldsymbol{S}_0) - K\,(\boldsymbol{S}_0 \cdot g\boldsymbol{S}_0)^2\ . \tag{3.15}$$

4. Exact evaluation by Fourier analysis

In this section we will perform the calculation of the partition function and certain expectation values for models belonging to the class defined in Section 3. We will utilize the symmetry of these models by applying abstract Fourier analysis. This idea dates back at least to the pioneering works of Joyce [7] and Romerio and Vuillermot [8].

For a simple presentation of Fourier analysis on $M = G/G_0$ we will make the further (technical) assumption that M is a symmetric homogeneous space. For such spaces it is known [19] that the Hilbert space $L^2(M)$ can be uniquely decomposed into an orthogonal sum of invariant subspaces $\mathscr{D}^l$, $L^2(M) = \oplus_{l\in\Lambda}\mathscr{D}^l$. Each of these subspaces carries a unitary irreducible representation $D^l(g)$. These are called *representations of class one relative to* G_0 [17]. The set Λ is the equivalence class of all unitary irreducible representations of class one of the group G. A further property of these subspaces $\mathscr{D}^l$ is that they contain exactly one vector, denoted by $|l,0\rangle$, being invariant under transformations of the subgroup G_0, that is, $D^l(h)|l,0\rangle = |l,0\rangle$ for all $h \in G_0$. The set of diagonal matrix elements $D^l_{00}(g) := \langle l,0|D^l(g)|l,0\rangle = \left(D^l_{00}(g^{-1})\right)^*$, $l \in \Lambda$, forms a complete set in the linear subspace of zonal spherical functions and obeys the orthonormality relation [17, p. 47]

$$\int_G \mathrm{d}g'\, D^l_{00}(g^{-1}g')\,D^{l'}_{00}(g'^{-1}g'') = \frac{\delta_{ll'}}{d_l}\,D^l_{00}(g^{-1}g'')\,, \qquad d_l := \dim\mathscr{D}^l\ . \tag{4.1}$$

Throughout this paper, we will reserve the value $l = 0$ for the one-dimensional trivial representation which is always contained in the set Λ. This implies $D^0_{00}(g) = 1$ for all g and hence by unitarity

$$|D^l_{00}(g)| \leqslant D^0_{00}(g)\,. \tag{4.2}$$

By the completeness of the set $\{D^l_{00}\}$ the zonal spherical function $\exp\{-\beta v(g)\}$ can be (abstractly) Fourier expanded as follows:

$$\exp\{-\beta v(g)\} = \sum_{l\in\Lambda} d_l\,\lambda_l(\beta)\,D^l_{00}(g)\,, \tag{4.3}$$

where the Fourier coefficients are defined by

$$\lambda_l(\beta) := \int_G \mathrm{d}g \, \exp\{-\beta v(g)\} D^l_{00}(g^{-1}) \,, \qquad l \in \Lambda \,. \tag{4.4}$$

These coefficients obey the strict inequality

$$|\lambda_l(\beta)| < \lambda_0(\beta), \qquad l \neq 0 \,. \tag{4.5}$$

This is a consequence of (4.2) in combination with (4.1) for $l' = 0$ and $l \neq 0$. It should also be noted that despite the fact that the matrix elements $D^l_{00}(g)$ are in general complex, the Fourier coefficients (4.4) are real. This is a direct consequence of the symmetry (3.10).

With the decomposition (4.3) we can put the partition function (3.13) into the form

$$Z = \int_G \mathrm{d}g_1 \cdots \int_G \mathrm{d}g_{N+1} \prod_{j=1}^{N} \sum_{l_j \in \Lambda} d_{l_j} \lambda_{l_j}(\beta) D^{l_j}_{00}(g_j^{-1} g_{j+1}) \,. \tag{4.6}$$

Using the orthonormality (4.1) we can immediately perform $(N-1)$ integrations to obtain

$$Z = \int_G \mathrm{d}g_1 \int_G \mathrm{d}g_{N+1} \sum_{l \in \Lambda} d_l \, [\lambda_l(\beta)]^N \, D^l_{00}(g_1^{-1} g_{N+1}) \,. \tag{4.7}$$

Using again (4.1) in combination with $D^0_{00}(g) = 1$ we can perform the remaining two integrations to arrive at the simple expression

$$Z = [\lambda_0(\beta)]^N \,. \tag{4.8}$$

As a consequence, the basic thermostatic properties of the corresponding spin chain are completely determined by the Fourier coefficient $\lambda_0(\beta)$ of the trivial representation which is just the average of the Boltzmann weight $\exp\{-\beta v(g)\}$ for the spin-pair interaction with respect to the normalized Haar measure:

$$\lambda_0(\beta) = \int_G \mathrm{d}g \, \exp\{-\beta v(g)\} = \int_M \mathrm{d}S \, \exp\{-\beta V(S_0, S)\} \,. \tag{4.9}$$

Fourier analysis is not only useful for the calculation of the partition function but also allows for simple and straightforward calculations of equilibrium expectation values. For simplicity we will consider only two-spin functions $A : M \times M \to \mathbb{C}$. The calculation of their expectation values can be done similarly to that of the partition function. The result is

$$\langle A(S_j, S_{j+r}) \rangle = \sum_{l \in \Lambda} d_l \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)} \right)^r \int_G \mathrm{d}g \int_G \mathrm{d}g' \, D^l_{00}(g^{-1} g') A(gS_0, g'S_0) \,, \tag{4.10}$$

where $1 \leqslant j < j + r \leqslant N + 1$. This expression can be simplified further by introducing a function as in (3.9):

$$a(g) := \int_G d\tilde{g}\, A(\tilde{g}gS_0, \tilde{g}S_0)\,. \tag{4.11}$$

Obviously, a is a zonal spherical function with Fourier coefficients

$$a_l := \int_G dg\, a(g)\, D^l_{00}(g^{-1})\,. \tag{4.12}$$

Making the substitution $g \mapsto g'g$ in (4.10) one arrives at the simple relation

$$\langle A(S_j, S_{j+r})\rangle = \sum_{l\in A} d_l\, a_l \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)}\right)^r\,. \tag{4.13}$$

Let us also briefly consider expectation values of spin-one functions $A(S,S') = A_1(S)$ which may be called "generalized magnetizations". In this case the function (4.11) is a constant, $a(g) = a_0$, and the magnetization explicitly reads

$$\langle A_1(S_j)\rangle = a_0 = \int_M dS\, A_1(S)\,. \tag{4.14}$$

This expectation value is independent of the spin "position" j and, more importantly, does not depend on the temperature. It is just the uniform average of $A_1(S)$ over the spin space M. The reason for this result is, of course, the symmetry (3.11) of the pair interaction. A non-trivial magnetization can only arise if one allows for an explicit breaking of the postulated symmetry of the Hamiltonian, for example, by switching on an external magnetic field. The relation (3.11), which was essential in the derivation of (4.14), is then no longer sufficient to arrive at (4.14).

The expressions derived so far in this section are valid for the finite chain as they stand. The simple dependence of the partition function (4.8) on the chain length N and the N-independence of the expectation value (4.13) are direct consequences of our choice of open boundary conditions. Results for other boundary conditions are a bit more complicated and some of them will be given in Appendix A for illustrative purposes.

The basic thermostatic properties of the spin chain are determined by the free energy per spin in the macroscopic limit $N \to \infty$,

$$F(\beta) := -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N+1} \ln Z = -\frac{1}{\beta} \ln \lambda_0(\beta)\,, \tag{4.15}$$

which only depends on the Fourier coefficient of the trivial representation. In contrast, to the general two-spin expectation values (4.13) all other Fourier coefficients contribute.

The general result (4.13) also allows to obtain a fairly explicit expression for the (inverse) correlation length defined as follows:

$$\frac{1}{\xi_A(\beta)} := -\lim_{r\to\infty}\lim_{N\to\infty}\left[\frac{1}{r}\ln\left|\langle A(S_j,S_{j+r})\rangle - a_0\right|\right] . \tag{4.16}$$

Obviously, it can be put into the form

$$\xi_A(\beta) = \left[\ln\left(\frac{\lambda_0(\beta)}{\rho_A(\beta)}\right)\right]^{-1} , \tag{4.17}$$

where $\rho_A(\beta) := \sup_{l\neq 0, a_l\neq 0}|\lambda_l(\beta)| < \lambda_0(\beta)$.

Let us now make use of the results of this section to derive thermal equilibrium properties of the n-vector model introduced in Section 2.

5. Explicit results for the n-vector model on the harmonic chain

The spins of the n-vector model defined by H_{spin} in (2.8) take values in the $(n-1)$-dimensional unit sphere which may be represented by the group quotient $SO(n)/SO(n-1)$. Let us choose for the fixed vector $\boldsymbol{S}_0$ the unit vector pointing in the direction of the nth coordinate axis in the embedding space $\mathbb{R}^n$. We may obtain any vector $\boldsymbol{S}_j$ via a rotation in $\mathbb{R}^n$. Let g_j be the corresponding $(n\times n)$-rotation matrix being an element of $SO(n)$. Then any spin configuration on the chain can be obtained from the fixed vector $\boldsymbol{S}_0$ by

$$\boldsymbol{S}_j = g_j\boldsymbol{S}_0 , \quad j = 1,\ldots,N+1 . \tag{5.1}$$

Obviously, the Hamiltonian H_{spin} is of the form (3.12). Note that

$$\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1} = (g_j\boldsymbol{S}_0)\cdot(g_{j+1}\boldsymbol{S}_{j+1}) = \boldsymbol{S}_0\cdot(g_j^{-1}g_{j+1}\boldsymbol{S}_0) . \tag{5.2}$$

Furthermore, the vector $\boldsymbol{S}_0$ is invariant under all rotations about itself which form the subgroup $G_0(\boldsymbol{S}_0) = SO(n-1)$. In other words, the spin space may, indeed, be identified with the group quotient $SO(n)/SO(n-1)$.

Before we start to calculate the Fourier coefficients $\lambda_l(\beta)$ defined in (4.4) we recall some basic properties of the unitary irreducible class-one representations of $SO(n)$ [15, 17, 19]. The complete set of such representations is given by $\Lambda = \{0,1,2,\ldots\}$ and the Hilbert space decomposes into an orthogonal sum of irreducible subspaces as follows, $L^2(SO(n)/SO(n-1)) = \oplus_{l=0}^{\infty}\mathscr{D}^l$. The representation $D^l(g)$ in each of these subspaces has dimension

$$d_l = (2l+n-2)\frac{\Gamma(l+n-2)}{\Gamma(l+1)\Gamma(n-1)} , \tag{5.3}$$

where Γ denotes Euler's gamma function. Let us choose a complete orthonormal basis in $\mathscr{D}^l$ by $|l,\nu\rangle$, $\nu = 0,1,\ldots,d_l-1$ where, according to the general procedure of

Section 4, we have defined $|l,0\rangle$ such that $D(h)|l,0\rangle = |l,0\rangle$ for all $h \in SO(n-1)$. The corresponding matrix element explicitly reads

$$D^l_{00}(g) = \frac{\Gamma(l+1)\,\Gamma(n-2)}{\Gamma(l+n-2)}\, C_l^{(n-2)/2}(\cos\theta)\,, \tag{5.4}$$

where C_l^ν are Gegenbauer polynomials and θ is the angle of the rotation represented by the group element g. In particular, the $l = 1$ representation has dimension n and thus represents the matrices in (5.1) which map $\boldsymbol{S}_0$ to $\boldsymbol{S}_j$, i.e., $D^1(g) = g$. In this representation space $|1,0\rangle = \boldsymbol{S}_0$ and the scalar product reads

$$\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} = \boldsymbol{S}_0 \cdot D^1(g_j^{-1} g_{j+1})\boldsymbol{S}_0 = D^1_{00}(g_j^{-1} g_{j+1})\,. \tag{5.5}$$

We are now prepared for the calculation of the Fourier coefficients. From the general expression (4.4) we read off

$$\begin{aligned}\lambda_l(\beta) &= \int\limits_{SO(n)} \mathrm{d}g \exp\{\beta J D^1_{00}(g) + \beta K [D^1_{00}(g)]^2\}\, D^l_{00}(g)\\ &= \frac{\Gamma(n/2)\Gamma(l+1)\,\Gamma(n-2)}{\sqrt{\pi}\,\Gamma(\frac{n-1}{2})\Gamma(l+n-2)} \int\limits_0^\pi \mathrm{d}\theta \sin^{n-2}\theta \exp\left\{\beta J \cos\theta + \beta K \cos^2\theta\right\}\\ &\quad \times C_l^{(n-2)/2}(\cos\theta)\\ &= \frac{\Gamma(l+1)\,\Gamma(n-2)}{\Gamma(l+n-2)}\, C_l^{(n-2)/2}\left(\frac{1}{\beta}\frac{\partial}{\partial J}\right)\lambda_0(\beta)\,.\end{aligned} \tag{5.6}$$

For the second step we have made use of the explicit form of the real matrix elements (5.4) and of the normalized Haar measure $\mathrm{d}g$ on $SO(n)$ [17]. As they stand, the above expressions are only valid for $n > 2$. However, by setting $n = 2$ in the final results derived below one gets correct expressions for the planar–rotator chain, too. For the Ising limit $n \downarrow 1$ some more care has to be taken. Actually, it is better and simpler to discuss the Ising model separately, as for this case the (two) Fourier coefficients can be obtained in closed form (see Appendix B). Closed-form expressions of (5.6) for arbitrary $n > 1$ and $l \geqslant 0$ we know only for $K = 0$,

$$\lambda_l(\beta) = \Gamma(n/2)\left(\frac{2}{\beta J}\right)^{\frac{n-2}{2}} \mathrm{I}_{l+(n-2)/2}(\beta J)\,, \tag{5.7}$$

or for $J = 0$,

$$\begin{aligned}\lambda_{2p}(\beta) &= \frac{\Gamma(n/2)\,\Gamma(p+1/2)}{\sqrt{\pi}\,\Gamma(2p+n/2)}\,(\beta K)^p\, {}_1F_1(p+1/2; 2p+n/2; \beta K)\,,\\ \lambda_{2p+1}(\beta) &= 0\,, \quad p = 0,1,2,\ldots\,.\end{aligned} \tag{5.8}$$

Here I_ν denotes the modified Bessel function of order ν and ${}_1F_1(a;b;\cdot)$ stands for the confluent hypergeometric function with parameters a and b. The result (5.7), which has already been given by Stanley [6,20], can be obtained from standard integral tables.

See, for example, formula (7.321) of [21]. The result (5.8) for $l = 2p = 0$ can be obtained from an integral representation of the confluent hypergeometric function (see, for example, Eq. (9.211.2) in [21]) and has already been given for $n = 2$ and 3 in [12]. The general result for odd l is obvious and for even $l = 2p > 0$ is obtained by expressing the Gegenbauer polynomial in terms of a hypergeometric function and using the integral (7.523) of [21]. In addition we have made use of the following two properties of a generalized hypergeometric function:

$$\lim_{b_2\to 1-p} \frac{1}{\Gamma(b_2)}\, {}_2F_2(a_1,a_2;b_1,b_2;z) = \frac{\Gamma(a_1+p)\Gamma(a_2+p)\Gamma(b_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1+p)\Gamma(p+1)} z^p \times {}_2F_2(a_1+p,a_2+p;b_1+p,p+1;z)\,, \tag{5.9}$$

$${}_2F_2(a,p+1;b,p+1;z) = {}_1F_1(a;b;z)\,.$$

5.1. Basic thermostatic properties

Basic thermostatic properties of the Hamiltonian (2.8) can be obtained from (5.6) for $l = 0$ (see (4.15)):

$$\lambda_0(\beta) = \frac{\Gamma(n/2)}{\sqrt{\pi}\,\Gamma(\frac{n-1}{2})} \int_{-1}^{+1} \mathrm{d}t\, \mathrm{e}^{\beta(Jt+Kt^2)}(1-t^2)^{(n-3)/2}\,. \tag{5.10}$$

An expansion in powers of $\beta|J|$, βK and $K/|J|$, respectively, allows for an explicit integration and leads to the following series representations:

$$\begin{aligned}\lambda_0(\beta) &= \sum_{r=0}^{\infty} \frac{\Gamma(n/2)(\beta J/2)^{2r}}{\Gamma(n/2+r)\Gamma(r+1)}\, {}_1F_1\left(r+\tfrac{1}{2}; r+\tfrac{n}{2}; \beta K\right)\\ &= \sum_{r=0}^{\infty} \frac{\Gamma(n/2)\Gamma(r+1/2)(\beta K)^r}{\sqrt{\pi}\,\Gamma(n/2+r)\Gamma(r+1)}\, {}_1F_2\left(r+\tfrac{1}{2}; \tfrac{1}{2}, r+\tfrac{n}{2}; \tfrac{\beta^2 J^2}{4}\right)\\ &= \mathrm{e}^{\beta K}\left(\frac{2}{\beta|J|}\right)^{\frac{n-2}{2}} \sum_{r=0}^{\infty} \frac{\Gamma(n/2)\Gamma(r+\frac{n-1}{2})}{\Gamma(\frac{n-1}{2})\Gamma(r+1)}\left(-\frac{2K}{|J|}\right)^r \mathrm{I}_{r+\frac{n-2}{2}}(\beta|J|)\,,\end{aligned} \tag{5.11}$$

where ${}_1F_2(a;b,c;\cdot)$ is a generalized hypergeometric function [22, 23]. The first sum can explicitly be performed [24] leading to another generalized hypergeometric function of two variables [22, 23]:

$$\lambda_0(\beta) = \exp\left\{-\tfrac{\beta J^2}{4K}\right\} \Psi_2\left(\tfrac{1}{2}; \tfrac{n}{2}, \tfrac{1}{2}; \beta K, \tfrac{\beta J^2}{4K}\right)\,. \tag{5.12}$$

Somewhat more illuminating representations can be found in the particular cases $n = 1, 2$ and 3, where $\lambda_0(\beta)$ can be expressed in terms of hyperbolic, Bessel and confluent hypergeometric functions, respectively [25]:

$$\begin{aligned}
\lambda_0(\beta) &= \mathrm{e}^{\beta K}\cosh(\beta J) && \text{for } n=1\,,\\
\lambda_0(\beta) &= \mathrm{e}^{\beta K}\sum_{r=0}^{\infty}\frac{\Gamma(r+1/2)}{\Gamma(1/2)\Gamma(r+1)}\left(-\frac{2K}{|J|}\right)^{r} \mathrm{I}_r(\beta|J|) && \text{for } n=2\,,\\
\lambda_0(\beta) &= \frac{1}{2}\mathrm{e}^{-\beta J^2/4K}\left[\left(1+\frac{J}{2K}\right) {}_1F_1\left(\frac{1}{2};\frac{3}{2};\beta K\left(1+\frac{J}{2K}\right)^2\right)\right.\\
&\quad\left.+\left(1-\frac{J}{2K}\right) {}_1F_1\left(\frac{1}{2};\frac{3}{2};\beta K\left(1-\frac{J}{2K}\right)^2\right)\right] && \text{for } n=3\,.
\end{aligned} \tag{5.13}$$

In the following we list some of the relevant thermostatic quantities (per spin, in the macroscopic limit) and their dependence on the function $\beta \mapsto \lambda_0(\beta)$:

$$\text{Free energy:}\quad F(\beta) = -\frac{1}{\beta}\ln\lambda_0(\beta)\,, \tag{5.14}$$

$$\text{Internal energy:}\quad E(\beta) = \frac{\partial}{\partial\beta}\left[\beta F(\beta)\right] = -\lambda_0'(\beta)/\lambda_0(\beta)\,, \tag{5.15}$$

$$\text{Entropy:}\quad S(\beta) = k_B\beta\left[E(\beta)-F(\beta)\right] = k_B\left[\ln\lambda_0(\beta) - \beta\lambda_0'(\beta)/\lambda_0(\beta)\right]\,, \tag{5.16}$$

$$\text{Heat capacity:}\quad C(\beta) = -k_B\beta^2\,\frac{\partial E(\beta)}{\partial\beta} = k_B\beta^2\left[\frac{\lambda_0''(\beta)}{\lambda_0(\beta)} - \left(\frac{\lambda_0'(\beta)}{\lambda_0(\beta)}\right)^2\right]\,. \tag{5.17}$$

As $\lambda_0(\beta)$ is an even function of the spin-coupling constant J, all quantities listed above depend only on the absolute value $|J|$, that is, they cannot discriminate between ferromagnetic and antiferromagnetic coupling. Note that $\lambda_0'(\beta) := \partial\lambda_0(\beta)/\partial\beta$ and $\lambda_0''(\beta) := \partial^2\lambda_0(\beta)/\partial\beta^2$ have integral representations similar to that of (5.10).

The behaviour of these thermostatic quantities as functions of $\beta|J|$ and $K/|J|$ can be studied by a numerically exact integration and by expansions of the integral (5.10) for small and large $\beta|J|$.

We have performed a numerical calculation for the internal energy and the heat capacity. Fig. 1 shows the internal energy versus the temperature $1/k_B\beta$ for spin dimension $n=3$ and various values of the spin-vibrational-coupling parameter K. Fig. 2 displays the temperature dependence of the internal energy for fixed parameter $K=|J|$ and various spin dimensions n. In Figs. 3–5 we plot the heat capacity as a function over the $1/\beta|J|$–$K/|J|$-plane for spin dimension $n=2$, 3 and 4, respectively. All three figures show the common feature that the specific heat attains a global maximum near the point $(1/\beta|J|, K/|J|) \approx (1,4)$. For a fixed $K \geqslant K_0$ the heat capacity as a function of the temperature shows two maxima. The first maximum is located near $1/\beta|J| \approx 1$ whereas the location of the second one appears to depend linearly on the value of K. For $n=2$ and 3 the first maximum (near $1/\beta|J|$) acquires a value for the heat capacity

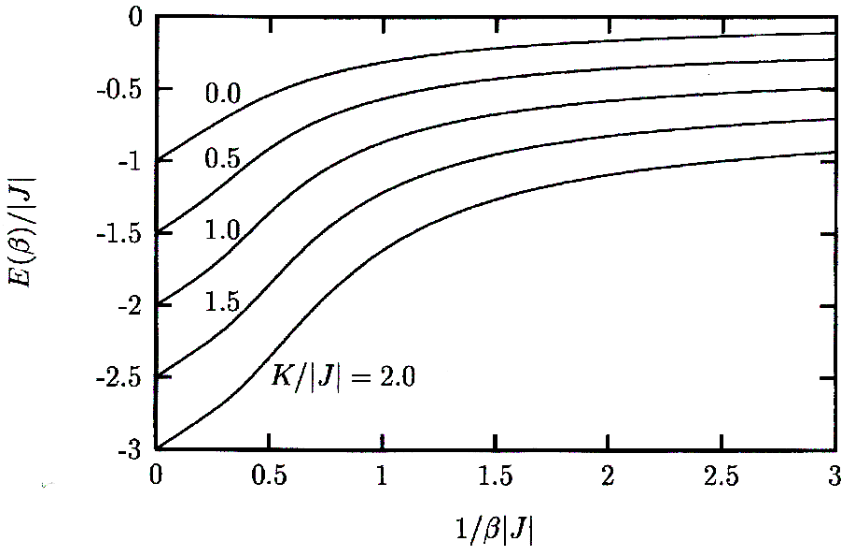

Fig. 1. The internal energy (5.15) as a function of the temperature for spin dimension $n = 3$ and various values of the spin-vibrational-coupling constant K as indicated.

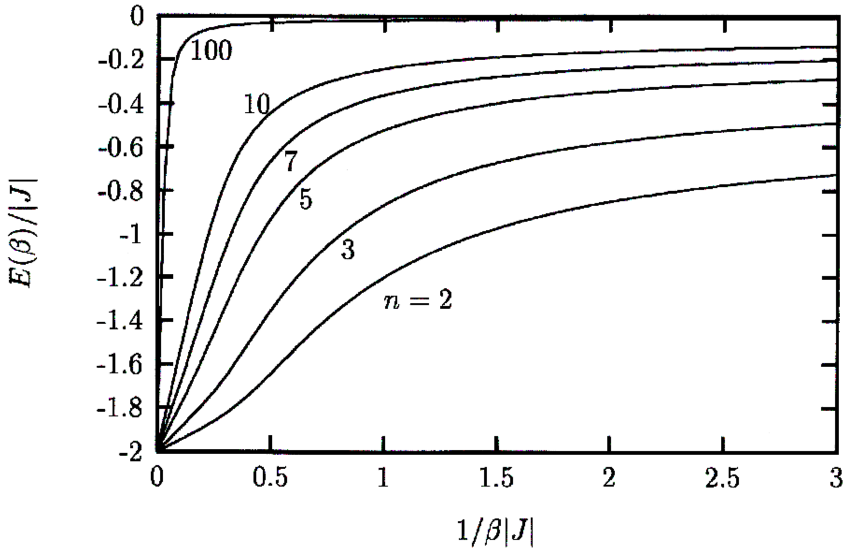

Fig. 2. Same as Fig. 1 but for fixed spin-vibrational coupling $K/|J| = 1$ and various spin dimensions n.

which is larger than the value of the second maximum. However, for $n = 4$ the situation is reversed. The value of K_0 for the three cases $n = 2$, 3 and 4 is approximately given by 25, 15 and 10, respectively.

A Taylor-series expansion of the integrand in (5.10) in powers of βJ leads to the following high-temperature series:

$$\lambda_0(\beta) = \sum_{k=0}^{\infty} \gamma_k \left(\frac{\beta J}{2}\right)^k \tag{5.18}$$

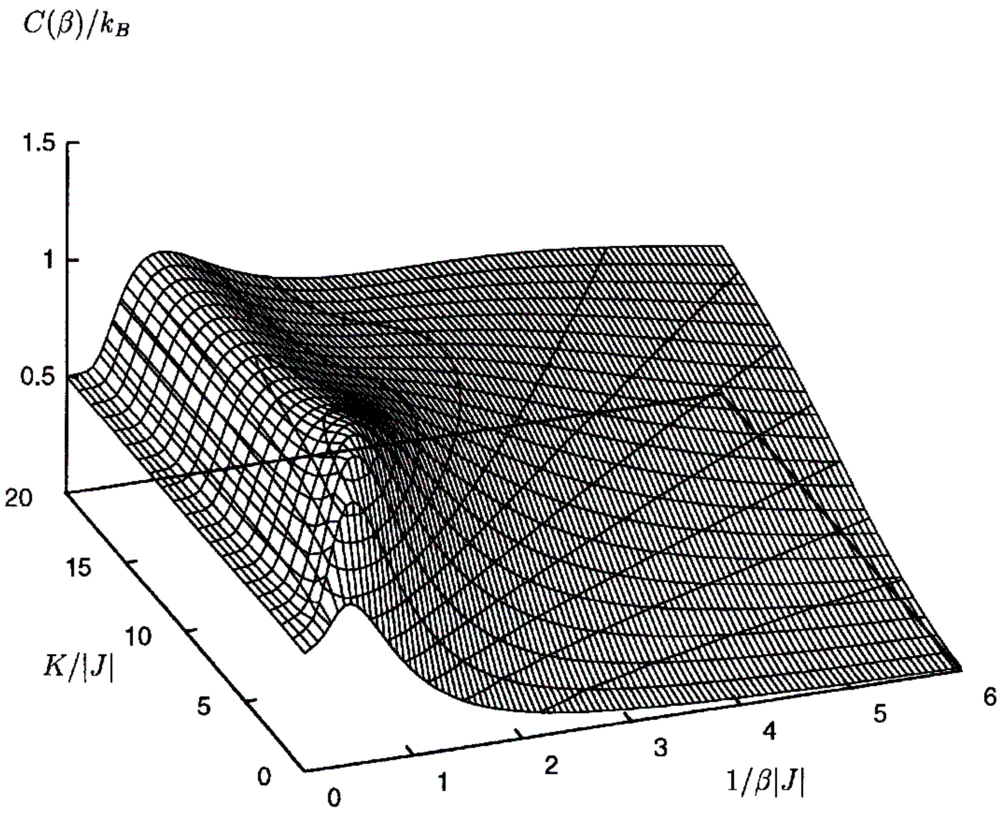

Fig. 3. The heat capacity (5.17) as a function of the temperature and the spin-vibrational coupling constant K for spin dimension $n = 2$.

with coefficients

$$\gamma_{2p} := \Gamma\left(\frac{n}{2}\right) \sum_{j=0}^{p} \frac{\Gamma(2j+2p+1)\left(\frac{K}{2J}\right)^{2j}}{\Gamma(2j+1)\,\Gamma(2p-2j+1)\,\Gamma(j+p+1)\Gamma(j+p+n/2)}\,,$$

$$\gamma_{2p+1} := \Gamma\left(\frac{n}{2}\right) \sum_{j=0}^{p} \frac{\Gamma(2j+2p+3)\left(\frac{K}{2J}\right)^{2j+1}}{\Gamma(2j+2)\,\Gamma(2p-2j+1)\,\Gamma(j+p+2)\Gamma(j+p+1+n/2)}\,. \tag{5.19}$$

The first few coefficients explicitly read

$$\gamma_0 = 1\,, \qquad \gamma_1 = \frac{2K}{nJ}\,, \qquad \gamma_2 = \frac{2}{n} + \left(\frac{K}{2J}\right)^2 \frac{24}{n(n+2)}\,,$$
$$\gamma_3 = \frac{K}{2J}\,\frac{24}{n(n+2)} + \left(\frac{K}{2J}\right)^3 \frac{160}{n(n+2)(n+4)}\,. \tag{5.20}$$

With this power series in βJ we have, for example, a complete high-temperature expansion for the quantities listed in (5.14)–(5.17). The leading terms are

$$F(\beta) = -\frac{K}{n} - \frac{\nu}{2n}\,\beta J^2 + O(\beta^2 J^2)\,, \qquad E(\beta) = -\frac{K}{n} - \frac{\nu}{n}\,\beta J^2 + O(\beta^2 J^2)\,,$$

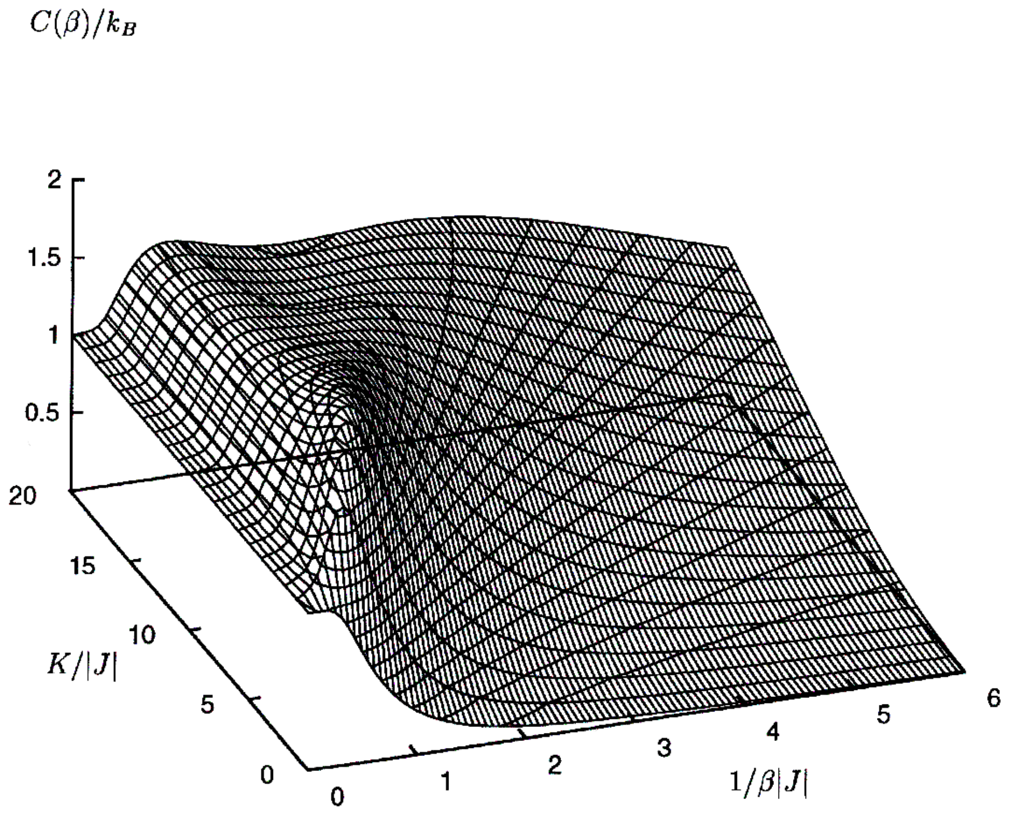

Fig. 4. Same as Fig. 3 but for spin dimension $n = 3$.

$$S(\beta) = -k_B \frac{v}{2n}\,\beta^2 J^2 + O(\beta^3 J^3)\,, \qquad C(\beta) = k_B \frac{v}{n}\,\beta^2 J^2 + O(\beta^3 J^3)\,, \tag{5.21}$$

where $v := 1 + 2(K^2/J^2)(n-1)/n(n+2)$. The free and internal energies approach in the high-temperature limit the constant value $-K/n$. This can also be seen in Fig. 1. The heat capacity goes to zero for high temperatures (cf. Figs. 3–5). The entropy also vanishes at $\beta J = 0$.

The integral (5.10) does also allow for a low-temperature expansion which is, in essence, an asymptotic expansion in powers of $1/\beta|J|$. The derivation of this expansion is based on the third series representation of λ_0 given in (5.11). Using the asymptotic form of the modified Bessel function for large argument one obtains:

$$\lambda_0(\beta) = \frac{\Gamma(n/2)}{\sqrt{\pi}} \left(\frac{2}{\beta|J|}\right)^{\frac{n-1}{2}} \frac{e^{\beta K}}{2} \times \left[\frac{e^{\beta|J|}}{(2K/|J|+1)^{\frac{n-1}{2}}} \sum_{k=0}^{\infty} \mu_k^+ \,(\beta|J|)^{-k} + \frac{e^{-\beta|J|}}{(2K/|J|-1)^{\frac{n-1}{2}}} \sum_{k=0}^{\infty} \mu_k^- \,(\beta|J|)^{-k} \right] \tag{5.22}$$

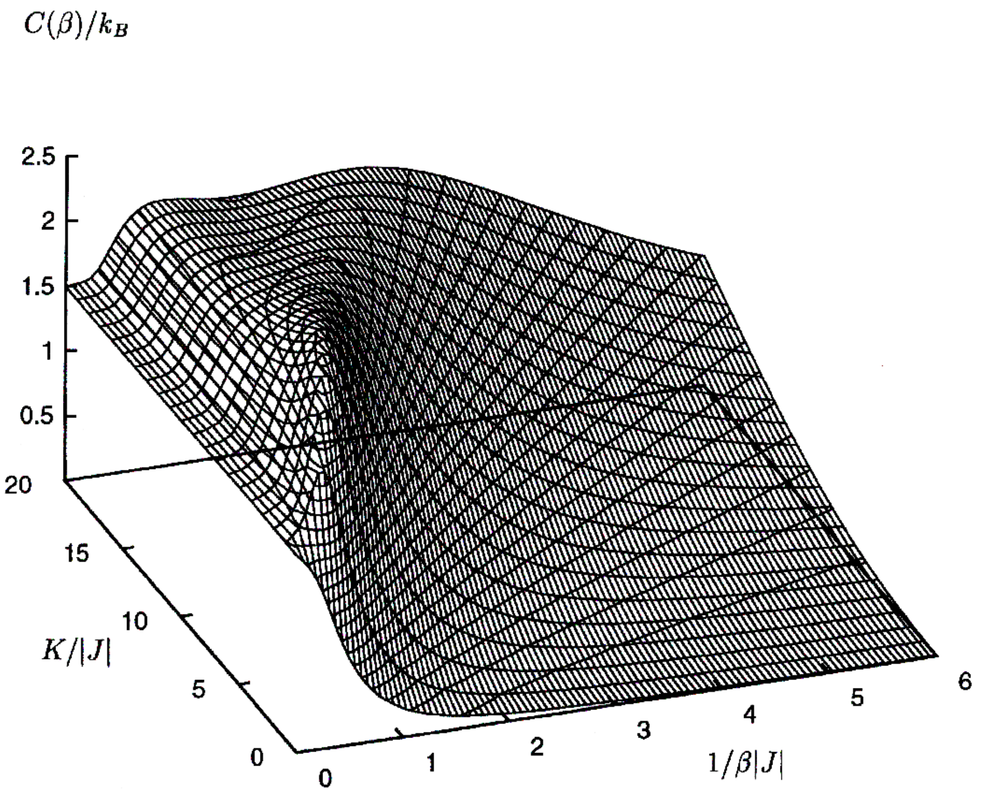

Fig. 5. Same as Fig. 3 but for spin dimension $n = 4$.

with coefficients $\mu_k^\pm$ defined in terms of hypergeometric functions

$$\mu_k^\pm := \left(\frac{-1/2}{2K/|J| \pm 1}\right)^k \frac{\Gamma([(n-1)/2]+k)}{\Gamma([(n-1)/2]-k)\Gamma(k+1)} \times {}_2F_1\left(-k, \tfrac{n-1}{2}+k; \tfrac{n-1}{2}-k; \tfrac{2K}{2K\pm|J|}\right) . \tag{5.23}$$

The hypergeometric function in (5.23) is simply a polynomial of degree k in its last argument. The poles appearing for odd spin dimensions n due to the third argument are cancelled by those of the first gamma function appearing in the denominator of the prefactor. The first coefficients explicitly read

$$\mu_0^\pm = 1 , \qquad \mu_1^\pm = \frac{(n-1)(n+1)K/|J|}{4(2K/|J| \pm 1)^2} - \frac{(n-3)(n-1)}{8(2K/|J| \pm 1)} ,$$

$$\mu_2^\pm = \frac{(n-1)(n+1)(n+3)(n+5)K^2/|J|^2}{2^5(2K/|J| \pm 1)^4} - \frac{(n-3)(n-1)(n+1)(n+3)K/|J|}{2^5(2K/|J| \pm 1)^3} + \frac{(n-5)(n-3)(n-1)(n+1)}{2^7(2K/|J| \pm 1)^2} . \tag{5.24}$$

Note that for $n = 1$ all $\mu_k^{\pm}$ vanish for $k \geqslant 1$ in accordance with the exact closed-form result $\lambda_0(\beta) = \mathrm{e}^{\beta K} \cosh(\beta J)$ for the Ising limit $n \downarrow 1$. See (5.13) and (B.10) of Appendix B.

With the asymptotic expansion of $\lambda_0(\beta)$ we have also obtained low-temperature expansions of the quantities (5.14)–(5.17). Note that only the first sum in (5.22) needs to be considered for $\beta|J| \to \infty$. For $n > 1$ the leading terms read

$$
\begin{aligned}
F(\beta) &= -(|J| + K) + \frac{n-1}{2\beta} \ln[\beta(|J|/2 + K)] - \frac{1}{\beta} \ln \frac{\Gamma(n/2)}{2\sqrt{\pi}} \\
&\quad - \frac{\mu_1^+}{\beta^2 |J|} + O(\beta^{-3} J^{-3}) \,, \\
E(\beta) &= -(|J| + K) + \frac{n-1}{2\beta} + \frac{\mu_1^+}{\beta^2 |J|} + O(\beta^{-3} J^{-3}) \,, \\
S(\beta) &= k_B \bigg(-\frac{n-1}{2} \ln[\beta(|J|/2 + K)] + \frac{n-1}{2} + \ln \frac{\Gamma(n/2)}{2\sqrt{\pi}} + \frac{2\mu_1^+}{\beta |J|} \\
&\quad + O(\beta^{-2} J^{-2}) \bigg) \,, \\
C(\beta) &= k_B \left(\frac{n-1}{2} + \frac{2\mu_1^+}{\beta |J|} + O(\beta^{-2} J^{-2}) \right) .
\end{aligned}
\tag{5.25}
$$

With decreasing temperature the free and internal energies approach the ground-state energy $E(\infty) = -(|J| + K)$. The entropy diverges logarithmically and the heat capacity approaches a constant value independent of the spin-vibrational coupling and in agreement with the equipartition theorem.

5.2. *Some expectation values*

In this section we are going to calculate expectation values of certain one-spin and two-spin functions explicitly.

For the one-spin function we choose $A_1(S) = (S_0 \cdot S)^k = [D_{00}^1(g)]^k$. The thermal expectation value of this function is, according to the general results of Section 4, given by

$$
\langle (S_0 \cdot S_j)^k \rangle = \int_G \mathrm{d}g \, [D_{00}^1(g)]^k \,, \quad j \geqslant 1 \,. \tag{5.26}
$$

With the help of the decomposition (see, for example, [26,27])

$$
[D_{00}^1(g)]^k = \frac{\Gamma(k+1)}{2^k} \sum_{r=0}^{[k/2]} \frac{d_{k-2r}\, \Gamma(n/2)}{\Gamma(r+1)\, \Gamma(n/2 + k - r)} D_{00}^{k-2r}(g) \tag{5.27}
$$

this expectation value is easily found to be

$$\langle (\boldsymbol{S}_0 \cdot \boldsymbol{S}_j)^{2p} \rangle = \frac{\Gamma(p+\frac{1}{2})\,\Gamma(n/2)}{\sqrt{\pi}\,\Gamma(p+\frac{n}{2})}\,, \qquad \langle (\boldsymbol{S}_0 \cdot \boldsymbol{S}_j)^{2p+1} \rangle = 0\,. \tag{5.28}$$

Here we have used the fact that only the trivial representation in the sum (5.27) survives the integration (5.26).

For the two-spin function we choose

$$A(S,S') = \boldsymbol{S} \cdot \boldsymbol{S}' = D^{1}_{00}(g^{-1}g') \tag{5.29}$$

in the general formalism of Section 4. This leads to $a(g) = D^{1}_{00}(g)$, $a_l = \delta_{l,1}/d_1$ and, therefore, to

$$\langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+r} \rangle = \left(\frac{\lambda_1(\beta)}{\lambda_0(\beta)} \right)^{r}, \quad r \geqslant 0\,. \tag{5.30}$$

The corresponding correlation length is given by (4.17) with $\rho_A(\beta) = \lambda_1(\beta)$. The Fourier coefficient $\lambda_1(\beta)$ may be expressed by an integral similar to that for $\lambda_0(\beta)$:

$$\lambda_1(\beta) = \frac{1}{\beta}\frac{\partial}{\partial J}\lambda_0(\beta) = \frac{\Gamma(n/2)}{\sqrt{\pi}\,\Gamma(\frac{n-1}{2})} \int\limits_{-1}^{1} \mathrm{d}t\, e^{\beta(Jt+Kt^2)}\, t(1-t^2)^{(n-3)/2}\,. \tag{5.31}$$

Whereas $\lambda_0(\beta)$ is even $\lambda_1(\beta)$ is odd in J. By combining (5.14) and (5.31) the quotient of these two Fourier coefficients can be expressed in terms of the free energy as follows:

$$\frac{\lambda_1(\beta)}{\lambda_0(\beta)} = -\frac{\partial}{\partial J} F(\beta)\,. \tag{5.32}$$

We can also calculate the zero-field susceptibility which is given by

$$\chi_0(\beta) := \beta \left(1 + 2\sum_{r=1}^{\infty} \langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+r} \rangle \right) = \beta\, \frac{1+\lambda_1(\beta)/\lambda_0(\beta)}{1-\lambda_1(\beta)/\lambda_0(\beta)}\,. \tag{5.33}$$

Here we have used (5.30) and the strict inequality (4.7) for $l = 1$. For $n \geqslant 2$ the susceptibility depends on the parameter K. We have calculated numerically the excess zero-field susceptibility

$$\Delta\chi_0(\beta) := \chi_0(\beta) - \chi_0(\beta)\Big|_{K=0}\,. \tag{5.34}$$

In Fig. 6 we present results for the dimensionless quantity $\Delta\chi_0(\beta)/\beta^2 J$, for ferromagnetic coupling ($J > 0$), $n = 3$ and various values of the parameter K, as a function of the temperature. In the ferromagnetic case the spin–vibrational coupling leads to an increase in the zero-field susceptibility. In contrast to this, we observe for the

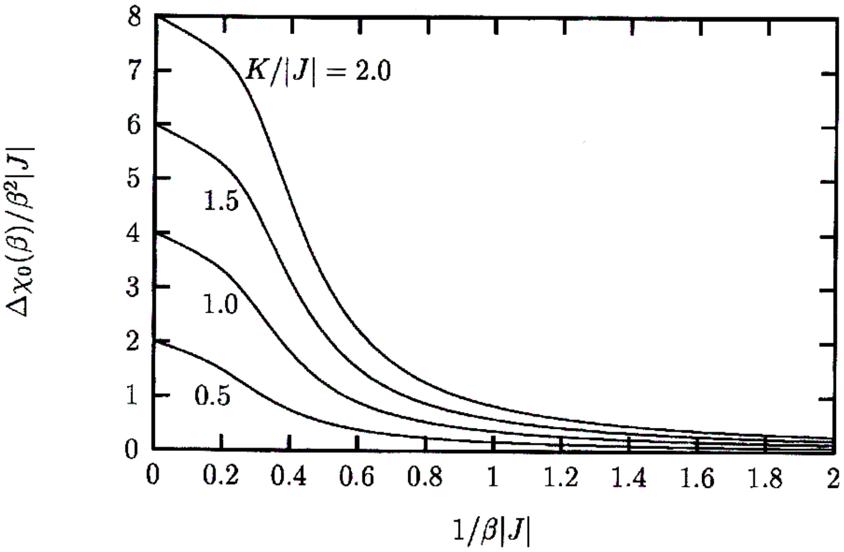

Fig. 6. Temperature dependence of the excess zero-field susceptibility (5.34) for $n = 3$, $J > 0$ and $K/|J| = 0.5, 1.0, 1.5$ and 2.0. Note that we have plotted $\Delta\chi_0(\beta)/\beta^2|J|$.

antiferromagnetic case ($J < 0$) a decreasing susceptibility as K is increasing. This is explicitly shown in Fig. 7 where we plot $\Delta\chi_0(\beta)|J|$ as a function over the $1/\beta|J|$–$K/|J|$–plane. It should be noted that for $K/|J| > 5$ the susceptibility is approximately independent of the parameter K.

Using the high-temperature expansion (5.18) the susceptibilty reads for small β:

$$\chi_0(\beta) = \beta\left[1 + \frac{2}{n}\beta J + \frac{2}{n^2}\left(1 + 2\frac{n-1}{n+2}\frac{K}{J}\right)\beta^2 J^2 + O(\beta^3 J^3)\right] . \tag{5.35}$$

For low temperatures we find for ferromagnetic coupling $J > 0$ and $n \geqslant 2$:

$$\chi_0(\beta) = \beta^2\,\frac{4(J + 2K)}{n-1}\left[1 - \frac{J + 2(n+2)K}{2\beta(J + 2K)^2} + O(\beta^{-2}J^{-2})\right] . \tag{5.36}$$

The susceptibility diverges for ferromagnetic coupling at zero temperature with a critical exponent of value 2 independent of the spin dimension n and the spin-vibrational-coupling constant K. For antiferromagnetic coupling $J < 0$ the susceptibility remains finite at low temperatures ($n \geqslant 2$):

$$\chi_0(\beta) = \frac{n-1}{4(|J| + 2K)}\left[1 + \frac{|J| + 2(n+2)K}{2\beta(|J| + 2K)^2} + O(\beta^{-2}J^{-2})\right] . \tag{5.37}$$

For the particular case $J = 0$ we find $\chi_0(\beta) = \beta$, because $\lambda_1(\beta)$ vanishes due to the result (5.8).

The Fourier coefficient $\lambda_1(\beta)$ allows also for a discussion of the magnetostrictive effect of the spin-vibrational interaction on the length of the chain. The mean

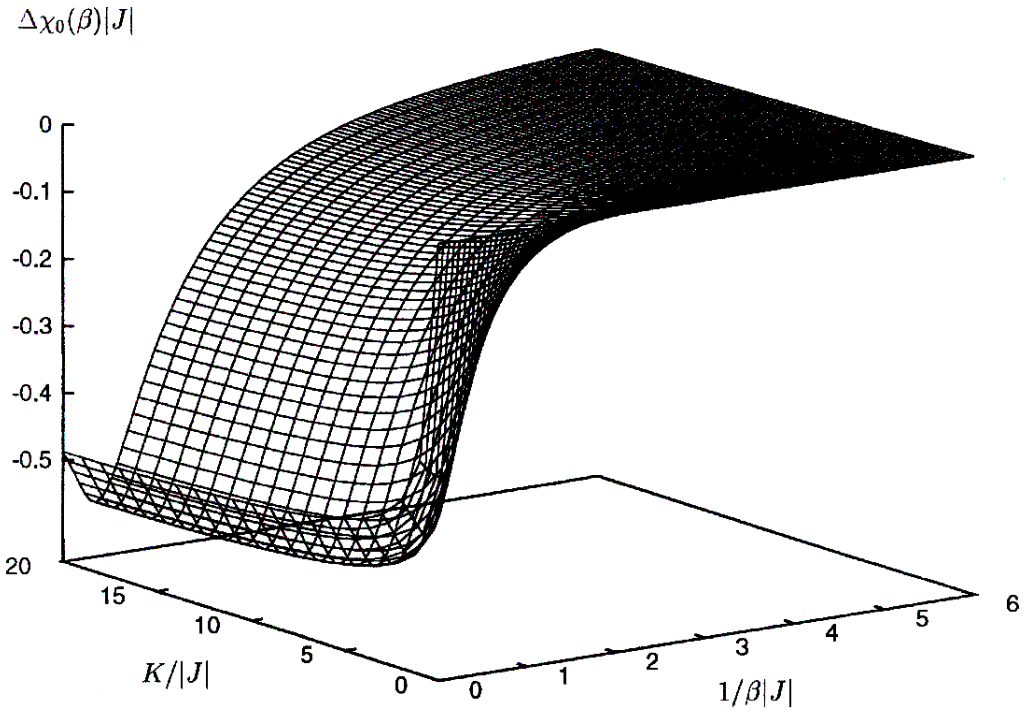

Fig. 7. The excess zero-field susceptibility for $n = 3$ and $J < 0$ as a function of the temperature and the spin-vibrational coupling K.

interparticle distance in the presence of the spin-vibrational interaction is given by

$$L(\beta) := \ell + \frac{1}{N}\sum_{j=1}^{N} \langle q_{j+1} - q_j \rangle_H \ , \tag{5.38}$$

where $\langle\cdot\rangle_H$ stands for the thermal average associated with the total Hamiltonian H given in (2.4), respectively, (2.6). The substitution (2.5) leads to

$$L(\beta) = \ell + \frac{1}{N}\sum_{j=1}^{N} \langle x_{j+1} - x_j \rangle_H + \frac{\eta}{m\omega_0^2}\frac{1}{N}\sum_{j=1}^{N} \langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \rangle \ . \tag{5.39}$$

The first sum vanishes because of the harmonicity of the vibrational part H_{vib} of the total Hamiltonian H. By (5.30) and (5.32) for the nearest-neighbour spin correlation we therefore get

$$L(\beta) = \ell + \frac{\eta}{m\omega_0^2}\frac{\lambda_1(\beta)}{\lambda_0(\beta)} = \ell - \frac{\eta}{m\omega_0^2}\frac{\partial}{\partial J}F(\beta) \, . \tag{5.40}$$

In particular, at zero temperature, where F equals the ground-state energy $E(\infty) = -|J| - K$, we have $L(\infty) = \ell + (\eta/m\omega^2)\mathrm{sgn}\,(J)$. It follows that $L(\infty) < \ell$ when the spin-coupling function W decreases with the actual distance of the spins. As it should do, the result (5.40) reduces for the Ising case to that of Mattis and Schultz [4]

$$L(\beta) = \ell - \frac{\eta}{m\omega_0^2}\tanh(\beta J)\,, \qquad n = 1\,. \tag{5.41}$$

Note that in general the derivative $\partial F(\beta)/\partial J$ appearing in (5.40) may, even for the Ising case, not be identified with the energy $E(\beta)$ as suggested in [5].

5.3. *Relation between susceptibility and nearest–neigbour correlation*

Combining formulas (5.30) and (5.33) for the n-vector model on the harmonic chain relates its zero-field susceptibility $\chi_0(\beta)$ to its nearest-neighbour spin correlation $\langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle$ as follows

$$\chi_0(\beta) = \beta\,\frac{1 + \langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle}{1 - \langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle}\,. \tag{5.42}$$

Since $\langle \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle$ is an odd function of the spin-coupling constant J, this implies

$$X(\beta J)X(-\beta J) = 1 \tag{5.43}$$

for the “dimensionless susceptibility”

$$X(\beta J) := \chi_0(\beta)/\beta\,. \tag{5.44}$$

Relation (5.42) generalizes the result (20) of [6] to non-zero spin-vibrational-coupling constant K. The interesting relation (5.43) between the susceptibility of the ferromagnetic and the antiferromagnetic chain generalizes an observation of Mattis [28, 5] for $K = 0$ and $n = 1, 2, 3$ and, therefore, supports his suggestion that (5.43) may hold for a wider class of classical chains [28, 5].

6. Concluding remarks

We have obtained explicit thermostatic properties and certain expectation values for the n-vector model on a harmonic chain, effectively described by the Hamiltonian (2.8). We have shown that this model belongs to a rather general class of spin models previously considered by Romerio and Vuillermot [8]. Subsets of the class associated with discrete symmetry groups, even in more than one space dimension, have extensively been discussed by Moraal [18].

To obtain the explicit results we have used the elegant method of abstract Fourier analysis the application of which to the statistical mechanics of classical spin models appears to date back to Jocye [7] and Romerio and Vuillermot [8]. Our approach may be understood as a direct generalization of that in [7]. Nevertheless, it is equivalent to that of [8], where Fourier analysis is used to derive the spectral properties of the self-adjoint, compact and positivity improving transfer operator $T : L^2(G) \to L^2(G)$ defined by

$$(Tf)(g) := \int_G dg' \exp\{-\beta v(g^{-1}g')\} f(g') , \qquad f \in L^2(G) . \tag{6.1}$$

For example, it follows from (4.1) and (4.3) that the Fourier coefficients $\lambda_l(\beta)$ defined in (4.4) are the (d_l-fold degenerate) eigenvalues of T. As a consequence, the strict inequality (4.5) may be viewed as a special case of Jentzsch's extension [29] of the Perron–Frobenius theorem [30] to infinite-dimensional spaces.

As is well known [31], the statistical mechanics of classical spin chains (with finite-range interactions) can generally be formulated in terms of a suitably defined transfer operator. This is also true for chains with interactions which are not G-invariant, as happens, for example, when the spin-pair interaction shows an anisotropy or when an external field is present. In such cases, the spectral properties of the transfer operator can be obtained in general only numerically. See, for example, [32, 33] and references therein. In contrast, for G-invariant interactions as considered in the present paper, the eigenfunctions are simply the so-called *spherical functions of representation* $D^l(g)$ *relative to* G_0 [17] and hence independent of the actual interaction. The eigenvalues of the transfer operator are then obtainable by a simple integration, see (4.4).

A final remark is devoted to the case of a G-invariant pair interaction in more than one space dimension where there is no natural analogue of a transfer operator. While abstract Fourier analysis is still applicable (in the sense of Joyce [7]), by itself it can in general no longer be expected to yield exact closed-form expressions. However, it appears to be very efficient in deriving high-temperature expansions and mean-field type of approximations [7, 9, 27].

Appendix A. Discussion of boundary conditions

This appendix is devoted to the effect of boundary conditions on the thermostatic properties and expectation values of models belonging to the class characterized in Section 3. We begin with the definition of the partition function of a finite chain with fixed spins at its endpoints:

$$Z_{\text{fixed}}(S_1, S_{N+1}) := \int_G dg_2 \cdots \int_G dg_N \prod_{j=1}^{N} \exp\left\{-\beta v(g_j^{-1} g_{j+1})\right\} . \tag{A.1}$$

This is the most convenient choice, as the partition function for other boundary conditions can be derived from it by integration. For example, the partition function for the cyclic boundary condition is given by

$$Z_{\text{cycl.}} := \int_M dS_1\, Z_{\text{fixed}}(S_1, S_1) \tag{A.2}$$

and the one with open ends, which we have used in the main text, follows from (A.1) via

$$Z = \int_M \mathrm{d}S_1 \int_M \mathrm{d}S_{N+1}\, Z_{\text{fixed}}(S_1, S_{N+1})\,. \tag{A.3}$$

The calculation of the partition function (A.1) is similar to that in Section 4 for open ends and directly leads to [cf. eq. (4.7)]

$$\begin{aligned} Z_{\text{fixed}}(S_1, S_{N+1}) &= \sum_{l\in\Lambda} d_l\, [\lambda_l(\beta)]^N\, D^l_{00}(g_1^{-1} g_{N+1}) \\ &= Z\left[1 + \sum_{l\neq 0} d_l \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)}\right)^N D^l_{00}(g_1^{-1} g_{N+1})\right]. \end{aligned} \tag{A.4}$$

For the cyclic boundary condition the result reads

$$Z_{\text{cycl.}} = Z\left[1 + \sum_{l\neq 0} d_l \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)}\right)^N\right]. \tag{A.5}$$

It can be seen from (A.4) and (A.5) in combination with (4.5) that the particular choice of the boundary condition becomes irrelevant in the macroscopic limit $N \to \infty$.

The expectation values of two–spin functions on a cyclic chain are given as follows

$$\langle A(S_j, S_{j+r})\rangle_{\text{cycl.}} = \frac{1}{Z_{\text{cycl.}}} \sum_{l_1, l_2, l_3 \in \Lambda} d_{l_1}\, d_{l_2}\, d_{l_3}\, a_{l_1}\, \lambda_{l_2}^{N-r}(\beta)\, \lambda_{l_3}^{r}(\beta)\, C(l_1, l_2; l_3) \tag{A.6}$$

where we have defined

$$C(l_1, l_2; l_3) := \int_G \mathrm{d}g\, D^{l_1}_{00}(g) D^{l_2}_{00}(g) D^{l_3}_{00}(g^{-1}) \tag{A.7}$$

and the coefficients a_l are given in (4.12). Note that the integral (A.7) is related to coupling coefficients of class-one representations. Explicit expressions for the group $SO(n)$ can be found in Ref. [34]. The result for fixed ends is more complicated and will not be given. In any case, it will as (A.6) approach the expression (4.13) in the macroscopic limit.

Appendix B. The special case of a trivial isotropy group

In this appendix we present results for the special case of a trivial isotropy group $G_0 = \{e\}$. That is, the spin space M can be identified with the group G. Therefore, the spins S are elements of this group. We will choose $S_0 = e$, the unit element of G, which implies $S_j = g_j$ for the spin at lattice site j.

On the other hand, G can be viewed as the quotient $(G \times G)/G$ which explicitly shows that this is a special case of the general formulation given in Sections 3 and

4. Let us note that zonal spherical functions defined on the product group $G \times G$ are central functions on the group G [14]. In particular, the function $v(g)$ characterizing the exchange-invariant spin-pair interaction (3.8) becomes a central function, i.e.,

$$v(g) = v(g'^{-1} g g') \quad \text{for all } g' \in G\,. \tag{B.1}$$

A complete set in the subspace of $L^2(G)$ formed by central functions is the set of all characters of non-equivalent unitary irreducible representation of G, $\chi^l(g) := \operatorname{Tr} D^l(g)$. For the weight $\mathrm{e}^{-\beta v(g)}$ the decomposition in characters explicitly reads [17, p. 57]:

$$\mathrm{e}^{-\beta v(g)} = \sum_{l \in \Lambda} d_l\, \lambda_l(\beta)\, \chi^l(g) \tag{B.2}$$

with Fourier coefficients given by

$$\lambda_l(\beta) := \frac{1}{d_l} \int_G \mathrm{d}g\, \mathrm{e}^{-\beta v(g)} \chi^l(g^{-1})\,, \quad l \in \Lambda\,. \tag{B.3}$$

Note that Λ stands for the set of *all* non-equivalent unitary irreducible representations. This set is indeed identical with the set of all irreducible unitary class-one representations of the product group $G \times G$. Again we will reserve the value $l = 0$ for the trivial representation.

The evaluation of the partition function is similar to that in Section 4 as the characters obey the orthogonality relation [17, p. 47]

$$\int_G \mathrm{d}g'\, \chi^l(g^{-1}g')\chi^{l'}(g'^{-1}g'') = \frac{\delta_{ll'}}{d_l}\, \chi^l(g^{-1}g'') \tag{B.4}$$

which may be compared with (4.1).

For the various boundary conditions discussed in the main text and in Appendix A the partition functions read,

$$\begin{aligned} Z &= \lambda_0^N(\beta)\,, \\ Z_{\text{fixed}}(g_1, g_{N+1}) &= Z \left[1 + \sum_{l \neq 0} d_l \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)} \right)^N \chi^l(g_1^{-1} g_{N+1}) \right]\,, \\ Z_{\text{cycl.}} &= Z \left[1 + \sum_{l \neq 0} d_l^2 \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)} \right)^N \right]\,. \end{aligned} \tag{B.5}$$

For completeness we also present expressions for expectation values of two-spin functions which we assume, for simplicity, to be exchange invariant, $A(g, g') = A(g', g)$. Under this assumption

$$a(g) := \int_G \mathrm{d}g'\, A(g', g'g) \tag{B.6}$$

is central and its Fourier coefficients read

$$a_l := \frac{1}{d_l}\int_G \mathrm{d}g\, a(g)\,\chi^l(g^{-1})\,. \tag{B.7}$$

The results for the open and cyclic chain, are respectively,

$$\begin{aligned} \langle A(g_j, g_{j+r})\rangle &= \sum_{l\in\Lambda} d_l^2\, a_l \left(\frac{\lambda_l(\beta)}{\lambda_0(\beta)}\right)^r , \\ \langle A(g_j, g_{j+r})\rangle_{\text{cycl.}} &= \frac{1}{Z_{\text{cycl.}}} \sum_{l_1,l_2,l_3\in\Lambda} d_{l_1}\, d_{l_2}\, d_{l_3}\, a_{l_1}\, \lambda_{l_2}^{N-r}(\beta)\,\lambda_{l_3}^{r}(\beta)\,\mathcal{N}(l_1,l_2;l_3) \end{aligned} \tag{B.8}$$

where

$$\mathcal{N}(l_1,l_2;l_3) := \int_G \mathrm{d}g\,\chi^{l_1}(g)\chi^{l_2}(g)\chi^{l_3}(g^{-1}) \tag{B.9}$$

is the multiplicity of the representation D^{l_3} appearing in the decomposition of the tensor product $D^{l_1}\otimes D^{l_2}$ [17, p. 59]

A similar reasoning as in Appendix A shows that the expressions in (B.8) and in (B.9) asymptotically coincide, respectively, in the limit $N\to\infty$.

In the following we give two simple models where the spin space is a group:

Example 1: The Ising model on the harmonic chain [4]. Here, the group elements which represent the spins take values in $Z_2 := \{-1,+1\}$. Besides the trivial representation $\chi^0(S) = 1$ the group Z_2 has only one non-trivial unitary irreducible representation $\chi^1(S) = S$ which is also one-dimensional. The normalized group measure is $\frac{1}{2}\sum_{S=\pm1}(\cdot)$. For the nearest-neighbor interaction we have, according to Section 2, $V(S,S') := -\left(JSS' + K(SS')^2\right)$ from which $v(S) = -(JS+K)$ follows. The Fourier coefficients are easily found to be

$$\lambda_0(\beta) = \mathrm{e}^{\beta K}\cosh(\beta J)\,, \qquad \lambda_1(\beta) = \mathrm{e}^{\beta K}\sinh(\beta J)\,. \tag{B.10}$$

Inserting these results in (B.5) we immediately find

$$\begin{aligned} &Z = \mathrm{e}^{\beta K N}\cosh^N(\beta J)\,, \qquad Z_{\text{cycl.}} = Z\left[1+\tanh^N(\beta J)\right]\,, \\ &Z_{\text{fixed}}(S_1,S_{N+1}) = Z\left[1\pm\tanh^N(\beta J)\right] \quad \text{for } S_{N+1} = \pm S_1\,. \end{aligned} \tag{B.11}$$

The magnetization, that is, the expectation value of $A_1(S) = S$, obviously vanishes for the open and the cyclic chain. Since the two–spin function $A(S,S') := SS'$ leads to the Fourier coefficients $a_l = \delta_{l,1}$ of the associated central function $a(S) = S$, the corresponding correlation length for the infinite chain is given by $\xi_A(\beta) = 1/\ln(\coth\beta|J|)$.

Example 2: The SU(2)-matrix model. Another example which is immediately solvable is one with spin space $M = SU(2)$. That is, the spins are represented by non-commuting unitary 2×2 matrices. The unitary irreducible representations of $SU(2)$

are enumerated by $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, their dimension is given by $d_l = 2l + 1$, and the corresponding characters are $\chi^l(g) = \sin[(l+\frac{1}{2})\theta]/\sin(\theta/2)$ where θ is the angle of the rotation represented by the group element $g \in SU(2)$ [17]. Let us assume a pair interaction characterized by $v(g) := -(J/2)\chi^{(1/2)}(g)$. This leads to Fourier coefficients [9]

$$\lambda_l(\beta) = \frac{2}{\beta J}\,\mathrm{I}_{2l+1}(\beta J)\,, \quad l = 0, \tfrac{1}{2}, 1, \ldots\,. \tag{B.12}$$

The partition functions for this model read

$$Z = \left[\frac{2}{\beta J}\,\mathrm{I}_1(\beta J)\right]^N, \qquad Z_{\text{cycl.}} = Z\left[1 + \sum_{k=1}^{\infty}(k+1)^2\left(\frac{\mathrm{I}_{k+1}(\beta J)}{\mathrm{I}_1(\beta J)}\right)^N\right], \tag{B.13}$$

for open and cyclic boundary condition, respectively. The magnetization, which is the expectation value of $A_1(g) := \chi^{(1/2)}(g)$, also vanishes for these boundary conditions. For the two-spin function defined by $A(g,g') := \chi^{(1/2)}(g^{-1}g')$, i.e. $a_l = \frac{1}{2}\,\delta_{2l,1}$, the correlation length is found to be

$$\xi_A(\beta) = \left[\ln\left|\frac{\mathrm{I}_1(\beta J)}{\mathrm{I}_2(\beta J)}\right|\right]^{-1} \tag{B.14}$$

in the macroscopic limit.

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[24] See Ref. [22, formula (6.6.2.2)] with $a = b' = 1/2$, $b = n/2$, $x = \beta K$, $y = \beta^2 J^2/4x$ and ${}_1F_1(a;a;y) = e^y$.

[25] For $n = 1$ see Ref. [22, formula (7.2.4.91)]. The case $n = 2$ is directly obtained from the last expression in (5.11). For $n = 3$ the integral (5.10) reduces to the sum of two error functions with complex argument which are expressed in terms of confluent hypergeometric functions.

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