JOINT INSTITUTE FOR NUCLEAR RESEARCH

International Workshop

SYMMETRY METHODS IN PHYSICS

IN MEMORY OF PROFESSOR YA.A.SMORODINSKY

Dubna, Russia July 6 – 10 1993

Edited by
A.N.Sissakian
G.S.Pogosyan
S.I.Vinitsky

Volume 1

Dubna 1994

Published by

Publishing Department
Joint Institute For Nuclear Research
Joliot Curie, 6
141980, Dubna, Moscow Region
Russia

PROCEEDINGS OF THE INTERNATIONAL WORKSHOP
ON SYMMETRY METHODS IN PHYSICS
IN MEMORY OF PROFESSOR YA.A.SMORODINSKY

Photographs: By Yu.A.Tumanov

EXPLICIT THERMOSTATICS OF CERTAIN CLASSICAL ONE-DIMENSIONAL LATTICE MODELS BY HARMONIC ANALYSIS

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Abstract

A certain class of one-dimensional classical lattice models is considered. Using the method of abstract harmonic analysis explicit thermostatic properties of such models are derived. In particular, we discuss the low-temperature behavior of some of these models.

1. A class of one-dimensional models

In this section we will characterize a certain class of lattice models in one dimension. This class of models has already been considered by Romerio and Vuillermot [1] in connection with the transfer-matrix method. See also the book by Moraal [2] where discrete spin models of this class are discussed.

First, we begin with the definition of the "spin space" denoted by M. We will assume that M is a homogeneous space and thus can be identified with a group quotient G/H, i.e. $M = G/H$. Here G is the transformation group acting transitively on M, i.e. for each pair $(S, S_0) \in M \times M$ there exists a group element $g \in G$ such that $S = gS_0$ (see for example ref. [3] for details). The subgroup $H \subset G$ is the stability group of some spin-direction in M. We will keep this direction fixed throughout this paper and denote it by S_0. Hence, $hS_0 = S_0$ for all $h \in H$. For simplicity we will assume that M has a finite volume and hence G is a compact group. However, all results presented below can be generalized to the case of non-compact unimodular groups. With the help of the unique normalized invariant Haar measure dg on G we can define a G-invariant probability measure dS on the spin space M [4, 5]:

$$\int_M dS\, F(S) := \int_G dg\, F(gS_0) \tag{1}$$

for any integrable function F. The normalization and G-invariance guarantee a uniform a priori probability distribution on the spin space M.

In a second step, we will introduce a G-invariant and exchange-invariant spin-pair interaction:

$$V(gS, gS') = V(S, S') = V(S', S), \quad \text{for all } g \in G. \tag{2}$$

In addition we define the function

$$v(g) := V(S_0, gS_0). \tag{3}$$

Obviously, $V(S, S') = v(g^{-1}g')$ where $S = gS_0$ and $S' = g'S_0$. Furthermore, we note that v is a zonal spherical function, that is, it is invariant under left and right shifts of the subgroup H:

$$v(hgh') = v(g) \quad \text{for all } h, h' \in H. \tag{4}$$

With the help of the spin-pair interaction (2) we can introduce a Hamiltonian describing the interaction energy of a set of $N+1$ spins $\{S_1, \ldots, S_{N+1}\}$:

$$\mathcal{H} := \sum_{j=1}^{N} V(S_j, S_{j+1}) = \sum_{j=1}^{N} v(g_j^{-1} g_{j+1}), \quad S_j =: g_j S_0. \tag{5}$$

Viewing S_j as the spin being attached to the j-th site of a one-dimensional lattice the Hamiltonian (5) can be interpreted to characterize a classical spin chain with nearest-neighbor coupling given by the spin-pair interaction V.

The thermostatic (i.e. equilibrium thermodynamic) properties of such a chain can be derived from the canonical partition function in the macroscopic limit $N \to \infty$. The partition function, as a function of the inverse temperature $\beta = 1/k_B T$, is defined as follows:

$$\begin{aligned} Z_N(\beta) &:= \int_M dS_1 \cdots \int_M dS_{N+1} \exp\{-\beta\mathcal{H}\} \\ &= \int_G dg_1 \cdots \int_G dg_{N+1} \prod_{j=1}^{N} \exp\{-\beta v(g_j^{-1} g_{j+1})\}. \end{aligned} \tag{6}$$

Note that we have used open boundary conditions for the finite chain.

In the next section we will explicitly perform the calculation of this partition function using the method of abstract harmonic analysis and thus obtain the free energy per spin in the macroscopic limit,

$$F(\beta) := -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N+1} \ln Z_N(\beta), \tag{7}$$

from which further thermostatic properties can be derived.

2. Explicit thermostatic properties

The basic fact which we will utilize for the abstract harmonic analysis on homogeneous spaces is that the Hilbert space $L^2(M)$ decomposes, e.g., uniquely into an orthogonal sum of invariant subspaces, $L^2(M) = \bigoplus_{l\in\Lambda} H^l$. Each of these subspaces H^l carries a unitary irreducible representation which associates with each group element $g \in G$ an operator $D^l(g)$ acting on H^l. The set Λ of pairwise non-equivalent representations consists of all so-called representations of class one relative to H [3]. Each of these representation spaces H^l contains vectors which are invariant under arbitrary transformations $D^l(h)$, $h \in H$, of the subgroup H. In the following we will make the further assumption that the subgroup H is massive, that is, there exists one and only one vector, say $|l, 0\rangle$, which is invariant in this sense [3]:

$$D^l(h)|l, 0\rangle = |l, 0\rangle, \quad \text{for all } h \in H. \tag{8}$$

A sufficient condition for H being massive is that M is a symmetric space [4]. Let us denote by $\{|l, m\rangle\}$, $m = 0, 1, 2, \ldots, d_l - 1$, $d_l := \dim H^l$, a complete orthonormal basis in the irreducible subspace H^l. Note that we have chosen the basis such that the invariant vector (8) is one of these basis vectors. It follows from the Peter-Weyl theorem that the matrix elements $D^l_{00}(g) := \langle l, 0|D^l(g)|l, 0\rangle$, $l \in \Lambda$, form a complete set for zonal spherical functions such as $\exp\{v(g)\}$ [3]:

$$\exp\{v(g)\} = \sum_{l\in\Lambda} d_l\, \lambda_l(\beta)\, D^l_{00}(g). \tag{9}$$

The "Fourier coefficients" are given by

$$\lambda_l(\beta) := \int_G dg\, \exp\{v(g)\}\, D^{l*}_{00}(g). \tag{10}$$

Using the decomposition (9) we can put the partition function (6) into the form

$$Z_N(\beta) := \int_G \mathrm{d}g_1 \cdots \int_G \mathrm{d}g_{N+1} \prod_{j=1}^{N} \sum_{l_j \in \Lambda} d_{l_j}\, \lambda_{l_j}(\beta)\, D^{l_j}_{00}(g_j^{-1} g_{j+1}). \tag{11}$$

Due to the orthonormality relation

$$\int_G \mathrm{d}g_j\, D^{l_{j-1}}_{00}(g_{j-1}^{-1} g_j) D^{l_j}_{00}(g_j^{-1} g_{j+1}) = \frac{\delta_{l_{j-1} l_j}}{d_{l_j}}\, D^{l_j}_{00}(g_{j-1}^{-1} g_{j+1}) \tag{12}$$

the calculation is straightforward. Because of the open boundary conditions we have used, only the trivial representation, denoted by the label $l = 0 \in \Lambda$, survives. The resulting partition function is explicitly given by

$$Z_N(\beta) = [\lambda_0(\beta)]^N . \tag{13}$$

The Fourier coefficient for the trivial representation is the average of the statistical weight $\exp\{-\beta v(g)\} = \exp\{-\beta V(S_0, S)\}$ with respect to the normalized measures $\mathrm{d}g$ and $\mathrm{d}S$, respectively:

$$\lambda_0(\beta) = \int_G \mathrm{d}g\, \exp\{-\beta v(g)\} = \int_M \mathrm{d}S\, \exp\{-\beta V(S_0, S)\}. \tag{14}$$

Let us note that these integral expressions can be further simplified. As zonal spherical functions do not depend on all but only r group parameters, where r is the rank of the spin space M [6], the trivial Fourier coefficient (14) can be expressed as a r-fold integral. In particular, for spin spaces of rank one all thermostatic properties can be obtained from one single integral expression. Important examples are so-called n-vector models where the spin space is given by the unit sphere $S^{n-1} = SO(n)/SO(n-1)$ which is of rank one. For an explicit application of the method of harmonic analysis to such models see ref. [7].

The presented method of abstract harmonic analysis can be extended to calculate also expectation values such as magnetization and two-spin correlations [7].

3. Discussion for low temperatures

We are finally turning to the discussion of the low-temperature behavior of the Fourier coefficient (14). For this we consider only the special case where the spin space is isomorphic to a group manifold, $M \simeq G$. This case can be embedded into the general approach of the previous section by noting that $M = G \times G/G$. The zonal spherical functions of the product group $G \times G$ are identical with the characters of the representations of the group G [4]. The set of all class-one representations of $G \times G$ with respect to the subgroup G can be identified with the set of all non-equivalent unitary irreducible representations of the group G. Let us stress that the function v which characterizes the spin-pair interaction (2) is now a central function, that is, it can be decomposed into characters $\chi^l(g) := \mathrm{Tr}\, D^l(g)$ of unitary irreducible representations of G:

$$v(g) = \sum_{l \in \Lambda} v_l\, \chi^l(g) \tag{15}$$

where the Fourier coefficients are given by

$$v_l := \int_G \mathrm{d}g\, v(g) \chi^l(g^{-1}). \tag{16}$$

In the following we will study the low-temperature behavior of the trivial Fourier coefficient (14). We will first consider the case of a finite group, hence a discrete spin model. In this case

the group integrals have to be replaced by appropriate sums:

$$\lambda_0(\beta) = \frac{1}{|G|} \sum_{g \in G} \exp\{-\beta v(g)\}. \tag{17}$$

Here $|G|$ stands for the order of the group, that is, the number of its elements. Similarly, we will use the notation $|\mathcal{P}|$ for the number of elements of any subset $\mathcal{P} \subset G$. We will make the following further definitions:

$$\begin{aligned} J &:= \inf_{g \in G} v(g), & \mathcal{J} &:= \{g \in G | v(g) = J\}, \\ K &:= \inf_{g \in G \setminus \mathcal{J}} v(g), & \mathcal{K} &:= \{g \in G | v(g) = K\}. \end{aligned} \tag{18}$$

Obviously, $\Delta := K - J > 0$ is the energy gap between the ground state and the first excited state of the chain. The numbers $|\mathcal{J}|$ and $|\mathcal{K}|$ are the degeneracies of the ground state and the first exited state, respectively. With these definitions it is obvious that the leading asymptotic behavior of (17) for large β is given by

$$\lambda_0(\beta) \approx \frac{|\mathcal{J}|}{|G|} \mathrm{e}^{-\beta J} \left(1 + \frac{|\mathcal{K}|}{|\mathcal{J}|} \mathrm{e}^{-\beta\Delta} + \cdots\right). \tag{19}$$

Consequently, the low-temperature behavior of the free energy, the internal energy and the heat capacity per spin, respectively, read in the macroscopic limit

$$F(\beta) = -\frac{1}{\beta} \ln \lambda_0(\beta) = J - \frac{1}{\beta} \ln \frac{|\mathcal{J}|}{|G|} - \frac{1}{\beta} \frac{|\mathcal{K}|}{|\mathcal{J}|} \mathrm{e}^{-\beta\Delta} + \cdots, \tag{20}$$

$$E(\beta) = \frac{\partial}{\partial\beta} [\beta F(\beta)] = J + \Delta \frac{|\mathcal{K}|}{|\mathcal{J}|} \mathrm{e}^{-\beta\Delta} + \cdots, \tag{21}$$

$$c(\beta) = -k_B \beta^2 \frac{\partial E(\beta)}{\partial \beta} = k_B (\beta\Delta)^2 \frac{|\mathcal{K}|}{|\mathcal{J}|} \mathrm{e}^{-\beta\Delta} + \cdots. \tag{22}$$

In the case of a continuous group $G \simeq M$ we can find explicit expressions if we allow only for ferromagnetic interaction, that is,

$$\inf_{g \in G} v(g) = v(e) \quad \Longleftrightarrow \quad \inf_{S \in M} V(S_0, S) = V(S_0, S_0) \tag{23}$$

where $e \in G$ stands for the unit element of the group. Let us introduce a parameterization of the group such that $g = g(\theta_1, \cdots, \theta_f)$ with $f := \dim G = \dim M$. The parameters are supposed to take values in closed intervals (for compact groups): $\theta_a \in [0, \theta_a^{\max}]$. The parameterization is chosen such that the unit element is given by $e = g(0, \ldots, 0)$. Finally, if the normalized Haar measure is characterized by a probability density $\mu(\theta_1, \ldots, \theta_f)$, the integral (14) explicitly reads

$$\lambda_0(\beta) = \int_0^{\theta_1^{\max}} \mathrm{d}\theta_1 \cdots \int_0^{\theta_f^{\max}} \mathrm{d}\theta_f \mu(\theta_1, \cdots, \theta_f) \exp\{-\beta v(g(\theta_1, \cdots, \theta_f))\}. \tag{24}$$

Obviously, the main contribution to this integral in the limit $\beta \to \infty$ comes from the region with small θ's. Hence, using Laplace's method, we expand v up to second order in the group parameters. If $\{L_a\}$ denotes the set of generators of G we have

$$\begin{aligned} v(g) &= \sum_{l \in \Lambda} v_l\, \chi^l(g) = \sum_{l \in \Lambda} v_l\, \mathrm{Tr} \exp\left\{ \mathrm{i} \sum_{a=1}^{f} \theta_a L_a \right\} \\ &\approx \sum_{l \in \Lambda} v_l\, \mathrm{Tr} \left(1 + \mathrm{i} \sum_{a=1}^{f} \theta_a L_a - \frac{1}{2} \sum_{a,b=1}^{f} \theta_a \theta_b L_a L_b \right). \end{aligned} \tag{25}$$

Using the identities

$$\mathrm{Tr}\,1 = d_l, \qquad \mathrm{Tr}\,L_a = 0, \qquad \mathrm{Tr}\,L_a L_b = \gamma_l \delta_{ab}, \tag{26}$$

where γ_l is the Dynkin index [8] of the representation carrying label l, we arrive at

$$v(g) \approx J + \frac{k}{2}\sum_{a=1}^{f} \theta_a^2 \tag{27}$$

with

$$J := v(e) = \sum_{l\in\Lambda} v_l d_l, \qquad k := -\sum_{l\in\Lambda} v_l \gamma_l. \tag{28}$$

The integration may now be performed and leads to

$$\lambda_0(\beta) \approx \mu_0 \left(\frac{2\pi}{\beta k}\right)^{f/2} \mathrm{e}^{-\beta J}. \tag{29}$$

Here we have assumed that $\mu_0 := \mu(0,\ldots,0) \neq 0$. Otherwise, the leading non-vanishing term for small θ's has to be kept in μ. In the latter case, we would arrive at the same result with some positive constant replacing μ_0.

From this result we obtain the leading low-temperature behavior of the free energy, the internal energy and the heat capacity, respectively:

$$F(\beta) = J - \frac{f}{2\beta}\ln\frac{2\pi}{\beta k} - \frac{\ln\mu_0}{\beta} + \cdots, \tag{30}$$

$$E(\beta) = J + \frac{f}{2\beta} + \cdots, \tag{31}$$

$$c(\beta) = k_{\mathrm{B}}\frac{f}{2} + \cdots. \tag{32}$$

As it should be, because of the quadratic nature of (27), the low-temperature behavior of the heat capacity is in agreement with the equipartition theorem. This property is not restricted to the class of models discussed here, but also holds for some anisotropic spin chains [9].

Finally, we note that the results for continuous spin models remain valid for the general case $M = G/H$ if we set $f = \dim M$, $\gamma_l = ||L_a|l,0)||^2$ and μ_0 is some positive constant.

Acknowledgement

I would like to thank the organizers for their kind invitation to this enjoyable and inspiring conference. I am also thankful to Hajo Leschke for his comments. Finally, support by the Heisenberg – Landau Program is gratefully acknowledged.

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